Supporting Information

Insights on Absolute and Relative Stereocontrol in Stereodivergent Cooperative Catalysis

Avtar Changotra,[a] Bangaru Bhaskararao,[a] Christopher M. Hadad,[b] and Raghavan B. Sunoj [a,]*

[a] Department of Chemistry, Indian Institute of Technology Bombay,

Powai, Mumbai 400076, India

[b] Department of Chemistry and Biochemistry, The Ohio State University,

Columbus, OH 43210, USA

E-mail: sunoj@chem.iitb.ac.in

Part-A

Section	Table of Contents	Page No.
1.1	Generation of Ir-π-allyl intermediate	S3
	(i) Activation of cinnamyl methyl carbonate	S3
	(ii) Optimized geometries of transition states (TSs)	S5
	(iii) Formation of CO_2 and CH_3OH by the action of $[DBU\text{-}H]^+$	S7
1.2	Activation strain analysis of TSs **[12-13]**$_{endo\text{-}re}^{‡}$ and **[12-13]**$_{exo\text{-}si}^{‡}$	S7
1.3	Generation of Cu-enolate	S8
	(i) Activation of azaaryl acetamide	S8
	(ii) Product release and the catalyst regeneration	S9
1.4	Energetic Span Model	S12
1.5	Kinetic Analysis	S12
1.6	Reaction between Cu-enolate and Ir-π-allyl	S17
	(i) Configurational and conformational study for the C–C bond formation transition states	S17
	(ii) Energetic details of stereodivergence	S18
	(iii) Conformational analysis of the C–C bond formation transition states	S19
1.7	Space filling model for **C2-P1** catalytic dyad	S24
1.8	Global contact surface area, catalyst cavity volume and solvent accessible surface area	S24
1.9	Activation strain analysis for various modes of additions between the nucleophile (Cu-enolate) and the electrophile (Ir-π-allyl)	S27
1.10	Optimized geometries of stereocontrolling transition states	S29
	(i) **C1-P1** catalyst dyad	S29
	(ii) **C2-P1** catalyst dyad	S32
1.11	Space filling model for the lowest energy TS for all catalyst dyads	S35
1.12	Interaction wheel diagram	S36
1.13	Quantification of Noncovalent Interactions	S38

Part-B

Optimized Cartesian Coordinates of All Stationary Points (pp S42-S386)

1.1. Generation of Ir-π-allyl intermediate

(i) Activation of cinnamyl methyl carbonate

Cinnamyl methyl carbonate (**10**) gets activated in the form of Ir-π-allyl intermediate with the assistance of prononated base, $[DBU\text{-}H]^+$, generated during the Cu-Walphos enolate formation (Figure S1(a)). Depending on the mode of binding of the allyl moiety to the Ir center, an *endo* or an *exo* diastereomer of the Ir-π-allyl intermediate can be envisaged. A *syn* disposition of the allyl C4–H and the Ir–C bond of the phosphoramidite ligand is denoted as *endo* whereas an *anti* orientation is designated as *exo* Figure S1(b). These notations are followed for both the **P1** (*R*,*R*,*R*) and **P2** (*S*,*S*,*S*) Ir-phosphoramidite catalysts. The elementary step barrier for the formation of the *exo* Ir-π-allyl intermediate is only about a kcal/mol higher than that for the *endo* intermediate in the case of **P1** catalyst, suggesting that both *endo* and *exo* intermediates could be produced under the reaction conditions (Figure S1(a)). The relative Gibbs free energy of the transition states for the formation of an *endo* and an *exo* Ir-π-allyl intermediate is provided in Tables S1.

(a)

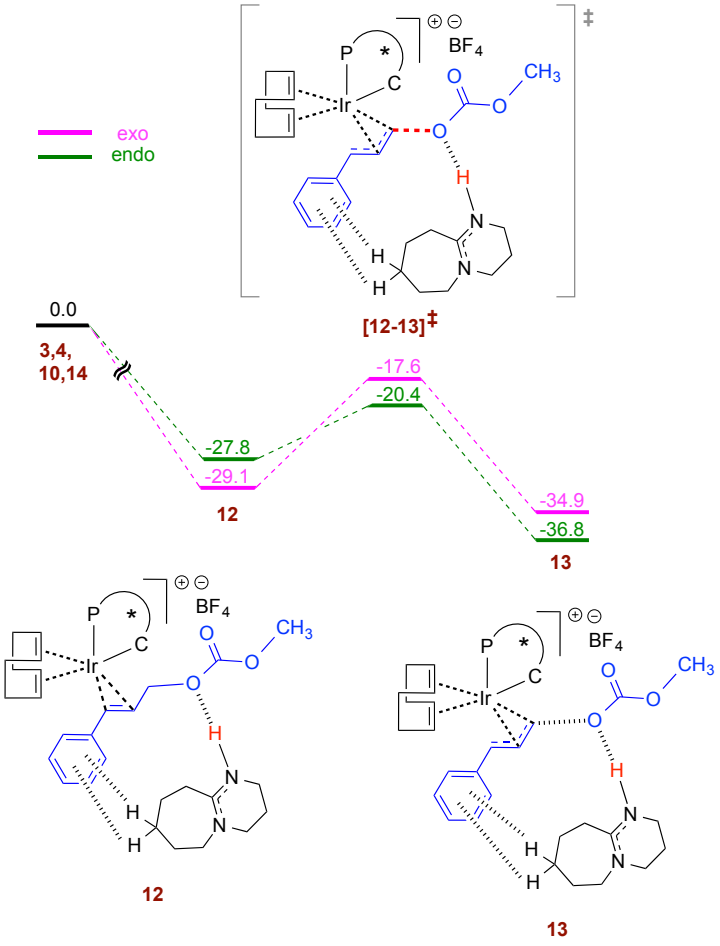
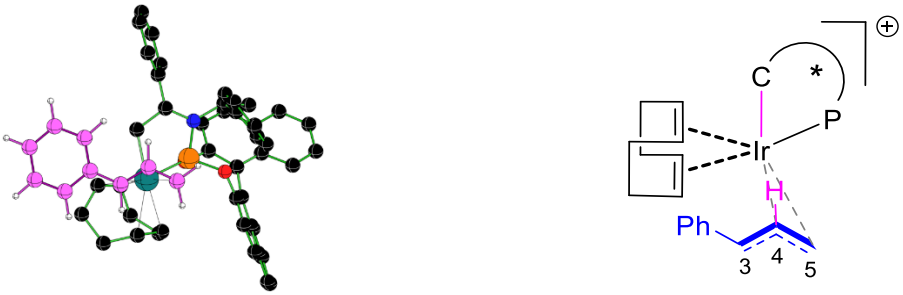


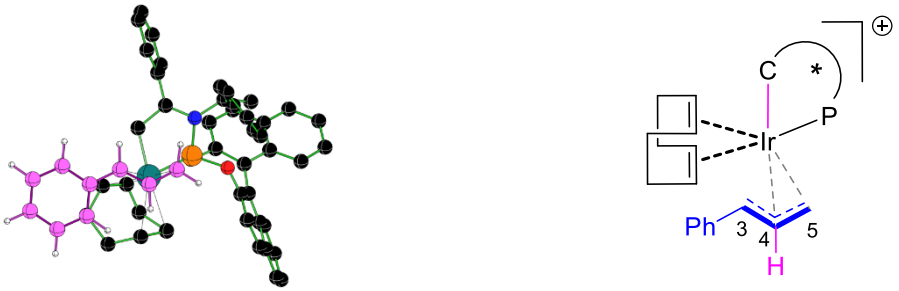
Figure S1 continued…

(b)

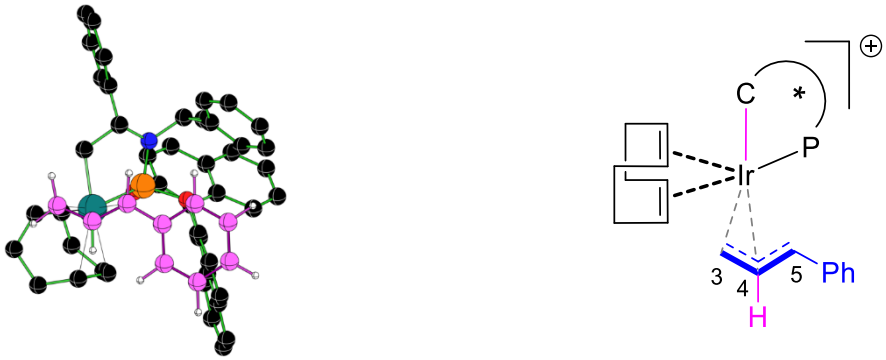


endo-re

endo-si



exo-si



exo-re

C H Ir P O N Allyl moiety is shown in pink color

Figure S1. (a) Gibbs free energy profile for the formation of Ir-π-allyl intermediate with **P1** catalyst. (b) Optimized geometries and qualitative representation of an *endo* and an *exo* diastereomer of the Ir-π-allyl intermediates with the **P1** catalyst. The *re* and *si* notations represents the prochiral face of the substrate which is readily available for bond formation with the incoming nucleophile. Although the transition states consist of the counter ion ($BF4^-$) in the actual computations, it is removed from this figure for improved clarity.

Table S1. Relative Gibbs Free Energies (kcal/mol) of *endo* and *exo* Transition States **[12-13]**‡ for the Formation of Ir-π-allyl Intermediate with Respect to the Lowest Energy Transition State for **P1** and **P2** catalysts

(a) without BF_4^- Counter Ion

P1		**P2**	
endo-re[a]	0.0	*endo-si*	0.0
endo-si	9.5	*endo-re*	9.5
exo-re	2.8	*exo-si*	2.8
exo-si	1.8	*exo-re*	1.8

(b) with BF_4^- Counter Ion

P1		**P2**	
endo-re[a]	0.0	*endo-si*	0.0
endo-si	10.8	*endo-re*	10.8
exo-re	6.2	*exo-si*	6.2
exo-si	3.6	*exo-re*	3.6

[a-] The *re* and *si* notations represent the prochiral faces of the substrate, which is available for the bond formation with the incoming nucleophile

(ii) Optimized geometries of transition states for the formation of *endo* and *exo* Ir-π-allyl intermediate

(a)

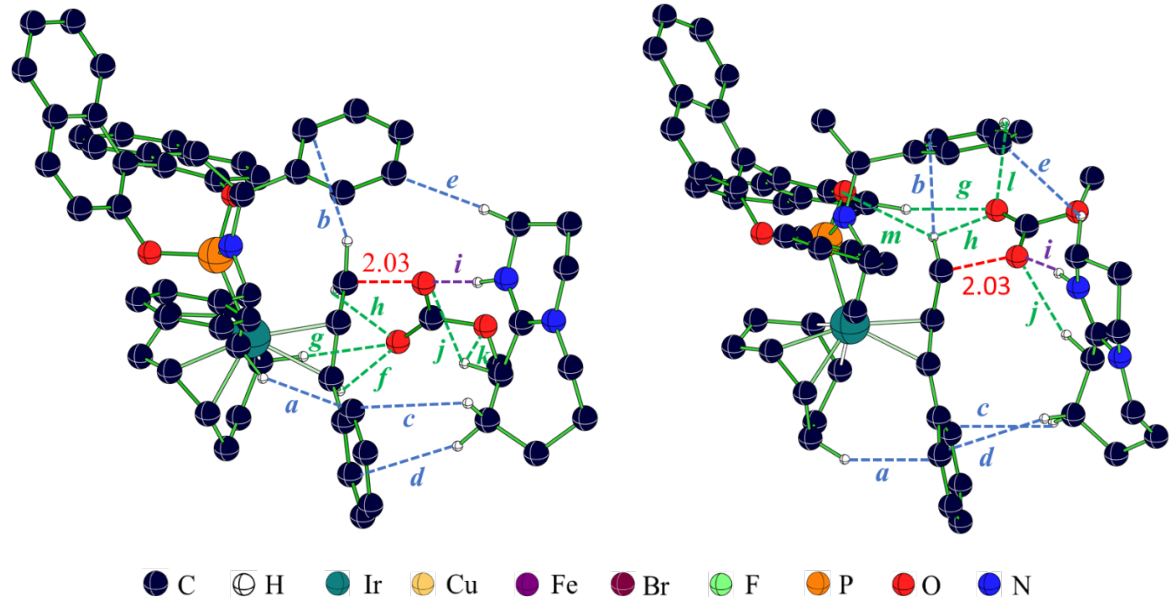
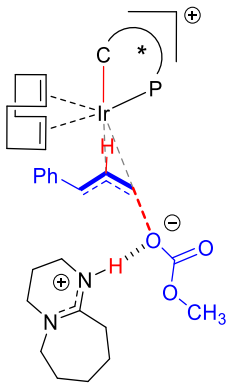
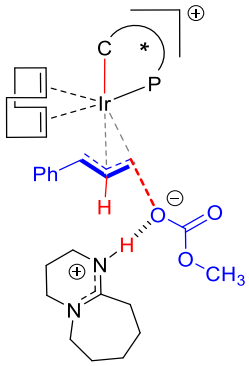


Figure S2 continued…

(b)



[12-13]$_{endo\text{-}re}^{‡}$ (0.0)



[12-13]$_{exo\text{-}si}^{‡}$ (1.8)

Bond path	Type of interaction	**[12-13]**$_{endo\text{-}re}^{‡}$ (Å)	ρ x 10^{-2}	(θ)	**[12-13]**$_{exo\text{-}si}^{‡}$ (Å)	ρ x 10^{-2}	(θ)
a	C–H···π	2.37	1.4	23.8	2.64	0.9	25.4
b	C–H···π	3.57	0.1	25.5	2.88	0.5	66.8
c	C–H···π	2.89	0.6	68.6	2.89	0.6	60.1
d	C–H···π	2.83	0.7	37.3	2.85	0.6	47.3
e	C–H···π	2.74	0.7	17.8	2.86	0.6	47.6
f	C–H···O	2.65	0.7	130.2	-[a]	-[a]	-[a]
g	C–H···O	2.39	1.1	175.8	2.42	1.0	170.1
h	C–H···O	2.31	1.5	115.1	2.33	1.5	117.4
i	C–H···O	1.75	4.1	172.5	1.72	4.3	169.2
j	C–H···O	2.61	0.8	140.7	2.40	1.2	146.5
k	C–H···O	2.70	0.7	12.4	-[a]	-[a]	-[a]
l	C–H···O	-[a]	-[a]	-[a]	2.59	0.8	122.9
m	C–H···O	-[a]	-[a]	-[a]	2.89	0.5	112.5

Figure S2. Optimized geometries of the transition states in the case of **P1** catalyst, highlighting important noncovalent interactions in the **[12-13]**$_{endo\text{-}re}^{‡}$ and **[12-13]**$_{exo\text{-}si}^{‡}$. Interatomic contacts that correspond to the NCIs are in Å, and the corresponding electron densities ($\rho \times 10^{-2}$) at the bond critical points as well as the angle of interaction (θ, in °) for various NCIs are provided in the table. Only selected hydrogen atoms are shown. Although the transition states consist of the counter ion ($BF4^-$) in the actual computations, it is removed from this figure for improved clarity. [a-] No *bcp* found

(iii) Formation of CO_2 and CH_3OH by the action of $[DBU\text{-}H]^+$

Intermediate **13**, produced via the C–O bond breaking TS **[12-13]**‡, can provide the vital Ir-π-allyl intermediate and a carbonate-DBU adduct. The protonation of the carbonate oxygen of the $–OCH_3$ group of the Ir-bound carbonate ester by $[DBU\text{-}H]^+$ via **TS[13'-14']** is key to substrate activation. The action of $[DBU\text{-}H]^+$ on methyl carbonate ester can then lead to CO_2 and CH_3OH (**14'**) as shown in Figure S3.

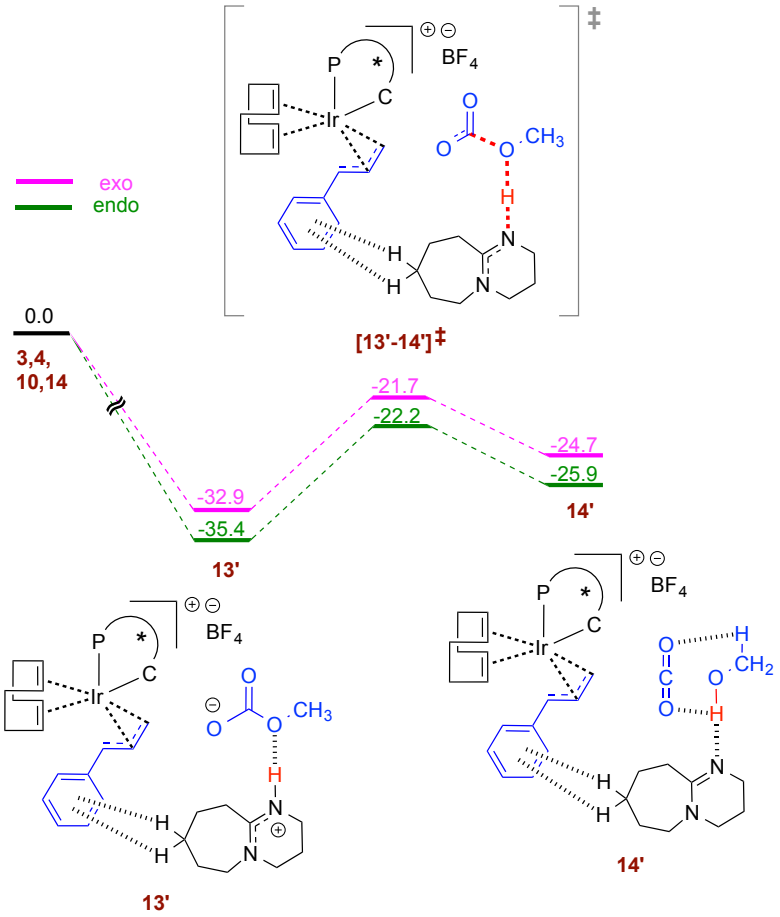


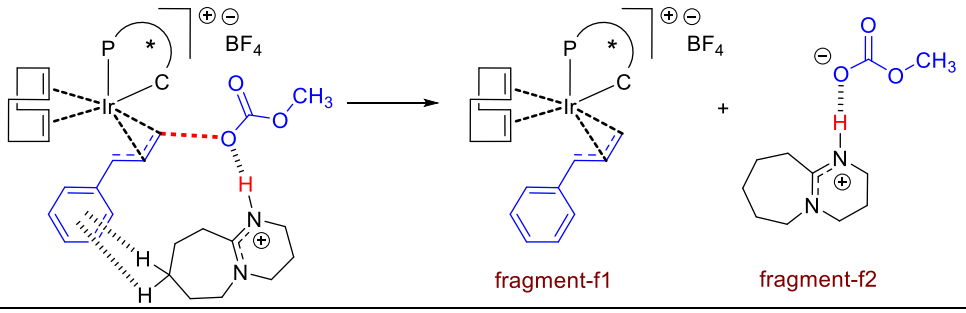
Figure S3. Gibbs free energy profile for the $[DBU\text{-}H]^+$ assisted removal of methyl carbonate as CO_2 and MeOH.

1.2. Activation strain analysis

The activation strain analysis is applied to rationalize the origin of the energy difference between the TSs **[12-13]**$_{endo\text{-}re}^{‡}$ and **[12-13]**$_{exo\text{-}si}^{‡}$ for the formation of the *endo* and *exo* Ir-π-allyl intermediates. The activation strain energy ($\Delta\Delta E^{‡}$) is partitioned to the (a) destabilizing distortion energy in the reacting partners ($\Delta\Delta E^{‡}_{d}$) while going from their respective ground state geometries to that in the transition states, and (b) stabilizing interaction energy between the deformed reactants ($\Delta\Delta E^{‡}_{i}$) in the TS geometry. Here, the TS is divided into two

fragments, f1= [Ir-π-allyl]$^{+}$BF$_4^{-}$ and f2= [DBU-H]$^{+}$OCO$_2$CH$_3^{-}$. The distortion energy of each fragment and the total interaction energy between the two fragments with respect to the lower energy **[12-13]**$_{endo\text{-}re}^{‡}$ are given in Table S2.

Table S2. Computed Relative Distortion Energies in each Fragment, Total Relative Distortion Energies ($\Delta\Delta E^{‡}_{d}$) and Relative Interaction Energies ($\Delta\Delta E^{‡}_{i}$) (in kcal/mol) in the TSs **[12-13]**$_{endo\text{-}re}^{‡}$ and **[12-13]**$_{exo\text{-}si}^{‡}$ with **P1** Catalyst Obtained at the SMD$_{(THF)}$/B3LYP-D3/6-31G**,SDD(Ir,Cu,Fe,Br) Level of Theory.[a] All Energies are in kcal/mol



TS	$\Delta\Delta E^{‡}_{d}$ (f1)	$\Delta\Delta E^{‡}_{d}$ (f2)	total $\Delta\Delta E^{‡}_{d}$ [$\Delta\Delta E^{‡}_{d}$ (f1) + $\Delta\Delta E^{‡}_{d}$ (f2)]	$\Delta\Delta E^{‡}_{i}$	$\Delta\Delta E^{‡}$ [$\Delta\Delta E^{‡}_{d}$ + $\Delta\Delta E^{‡}_{i}$]
[12-13]$_{endo\text{-}re}^{‡}$	0.0	0.0	0.0	0.0	0.0
[12-13]$_{exo\text{-}si}^{‡}$	1.9	0.3	2.2	-0.3	1.9

[a] Relative energies with respect to lower energy TS

The distortion energies of fragments, f1 and f2 are 1.9 kcal/mol and 0.3 kcal/mol higher in **[12-13]**$_{exo\text{-}si}^{‡}$ compared to **[12-13]**$_{endo\text{-}re}^{‡}$. On the other hand, the stabilizing interaction between the deformed fragments at the transition state geometry is 0.3 kcal/mol more in the higher energy **[12-13]**$_{exo\text{-}si}^{‡}$ than that in the lower energy **[12-13]**$_{endo\text{-}re}^{‡}$. The overall balance between the destabilizing distortion and stabilization interaction energies is found to be in favor of **[12-13]**$_{endo\text{-}re}^{‡}$ by 1.9 kcal/mol. The higher distortion energy (1.9 kcal/mol) in the Ir-π-allyl moiety is a major factor contributing to the energy difference between the stereo-determining transition states.

1.3. Generation of Cu-enolate

(i) Activation of azaaryl acetamide

Azaaryl acetamide **2** gets activated in the form of Cu-Walphos enolate by the action of base DBU that then serves as the nucleophilic component in the reaction. Subsequent action of DBU generates a chiral Cu-enolate intermediate **6** via **[5-6]**‡ (as described in the main text). Ir-π-allyl intermediate enters the primary catalytic cycle, centered around the Cu-Walphos enolate, by displacing [DBU-H]$^{+}$PF$_6^{-}$ (**7**) and thereby leading to a lower energy intermediate **8**

(Figure S4). Alternatively, the release of the $[DBU\text{-}H]^{+}PF_6^{-}$ from intermediate **6** leads to **6'**, which is 9.9 kcal/mol higher in energy than **6**. In the next step, the addition of the Cu-Walphos enolate to the Ir-π-allyl intermediate leads to a lower energy intermediate **8**.

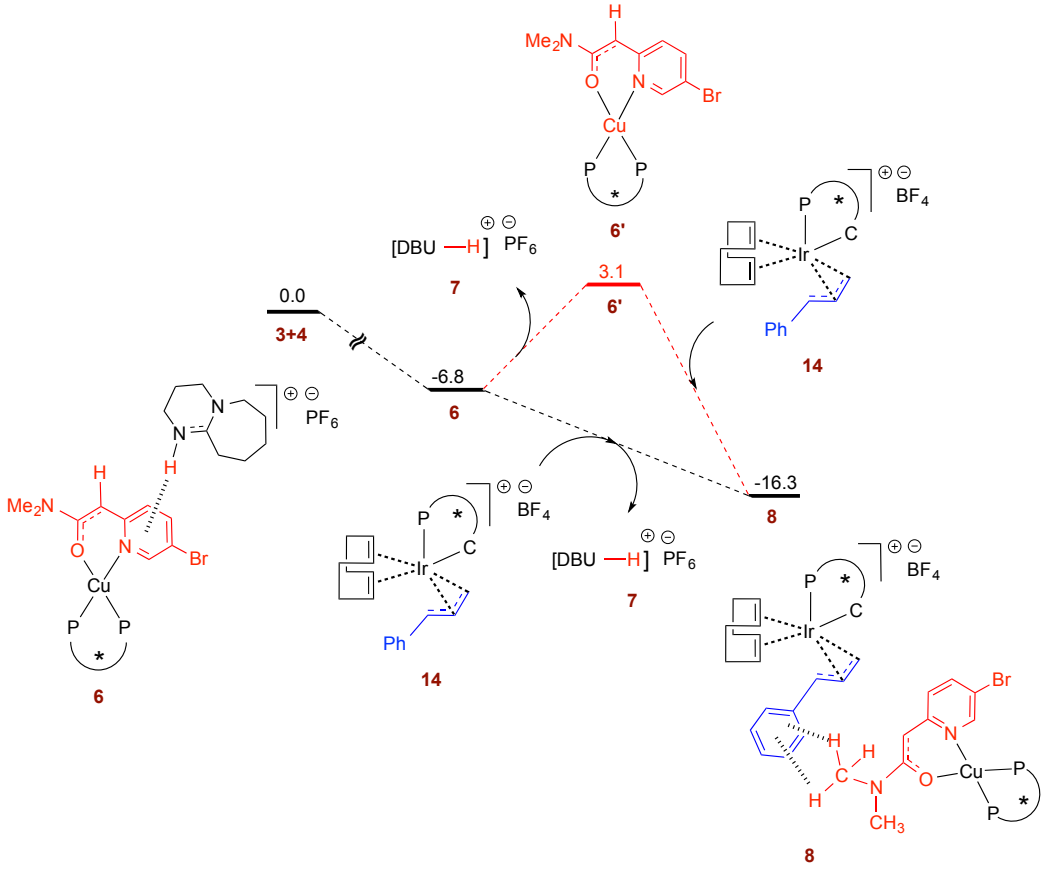


Figure S4. Gibbs Free energy profile for the formation of an intermediate **6'** from **6**.

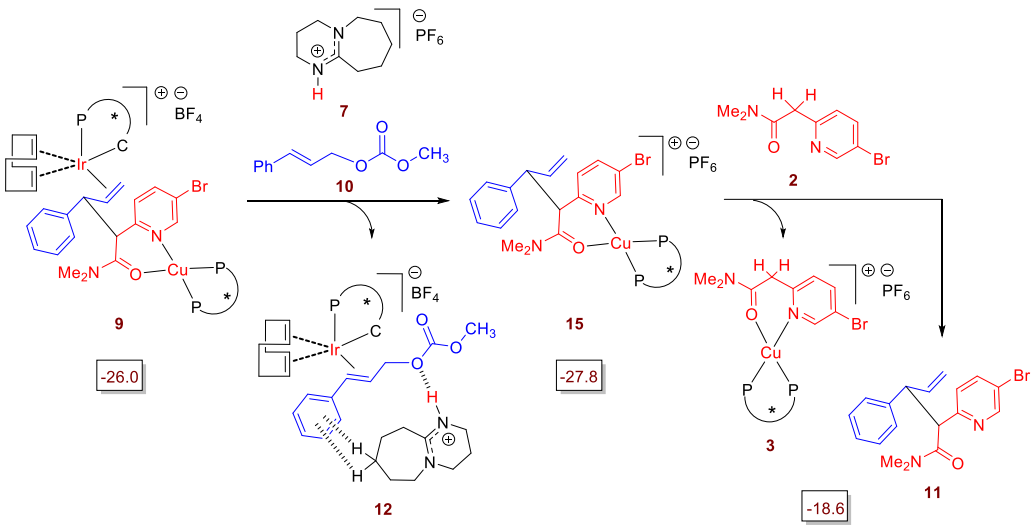
(ii) Different Possibilities for Product Release and the Catalyst Regeneration

One can envisage a step-wise process for the release of the final product **11** from the catalyst-product complex **9**. For instance, incorporation of a molecule of acetonitrile (native ligand in the catalyst precursor) can weaken the binding of **11** to the copper center and thereby open up a coordination site to generate more room for a new molecule of aryl amide (**2**). Similarly, allyl carbonate **10** uptake can help displace the Ir(cod)phosphoramidite from the product complex **9**. Details of different possibilities considered for product release and catalyst regeneration are provided in the following section.

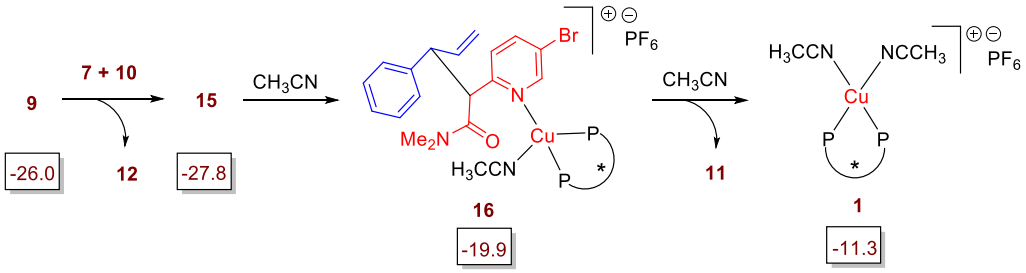
(I) Cinnamyl methyl carbonate **10** uptake along with **7** (protonated DBU) can help displace the Ir(cod)phophoramidite from the product complex **9** thereby resulting in the formation of complex **15** and **12** as shown in Scheme S1(a)-(c). Further uptake by the azaaryl acetamide **2** as shown in Scheme S1(a) or by two molecules of acetonitrile in consecutive steps as in Scheme S1(b) results in the release of the product **11** along with regeneration of the Walphos-

ligated catalyst-substrate adduct **3** and catalyst precursor **1** respectively. The formation of a new catalyst-substrate complex **12** (Scheme 1(c), wherein allyl carbonate **10** is bound to the iridium center is relevant to the ensuing steps furnishing the Ir-π-allyl required for sustaining the catalytic cycle. The intermediate **13** produced via the C–O bond breaking TS **[12-13]**‡ can provide the vital Ir-π-allyl intermediate and a carbonate-DBU adduct.

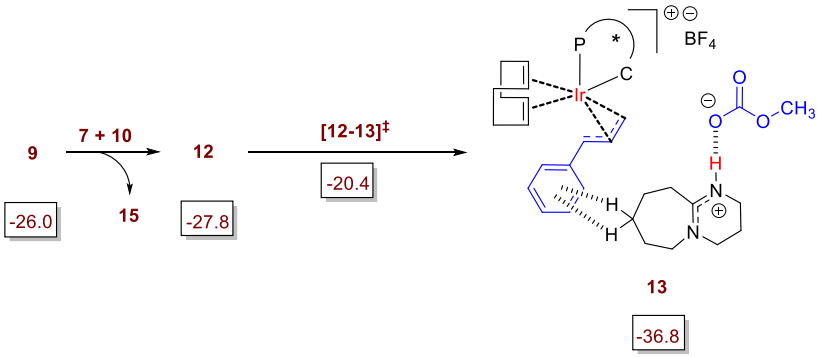
(a)



(b)

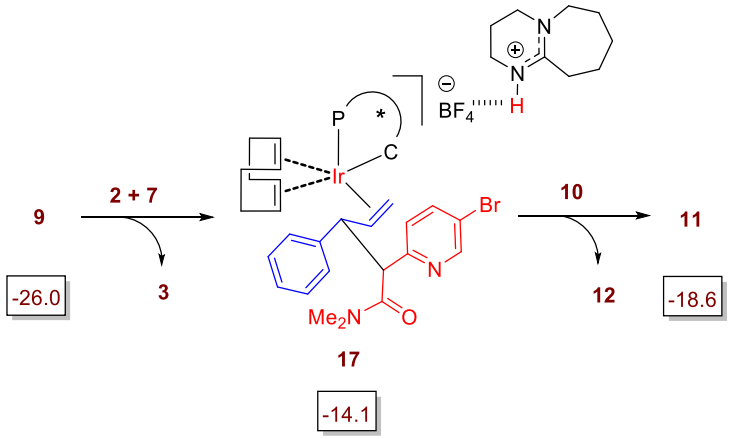


(c)



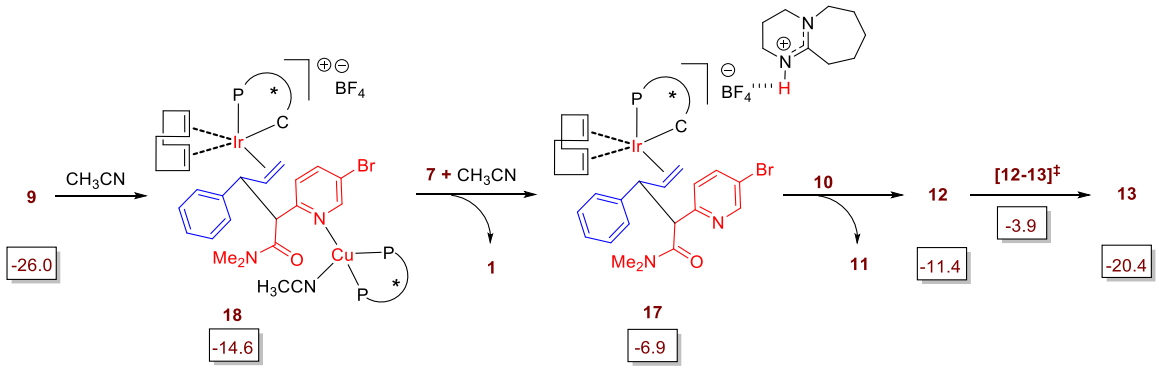
Scheme S1. Step-wise process for the release of the final product **11** from the catalyst-product complex **9** by the uptake of cinnamyl methyl carbonate **10** along with **7** (protonated DBU). The relative Gibbs free energies (in kcal/mol) of the intermediates are provided in the square boxes.

(II) Alternatively, an uptake of azaaryl acetamide **2** along with **7** (protonated DBU) by the catalyst-product complex **9**, as shown in Scheme S2, results in the formation of an intermediate **17** which upon the incorporation of cinnamyl methyl carbonate **10** results in the final release of the product **11** and catalyst-substrate complex **12**.



Scheme S2. Step-wise process for the release of the final product **11** from the catalyst-product complex **9** by the uptake of azaaryl acetamide **2** along with **7** (protonated DBU). The relative Gibbs free energies (in kcal/mol) of the intermediates are provided in the square boxes. Refer to Scheme S1 for additional details of numbering of various species shown here.

(III) Incorporation of a molecule of acetonitrile can weaken the binding of **11** to the copper center and thereby open up a coordination site to generate an intermediate **18** which subsequently takes up another molecule of acetonitrile along with **7** to generate intermediate **17** as shown in Scheme S3. Intermediate **17** provides the key Ir-π-allyl intermediate and a carbonate-DBU adduct **13**, produced via the C–O bond breaking TS **[12-13]**‡ after the incorporation of cinnamyl methyl carbonate **10**.



Scheme S3. Step-wise process for the release of the final product **11** from the catalyst-product complex **9** by the consecutive uptake of two molecules of acetonitrile followed by cinnamyl methyl carbonate **10**. The relative Gibbs free energies (in kcal/mol) of the intermediates are provided in the square boxes. Refer to Scheme S1 for additional details of

numbering of various species shown here.

Comparison of the different possibilities for the final release of the product **11**, reveals that the uptake of substrate, cinnamyl methyl carbonate **10** along with **7** (protonated DBU) resulting in the formation of complexes **15** and **12** as shown as Scheme S1(c) is energetically more feasible. Complex **15** results in the regeneration of the Walphos-ligated catalyst-substrate adduct **3** (Scheme S1(a)) and catalyst precursor **1** (Scheme S1(b)) respectively. To sustain the catalytic process, the regeneration of the Ir-catalyst, should therefore involve the displacement of the product **11** from the product-catalyst complex **9** by a molecule of unreacted substrate **10** (cinnamyl carbonate).

1.4. Energetic Span Model

The energetic span (δE) can be calculated from TOF-determining transition state (TDTS) and TOF-determining intermediate (TDI) as follows,

δE= TDTS – TDI, if TDTS appears after the TDI

δE= TDTS – TDI + ΔG_r, if TDTS appears before the TDI

ΔG_r is the Gibbs free energy of the reaction.

Table S3. Calculation of Energetic Span (δE, in kcal/mol) using Different Likely Combinations of TDI and TDTS for Asymmetric Allylation of Azaaryl Acetamide using Cinnamyl Methyl Carbonate under Dual Catalytic Condition[a]

TDI	TDTS	δE	TDI	TDTS	δE	TDI	TDTS	δE
5	**[5-6]**‡	7.3	**6**	**[5-6]**‡	-13.0	**8**	**[5-6]**‡	-3.5
	[8-9]‡	-5.5		**[8-9]**‡	-5.6		**[8-9]**‡	3.9
	[12-13]‡	-13.5		**[12-13]**‡	-13.6		**[12-13]**‡	-4.1
9	**[5-6]**‡	6.2	**12**	**[5-6]**‡	8.0	**13**	**[5-6]**‡	17.0
	[8-9]‡	-6.6		**[8-9]**‡	-4.8		**[8-9]**‡	4.2
	[12-13]‡	5.6		**[12-13]**‡	7.4		**[12-13]**‡	-3.8

[a]- The *energy span* calculations were done using the Gibbs free energy profile diagram (Figure 1) shown in main text.

1.5. Details of Kinetic Analysis

Kinetic analysis was applied to this catalytic reaction consisting of the Cu-enolate formation, C–C bond formation, generation of Ir-π-allyl intermediate, and Cu-walphos-substrate complex (**3**). Table S4 provides a list of the reactions steps of significance to the kinetic model along with the corresponding free energies of activation for the forward and backward

reactions, and the respective rate constants. The rate constants were calculated using the Eyring equation, at 24.85 °C (298.15 K) as follows,

$$k = \frac{k_B T}{h} e^{\frac{-\Delta G^{\ddagger}}{RT}}$$

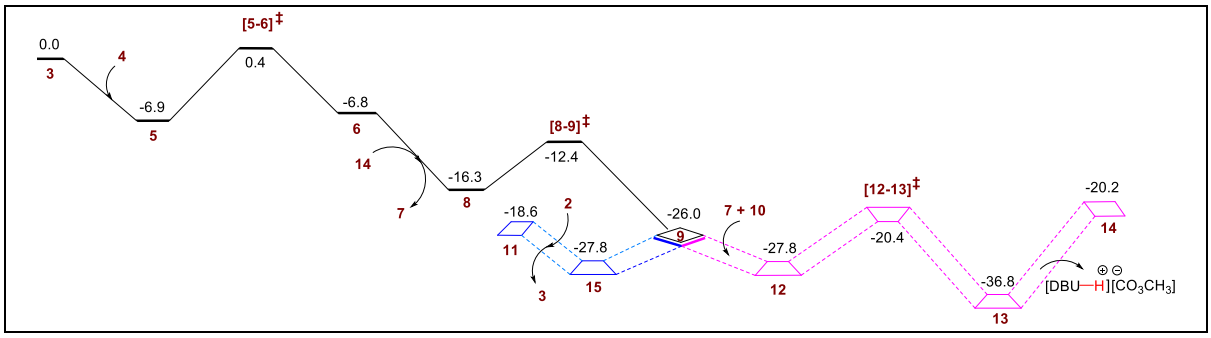
where k is the rate constant, k_B is the Boltzmann constant (kcal K^{-1}), T is the temperature (K), h is the Plank's constant (kcal s), $\Delta G^{\ddagger}$ is the free energy of activation (kcal mol^{-1}), R is the gas constant (kcal mol^{-1} K^{-1}). For barrierless steps, the rate constants were assumed to be equal to the pre-exponential factor in the Eyring equation, $k_BT/h = 6.212\times10^{12}$ $s^{-1}mol^{-2}$ (at 24.85 °C).[1]

Table S4. Rate Constants[2] and Gibbs Free Energies of Activation (kcal mol^{-1})

reaction step		kinetic model	$\Delta G^{\ddagger}_f$	$\Delta G^{\ddagger}_b$	k_f forward	k_b backward
	1	**3 + 4** $\underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}}$ **5**	barrier-less	6.9	6.212×10^{12} ($s^{-1}mol^{-1}$)	5.411×10^{7} (s^{-1})
formation of Cu-enolate	2	**5 + 14** $\underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}}$ **7 + 8**	7.3	16.7	2.754×10^{7} ($s^{-1}mol^{-1}$)	3.522 ($s^{-1}mol^{-1}$)
C–C bond formation	3	**7 + 8 + 10** $\underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}}$ **12 + 15**	3.9	15.4	8.576×10^{9} ($s^{-1}mol^{-2}$)	3.163×10^{1} ($s^{-1}mol^{-1}$)
formation of Ir-π-allyl	4	**12** $\underset{k_{-4}}{\overset{k_4}{\rightleftharpoons}}$ **13**	7.4	16.4	2.326×10^{7} (s^{-1})	5.845 (s^{-1})
regeneration of **14**	5	**13** $\underset{k_{-5}}{\overset{k_5}{\rightleftharpoons}}$ **14** + $[DBU\text{-}H][OCO_2CH_3]$	16.6	barrier -less	4.170 (s^{-1})	6.212×10^{12} ($s^{-1}mol^{-1}$)
regeneration of **3**	6	**15 + 2** $\underset{k_{-6}}{\overset{k_6}{\rightleftharpoons}}$ **3 + 11**	9.2	barrier -less	1.113×10^{6} ($s^{-1}mol^{-1}$)	6.212×10^{12} ($s^{-1}mol^{-1}$)

1) (a) Kalek, M.; Himo, F. Mechanism and selectivity of cooperatively catalyzed Meyer−Schuster rearrangement/Tsuji−Trost allylic substitution. Evaluation of synergistic catalysis by means of combined DFT and kinetics simulations. *J. Am. Chem. Soc*. **2017**, *139*, 10250−10266. (b) Kefalidis, C. E.; Davi, M.; Holstein, P. M.; Clot, E.; Baudoin, O. Mechanistic study of the selectivity of olefin versus cyclobutene formation by palladium(0)-catalyzed intramolecular C(sp^3)−H activation. *J. Org. Chem*. **2014**, *79*, 11903−11910.

2) (a) The calculated rate constants should be regarded only as a decent estimate of the actual rate constants, as the errors in the computed entropies (i) that relies on harmonic oscillator and rigid rotor approximations besides (ii) those in translation entropy introduced through DFT calculations could be large. (b) Harvey, J. N.; Himo, F.; Maseras, F.; Perrin, L. *ACS Catal*. **2019**, *9*, 6803−6813. (c) Besora, M.; Vidossich, P.; Lledos, A.; Ujaque, G.; Maseras, F. Calculation of reaction free energies in solution: A comparison of current approaches. *J. Phys. Chem*. A **2018**, *122*, 1392−1399. (d) Grimme, S. Supramolecular binding thermodynamics by dispersion-corrected density functional theory. *Chem.- Eur. J*. **2012**, *18*, 9955−9964. (e) Marenich, A. V.; Olson, R. M.; Kelly, C. P.; Cramer, C. J.; Truhlar, D. G. Self-consistent reaction field model for aqueous and nonaqueous solutions based on accurate polarized partial charges. J. *Chem. Theory Comput*. **2007**, *3*, 2011−2033. (f) Piccini, G. M.; Sauer, J. Effect of anharmonicity on adsorption thermodynamics. *J. Chem. Theory Comput*. **2014**, *10*, 2479−2487.



It can be noted from Table S4 that the rate constants of most of the forward reactions (entries 1-4, Table S4) are higher than the corresponding backward reactions, except that for **13** and **15**. According to this analysis, complex **13** is the rate-limiting intermediate, which is in line with the TDI identified through the energetic span model.[3] We have carried out microkinetic modeling[4] to examine the concentration evolution of various species with time by using the rate constants of elementary reactions shown in entries 1-6 in Table S4. Shown below are the differential equations (1) to (13) associated with the kinetic model, which were solved for the initial concentrations as given in the experimental procedure.[5] These concentrations are **3** (0.100 mmol), **10** (0.110 mmol), **4** (0.0020 mmol), **14** (0.0010 mmol), and **2** (0.100 mmol). The time evolution obtained using the Euler's numerical integration[6] as shown in Figure S5 indicates the change in the concentration of various species with respect to time. The change in concentration can be expressed as,

$$\{\mathrm{C}(t_{n+1}) = \mathrm{C}(t_n) + \Delta t \times \frac{d}{dt}\mathrm{C}(t_n)\}$$

where, $\mathrm{C}(t_n)$ is the concentration of any species at time t_n, Δt is the time interval between t_n and t_{n+1}, d/dt is the rate of change of concentration of respective species given by the differential equations below,

$$\frac{d[\mathbf{3}]}{dt} = -k_1[\mathbf{3}][\mathbf{4}] + k_{-1}[\mathbf{5}] + k_6[\mathbf{15}][\mathbf{2}] - k_{-6}[\mathbf{3}][\mathbf{11}] \quad (1)$$

$$\frac{d[\mathbf{4}]}{dt} = -k_1[\mathbf{3}][\mathbf{4}] + k_{-1}[\mathbf{5}] \quad (2)$$

3) For energetic span model, see Table S3.

4) (a) Fernandez-Alvarez, V. M.; Nappi, M.; Melchiorre, P.; Maseras, F. Computational study with DFT and kinetic models on the mechanism of photoinitiated aromatic perfluoroalkylations. *Org. Lett.* **2015**, *17*, 2676−2679. (g) Guo, W.; Kuniyil, R.; Gomez, J. E.; Maseras, F.; Kleij, A. W. A domino process toward functionally dense quaternary carbons through Pd-catalyzed decarboxylative C(sp^3)−C(sp^3) bond formation. *J. Am. Chem. Soc*. **2018**, *140*, 3981−3987. (c) Rush, L. E.; Pringle, P. G.; Harvey, J. N. Computational kinetics of cobalt-catalyzed alkene hydroformylation. *Angew. Chem., Int. Ed*. **2014**, *53*, 8672–8676. (d) Besora, M.; Maseras, F. Microkinetic modeling in homogeneous catalysis. *WIREs Comput Mol Sci*. **2018**, e1372.

5) Jiang, X.; Boehm, P.; Hartwig, J. F. Stereodivergent allylation of azaaryl acetamides and acetates by synergistic iridium and copper catalysis. *J. Am. Chem. Soc*. **2018**, *140*, 1239−1242.

6) Chapra, Steven C.; Raymond P. Canale. Numerical methods for engineers. Vol. 2. New York: Mcgraw-hill, 2011.

$$\frac{d[\mathbf{5}]}{dt} = k_1[\mathbf{3}][\mathbf{4}] - k_{-1}[\mathbf{5}] - k_2[\mathbf{5}][\mathbf{14}] + k_{-2}[\mathbf{7}][\mathbf{8}] \quad (3)$$

$$\frac{d[\mathbf{14}]}{dt} = -k_2[\mathbf{5}][\mathbf{14}] + k_{-2}[\mathbf{7}][\mathbf{8}] + k_5[\mathbf{13}] - k_{-5}[\mathbf{14}][(\mathrm{DBUH})(\mathrm{CO_3CH_3})] \quad (4)$$

$$\frac{d[\mathbf{7}]}{dt} = k_2[\mathbf{5}][\mathbf{14}] - k_{-2}[\mathbf{7}][\mathbf{8}] - k_3[\mathbf{7}][\mathbf{8}][\mathbf{10}] + k_{-3}[\mathbf{12}][\mathbf{15}] \quad (5)$$

$$\frac{d[\mathbf{8}]}{dt} = k_2[\mathbf{5}][\mathbf{14}] - k_{-2}[\mathbf{7}][\mathbf{8}] - k_3[\mathbf{7}][\mathbf{8}][\mathbf{10}] + k_{-3}[\mathbf{12}][\mathbf{15}] \quad (6)$$

$$\frac{d[\mathbf{10}]}{dt} = -k_3[\mathbf{7}][\mathbf{8}][\mathbf{10}] + k_{-3}[\mathbf{12}][\mathbf{15}] \quad (7)$$

$$\frac{d[\mathbf{15}]}{dt} = k_3[\mathbf{7}][\mathbf{8}][\mathbf{10}] - k_{-3}[\mathbf{12}][\mathbf{15}] - k_6[\mathbf{15}][\mathbf{2}] + k_{-6}[\mathbf{3}][\mathbf{11}] \quad (8)$$

$$\frac{d[\mathbf{12}]}{dt} = k_3[\mathbf{7}][\mathbf{8}][\mathbf{10}] - k_{-3}[\mathbf{12}][\mathbf{15}] - k_4[\mathbf{12}] + k_{-4}[\mathbf{13}] \quad (9)$$

$$\frac{d[\mathbf{13}]}{dt} = k_4[\mathbf{12}] - k_{-4}[\mathbf{13}] - k_5[\mathbf{13}] + k_{-5}[\mathbf{14}][(\mathrm{DBUH})(\mathrm{CO_3CH_3})] \quad (10)$$

$$\frac{d[(\mathrm{DBUH})(\mathrm{CO_3CH_3})]}{dt} = k_5[\mathbf{13}] - k_{-5}[\mathbf{14}][(\mathrm{DBUH})(\mathrm{CO_3CH_3})] \quad (11)$$

$$\frac{d[\mathbf{2}]}{dt} = -k_6[\mathbf{15}][\mathbf{2}] + k_{-6}[\mathbf{3}][\mathbf{11}] \quad (12)$$

$$\frac{d[\mathbf{11}]}{dt} = k_6[\mathbf{15}][\mathbf{2}] - k_{-6}[\mathbf{3}][\mathbf{11}] \quad (13)$$

For example, the concentration profile shown in Figure S5(c) for specie **3** is calculated as follows,

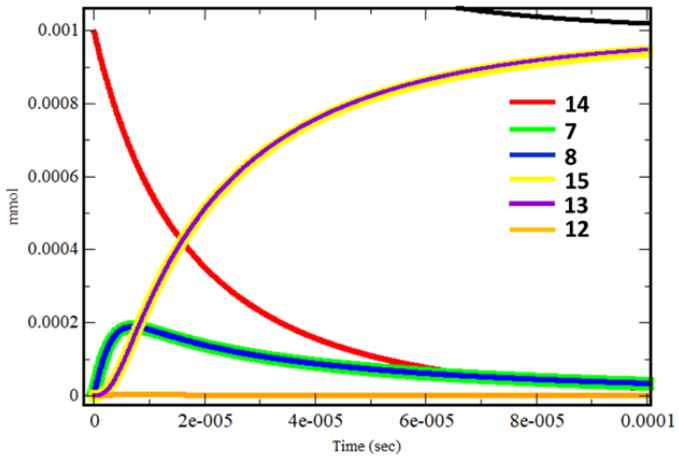
$$[\mathbf{3}]_{t_{n+1}} = [\mathbf{3}]_{t_n} + \Delta t \times (-k_1[\mathbf{3}][\mathbf{4}] + k_{-1}[\mathbf{5}] + k_6[\mathbf{15}][\mathbf{2}] - k_{-6}[\mathbf{3}][\mathbf{11}]) \quad (14)$$

t_n is the current time, t_{n+1} is the next time, Δt is time interval. The equation (14) is solved from time t = 0 to t = 5×10^{-5} as shown in Figure S5(c).

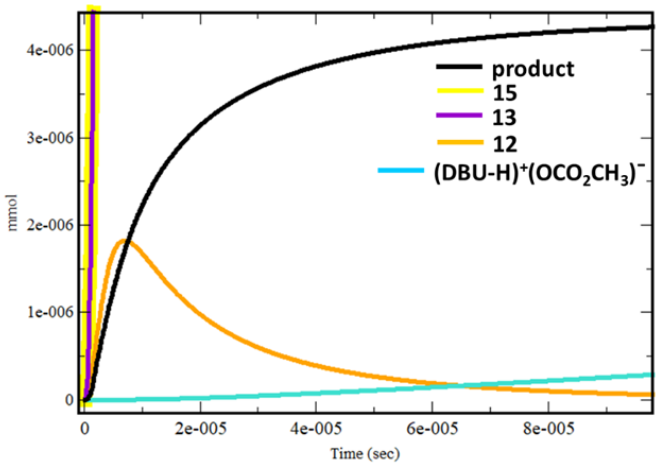
Figure S5(a) depicts the variation in concentration of various intermediates (**7**, **8**, **12**, **13** and **15**) generated during the course of the reaction. The nearly overlapping curves for species **7** (green) and **8** (blue), indicate a rapid increase in concentration and then a gradual decrease, consistent with their consumption as the reaction proceeds. The concentration of species **15** and **13**, shown using overlapping yellow and indigo colored curves, indicates a gradual increase as both of these species are generated in the forward reactions. To inspect the evolution of species **12** (orange) and buildup of the final product **11** (black), an expanded scale of the Y-axis as shown in Figure S5(b) was employed. The concentration of product (**11**) shows a sharp increase. It is noted that **12** is readily consumed as soon as it is formed, thereby making it appear in near-zero concentrations in Figure S5(a). A zoomed out representation of the concentration variation for the primary reactants such as **3**, **4**, **10** and **2** is provided in Figure S5(c-f). A drop in concentration of these species suggests their consumption as the reaction proceeds in the forward direction. Zoomed out picture shown in

Figure S5(g-h) shows a gradual increase in the concentration of species such as **14** and **3** as both of these catalytic active species are regenerated in the later part of the reaction.

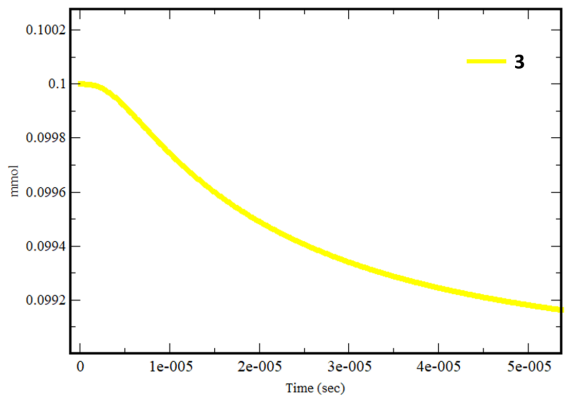
(a)



(b)



(c)



(d)

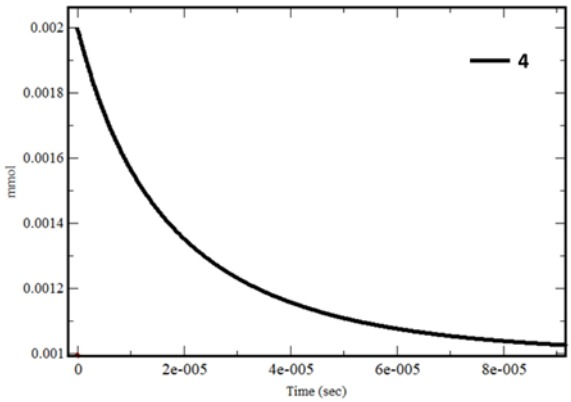


Figure S5 continued…

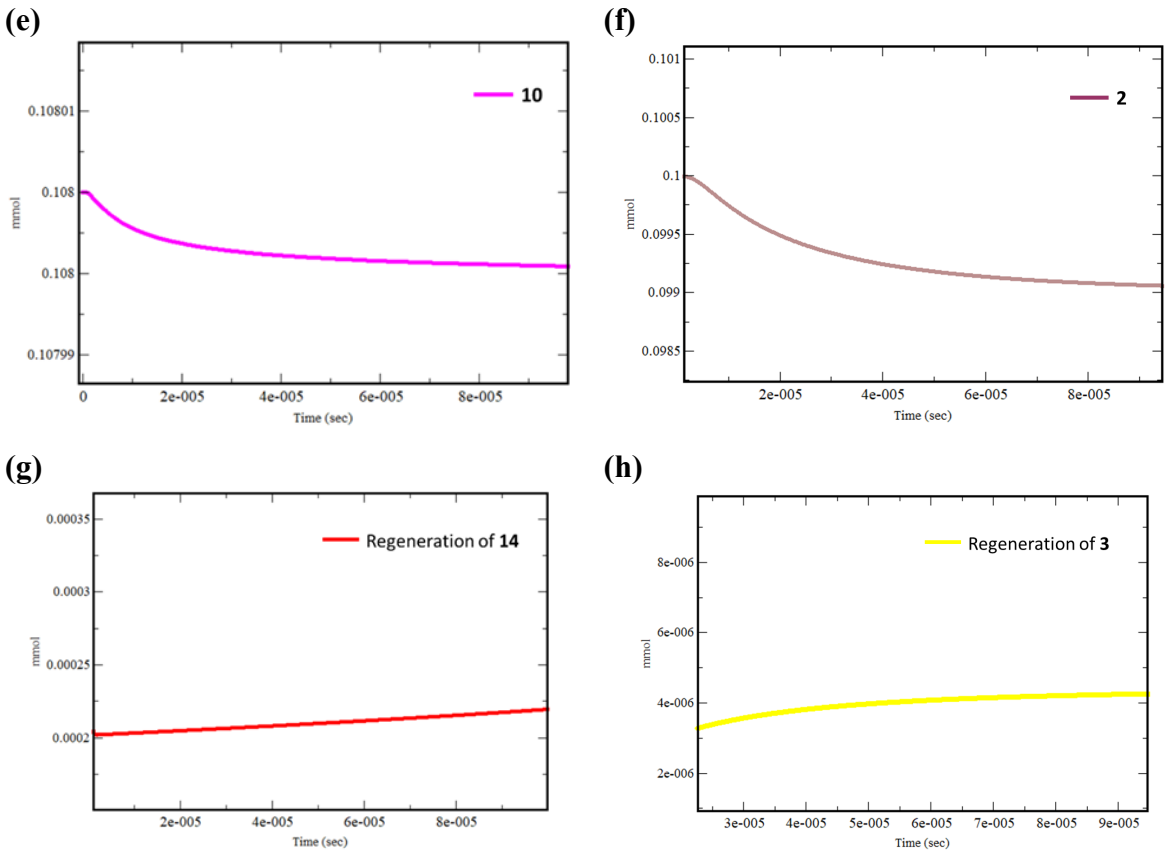


Figure S5. (a) Computed concentration (mmol) of various species and product over time (sec) obtained with DFT method. (b) Zoomed out region of the concentration variation for some selected species.

1.6. Reaction between Cu-enolate and Ir-π-allyl

(i) Different stereochemical modes of addition for the C–C bond formation transition states between Cu-enolate and Ir-π-allyl: Configurational and conformational study

The two reacting partners or substrates are activated by different transition-metal catalysts in separate catalytic events, which resulted in the formation of Cu-enolate and Ir-π-allyl intermediates. These transition-metal catalytic cycles converge in the stereocontrolling C–C bond formation step wherein the nucleophilic and electrophilic reacting partners react through their prochiral faces. This C–C bond formation furnishes two new stereogenic carbon centers in the product. We have considered different stereochemical modes of addition for the C–C bond formation that differ primarily in terms of the open prochiral face provided by the nucleophilic and the electrophilic partners (Figure S6).

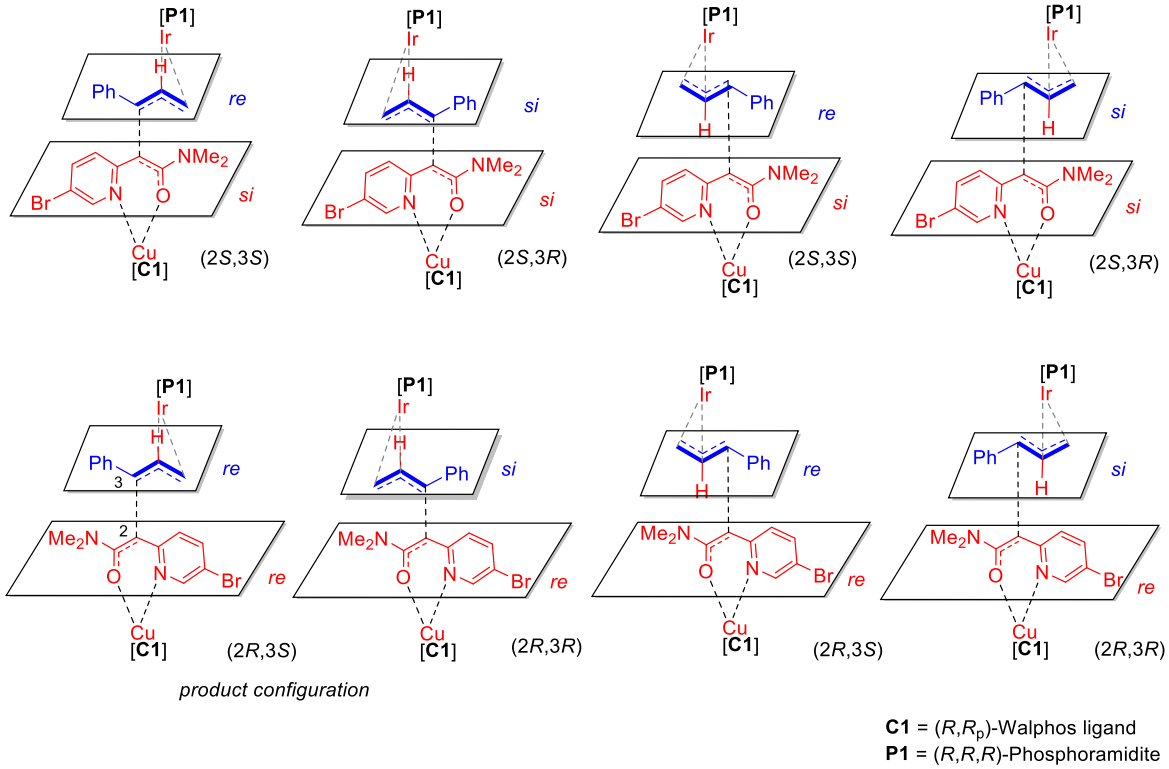


Figure S6. Qualitative representation of different modes of C−C bond formation transition states between Cu-enolate and Ir-π-allyl for the **C1-P1** catalyst dyad. Product configuration at the ensuing stereogenic carbon centers is provided in parentheses. Although the transition states consist of the counter ion (BF_4^-) in the actual computations, it is removed from this figure for improved clarity.

(ii) Energetic details of stereodivergence

Table S5. Relative Gibbs Free Energies (kcal/mol) for the C–C Bond Formation Transition States Involving Different Prochiral Faces of the Cu-enolate (nucleophile) and the Ir-π-allyl Intermediate (electrophile) for Different Catalyst Dyads (Cu-Walphos (**C**) and Ir-Phosphoramidite (**P**)) without BF_4^- Counter Ion Obtained at Different Level of Theories[a]

(a) C1-P1

prochiral faces of **C-P**	product configuration	orientation of Ir-π-allyl	**L1**	**L2**	**L3**	**L4**	**L5**
re-re	(2*R*,3*S*)	*endo*	**0.0**	**0.0**	**0.0**	**0.0**	**0.0**
si-re	(2*S*,3*S*)	*endo*	6.4	5.7	3.7	6.3	3.0
si-si	(2*S*,3*R*)	*endo*	6.7	6.4	4.3	5.9	5.3
re-si	(2*R*,3*R*)	*endo*	6.1	8.1	7.6	7.0	7.5
si-si	(2*S*,3*R*)	*exo*	7.7	4.8	3.0	4.5	4.1
re-si	(2*R*,3*R*)	*exo*	1.2	1.6	1.5	1.8	2.2
si-re	(2*S*,3*S*)	*exo*	16.3	17.1	12.9	17.0	14.8
re-re	(2*R*,3*S*)	*exo*	9.4	10.7	8.9	10.6	10.5

Table S5 continued…

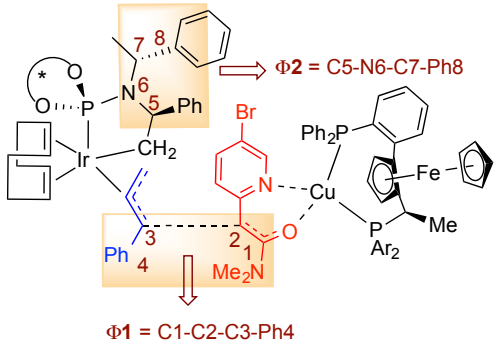
(b) C2-P1							
prochiral faces of **C-P**	product configuration	orientation of Ir-π-allyl	**L1**	**L2**	**L3**	**L4**	**L5**
re-re	(2*R*,3*S*)	*endo*	6.8	7.4	5.6	5.7	6.1
si-re	(2*S*,3*S*)	*endo*	**0.0**	**0.0**	**0.0**	**0.0**	**0.0**
si-si	(2*S*,3*R*)	*endo*	5.8	7.4	6.9	4.4	6.2
re-si	(2*R*,3*R*)	*endo*	13.1	14.0	11.4	11.8	10.8
si-si	(2*S*,3*R*)	*exo*	2.7	4.1	2.2	2.9	3.0
re-si	(2*R*,3*R*)	*exo*	11.6	12.5	8.7	12.6	8.7
si-re	(2*S*,3*S*)	*exo*	11.8	13.0	13.1	13.0	12.0
re-re	(2*R*,3*S*)	*exo*	9.9	10.0	8.8	9.5	10.1
(c) C2-P2							
prochiral faces of **C-P**	product configuration	orientation of Ir-π-allyl	**L1**	**L2**	**L3**	**L4**	**L5**
re-re	(2*R*,3*S*)	*endo*	6.7	6.4	4.3	5.9	5.3
si-re	(2*S*,3*S*)	*endo*	6.1	8.1	7.6	7.0	7.5
si-si	(2*S*,3*R*)	*endo*	**0.0**	**0.0**	**0.0**	**0.0**	**0.0**
re-si	(2*R*,3*R*)	*endo*	6.4	5.7	3.7	6.3	3.0
si-si	(2*S*,3*R*)	*exo*	9.4	10.7	8.9	10.6	10.5
re-si	(2*R*,3*R*)	*exo*	16.3	17.1	12.9	17.0	14.8
si-re	(2*S*,3*S*)	*exo*	1.2	1.6	1.5	1.8	2.2
re-re	(2*R*,3*S*)	*exo*	7.7	4.8	3.0	4.5	4.1
(d) C1-P2							
prochiral faces of **C-P**	product configuration	orientation of Ir-π-allyl	**L1**	**L2**	**L3**	**L4**	**L5**
re-re	(2*R*,3*S*)	*endo*	5.8	7.4	6.9	4.4	6.2
si-re	(2*S*,3*S*)	*endo*	13.1	14.0	11.4	11.8	10.8
si-si	(2*S*,3*R*)	*endo*	6.8	7.4	5.6	5.7	6.1
re-si	(2*R*,3*R*)	*endo*	**0.0**	**0.0**	**0.0**	**0.0**	**0.0**
si-si	(2*S*,3*R*)	*exo*	9.9	10.0	8.8	9.5	10.1
re-si	(2*R*,3*R*)	*exo*	11.8	13.0	13.1	13.0	12.0
si-re	(2*S*,3*S*)	*exo*	11.6	12.5	8.7	12.6	8.7
re-re	(2*R*,3*S*)	*exo*	2.7	4.1	2.2	2.9	3.0

[a]-**L1** = $SMD_{(THF)}$/B3LYP-D3/6-31G**,SDD(Ir,Cu,Fe,Br); **L2**=$SMD_{(THF)}$/wB97X-D/6-311G**,def2-TZVP(Ir,Br,Fe,Cu)//**L1**; **L3**=$SMD_{(THF)}$/M06-L/6-311G**,def2-TZVP(Ir,Br,Fe,Cu)//**L1**; **L4**=$SMD_{(THF)}$/M06-D3/6-311G**,def2-TZVP(Ir,Br,Fe,Cu)//**L1**; **L5**=$SMD_{(THF)}$/M06/6-311G**,def2-TZVP(Ir,Br,Fe,Cu)//**L1**

(iii) Conformational analysis of transition states for the C–C bond formation between Cu-enolate and Ir-π-allyl intermediate

Key dihedral angles Φ1, Φ2, Φ3, Φ4, Φ5 and Φ6 are employed in the conformational sampling for the stereoselective C–C bond formation transition states.

Table S6. Relative Gibbs Free Energies (kcal/mol) for the C–C Bond Formation Transition States Involving Different Prochiral Faces of the Cu-enolate (nucleophile) and the Ir-π-allyl Intermediate (electrophile) Obtained at the $SMD_{(THF)}$/B3LYP-D3/6-31G**,SDD(Ir,Cu,Fe,Br) Level of Theory for Different Catalyst Dyad (Cu-Walphos (**C**) and Ir-Phosphoramidite (**P**)) without BF_4^- Counter Ion

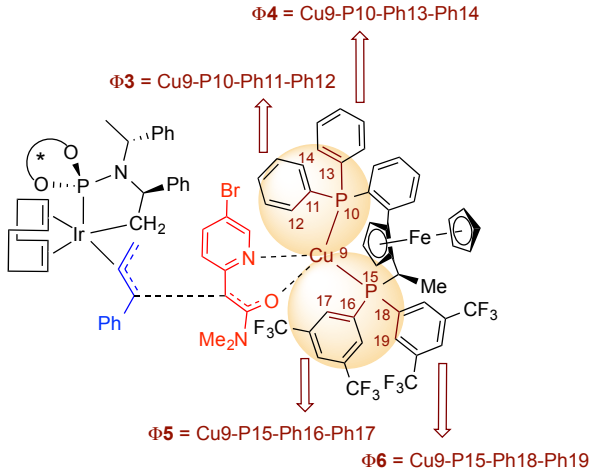


prochiral faces of **C-P**	Dihedral angel (Φ1)	Dihedral angel (Φ2)	ΔG (kcal/mol)
	C1-P1		
*re-re*_1	47.9	74.4	0.0
*re-re*_2	92.1	-85.9	0.8
*re-re*_3	48.5	-73.0	3.8
*re-re*_4	91.4	-86.2	0.6
*re-re*_5	-97.3	70.6	5.9
*re-re*_6	-94.8	65.9	1.8
*si-re*_1	164.8	70.1	7.3
*si-re*_3	165.3	-72.9	8.6
*si-re*_6	166.2	-135.9	11.5
*si-re*_8	164.9	70.4	6.4
*si-si*_1	46.1	67.6	12.0
*si-si*_2	179.2	72.3	7.8
*si-si*_3	151.3	69.1	8.1
*si-si*_4	-169.4	-88.7	7.7
*si-si*_5	150.8	-73.1	9.3
*si-si*_6	151.1	-70.7	8.4
*si-si*_7	-169.4	-88.7	7.6
*si-si*_8	179.1	72.2	7.8
*si-si*_9	105.6	70.1	11.9
*re-si*_1	-103.1	-67.1	5.4
*re-si*_2	45.9	54.8	3.2
*re-si*_3	-169.4	-88.6	7.7
*re-si*_4	68.1	56.4	1.1
*re-si*_5	27.9	75.4	2.4
	C2-P1		
*re-re*_1	-99.8	64.5	14.4
*re-re*_2	-178.0	-135.8	16.9
*re-re*_3	-118.2	69.7	15.5
*re-re*_4	56.9	74.6	6.7

Table S6 continued…

re-re_5	56.4	-76.9	11.2
si-re_1	172.5	76.2	0
si-re_2	172.8	-87.6	4.5
si-re_3	173.2	-71.6	3.9
si-re_4	-32.5	128.2	7.6
si-re_5	75.4	67.4	6.7
si-re_6	107.7	74.9	6.5
si-re_7	171.6	-141.4	6.2
si-re_8	173.2	-71.6	3.8
si-si_1	158.1	-88.9	7.4
si-si_2	150.9	72.6	2.7
si-si_3	158.6	-68.6	6.9
si-si_4	79.0	71.4	5.7
si-si_5	150.9	72.6	2.7
si-si_6	152.1	-72.8	5.1
re-si_1	143.4	44.3	19.9
re-si_2	-56.2	-142.3	17.4
re-si_3	-55.7	65.9	11.6
re-si_4	152.5	-83.7	13.9
re-si_5	-58.9	-68.7	14.6

Table S7. Relative Gibbs Free Energies (kcal/mol) for the C–C Bond Formation Transition States Involving Different Prochiral Faces of the Cu-enolate (nucleophile) and the Ir-π-allyl Intermediate (electrophile) and Different Conformers of Walphos-ligated Cu-enolate Obtained at the $SMD_{(THF)}$/B3LYP-D3/6-31G**,SDD(Ir,Cu,Fe,Br) Level of Theory for **C1-P1** Catalyst Dyad (Cu-Walphos (**C**) and Ir-Phosphoramidite (**P**)) without BF_4^- Counter Ion



Conformer	ΔG (kcal/mol)
Conformer_1	-0.01
Conformer_2	0.00
Conformer_3	-0.02
Conformer_4	1.14

Table S7 continued…

*Conformer*_5	-0.01
*Conformer*_6	-0.01
*Conformer*_7	-0.01
*Conformer*_8	-0.01
*Conformer*_9	0.00
*Conformer*_10	0.00
*Conformer*_11	-0.01
*Conformer*_12	0.01
*Conformer*_13	0.01
*Conformer*_14	0.00
*Conformer*_15	0.00
*Conformer*_16	-0.01
*Conformer*_17	-0.01
*Conformer*_18	-0.01
Walphos-ligated Cu-enolate Conformers	
*Conformer*_1	1.47
*Conformer*_2	0.73
*Conformer*_3	0.02
*Conformer*_4	0.01
*Conformer*_5	0.00
*Conformer*_6	0.87
*Conformer*_7	0.60
*Conformer*_8	0.59
*Conformer*_9	0.61
*Conformer*_10	0.22
*Conformer*_11	0.22
*Conformer*_12	0.60
*Conformer*_13	0.61
*Conformer*_14	0.59
*Conformer*_15	0.74
*Conformer*_16	0.63
*Conformer*_17	0.60
*Conformer*_18	0.60
*Conformer*_19	0.60
*Conformer*_20	0.76
*Conformer*_21	0.60
*Conformer*_22	0.60
*Conformer*_23	0.61
*Conformer*_24	0.62
*Conformer*_25	0.60
*Conformer*_26	0.60
*Conformer*_27	0.60
*Conformer*_28	0.60
*Conformer*_29	0.87
*Conformer*_30	0.59

Table S8. Relative Gibbs Free Energies (kcal/mol) for the C–C Bond Formation Transition States Involving Different Prochiral Faces of the Cu-enolate (nucleophile) and the Ir-π-allyl Intermediate (electrophile) for Different Catalyst Dyads (Cu-Walphos (**C**) and Ir-Phosphoramidite (**P**)) with BF_4^- Counter Ion Obtained at Different Level of Theories[a]

(a) C1-P1

prochiral faces of **C-P**	product configuration	orientation of Ir-π-allyl	**L1**	**L2**	**L3**	**L4**	**L5**
re-re	(2*R*,3*S*)	*endo*	**0.0**	**0.0**	**0.0**	**0.0**	**0.0**
si-re	(2*S*,3*S*)	*endo*	7.6	6.0	6.5	6.4	5.3
si-si	(2*S*,3*R*)	*exo*	12.8	8.2	6.6	6.9	8.2
re-si	(2*R*,3*R*)	*exo*	2.7	5.2	2.2	2.0	5.4

(b) C2-P1

prochiral faces of **C-P**	product configuration	orientation of Ir-π-allyl	**L1**	**L2**	**L3**	**L4**	**L5**
re-re	(2*R*,3*S*)	*endo*	4.8	5.5	4.9	5.6	3.7
si-re	(2*S*,3*S*)	*endo*	**0.0**	**0.0**	**0.0**	**0.0**	**0.0**
si-si	(2*S*,3*R*)	*exo*	1.5	3.1	3.2	4.6	3.1
re-si	(2*R*,3*R*)	*exo*	9.3	11.2	7.3	6.1	10.3

(c) C2-P2

prochiral faces of **C-P**	product configuration	orientation of Ir-π-allyl	**L1**	**L2**	**L3**	**L4**	**L5**
re-re	(2*R*,3*S*)	*exo*	12.8	8.2	6.5	6.8	8.1
si-re	(2*S*,3*S*)	*exo*	2.7	5.2	2.2	2.0	5.3
si-si	(2*S*,3*R*)	*endo*	**0.0**	**0.0**	**0.0**	**0.0**	**0.0**
re-si	(2*R*,3*R*)	*endo*	7.6	6.0	6.5	6.4	5.3

(d) C1-P2

prochiral faces of **C-P**	product configuration	orientation of Ir-π-allyl	**L1**	**L2**	**L3**	**L4**	**L5**
re-re	(2*R*,3*S*)	*exo*	1.5	3.1	3.2	4.6	3.1
si-re	(2*S*,3*S*)	*exo*	9.3	11.2	7.3	6.1	10.3
si-si	(2*S*,3*R*)	*endo*	4.8	5.5	4.9	5.6	3.7
re-si	(2*R*,3*R*)	*endo*	**0.0**	**0.0**	**0.0**	**0.0**	**0.0**

[a]-**L1** = $SMD_{(THF)}$/B3LYP-D3/6-31G**,SDD(Ir,Cu,Fe,Br); **L2**=$SMD_{(THF)}$/wB97X-D/6-311G**,def2-TZVP(Ir,Br,Fe,Cu)//**L1**; **L3**=$SMD_{(THF)}$/M06-L/6-311G**,def2-TZVP(Ir,Br,Fe,Cu)//**L1**; **L4**=$SMD_{(THF)}$/M06-D3/6-311G**,def2-TZVP(Ir,Br,Fe,Cu)//**L1**; **L5**=$SMD_{(THF)}$/M06/6-311G**,def2-TZVP(Ir,Br,Fe,Cu)//**L1**

1.7. Space filling model for C2-P1 catalytic dyad

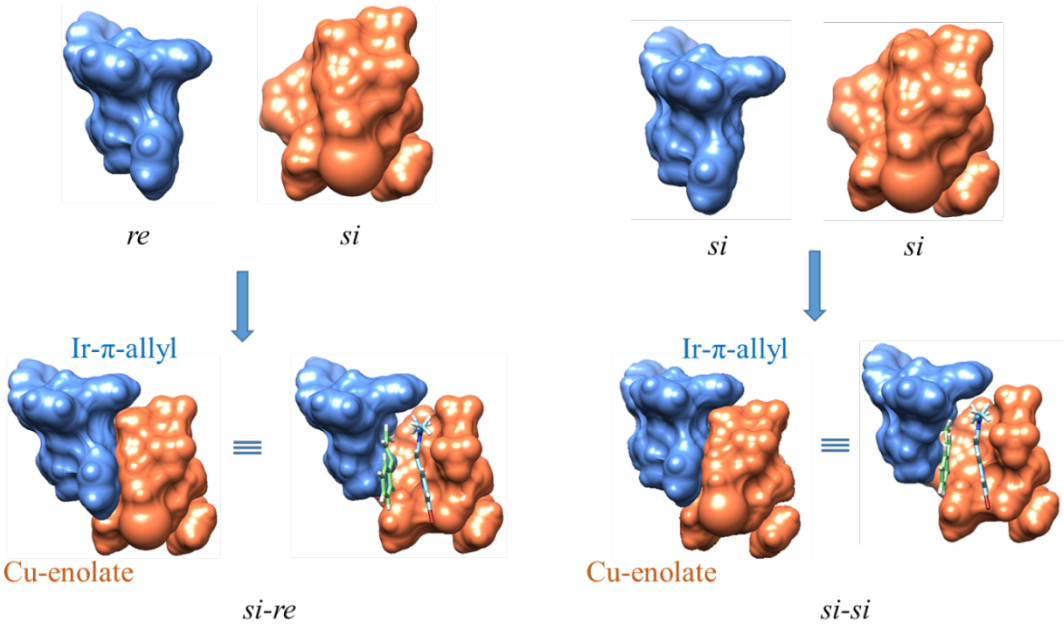


Figure S7. The space-filling representations for the **C2-P1** catalytic dyad for the reacting partners (Cu-enolate and Ir-π-allyl) are shown in the top row and the corresponding C–C bond formation TSs conveying the contact between the chiral catalysts and the chiral cavity provided by the catalysts in the bottom row. In the second row, chiral catalysts are shown using space-filling model and a stick model is used for the substrates. Although the transition states consist of the counter ion (BF_4^-) in the actual computations, it is removed from this figure for improved clarity.

1.8. Global Contact Surface Area, Catalyst Cavity Volume, and Solvent Accessible Surface Area

Global contact surface area[7] between the two interacting catalysts, namely, chiral Cu-Walphos and Ir-phosphoramidite catalysts is calculated as follows,

Contact_area = [(Cu-Walphos_area + Ir-phosphoramidite_area) – (Complex_area)]/2

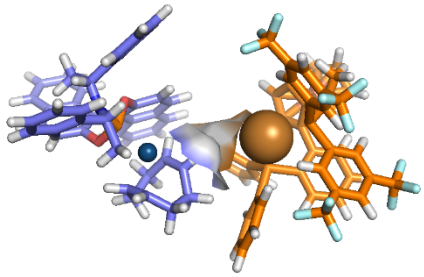
If only a single global contact surface is calculated, a selection named "contact" is created that includes all receptor atoms within 3.9 Å of any atom of the catalyst. The area has to be normalized since it is counted twice (once on Cu-Walphos and once on Ir-phosphoramidite).

7) (a) Ribeiro, J.; Rıos-Vera, C.; Melo, F.; Schuller, A. Calculation of accurate interatomic contact surface areas for the quantitative analysis of non-bonded molecular interactions. *Bioinformatics* **2019**, *35*, 3499–3501. (b) Klenin, K. V.; Tristram, F.; Strunk, T.; Wenzel, W. Derivatives of molecular surface area and volume: Simple and exact analytical formulas. *J. Comput. Chem*. **2011**, *32*, 2647–2653. (c) Bauer, T. L.; Buchholz, P. C. F.; Pleiss, J. *FEBS J*. **2019**. https://doi.org/10.1111/febs.15071

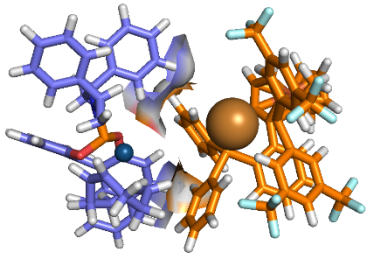
The complex area takes into account the non-normal portions of the area that lie buried inside the other catalyst surface and hence need not be counted (Table S9).

Table S9. Calculation of Global Contact Surface Area (in Å^2) between the two chiral Cu-Walphos and Ir-phosphoramidite catalysts for all the catalyst dyads[a]

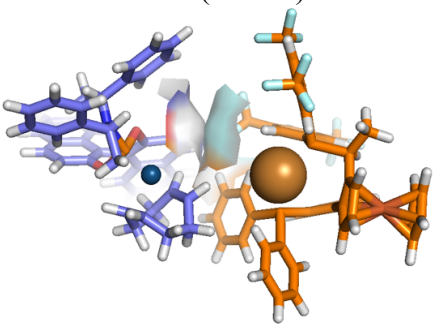
prochiral faces of **C-P**	product confign.	**C1-P1**	**C2-P1**	**C2-P2**	**C1-P2**
re-re	(2*R*,3*S*)	123.8	127.1	126.8	135.6
si-re	(2*S*,3*S*)	101.6	142.7	135.7	44.4
si-si	(2*S*,3*R*)	126.8	135.6	123.8	127.1
re-si	(2*R*,3*R*)	135.7	44.4	101.6	142.7



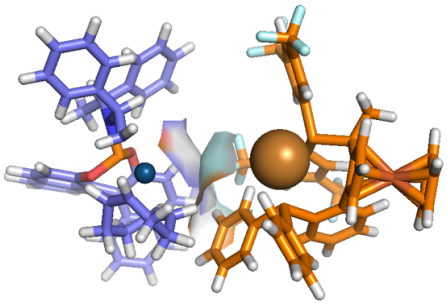
re-re **(C1-P1)**



re-si **(C1-P1)**



si-re **(C2-P1)**



si-si **(C2-P1)**

[a] counter ion (BF_4^-) is removed from figures for improved clarity.

Analysis of contact surface area reveals that the contact region between the chiral catalysts in the lower energy *re-re* mode of addition is lesser than that in the *re-si* mode for the **C1-P1** catalyst dyad whereas an opposite trend is noticed for the **C2-P1** catalyst dyad where the lower energy *si-re* mode of addition have larger contact area than that in the corresponding higher energy *si-si* mode of addition. The same is evident from the noncovalent interactions mapped through AIM analysis wherein examples with lower contact area exhibited lesser number of favourable interactions as compared to the ones with higher contact area results in more number of favourable interactions between the two chiral catalysts as shown in Figures S9 and S10.

Table S10. Calculation of Catalyst Cavity Volume (Å^3) for *re-re* (low) and *re-si* (high) TSs with **C1-P1** Catalyst

Both catalyst of *re-re* at probe 6 Shell volume (probe radius of 6.0 Å)	Both catalyst of *re-re* at probe 1.5 Solvent-excluded volume (probe radius of 1.5 Å)
2226	1912
Solvent Volume = shell volume–solvent-excluded volume	
Solvent Volume	314
Both catalyst of *re-si* at probe 6 Shell volume (probe radius of 6.0 Å)	Both catalyst of *re-si* at probe 1.5 Solvent-excluded volume (probe radius of 1.5 Å)
2199	1895
Solvent Volume = shell volume–solvent-excluded volume	
Solvent Volume	304

Table S11. Calculation of Catalyst Cavity Volume (Å^3) for *si-re* (low) and *si-si* (high) with **C2-P1** Catalyst

Both catalyst of *si-re* at probe 6 shell volume (probe radius of 6.0 Å)	Both catalyst of *si-re* at probe 1.5 solvent-excluded volume (probe radius of 1.5 Å)
2217	1911
Solvent Volume = shell volume–solvent-excluded volume	
Solvent Volume	306
Both catalyst of *si-si* at probe 6 shell volume (probe radius of 6.0 Å)	Both catalyst of *si-si* at probe 1.5 solvent-excluded volume (probe radius of 1.5 Å)
2245	1936
solvent solume = shell volume–solvent-excluded volume	
Solvent Volume	309

Table S12. Calculation of Solvent Accessible Surface Area (Å^2) for **C1-P1** and **C2-P1**

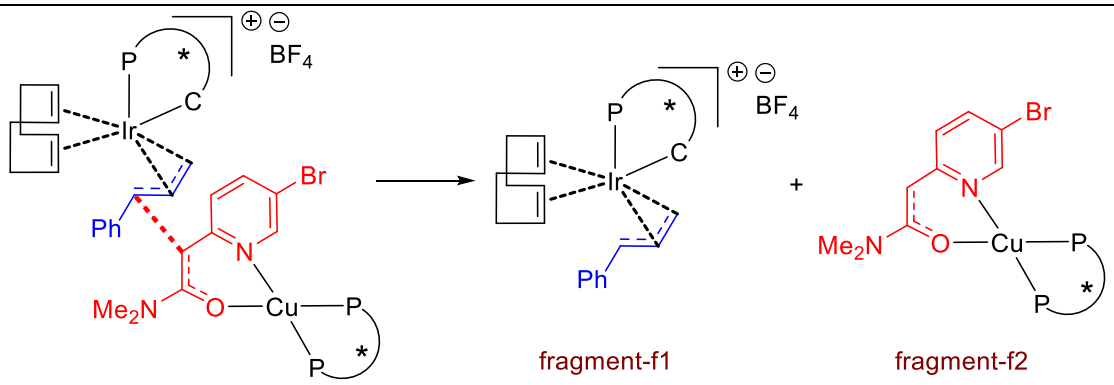
	C1-P1			**C2-P1**	
	re-re	*re-si*		*si-re*	*si-si*
TS	1046	1029	TS	1039	1035
catalyst	1038	1003	catalyst	1009	1013
substrates	295	302	substrates	293	297

Solvent Accessible Surface Area = (Catalyst + Substrates) – TS at probe 3 Å^2			
re-re	*re-si*	*si-re*	*si-si*
287	276	263	275

1.9. Activation strain analysis

For rationalizing the energetic preference for various modes of additions between the nucleophile (Cu-enolate) and electrophile (Ir-π-allyl), the activation strain analysis is applied to the stereo-determining transition states. Following fragments, f1=Ir-π-allyl and f2=Cu-enolate are used in our computations (Table S13).

Table S13. Computed Relative Distortion Energies in each Fragment, Total Relative Distortion Energies ($\Delta\Delta E^{\ddagger}_{d}$) and Relative Interaction Energies ($\Delta\Delta E^{\ddagger}_{i}$) (in kcal/mol) in the Stereocontrolling TSs at the $SMD_{(THF)}$/B3LYP-D3/6-31G**,SDD(Ir,Cu,Fe,Br) Level of Theory[a] All Energies are in kcal/mol



mode of addition	$\Delta\Delta E^{\ddagger}_{d}$ (f1)	$\Delta\Delta E^{\ddagger}_{d}$ (f2)	total $\Delta\Delta E^{\ddagger}_{d}$ [$\Delta\Delta E^{\ddagger}_{d}$ (f1) + $\Delta\Delta E^{\ddagger}_{d}$ (f2)]	$\Delta\Delta E^{\ddagger}_{i}$	$\Delta\Delta E^{\ddagger}$ [$\Delta\Delta E^{\ddagger}_{d}$ + $\Delta\Delta E^{\ddagger}_{i}$]
			C1-P1		
re-re	0.0	0.0	0.0	0.0	0.0
re-si	5.5	0.6	6.1	-3.5	2.6
si-si	8.8	7.6	16.4	-3.0	13.4
			C2-P1		
si-re	0.0	0.0	0.0	0.0	0.0
si-si	6.7	-0.1	6.6	-4.5	2.1
re-si	0.5	5.4	5.9	5.7	11.6
			C2-P2		
si-si	0.0	0.0	0.0	0.0	0.0
si-re	5.5	0.6	6.1	-3.5	2.6
re-re	8.8	7.6	16.4	-3.0	13.4
			C1-P2		
re-si	0.0	0.0	0.0	0.0	0.0
re-re	6.7	-0.1	6.6	-4.5	2.1
si-re	0.5	5.4	5.9	5.7	11.6

[a]-Relative energies with respect to lower energy TS in each catalyst dyad.

The distortion energy of both the fragments f1 and f2 of the higher energy transition state is presented with respect to the fragments f1 and f2 of the lowest energy transition state

(Table S13). For the **C1-P1** catalyst combination, the distortion energies of f1 and f2 are 5.5 kcal/mol and 0.6 kcal/mol higher in *re-si* TS compared to *re-re* TS. However, the interaction energy between the two fragments in the *re-si* TS is 3.5 kcal/mol lower than in the *re-re* TS. Thus, the net balance between the destabilizing distortion and stabilization interaction results in an overall stabilization of *re-re* TS by 2.6 kcal/mol. Similarly in the case of **C2-P1** catalyst combination, the fragment f1of *si-si* TS is distorted by 6.7 kcal/mol as compared to the f1 of *si-re* TS whereas f2 of *si-re* TS is distorted by only 0.1 kcal/mol as compared to f2 of *si-si* TS. In *si-si* TS, an improved interaction energy by 4.5 kcal/mol is noted than that in *si-re* TS. The net balance between the destabilizing distortion and stabilizing interaction energies results in an overall stabilization of *si-re* TS by 2.1 kcal/mol. It can be noted from Figure 8 that Ir-π-allyl fragment experiences a higher distortion and thus can be considered as a major factor contributing to the energy difference between the stereo-determining TSs in both the catalyst combination.

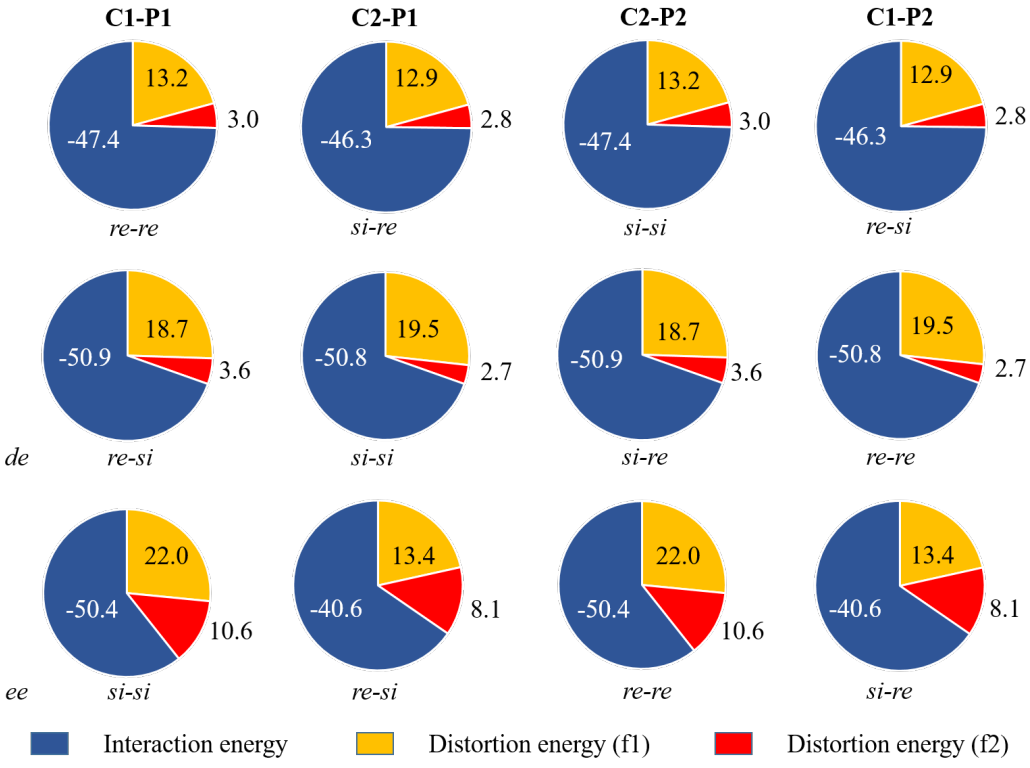
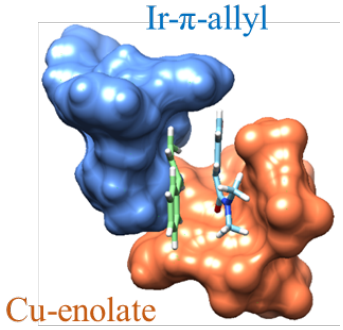


Figure 8. Computed distortion ($\Delta\Delta E^{\ddagger}_{d}$) and interaction ($\Delta\Delta E^{\ddagger}_{i}$) energies (kcal/mol) for the stereocontrolling TSs with respect to the separated reactants for each of the catalyst dyad.

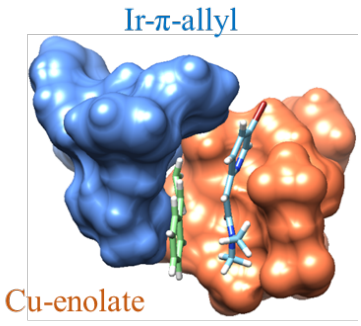
1.10. Optimized Geometries of Stereocontrolling Transition States

(i) C1-P1 Catalyst Dyad

(a) Space filling models of TSs $[8\text{-}9]_{re\text{-}re}^{\ddagger}$ and $[8\text{-}9]_{re\text{-}si}^{\ddagger}$ for the *re-re* and *re-si* modes of addition between Cu-enolate (nucleophile) and Ir-π-allyl intermediate (electrophile)



re-re



re-si

(b) NCIs interactions in the TSs

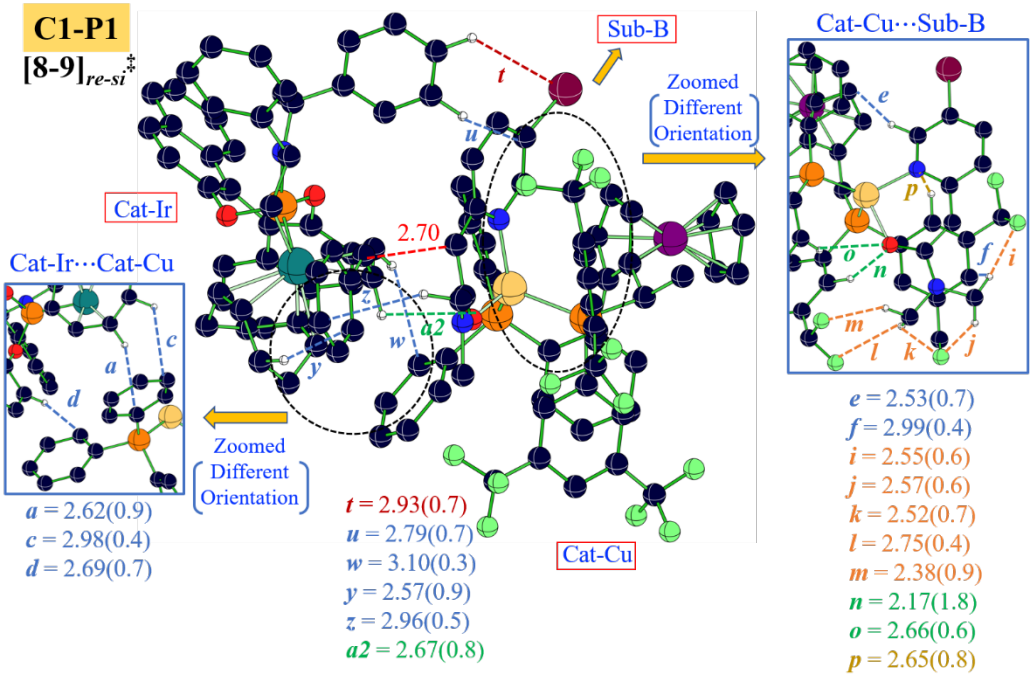
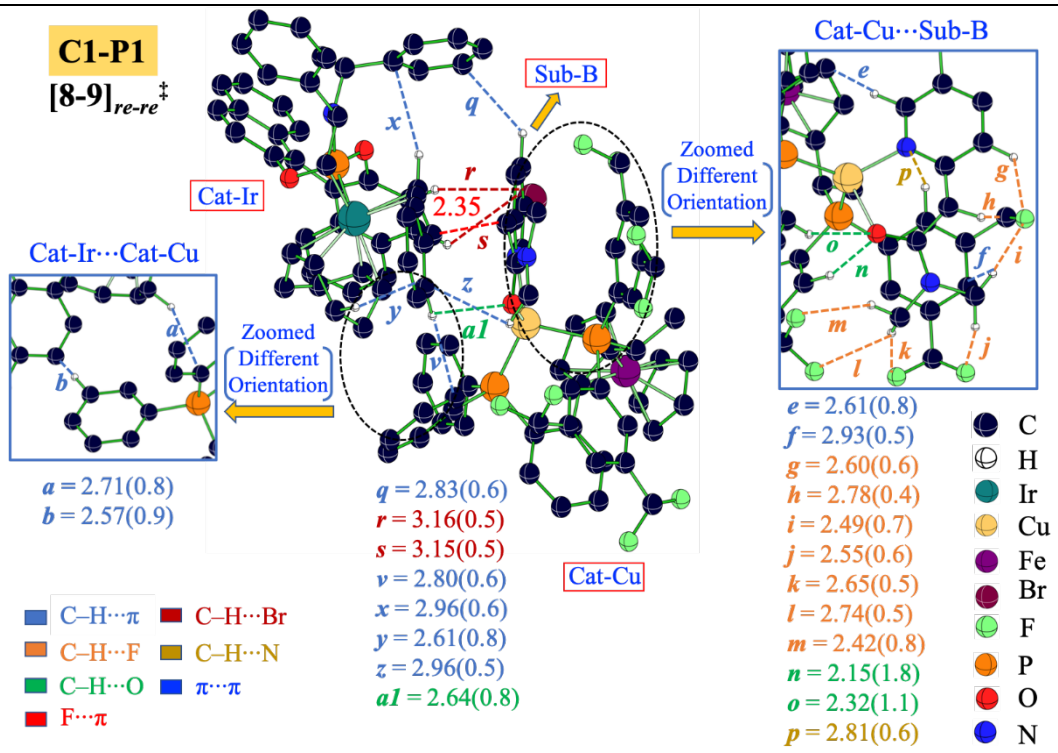


Figure S9 continued…



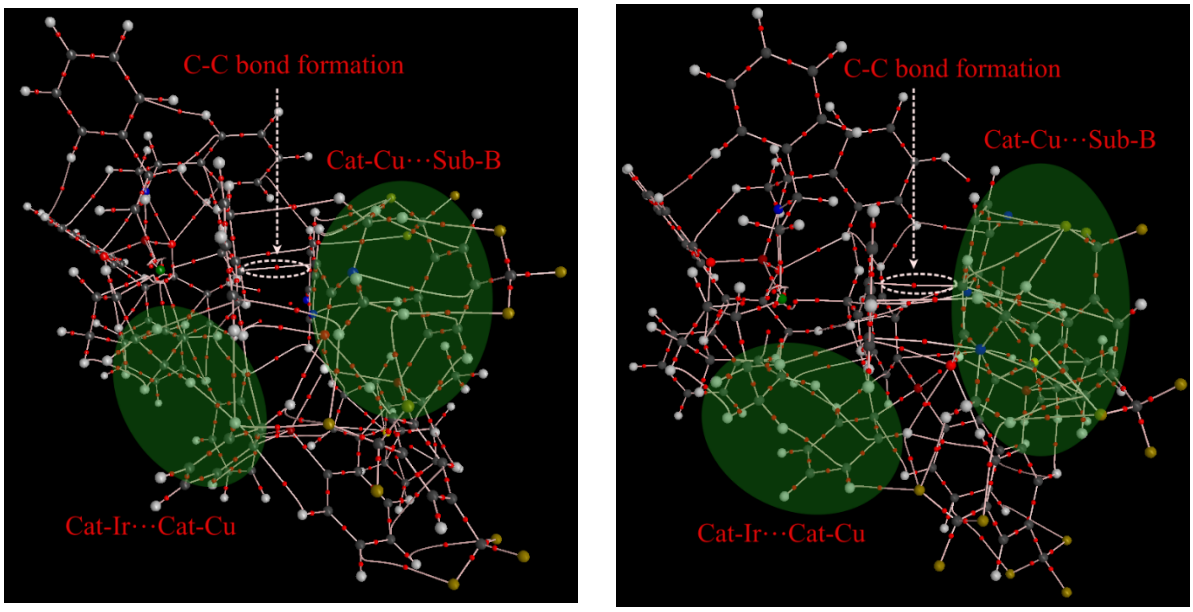
Bond Path	Type of Interaction	*re-re* (Å)	*re-re* ρ x 10^{-2}	*re-re* (θ)	*re-si* (Å)	*re-si* ρ x 10^{-2}	*re-si* (θ)
a	C–H···π	2.71	0.8	20.7	2.62	0.94	35.8
b	C–H···π	2.57	0.9	5.4	-[a]	-[a]	-[a]
c	C–H···π	-[a]	-[a]	-[a]	2.98	0.47	63.5
d	C–H···π	-[a]	-[a]	-[a]	2.69	0.79	30.9
e	C–H···π	2.61	0.8	31.2	2.53	0.7	20.0
f	C–H···π	2.93	0.5	62.2	2.99	0.4	50.9
g	C–H···F	2.60	0.6	107.1	-[a]	-[a]	-[a]
h	C–H···F	2.78	0.4	111.6	-[a]	-[a]	-[a]
i	C–H···F	2.49	0.7	172.8	2.55	0.6	173.5
j	C–H···F	2.55	0.6	150.5	2.55	0.6	142.7
k	C–H···F	2.65	0.5	162.2	2.52	0.7	128.0
l	C–H···F	2.74	0.5	104.6	2.75	0.4	105.9
m	C–H···F	2.42	0.8	144.1	2.38	0.9	142.2
n	C–H···O	2.15	1.8	153.3	2.17	1.8	152.9
o	C–H···O	2.32	1.1	150.0	2.66	0.6	139.6
p	C–H···N	2.81	0.6	34.1	2.65	0.8	33.14
q	C–H···π	2.83	0.6	46.2	-[a]	-[a]	-[a]
r	C–H···Br	3.16	0.5	121.4	-[a]	-[a]	-[a]
s	C–H···Br	3.15	0.5	122.7	-[a]	-[a]	-[a]
t	C–H···Br	-[a]	-[a]	-[a]	2.93	0.7	129.7
u	C–H···π	-[a]	-[a]	-[a]	2.79	0.7	57.5
v	C–H···π	2.80	0.6	16.8	-[a]	-[a]	-[a]
w	C–H···π	-[a]	-[a]	-[a]	3.10	0.3	39.7

Figure S9 continued…

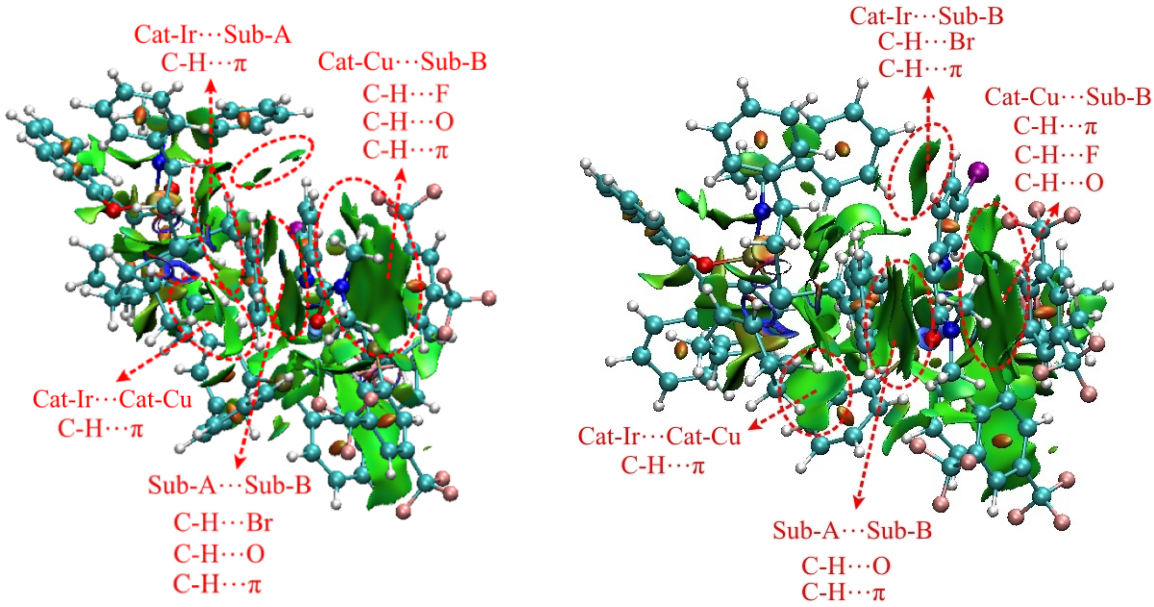
x	C–H···π	2.96	0.6	8.3	-[a]	-[a]	-[a]
y	C–H···π	2.61	0.8	18.3	2.57	0.9	21.6
z	C–H···π	2.96	0.5	73.5	2.96	0.5	33.2
a1	C–H···O	2.64	0.8	107.5	-[a]	-[a]	-[a]
a2	C–H···O	-[a]	-[a]	-[a]	2.67	0.8	105.0

[a]- No *bcp* found

(c) Topological analysis of the electron density



(d) NCI plots

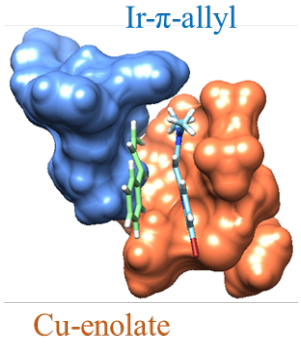


re-re *re-si*

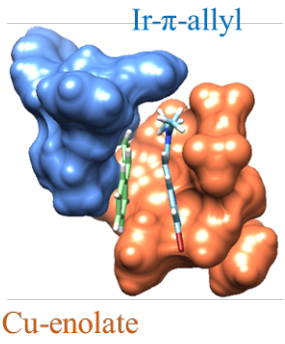
Figure S9. (a) Space-filling models for *re-re* and *re-si* diastereomeric TSs, (b) Important NCIs in the stereocontrolling TSs, (c) The bond critical points and the bond paths obtained using the *atoms-in-molecules* formalism, and (d) NCI plots highlighting the different interactions. Distances (Å), electron densities ($\rho \times 10^{-2}$) at the bond critical points as well as the angle of interaction (θ, in °) for various NCIs for **C1-P1** catalyst dyad are provided. Although the transition states consist of the counter ion (BF_4^-) in the actual computations, it is removed from this figure for improved clarity.

(ii) C2-P1 Catalyst Dyad

(a) Space filling models of TSs **[8-9]**$_{si\text{-}re}^{\ddagger}$ and **[8-9]**$_{si\text{-}si}^{\ddagger}$ for the *si-re* and *si-si* modes of addition between Cu-enolate (nucleophile) and Ir-π-allyl intermediate (electrophile)



si-re



si-si

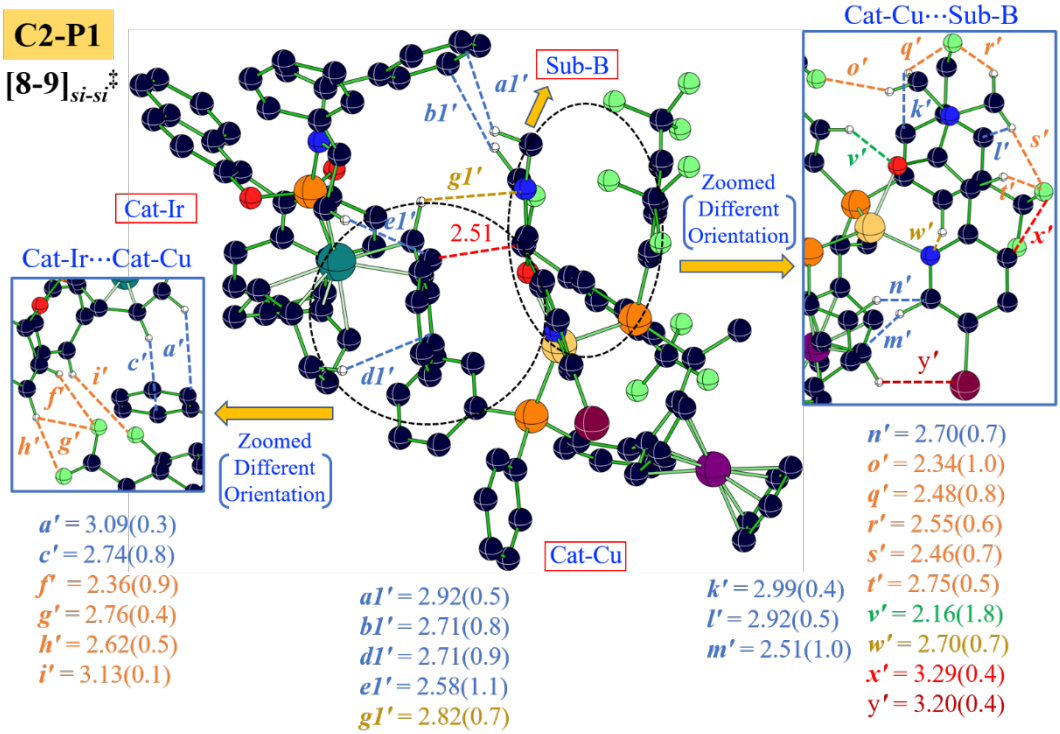
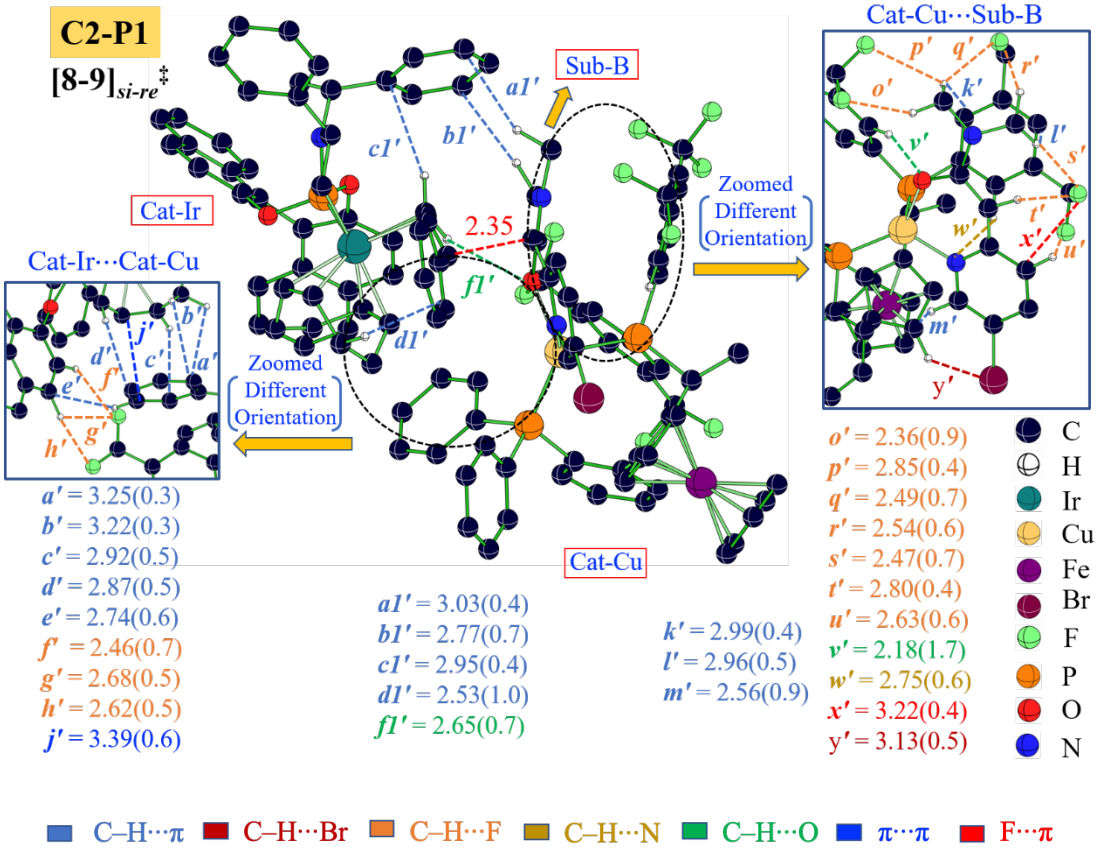


Figure S10 continued…



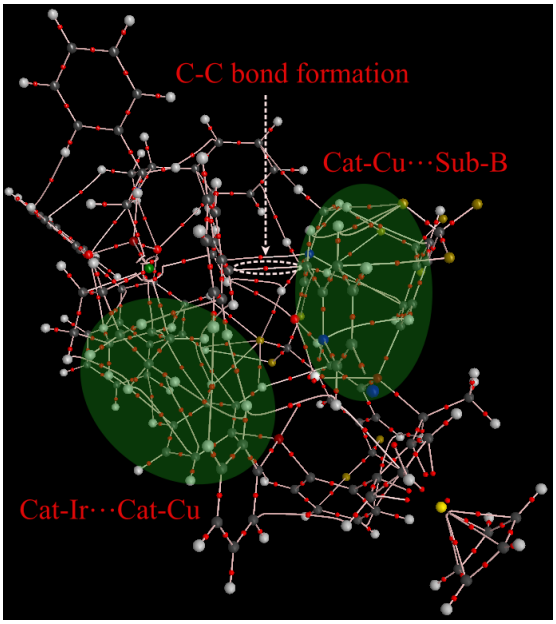
Bond Path	Type of Interaction	*si-re*			*si-si*		
		(Å)	ρ x 10^{-2}	(θ)	(Å)	ρ x 10^{-2}	(θ)
a′	C–H···π	3.25	0.3	74.7	3.09	0.3	55.5
b′	C–H···π	3.22	0.3	65.0	-[a]	-[a]	-[a]
c′	C–H···π	2.92	0.5	50.2	2.74	0.8	36.8
d′	C–H···π	2.87	0.5	50.4	-[a]	-[a]	-[a]
e′	C–H···π	2.74	0.6	39.9	-[a]	-[a]	-[a]
f′	C–H···F	2.46	0.7	120.9	2.36	0.9	125.2
g′	C–H···F	2.68	0.5	112.9	2.76	0.4	110.2
h′	C–H···F	2.62	0.5	154.8	2.62	0.5	148.6
i′	C–H···F	-[a]	-[a]	-[a]	3.13	0.1	128.2
j′	π···π	3.39	0.6	-[a]	-[a]	-[a]	-[a]
k′	C–H···π	2.99	0.4	55.5	2.99	0.4	84.5
l′	C–H···π	2.96	0.5	60.1	2.92	0.5	59.0
m′	C–H···π	2.56	0.9	34.9	2.51	1.0	31.0
n′	C–H···π	-[a]	-[a]	-[a]	2.70	0.7	28.0
o′	C–H···F	2.36	0.9	145.8	2.34	1.0	145.9
p′	C–H···F	2.85	0.4	103.1	-[a]	-[a]	-[a]
q′	C–H···F	2.49	0.7	129.8	2.48	0.8	129.5
r′	C–H···F	2.54	0.6	143.3	2.55	0.6	139.7

Figure S10 continued…

s'	C–H···F	2.47	0.7	174.4	2.46	0.7	171.3
t'	C–H···F	2.80	0.4	111.4	2.75	0.5	110.0
u'	C–H···F	2.63	0.6	107.8	-[a]	-[a]	-[a]
v'	C–H···O	2.18	1.7	150.5	2.16	1.8	148.5
w'	C–H···N	2.75	0.6	31.9	2.70	0.7	125.3
x'	C–F···π	3.22	0.4	51.8	3.29	0.4	49.7
y'	C–H···Br	3.13	0.5	121.9	3.20	0.4	123.3
a1'	C–H···π	3.03	0.4	45.8	2.92	0.5	54.5
b1'	C–H···π	2.77	0.7	14.2	2.71	0.8	11.1
c1'	C–H···π	2.95	0.4	5.9	-[a]	-[a]	-[a]
d1'	C–H···π	2.53	1.0	17.9	2.71	0.9	20.9
e1'	C–H···π	-[a]	-[a]	-[a]	2.58	1.1	109.6
f1'	C–H···O	2.65	0.7	128.5	-[a]	-[a]	-[a]
g1'	C–H···N	-[a]	-[a]	-[a]	2.82	0.7	110.9

[a]- No *bcp* found

(c) Topological analysis of the electron density



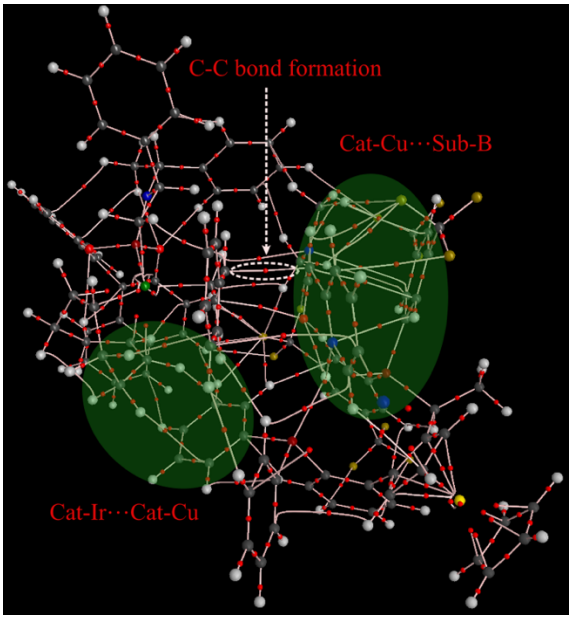
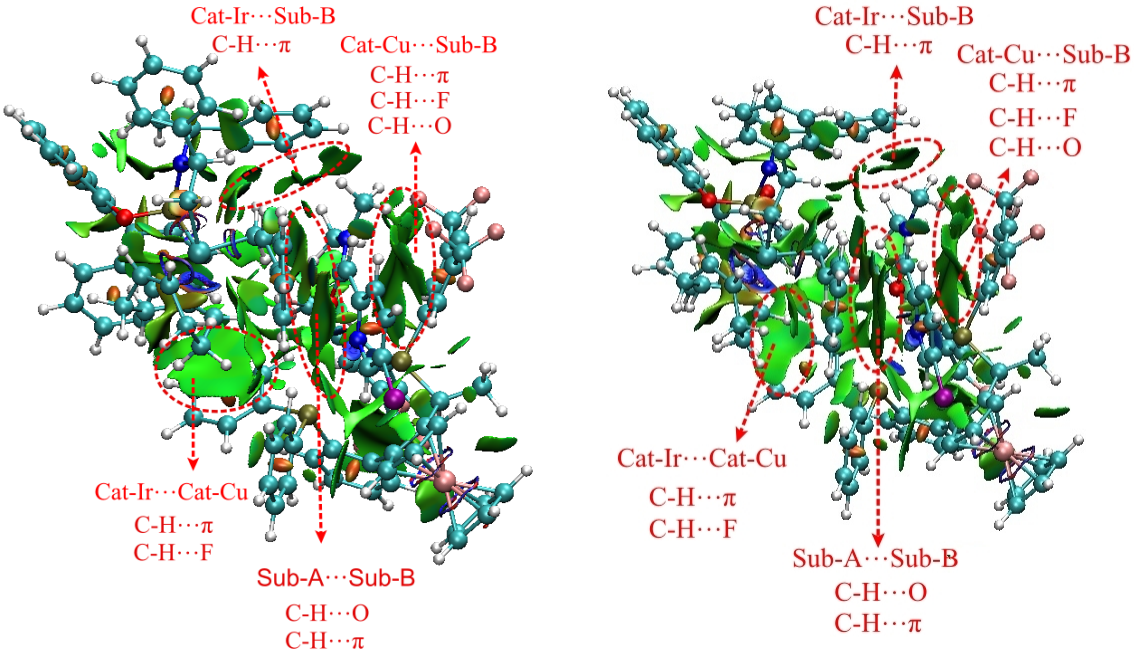


Figure S10 continued…

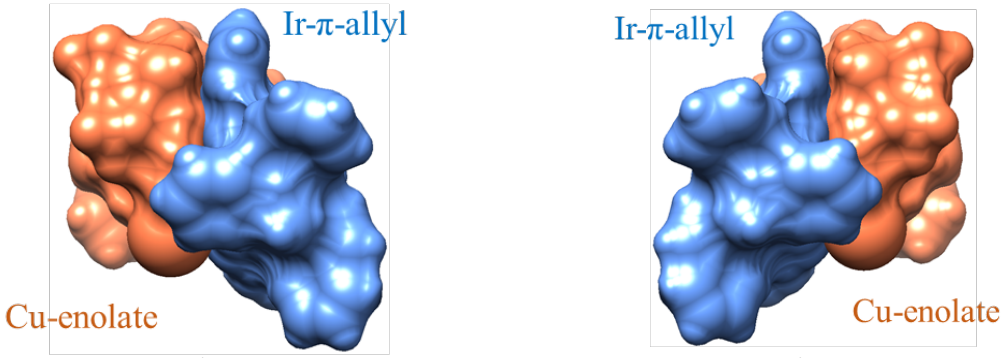
(d) NCI plots



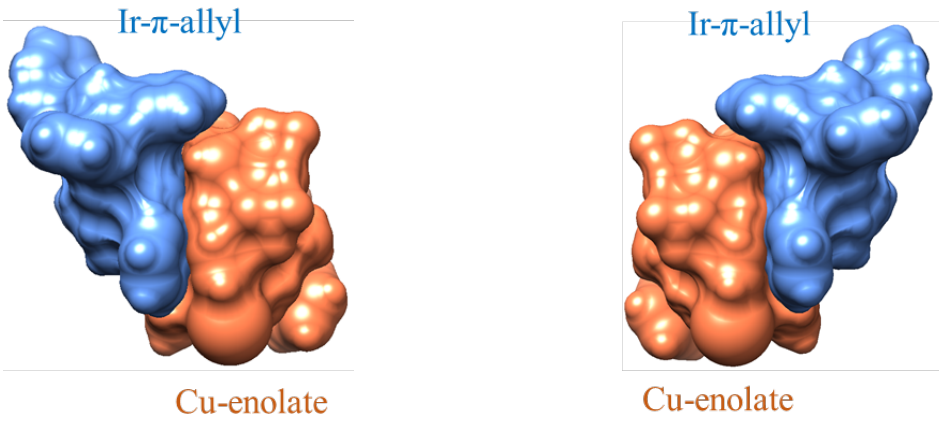
si-re *si-si*

Figure S10. (a) Space-filling models for *si-re* and *si-si* diastereomeric TSs, (b) Important NCIs in the stereocontrolling TSs, (c) The bond critical points and the bond paths obtained using the *atoms-in-molecules* formalism, and (d) NCI plots highlighting the different interactions. Distances (Å), electron densities ($\rho \times 10^{-2}$) at the bond critical points as well as the angle of interaction (θ, in °) for various NCIs for **C2-P1** catalyst combination are provided. Although the transition states consist of the counter ion (BF_4^-) in the actual computations, it is removed from this figure for improved clarity.

1.11. Space filling model for the lowest energy TS for all catalyst dyads



[8-9]$_{re\text{-}re}^{‡}$ (C1-P1) **[8-9]$_{si\text{-}si}^{‡}$ (C2-P2)**



[8-9]$_{si\text{-}re}^{‡}$ (C2-P1) **[8-9]$_{re\text{-}si}^{‡}$ (C1-P2)**

Figure S11. The space-filling representations for all the catalyst dyads for the lowest energy stereocontrolling C–C bond formation TSs conveying the contact between the chiral catalysts. Although the transition states consist of the counter ion (BF_4^-) in the actual computations, it is removed from this figure for improved clarity.

1.12. *Interaction wheel* diagram: *Interaction wheel* diagram capturing all NCIs in the stereocontrolling TSs in each catalyst dyad is provided in Figures S12 and S13. As shown in the Figure 4 of the main text, the key NCIs are categorized into six types. Each such type of NCI could differ in nature (such as C–H···π, C–H···F, C–H···O, C–H···N, C–H···Br, π···π and lone pair···π) and number of times it appears in a given TS geometry. Inspection of these NCIs in the stereocontrolling TSs conveys important molecular insights. This diagram helps us directly compare the key differences in the pattern of NCIs upon changing the catalyst configuration without having to inspect complex geometries of the TSs. It can be noticed from the total number of NCIs that the lowest energy TSs for each catalyst dyads exhibit more number of NCIs as compared to the corresponding higher energy TSs. Among the different categories of major NCIs in the stereocontrolling TSs, an important interaction is Cat–Ir···Cat–Cu operating between two chiral catalysts. In **C2-P1** and **C1-P2** catalyst dyads, the catalyst interact through C–H···π, C–H···F and π···π NCIs whereas C–H···π interactions are noticed in the case of **C1-P1**and **C2-P2** catalyst dyads.

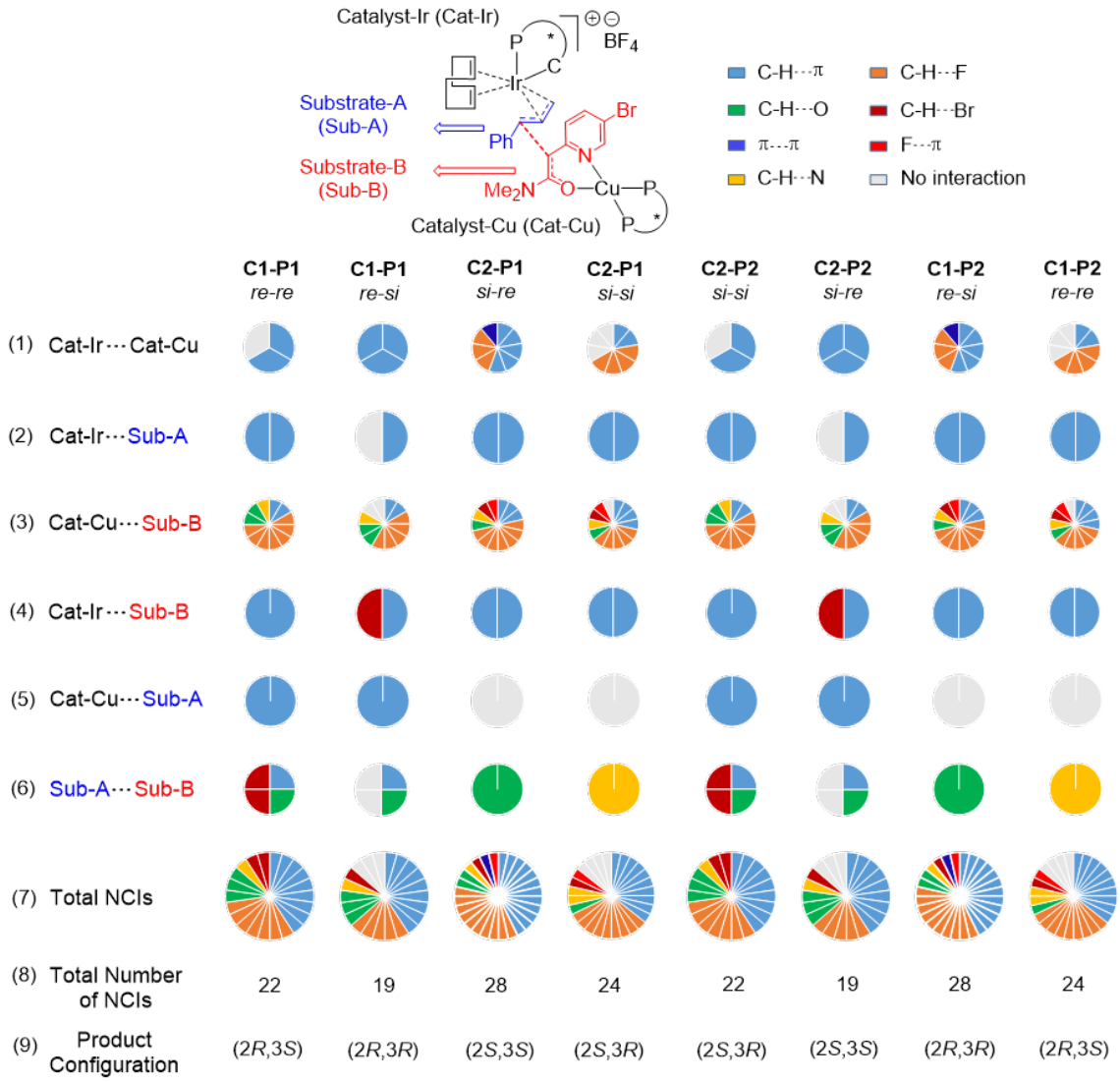


Figure S12. *Interaction wheel* diagram capturing all NCIs in the stereocontrolling TSs in each catalyst dyad.

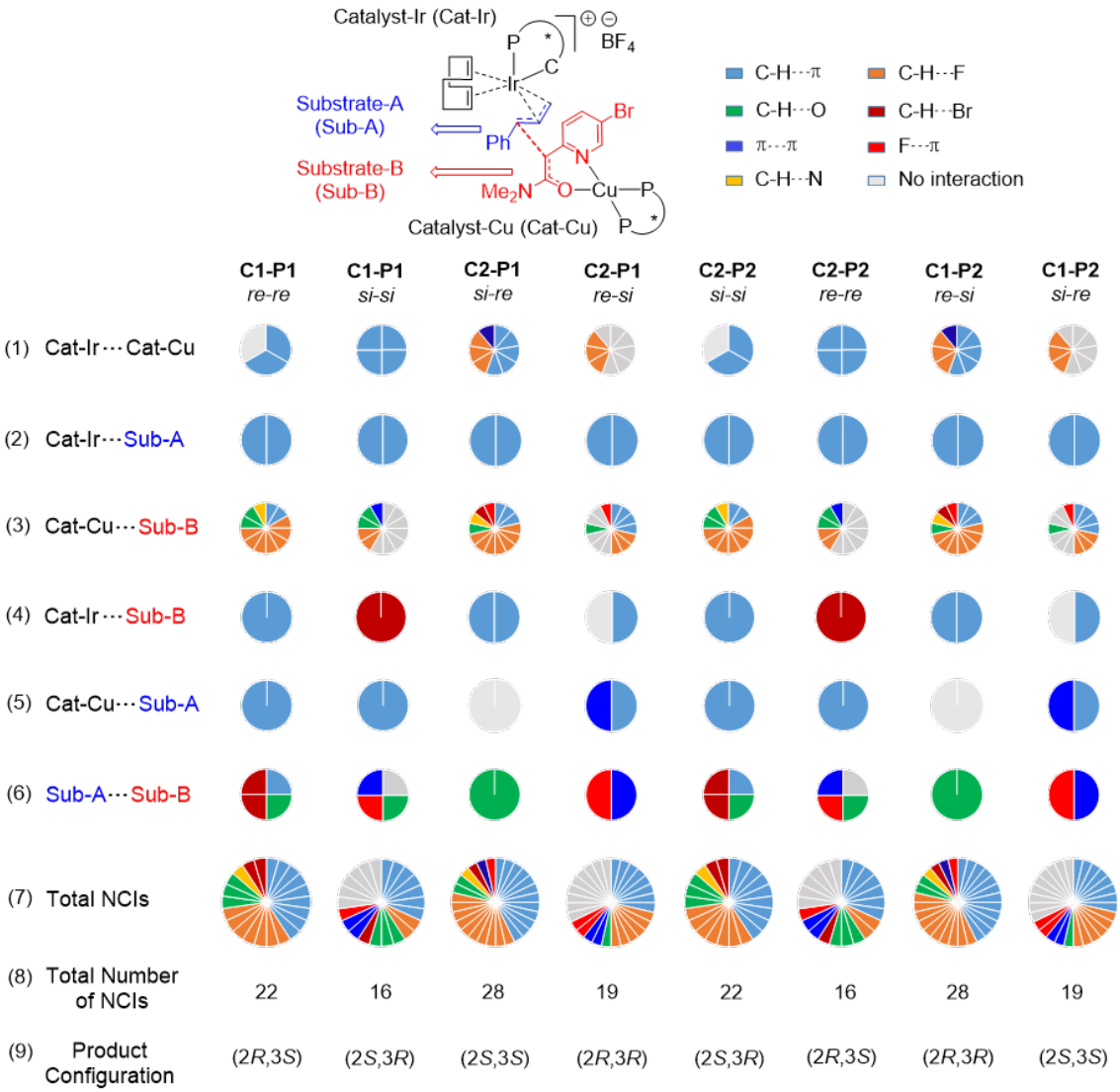


Figure S13. *Interaction wheel* diagram capturing all NCIs in the stereocontrolling TSs in each catalyst dyad.

1.13. Quantification of Noncovalent Interactions using the Espinosa's Formulation

We have employed Espinosa's formulation, that relies the topological parameters such as the electron density at the bond critical point (ρ_{bcp}), the corresponding Laplacian of the electron density ($V^2\rho$), and kinetic energy (G) toward quantification of the overall strength of the NCIs. Sum of the strength of key NCIs (in kcal/mol) calculated using Espinosa's method for the stereocontrolling transition states is provided in Table S14.

Table S14. Estimated Strengths of the Important Noncovalent Interactions in the Stereocontrolling TSs for the **C1-P1** and **C2-P1** catalyst dyad. The Topological Quantities are Derived from the *Atoms-in-Molecules* (AIM) Analysis[a]

C1-P1

re-re		ρ	$\nabla^2\rho$	G	$V=1/4\nabla^2\rho-2G$	E=1/2(V)(kcal/mol)
	a	0.008	-0.006	0.005	-0.012	-3.8
	b	0.009	-0.007	0.006	-0.014	-4.3
	e	0.009	-0.007	0.006	-0.013	-4.1
	f	0.005	-0.004	0.003	-0.008	-2.5
C–H···π	***q***	0.006	-0.005	0.004	-0.009	-2.8
	v	0.006	-0.005	0.004	-0.009	-2.8
	x	0.005	-0.004	0.003	-0.007	-2.1
	y	0.009	-0.007	0.005	-0.013	-4.0
	z	0.006	-0.005	0.004	-0.008	-2.6
	g	0.007	-0.008	0.007	-0.015	-4.8
	h	0.005	-0.006	0.004	-0.010	-3.2
	i	0.007	-0.008	0.006	-0.015	-4.7
C–H···F	***j***	0.006	-0.007	0.006	-0.013	-4.2
	k	0.005	-0.006	0.005	-0.011	-3.3
	l	0.005	-0.006	0.005	-0.011	-3.6
	m	0.009	-0.009	0.008	-0.018	-5.7
	a1	0.009	-0.008	0.007	-0.015	-4.7
C–H···O	***n***	0.019	-0.014	0.014	-0.031	-9.8
	o	0.012	-0.010	0.010	-0.022	-6.9
C–H···Br	***r***	0.005	-0.005	0.003	-0.008	-2.5
	s	0.005	-0.004	0.003	-0.008	-2.4
C–H···N	***p***	0.006	-0.005	0.004	-0.010	-3.2
		Total Strength				-88.2

C1-P1

re-si		ρ	$\nabla^2\rho$	G	$V=1/4\nabla^2\rho-2G$	E=1/2(V)(kcal/mol)
	a	0.009	-0.007	0.006	-0.014	-4.5
	c	0.005	-0.004	0.003	-0.007	-2.2
	d	0.008	-0.006	0.005	-0.012	-3.6
	e	0.007	-0.006	0.005	-0.011	-3.5
C–H···π	***f***	0.005	-0.004	0.003	-0.007	-2.2
	u	0.007	-0.006	0.005	-0.011	-3.5
	w	0.004	-0.003	0.002	-0.005	-1.6
	y	0.009	-0.007	0.006	-0.014	-4.3
	z	0.005	-0.004	0.003	-0.008	-2.4
	i	0.006	-0.007	0.006	-0.013	-4.1
	j	0.006	-0.007	0.006	-0.013	-4.2
C–H···F	***k***	0.007	-0.008	0.007	-0.015	-4.8
	l	0.005	-0.006	0.005	-0.011	-3.5
	m	0.010	-0.010	0.009	-0.020	-6.3
	n	0.018	-0.013	0.013	-0.030	-9.4
C–H···O	***o***	0.006	-0.006	0.005	-0.011	-3.6
	a2	0.008	-0.008	0.006	-0.015	-4.6
C–H···Br	***t***	0.008	-0.007	0.005	-0.012	-3.8
C–H···N	***p***	0.008	-0.007	0.006	-0.013	-4.2

Total Strength						-76.3
C2-P1						
si-re		ρ	$\nabla^2\rho$	G	V=1/4$\nabla^2\rho$-2G	E=1/2(V)(kcal/mol)
C–H···π	***a'***	0.004	-0.003	0.002	-0.005	-1.7
	b'	0.004	-0.003	0.002	-0.005	-1.7
	c'	0.006	-0.004	0.003	-0.008	-2.5
	d'	0.005	-0.004	0.003	-0.008	-2.5
	e'	0.007	-0.006	0.005	-0.011	-3.4
	a1'	0.004	-0.003	0.002	-0.006	-1.8
	b1'	0.007	-0.005	0.004	-0.010	-3.1
	c1'	0.005	-0.004	0.003	-0.007	-2.1
	d1'	0.010	-0.008	0.006	-0.015	-4.6
	k'	0.004	-0.004	0.003	-0.006	-2.0
	l'	0.005	-0.004	0.003	-0.008	-2.4
	m'	0.009	-0.008	0.006	-0.015	-4.7
C–H···F	***f'***	0.008	-0.009	0.008	-0.017	-5.5
	g'	0.005	-0.007	0.005	-0.012	-3.8
	h'	0.005	-0.006	0.005	-0.011	-3.4
	o'	0.010	-0.010	0.009	-0.021	-6.5
	p'	0.004	-0.005	0.004	-0.009	-2.9
	q'	0.008	-0.008	0.007	-0.016	-5.1
	r'	0.006	-0.007	0.006	-0.014	-4.3
	s'	0.007	-0.008	0.007	-0.016	-4.9
	t'	0.005	-0.006	0.004	-0.010	-3.1
	u'	0.006	-0.008	0.006	-0.014	-4.4
C–H···O	***v'***	0.018	-0.013	0.013	-0.030	-9.3
	f1'	0.008	-0.007	0.006	-0.014	-4.4
C–H···Br	***y'***	0.005	-0.005	0.003	-0.008	-2.5
C–H···N	***w'***	0.007	-0.006	0.005	-0.011	-3.5
π···π	***j'***	0.006	-0.005	0.004	-0.008	-2.6
C–F···π	***x'***	0.005	-0.005	0.004	-0.010	-3.1
Total Strength						-101.7
C2-P1						
si-si		ρ	$\nabla^2\rho$	G	V=1/4$\nabla^2\rho$-2G	E=1/2(V)(kcal/mol)
C–H···π	***a'***	0.004	-0.003	0.002	-0.006	-1.7
	c'	0.008	-0.006	0.005	-0.012	-3.8
	a1'	0.006	-0.004	0.003	-0.008	-2.5
	b1'	0.008	-0.006	0.005	-0.011	-3.5
	d1'	0.007	-0.005	0.004	-0.010	-3.1
	e1'	0.011	-0.011	0.009	-0.020	-6.4
	k'	0.004	-0.004	0.003	-0.006	-2.0
	l'	0.005	-0.004	0.003	-0.008	-2.5
	m'	0.010	-0.008	0.007	-0.016	-5.0
	n'	0.007	-0.007	0.005	-0.012	-3.8
C–H···F	***f'***	0.010	-0.011	0.009	-0.021	-6.6
	g'	0.005	-0.006	0.005	-0.011	-3.3

	h′	0.005	-0.006	0.005	-0.011	-3.4
	I′	0.001	-0.002	0.001	-0.003	-1.0
	o′	0.010	-0.010	0.009	-0.021	-6.7
	q′	0.008	-0.009	0.007	-0.017	-5.3
	r′	0.006	-0.007	0.006	-0.013	-4.2
	s′	0.008	-0.008	0.007	-0.016	-5.0
	t′	0.005	-0.006	0.005	-0.011	-3.5
C–H···O	***v′***	0.019	-0.014	0.014	-0.031	-9.8
C–H···Br	***y′***	0.005	-0.004	0.003	-0.007	-2.2
C–H···N	***g1′***	0.007	-0.006	0.005	-0.011	-3.6
	w′	0.007	-0.006	0.005	-0.012	-3.7
C–F···π	***x′***	0.005	-0.006	0.004	-0.010	-3.1
			Total Strength			-96.1

[a-] ρ= electron density, $\nabla^2\rho$ = Laplacian of the electron density; G, V, and H are respectively the kinetic, potential, and total electron energy densities at the bond critical points.

----------Part B----------

Cartesian Coordinates of the optimized geometries of various stationary points obtained at the $SMD_{(THF)}$/B3LYP-D3/6-31G**,SDD(Ir,Cu,Fe,Br) Level of Theory.

Cinnamyl methyl carbonate (**10**)

Number of imaginary frequencies= 0
The smallest frequencies are= 23.7470 31.5764 57.9605 cm(-1)
Electronic energy= -652.1010016
Zero-point correction= 0.210817
(Hartree/Particle)
Thermal correction to Energy= 0.224114
Thermal correction to Enthalpy= 0.225058
Thermal correction to Gibbs Free Energy= 0.168302
Sum of electronic and zero-point Energies= -651.890185
Sum of electronic and thermal Energies= -651.876888
Sum of electronic and thermal Enthalpies= -651.875943
Sum of electronic and thermal Free Energies= -651.932700

Cartesian Coordinates

6	1.516024	1.780614	-0.550798
6	0.193960	1.358750	0.007132
1	-0.006454	1.671078	1.029984
6	-0.696249	0.640132	-0.693749
1	-0.423230	0.343237	-1.706136
6	-2.025882	0.191147	-0.254591
6	-2.798699	-0.589059	-1.134469
6	-2.568863	0.501693	1.008087
6	-4.065313	-1.046754	-0.770139
1	-2.396187	-0.838589	-2.113245
6	-3.832777	0.044346	1.371891
1	-2.001430	1.105533	1.709843
6	-4.588228	-0.731937	0.485539
1	-4.642523	-1.648175	-1.467041
1	-4.233150	0.295194	2.350421
1	-5.574417	-1.085416	0.772962
8	2.614595	1.211153	0.224168
6	2.943114	-0.051114	-0.085806
8	2.492483	-0.714081	-0.997779
8	3.876975	-0.453476	0.786918
6	4.362124	-1.794071	0.575967
1	4.830872	-1.886997	-0.407626
1	5.098930	-1.964469	1.361511
1	3.547244	-2.518447	0.658483
1	1.625263	1.496823	-1.600119
1	1.667398	2.858977	-0.449882

Azaaryl acetamide (**2**)

Number of imaginary frequencies= 0
The smallest frequencies are= 35.4026 38.1643 58.7669 cm(-1)
Electronic energy= -547.7347365
Zero-point correction= 0.190565
(Hartree/Particle)
Thermal correction to Energy= 0.203811
Thermal correction to Enthalpy= 0.204755
Thermal correction to Gibbs Free Energy= 0.147968
Sum of electronic and zero-point Energies= -547.544171
Sum of electronic and thermal Energies= -547.530926
Sum of electronic and thermal Enthalpies= -547.529982
Sum of electronic and thermal Free Energies= -547.586768

Cartesian Coordinates

6	3.063768	-0.616644	0.135642
6	2.129034	-0.552623	1.352389
6	0.686016	-0.417611	0.914638
7	3.487392	0.561267	-0.405151
6	4.435623	0.541625	-1.512704
1	5.352217	1.076327	-1.234687
1	4.678485	-0.490840	-1.757834
1	4.003915	1.031905	-2.393449
6	3.150228	1.888097	0.101198
1	2.203748	1.889284	0.639787
1	3.940283	2.279271	0.756155
1	3.045247	2.570640	-0.748085
8	3.369506	-1.717899	-0.330852
6	0.074858	-1.432052	0.163867
6	-1.246894	-1.277690	-0.242943
1	0.638235	-2.320605	-0.101011
6	-1.896905	-0.102797	0.123857
6	-1.231446	0.868710	0.864616
1	-1.725551	1.791938	1.155077
7	0.041099	0.710439	1.251338
1	-1.746648	-2.045926	-0.822909
35	-3.762217	0.197569	-0.402444
1	2.268529	-1.504417	1.870385
1	2.377937	0.254659	2.042279

CH_3CN

Number of imaginary frequencies= 0
The smallest frequencies are= 398.1343 399.5145 933.8101 cm(-1)
Electronic energy= -132.7645774
Zero-point correction= 0.045316
(Hartree/Particle)
Thermal correction to Energy= 0.048895
Thermal correction to Enthalpy= 0.049839
Thermal correction to Gibbs Free Energy= 0.022356
Sum of electronic and zero-point Energies= -132.719261
Sum of electronic and thermal Energies= -132.715682
Sum of electronic and thermal Enthalpies= -132.714738
Sum of electronic and thermal Free Energies= -132.742221

Cartesian Coordinates

7	0.000000	-0.000000	1.438627
6	0.000000	-0.000000	0.277792
6	-0.000000	0.000000	-1.179680
1	0.000000	1.028348	-1.553019
1	0.890576	-0.514174	-1.553019
1	-0.890576	-0.514174	-1.553019

$[CH_3OCO^-]^-$

Number of imaginary frequencies= 0
The smallest frequencies are= 126.8441 185.6375 331.5602 cm(-1)
Electronic energy= -303.8128844
Zero-point correction= 0.053897
(Hartree/Particle)
Thermal correction to Energy= 0.058925
Thermal correction to Enthalpy= 0.059869
Thermal correction to Gibbs Free Energy= 0.025702
Sum of electronic and zero-point Energies= -303.758988
Sum of electronic and thermal Energies= -303.753959
Sum of electronic and thermal Enthalpies= -303.753015
Sum of electronic and thermal Free Energies= -303.787183

Cartesian Coordinates

6	-0.653008	0.063605	-0.000069
8	-0.469461	1.298797	0.000012
8	-1.687919	-0.625132	0.000033
8	0.542265	-0.753014	-0.000008
6	1.755987	-0.033604	0.000007
1	1.866739	0.612772	0.883079
1	2.569882	-0.771298	-0.000321
1	1.866426	0.613304	-0.882691

Phosphoramidite-**P1**(*R*,*R*,*R*)

Number of imaginary frequencies= 0
The smallest frequencies are= 17.4818 27.8028 32.7869 cm(-1)
Electronic energy= -1936.6379935
Zero-point correction= 0.566984
(Hartree/Particle)
Thermal correction to Energy= 0.599224
Thermal correction to Enthalpy= 0.600168
Thermal correction to Gibbs Free Energy= 0.503286
Sum of electronic and zero-point Energies= -1936.071010
Sum of electronic and thermal Energies= -1936.038770
Sum of electronic and thermal Enthalpies= -1936.037826
Sum of electronic and thermal Free Energies= -1936.134707

.....

Cartesian Coordinates

.....

15	0.536829	0.719506	-1.489924
8	-0.191709	1.120005	-0.021840
8	-0.703125	-0.293299	-2.097632
7	1.804568	-0.203168	-0.867103
6	-1.477501	1.637790	-0.078417
6	-1.625725	3.033205	0.085539
1	-0.735381	3.634407	0.238244
6	-2.880002	3.591409	0.061109
1	-3.008463	4.661225	0.200571
6	-4.024852	2.784354	-0.177340
6	-5.321746	3.360777	-0.265305
1	-5.423441	4.432548	-0.114547
6	-6.423661	2.586332	-0.548818
1	-7.408867	3.038274	-0.618270
6	-6.267459	1.196438	-0.768040
1	-7.134225	0.590848	-1.017461
6	-5.026635	0.604317	-0.675683
1	-4.926576	-0.458999	-0.858119
6	-3.867699	1.368099	-0.357728
6	-2.557103	0.783173	-0.248853
6	-2.323610	-0.684383	-0.363717
6	-2.966482	-1.637094	0.500830
6	-3.760269	-1.246754	1.616555
1	-3.883408	-0.192491	1.834875
6	-4.358799	-2.185046	2.429159
1	-4.953316	-1.859505	3.278176
6	-4.201292	-3.568543	2.173646
1	-4.684099	-4.296955	2.818734
6	-3.422625	-3.983028	1.116783
1	-3.276997	-5.042065	0.919008
6	-2.778749	-3.041600	0.268240
6	-1.934604	-3.465784	-0.793484
1	-1.809654	-4.529910	-0.975029
6	-1.258808	-2.546425	-1.556903
1	-0.579981	-2.849822	-2.346880
6	-1.433161	-1.162316	-1.317913
6	2.825421	-0.493564	-1.922818
1	2.612122	0.212976	-2.736666
6	4.233335	-0.171579	-1.432953
6	4.556800	1.165401	-1.158220
1	3.804441	1.934181	-1.313593
6	5.810725	1.510719	-0.660654
1	6.038932	2.550281	-0.442627
6	6.770621	0.518351	-0.432466
1	7.747782	0.784302	-0.039030
6	6.465055	-0.812585	-0.715334
1	7.204701	-1.590292	-0.545083
6	5.203175	-1.154774	-1.213892
1	4.981232	-2.196768	-1.419853
6	2.640711	-1.900983	-2.500892
1	2.743924	-2.681893	-1.741107
1	3.374569	-2.095537	-3.289521
6	2.059358	-0.851482	0.453855
1	2.707732	-1.703007	0.226591
6	2.851751	0.047152	1.405529
6	3.999748	-0.462661	2.025185
1	4.327706	-1.472089	1.791414
6	4.744991	0.315766	2.913219
1	5.641207	-0.095975	3.369643
6	4.347384	1.623166	3.199536
1	4.927932	2.235502	3.884177
6	3.197543	2.138086	2.594550
1	2.877945	3.154072	2.812167
6	2.455358	1.357020	1.706919
1	1.568032	1.768500	1.241489
6	0.829988	-1.441126	1.158117
1	0.315681	-2.155629	0.513194
1	0.123820	-0.673344	1.470486
1	1.173641	-1.973550	2.050993
1	1.640175	-1.984324	-2.933694

Walphos-**C1**(R,R_p)

Number of imaginary frequencies= 0
The smallest frequencies are= 10.4583 14.0513 16.9985 cm(-1)
Electronic energy= -3777.10338
Zero-point correction= 0.673765
(Hartree/Particle)
Thermal correction to Energy= 0.727139
Thermal correction to Enthalpy= 0.728083
Thermal correction to Gibbs Free Energy= 0.580332
Sum of electronic and zero-point Energies= -3776.429615
Sum of electronic and thermal Energies= -3776.376242
Sum of electronic and thermal Enthalpies= -3776.375297
Sum of electronic and thermal Free Energies= -3776.523048

.....

Cartesian Coordinates

.....

26	-1.460011	-3.999265	0.460496
15	-3.295172	0.449487	-1.140468
15	1.462048	-0.471072	-1.034055
6	-1.695627	-1.961604	0.080355
6	-0.363545	-2.394101	-0.278461
6	-0.497618	-3.412716	-1.275251
1	0.319974	-3.949892	-1.736711
6	-1.883416	-3.626626	-1.526460
1	-2.302605	-4.364708	-2.197484
6	-2.621729	-2.742207	-0.689198
1	-3.697017	-2.691975	-0.611306
6	-0.678462	-4.641360	2.271135
1	0.090908	-4.120295	2.825220
6	-0.462643	-5.629507	1.261211
1	0.497561	-5.984799	0.911577
6	-1.737768	-6.030607	0.757589
1	-1.911045	-6.741714	-0.039432
6	-2.741368	-5.291400	1.455476
1	-3.807632	-5.341527	1.277938
6	-2.087587	-4.433423	2.389913
1	-2.572798	-3.720926	3.043196
6	-2.025809	-0.870247	1.033539
6	-1.576944	-0.957089	2.361845
1	-1.031205	-1.843441	2.664133
6	-1.824814	0.056440	3.284740
1	-1.458371	-0.034926	4.302509
6	-2.535722	1.188470	2.888162
1	-2.726705	1.991873	3.591787
6	-2.988896	1.293965	1.573628
1	-3.533680	2.184091	1.278907
6	-2.748532	0.282145	0.629457
6	0.944190	-1.826119	0.213582
1	0.783299	-1.358561	1.186573
6	2.032302	-2.899380	0.371014
1	2.924988	-2.490573	0.849920
1	2.335163	-3.327961	-0.589690

1	1.646433	-3.712257	0.990237
6	-3.843691	2.216358	-1.234871
6	-2.932039	3.139034	-1.771542
1	-1.958113	2.798685	-2.107078
6	-3.263845	4.490664	-1.885143
1	-2.541887	5.188440	-2.295445
6	-4.522451	4.936370	-1.475986
1	-4.786079	5.986306	-1.569735
6	-5.444971	4.025926	-0.952890
1	-6.427651	4.366402	-0.637426
6	-5.109128	2.676087	-0.832036
1	-5.834423	1.980379	-0.421750
6	-4.931098	-0.422175	-1.120340
6	-5.629854	-0.752934	0.051707
1	-5.220735	-0.483377	1.020544
6	-6.849217	-1.431987	-0.016260
1	-7.377053	-1.683249	0.899913
6	-7.390124	-1.783581	-1.255584
1	-8.337320	-2.313189	-1.307252
6	-6.705132	-1.454417	-2.428569
1	-7.118063	-1.727168	-3.395945
6	-5.482209	-0.784963	-2.360387
1	-4.947858	-0.548986	-3.277671
6	0.961950	1.123769	-0.229528
6	0.775531	2.211057	-1.093114
1	0.846473	2.069342	-2.167037
6	0.504532	3.485316	-0.587208
6	0.401296	3.698063	0.783802
1	0.187593	4.686647	1.174899
6	0.581802	2.616461	1.647830
6	0.857613	1.342390	1.153397
1	1.005135	0.532762	1.856534
6	3.304601	-0.387603	-0.786489
6	4.086099	-1.171553	-1.646468
1	3.611178	-1.769379	-2.418706
6	5.476939	-1.203091	-1.517637
6	6.119557	-0.438036	-0.547847
1	7.199144	-0.455405	-0.454892
6	5.345307	0.357832	0.298005
6	3.955398	0.383553	0.187259
1	3.390291	1.015348	0.861509
6	6.028413	1.145864	1.382050
6	6.279026	-2.030825	-2.483922
6	0.399263	4.651126	-1.531019
6	0.540464	2.882641	3.127922
9	-0.602285	3.509912	3.496061
9	0.641325	1.756871	3.866281
9	1.558033	3.695825	3.505102
9	1.612620	5.193997	-1.790977
9	-0.374224	5.642262	-1.033835
9	-0.125688	4.292117	-2.728535
9	6.321109	0.367692	2.453464
9	5.263935	2.163762	1.834780
9	7.198777	1.675169	0.957951
9	7.517788	-2.303530	-2.018788
9	5.676047	-3.213438	-2.748370
9	6.433557	-1.401437	-3.673951

DBU (**4**)

Number of imaginary frequencies= 0
The smallest frequencies are= 67.2608 88.1080 194.8032 cm(-1)
Electronic energy= -462.138808
Zero-point correction= 0.246331
(Hartree/Particle)
Thermal correction to Energy= 0.256112
Thermal correction to Enthalpy= 0.257056
Thermal correction to Gibbs Free Energy= 0.211362
Sum of electronic and zero-point Energies= -461.892477
Sum of electronic and thermal Energies= -461.882696
Sum of electronic and thermal Enthalpies= -461.881752
Sum of electronic and thermal Free Energies= -461.927446

.....

Cartesian Coordinates

.....

6	-2.730189	-0.839767	0.176709
6	-2.789792	0.611025	-0.296098
1	-2.970881	-0.890921	1.250188
1	-3.493317	-1.441828	-0.333116
6	-1.594441	1.357094	0.280721
1	-3.720847	1.098316	0.012780
1	-2.743406	0.644061	-1.391489
1	-1.537681	2.370795	-0.131187
1	-1.701700	1.457805	1.372914
7	-1.429281	-1.462817	-0.051726
6	-0.369569	-0.722659	-0.127192
7	-0.340664	0.664314	-0.046791
6	0.923317	-1.482992	-0.400595
1	0.643092	-2.534900	-0.322804
1	1.228764	-1.317644	-1.442416
6	2.102790	-1.173922	0.539847
1	1.715763	-0.974053	1.546641
6	0.850039	1.467581	0.282305
6	2.959669	0.006540	0.059149
1	3.566662	0.377187	0.894665
6	2.118929	1.155871	-0.518217
1	2.729482	2.065509	-0.553243
1	1.827113	0.943678	-1.553004
1	0.563438	2.502776	0.074730
1	1.062671	1.418768	1.362801
1	3.663948	-0.336364	-0.709239
1	2.731992	-2.066281	0.631609

$[DBU\text{-}H]^+$

Number of imaginary frequencies= 0
The smallest frequencies are= 62.3384 90.0186 176.0142 cm(-1)
Electronic energy= -462.6281218
Zero-point correction= 0.261261
(Hartree/Particle)
Thermal correction to Energy= 0.271195
Thermal correction to Enthalpy= 0.272139
Thermal correction to Gibbs Free Energy= 0.226194
Sum of electronic and zero-point Energies= -462.366861
Sum of electronic and thermal Energies= -462.356927
Sum of electronic and thermal Enthalpies= -462.355983
Sum of electronic and thermal Free Energies= -462.401928

.....

Cartesian Coordinates

.....

6	-2.801083	0.775280	-0.051813
6	-2.742659	-0.696100	0.327110
1	-3.148163	0.905295	-1.082967
1	-3.467795	1.336491	0.606957
6	-1.575810	-1.357535	-0.394627
1	-3.673743	-1.195420	0.049098
1	-2.610317	-0.800336	1.409031
1	-1.457759	-2.389065	-0.060865
1	-1.736384	-1.369064	-1.479135
7	-1.456816	1.345398	0.075834
6	-0.310051	0.666630	0.063758
7	-0.301077	-0.651490	-0.115485
6	0.933187	1.505036	0.278244
1	0.646536	2.539711	0.075768
1	1.189872	1.461783	1.343523
6	2.148086	1.126988	-0.584706
1	1.804455	0.847761	-1.587296
6	0.911430	-1.504030	-0.245576
6	2.980500	-0.005030	0.030787
1	3.639574	-0.423854	-0.738220
6	2.105455	-1.116002	0.627247
1	2.707896	-2.018790	0.771541
1	1.735777	-0.836014	1.620270
1	0.580131	-2.504010	0.038075
1	1.192014	-1.545898	-1.304951
1	3.628031	0.397242	0.818530
1	2.768117	2.019329	-0.712627
1	-1.387327	2.346064	0.208277

$[DBU\text{-}H]^+PF_6^-$ (**7**)

Number of imaginary frequencies= 0
The smallest frequencies are= 24.2448 46.9590 56.9877 cm(-1)
Electronic energy= -1403.3760898
Zero-point correction= 0.281777
(Hartree/Particle)
Thermal correction to Energy= 0.299642
Thermal correction to Enthalpy= 0.300586
Thermal correction to Gibbs Free Energy= 0.235422
Sum of electronic and zero-point Energies= -1403.094313
Sum of electronic and thermal Energies= -1403.076448
Sum of electronic and thermal Enthalpies= -1403.075504
Sum of electronic and thermal Free Energies= -1403.140668

.....

Cartesian Coordinates

.....

6	-0.633493	2.841783	0.867752
6	-1.352312	3.047155	-0.456565
1	0.450706	2.825219	0.726586
1	-0.884619	3.623705	1.589052
6	-1.233388	1.780102	-1.293870
1	-0.907254	3.885997	-0.997415
1	-2.409090	3.276812	-0.282835
1	-1.817043	1.871137	-2.210910
1	-0.192190	1.577092	-1.558605
7	-1.046939	1.556092	1.432108
6	-1.529073	0.516059	0.753462
7	-1.747165	0.602647	-0.554599
6	-1.820598	-0.714317	1.588780
1	-1.229852	-0.609218	2.500964
1	-2.873116	-0.678579	1.895257
6	-1.490205	-2.060397	0.924686
1	-0.560971	-1.954111	0.362128
6	-2.236855	-0.489456	-1.432130
6	-2.621419	-2.570519	0.023664
1	-2.226512	-3.348113	-0.640660
6	-3.252628	-1.449189	-0.812473
1	-3.830403	-1.885504	-1.634341
1	-3.965562	-0.868673	-0.215478
1	-2.706893	0.020998	-2.275046
1	-1.364908	-1.027366	-1.818316
1	-3.403679	-3.040916	0.631761
1	-1.289761	-2.788918	1.716763
1	-0.796427	1.381750	2.395562
15	2.135173	-0.334644	-0.105164
9	2.387260	-1.932406	0.102813
9	0.830128	-0.670356	-1.051599
9	3.417250	0.016308	0.838463
9	1.844537	1.272193	-0.316216
9	3.088243	-0.336788	-1.428504
9	1.161308	-0.322300	1.218442

[PF_6^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 288.2990 292.0495 292.6025
cm(-1)
Electronic energy= -940.7146345
Zero-point correction= 0.019013
(Hartree/Particle)
Thermal correction to Energy= 0.025167
Thermal correction to Enthalpy= 0.026111
Thermal correction to Gibbs Free Energy= -0.011213
Sum of electronic and zero-point Energies= -940.695634
Sum of electronic and thermal Energies= -940.689479
Sum of electronic and thermal Enthalpies= -940.688535
Sum of electronic and thermal Free Energies= -940.725860

.....

Cartesian Coordinates

.....

15	0.000000	0.000000	0.000000
9	1.378879	-0.212263	-0.856835
9	-0.862365	-0.664515	-1.222685
9	-0.189284	1.481211	-0.671320
9	0.862365	0.664515	1.222685
9	-1.378879	0.212263	0.856835
9	0.189284	-1.481211	0.671320

---

12 P1 *endo-re* [BF_4^-]

Number of imaginary frequencies=0
The smallest frequencies are= 17.8039 18.4279 23.4608 cm(-1)
Electronic energy= -3892.024528
Zero-point correction= 1.235566
(Hartree/Particle)
Thermal correction to Energy= 1.307751
Thermal correction to Enthalpy= 1.308695
Thermal correction to Gibbs Free Energy= 1.126716
Sum of electronic and zero-point Energies= -3890.788962
Sum of electronic and thermal Energies= -3890.716778
Sum of electronic and thermal Enthalpies= -3890.715833
Sum of electronic and thermal Free Energies= -3890.897812

.....

Cartesian Coordinates

.....

77	0.415599	-0.950357	-1.679610
15	1.847695	0.324431	-0.412166
8	2.336083	0.082439	1.164795
8	3.368986	0.385324	-1.142132
7	1.204835	1.856749	-0.243591
6	3.230557	-0.932877	1.466050
6	2.716606	-2.054362	2.155567
1	1.666850	-2.056252	2.425911
6	3.546375	-3.104477	2.460948
1	3.164149	-3.969690	2.995435
6	4.908030	-3.089197	2.054282
6	5.757251	-4.203927	2.292286
1	5.347782	-5.063728	2.816319
6	7.063396	-4.204595	1.857635
1	7.701724	-5.064200	2.040080
6	7.570656	-3.085592	1.154843
1	8.593819	-3.098191	0.790188
6	6.778196	-1.982369	0.922234
1	7.181289	-1.139319	0.373829
6	5.430188	-1.936034	1.376618
6	4.573141	-0.802173	1.143263
6	5.079614	0.465041	0.547225
6	6.164433	1.205799	1.138028
6	6.737596	0.859741	2.394418
1	6.345129	0.010075	2.940301
6	7.769997	1.596042	2.934272
1	8.183021	1.314114	3.898727
6	8.292850	2.719015	2.249695
1	9.111204	3.285700	2.684238
6	7.748301	3.096546	1.043042
1	8.124950	3.968351	0.514125
6	6.671935	2.369170	0.466482
6	6.075483	2.788059	-0.753613
1	6.476658	3.658364	-1.265499
6	4.985210	2.126068	-1.259206
1	4.490750	2.449364	-2.169012
6	4.476278	0.991509	-0.586267
6	0.063619	2.124954	-1.162461
1	-0.857211	2.112406	-0.570727
6	0.198019	3.495410	-1.811726
6	1.434295	3.930380	-2.313488
1	2.307863	3.299366	-2.180049
6	1.546794	5.161045	-2.959809
1	2.512605	5.486852	-3.337643
6	0.420402	5.975439	-3.119000
1	0.506538	6.935180	-3.621288
6	-0.813055	5.549085	-2.622282
1	-1.692109	6.178442	-2.734330
6	-0.924239	4.317988	-1.968554
1	-1.880128	3.998626	-1.566790
6	-0.029422	1.048594	-2.261908
1	0.675794	1.320092	-3.056903
1	-1.027725	1.107511	-2.698554
6	1.340775	2.822481	0.892652
1	0.876986	3.731527	0.500590

6	0.514971	2.424099	2.115494
6	-0.841676	2.775714	2.160816
1	-1.295477	3.307921	1.331351
6	-1.632080	2.461573	3.269106
1	-2.675927	2.755023	3.267321
6	-1.072913	1.787818	4.356384
1	-1.680885	1.548197	5.224906
6	0.279635	1.434608	4.326527
1	0.727524	0.918832	5.172212
6	1.066187	1.753999	3.218308
1	2.114188	1.479425	3.215598
6	2.786943	3.198534	1.212303
1	3.275905	3.592268	0.319114
1	3.374569	2.357629	1.579286
1	2.791010	3.978355	1.980506
6	-0.915498	-1.786142	1.036857
1	-0.284866	-2.645809	0.828984
1	-0.482212	-1.199110	1.846847
6	-1.183656	-0.918335	-0.160136
1	-1.474076	0.089622	0.127134
6	-1.763869	-1.445409	-1.365414
1	-1.865634	-2.524627	-1.418835
6	1.820420	-1.070098	-3.374078
1	2.160061	-0.063998	-3.609343
6	0.509480	-1.411283	-3.822833
1	-0.036468	-0.643061	-4.371103
6	0.064782	-2.820786	-4.175433
1	0.455494	-3.103462	-5.165778
1	-1.024429	-2.807489	-4.272756
6	0.468669	-3.886573	-3.133052
1	1.425485	-4.341094	-3.409102
1	-0.265821	-4.699032	-3.148716
6	0.567011	-3.361586	-1.705449
1	-0.219427	-3.684374	-1.032111
6	1.732970	-2.894686	-1.129948
1	1.792430	-2.903497	-0.046066
6	3.060879	-2.746118	-1.845223
1	3.712586	-2.141031	-1.212841
1	3.534935	-3.736052	-1.926269
6	2.960630	-2.084980	-3.238424
1	2.857084	-2.850532	-4.015424
1	3.906946	-1.575089	-3.444249
6	-2.790816	-0.759606	-2.182567
6	-3.214648	0.561719	-1.951824
6	-3.396124	-1.461522	-3.244796
6	-4.172080	1.165895	-2.766648
1	-2.824193	1.118103	-1.112457
6	-4.353360	-0.859147	-4.061415
1	-3.109739	-2.495071	-3.424716
6	-4.742986	0.465117	-3.831752
1	-4.491988	2.177263	-2.534665
1	-4.800682	-1.426320	-4.873956
1	-5.492441	0.935039	-4.462601
8	-1.974633	-4.283907	0.467015
6	-2.553368	-3.542462	1.235678
8	-2.167530	-2.324811	1.634992
8	-3.715057	-3.813847	1.849191
6	-4.338297	-5.059257	1.471590
1	-3.688980	-5.903998	1.714037
1	-5.258611	-5.109879	2.053378
1	-4.564181	-5.064728	0.402074
6	-4.258411	-0.208393	4.007465
6	-5.552041	0.331450	4.594393
1	-3.553810	0.600239	3.794171
1	-3.772338	-0.920635	4.679674
6	-6.313442	1.088312	3.513422
1	-5.337235	1.005446	5.427745
1	-6.166123	-0.492678	4.973581
1	-7.299863	1.380182	3.878271
1	-5.774741	1.990362	3.207945
7	-4.558717	-0.898895	2.757694
6	-5.579213	-0.625244	1.950694
7	-6.517529	0.248907	2.307518
6	-5.581463	-1.408452	0.651309
1	-4.537389	-1.659717	0.458898
1	-6.101659	-2.358215	0.828814
6	-6.146878	-0.693146	-0.580699
1	-5.800914	0.341163	-0.571778
6	-7.668144	0.667204	1.467725
6	-7.673940	-0.751398	-0.669852
1	-8.011017	-0.023741	-1.417705
6	-8.343941	-0.457179	0.679486
1	-9.389294	-0.171379	0.520014
1	-8.366871	-1.355227	1.308822
1	-8.389127	1.086529	2.171471
1	-7.334512	1.480060	0.814647
1	-7.996208	-1.739188	-1.022717
1	-5.703029	-1.151636	-1.468709
1	-3.813964	-1.467622	2.370723
5	-4.241391	2.595743	0.758064
9	-5.428019	2.546514	-0.000666
9	-4.474309	3.322277	1.945486
9	-3.229787	3.229096	0.004838
9	-3.822177	1.292051	1.084775

[12-13]‡ P1 *endo-re* [BF_4^-]

Number of imaginary frequencies= 1
The smallest frequencies are= -255.1672 2.7472 17.2882 cm(-1)
Electronic energy= -3892.0082688
Zero-point correction= 1.232693
(Hartree/Particle)
Thermal correction to Energy= 1.305191
Thermal correction to Enthalpy= 1.306135
Thermal correction to Gibbs Free Energy= 1.120481
Sum of electronic and zero-point Energies= -3890.775575
Sum of electronic and thermal Energies= -3890.703078
Sum of electronic and thermal Enthalpies= -3890.702134
Sum of electronic and thermal Free Energies= -3890.887788

.....

Cartesian Coordinates

.....

77	0.345172	-0.749393	-1.663200
15	1.865085	0.399471	-0.366913
8	2.367387	0.028979	1.173071
8	3.361442	0.460262	-1.128141
7	1.250107	1.921557	-0.080379
6	3.216797	-1.049475	1.377807
6	2.659084	-2.194612	1.988527
1	1.615950	-2.167761	2.283603
6	3.442969	-3.304019	2.188646
1	3.029502	-4.190434	2.661333
6	4.794290	-3.321466	1.747992
6	5.589789	-4.493100	1.870408
1	5.148598	-5.371741	2.333779
6	6.883067	-4.523203	1.399942
1	7.479317	-5.426260	1.492462
6	7.431944	-3.376397	0.777798
1	8.444332	-3.410112	0.385495
6	6.693227	-2.219243	0.658219
1	7.126886	-1.354466	0.170151
6	5.360210	-2.144250	1.151163
6	4.556033	-0.955658	1.031123
6	5.107313	0.332235	0.524846
6	6.237819	0.973944	1.145270
6	6.828208	0.494858	2.348843
1	6.413907	-0.382138	2.831668
6	7.907706	1.135485	2.917543
1	8.334311	0.751798	3.839980
6	8.461626	2.291139	2.317016
1	9.316497	2.781798	2.773166
6	7.901898	2.796756	1.165553
1	8.303722	3.694650	0.702988
6	6.778591	2.169147	0.561463
6	6.170055	2.717418	-0.599653
1	6.594225	3.612529	-1.045837
6	5.042032	2.145240	-1.131916
1	4.541396	2.565470	-1.997589
6	4.504896	0.976953	-0.546153
6	0.103443	2.286204	-0.957887

1	-0.807465	2.267591	-0.352441
6	0.279870	3.687233	-1.528283
6	1.526876	4.106158	-2.016698
1	2.378056	3.437738	-1.930226
6	1.678559	5.367828	-2.591139
1	2.652283	5.680619	-2.959304
6	0.581152	6.229788	-2.689884
1	0.697826	7.214070	-3.135181
6	-0.662862	5.819223	-2.206548
1	-1.519333	6.485058	-2.272460
6	-0.813595	4.556574	-1.625068
1	-1.777359	4.247306	-1.235075
6	-0.046841	1.284463	-2.117512
1	0.650242	1.575718	-2.911331
1	-1.050477	1.388480	-2.529976
6	1.428969	2.798384	1.123797
1	0.968895	3.740363	0.813496
6	0.623891	2.307402	2.326377
6	-0.738227	2.630915	2.409315
1	-1.206136	3.226824	1.632868
6	-1.517272	2.199320	3.485622
1	-2.567881	2.466814	3.509668
6	-0.940194	1.441041	4.505731
1	-1.540073	1.107665	5.348376
6	0.420218	1.124798	4.443317
1	0.882480	0.545029	5.238140
6	1.194648	1.557190	3.365281
1	2.247528	1.303700	3.334259
6	2.890210	3.123840	1.427729
1	3.358559	3.581610	0.553939
1	3.473021	2.245857	1.705269
1	2.933011	3.837335	2.256630
6	-0.851757	-1.559771	0.737787
1	-0.468930	-2.540368	0.514719
1	-0.480045	-1.078942	1.634681
6	-1.429154	-0.742545	-0.260370
1	-1.749904	0.241068	0.063647
6	-1.863349	-1.245447	-1.537543
1	-1.926323	-2.324934	-1.623625
6	1.712052	-0.792680	-3.384965
1	2.065244	0.221436	-3.554053
6	0.385367	-1.070559	-3.828446
1	-0.152138	-0.249052	-4.302797
6	-0.119228	-2.432369	-4.267230
1	0.185656	-2.616676	-5.308908
1	-1.210766	-2.388695	-4.273312
6	0.332592	-3.612794	-3.379527
1	1.279277	-4.020643	-3.745861
1	-0.401044	-4.420695	-3.470065
6	0.481916	-3.269912	-1.906858
1	-0.315692	-3.607419	-1.251121
6	1.655748	-2.864922	-1.321173
1	1.726754	-2.936059	-0.240332
6	2.964936	-2.625006	-2.041913
1	3.619984	-2.077699	-1.363668
1	3.450394	-3.593659	-2.231094
6	2.839717	-1.829324	-3.359426
1	2.708730	-2.511937	-4.205758
1	3.786785	-1.309977	-3.532985
6	-2.888593	-0.554450	-2.351258
6	-3.306159	0.769412	-2.115451
6	-3.526448	-1.266058	-3.386778
6	-4.299895	1.360077	-2.894878
1	-2.889915	1.337783	-1.296167
6	-4.515689	-0.673616	-4.172116
1	-3.255788	-2.304545	-3.559585
6	-4.906168	0.647664	-3.932791
1	-4.618050	2.371627	-2.660406
1	-4.991128	-1.248844	-4.962286
1	-5.683787	1.108392	-4.535533
8	-2.075980	-4.191779	0.261948
6	-2.674533	-3.592988	1.159182
8	-2.351052	-2.487712	1.745757
8	-3.854337	-4.078724	1.667474
6	-4.363488	-5.253991	1.026634
1	-3.659111	-6.087914	1.103893
1	-5.290258	-5.501843	1.548827
1	-4.573006	-5.067658	-0.031865
6	-4.227563	-0.458300	4.064739
6	-5.517976	0.076815	4.663464
1	-3.499875	0.345379	3.917012
1	-3.768168	-1.220006	4.700977
6	-6.244236	0.910651	3.615346
1	-5.303713	0.696271	5.538515
1	-6.156305	-0.753932	4.984170
1	-7.229094	1.206297	3.982257
1	-5.680110	1.815775	3.369987
7	-4.512901	-1.065720	2.770222
6	-5.520907	-0.735840	1.975976
7	-6.448270	0.143985	2.363939
6	-5.534675	-1.458412	0.642029
1	-4.499931	-1.749034	0.460486
1	-6.097023	-2.391913	0.766489
6	-6.047361	-0.660679	-0.562315
1	-5.666121	0.358947	-0.494406
6	-7.564035	0.645309	1.523997
6	-7.573198	-0.657041	-0.685823
1	-7.866744	0.121105	-1.400784
6	-8.262595	-0.410310	0.663219
1	-9.293246	-0.077785	0.497653
1	-8.331673	-1.338863	1.242714
1	-8.286476	1.053424	2.233363
1	-7.191628	1.479278	0.919450
1	-7.922678	-1.612156	-1.097881
1	-5.604138	-1.088595	-1.465537
1	-3.765447	-1.656066	2.374982
5	-4.092145	2.513634	0.882186
9	-5.273454	2.566180	0.118187
9	-4.309797	3.123722	2.134319
9	-3.060909	3.196992	0.195695
9	-3.698369	1.176428	1.072420

---

13 P1 *endo-re* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 14.9609 21.2149 24.3543 cm(-1)
Electronic energy= -3892.037264
Zero-point correction= 1.234079
(Hartree/Particle)
Thermal correction to Energy= 1.306566
Thermal correction to Enthalpy= 1.307511
Thermal correction to Gibbs Free Energy= 1.125672
Sum of electronic and zero-point Energies= -3890.803185
Sum of electronic and thermal Energies= -3890.730697
Sum of electronic and thermal Enthalpies= -3890.729753
Sum of electronic and thermal Free Energies= -3890.911592

.....

Cartesian Coordinates

.....

77	0.081108	-0.765564	-1.177739
15	1.898081	0.304239	-0.336870
8	2.545166	0.017399	1.146451
8	3.230861	0.054672	-1.303845
7	1.541035	1.924671	-0.175895
6	3.401344	-1.050882	1.391500
6	2.906897	-2.065528	2.238591
1	1.911145	-1.952804	2.654311
6	3.691326	-3.158912	2.509198
1	3.327342	-3.947302	3.161667
6	4.975891	-3.289533	1.915375
6	5.764655	-4.452578	2.128440
1	5.372498	-5.232033	2.776402
6	6.990360	-4.597758	1.519174
1	7.582416	-5.492966	1.685142
6	7.472864	-3.582288	0.659474
1	8.428767	-3.710318	0.159702
6	6.740087	-2.435300	0.443850
1	7.122110	-1.673997	-0.225681
6	5.479555	-2.239778	1.074611
6	4.684667	-1.056073	0.867773

6	5.188786	0.115340	0.096664
6	6.401469	0.804764	0.456086
6	7.132289	0.505513	1.640197
1	6.768835	-0.266047	2.308380
6	8.284163	1.191934	1.958210
1	8.818351	0.949056	2.872338
6	8.774305	2.214318	1.111187
1	9.687176	2.741942	1.371604
6	8.080984	2.546278	-0.030509
1	8.433696	3.342583	-0.680654
6	6.880608	1.869855	-0.379488
6	6.138554	2.245323	-1.531680
1	6.519110	3.036203	-2.171671
6	4.940324	1.639022	-1.816275
1	4.344273	1.924314	-2.675878
6	4.466246	0.606415	-0.979111
6	0.353408	2.335476	-0.970103
1	-0.483813	2.470332	-0.282354
6	0.586092	3.650289	-1.698737
6	1.823891	3.946264	-2.285807
1	2.646803	3.250928	-2.162385
6	2.006571	5.131219	-2.999331
1	2.974267	5.349972	-3.443324
6	0.950216	6.036664	-3.138522
1	1.091788	6.960559	-3.692513
6	-0.284903	5.750015	-2.552332
1	-1.108628	6.452617	-2.646146
6	-0.466554	4.565850	-1.832910
1	-1.422219	4.353690	-1.363955
6	-0.016703	1.231628	-1.970625
1	0.652264	1.289833	-2.836860
1	-1.029778	1.408615	-2.337288
6	1.873130	2.837923	0.973830
1	1.535547	3.812520	0.610240
6	1.030984	2.515419	2.209114
6	-0.281996	3.005693	2.286816
1	-0.673288	3.643761	1.501281
6	-1.113626	2.682270	3.361658
1	-2.125515	3.070797	3.376824
6	-0.636077	1.870715	4.392062
1	-1.276851	1.619021	5.232941
6	0.679409	1.399456	4.343707
1	1.067127	0.781523	5.149425
6	1.504915	1.721872	3.264768
1	2.520071	1.344821	3.246445
6	3.373320	2.973530	1.226001
1	3.880133	3.273139	0.305634
1	3.832386	2.051579	1.580122
1	3.538275	3.748729	1.980782
6	-0.797901	-0.556323	0.832504
1	-0.909992	-1.557046	1.241357
1	-0.359438	0.167964	1.513359
6	-1.792780	-0.060783	-0.062755
1	-1.937868	1.007780	-0.113934
6	-2.494227	-0.890914	-0.942858
1	-2.550465	-1.943718	-0.707468
6	1.215118	-1.334645	-3.054527
1	1.718759	-0.425451	-3.366964
6	-0.160638	-1.424467	-3.331261
1	-0.626276	-0.586558	-3.847826
6	-0.935344	-2.725354	-3.428599
1	-0.742413	-3.177583	-4.412996
1	-1.997908	-2.476435	-3.413006
6	-0.638725	-3.754565	-2.312720
1	0.147978	-4.445391	-2.633138
1	-1.528492	-4.365218	-2.136830
6	-0.239322	-3.153104	-0.972415
1	-0.963134	-3.249632	-0.171644
6	1.060643	-2.871623	-0.598456
1	1.254491	-2.787459	0.466280
6	2.288174	-3.064335	-1.463835
1	3.122846	-2.546139	-0.989103
1	2.548761	-4.132301	-1.470979
6	2.131862	-2.548233	-2.909982
1	1.760699	-3.346449	-3.559908
1	3.120577	-2.276680	-3.290732
6	-3.446594	-0.415410	-1.949106
6	-3.678550	0.949348	-2.219405
6	-4.203636	-1.374250	-2.653023
6	-4.617960	1.330121	-3.175924
1	-3.158207	1.718427	-1.661701
6	-5.134834	-0.989355	-3.615961
1	-4.070459	-2.423941	-2.412918
6	-5.342773	0.366720	-3.885055
1	-4.793032	2.386599	-3.358053
1	-5.706164	-1.746243	-4.146285
1	-6.072830	0.671070	-4.629641
8	-2.592960	-5.278050	0.062653
6	-3.149945	-4.217242	0.371099
8	-2.792918	-3.327258	1.200019
8	-4.346546	-3.871142	-0.285703
6	-4.836628	-4.824285	-1.225002
1	-5.028652	-5.793919	-0.752585
1	-5.773168	-4.415682	-1.615719
1	-4.134005	-4.982715	-2.051243
6	-3.219964	-0.805930	3.383365
6	-4.056176	-0.219466	4.510655
1	-2.525191	-0.057396	2.990493
1	-2.645054	-1.675655	3.709805
6	-5.006721	0.825854	3.941938
1	-3.413741	0.247347	5.262282
1	-4.627402	-1.015278	5.001437
1	-5.731052	1.127713	4.702915
1	-4.465115	1.715692	3.608039
7	-4.105137	-1.239039	2.306228
6	-5.262891	-0.666938	2.021548
7	-5.774864	0.303675	2.790745
6	-5.971478	-1.206999	0.797595
1	-5.259251	-1.849139	0.278656
1	-6.785431	-1.863395	1.129117
6	-6.507039	-0.127540	-0.159919
1	-5.816658	0.719841	-0.172521
6	-6.888151	1.203517	2.397949
6	-7.917491	0.348166	0.210460
1	-8.120158	1.295256	-0.304045
6	-8.090239	0.537106	1.724749
1	-8.967173	1.164746	1.918448
1	-8.285642	-0.420225	2.221563
1	-7.218882	1.662471	3.332043
1	-6.480024	2.001578	1.767826
1	-8.664130	-0.372466	-0.146409
1	-6.505459	-0.535221	-1.174321
1	-3.751751	-2.034506	1.726647
5	-3.794071	2.881229	0.938245
9	-4.987295	2.926385	0.197786
9	-3.858625	3.774108	2.018488
9	-2.703408	3.226892	0.091625
9	-3.585717	1.577272	1.422688

---

12 P1 *exo-si* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 8.0590 14.0000 20.0176 cm(-1)
Electronic energy= -3892.0254436
Zero-point correction= 1.235436
(Hartree/Particle)
Thermal correction to Energy= 1.307835
Thermal correction to Enthalpy= 1.308780
Thermal correction to Gibbs Free Energy= 1.123718
Sum of electronic and zero-point Energies= -3890.790007
Sum of electronic and thermal Energies= -3890.717608
Sum of electronic and thermal Enthalpies= -3890.716664
Sum of electronic and thermal Free Energies= -3890.901726

.....

Cartesian Coordinates

.....

77	0.280289	-0.887088	-1.457943
15	1.823501	0.525010	-0.502219
8	2.409054	0.389417	1.059551
8	3.287942	0.500013	-1.327303

7	1.222260	2.089228	-0.419812
6	3.162010	-0.732651	1.372839
6	2.542044	-1.720402	2.170526
1	1.533244	-1.544301	2.528410
6	3.229125	-2.872370	2.466531
1	2.771449	-3.639934	3.084578
6	4.529178	-3.096518	1.935699
6	5.211000	-4.324244	2.156739
1	4.725455	-5.083756	2.764153
6	6.449583	-4.556794	1.602502
1	6.957788	-5.501596	1.772390
6	7.055511	-3.565672	0.793661
1	8.021433	-3.761095	0.336551
6	6.429749	-2.357506	0.574803
1	6.904126	-1.613694	-0.054571
6	5.158222	-2.074055	1.147539
6	4.471338	-0.827801	0.928032
6	5.113062	0.329719	0.243388
6	6.348849	0.897768	0.722964
6	6.964766	0.483636	1.937967
1	6.488786	-0.280074	2.541120
6	8.146206	1.048102	2.368682
1	8.589026	0.716952	3.303819
6	8.783774	2.058771	1.610798
1	9.718036	2.489745	1.958841
6	8.204461	2.502358	0.443500
1	8.670063	3.292571	-0.140083
6	6.978593	1.952445	-0.020288
6	6.354075	2.446828	-1.197223
1	6.843652	3.233658	-1.764330
6	5.133790	1.962004	-1.593031
1	4.620897	2.348275	-2.467641
6	4.509106	0.931039	-0.853055
6	-0.096578	2.247768	-1.089002
1	-0.867912	2.286071	-0.316724
6	-0.196137	3.541765	-1.880318
6	0.894082	4.057442	-2.594448
1	1.854240	3.552659	-2.529977
6	0.754068	5.211183	-3.367756
1	1.609577	5.603994	-3.911281
6	-0.481726	5.861064	-3.443100
1	-0.591106	6.758869	-4.045329
6	-1.574600	5.348135	-2.739217
1	-2.540306	5.843577	-2.795584
6	-1.432801	4.197847	-1.959703
1	-2.285540	3.787990	-1.425734
6	-0.401965	1.067247	-2.027742
1	0.069062	1.287118	-2.993278
1	-1.476905	1.059331	-2.195684
6	1.552378	3.173464	0.563456
1	1.199505	4.081610	0.067117
6	0.732530	3.042683	1.846937
6	-0.518730	3.672914	1.914289
1	-0.856312	4.277230	1.076123
6	-1.335074	3.537141	3.039381
1	-2.292569	4.047273	3.070770
6	-0.915439	2.756908	4.118545
1	-1.553706	2.635561	4.989619
6	0.342528	2.148973	4.076587
1	0.687108	1.551825	4.916268
6	1.163042	2.301321	2.957122
1	2.132120	1.819237	2.941243
6	3.047649	3.382500	0.795249
1	3.551889	3.586202	-0.151746
1	3.534633	2.528556	1.264544
1	3.181278	4.252034	1.446486
6	-0.961835	0.017795	1.320345
6	-0.887734	-1.154229	0.391660
1	-0.578646	-2.065297	0.903770
6	-1.822406	-1.251346	-0.688526
1	-2.352666	-0.334528	-0.914939
6	1.306264	-0.972740	-3.419171
1	1.545197	0.041971	-3.729282
6	-0.050527	-1.379777	-3.584972
1	-0.734935	-0.649375	-4.016010
6	-0.489957	-2.816892	-3.807362
1	-0.290737	-3.116922	-4.848306
1	-1.573860	-2.850019	-3.677060
6	0.155301	-3.822045	-2.831345
1	1.053839	-4.265174	-3.273324
1	-0.541450	-4.649136	-2.661630
6	0.516843	-3.220289	-1.476527
1	-0.078368	-3.572446	-0.643202
6	1.764550	-2.694567	-1.165032
1	2.056869	-2.696261	-0.120841
6	2.908351	-2.542082	-2.149089
1	3.655563	-1.894012	-1.689333
1	3.389410	-3.521550	-2.294204
6	2.489028	-1.941601	-3.508108
1	2.247174	-2.740792	-4.217831
1	3.346816	-1.410861	-3.933784
6	-2.616872	-2.439120	-1.065867
6	-2.561920	-3.673620	-0.392732
6	-3.544054	-2.307767	-2.120588
6	-3.359333	-4.748872	-0.792333
1	-1.908931	-3.790534	0.466704
6	-4.347774	-3.376092	-2.511694
1	-3.635255	-1.343888	-2.612787
6	-4.252488	-4.610268	-1.857969
1	-3.293112	-5.692734	-0.256837
1	-5.055358	-3.245141	-3.326420
1	-4.876945	-5.445007	-2.163981
8	-0.499159	-1.357947	3.673214
6	-1.583371	-0.846119	3.478640
8	-1.977030	-0.196112	2.380778
8	-2.612111	-0.843606	4.338932
6	-2.365656	-1.522679	5.587867
1	-1.540996	-1.048246	6.126033
1	-3.291043	-1.430454	6.156594
1	-2.130908	-2.576043	5.413907
6	-4.689821	2.458676	2.142115
6	-6.143169	2.904872	2.127427
1	-4.152301	2.813976	1.258921
1	-4.171316	2.814845	3.034690
6	-6.900305	2.110597	1.071811
1	-6.205484	3.971508	1.896961
1	-6.600096	2.742989	3.109927
1	-7.965064	2.348151	1.107850
1	-6.524349	2.335985	0.068599
7	-4.636140	0.997326	2.152839
6	-5.596641	0.178019	1.741127
7	-6.762293	0.654840	1.303344
6	-5.269631	-1.297499	1.861118
1	-4.183608	-1.362493	1.950035
1	-5.678458	-1.656476	2.814146
6	-5.734206	-2.183124	0.696248
1	-5.576038	-1.637460	-0.235301
6	-7.821276	-0.152172	0.652284
6	-7.191958	-2.636191	0.822780
1	-7.531010	-3.009935	-0.150766
6	-8.117385	-1.507503	1.297508
1	-9.157851	-1.763369	1.069834
1	-8.064734	-1.390314	2.386374
1	-8.719120	0.466302	0.706123
1	-7.561539	-0.257312	-0.407728
1	-7.266249	-3.475729	1.525247
1	-5.077346	-3.054881	0.647891
1	-3.738099	0.574635	2.374174
5	-4.260230	1.507815	-1.503559
9	-5.114480	0.494028	-1.024193
9	-4.985446	2.695822	-1.678470
9	-3.689714	1.091122	-2.719877
9	-3.231313	1.742844	-0.550796
1	-0.023692	0.229364	1.825980
1	-1.333832	0.905816	0.821690

[12-13]‡ P1 *exo-si* [BF_4^-]

Number of imaginary frequencies= 1
The smallest frequencies are=-270.0672 13.9445 20.2724cm(-1)

Electronic energy= -3892.005384
Zero-point correction= 1.233242
(Hartree/Particle)
Thermal correction to Energy= 1.305490
Thermal correction to Enthalpy= 1.306434
Thermal correction to Gibbs Free Energy= 1.123402
Sum of electronic and zero-point Energies= -3890.772142
Sum of electronic and thermal Energies= -3890.699894
Sum of electronic and thermal Enthalpies= -3890.698950
Sum of electronic and thermal Free Energies= -3890.881982

Cartesian Coordinates

77	0.226104	-1.203028	-1.187019
15	1.784042	0.389046	-0.548924
8	2.411021	0.541438	0.989640
8	3.206367	0.199570	-1.405077
7	1.154773	1.922685	-0.756350
6	3.223634	-0.469974	1.486275
6	2.675914	-1.294212	2.495926
1	1.680900	-1.077567	2.874760
6	3.422680	-2.339850	2.981476
1	3.023887	-2.979916	3.763500
6	4.709236	-2.623094	2.446122
6	5.448411	-3.759268	2.874352
1	5.017737	-4.398081	3.641128
6	6.674328	-4.055903	2.322605
1	7.226681	-4.930986	2.652462
6	7.209581	-3.224817	1.309592
1	8.165715	-3.474427	0.858443
6	6.527362	-2.105184	0.885014
1	6.948192	-1.485048	0.102216
6	5.266733	-1.756938	1.445445
6	4.519788	-0.603755	1.014034
6	5.088277	0.417516	0.088399
6	6.312577	1.114690	0.394044
6	6.989144	0.969362	1.638128
1	6.570137	0.321431	2.398368
6	8.158354	1.650992	1.898626
1	8.648957	1.526037	2.859786
6	8.721824	2.516982	0.931657
1	9.647297	3.042524	1.148441
6	8.082192	2.701601	-0.273114
1	8.490665	3.379063	-1.018576
6	6.866765	2.025902	-0.567328
6	6.179912	2.257105	-1.789773
1	6.612640	2.936828	-2.518447
6	4.970262	1.656803	-2.032142
1	4.408634	1.844297	-2.941418
6	4.424522	0.766948	-1.078959
6	-0.180027	1.931476	-1.416734
1	-0.934716	2.109685	-0.646888
6	-0.310641	3.045179	-2.443232
6	0.758367	3.406513	-3.274699
1	1.722493	2.924013	-3.136205
6	0.594210	4.385799	-4.255716
1	1.433809	4.663121	-4.887917
6	-0.645728	5.009908	-4.424056
1	-0.774287	5.772302	-5.187552
6	-1.717761	4.646712	-3.604600
1	-2.686906	5.121816	-3.731495
6	-1.551893	3.672003	-2.617735
1	-2.389626	3.382057	-1.991083
6	-0.482399	0.594145	-2.113088
1	-0.022378	0.630842	-3.106912
1	-1.556903	0.544887	-2.264413
6	1.464753	3.192150	-0.019329
1	1.203396	3.974081	-0.737171
6	0.542411	3.389548	1.183223
6	-0.538466	4.275632	1.072326
1	-0.704790	4.797377	0.133176
6	-1.405229	4.490889	2.146920
1	-2.235791	5.183043	2.038892
6	-1.207454	3.811649	3.350735
1	-1.883639	3.968060	4.186793
6	-0.136719	2.922370	3.470780
1	0.018609	2.374185	4.394949
6	0.733346	2.717581	2.399524
1	1.555272	2.021674	2.506453
6	2.940789	3.417972	0.313126
1	3.553644	3.354975	-0.588461
1	3.330879	2.716248	1.049082
1	3.043054	4.428847	0.719980
6	-0.826479	-0.140930	1.140646
6	-1.114599	-1.416769	0.610298
1	-0.814242	-2.272171	1.207641
6	-1.949144	-1.568267	-0.540812
1	-2.426095	-0.656985	-0.877742
6	1.313865	-1.590861	-3.060754
1	1.511096	-0.633022	-3.534977
6	-0.013368	-2.091387	-3.197379
1	-0.712044	-1.478540	-3.766102
6	-0.375163	-3.564946	-3.190760
1	-0.129277	-4.004194	-4.169714
1	-1.458517	-3.640895	-3.082858
6	0.300823	-4.371986	-2.063938
1	1.238433	-4.812388	-2.417670
1	-0.348091	-5.209479	-1.790496
6	0.581933	-3.560198	-0.806863
1	-0.045453	-3.786720	0.045568
6	1.782196	-2.925109	-0.546992
1	2.020823	-2.707639	0.488655
6	2.944901	-2.886581	-1.516710
1	3.680595	-2.179771	-1.134829
1	3.431248	-3.873076	-1.518567
6	2.553107	-2.484983	-2.957419
1	2.392025	-3.378224	-3.570836
1	3.396615	-1.954244	-3.407920
6	-2.735649	-2.764777	-0.888580
6	-2.685851	-3.981748	-0.185569
6	-3.644223	-2.655037	-1.960974
6	-3.488620	-5.059739	-0.562606
1	-2.040341	-4.083820	0.680625
6	-4.448162	-3.730299	-2.333695
1	-3.724049	-1.705551	-2.482428
6	-4.369295	-4.943721	-1.641654
1	-3.434215	-5.989496	-0.002332
1	-5.143532	-3.619243	-3.161463
1	-4.996082	-5.782747	-1.930362
8	-0.343981	-0.479937	4.069326
6	-1.480099	-0.047735	3.859124
8	-2.070146	0.119430	2.724091
8	-2.301057	0.323638	4.893457
6	-1.746189	0.161773	6.203469
1	-0.850380	0.776729	6.337961
1	-2.522954	0.485466	6.900082
1	-1.484300	-0.882967	6.399702
6	-4.492415	2.713465	1.843108
6	-5.930268	3.204398	1.789899
1	-3.978254	2.882165	0.892604
1	-3.922478	3.206066	2.633181
6	-6.737865	2.285312	0.882761
1	-5.968941	4.225207	1.400538
1	-6.364131	3.208806	2.796141
1	-7.797381	2.549225	0.919929
1	-6.395628	2.364530	-0.154079
7	-4.486799	1.279316	2.121443
6	-5.470991	0.441157	1.837015
7	-6.620918	0.872082	1.306293
6	-5.203621	-1.007660	2.194083
1	-4.137279	-1.074719	2.416808
1	-5.729896	-1.234112	3.129456
6	-5.575899	-2.020339	1.098048
1	-5.341072	-1.581035	0.126047
6	-7.666640	0.004262	0.714091
6	-7.046753	-2.451315	1.153918
1	-7.321450	-2.899226	0.191350
6	-7.992155	-1.284159	1.471518
1	-9.018807	-1.565574	1.212235
1	-7.999928	-1.066541	2.545760

1	-8.563353	0.626902	0.684434
1	-7.378599	-0.205511	-0.322096
1	-7.181158	-3.231078	1.914044
1	-4.929321	-2.896470	1.198544
1	-3.599918	0.872648	2.464171
5	-4.258677	1.229527	-1.691850
9	-5.217039	0.344604	-1.160393
9	-4.851359	2.471598	-1.966315
9	-3.717008	0.669986	-2.865220
9	-3.224498	1.425792	-0.738891
1	0.006544	-0.007203	1.811133
1	-1.243480	0.736347	0.669089

---

13 P1 *exo-si* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 17.2056 21.5980 24.4186 cm(-1)
Electronic energy= -3892.0341591
Zero-point correction= 1.233950
(Hartree/Particle)
Thermal correction to Energy= 1.306476
Thermal correction to Enthalpy= 1.307420
Thermal correction to Gibbs Free Energy= 1.125030
Sum of electronic and zero-point Energies= -3890.800210
Sum of electronic and thermal Energies= -3890.727683
Sum of electronic and thermal Enthalpies= -3890.726739
Sum of electronic and thermal Free Energies= -3890.909129

.....

Cartesian Coordinates

.....

77	-0.092677	-0.550660	-1.414377
15	1.724292	0.408089	-0.452712
8	2.330121	-0.049145	1.005987
8	3.084228	0.248169	-1.402666
7	1.377697	2.006248	-0.134633
6	3.155526	-1.164009	1.143497
6	2.600856	-2.273846	1.814801
1	1.567305	-2.236259	2.142528
6	3.363096	-3.403252	1.981787
1	2.949119	-4.268078	2.492757
6	4.678360	-3.477326	1.449698
6	5.443463	-4.670901	1.554054
1	5.012015	-5.516138	2.083933
6	6.693057	-4.763426	0.984661
1	7.266377	-5.682300	1.065923
6	7.224033	-3.660991	0.273328
1	8.198449	-3.744950	-0.199395
6	6.514996	-2.484055	0.167153
1	6.935213	-1.656365	-0.391433
6	5.231541	-2.341789	0.766158
6	4.459324	-1.128349	0.672922
6	5.004743	0.108351	0.046540
6	6.221111	0.727926	0.505867
6	6.903870	0.297984	1.678277
1	6.497283	-0.522716	2.257067
6	8.061192	0.918635	2.095638
1	8.558181	0.576303	2.998839
6	8.605083	2.001421	1.364158
1	9.521990	2.475975	1.701267
6	7.958660	2.459243	0.238486
1	8.352754	3.303162	-0.321715
6	6.753053	1.853727	-0.209317
6	6.055584	2.359221	-1.339767
1	6.475660	3.197623	-1.888080
6	4.849493	1.819492	-1.712200
1	4.280345	2.208519	-2.549468
6	4.324222	0.724003	-0.992862
6	0.183475	2.511130	-0.860039
1	-0.626135	2.637508	-0.136762
6	0.438112	3.859571	-1.517160
6	1.709974	4.235651	-1.968976
1	2.551972	3.574173	-1.793116
6	1.899954	5.457829	-2.617251
1	2.894080	5.739758	-2.954595
6	0.818589	6.317798	-2.826715
1	0.966227	7.269683	-3.329427
6	-0.453375	5.946734	-2.381224
1	-1.300163	6.609624	-2.538037
6	-0.643062	4.727641	-1.727273
1	-1.633960	4.432060	-1.394672
6	-0.286322	1.506985	-1.928331
1	0.298015	1.666256	-2.841844
1	-1.324133	1.744874	-2.161872
6	1.770627	2.832584	1.060260
1	1.483279	3.842454	0.755928
6	0.935771	2.503068	2.297333
6	-0.292388	3.154415	2.480142
1	-0.628207	3.883739	1.750165
6	-1.098923	2.877561	3.586018
1	-2.053008	3.384937	3.691425
6	-0.679817	1.953193	4.543113
1	-1.301727	1.736673	5.407228
6	0.551919	1.310936	4.383936
1	0.894302	0.598255	5.129079
6	1.350842	1.582585	3.272114
1	2.300509	1.072828	3.167570
6	3.275095	2.885700	1.318082
1	3.801516	3.209986	0.418329
1	3.691666	1.929692	1.631494
1	3.466981	3.614840	2.111423
6	-0.990672	-0.136245	0.566230
6	-1.942050	-0.949769	-0.112319
1	-2.036683	-1.976022	0.212869
6	-2.630170	-0.529879	-1.251041
1	-2.715538	0.527815	-1.455395
6	1.076643	-0.864021	-3.314059
1	1.506410	0.105795	-3.547407
6	-0.289807	-1.027791	-3.615240
1	-0.801673	-0.167622	-4.045661
6	-0.970171	-2.347763	-3.916634
1	-0.772709	-2.607717	-4.967404
1	-2.046689	-2.194412	-3.839574
6	-0.569473	-3.535468	-3.011342
1	0.293398	-4.056696	-3.437061
1	-1.395242	-4.253305	-3.005575
6	-0.251748	-3.161609	-1.578401
1	-1.001811	-3.365906	-0.823554
6	0.994161	-2.835432	-1.120988
1	1.125733	-2.847391	-0.045010
6	2.243401	-2.773419	-1.970206
1	3.032576	-2.304720	-1.382184
1	2.580236	-3.800189	-2.172191
6	2.091052	-2.009298	-3.307849
1	1.820331	-2.705805	-4.108415
1	3.067789	-1.597513	-3.575520
6	-3.559767	-1.380589	-1.999433
6	-3.792340	-2.735487	-1.685485
6	-4.261160	-0.811880	-3.079381
6	-4.673489	-3.495576	-2.451854
1	-3.307034	-3.188329	-0.827075
6	-5.144006	-1.574758	-3.842477
1	-4.107477	0.239056	-3.310547
6	-5.346849	-2.923579	-3.537551
1	-4.842216	-4.538139	-2.196480
1	-5.674506	-1.116949	-4.672667
1	-6.031340	-3.521953	-4.132084
8	-0.542092	-3.202564	1.797532
6	-1.644973	-3.021731	2.347505
8	-2.807431	-3.147623	1.865013
8	-1.664668	-2.595023	3.680181
6	-0.394670	-2.315317	4.265284
1	0.100112	-1.472144	3.771478
1	-0.589446	-2.052908	5.309393
1	0.270442	-3.184559	4.225305
6	-3.349668	0.153670	3.214971
6	-4.291371	1.017153	4.038671
1	-2.781112	0.773134	2.516840
1	-2.650435	-0.411742	3.829956
6	-5.353359	1.604428	3.120084
1	-3.743158	1.830321	4.520284

1	-4.762794	0.413756	4.822575
1	-6.138774	2.087216	3.707815
1	-4.922779	2.354933	2.449897
7	-4.143383	-0.811389	2.454596
6	-5.358471	-0.568152	1.993058
7	-6.007851	0.563232	2.296102
6	-5.959921	-1.668922	1.142396
1	-5.144839	-2.359002	0.916010
1	-6.681918	-2.224869	1.752885
6	-6.613456	-1.192974	-0.167735
1	-6.023588	-0.368529	-0.574023
6	-7.202962	1.072908	1.582551
6	-8.075859	-0.767744	0.012307
1	-8.383263	-0.177202	-0.859206
6	-8.301668	0.047688	1.294175
1	-9.249777	0.591447	1.218044
1	-8.399055	-0.611302	2.164767
1	-7.610990	1.846039	2.236787
1	-6.860989	1.570391	0.668489
1	-8.723380	-1.653181	0.036998
1	-6.548337	-2.004051	-0.898137
1	-3.704882	-1.735803	2.252817
5	-3.863585	2.584311	-0.063201
9	-4.531308	1.342272	-0.066773
9	-4.766417	3.596043	0.280623
9	-3.319403	2.816863	-1.347713
9	-2.813068	2.551496	0.883014
1	-0.500613	-0.593007	1.420278
1	-1.178418	0.926374	0.654774

---

12 P1 *endo-si* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 16.4564 19.7042 25.7201 cm(-1)
Electronic energy= -3892.0137547
Zero-point correction= 1.236467
(Hartree/Particle)
Thermal correction to Energy= 1.308353
Thermal correction to Enthalpy= 1.309298
Thermal correction to Gibbs Free Energy= 1.128982
Sum of electronic and zero-point Energies= -3890.777288
Sum of electronic and thermal Energies= -3890.705401
Sum of electronic and thermal Enthalpies= -3890.704457
Sum of electronic and thermal Free Energies= -3890.884773

.....

Cartesian Coordinates

.....

77	0.437709	-1.012148	-1.534254
15	1.602326	0.546412	-0.279050
8	2.125032	0.389506	1.301939
8	3.097934	0.877761	-0.999321
7	0.707371	1.933192	-0.135631
6	2.972578	-0.683353	1.552121
6	2.409924	-1.801576	2.203641
1	1.377073	-1.737439	2.521659
6	3.172762	-2.924530	2.404120
1	2.754028	-3.791210	2.908227
6	4.506652	-2.984509	1.914718
6	5.274208	-4.175928	2.024075
1	4.827447	-5.035004	2.518007
6	6.546100	-4.249883	1.502777
1	7.120379	-5.168063	1.585605
6	7.100170	-3.128335	0.840647
1	8.093958	-3.196470	0.407275
6	6.389711	-1.952156	0.734422
1	6.827069	-1.107485	0.215544
6	5.080274	-1.831420	1.279297
6	4.302029	-0.622877	1.166642
6	4.873956	0.642789	0.632130
6	6.054760	1.233430	1.214375
6	6.647471	0.741560	2.411702
1	6.194447	-0.099648	2.922454
6	7.777475	1.325988	2.942731
1	8.202393	0.933197	3.862215
6	8.384320	2.435358	2.308270
1	9.278250	2.881918	2.733955
6	7.825144	2.953165	1.161521
1	8.267009	3.817487	0.672081
6	6.651876	2.383249	0.597869
6	6.045901	2.945010	-0.558412
1	6.510827	3.803216	-1.035696
6	4.871299	2.433977	-1.045590
1	4.371808	2.873327	-1.902449
6	4.270395	1.310157	-0.426681
6	-0.397629	2.079083	-1.110835
1	-1.263440	2.429663	-0.541896
6	-0.071255	3.141846	-2.156301
6	1.208152	3.249866	-2.721776
1	2.006003	2.606744	-2.367969
6	1.466305	4.182722	-3.728284
1	2.464189	4.252682	-4.154282
6	0.449774	5.027859	-4.182646
1	0.650825	5.755867	-4.963912
6	-0.823517	4.936270	-3.614697
1	-1.617441	5.599237	-3.949034
6	-1.081271	4.003093	-2.606770
1	-2.064347	3.950034	-2.149236
6	-0.797251	0.734166	-1.793452
1	-0.841688	0.920722	-2.870256
1	-1.819334	0.517797	-1.486283
6	0.898748	3.131718	0.736590
1	0.473726	3.950811	0.149270
6	0.083074	3.060248	2.024215
6	-1.150140	3.722150	2.087766
1	-1.551897	4.200513	1.200729
6	-1.885161	3.756437	3.275753
1	-2.846717	4.261400	3.295011
6	-1.391333	3.131315	4.421230
1	-1.956229	3.161199	5.349205
6	-0.172603	2.448108	4.361533
1	0.211078	1.942604	5.243830
6	0.555958	2.408409	3.172413
1	1.497404	1.872270	3.136282
6	2.359661	3.512077	0.977842
1	2.859681	3.706443	0.027417
1	2.918034	2.744272	1.514128
1	2.390858	4.430173	1.572408
6	1.528747	-0.458461	-3.376994
1	1.451932	0.615264	-3.528807
6	0.371060	-1.214668	-3.726655
1	-0.474755	-0.651257	-4.118798
6	0.403646	-2.647938	-4.232393
1	0.779167	-2.667838	-5.267366
1	-0.628449	-3.007313	-4.280009
6	1.234814	-3.605212	-3.353791
1	2.247401	-3.702956	-3.760229
1	0.794686	-4.607190	-3.394346
6	1.335742	-3.179693	-1.893160
1	0.832860	-3.817752	-1.173470
6	2.370684	-2.395795	-1.408236
1	2.609816	-2.480813	-0.354045
6	3.463280	-1.818320	-2.286999
1	4.092001	-1.180555	-1.667503
1	4.103547	-2.646614	-2.625546
6	2.952991	-1.010687	-3.506222
1	3.007792	-1.627057	-4.412336
1	3.634403	-0.170756	-3.669383
6	-1.890596	-3.318538	-1.721643
1	-1.157496	-4.119335	-1.653084
1	-2.242639	-3.223162	-2.748749
6	-1.452934	-2.010493	-1.131343
1	-2.256499	-1.284698	-1.222429
6	-0.719836	-1.966008	0.111046
1	-0.201497	-2.888948	0.360870
6	-1.246648	-1.325034	1.344309
6	-1.960421	-0.114586	1.372576
6	-1.106026	-2.028837	2.557585
6	-2.485067	0.378380	2.565188
1	-2.133691	0.446243	0.465402
6	-1.631584	-1.535336	3.754142

1	-0.595109	-2.988136	2.553557
6	-2.321410	-0.322167	3.764029
1	-3.019854	1.318658	2.546144
1	-1.501094	-2.102047	4.672865
1	-2.724491	0.077393	4.690145
8	-1.913005	-4.892500	0.583070
6	-2.903806	-4.301281	0.212126
8	-3.108860	-3.738947	-0.988243
8	-4.015973	-4.100074	0.942104
6	-3.963554	-4.594760	2.297695
1	-3.722615	-5.660208	2.309876
1	-4.959267	-4.427097	2.708161
1	-3.218045	-4.037625	2.870718
6	-4.896682	-1.105971	-1.968094
6	-6.259201	-0.641281	-2.456253
1	-4.135602	-0.343635	-2.160513
1	-4.587692	-2.041688	-2.436945
6	-6.726084	0.525314	-1.597146
1	-6.200619	-0.317860	-3.498637
1	-6.976700	-1.466959	-2.395524
1	-7.767794	0.764205	-1.822109
1	-6.121679	1.417568	-1.767512
7	-4.980455	-1.338380	-0.527933
6	-5.793578	-0.694173	0.305311
7	-6.660254	0.206728	-0.148760
6	-5.678103	-1.118636	1.757749
1	-4.678812	-1.544676	1.869262
1	-6.391079	-1.938049	1.916952
6	-5.870530	-0.023668	2.817238
1	-5.363794	0.883326	2.481457
6	-7.483992	1.098296	0.709318
6	-7.340909	0.270508	3.132549
1	-7.396124	1.204335	3.704453
6	-8.198725	0.390550	1.863895
1	-9.113979	0.948493	2.088988
1	-8.520849	-0.598078	1.516041
1	-8.226005	1.527038	0.035232
1	-6.854815	1.922603	1.055248
1	-7.754778	-0.517660	3.773641
1	-5.351433	-0.345707	3.725102
1	-4.390613	-2.062467	-0.138562
5	-4.285918	2.826601	-0.044722
9	-4.451226	2.641235	1.344366
9	-5.511967	3.228679	-0.603986
9	-3.312679	3.819268	-0.276556
9	-3.870399	1.614627	-0.641426

[**12-13**]‡ **P1** *endo-si* [BF_4^-]

Number of imaginary frequencies= 1
The smallest frequencies are= -296.0596 7.6177 12.5028 cm(-1)
Electronic energy= -3891.9933958
Zero-point correction= 1.232937
(Hartree/Particle)
Thermal correction to Energy= 1.305136
Thermal correction to Enthalpy= 1.306081
Thermal correction to Gibbs Free Energy= 1.122892
Sum of electronic and zero-point Energies= -3890.760459
Sum of electronic and thermal Energies= -3890.688260
Sum of electronic and thermal Enthalpies= -3890.687315
Sum of electronic and thermal Free Energies= -3890.870504

.....

Cartesian Coordinates

.....

77	0.269459	-0.838541	-1.564084
15	1.698583	0.513268	-0.374822
8	2.242742	0.305578	1.186499
8	3.183851	0.528667	-1.162115
7	1.092388	2.055708	-0.264265
6	2.979719	-0.839862	1.467945
6	2.325853	-1.848747	2.207038
1	1.316197	-1.656432	2.546851
6	2.975306	-3.029414	2.467275
1	2.485111	-3.811520	3.040346
6	4.281287	-3.259787	1.955078
6	4.926766	-4.514117	2.130024
1	4.409826	-5.288082	2.691466
6	6.169143	-4.752982	1.587420
1	6.649982	-5.717657	1.721147
6	6.814138	-3.741071	0.837187
1	7.782574	-3.939900	0.386974
6	6.223981	-2.507368	0.666128
1	6.729564	-1.749612	0.079645
6	4.950287	-2.216365	1.230504
6	4.297669	-0.942841	1.053293
6	4.985491	0.214555	0.419257
6	6.240142	0.714578	0.925925
6	6.813794	0.252768	2.144117
1	6.290570	-0.494932	2.728160
6	8.013300	0.753399	2.603302
1	8.422432	0.388968	3.541387
6	8.712296	1.742068	1.871323
1	9.659763	2.122470	2.241840
6	8.176322	2.228997	0.700359
1	8.690067	3.003518	0.136537
6	6.933619	1.746017	0.208521
6	6.354044	2.283971	-0.972690
1	6.892143	3.049868	-1.524263
6	5.114931	1.870890	-1.388867
1	4.632191	2.298234	-2.261548
6	4.422343	0.869084	-0.667807
6	-0.153727	2.297525	-1.037682
1	-0.971132	2.413785	-0.323843
6	-0.051609	3.583446	-1.848548
6	1.086761	3.849038	-2.626417
1	1.917601	3.148468	-2.603554
6	1.162513	5.003073	-3.404867
1	2.052860	5.199398	-3.996701
6	0.094977	5.908095	-3.422944
1	0.152189	6.807669	-4.029729
6	-1.039782	5.650637	-2.651757
1	-1.870441	6.351540	-2.654216
6	-1.112157	4.496896	-1.864032
1	-1.985654	4.307376	-1.248736
6	-0.461968	1.132555	-2.006279
1	-0.022090	1.389570	-2.974612
1	-1.541866	1.110382	-2.146042
6	1.493232	3.174045	0.644083
1	1.149496	4.063851	0.111592
6	0.765262	3.191210	1.986318
6	-0.364783	4.007625	2.129180
1	-0.760263	4.528227	1.262445
6	-0.987422	4.164659	3.369675
1	-1.861884	4.803952	3.455041
6	-0.486697	3.500954	4.490599
1	-0.963262	3.624745	5.459360
6	0.625569	2.664854	4.355176
1	1.014992	2.133637	5.219564
6	1.245613	2.511073	3.114907
1	2.113030	1.867900	3.028457
6	3.004287	3.346539	0.793098
1	3.465926	3.493600	-0.184692
1	3.486882	2.499124	1.279905
1	3.196184	4.237322	1.398623
6	1.571138	-0.629194	-3.375351
1	1.760843	0.432514	-3.506815
6	0.304620	-1.100795	-3.801680
1	-0.380009	-0.369936	-4.229347
6	0.054570	-2.522972	-4.274651
1	0.483786	-2.647656	-5.280692
1	-1.023811	-2.657693	-4.387847
6	0.611680	-3.617246	-3.334896
1	1.599687	-3.939163	-3.679170
1	-0.032071	-4.500725	-3.397270
6	0.719383	-3.209838	-1.869072
1	0.024912	-3.697004	-1.191402
6	1.857085	-2.649123	-1.320346
1	1.993378	-2.735147	-0.246941
6	3.099010	-2.321069	-2.122981
1	3.791149	-1.781654	-1.479368

1	3.596500	-3.266467	-2.385061
6	2.835758	-1.492124	-3.402591
1	2.786618	-2.153476	-4.275181
1	3.693600	-0.834216	-3.566261
6	-2.229193	-2.192571	-1.994022
1	-1.702729	-3.119794	-2.117598
1	-2.768039	-1.822089	-2.858633
6	-1.876915	-1.264915	-0.988627
1	-2.476723	-0.362032	-0.948350
6	-1.028614	-1.554196	0.132927
1	-0.746684	-2.595457	0.256451
6	-1.278462	-0.900654	1.441363
6	-1.755746	0.413110	1.558504
6	-1.142161	-1.662880	2.615820
6	-2.082267	0.948788	2.800080
1	-1.905121	1.010583	0.671630
6	-1.453807	-1.121810	3.865939
1	-0.806476	-2.694958	2.543695
6	-1.924629	0.189163	3.963178
1	-2.461011	1.961969	2.844679
1	-1.336992	-1.729704	4.759454
1	-2.171115	0.614398	4.931770
8	-2.299362	-4.608885	-0.390845
6	-3.414903	-4.096089	-0.485295
8	-3.806005	-3.179503	-1.314709
8	-4.442337	-4.469129	0.342130
6	-4.100878	-5.431251	1.348266
1	-3.735329	-6.361227	0.902499
1	-5.021891	-5.621245	1.903541
1	-3.334440	-5.038813	2.024557
6	-5.799579	-0.356017	-2.065591
6	-7.187822	0.263245	-2.006793
1	-5.032114	0.415849	-2.178618
1	-5.706912	-1.068972	-2.888719
6	-7.336281	1.034086	-0.701418
1	-7.338048	0.945568	-2.847484
1	-7.949008	-0.522558	-2.065737
1	-8.370081	1.364845	-0.574954
1	-6.690216	1.917719	-0.690028
7	-5.552393	-1.079362	-0.818606
6	-6.093727	-0.779396	0.353825
7	-6.998893	0.195417	0.471330
6	-5.628640	-1.634163	1.514199
1	-4.771910	-2.203368	1.156151
1	-6.407206	-2.371571	1.740664
6	-5.238592	-0.839269	2.771336
1	-4.765750	0.094336	2.459444
6	-7.467257	0.782591	1.750532
6	-6.434558	-0.558213	3.689611
1	-6.175368	0.257631	4.375006
6	-7.703216	-0.191675	2.906497
1	-8.425316	0.278556	3.583206
1	-8.196449	-1.089161	2.515703
1	-8.415600	1.265347	1.505123
1	-6.760791	1.570659	2.031433
1	-6.646456	-1.437345	4.310798
1	-4.472062	-1.401223	3.313085
1	-4.921753	-1.893595	-0.871295
5	-4.024215	2.582128	-0.049192
9	-4.696942	1.837997	0.938205
9	-4.918706	3.460463	-0.674752
9	-2.971864	3.304000	0.548911
9	-3.488023	1.694593	-1.018510

---

13 P1 *endo-si* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 11.3558 16.2534 19.6476 cm(-1)
Electronic energy= -3892.021813
Zero-point correction= 1.233645
(Hartree/Particle)
Thermal correction to Energy= 1.306443
Thermal correction to Enthalpy= 1.307387
Thermal correction to Gibbs Free Energy= 1.122445
Sum of electronic and zero-point Energies= -3890.788168
Sum of electronic and thermal Energies= -3890.715370
Sum of electronic and thermal Enthalpies= -3890.714426
Sum of electronic and thermal Free Energies= -3890.899368

.....

Cartesian Coordinates

.....

77	-0.006548	-0.626941	-1.664708
15	1.656638	0.530226	-0.463480
8	2.192144	0.258133	1.084798
8	3.110657	0.388282	-1.279410
7	1.177141	2.114969	-0.318685
6	2.888299	-0.918199	1.353740
6	2.198726	-1.906076	2.088034
1	1.194774	-1.685190	2.428715
6	2.811121	-3.105569	2.352560
1	2.293740	-3.871697	2.923382
6	4.113951	-3.375336	1.852016
6	4.721141	-4.647308	2.036060
1	4.178412	-5.403781	2.596922
6	5.959298	-4.924586	1.502252
1	6.410607	-5.902474	1.642423
6	6.638381	-3.935294	0.752175
1	7.603166	-4.164354	0.308662
6	6.085769	-2.685649	0.572057
1	6.616970	-1.946311	-0.015069
6	4.818088	-2.354980	1.127724
6	4.202834	-1.064061	0.940506
6	4.922111	0.061032	0.283030
6	6.192803	0.537307	0.769657
6	6.761749	0.086925	1.994098
1	6.222821	-0.634602	2.596630
6	7.976933	0.566088	2.434006
1	8.383576	0.211986	3.377032
6	8.696150	1.519703	1.675189
1	9.655748	1.883094	2.031166
6	8.165839	1.994593	0.496937
1	8.696056	2.742426	-0.087187
6	6.907401	1.533783	0.023755
6	6.334526	2.060333	-1.165595
1	6.889015	2.799154	-1.737342
6	5.081513	1.671649	-1.565057
1	4.604102	2.092572	-2.443612
6	4.372043	0.706027	-0.815036
6	-0.092803	2.451080	-1.028884
1	-0.902216	2.471395	-0.294359
6	-0.008847	3.821943	-1.688416
6	1.092398	4.166071	-2.488047
1	1.912991	3.461002	-2.593431
6	1.147714	5.405191	-3.124569
1	2.009613	5.662008	-3.734808
6	0.096438	6.317064	-2.976508
1	0.138427	7.283029	-3.472161
6	-1.002695	5.980212	-2.184618
1	-1.821036	6.684343	-2.060183
6	-1.054989	4.740006	-1.540597
1	-1.902100	4.479761	-0.915259
6	-0.411199	1.415403	-2.119011
1	0.180269	1.660717	-3.006594
1	-1.461640	1.541382	-2.387116
6	1.664238	3.158587	0.640860
1	1.323446	4.089303	0.184176
6	1.008448	3.121743	2.020389
6	-0.156914	3.872933	2.230113
1	-0.627716	4.375383	1.391193
6	-0.710043	4.001218	3.505944
1	-1.610734	4.592962	3.644047
6	-0.100716	3.377757	4.596677
1	-0.519814	3.484925	5.593550
6	1.042535	2.599708	4.394506
1	1.514660	2.097869	5.234917
6	1.590599	2.470757	3.117533
1	2.485741	1.875313	2.980314
6	3.185777	3.272306	0.706351
1	3.593327	3.450734	-0.290288
1	3.665523	2.387117	1.123160

1	3.445850	4.125243	1.340241
6	1.428138	-0.655055	-3.375624
1	1.794779	0.359979	-3.495472
6	0.126832	-0.905390	-3.871088
1	-0.396054	-0.064449	-4.322682
6	-0.368589	-2.253792	-4.353556
1	0.034642	-2.423926	-5.362554
1	-1.454127	-2.193725	-4.466891
6	-0.013165	-3.446967	-3.437076
1	0.921061	-3.910624	-3.768712
1	-0.797124	-4.203717	-3.522531
6	0.104858	-3.105716	-1.961320
1	-0.719335	-3.462948	-1.355984
6	1.272538	-2.746522	-1.333312
1	1.313257	-2.832258	-0.250466
6	2.599252	-2.556468	-2.035114
1	3.286712	-2.079744	-1.339205
1	3.020371	-3.546969	-2.259075
6	2.530881	-1.715168	-3.330090
1	2.408605	-2.369279	-4.199798
1	3.490615	-1.208155	-3.457018
6	-2.127190	-1.018911	-2.111282
1	-2.319165	-2.069909	-2.282321
1	-2.563734	-0.366625	-2.863488
6	-2.124127	-0.529901	-0.764722
1	-2.470465	0.473926	-0.559011
6	-1.564992	-1.297345	0.258118
1	-1.432081	-2.355623	0.070034
6	-1.491824	-0.937084	1.675494
6	-1.726063	0.360685	2.163625
6	-1.265357	-1.977215	2.598610
6	-1.774589	0.590706	3.535503
1	-1.908391	1.183084	1.484892
6	-1.292690	-1.737280	3.971612
1	-1.077594	-2.980837	2.229444
6	-1.556633	-0.449652	4.444337
1	-1.979931	1.591645	3.893805
1	-1.118006	-2.553195	4.667271
1	-1.590658	-0.254888	5.512533
8	-2.523274	-4.899215	-1.673397
6	-3.361327	-4.162840	-1.127568
8	-4.214449	-3.392014	-1.642950
8	-3.397418	-4.139376	0.283223
6	-2.509448	-5.036134	0.941737
1	-2.701960	-6.076776	0.657377
1	-2.686235	-4.912756	2.013896
1	-1.458791	-4.816493	0.716918
6	-5.640663	-0.316534	-1.863089
6	-7.031126	0.295391	-1.763084
1	-4.874810	0.466228	-1.848460
1	-5.515280	-0.911502	-2.770114
6	-7.184343	0.951412	-0.397200
1	-7.181945	1.048540	-2.541357
1	-7.787022	-0.486643	-1.896252
1	-8.231582	1.216151	-0.220614
1	-6.587506	1.865678	-0.333318
7	-5.437840	-1.204994	-0.720857
6	-5.941964	-0.973259	0.478171
7	-6.775962	0.051644	0.704582
6	-5.531731	-1.943564	1.562550
1	-4.802516	-2.625198	1.122404
1	-6.400838	-2.549210	1.843808
6	-4.926675	-1.252605	2.800354
1	-4.373490	-0.368629	2.472818
6	-7.029499	0.652105	2.036513
6	-5.985898	-0.860169	3.839202
1	-5.562190	-0.104601	4.512046
6	-7.271222	-0.318056	3.195979
1	-7.856935	0.217064	3.951821
1	-7.908838	-1.136197	2.842326
1	-7.923218	1.265354	1.903219
1	-6.197781	1.331561	2.256000
1	-6.241939	-1.727737	4.460225
1	-4.187416	-1.920817	3.251132
1	-4.914199	-2.097306	-0.908272
5	-3.922307	2.635567	0.095506
9	-4.253639	1.428106	0.746142
9	-5.037221	3.481813	0.071631
9	-2.855657	3.254789	0.781676
9	-3.512705	2.341007	-1.228200

---

12 P1 *exo-re* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 12.4762 18.6409 21.2242 cm(-1)
Electronic energy= -3892.02497
Zero-point correction= 1.234541
(Hartree/Particle)
Thermal correction to Energy= 1.306842
Thermal correction to Enthalpy= 1.307787
Thermal correction to Gibbs Free Energy= 1.124579
Sum of electronic and zero-point Energies= -3890.790429
Sum of electronic and thermal Energies= -3890.718128
Sum of electronic and thermal Enthalpies= -3890.717183
Sum of electronic and thermal Free Energies= -3890.900391

.....

Cartesian Coordinates

.....

77	0.283642	-1.076457	-1.560082
15	1.811814	0.251717	-0.447251
8	2.428580	0.106688	1.093736
8	3.272360	0.267477	-1.298908
7	1.187064	1.800674	-0.320672
6	3.388416	-0.853439	1.380846
6	2.975322	-1.954511	2.163446
1	1.945898	-1.989289	2.499775
6	3.873678	-2.945121	2.472150
1	3.567202	-3.793394	3.077950
6	5.204955	-2.892557	1.978046
6	6.122044	-3.949918	2.226143
1	5.789898	-4.791923	2.828099
6	7.396180	-3.919219	1.706052
1	8.087020	-4.735165	1.897700
6	7.800566	-2.826029	0.903083
1	8.797424	-2.815558	0.471486
6	6.940867	-1.777353	0.656988
1	7.266373	-0.955385	0.030569
6	5.624302	-1.761942	1.198513
6	4.698714	-0.684845	0.956638
6	5.099276	0.555297	0.236793
6	6.185781	1.386732	0.685200
6	6.865301	1.163845	1.916047
1	6.556052	0.341522	2.550420
6	7.896630	1.984049	2.319727
1	8.393091	1.795605	3.267505
6	8.310603	3.073419	1.516413
1	9.129297	3.707626	1.843906
6	7.661208	3.332725	0.330567
1	7.955233	4.177046	-0.287744
6	6.583555	2.515941	-0.107509
6	5.881795	2.808140	-1.308350
1	6.202078	3.650024	-1.915840
6	4.794168	2.058162	-1.679866
1	4.227207	2.279626	-2.577529
6	4.389329	0.962109	-0.884003
6	0.023753	2.030938	-1.219447
1	-0.889431	2.019137	-0.614401
6	0.109218	3.375422	-1.926864
6	1.334729	3.882107	-2.381731
1	2.244492	3.334510	-2.160794
6	1.389547	5.080419	-3.094734
1	2.348831	5.463321	-3.433776
6	0.214747	5.786581	-3.370839
1	0.255069	6.720611	-3.924769
6	-1.010606	5.284511	-2.924879
1	-1.928815	5.828990	-3.129648
6	-1.064543	4.088584	-2.204271
1	-2.016490	3.708910	-1.849186
6	-0.063315	0.913045	-2.276691
1	0.689150	1.119825	-3.049706

1	-1.028903	1.008757	-2.774766
6	1.363874	2.797551	0.785485
1	0.820706	3.671594	0.416267
6	0.665446	2.384419	2.082274
6	-0.718461	2.577257	2.193734
1	-1.271419	3.031674	1.380537
6	-1.405016	2.204220	3.351261
1	-2.478365	2.356677	3.403968
6	-0.714039	1.650067	4.429679
1	-1.245451	1.359455	5.331985
6	0.670095	1.474233	4.339434
1	1.221603	1.051176	5.175176
6	1.351969	1.835955	3.175813
1	2.422826	1.679336	3.120660
6	2.812682	3.245438	0.973973
1	3.209417	3.640301	0.036813
1	3.463234	2.435968	1.303030
1	2.848517	4.039688	1.726556
6	1.636331	-1.427519	-3.281295
1	2.035212	-0.468409	-3.602342
6	0.292782	-1.705418	-3.666846
1	-0.205743	-0.945226	-4.270399
6	-0.305465	-3.091367	-3.842844
1	-0.036427	-3.504464	-4.827907
1	-1.394164	-2.979157	-3.836675
6	0.096749	-4.082073	-2.729990
1	1.016781	-4.607901	-3.001813
1	-0.676337	-4.853125	-2.641589
6	0.279852	-3.427971	-1.363722
1	-0.494136	-3.640502	-0.634315
6	1.490767	-2.984497	-0.854907
1	1.570232	-2.908899	0.225635
6	2.810736	-2.994563	-1.603789
1	3.505448	-2.349828	-1.061335
1	3.235304	-4.009410	-1.571107
6	2.708664	-2.499903	-3.063486
1	2.524281	-3.342602	-3.738492
1	3.679270	-2.086921	-3.356205
6	-2.822550	-0.581163	-2.152972
6	-1.866037	-1.389723	-1.326321
1	-2.085980	-2.448164	-1.418639
6	-1.356021	-0.908812	-0.072611
1	-1.539250	0.138959	0.147126
6	-1.308765	-1.726076	1.169380
6	-2.024954	-2.927110	1.319496
6	-0.603886	-1.240708	2.286748
6	-2.019841	-3.626152	2.530502
1	-2.621174	-3.301707	0.492497
6	-0.605176	-1.930877	3.497771
1	-0.056868	-0.308739	2.201084
6	-1.309603	-3.133591	3.627480
1	-2.587148	-4.549383	2.618657
1	-0.059358	-1.521511	4.343327
1	-1.312545	-3.671123	4.571609
8	-3.984331	-2.901416	-3.083684
6	-4.607373	-2.180320	-2.332196
8	-4.209298	-0.995919	-1.848801
8	-5.829322	-2.426096	-1.838898
6	-6.426914	-3.663970	-2.277527
1	-6.548881	-3.669725	-3.363742
1	-7.399995	-3.705600	-1.788065
1	-5.813391	-4.516344	-1.974165
6	-7.068959	1.144614	-0.799140
6	-8.286631	1.349258	0.088299
1	-6.565523	2.089187	-1.017211
1	-7.334490	0.662673	-1.744087
6	-7.831838	1.706901	1.498696
1	-8.913313	2.152640	-0.307449
1	-8.888600	0.434316	0.119033
1	-8.688306	1.749447	2.174077
1	-7.327389	2.677441	1.512885
7	-6.122083	0.274750	-0.108556
6	-6.033107	0.099924	1.201686
7	-6.893713	0.692767	2.032702
6	-4.916232	-0.821834	1.646950
1	-4.198564	-0.843420	0.827439
1	-5.319478	-1.837596	1.739586
6	-4.197414	-0.397092	2.934691
1	-4.104724	0.691365	2.933073
6	-6.855945	0.628028	3.513842
6	-4.903521	-0.889794	4.200050
1	-4.510202	-0.344509	5.066603
6	-6.425352	-0.709755	4.119425
1	-6.860674	-0.770620	5.122871
1	-6.885607	-1.517730	3.538772
1	-7.878867	0.842421	3.829967
1	-6.226722	1.447537	3.883735
1	-4.674782	-1.949892	4.364245
1	-3.177455	-0.782899	2.902666
1	-5.381207	-0.128063	-0.676228
5	-3.894855	2.637886	0.121432
9	-5.119102	2.932846	0.752909
9	-4.117661	2.337286	-1.241577
9	-3.039196	3.749333	0.222674
9	-3.301018	1.521755	0.745506
1	-2.676457	-0.718767	-3.226457
1	-2.836277	0.475393	-1.899457

[12-13]‡ P1 *exo-re* [BF_4^-]

Number of imaginary frequencies= 1
The smallest frequencies are=-282.7290 12.8632 15.5595cm(-1)
Electronic energy= -3891.9994043
Zero-point correction= 1.232196
(Hartree/Particle)
Thermal correction to Energy= 1.304676
Thermal correction to Enthalpy= 1.305620
Thermal correction to Gibbs Free Energy= 1.121500
Sum of electronic and zero-point Energies= -3890.767209
Sum of electronic and thermal Energies= -3890.694729
Sum of electronic and thermal Enthalpies= -3890.693785
Sum of electronic and thermal Free Energies= -3890.877904

.....

Cartesian Coordinates

.....

77	0.257279	-0.999197	-1.604095
15	1.706408	0.380305	-0.478071
8	2.257166	0.230394	1.079584
8	3.184543	0.406234	-1.276050
7	1.047438	1.899782	-0.367617
6	3.143873	-0.785352	1.413337
6	2.627496	-1.835889	2.201127
1	1.595096	-1.778069	2.516523
6	3.437442	-2.889551	2.541928
1	3.050764	-3.700856	3.152339
6	4.776540	-2.951218	2.069251
6	5.597138	-4.080519	2.336767
1	5.185934	-4.887026	2.938475
6	6.875965	-4.162479	1.833884
1	7.491553	-5.033381	2.039548
6	7.383034	-3.113389	1.030701
1	8.382563	-3.191210	0.612439
6	6.619854	-1.996071	0.768319
1	7.022744	-1.208436	0.142897
6	5.302317	-1.865211	1.290374
6	4.472228	-0.716786	1.022455
6	4.992149	0.487807	0.318548
6	6.144025	1.209471	0.799045
6	6.765579	0.919927	2.046409
1	6.357620	0.135506	2.672558
6	7.864373	1.631282	2.477992
1	8.313368	1.394218	3.438405
6	8.408888	2.671307	1.687765
1	9.279717	3.218281	2.037188
6	7.818948	2.995414	0.486916
1	8.211740	3.805608	-0.121960
6	6.674255	2.293553	0.021263
6	6.031952	2.663205	-1.191551
1	6.448319	3.473075	-1.784104
6	4.879688	2.033710	-1.587767

1	4.345769	2.327494	-2.485471
6	4.351506	0.976968	-0.811120
6	-0.147833	2.115463	-1.222177
1	-1.014765	2.203870	-0.562708
6	0.000989	3.395888	-2.033904
6	1.207798	3.676756	-2.694535
1	2.045685	2.995169	-2.577401
6	1.339230	4.822159	-3.478194
1	2.281607	5.030016	-3.978585
6	0.261313	5.703894	-3.617447
1	0.362414	6.598062	-4.226537
6	-0.941225	5.430090	-2.963336
1	-1.780980	6.113405	-3.059554
6	-1.071556	4.283659	-2.172283
1	-1.999978	4.083309	-1.648175
6	-0.385008	0.940726	-2.198088
1	0.152676	1.152275	-3.128405
1	-1.447512	0.965488	-2.440742
6	1.313570	2.992204	0.627118
1	0.822553	3.857259	0.174420
6	0.619157	2.772120	1.969245
6	-0.711729	3.185215	2.113605
1	-1.237391	3.628085	1.276210
6	-1.389189	3.017507	3.323585
1	-2.428105	3.325570	3.400622
6	-0.730604	2.463888	4.422419
1	-1.250062	2.340600	5.369047
6	0.604765	2.067484	4.295831
1	1.127141	1.635516	5.145301
6	1.270477	2.212904	3.078438
1	2.300042	1.885201	2.994586
6	2.788317	3.368798	0.749513
1	3.186806	3.645782	-0.228180
1	3.401379	2.564296	1.155229
1	2.879180	4.232386	1.415748
6	1.659588	-1.023922	-3.363291
1	1.865756	0.017073	-3.597556
6	0.402761	-1.514425	-3.787223
1	-0.242848	-0.812387	-4.313887
6	0.087630	-2.964538	-4.107207
1	0.423876	-3.188316	-5.131176
1	-0.999913	-3.079319	-4.115065
6	0.694935	-4.001957	-3.136845
1	1.697314	-4.284524	-3.471255
1	0.090654	-4.913933	-3.178329
6	0.772441	-3.546110	-1.692510
1	0.013527	-3.934988	-1.025441
6	1.864132	-2.944324	-1.130629
1	1.920454	-2.904811	-0.046758
6	3.130084	-2.599718	-1.884759
1	3.743765	-1.968740	-1.244257
1	3.700829	-3.526496	-2.042323
6	2.918610	-1.886324	-3.242541
1	2.911790	-2.621018	-4.055175
1	3.785564	-1.244152	-3.419668
6	-2.479398	-1.447392	-2.148939
6	-1.744504	-1.867286	-1.025413
1	-1.708355	-2.940396	-0.893634
6	-1.269332	-1.012120	0.027780
1	-1.681751	-0.008864	0.061182
6	-0.971518	-1.554689	1.379139
6	-0.766289	-2.923170	1.639557
6	-0.937996	-0.668205	2.471268
6	-0.551907	-3.388496	2.936796
1	-0.782518	-3.640800	0.827818
6	-0.725103	-1.133859	3.770177
1	-1.106307	0.389226	2.298060
6	-0.533150	-2.496478	4.013240
1	-0.400728	-4.451469	3.106030
1	-0.714019	-0.424759	4.591266
1	-0.369409	-2.857822	5.024581
8	-3.888501	-4.004140	-1.733525
6	-4.626700	-3.050896	-1.490700
8	-4.430958	-1.799393	-1.754330
8	-5.835210	-3.224620	-0.855592
6	-6.136733	-4.570760	-0.474794
1	-6.168978	-5.235008	-1.344293
1	-7.120032	-4.535338	-0.000063
1	-5.397431	-4.958313	0.234048
6	-6.899990	0.806217	-1.435552
6	-8.211204	1.191948	-0.769071
1	-6.289061	1.684823	-1.664599
1	-7.064047	0.249232	-2.361979
6	-7.925469	1.700360	0.638068
1	-8.718768	1.973198	-1.341185
1	-8.874877	0.321522	-0.721288
1	-8.860450	1.862555	1.179915
1	-7.373493	2.645719	0.606094
7	-6.141414	-0.050369	-0.530748
6	-6.224548	-0.034627	0.786370
7	-7.123798	0.733038	1.417738
6	-5.258395	-0.961424	1.499741
1	-4.517365	-1.252380	0.754280
1	-5.795254	-1.877007	1.774084
6	-4.547539	-0.352502	2.719413
1	-4.303306	0.688124	2.496400
6	-7.098329	1.040843	2.865172
6	-5.364668	-0.465252	4.011222
1	-4.946540	0.220741	4.758065
6	-6.851381	-0.150019	3.794698
1	-7.324687	0.073444	4.757124
1	-7.380740	-1.020239	3.389454
1	-8.083619	1.458360	3.082423
1	-6.363679	1.838165	3.033054
1	-5.272207	-1.476488	4.426631
1	-3.588459	-0.861808	2.843356
1	-5.463741	-0.702564	-0.962936
5	-3.780778	2.501141	0.171625
9	-4.999817	2.539161	0.876944
9	-3.990363	2.073134	-1.152833
9	-3.215811	3.794163	0.167400
9	-2.901631	1.603566	0.815475
1	-2.549606	-2.110958	-2.997726
1	-2.693733	-0.402947	-2.317522

---

13 P1 *exo-re* [BF_4^-]

Number of imaginary frequencies=0
The smallest frequencies are= 17.5057 23.4218 24.2100 cm(-1)
Electronic energy= -3892.0269636
Zero-point correction= 1.234003
(Hartree/Particle)
Thermal correction to Energy= 1.306562
Thermal correction to Enthalpy= 1.307506
Thermal correction to Gibbs Free Energy= 1.126267
Sum of electronic and zero-point Energies= -3890.792960
Sum of electronic and thermal Energies= -3890.720402
Sum of electronic and thermal Enthalpies= -3890.719457
Sum of electronic and thermal Free Energies= -3890.900697

.....

Cartesian Coordinates

.....

77	-0.322562	-0.488929	-1.507096
15	1.518730	0.483351	-0.447623
8	2.152032	0.134077	1.036977
8	2.873891	0.241120	-1.394470
7	1.198051	2.091871	-0.204835
6	2.876920	-1.033819	1.253740
6	2.263798	-2.001343	2.075820
1	1.300199	-1.768399	2.507892
6	2.900349	-3.194431	2.307960
1	2.440034	-3.945403	2.943895
6	4.152060	-3.473825	1.695402
6	4.780342	-4.738522	1.856388
1	4.292330	-5.482586	2.480547
6	5.970656	-5.023140	1.226328
1	6.439048	-5.994994	1.351722
6	6.577273	-4.049272	0.397883
1	7.503093	-4.284503	-0.119347
6	6.003198	-2.806863	0.235226

1	6.479510	-2.078902	-0.410654
6	4.784925	-2.468427	0.888547
6	4.151340	-1.182925	0.729323
6	4.811961	-0.061442	0.006683
6	6.112040	0.428854	0.390717
6	6.784758	-0.016815	1.563196
1	6.307218	-0.748794	2.203289
6	8.023929	0.479472	1.905949
1	8.510563	0.128431	2.811471
6	8.665095	1.446543	1.095792
1	9.644740	1.823317	1.374897
6	8.034215	1.917660	-0.033220
1	8.504298	2.675700	-0.654341
6	6.748327	1.440051	-0.405503
6	6.072830	1.966335	-1.539719
1	6.568379	2.717799	-2.147856
6	4.796495	1.561741	-1.838891
1	4.243166	1.980103	-2.672985
6	4.168306	0.580006	-1.040730
6	0.010881	2.603770	-0.932674
1	-0.785443	2.783634	-0.206621
6	0.325796	3.914189	-1.642499
6	1.508600	4.053691	-2.385634
1	2.219567	3.232317	-2.409353
6	1.779766	5.236634	-3.071655
1	2.702920	5.334722	-3.636872
6	0.866666	6.296156	-3.029472
1	1.077251	7.219196	-3.562649
6	-0.312372	6.162549	-2.293719
1	-1.022789	6.983822	-2.250385
6	-0.581597	4.978948	-1.598900
1	-1.487506	4.880986	-1.009125
6	-0.482739	1.591639	-1.977518
1	0.096453	1.734534	-2.895417
1	-1.511905	1.865048	-2.204685
6	1.764278	3.033094	0.820584
1	1.430770	4.007507	0.456548
6	1.147211	2.876743	2.208433
6	-0.061739	3.529934	2.486204
1	-0.571831	4.084046	1.706767
6	-0.633512	3.473064	3.759488
1	-1.579256	3.974866	3.942869
6	0.010977	2.778264	4.784442
1	-0.422890	2.742323	5.780049
6	1.217433	2.123883	4.518583
1	1.723351	1.574245	5.307784
6	1.776787	2.166982	3.240820
1	2.709915	1.648591	3.052512
6	3.289679	3.096310	0.828531
1	3.659588	3.336759	-0.169479
1	3.755597	2.166446	1.153091
1	3.605021	3.889067	1.513754
6	0.984375	-0.727007	-3.325820
1	1.424658	0.248889	-3.505731
6	-0.356846	-0.882895	-3.727492
1	-0.839579	-0.013042	-4.169430
6	-0.997676	-2.200249	-4.118389
1	-0.696373	-2.431128	-5.150833
1	-2.080298	-2.060792	-4.144412
6	-0.661279	-3.397992	-3.202587
1	0.235925	-3.907148	-3.567633
1	-1.480033	-4.120387	-3.245878
6	-0.453783	-3.039225	-1.743356
1	-1.265658	-3.299113	-1.076831
6	0.760293	-2.728925	-1.186246
1	0.852461	-2.773876	-0.104046
6	2.056547	-2.682964	-1.968438
1	2.830417	-2.267182	-1.325380
1	2.360028	-3.716114	-2.188658
6	2.000373	-1.869617	-3.284814
1	1.795686	-2.534223	-4.130474
1	2.990592	-1.442787	-3.460142
6	-2.584029	-0.471786	-1.830342
6	-2.328039	-0.933019	-0.526498
1	-2.547562	-1.973046	-0.323480
6	-1.602941	-0.199338	0.441134
1	-1.719120	0.877091	0.468075
6	-1.279457	-0.838111	1.739700
6	-1.216953	-2.235780	1.899483
6	-1.121311	-0.031686	2.876734
6	-1.032573	-2.806412	3.157054
1	-1.318064	-2.888989	1.043380
6	-0.928903	-0.603706	4.135741
1	-1.194247	1.044634	2.777275
6	-0.888474	-1.991549	4.285201
1	-0.991647	-3.887881	3.253343
1	-0.818956	0.042719	5.000056
1	-0.743371	-2.434240	5.266582
8	-3.160837	-5.197594	-1.940024
6	-3.649834	-4.197325	-1.401633
8	-4.275014	-3.221286	-1.899766
8	-3.491933	-4.058957	0.003595
6	-2.854141	-5.146283	0.669024
1	-3.391245	-6.086699	0.505695
1	-2.861074	-4.900093	1.734216
1	-1.820570	-5.282734	0.329715
6	-6.086163	-0.477983	-2.084700
6	-7.117146	0.579789	-1.722981
1	-5.233198	-0.023631	-2.601700
1	-6.501124	-1.247561	-2.741701
6	-6.578153	1.398716	-0.557433
1	-7.307386	1.231813	-2.579631
1	-8.064361	0.108731	-1.437791
1	-7.305073	2.143215	-0.231729
1	-5.659855	1.924416	-0.830682
7	-5.607749	-1.141614	-0.872181
6	-5.743630	-0.679434	0.363630
7	-6.287493	0.519082	0.599272
6	-5.250303	-1.606776	1.454762
1	-4.559414	-2.307033	0.980945
1	-6.101263	-2.214338	1.788926
6	-4.575889	-0.917554	2.650605
1	-3.997814	-0.060194	2.295553
6	-6.479167	1.150020	1.931494
6	-5.583581	-0.461351	3.711850
1	-5.090982	0.243775	4.392052
6	-6.816929	0.200414	3.081690
1	-7.350210	0.783727	3.840487
1	-7.527581	-0.553365	2.723225
1	-7.311234	1.843457	1.793173
1	-5.595600	1.751402	2.158592
1	-5.905305	-1.316852	4.318972
1	-3.852401	-1.610161	3.090432
1	-5.078031	-2.028075	-1.049828
5	-3.508248	3.096797	0.706736
9	-4.840984	3.527291	0.758643
9	-3.275042	2.420481	-0.516414
9	-2.647918	4.212380	0.788403
9	-3.245634	2.217853	1.778632
1	-3.042864	-1.191488	-2.497118
1	-2.806596	0.569487	-2.017161

[12-13]‡ P2 *endo-re* [BF_4^-]

Number of imaginary frequencies= 1
The smallest frequencies are=-274.2592 12.5189 15.7429cm(-1)
Electronic energy= -3891.9936916
Zero-point correction= 1.233376
(Hartree/Particle)
Thermal correction to Energy= 1.305602
Thermal correction to Enthalpy= 1.306546
Thermal correction to Gibbs Free Energy= 1.123316
Sum of electronic and zero-point Energies= -3890.760316
Sum of electronic and thermal Energies= -3890.688090
Sum of electronic and thermal Enthalpies= -3890.687145
Sum of electronic and thermal Free Energies= -3890.870376
.....
Cartesian Coordinates
.....

77	-0.218836	-0.826181	-1.527954

15	-1.590640	0.544221	-0.295903
8	-2.153721	0.299464	1.251626
8	-3.066076	0.690186	-1.091735
7	-0.883201	2.026372	-0.099885
6	-2.931682	-0.833526	1.472604
6	-2.318879	-1.895498	2.170780
1	-1.311873	-1.747306	2.538687
6	-3.001713	-3.071845	2.353088
1	-2.542444	-3.895730	2.892196
6	-4.300011	-3.242286	1.799289
6	-4.976692	-4.489220	1.886685
1	-4.490322	-5.305479	2.414501
6	-6.210189	-4.668073	1.302290
1	-6.714706	-5.627592	1.368612
6	-6.814740	-3.600472	0.596722
1	-7.775584	-3.751282	0.112875
6	-6.194218	-2.372825	0.511033
1	-6.667823	-1.571088	-0.042919
6	-4.928590	-2.144321	1.120589
6	-4.243246	-0.879038	1.028983
6	-4.892069	0.330598	0.454503
6	-6.141984	0.829316	0.974785
6	-6.746430	0.304862	2.152012
1	-6.251255	-0.491244	2.695024
6	-7.941588	0.803904	2.624161
1	-8.374891	0.389558	3.530123
6	-8.605075	1.854168	1.947150
1	-9.549562	2.232854	2.326871
6	-8.038449	2.401667	0.818079
1	-8.524964	3.222340	0.297093
6	-6.799866	1.920425	0.314563
6	-6.189877	2.516012	-0.822777
1	-6.700548	3.328257	-1.332524
6	-4.956523	2.096995	-1.249495
1	-4.453206	2.565416	-2.088656
6	-4.298821	1.034389	-0.584590
6	0.262799	2.312615	-0.993049
1	1.094121	2.606844	-0.350427
6	-0.058862	3.477443	-1.923128
6	-1.293205	3.544278	-2.588910
1	-2.044329	2.784295	-2.395915
6	-1.564229	4.581730	-3.481122
1	-2.525893	4.622366	-3.986438
6	-0.603885	5.570561	-3.721070
1	-0.815184	6.381065	-4.413239
6	0.624406	5.512333	-3.059420
1	1.372954	6.281020	-3.233132
6	0.895097	4.473856	-2.162596
1	1.843971	4.433965	-1.636819
6	0.705480	1.084998	-1.841557
1	0.509537	1.324238	-2.889471
1	1.786502	1.002350	-1.736778
6	-1.240040	3.155903	0.813880
1	-0.850602	4.034156	0.292481
6	-0.516574	3.111125	2.156644
6	0.656321	3.861683	2.320607
1	1.090638	4.374443	1.468341
6	1.285382	3.947373	3.565192
1	2.194789	4.533099	3.667826
6	0.749270	3.279009	4.667049
1	1.232173	3.347698	5.638105
6	-0.406156	2.508393	4.508881
1	-0.823287	1.972847	5.357554
6	-1.033499	2.425289	3.265240
1	-1.932928	1.830148	3.158955
6	-2.742559	3.397259	0.956718
1	-3.187234	3.579989	-0.022920
1	-3.267175	2.565373	1.427507
1	-2.898572	4.286840	1.574256
6	-1.456479	-0.434333	-3.353165
1	-1.541345	0.645077	-3.447731
6	-0.229253	-1.003308	-3.770830
1	0.528410	-0.322598	-4.154879
6	-0.083625	-2.422486	-4.296119
1	-0.481707	-2.466849	-5.321424
1	0.984304	-2.643251	-4.375076
6	-0.763101	-3.511556	-3.432831
1	-1.764510	-3.723408	-3.821501
1	-0.197009	-4.443574	-3.529728
6	-0.882846	-3.175865	-1.951939
1	-0.244901	-3.737844	-1.275864
6	-1.979192	-2.541243	-1.411836
1	-2.146913	-2.645299	-0.344738
6	-3.159035	-2.068998	-2.234790
1	-3.839386	-1.529497	-1.579617
1	-3.707334	-2.957203	-2.580954
6	-2.792847	-1.176289	-3.446874
1	-2.787815	-1.775808	-4.364638
1	-3.584969	-0.433594	-3.572786
6	2.164955	-2.436229	-1.927774
1	1.577035	-3.327829	-2.049081
1	2.769173	-2.132392	-2.774395
6	1.860105	-1.476446	-0.944099
1	2.537861	-0.631515	-0.878005
6	0.958466	-1.690129	0.158588
1	0.581228	-2.703140	0.263283
6	1.264540	-1.091710	1.481311
6	1.789087	0.199954	1.638260
6	1.122921	-1.897574	2.625831
6	2.159958	0.666799	2.896081
1	1.938351	0.832894	0.773234
6	1.477828	-1.423075	3.890599
1	0.744481	-2.910937	2.516431
6	1.997392	-0.134905	4.029810
1	2.587751	1.656795	2.977812
1	1.355883	-2.063779	4.760188
1	2.279227	0.241943	5.008865
8	2.033727	-4.755670	-0.135604
6	3.151871	-4.241768	-0.183410
8	3.662019	-3.533027	-1.139452
8	4.039627	-4.372662	0.855663
6	3.551911	-5.081902	2.001197
1	3.211255	-6.086416	1.733372
1	4.394257	-5.146183	2.693537
1	2.726765	-4.539771	2.474289
6	5.368216	-0.748481	-2.276559
6	6.727268	-0.093964	-2.471896
1	4.565892	-0.009679	-2.377067
1	5.196502	-1.555651	-2.992174
6	6.985102	0.869399	-1.321833
1	6.758389	0.457549	-3.415243
1	7.505180	-0.864829	-2.502596
1	8.025207	1.205149	-1.341042
1	6.341109	1.748668	-1.384960
7	5.317087	-1.321941	-0.934349
6	5.945468	-0.815949	0.119230
7	6.760766	0.233674	-0.000408
6	5.692391	-1.536996	1.426773
1	4.824432	-2.176837	1.266937
1	6.536240	-2.213041	1.612355
6	5.452302	-0.624442	2.640671
1	4.885883	0.252414	2.319093
6	7.323199	1.014813	1.132732
6	6.754427	-0.193286	3.325647
1	6.545316	0.658706	3.983663
6	7.844162	0.191385	2.313472
1	8.616757	0.784663	2.814915
1	8.350170	-0.699772	1.923927
1	8.152785	1.575660	0.699406
1	6.571182	1.741311	1.453722
1	7.130532	-1.002414	3.964150
1	4.811976	-1.157463	3.349863
1	4.754250	-2.178843	-0.818277
5	4.116792	2.724809	0.171245
9	4.364531	2.366822	1.511571
9	5.253490	3.347718	-0.367260
9	3.024495	3.616064	0.123818
9	3.815135	1.562917	-0.582137

[12-13]‡ P2 *exo-re* [BF_4^-]

Number of imaginary frequencies= 1
The smallest frequencies are=-269.9824 13.9417 20.1960cm(-1)
Electronic energy= -3892.0053835
Zero-point correction= 1.233234
(Hartree/Particle)
Thermal correction to Energy= 1.305488
Thermal correction to Enthalpy= 1.306432
Thermal correction to Gibbs Free Energy= 1.123336
Sum of electronic and zero-point Energies= -3890.772149
Sum of electronic and thermal Energies= -3890.699895
Sum of electronic and thermal Enthalpies= -3890.698951
Sum of electronic and thermal Free Energies= -3890.882048

.....

Cartesian Coordinates

.....

77	-0.225847	-1.202815	-1.187036
15	-1.783968	0.389027	-0.548797
8	-2.411093	0.541217	0.989707
8	-3.206187	0.199520	-1.405114
7	-1.154793	1.922724	-0.755996
6	-3.223733	-0.470242	1.486202
6	-2.676105	-1.294501	2.495885
1	-1.681146	-1.077834	2.874856
6	-3.422902	-2.340173	2.981313
1	-3.024185	-2.980254	3.763364
6	-4.709389	-2.623433	2.445801
6	-5.448579	-3.759646	2.873900
1	-5.017976	-4.398477	3.640701
6	-6.674424	-4.056295	2.322000
1	-7.226789	-4.931407	2.651759
6	-7.209582	-3.225186	1.308957
1	-8.165653	-3.474809	0.857683
6	-6.527348	-2.105514	0.884503
1	-6.948106	-1.485363	0.101680
6	-5.266797	-1.757250	1.445097
6	-4.519837	-0.604025	1.013822
6	-5.088264	0.417280	0.088187
6	-6.312637	1.114370	0.393736
6	-6.989329	0.968941	1.637741
1	-6.570360	0.321008	2.398000
6	-8.158616	1.650477	1.898141
1	-8.649314	1.525447	2.859243
6	-8.722042	2.516470	0.931149
1	-9.647577	3.041935	1.147854
6	-8.082287	2.701193	-0.273540
1	-8.490723	3.378663	-1.019016
6	-6.866780	2.025594	-0.567651
6	-6.179803	2.256910	-1.790006
1	-6.612493	2.936646	-2.518690
6	-4.970090	1.656697	-2.032271
1	-4.408367	1.844283	-2.941470
6	-4.424406	0.766815	-1.079081
6	0.179974	1.931709	-1.416444
1	0.934707	2.109820	-0.646616
6	0.310389	3.045590	-2.442778
6	-0.758758	3.406895	-3.274084
1	-1.722795	2.924225	-3.135560
6	-0.594855	4.386372	-4.254950
1	-1.434557	4.663659	-4.887029
6	0.644962	5.010722	-4.423290
1	0.773324	5.773272	-5.186663
6	1.717128	4.647569	-3.603991
1	2.686173	5.122877	-3.730883
6	1.551518	3.672652	-2.617286
1	2.389345	3.382713	-1.990760
6	0.482350	0.594497	-2.113030
1	0.022166	0.631280	-3.106774
1	1.556836	0.545310	-2.264513
6	-1.464911	3.192041	-0.018771
1	-1.203569	3.974103	-0.736478
6	-0.542665	3.389283	1.183873
6	0.538352	4.275216	1.073102
1	0.704839	4.796959	0.133979
6	1.405048	4.490303	2.147783
1	2.235742	5.182311	2.039846
6	1.207043	3.811071	3.351565
1	1.883174	3.967356	4.187690
6	0.136158	2.921960	3.471489
1	-0.019338	2.373761	4.395619
6	-0.733816	2.717312	2.400136
1	-1.555841	2.021507	2.506959
6	-2.940988	3.417718	0.313606
1	-3.553768	3.354788	-0.588037
1	-3.331096	2.715887	1.049447
1	-3.043346	4.428541	0.720564
6	0.826263	-0.141132	1.140591
6	1.115001	-1.416749	0.610166
1	0.814914	-2.272378	1.207314
6	1.949597	-1.567744	-0.540960
1	2.426239	-0.656242	-0.877761
6	-1.313638	-1.590701	-3.060713
1	-1.510950	-0.632866	-3.534911
6	0.013634	-2.091106	-3.197436
1	0.712201	-1.478168	-3.766196
6	0.375620	-3.564617	-3.190859
1	0.129990	-4.003840	-4.169888
1	1.458962	-3.640429	-3.082757
6	-0.300450	-4.371819	-2.064209
1	-1.238090	-4.812069	-2.418037
1	0.348389	-5.209418	-1.790914
6	-0.581512	-3.560220	-0.807010
1	0.046013	-3.786724	0.045323
6	-1.781755	-2.925184	-0.546988
1	-2.020289	-2.707760	0.488691
6	-2.944524	-2.886599	-1.516630
1	-3.680198	-2.179824	-1.134653
1	-3.430866	-3.873094	-1.518528
6	-2.552835	-2.484886	-2.957339
1	-2.391757	-3.378074	-3.570831
1	-3.396396	-1.954150	-3.407744
6	2.736242	-2.764038	-0.889123
6	2.686558	-3.981230	-0.186481
6	3.644718	-2.653912	-1.961555
6	3.489334	-5.059069	-0.563923
1	2.041131	-4.083603	0.679738
6	4.448659	-3.729036	-2.334682
1	3.724520	-1.704265	-2.482701
6	4.369902	-4.942680	-1.643019
1	3.435016	-5.989002	-0.003932
1	5.143954	-3.617692	-3.162474
1	4.996692	-5.781592	-1.932051
8	0.343626	-0.480232	4.069378
6	1.479828	-0.048110	3.859399
8	2.069962	0.119413	2.724496
8	2.300750	0.322753	4.893977
6	1.745665	0.160642	6.203860
1	0.849309	0.774867	6.338019
1	2.521969	0.485072	6.900647
1	1.484603	-0.884295	6.400191
6	4.492098	2.713187	1.844292
6	5.929911	3.204149	1.790315
1	3.977373	2.882015	0.894110
1	3.922622	3.205687	2.634763
6	6.737015	2.285141	0.882658
1	5.968348	4.224991	1.401015
1	6.364336	3.208481	2.796315
1	7.796534	2.549117	0.919182
1	6.394139	2.364320	-0.153970
7	4.486633	1.278995	2.122420
6	5.470711	0.440877	1.837435
7	6.620380	0.871895	1.306254
6	5.203446	-1.008001	2.194371
1	4.137087	-1.075146	2.417005
1	5.729648	-1.234462	3.129787
6	5.575897	-2.020594	1.098321
1	5.341110	-1.581279	0.126305
6	7.666210	0.004198	0.714095
6	7.046784	-2.451408	1.154333
1	7.321556	-2.899499	0.191870

6	7.992007	-1.284041	1.471705
1	9.018701	-1.565311	1.212433
1	7.999772	-1.066243	2.545912
1	8.562808	0.626994	0.684274
1	7.378121	-0.205794	-0.322011
1	7.181254	-3.230981	1.914642
1	4.929392	-2.896789	1.198709
1	3.599787	0.872262	2.465218
5	4.259057	1.229798	-1.692465
9	5.216392	0.343814	-1.160922
9	4.853201	2.471141	-1.967010
9	3.716788	0.670848	-2.865847
9	3.225028	1.427290	-0.739575
1	-0.006743	-0.007798	1.811175
1	1.243045	0.736398	0.669312

[12-13]‡ P2 *endo-si* [BF_4^-]

Number of imaginary frequencies= 1
The smallest frequencies are= -255.1672 2.7472 17.2882 cm(-1)
Electronic energy= -3892.0082688
Zero-point correction= 1.232693
(Hartree/Particle)
Thermal correction to Energy= 1.305191
Thermal correction to Enthalpy= 1.306135
Thermal correction to Gibbs Free Energy= 1.120481
Sum of electronic and zero-point Energies= -3890.775575
Sum of electronic and thermal Energies= -3890.703078
Sum of electronic and thermal Enthalpies= -3890.702134
Sum of electronic and thermal Free Energies= -3890.887788
.....
Cartesian Coordinates
.....

77	-0.419600	-0.945471	-1.678424
15	-1.853109	0.327691	-0.412251
8	-2.343180	0.082196	1.163651
8	-3.373646	0.390573	-1.143701
7	-1.209938	1.859478	-0.239721
6	-3.238937	-0.932406	1.462986
6	-2.726887	-2.054525	2.152940
1	-1.677572	-2.057194	2.424907
6	-3.557951	-3.104041	2.456808
1	-3.177222	-3.969693	2.991653
6	-4.918991	-3.087527	2.048126
6	-5.769496	-4.201598	2.284594
1	-5.361459	-5.061969	2.808810
6	-7.075108	-4.200908	1.848335
1	-7.714444	-5.060003	2.029655
6	-7.580493	-3.081157	1.145383
1	-8.603226	-3.092678	0.779487
6	-6.786751	-1.978550	0.914208
1	-7.188385	-1.134869	0.365687
6	-5.439269	-1.933620	1.370279
6	-4.581028	-0.800293	1.138735
6	-5.085940	0.468253	0.544173
6	-6.170675	1.208842	1.135437
6	-6.745177	0.860985	2.390728
1	-6.353868	0.010034	2.935425
6	-7.777404	1.597160	2.931091
1	-8.191427	1.313816	3.894704
6	-8.298770	2.721811	2.248149
1	-9.117026	3.288369	2.683046
6	-7.752863	3.101123	1.042670
1	-8.128327	3.974223	0.515045
6	-6.676597	2.373931	0.465691
6	-6.078672	2.794677	-0.753037
1	-6.478694	3.666242	-1.263680
6	-4.988458	2.132765	-1.258856
1	-4.493056	2.457284	-2.167705
6	-4.481039	0.996477	-0.587665
6	-0.066882	2.128842	-1.156284
1	0.852631	2.116360	-0.562683
6	-0.200911	3.499706	-1.804869
6	-1.437344	3.935823	-2.305215
1	-2.311245	3.305521	-2.170835
6	-1.549587	5.166615	-2.951361
1	-2.515579	5.493192	-3.328077
6	-0.422745	5.980085	-3.111845
1	-0.508652	6.939905	-3.614022
6	0.810932	5.552634	-2.616588
1	1.690398	6.181222	-2.729740
6	0.921880	4.321424	-1.963056
1	1.878055	4.001018	-1.562787
6	0.030007	1.053350	-2.256778
1	-0.671368	1.326155	-3.054743
1	1.030385	1.111935	-2.688963
6	-1.345457	2.821894	0.899632
1	-0.884186	3.732953	0.509214
6	-0.515870	2.420537	2.119032
6	0.839222	2.777879	2.163170
1	1.287537	3.318898	1.336664
6	1.635298	2.456605	3.265301
1	2.678175	2.753749	3.261929
6	1.083234	1.770195	4.348223
1	1.695757	1.523969	5.211691
6	-0.268427	1.413273	4.320733
1	-0.711235	0.888572	5.163597
6	-1.060594	1.739555	3.218428
1	-2.107632	1.461461	3.217639
6	-2.791570	3.194359	1.223718
1	-3.283516	3.589477	0.332756
1	-3.376745	2.351489	1.590030
1	-2.795088	3.972289	1.993853
6	0.901324	-1.770982	1.046882
1	0.263962	-2.626614	0.842369
1	0.471926	-1.176896	1.853784
6	1.175531	-0.910780	-0.154508
1	1.468306	0.098074	0.126839
6	1.757192	-1.447408	-1.354617
1	1.854273	-2.527429	-1.400286
6	-1.817916	-1.063099	-3.377810
1	-2.155010	-0.056419	-3.614424
6	-0.505496	-1.406227	-3.821306
1	0.043683	-0.638756	-4.367446
6	-0.061367	-2.816340	-4.172380
1	-0.448202	-3.098344	-5.164451
1	1.028307	-2.804570	-4.265025
6	-0.471298	-3.882110	-3.132144
1	-1.427293	-4.335473	-3.412983
1	0.262377	-4.695373	-3.144821
6	-0.575865	-3.358051	-1.704695
1	0.206573	-3.681777	-1.027164
6	-1.743359	-2.889066	-1.134495
1	-1.807124	-2.897470	-0.050850
6	-3.067907	-2.737717	-1.855280
1	-3.721306	-2.131776	-1.225467
1	-3.543302	-3.726810	-1.938775
6	-2.960289	-2.076316	-3.247734
1	-2.854260	-2.841885	-4.024393
1	-3.904927	-1.565060	-3.457911
6	2.791959	-0.774246	-2.172438
6	3.220179	0.547831	-1.954518
6	3.402854	-1.492107	-3.220878
6	4.188944	1.136456	-2.767501
1	2.823961	1.117521	-1.126812
6	4.370521	-0.904990	-4.036269
1	3.112776	-2.526441	-3.390265
6	4.765809	0.419642	-3.818678
1	4.512746	2.148612	-2.544782
1	4.821820	-1.484419	-4.837900
1	5.523787	0.877763	-4.448037
8	1.935613	-4.282494	0.492926
6	2.523032	-3.537765	1.251741
8	2.149404	-2.315854	1.645889
8	3.689014	-3.811840	1.858439
6	4.307731	-5.059181	1.479959
1	3.658706	-5.902070	1.729278
1	5.231989	-5.109533	2.055439
1	4.526197	-5.067554	0.408945
6	4.270413	-0.208789	3.977487

6	5.544958	0.359104	4.579675
1	3.564846	0.586440	3.721669
1	3.774009	-0.906197	4.657404
6	6.321204	1.102576	3.500039
1	5.305322	1.048671	5.393266
1	6.158855	-0.450041	4.990086
1	7.300747	1.402844	3.877159
1	5.784533	1.998653	3.174522
7	4.610587	-0.932117	2.756897
6	5.636546	-0.653514	1.958677
7	6.549763	0.249960	2.307534
6	5.681224	-1.462798	0.677179
1	4.660267	-1.804241	0.504227
1	6.280585	-2.363215	0.861511
6	6.172683	-0.715988	-0.569216
1	5.774887	0.299328	-0.546491
6	7.679515	0.707188	1.458063
6	7.698570	-0.691765	-0.693383
1	7.980019	0.063523	-1.436781
6	8.382519	-0.382373	0.645755
1	9.410834	-0.049597	0.467530
1	8.458798	-1.284528	1.264649
1	8.395975	1.140675	2.158089
1	7.312879	1.516104	0.817624
1	8.064356	-1.656051	-1.067997
1	5.731128	-1.193292	-1.448376
1	3.887864	-1.530760	2.375749
5	4.237095	2.576399	0.748688
9	5.412397	2.540281	-0.028078
9	4.475113	3.316651	1.926521
9	3.204162	3.188177	0.006140
9	3.845180	1.268503	1.091348

[12-13]‡ P1 *endo-re* [BF_4^-] conf2

Number of imaginary frequencies= 1
The smallest frequencies are=-186.7290 21.2888 23.2630cm(-1)
Electronic energy= -3891.974268
Zero-point correction= 1.233459
(Hartree/Particle)
Thermal correction to Energy= 1.305441
Thermal correction to Enthalpy= 1.306385
Thermal correction to Gibbs Free Energy= 1.125899
Sum of electronic and zero-point Energies= -3890.740809
Sum of electronic and thermal Energies= -3890.668827
Sum of electronic and thermal Enthalpies= -3890.667883
Sum of electronic and thermal Free Energies= -3890.848369

.....

Cartesian Coordinates

.....

77	-0.988681	-0.952320	-1.148636
15	-1.415841	1.014355	0.057077
8	-0.558353	1.613307	1.356140
8	-1.334703	2.360433	-0.947464
7	-2.955665	0.927735	0.684750
6	0.790181	1.846682	1.114195
6	1.709934	0.941265	1.686349
1	1.322906	0.183277	2.354767
6	3.044088	1.054212	1.385745
1	3.759652	0.361517	1.814968
6	3.497024	2.048338	0.475619
6	4.857818	2.111236	0.070550
1	5.555272	1.392733	0.488804
6	5.283985	3.045578	-0.847187
1	6.325324	3.076355	-1.154550
6	4.356200	3.958193	-1.403460
1	4.688507	4.678980	-2.144936
6	3.033761	3.938774	-1.014811
1	2.334467	4.640218	-1.454778
6	2.561596	2.998307	-0.056642
6	1.180963	2.935271	0.348436
6	0.195375	3.986917	-0.020382
6	0.424943	5.373061	0.308061
6	1.526992	5.804277	1.099561
1	2.218219	5.069784	1.494518
6	1.720742	7.138102	1.388738
1	2.566733	7.435824	2.001849
6	0.825968	8.121385	0.904898
1	0.995000	9.169310	1.134933
6	-0.266633	7.739000	0.159841
1	-0.976851	8.478339	-0.201609
6	-0.502898	6.370851	-0.143012
6	-1.658380	5.971584	-0.867449
1	-2.350766	6.731515	-1.218948
6	-1.913257	4.643935	-1.094783
1	-2.804423	4.317966	-1.619705
6	-1.000123	3.658795	-0.644801
6	-3.777983	-0.141818	0.075417
1	-4.439020	-0.498498	0.875069
6	-4.701007	0.343305	-1.041724
6	-4.624425	1.623258	-1.604531
1	-3.870638	2.316767	-1.251598
6	-5.488752	2.008330	-2.633748
1	-5.407499	3.006026	-3.057406
6	-6.448025	1.117288	-3.117011
1	-7.118871	1.413641	-3.918529
6	-6.544235	-0.158816	-2.552540
1	-7.293379	-0.858925	-2.912553
6	-5.684655	-0.535977	-1.520628
1	-5.775168	-1.525828	-1.079792
6	-2.892001	-1.348419	-0.294858
1	-3.448587	-2.009814	-0.961475
1	-2.709765	-1.878522	0.638717
6	-3.721545	1.843098	1.580179
1	-4.563495	2.219153	0.986838
6	-4.297858	1.055502	2.750770
6	-5.658307	1.153304	3.064192
1	-6.308688	1.767443	2.444981
6	-6.184735	0.462839	4.159531
1	-7.243375	0.544266	4.392057
6	-5.352423	-0.339795	4.943408
1	-5.761226	-0.885865	5.789534
6	-3.993959	-0.447046	4.629594
1	-3.334491	-1.079292	5.214062
6	-3.468556	0.251315	3.541653
1	-2.417662	0.154051	3.292738
6	-2.959741	3.064002	2.105221
1	-2.573237	3.690092	1.300374
1	-2.135098	2.777230	2.758227
1	-3.664901	3.666013	2.686278
6	0.991199	-2.098481	0.558391
1	1.722319	-1.827313	-0.180345
1	1.086356	-1.656730	1.533418
6	-0.251985	-2.642823	0.213463
1	-0.919291	-2.815201	1.045686
6	-0.593858	-3.182743	-1.074462
6	-1.785700	0.143742	-2.916547
1	-2.756187	0.550380	-2.663711
6	-1.762325	-1.248020	-3.189629
1	-2.710210	-1.778425	-3.100351
6	-0.804282	-1.908220	-4.164174
1	-1.162413	-1.724081	-5.188371
1	-0.865621	-2.985415	-4.014139
6	0.672965	-1.465971	-4.049607
1	0.865524	-0.622047	-4.719176
1	1.311688	-2.283760	-4.399315
6	1.103180	-1.088665	-2.646109
1	1.674800	-1.832036	-2.104117
6	1.063156	0.188688	-2.157081
1	1.617095	0.427425	-1.252241
6	0.555515	1.354427	-2.977814
1	0.562058	2.244528	-2.352221
1	1.278301	1.541011	-3.785219
6	-0.858807	1.161820	-3.591951
1	-0.769185	0.880771	-4.648148
1	-1.363126	2.130993	-3.575000
6	-1.673051	-4.195422	-1.221156
6	-2.592529	-4.510066	-0.198958
6	-1.767959	-4.924270	-2.422390
6	-3.589134	-5.465008	-0.398860

1	-2.525348	-4.026572	0.768358
6	-2.766112	-5.877282	-2.624345
1	-1.031648	-4.756563	-3.202513
6	-3.694163	-6.144683	-1.615418
1	-4.282316	-5.684641	0.408861
1	-2.809712	-6.418869	-3.565685
1	-4.473331	-6.886748	-1.765733
6	6.524152	-1.380286	2.405057
6	7.547558	-0.417016	1.824562
1	6.988961	-2.334825	2.676648
1	6.046537	-0.972693	3.299384
6	7.926743	-0.865396	0.418105
1	8.441566	-0.391065	2.452349
1	7.133235	0.595402	1.788399
1	8.575721	-0.126840	-0.054439
1	8.464599	-1.820608	0.441689
7	5.475841	-1.628373	1.412656
6	5.589803	-1.454781	0.099317
7	6.728912	-1.019093	-0.440870
6	4.339279	-1.766334	-0.691075
1	3.739394	-2.428913	-0.062977
1	3.769734	-0.835064	-0.799108
6	4.561247	-2.432606	-2.057078
1	5.386588	-3.149220	-1.977481
6	6.978960	-0.804367	-1.890528
6	4.835591	-1.420505	-3.173485
1	5.254444	-1.941251	-4.042445
6	5.788759	-0.309085	-2.715639
1	6.195459	0.211538	-3.589253
1	5.254132	0.448445	-2.133321
1	7.765667	-0.048152	-1.926843
1	7.400183	-1.724859	-2.313375
1	3.892526	-0.964671	-3.498098
1	3.672422	-3.024861	-2.296967
1	4.560036	-1.925494	1.773333
8	2.255401	-3.673205	1.061561
6	2.700343	-3.639694	2.255988
8	2.939576	-4.555056	3.032157
8	3.010215	-2.304189	2.653140
6	3.168720	-2.115867	4.065562
1	4.003540	-2.704204	4.458897
1	3.357423	-1.049347	4.214075
1	2.249674	-2.403060	4.581467
1	0.225066	-3.365340	-1.763574
5	-0.894484	-2.179665	3.609033
9	0.154041	-3.102015	3.499907
9	-1.219315	-1.971485	4.957251
9	-0.490569	-0.947901	3.027531
9	-2.028809	-2.658516	2.909893

[12-13]‡ P1 *exo-si* [BF_4^-] conf2

Number of imaginary frequencies= 1
The smallest frequencies are=-276.4384 17.1358 20.9824cm(-1)
Electronic energy= -3891.9790924
Zero-point correction= 1.234326
(Hartree/Particle)
Thermal correction to Energy= 1.306301
Thermal correction to Enthalpy= 1.307245
Thermal correction to Gibbs Free Energy= 1.125898
Sum of electronic and zero-point Energies= -3890.744766
Sum of electronic and thermal Energies= -3890.672792
Sum of electronic and thermal Enthalpies= -3890.671848
Sum of electronic and thermal Free Energies= -3890.853194

.....

Cartesian Coordinates

.....

77	1.663330	-1.477615	0.248704
15	-0.377807	-0.520652	0.745886
8	-1.545644	-0.357906	-0.455652
8	-1.340781	-1.300088	1.889970
7	-0.139436	1.071939	1.211104
6	-2.168594	-1.521306	-0.900078
6	-1.767950	-2.062409	-2.143938
1	-1.002209	-1.562557	-2.721774
6	-2.357106	-3.214513	-2.605156
1	-2.064236	-3.630994	-3.564728
6	-3.330898	-3.893309	-1.824539
6	-3.896059	-5.122678	-2.260272
1	-3.584176	-5.525038	-3.220534
6	-4.806680	-5.797438	-1.479322
1	-5.228534	-6.738849	-1.818808
6	-5.183222	-5.269767	-0.220679
1	-5.884558	-5.816595	0.403000
6	-4.665564	-4.072705	0.224177
1	-4.959687	-3.687097	1.193361
6	-3.737742	-3.337318	-0.565333
6	-3.175041	-2.085924	-0.133736
6	-3.619563	-1.391496	1.103132
6	-4.987881	-0.985819	1.293749
6	-5.978034	-1.128401	0.280608
1	-5.705187	-1.563520	-0.673196
6	-7.274726	-0.709545	0.488954
1	-8.009301	-0.824359	-0.303134
6	-7.658049	-0.129277	1.721704
1	-8.685321	0.188332	1.874443
6	-6.721580	0.042639	2.716175
1	-6.996444	0.503140	3.661582
6	-5.372029	-0.361197	2.526899
6	-4.388724	-0.133030	3.527243
1	-4.687798	0.321893	4.467355
6	-3.072708	-0.449832	3.301041
1	-2.309621	-0.245806	4.043173
6	-2.692690	-1.042597	2.074644
6	1.254678	1.314269	1.685894
1	1.499232	2.336688	1.401901
6	1.429568	1.252078	3.197105
6	0.629349	0.481691	4.047038
1	-0.171948	-0.116321	3.632707
6	0.865380	0.457044	5.425648
1	0.231945	-0.149114	6.068419
6	1.909742	1.204142	5.972217
1	2.093670	1.188197	7.042970
6	2.718549	1.974493	5.129106
1	3.535006	2.559853	5.543629
6	2.477457	2.001394	3.756118
1	3.104742	2.597120	3.097753
6	2.272353	0.446893	0.914783
1	3.157652	0.337657	1.539686
1	2.589185	1.034969	0.059404
6	-1.185600	2.026340	1.710812
1	-1.510005	1.691920	2.701866
6	-0.605965	3.425207	1.874304
6	-0.656837	4.057413	3.119593
1	-1.073765	3.526213	3.971138
6	-0.162372	5.354982	3.281564
1	-0.206766	5.831066	4.257104
6	0.403653	6.027254	2.198037
1	0.803280	7.029499	2.323641
6	0.467608	5.397744	0.950438
1	0.928492	5.908020	0.109670
6	-0.042509	4.110137	0.786898
1	0.032183	3.613248	-0.175997
6	-2.421492	2.118459	0.804499
1	-2.971364	1.182409	0.742744
1	-2.132524	2.417564	-0.203759
1	-3.092289	2.880115	1.212988
6	1.149446	0.065674	-1.983420
1	1.407647	0.960458	-1.442988
1	0.116919	-0.048537	-2.253545
6	1.983991	-1.072679	-1.974848
1	1.668417	-1.918209	-2.580733
6	3.273427	-1.065875	-1.361001
6	1.975357	-2.265943	2.286751
1	1.896041	-1.438253	2.984025
6	3.205695	-2.358081	1.580237
1	3.943272	-1.583251	1.780653
6	3.816162	-3.660132	1.097886
1	4.226327	-4.200184	1.964902
1	4.666725	-3.419223	0.460833

6	2.845250	-4.573837	0.321961
1	2.395834	-5.308716	0.998326
1	3.413535	-5.142192	-0.420001
6	1.726778	-3.834077	-0.397518
1	1.795401	-3.785135	-1.477959
6	0.490393	-3.613778	0.171079
1	-0.348906	-3.429875	-0.490749
6	0.138782	-3.988552	1.596838
1	-0.848935	-3.584075	1.814224
1	0.048733	-5.083172	1.653769
6	1.140526	-3.491186	2.670957
1	1.826569	-4.300875	2.946361
1	0.577052	-3.250148	3.577488
6	4.383778	-1.980196	-1.684179
6	4.270182	-3.121778	-2.497051
6	5.651312	-1.664683	-1.152569
6	5.372897	-3.943896	-2.731109
1	3.322269	-3.367209	-2.964257
6	6.752137	-2.485312	-1.389944
1	5.756946	-0.766685	-0.548889
6	6.616249	-3.637782	-2.170509
1	5.262095	-4.822872	-3.360754
1	7.718323	-2.224311	-0.966508
1	7.472790	-4.280352	-2.354297
1	3.642363	-0.094669	-1.055837
5	4.854591	2.415928	0.064560
9	4.329602	2.014970	-1.187225
9	5.914220	3.305973	-0.132128
9	3.833766	3.049145	0.814370
9	5.310080	1.269239	0.755950
6	-1.092120	5.233263	-2.445679
6	-2.340529	5.580151	-1.652843
1	-1.050686	5.795038	-3.385904
1	-0.183953	5.449547	-1.882937
6	-3.560248	5.015885	-2.367859
1	-2.443451	6.663672	-1.555779
1	-2.267688	5.153815	-0.647585
1	-4.451093	5.138631	-1.749829
1	-3.736751	5.532984	-3.318633
7	-1.103885	3.799741	-2.744090
6	-2.196212	3.047626	-2.844837
7	-3.409007	3.566085	-2.640802
6	-1.939398	1.587823	-3.149222
1	-0.934239	1.531538	-3.575916
1	-1.893818	1.061724	-2.190578
6	-2.940797	0.898949	-4.091537
1	-3.212365	1.589112	-4.898334
6	-4.696092	2.840307	-2.800849
6	-4.199056	0.393226	-3.371893
1	-4.984711	0.204104	-4.112975
6	-4.705978	1.387470	-2.321246
1	-5.734159	1.136834	-2.040402
1	-4.118523	1.318596	-1.399811
1	-5.413180	3.411135	-2.209639
1	-5.013919	2.913137	-3.848131
1	-3.986322	-0.562721	-2.883108
1	-2.427823	0.059584	-4.571635
1	-0.191382	3.335574	-2.803929
8	1.417288	1.038121	-3.769409
6	2.020584	2.164629	-3.701853
8	2.829165	2.657652	-4.478764
8	1.612951	2.906850	-2.565830
6	2.396594	4.076261	-2.275671
1	2.120567	4.906492	-2.935325
1	2.191375	4.331155	-1.234716
1	3.457228	3.858478	-2.387918

---

12 P1 *endo-re*

Number of imaginary frequencies= 0
The smallest frequencies are= 16.2211 18.5650 21.2891 cm(-1)
Electronic energy= -3467.4000971
Zero-point correction= 1.219937
(Hartree/Particle)
Thermal correction to Energy= 1.285729
Thermal correction to Enthalpy= 1.286673
Thermal correction to Gibbs Free Energy= 1.118570
Sum of electronic and zero-point Energies= -3466.180160
Sum of electronic and thermal Energies= -3466.114368
Sum of electronic and thermal Enthalpies= -3466.113424
Sum of electronic and thermal Free Energies= -3466.281527

.....

Cartesian Coordinates

.....

77	-0.024864	-0.879720	-1.413916
15	1.643334	0.282848	-0.358817
8	2.299089	-0.077066	1.132474
8	3.050848	0.311222	-1.269337
7	1.115267	1.847376	-0.061224
6	3.252441	-1.077501	1.275108
6	2.848695	-2.238724	1.971216
1	1.837458	-2.281698	2.361031
6	3.732146	-3.276690	2.133352
1	3.435170	-4.172332	2.671738
6	5.035568	-3.207823	1.571560
6	5.931316	-4.307962	1.660597
1	5.606283	-5.198893	2.191684
6	7.176220	-4.255790	1.075464
1	7.850525	-5.104476	1.143553
6	7.571960	-3.095995	0.367310
1	8.544751	-3.066468	-0.115094
6	6.733926	-2.005739	0.277249
1	7.051508	-1.131192	-0.277942
6	5.447955	-2.014821	0.887108
6	4.544140	-0.896240	0.803046
6	4.948734	0.403860	0.198370
6	6.073596	1.161395	0.681167
6	6.806889	0.792705	1.844067
1	6.512738	-0.090589	2.398422
6	7.873331	1.547365	2.282706
1	8.411537	1.247250	3.177333
6	8.271068	2.712217	1.583881
1	9.118171	3.292836	1.937203
6	7.571677	3.110867	0.467432
1	7.853572	4.012841	-0.069607
6	6.457012	2.364689	-0.002847
6	5.705205	2.802900	-1.126874
1	6.013991	3.703490	-1.650216
6	4.585803	2.116060	-1.526675
1	3.978295	2.445634	-2.362535
6	4.204124	0.942892	-0.838621
6	-0.143427	2.175228	-0.786599
1	-0.964604	2.133407	-0.061690
6	-0.114723	3.580959	-1.363974
6	1.020906	4.074456	-2.021742
1	1.915008	3.459602	-2.063622
6	1.013705	5.347601	-2.591871
1	1.903921	5.719911	-3.091855
6	-0.133100	6.145224	-2.518770
1	-0.137925	7.137196	-2.961670
6	-1.269469	5.660733	-1.867191
1	-2.163702	6.274797	-1.801546
6	-1.256231	4.388148	-1.289772
1	-2.139819	4.015718	-0.776838
6	-0.422934	1.157844	-1.907038
1	0.197171	1.423630	-2.772660
1	-1.463312	1.278232	-2.214306
6	1.392036	2.769890	1.083709
1	1.211743	3.763100	0.663245
6	0.377562	2.591108	2.212472
6	-0.616549	3.560894	2.400073
1	-0.662561	4.411640	1.724583
6	-1.536977	3.454708	3.446977
1	-2.290454	4.225846	3.583361
6	-1.480334	2.365746	4.319054
1	-2.189449	2.282463	5.137746
6	-0.503437	1.382844	4.131190
1	-0.452555	0.531409	4.804742
6	0.418836	1.495860	3.089507
1	1.180140	0.736281	2.960898

6	2.834650	2.803076	1.594531
1	3.527669	2.998651	0.774954
1	3.135023	1.885762	2.097736
1	2.916147	3.626870	2.310815
6	-0.964924	-1.702983	1.473936
1	-0.491988	-2.628466	1.157113
1	-0.329423	-1.198695	2.201444
6	-1.321360	-0.775027	0.345929
1	-1.458010	0.242351	0.705796
6	-2.155884	-1.193185	-0.750791
1	-2.369275	-2.254952	-0.828870
6	1.097376	-1.073366	-3.309855
1	1.464798	-0.087289	-3.584095
6	-0.285382	-1.318574	-3.553869
1	-0.852367	-0.507245	-4.011984
6	-0.877461	-2.691854	-3.823696
1	-0.673055	-2.994335	-4.862605
1	-1.963864	-2.602325	-3.741067
6	-0.387055	-3.787288	-2.853461
1	0.487071	-4.297772	-3.268572
1	-1.163953	-4.552976	-2.754973
6	-0.042543	-3.276206	-1.458651
1	-0.737187	-3.559827	-0.674149
6	1.227248	-2.891524	-1.063898
1	1.450862	-2.926163	-0.002020
6	2.442859	-2.815836	-1.966410
1	3.204063	-2.231202	-1.446549
1	2.856805	-3.827063	-2.096040
6	2.171413	-2.165533	-3.340577
1	1.890306	-2.928767	-4.074192
1	3.105814	-1.727662	-3.705247
6	-3.229854	-0.368885	-1.350897
6	-3.563889	0.925729	-0.908633
6	-3.965366	-0.890990	-2.434324
6	-4.549281	1.678187	-1.551009
1	-3.041774	1.355414	-0.061567
6	-4.947415	-0.141495	-3.079138
1	-3.748676	-1.899192	-2.776346
6	-5.242129	1.156658	-2.646308
1	-4.775559	2.679160	-1.193439
1	-5.488607	-0.572239	-3.917286
1	-6.003739	1.745996	-3.148501
8	-2.368462	-4.056260	1.126560
6	-2.773917	-3.202118	1.887472
8	-2.171193	-2.070524	2.247806
8	-3.959825	-3.248402	2.533899
6	-4.753909	-4.433837	2.290910
1	-4.221869	-5.320298	2.642813
1	-5.670581	-4.289694	2.862278
1	-4.976629	-4.537056	1.226453
6	-3.992805	0.643847	2.887108
6	-4.886883	1.833230	3.196447
1	-3.158232	0.931918	2.240253
1	-3.572910	0.197337	3.789737
6	-5.649722	2.228769	1.939337
1	-4.287234	2.679023	3.536697
1	-5.593889	1.572761	3.991023
1	-6.380719	3.005920	2.168147
1	-4.969397	2.617598	1.173929
7	-4.798694	-0.375357	2.214644
6	-5.916535	-0.154899	1.528223
7	-6.390840	1.078810	1.369617
6	-6.581626	-1.405387	0.986869
1	-5.800938	-2.167416	0.949071
1	-7.311842	-1.744607	1.732212
6	-7.234229	-1.288529	-0.397714
1	-6.590132	-0.685739	-1.043410
6	-7.555372	1.447240	0.523548
6	-8.649212	-0.701026	-0.350174
1	-8.938665	-0.393206	-1.361703
6	-8.751667	0.496195	0.604900
1	-9.652586	1.074317	0.374470
1	-8.860858	0.161669	1.643026
1	-7.858324	2.433604	0.876277
1	-7.210046	1.564345	-0.509804
1	-9.364518	-1.470204	-0.035932
1	-7.261152	-2.287609	-0.843990
1	-4.514281	-1.341990	2.330775

[**12-13**]‡ **P1** *endo-re*

Number of imaginary frequencies= 1
The smallest frequencies are= -284.6891 9.5713 18.2824 cm(-1)
Electronic energy= -3467.3771617
Zero-point correction= 1.217131
(Hartree/Particle)
Thermal correction to Energy= 1.283460
Thermal correction to Enthalpy= 1.284404
Thermal correction to Gibbs Free Energy= 1.113738
Sum of electronic and zero-point Energies= -3466.160031
Sum of electronic and thermal Energies= -3466.093702
Sum of electronic and thermal Enthalpies= -3466.092758
Sum of electronic and thermal Free Energies= -3466.263424

.....

Cartesian Coordinates

.....

77	-0.096659	-0.838861	-1.287414
15	1.654786	0.299371	-0.313796
8	2.353620	-0.055739	1.148765
8	3.010407	0.274415	-1.288046
7	1.155017	1.868291	-0.016817
6	3.277293	-1.090399	1.264369
6	2.856176	-2.234179	1.976345
1	1.857401	-2.242556	2.400262
6	3.711059	-3.300140	2.109676
1	3.403409	-4.185472	2.658737
6	4.996947	-3.273047	1.505386
6	5.859725	-4.401039	1.569945
1	5.524248	-5.279006	2.115762
6	7.085744	-4.390432	0.944369
1	7.734730	-5.259800	0.994687
6	7.494954	-3.246549	0.218063
1	8.452031	-3.249961	-0.295577
6	6.689656	-2.130437	0.149865
1	7.016709	-1.268254	-0.418971
6	5.425029	-2.096545	0.801638
6	4.553805	-0.951396	0.741445
6	4.968587	0.331221	0.106187
6	6.130434	1.064201	0.536200
6	6.900099	0.685879	1.672074
1	6.607224	-0.185686	2.245325
6	8.001209	1.417386	2.061241
1	8.567112	1.111106	2.936407
6	8.398573	2.566987	1.337379
1	9.272668	3.129437	1.652180
6	7.665434	2.974531	0.246185
1	7.947502	3.865588	-0.308502
6	6.515285	2.252158	-0.173293
6	5.730662	2.700301	-1.270451
1	6.039398	3.589565	-1.812620
6	4.579963	2.038037	-1.620340
1	3.947206	2.376459	-2.433575
6	4.199761	0.880249	-0.907595
6	-0.120481	2.214871	-0.703926
1	-0.916896	2.200184	0.049953
6	-0.080660	3.611310	-1.302987
6	1.026224	4.048950	-2.043942
1	1.889814	3.397271	-2.138511
6	1.031112	5.314659	-2.629678
1	1.898528	5.644419	-3.195069
6	-0.074841	6.159503	-2.487893
1	-0.070079	7.145933	-2.942813
6	-1.181531	5.731071	-1.751909
1	-2.041757	6.383838	-1.631045
6	-1.180527	4.465027	-1.159729
1	-2.038630	4.138746	-0.576375
6	-0.450284	1.191667	-1.802743
1	0.158460	1.425697	-2.683874
1	-1.491402	1.326993	-2.097518
6	1.499748	2.809569	1.097966

1	1.335130	3.797202	0.658936
6	0.512124	2.677738	2.255443
6	-0.450956	3.676102	2.452802
1	-0.483038	4.525034	1.774321
6	-1.360461	3.597731	3.511727
1	-2.090405	4.389775	3.655783
6	-1.326726	2.506707	4.382652
1	-2.032625	2.440849	5.205618
6	-0.375563	1.499918	4.189547
1	-0.342374	0.647264	4.862217
6	0.539954	1.588031	3.139535
1	1.282028	0.809597	3.008279
6	2.957990	2.808329	1.561836
1	3.631698	2.961945	0.717363
1	3.245555	1.896062	2.081424
1	3.085722	3.647355	2.253047
6	-0.941432	-1.308808	1.263265
1	-0.692001	-2.346221	1.120099
1	-0.382235	-0.754047	2.004741
6	-1.673278	-0.588937	0.298082
1	-1.874721	0.450926	0.529651
6	-2.315178	-1.197052	-0.833010
1	-2.435135	-2.274055	-0.791494
6	1.040843	-1.057630	-3.172155
1	1.422360	-0.073879	-3.431139
6	-0.338914	-1.284003	-3.429373
1	-0.896792	-0.460331	-3.874609
6	-0.946020	-2.642993	-3.720237
1	-0.734326	-2.914647	-4.765471
1	-2.029502	-2.538389	-3.648936
6	-0.480909	-3.782319	-2.785086
1	0.380079	-4.298232	-3.220284
1	-1.278749	-4.528772	-2.716947
6	-0.120513	-3.342727	-1.374554
1	-0.830245	-3.598416	-0.591740
6	1.145827	-2.984705	-0.976445
1	1.353099	-2.996266	0.089269
6	2.360553	-2.865506	-1.869636
1	3.119769	-2.304986	-1.322099
1	2.776189	-3.869033	-2.041021
6	2.100344	-2.161970	-3.218300
1	1.809957	-2.894310	-3.978733
1	3.041353	-1.722551	-3.561315
6	-3.387306	-0.529516	-1.601868
6	-3.745879	0.823016	-1.433387
6	-4.110649	-1.278397	-2.551627
6	-4.741272	1.409003	-2.216839
1	-3.246944	1.427811	-0.684663
6	-5.104114	-0.694653	-3.336457
1	-3.893691	-2.336872	-2.662478
6	-5.420145	0.658594	-3.181170
1	-4.984888	2.458087	-2.072343
1	-5.639596	-1.299786	-4.062693
1	-6.192014	1.117645	-3.791745
8	-2.390362	-3.858158	1.440567
6	-2.838274	-3.016869	2.225827
8	-2.323333	-1.932149	2.659650
8	-4.119881	-3.190738	2.759438
6	-4.796519	-4.395898	2.375261
1	-4.237273	-5.276894	2.703277
1	-5.768545	-4.368508	2.872651
1	-4.931713	-4.450974	1.290601
6	-3.987614	0.684722	3.103566
6	-4.733033	2.008584	3.134350
1	-3.052611	0.760935	2.541887
1	-3.735606	0.330696	4.104997
6	-5.336572	2.274942	1.761479
1	-4.048924	2.817428	3.395609
1	-5.530417	1.979438	3.884524
1	-5.941146	3.182593	1.774807
1	-4.551139	2.403795	1.006895
7	-4.839104	-0.324805	2.473327
6	-5.875490	-0.088118	1.678025
7	-6.213573	1.158295	1.341390
6	-6.601958	-1.323058	1.187781
1	-5.911776	-2.154246	1.333535
1	-7.455199	-1.511352	1.850312
6	-7.043573	-1.269192	-0.281820
1	-6.276531	-0.748450	-0.861587
6	-7.317902	1.557700	0.431305
6	-8.403736	-0.588284	-0.468404
1	-8.522965	-0.311085	-1.522404
6	-8.552582	0.656949	0.415747
1	-9.388917	1.265243	0.055079
1	-8.801394	0.381067	1.446751
1	-7.615408	2.551410	0.772370
1	-6.906005	1.669494	-0.578664
1	-9.211476	-1.290546	-0.230655
1	-7.078483	-2.290981	-0.672216
1	-4.596145	-1.299194	2.649563

---

13 P1 *endo-re*

Number of imaginary frequencies= 0
The smallest frequencies are= 14.4254 20.3832 21.2828 cm(-1)
Electronic energy= -3467.4048875
Zero-point correction= 1.218023
(Hartree/Particle)
Thermal correction to Energy= 1.284576
Thermal correction to Enthalpy= 1.285520
Thermal correction to Gibbs Free Energy= 1.115855
Sum of electronic and zero-point Energies= -3466.186865
Sum of electronic and thermal Energies= -3466.120312
Sum of electronic and thermal Enthalpies= -3466.119368
Sum of electronic and thermal Free Energies= -3466.289032

.....

Cartesian Coordinates

.....

77	-0.164312	-0.885604	-1.024073
15	1.634402	0.307852	-0.323868
8	2.359290	0.080127	1.135904
8	2.923217	0.092674	-1.345679
7	1.195202	1.910523	-0.189881
6	3.256569	-0.965552	1.354197
6	2.825848	-1.980199	2.234656
1	1.846658	-1.889004	2.693209
6	3.648363	-3.051634	2.479197
1	3.334745	-3.840368	3.156792
6	4.904469	-3.160555	1.823259
6	5.728806	-4.303313	2.009822
1	5.387791	-5.082011	2.686857
6	6.924548	-4.430013	1.340120
1	7.544287	-5.309677	1.486657
6	7.339895	-3.415928	0.444573
1	8.272042	-3.529702	-0.101246
6	6.571745	-2.288061	0.252455
1	6.902887	-1.527533	-0.444433
6	5.341082	-2.111565	0.944568
6	4.509877	-0.948496	0.763528
6	4.946777	0.221865	-0.049167
6	6.156962	0.946501	0.239571
6	6.954808	0.679365	1.387382
1	6.646551	-0.093405	2.081280
6	8.103502	1.398045	1.637507
1	8.690545	1.179305	2.524840
6	8.522921	2.421922	0.754905
1	9.434789	2.974335	0.961802
6	7.763571	2.723458	-0.352669
1	8.062453	3.520485	-1.028367
6	6.563829	2.013383	-0.631250
6	5.750580	2.361070	-1.743740
1	6.074008	3.159842	-2.404885
6	4.554436	1.722105	-1.959844
1	3.896502	1.994729	-2.778196
6	4.160169	0.680833	-1.092735
6	-0.113367	2.214763	-0.830470
1	-0.858207	2.310359	-0.030282
6	-0.077763	3.524944	-1.598644
6	0.984368	3.820557	-2.465421
1	1.818389	3.127325	-2.537543

6	0.983511	5.001829	-3.206405
1	1.815084	5.224365	-3.869386
6	-0.082450	5.901118	-3.094214
1	-0.082042	6.821662	-3.670829
6	-1.142850	5.613666	-2.232452
1	-1.970033	6.311274	-2.134310
6	-1.136222	4.432733	-1.484708
1	-1.955124	4.215591	-0.802590
6	-0.521199	1.075569	-1.773994
1	0.029346	1.187674	-2.714381
1	-1.581253	1.170374	-2.017045
6	1.654802	2.974700	0.764747
1	1.517298	3.899790	0.198651
6	0.737296	3.062366	1.981591
6	-0.120924	4.161468	2.117395
1	-0.135710	4.924381	1.343359
6	-0.949387	4.290214	3.236122
1	-1.600335	5.155276	3.329236
6	-0.939127	3.309583	4.230342
1	-1.583663	3.404679	5.099446
6	-0.094072	2.203220	4.099111
1	-0.079563	1.435364	4.867690
6	0.740779	2.083120	2.986754
1	1.401784	1.229124	2.901333
6	3.134440	2.944206	1.152543
1	3.768365	2.942519	0.265145
1	3.398393	2.093427	1.778556
1	3.345648	3.857816	1.716610
6	-0.853551	-0.757506	1.058369
1	-0.808569	-1.758284	1.478672
1	-0.429221	0.016430	1.691402
6	-1.988338	-0.378143	0.279741
1	-2.240757	0.675370	0.235724
6	-2.689783	-1.264513	-0.538596
1	-2.606744	-2.322702	-0.337471
6	0.900754	-1.363822	-2.989199
1	1.309146	-0.414701	-3.322305
6	-0.474094	-1.558389	-3.183592
1	-1.029311	-0.752987	-3.662165
6	-1.171339	-2.903280	-3.237100
1	-1.047834	-3.325234	-4.245491
1	-2.241144	-2.721768	-3.112138
6	-0.704548	-3.932695	-2.182696
1	0.121321	-4.530816	-2.579320
1	-1.524885	-4.633845	-1.997717
6	-0.279922	-3.339795	-0.846768
1	-0.946899	-3.501179	-0.003104
6	1.010283	-2.960448	-0.545574
1	1.260527	-2.871688	0.506750
6	2.193550	-3.032816	-1.485846
1	3.012327	-2.464989	-1.043386
1	2.533540	-4.076699	-1.538750
6	1.921749	-2.497116	-2.908501
1	1.589312	-3.308187	-3.563277
1	2.864981	-2.133078	-3.324573
6	-3.775111	-0.882968	-1.445839
6	-4.154045	0.453654	-1.692630
6	-4.496362	-1.905758	-2.094835
6	-5.196850	0.748641	-2.569282
1	-3.641654	1.270201	-1.195355
6	-5.535910	-1.608709	-2.974609
1	-4.240958	-2.941553	-1.890119
6	-5.889117	-0.279150	-3.219515
1	-5.470463	1.784914	-2.746128
1	-6.076301	-2.415300	-3.461299
1	-6.700062	-0.044472	-3.902466
8	-1.922487	-3.728516	1.939530
6	-2.942306	-3.068636	2.215081
8	-3.083599	-2.110497	3.019027
8	-4.134750	-3.396187	1.545262
6	-4.082189	-4.520528	0.671966
1	-3.806822	-5.434678	1.209231
1	-5.086423	-4.630399	0.253454
1	-3.363848	-4.380424	-0.144164
6	-3.526379	1.244963	2.964453
6	-4.254369	2.574082	2.831852
1	-2.599400	1.246273	2.383377
1	-3.252311	1.038487	4.002704
6	-4.963925	2.611655	1.484069
1	-3.544050	3.399349	2.906208
1	-4.995142	2.688106	3.630334
1	-5.525060	3.538819	1.362881
1	-4.238519	2.549086	0.661859
7	-4.385029	0.152332	2.502552
6	-5.525613	0.289774	1.841772
7	-5.912715	1.484951	1.375342
6	-6.324555	-0.983569	1.666833
1	-5.615579	-1.806719	1.777087
1	-7.019046	-1.057722	2.513453
6	-7.073548	-1.124564	0.334831
1	-6.447742	-0.724365	-0.466582
6	-7.157902	1.776903	0.625080
6	-8.439220	-0.429047	0.333091
1	-8.786049	-0.321282	-0.701761
6	-8.384330	0.947275	1.008287
1	-9.270794	1.528516	0.732177
1	-8.412275	0.849710	2.099388
1	-7.371163	2.828118	0.829130
1	-6.948328	1.690869	-0.448796
1	-9.179027	-1.050151	0.852216
1	-7.195837	-2.190623	0.118450
1	-4.027920	-0.816795	2.710242

---

12 P1 *exo-si*

Number of imaginary frequencies= 0
The smallest frequencies are= 12.1398 18.5421 25.5783 cm(-1)
Electronic energy= -3467.3991261
Zero-point correction= 1.220003
(Hartree/Particle)
Thermal correction to Energy= 1.285930
Thermal correction to Enthalpy= 1.286874
Thermal correction to Gibbs Free Energy= 1.118885
Sum of electronic and zero-point Energies= -3466.179123
Sum of electronic and thermal Energies= -3466.113196
Sum of electronic and thermal Enthalpies= -3466.112252
Sum of electronic and thermal Free Energies= -3466.280241

.....

Cartesian Coordinates

.....

77	-0.252516	-0.569104	-1.454371
15	1.484306	0.554870	-0.439404
8	2.132369	0.175996	1.050909
8	2.877306	0.502622	-1.363128
7	1.038704	2.141823	-0.125351
6	2.807576	-1.032202	1.178033
6	2.153401	-2.060320	1.892794
1	1.185844	-1.855001	2.339002
6	2.757521	-3.289090	2.001731
1	2.273965	-4.090543	2.553357
6	4.002062	-3.543079	1.362429
6	4.589643	-4.837160	1.389712
1	4.076913	-5.626847	1.932813
6	5.772072	-5.092139	0.732498
1	6.208158	-6.086579	0.754682
6	6.413649	-4.056851	0.011335
1	7.333850	-4.266716	-0.526437
6	5.879599	-2.786876	-0.021262
1	6.379396	-2.008455	-0.585793
6	4.669417	-2.481515	0.662295
6	4.076517	-1.169314	0.638047
6	4.771028	0.012409	0.051926
6	6.074468	0.425596	0.509862
6	6.726019	-0.179195	1.621855
1	6.227954	-0.974911	2.162640
6	7.973055	0.239671	2.033125
1	8.443020	-0.236337	2.889087
6	8.644173	1.286387	1.357725
1	9.629787	1.600813	1.688350
6	8.034206	1.911887	0.294071

1	8.527309	2.731027	-0.222993
6	6.742250	1.514820	-0.145543
6	6.091537	2.195199	-1.210011
1	6.608325	3.008778	-1.711421
6	4.815198	1.852440	-1.577331
1	4.283504	2.380278	-2.362164
6	4.157756	0.785144	-0.924251
6	-0.265178	2.528490	-0.716414
1	-0.990892	2.585425	0.100583
6	-0.202774	3.906214	-1.356628
6	0.865047	4.266942	-2.191343
1	1.681484	3.565345	-2.338989
6	0.888413	5.515235	-2.812892
1	1.724718	5.784070	-3.452596
6	-0.158593	6.421569	-2.612410
1	-0.138460	7.394359	-3.095391
6	-1.225574	6.070939	-1.782913
1	-2.039200	6.771564	-1.615411
6	-1.243130	4.821564	-1.156025
1	-2.069895	4.556262	-0.501021
6	-0.771384	1.493613	-1.743523
1	-0.377620	1.782100	-2.724187
1	-1.858424	1.609239	-1.808300
6	1.506917	3.062998	0.968730
1	1.219136	4.053168	0.604392
6	0.720812	2.831649	2.259381
6	-0.492011	3.514245	2.447057
1	-0.801083	4.255659	1.714629
6	-1.302741	3.255629	3.555358
1	-2.240957	3.790924	3.676156
6	-0.900384	2.319689	4.510658
1	-1.531507	2.104910	5.368369
6	0.328547	1.671333	4.361572
1	0.658947	0.953506	5.106834
6	1.132634	1.928073	3.248999
1	2.071855	1.400150	3.141082
6	3.022029	3.108509	1.150422
1	3.505919	3.381760	0.210553
1	3.444369	2.164064	1.490845
1	3.259881	3.876344	1.893130
6	-1.178848	0.070464	1.509438
6	-1.322481	-0.950251	0.424554
1	-1.106096	-1.954207	0.787393
6	-2.327407	-0.799920	-0.586539
1	-2.761485	0.194123	-0.661762
6	0.677258	-0.521288	-3.462554
1	1.002019	0.494883	-3.676368
6	-0.720143	-0.772508	-3.600637
1	-1.337557	0.067795	-3.919608
6	-1.320441	-2.121606	-3.958879
1	-1.205306	-2.311373	-5.037365
1	-2.394812	-2.064593	-3.767323
6	-0.737177	-3.294589	-3.146325
1	0.093608	-3.761231	-3.685277
1	-1.503918	-4.068210	-3.037962
6	-0.262295	-2.898448	-1.751959
1	-0.860888	-3.284190	-0.935331
6	1.044176	-2.539052	-1.445555
1	1.371017	-2.692581	-0.422892
6	2.157208	-2.386506	-2.463458
1	2.993538	-1.888212	-1.970699
1	2.514858	-3.386863	-2.750279
6	1.754527	-1.580327	-3.717743
1	1.410802	-2.255835	-4.509006
1	2.646239	-1.083015	-4.111668
6	-3.285597	-1.833917	-1.034368
6	-3.342225	-3.136854	-0.505138
6	-4.248320	-1.482960	-2.003057
6	-4.290438	-4.057862	-0.955492
1	-2.657830	-3.427678	0.284917
6	-5.202622	-2.397195	-2.446570
1	-4.232450	-0.478019	-2.417422
6	-5.224683	-3.697656	-1.929687
1	-4.308970	-5.057063	-0.528574
1	-5.927361	-2.096789	-3.198603
1	-5.964867	-4.413814	-2.274174
8	-0.830500	-1.637017	3.631865
6	-1.847047	-0.976308	3.559998
8	-2.176832	-0.128620	2.578888
8	-2.847747	-0.977712	4.449327
6	-2.659477	-1.856603	5.580069
1	-1.767847	-1.570004	6.143209
1	-3.551412	-1.733491	6.194231
1	-2.566103	-2.894149	5.249386
6	-3.940880	2.599569	0.759807
6	-5.109188	3.145660	-0.043671
1	-3.090765	2.378114	0.106272
1	-3.601923	3.303879	1.523553
6	-5.740501	2.006594	-0.834850
1	-4.762363	3.922018	-0.730071
1	-5.856900	3.588322	0.622331
1	-6.626855	2.352561	-1.367476
1	-5.036575	1.605427	-1.573689
7	-4.353636	1.368407	1.435624
6	-5.400404	0.608764	1.116913
7	-6.158968	0.904433	0.063584
6	-5.632065	-0.570664	2.039722
1	-4.672917	-0.775294	2.521384
1	-6.307642	-0.239535	2.838390
6	-6.158776	-1.849910	1.375241
1	-5.662037	-1.979821	0.411263
6	-7.343084	0.135483	-0.401347
6	-7.679804	-1.849385	1.191855
1	-7.949911	-2.635135	0.476796
6	-8.201906	-0.494748	0.696410
1	-9.212078	-0.615033	0.291219
1	-8.289226	0.219098	1.523791
1	-7.947530	0.859522	-0.949831
1	-7.002241	-0.617281	-1.121717
1	-8.174781	-2.096590	2.138489
1	-5.855749	-2.703667	1.989129
1	-3.745079	1.013236	2.167599
1	-0.199384	0.053978	1.976957
1	-1.394710	1.076663	1.165231

[**12-13**]‡ **P1** *exo-si*

Number of imaginary frequencies= 1
The smallest frequencies are=-255.4996 14.1858 19.1075cm(-1)
Electronic energy= -3467.3760757
Zero-point correction= 1.217512
(Hartree/Particle)
Thermal correction to Energy= 1.283614
Thermal correction to Enthalpy= 1.284558
Thermal correction to Gibbs Free Energy= 1.115566
Sum of electronic and zero-point Energies= -3466.158563
Sum of electronic and thermal Energies= -3466.092462
Sum of electronic and thermal Enthalpies= -3466.091518
Sum of electronic and thermal Free Energies= -3466.260510

.....

Cartesian Coordinates

.....

77	-0.266860	-0.779174	-1.283017
15	1.500190	0.503067	-0.509601
8	2.167085	0.346184	1.005538
8	2.857760	0.288763	-1.447764
7	1.048093	2.112566	-0.462613
6	2.843672	-0.828821	1.319525
6	2.214087	-1.706809	2.230658
1	1.276071	-1.411859	2.692822
6	2.815925	-2.906923	2.522114
1	2.355329	-3.593109	3.227190
6	4.028483	-3.284698	1.882496
6	4.605898	-4.564841	2.102888
1	4.110826	-5.245408	2.790615
6	5.757657	-4.943432	1.450828
1	6.186282	-5.926629	1.621449
6	6.377946	-4.052352	0.542716
1	7.273657	-4.362435	0.012218
6	5.855035	-2.796752	0.320888

1	6.339184	-2.130178	-0.383124
6	4.676053	-2.364812	0.989803
6	4.092315	-1.066914	0.768680
6	4.781361	-0.002212	-0.015497
6	6.100108	0.459369	0.343445
6	6.772294	0.024735	1.520402
1	6.279515	-0.671345	2.188036
6	8.032091	0.487274	1.834221
1	8.518085	0.143916	2.743003
6	8.695558	1.409473	0.990643
1	9.691168	1.759309	1.247274
6	8.066103	1.871235	-0.142904
1	8.552981	2.595555	-0.790774
6	6.760649	1.426712	-0.486925
6	6.090857	1.944581	-1.628086
1	6.602858	2.665434	-2.259238
6	4.802902	1.565693	-1.910226
1	4.257093	1.973413	-2.754488
6	4.154438	0.619904	-1.084925
6	-0.297411	2.380870	-1.029777
1	-0.979037	2.543491	-0.188416
6	-0.318228	3.644723	-1.874393
6	0.691753	3.906509	-2.810801
1	1.532523	3.222199	-2.888549
6	0.629183	5.040585	-3.620553
1	1.421865	5.236493	-4.337471
6	-0.448146	5.926078	-3.508943
1	-0.494812	6.810242	-4.138282
6	-1.458397	5.671968	-2.578858
1	-2.294286	6.359236	-2.480299
6	-1.390022	4.538664	-1.763731
1	-2.169111	4.349678	-1.028482
6	-0.819546	1.202517	-1.874223
1	-0.445595	1.332970	-2.894710
1	-1.907625	1.303128	-1.931238
6	1.536907	3.211081	0.443367
1	1.338437	4.119924	-0.131411
6	0.680812	3.298772	1.706450
6	-0.354879	4.243571	1.761375
1	-0.497805	4.922315	0.924412
6	-1.207628	4.315237	2.866956
1	-2.005199	5.053324	2.887025
6	-1.031717	3.440172	3.941007
1	-1.700934	3.477317	4.795702
6	0.012886	2.513207	3.908013
1	0.153486	1.818537	4.729693
6	0.862037	2.444270	2.803214
1	1.655329	1.708504	2.788902
6	3.041442	3.209375	0.709648
1	3.595213	3.216721	-0.231430
1	3.376608	2.359677	1.302719
1	3.289409	4.124592	1.255815
6	-1.069935	-0.008775	1.210132
6	-1.550106	-1.137504	0.523459
1	-1.337740	-2.103505	0.970715
6	-2.433708	-1.026949	-0.596673
1	-2.829134	-0.030175	-0.767876
6	0.697626	-0.982567	-3.264646
1	0.982552	0.014533	-3.590419
6	-0.679623	-1.312227	-3.396549
1	-1.327176	-0.546289	-3.822270
6	-1.210177	-2.720616	-3.584466
1	-1.054987	-3.026429	-4.630082
1	-2.290286	-2.694595	-3.429874
6	-0.591297	-3.764018	-2.632545
1	0.268867	-4.248925	-3.104480
1	-1.327174	-4.552071	-2.448595
6	-0.156668	-3.199684	-1.287444
1	-0.762092	-3.486822	-0.437197
6	1.120995	-2.753368	-1.011546
1	1.430385	-2.730703	0.028014
6	2.234682	-2.673858	-2.034107
1	3.059320	-2.116043	-1.592264
1	2.609281	-3.691160	-2.217683
6	1.826970	-2.011038	-3.369617
1	1.531492	-2.774818	-4.096911
1	2.705684	-1.512889	-3.788104
6	-3.380270	-2.066862	-1.044151
6	-3.437827	-3.369275	-0.515624
6	-4.330046	-1.711106	-2.022517
6	-4.390785	-4.283239	-0.967230
1	-2.758837	-3.666632	0.276023
6	-5.285194	-2.621832	-2.471154
1	-4.309350	-0.704216	-2.431984
6	-5.317349	-3.918424	-1.947525
1	-4.417669	-5.281601	-0.539558
1	-6.004238	-2.320243	-3.227747
1	-6.060077	-4.631410	-2.292919
8	-0.694161	-0.749025	4.093802
6	-1.774912	-0.170128	3.948454
8	-2.315542	0.222844	2.846994
8	-2.570205	0.127534	5.023995
6	-2.058949	-0.286013	6.296554
1	-1.106296	0.203281	6.523512
1	-2.809945	0.011606	7.031895
1	-1.911750	-1.370143	6.334923
6	-3.909388	2.478587	0.582448
6	-5.117911	3.006917	-0.172022
1	-3.118116	2.187448	-0.116936
1	-3.491190	3.220384	1.267665
6	-5.818860	1.841830	-0.860759
1	-4.807436	3.741820	-0.919072
1	-5.812518	3.496158	0.518559
1	-6.740585	2.177682	-1.337958
1	-5.179743	1.403951	-1.637788
7	-4.299034	1.309694	1.368404
6	-5.359118	0.543999	1.141554
7	-6.176009	0.782652	0.111569
6	-5.545092	-0.588152	2.132841
1	-4.569003	-0.739171	2.600569
1	-6.212250	-0.232609	2.927841
6	-6.060498	-1.909859	1.544211
1	-5.597077	-2.071912	0.567487
6	-7.356992	-0.032071	-0.272137
6	-7.586926	-1.953975	1.415563
1	-7.863413	-2.776148	0.745012
6	-8.159890	-0.634428	0.882607
1	-9.180691	-0.796289	0.520408
1	-8.235537	0.111675	1.681991
1	-8.001159	0.652181	-0.827061
1	-7.029583	-0.809761	-0.972936
1	-8.041496	-2.171065	2.389495
1	-5.714463	-2.729204	2.182043
1	-3.644068	0.997527	2.104145
1	-0.239924	-0.097071	1.891541
1	-1.346925	0.983948	0.893575

---

13 P1 *exo-si*

Number of imaginary frequencies= 0
The smallest frequencies are= 13.3735 20.0144 23.8465 cm(-1)
Electronic energy= -3467.4009901
Zero-point correction= 1.217939
(Hartree/Particle)
Thermal correction to Energy= 1.284253
Thermal correction to Enthalpy= 1.285197
Thermal correction to Gibbs Free Energy= 1.116099
Sum of electronic and zero-point Energies= -3466.183051
Sum of electronic and thermal Energies= -3466.116737
Sum of electronic and thermal Enthalpies= -3466.115793
Sum of electronic and thermal Free Energies= -3466.284891

.....

Cartesian Coordinates

.....

77	-0.548661	-0.080075	-1.507703
15	1.398268	0.445635	-0.505678
8	1.904927	-0.303295	0.866087
8	2.679468	0.150807	-1.517018
7	1.340096	2.031803	-0.012790
6	2.513374	-1.562714	0.834156

6	1.778769	-2.620004	1.411667
1	0.817952	-2.402815	1.871797
6	2.314357	-3.884841	1.405057
1	1.770130	-4.708898	1.858257
6	3.566326	-4.142072	0.784375
6	4.088080	-5.461822	0.704089
1	3.518871	-6.270880	1.154335
6	5.278566	-5.714527	0.061074
1	5.665533	-6.727563	0.001548
6	5.992684	-4.650353	-0.539503
1	6.918799	-4.855506	-1.068793
6	5.523034	-3.356848	-0.464833
1	6.080698	-2.557871	-0.938587
6	4.309092	-3.054126	0.213355
6	3.786662	-1.714135	0.307793
6	4.555719	-0.533624	-0.173954
6	5.871876	-0.221015	0.319386
6	6.478759	-0.935044	1.390321
1	5.935912	-1.744443	1.863529
6	7.736522	-0.602061	1.843690
1	8.174324	-1.157405	2.668133
6	8.461329	0.459842	1.251514
1	9.454873	0.705232	1.614939
6	7.896064	1.187251	0.229151
1	8.432213	2.018124	-0.221793
6	6.593335	0.881970	-0.251073
6	5.986795	1.667740	-1.268313
1	6.546850	2.489623	-1.704910
6	4.698083	1.414620	-1.669630
1	4.201016	2.019002	-2.420471
6	3.994377	0.335267	-1.094813
6	0.197277	2.797738	-0.582253
1	-0.528544	2.946334	0.224880
6	0.627742	4.168291	-1.079218
6	1.768783	4.317609	-1.880849
1	2.378543	3.446089	-2.101466
6	2.134609	5.573204	-2.364693
1	3.025843	5.677400	-2.977485
6	1.359591	6.696902	-2.057996
1	1.645578	7.675325	-2.433403
6	0.222204	6.556060	-1.260370
1	-0.379505	7.425560	-1.010556
6	-0.137868	5.297605	-0.769807
1	-1.011553	5.192140	-0.131323
6	-0.476708	2.022693	-1.725595
1	0.065909	2.226950	-2.654891
1	-1.485399	2.421811	-1.857468
6	1.996377	2.741256	1.137352
1	2.256214	3.721290	0.726849
6	0.990784	2.976072	2.259711
6	0.648516	4.288324	2.610181
1	1.095244	5.117743	2.068071
6	-0.265682	4.538956	3.636704
1	-0.520033	5.563338	3.895607
6	-0.851544	3.472296	4.320982
1	-1.563475	3.661511	5.120118
6	-0.518755	2.156939	3.979390
1	-0.977781	1.323140	4.499882
6	0.396609	1.911246	2.952542
1	0.645197	0.888463	2.686847
6	3.304556	2.150150	1.666048
1	4.042639	2.047867	0.870667
1	3.169814	1.189257	2.160575
1	3.701985	2.856281	2.401498
6	-1.358909	0.075460	0.521297
6	-2.525671	-0.389285	-0.178097
1	-2.791467	-1.433618	-0.053285
6	-3.256292	0.376451	-1.069195
1	-3.086686	1.448930	-1.077639
6	0.537825	-0.299630	-3.514464
1	1.139000	0.601818	-3.588861
6	-0.831212	-0.153011	-3.773810
1	-1.177240	0.845240	-4.039364
6	-1.792335	-1.252653	-4.173613
1	-1.757748	-1.372636	-5.266459
1	-2.803920	-0.912669	-3.937997
6	-1.560169	-2.623780	-3.501585
1	-0.817280	-3.196979	-4.062497
1	-2.494131	-3.191452	-3.556591
6	-1.131746	-2.555276	-2.047144
1	-1.897863	-2.756565	-1.307360
6	0.163512	-2.560369	-1.610318
1	0.336678	-2.774180	-0.560355
6	1.387443	-2.552623	-2.494749
1	2.246127	-2.289083	-1.877946
1	1.566664	-3.577467	-2.849309
6	1.326632	-1.594774	-3.708194
1	0.912657	-2.115824	-4.576466
1	2.352558	-1.325282	-3.972211
6	-4.379205	-0.085737	-1.881645
6	-4.678560	-1.449784	-2.084764
6	-5.212837	0.874905	-2.488704
6	-5.783219	-1.830947	-2.841960
1	-4.038467	-2.215973	-1.663694
6	-6.320251	0.490991	-3.244205
1	-4.989363	1.930301	-2.353929
6	-6.612855	-0.863542	-3.420786
1	-5.995533	-2.886434	-2.986045
1	-6.953072	1.249262	-3.696064
1	-7.473911	-1.164776	-4.009908
8	-0.941787	-1.969263	3.002218
6	-1.143092	-1.261248	4.012636
8	-2.199411	-0.657624	4.358035
8	-0.120143	-1.068497	4.927315
6	1.146204	-1.640379	4.612086
1	1.621865	-1.124978	3.770352
1	1.768343	-1.513259	5.502479
1	1.065962	-2.704402	4.369241
6	-3.972172	1.704619	2.460589
6	-5.403726	2.183846	2.277558
1	-3.364001	1.955104	1.582766
1	-3.493437	2.155956	3.332552
6	-6.082090	1.332268	1.211634
1	-5.424935	3.233454	1.972892
1	-5.949234	2.093701	3.222887
1	-7.146720	1.568855	1.159431
1	-5.651028	1.521688	0.221981
7	-3.966597	0.257455	2.644716
6	-4.903047	-0.562308	2.198334
7	-5.962978	-0.112818	1.510507
6	-4.665854	-2.024711	2.529868
1	-3.610188	-2.105077	2.799132
1	-5.233781	-2.267078	3.436405
6	-5.000165	-3.020888	1.408383
1	-4.710567	-2.588317	0.445386
6	-6.994371	-0.954118	0.853665
6	-6.481396	-3.416951	1.374294
1	-6.708316	-3.875322	0.404097
6	-7.409733	-2.217884	1.609418
1	-8.424938	-2.473875	1.287505
1	-7.479651	-1.980138	2.676671
1	-7.865825	-0.304634	0.754066
1	-6.659717	-1.196842	-0.161887
1	-6.681588	-4.177298	2.138393
1	-4.378517	-3.912065	1.542797
1	-3.208297	-0.158346	3.261401
1	-0.964643	-0.607712	1.268363
1	-1.338901	1.115111	0.837835

[**12-13**]‡ **P1** *exo-re*

Number of imaginary frequencies= 1
The smallest frequencies are=-258.3765 10.3488 17.7271cm(-1)
Electronic energy= -3467.373106
Zero-point correction= 1.216427
(Hartree/Particle)
Thermal correction to Energy= 1.282771
Thermal correction to Enthalpy= 1.283715
Thermal correction to Gibbs Free Energy= 1.114210
Sum of electronic and zero-point Energies= -3466.156679

Sum of electronic and thermal Energies= -3466.090335
Sum of electronic and thermal Enthalpies= -3466.089391
Sum of electronic and thermal Free Energies= -3466.258896

.....

Cartesian Coordinates

.....

77	-0.078328	-1.328132	-1.354641
15	1.268110	0.351534	-0.552403
8	1.958149	0.442552	0.949140
8	2.639965	0.468799	-1.493453
7	0.417265	1.795738	-0.546154
6	3.000282	-0.416925	1.291618
6	2.695582	-1.438672	2.215488
1	1.691587	-1.488794	2.614238
6	3.668099	-2.337980	2.573593
1	3.446645	-3.125581	3.288217
6	4.959728	-2.276637	1.983685
6	5.945043	-3.258772	2.275131
1	5.699467	-4.042063	2.987492
6	7.175208	-3.232308	1.658067
1	7.918115	-3.992012	1.882553
6	7.464916	-2.220216	0.712347
1	8.425582	-2.216839	0.205430
6	6.538792	-1.241769	0.422055
1	6.777199	-0.482557	-0.312913
6	5.265662	-1.222350	1.057602
6	4.267452	-0.223217	0.765049
6	4.557436	0.949115	-0.106380
6	5.640907	1.856932	0.177834
6	6.399412	1.792250	1.380400
1	6.156542	1.040079	2.121332
6	7.425242	2.679719	1.624480
1	7.982344	2.612983	2.554609
6	7.756035	3.680604	0.680343
1	8.571863	4.368149	0.883287
6	7.029478	3.787213	-0.483911
1	7.257599	4.563214	-1.209953
6	5.954173	2.899300	-0.758433
6	5.169911	3.042014	-1.934964
1	5.425981	3.819395	-2.649234
6	4.080512	2.235529	-2.145968
1	3.440636	2.351263	-3.014494
6	3.765183	1.224204	-1.211088
6	-0.950503	1.659123	-1.101798
1	-1.648994	1.512005	-0.267707
6	-1.403438	2.893434	-1.861341
6	-0.571097	3.523756	-2.796803
1	0.445370	3.162689	-2.928745
6	-1.036481	4.610913	-3.536805
1	-0.380052	5.096340	-4.253700
6	-2.344255	5.076008	-3.359623
1	-2.705269	5.921398	-3.938203
6	-3.179975	4.452198	-2.430936
1	-4.195484	4.810154	-2.283760
6	-2.706821	3.371154	-1.682359
1	-3.350649	2.891682	-0.949228
6	-1.025705	0.447859	-2.043234
1	-0.552448	0.723083	-2.993253
1	-2.082773	0.294357	-2.262536
6	0.636596	3.010566	0.308911
1	0.049356	3.778300	-0.199698
6	0.036984	2.889527	1.708546
6	-1.299665	3.268653	1.906814
1	-1.880659	3.624759	1.059871
6	-1.878083	3.229494	3.178633
1	-2.908119	3.544246	3.316527
6	-1.123279	2.814179	4.277219
1	-1.566382	2.789925	5.268753
6	0.212839	2.448318	4.093381
1	0.813181	2.137500	4.943746
6	0.786085	2.482104	2.821569
1	1.822640	2.192944	2.700060
6	2.073922	3.524850	0.304978
1	2.402180	3.718000	-0.717597
1	2.779749	2.836581	0.768069
1	2.107182	4.467295	0.859869
6	1.181073	-1.375223	-3.257803
1	1.237280	-0.344131	-3.596685
6	-0.030664	-2.046959	-3.503573
1	-0.809564	-1.482218	-4.014672
6	-0.191038	-3.551774	-3.624829
1	0.114665	-3.863412	-4.634868
1	-1.256217	-3.785653	-3.543749
6	0.586232	-4.383768	-2.579065
1	1.588585	-4.611369	-2.953474
1	0.081229	-5.346844	-2.455538
6	0.715883	-3.733164	-1.213027
1	0.089623	-4.133246	-0.426070
6	1.769253	-2.941606	-0.834132
1	1.917616	-2.781247	0.229029
6	2.928773	-2.579287	-1.738073
1	3.524886	-1.818521	-1.238463
1	3.575744	-3.463203	-1.832238
6	2.537248	-2.072734	-3.148087
1	2.555713	-2.902312	-3.862934
1	3.305871	-1.368842	-3.477563
6	-2.780642	-2.150541	-1.659657
6	-1.945506	-2.351877	-0.549354
1	-1.798543	-3.391113	-0.291384
6	-1.472632	-1.342246	0.365801
1	-1.999334	-0.391703	0.344652
6	-1.017935	-1.696157	1.738524
6	-0.718613	-3.010091	2.144410
6	-0.898304	-0.673503	2.696995
6	-0.324359	-3.288888	3.453490
1	-0.806702	-3.832586	1.444401
6	-0.516218	-0.952590	4.009565
1	-1.103313	0.352555	2.410117
6	-0.225919	-2.263027	4.397458
1	-0.102050	-4.314136	3.736860
1	-0.441330	-0.139922	4.724384
1	0.074205	-2.481419	5.418210
8	-4.255760	-4.350076	-0.202320
6	-4.928335	-3.327710	-0.306461
8	-4.732794	-2.327638	-1.105936
8	-6.038477	-3.112294	0.475688
6	-6.330353	-4.151980	1.417022
1	-6.500940	-5.109243	0.914729
1	-7.238570	-3.839482	1.937326
1	-5.514526	-4.274795	2.136961
6	-5.767933	1.000998	-1.977352
6	-6.816900	2.048404	-1.633625
1	-4.870840	1.472699	-2.396651
1	-6.139330	0.272339	-2.701337
6	-6.333798	2.884582	-0.455954
1	-7.003122	2.703783	-2.488108
1	-7.758028	1.552466	-1.373934
1	-7.151157	3.503675	-0.079066
1	-5.520042	3.555489	-0.751752
7	-5.407906	0.275025	-0.759952
6	-5.465504	0.785585	0.462966
7	-5.869695	2.042743	0.673066
6	-5.059991	-0.170208	1.568725
1	-4.505360	-0.972884	1.082884
1	-5.971280	-0.634908	1.962279
6	-4.217460	0.424335	2.706196
1	-3.490025	1.128701	2.289147
6	-5.775345	2.765777	1.966378
6	-5.054976	1.110219	3.790019
1	-4.395031	1.734137	4.404065
6	-6.187358	1.965668	3.204474
1	-6.539596	2.677160	3.958766
1	-7.051748	1.344991	2.942216
1	-6.439963	3.623945	1.860757
1	-4.759144	3.161966	2.072815
1	-5.487092	0.356056	4.458124
1	-3.625792	-0.380505	3.149650
1	-5.202375	-0.743013	-0.843679
1	-2.894130	-2.961154	-2.364822
1	-3.038540	-1.167160	-2.014478

[12-13]‡ P1 *endo-si*

Number of imaginary frequencies= 1
The smallest frequencies are=-318.6077 13.9405 17.0332cm(-1)
Electronic energy= -3467.3649174
Zero-point correction= 1.217795
(Hartree/Particle)
Thermal correction to Energy= 1.283606
Thermal correction to Enthalpy= 1.284550
Thermal correction to Gibbs Free Energy= 1.116649
Sum of electronic and zero-point Energies= -3466.147122
Sum of electronic and thermal Energies= -3466.081312
Sum of electronic and thermal Enthalpies= -3466.080368
Sum of electronic and thermal Free Energies= -3466.248269

.....

Cartesian Coordinates

.....

77	-0.128003	-1.185844	-1.423240
15	1.466482	0.237600	-0.513100
8	1.989831	0.376022	1.060634
8	2.925015	-0.131409	-1.248109
7	1.032365	1.829503	-0.808606
6	2.735092	-0.654320	1.629798
6	2.086041	-1.427537	2.616350
1	1.075429	-1.155313	2.892937
6	2.746478	-2.478526	3.201939
1	2.260977	-3.073092	3.970851
6	4.061677	-2.822371	2.788162
6	4.722985	-3.962178	3.320915
1	4.210427	-4.551552	4.076779
6	5.976026	-4.323550	2.880716
1	6.469677	-5.200235	3.289659
6	6.615295	-3.557745	1.876968
1	7.592219	-3.859863	1.510525
6	6.009314	-2.435845	1.354135
1	6.511871	-1.870093	0.579078
6	4.724882	-2.016993	1.801940
6	4.058382	-0.854953	1.266847
6	4.740500	0.070033	0.320790
6	5.989313	0.711992	0.644845
6	6.571387	0.646651	1.941834
1	6.059324	0.102955	2.726802
6	7.765516	1.276538	2.219408
1	8.182792	1.217903	3.220638
6	8.449882	2.003812	1.216749
1	9.393646	2.488879	1.448228
6	7.905773	2.106178	-0.043647
1	8.409388	2.676926	-0.819599
6	6.667277	1.483745	-0.358029
6	6.080099	1.629450	-1.644348
1	6.609350	2.195298	-2.405846
6	4.844050	1.096269	-1.909041
1	4.354731	1.230863	-2.868091
6	4.170963	0.357026	-0.909870
6	-0.218240	1.938113	-1.613412
1	-1.061523	2.037065	-0.921132
6	-0.222740	3.148038	-2.532435
6	0.855512	3.414661	-3.389710
1	1.735171	2.777643	-3.348299
6	0.811639	4.497222	-4.267481
1	1.656868	4.698337	-4.919918
6	-0.315900	5.324844	-4.308051
1	-0.349030	6.168232	-4.991855
6	-1.395093	5.064435	-3.461548
1	-2.272448	5.705160	-3.482974
6	-1.344258	3.983884	-2.576062
1	-2.178941	3.790703	-1.905706
6	-0.392744	0.672680	-2.462339
1	0.334452	0.713107	-3.280899
1	-1.382378	0.699992	-2.925770
6	1.487972	3.089658	-0.138730
1	1.272473	3.859418	-0.881559
6	0.694854	3.491984	1.104881
6	-0.300268	4.472819	0.981133
1	-0.549847	4.852509	-0.006418
6	-0.941641	4.995604	2.107531
1	-1.698939	5.766368	1.989227
6	-0.591788	4.543745	3.380811
1	-1.076250	4.956473	4.261539
6	0.382757	3.550811	3.514506
1	0.654467	3.186023	4.501156
6	1.017653	3.026912	2.388292
1	1.779134	2.266122	2.509039
6	2.996101	3.172556	0.098914
1	3.537387	3.043971	-0.839172
1	3.360272	2.437234	0.815282
1	3.226463	4.167792	0.490782
6	1.310470	-1.763552	-3.020301
1	1.740926	-0.846435	-3.411000
6	0.009880	-2.090788	-3.481613
1	-0.448880	-1.402268	-4.189992
6	-0.510609	-3.514268	-3.578630
1	-0.042908	-4.007999	-4.443943
1	-1.581305	-3.477430	-3.794738
6	-0.271961	-4.353713	-2.304727
1	0.653749	-4.929293	-2.399368
1	-1.077725	-5.087530	-2.204583
6	-0.210027	-3.539883	-1.015105
1	-1.047308	-3.686412	-0.341020
6	0.966541	-3.052252	-0.461439
1	0.978396	-2.858947	0.608291
6	2.327096	-3.192414	-1.114363
1	3.028042	-2.557412	-0.573947
1	2.676521	-4.226824	-0.982025
6	2.351812	-2.810035	-2.612655
1	2.218549	-3.701600	-3.234826
1	3.343475	-2.416003	-2.850638
6	-2.797086	-1.889995	-1.935795
1	-2.619058	-2.931307	-1.723879
1	-2.949872	-1.621879	-2.973302
6	-2.328463	-0.882787	-1.050242
1	-2.609091	0.136610	-1.291753
6	-1.733745	-1.133579	0.218989
1	-1.735760	-2.166780	0.552152
6	-1.812093	-0.213277	1.374603
6	-2.334716	1.089465	1.308422
6	-1.452035	-0.713948	2.639438
6	-2.479108	1.859689	2.460230
1	-2.664768	1.492089	0.357747
6	-1.583609	0.059384	3.791693
1	-1.087371	-1.735056	2.713963
6	-2.100696	1.353991	3.706944
1	-2.875286	2.866173	2.384564
1	-1.297353	-0.354163	4.754638
1	-2.207606	1.963300	4.598686
8	-4.378455	-4.101299	-0.789876
6	-5.074761	-3.125865	-1.058123
8	-4.717225	-2.025747	-1.655194
8	-6.401854	-3.072996	-0.728803
6	-6.900312	-4.219281	-0.023910
1	-6.789882	-5.129752	-0.620270
1	-7.958348	-4.020156	0.157969
1	-6.377722	-4.356690	0.928090
6	-5.266102	1.574804	-1.320655
6	-6.069210	2.699917	-0.687388
1	-4.225944	1.882479	-1.490485
1	-5.684547	1.267883	-2.282532
6	-5.650104	2.852726	0.770007
1	-5.896105	3.638393	-1.219913
1	-7.138875	2.472010	-0.738054
1	-6.271684	3.595317	1.271311
1	-4.606877	3.181646	0.844339
7	-5.275808	0.413204	-0.434076
6	-5.528348	0.431800	0.870019
7	-5.792308	1.575314	1.504395
6	-5.463305	-0.933345	1.531919
1	-4.713595	-1.483734	0.960111
1	-6.416988	-1.442580	1.352044
6	-5.075917	-0.983012	3.012743

1	-4.235081	-0.306502	3.183309
6	-6.130463	1.703232	2.943628
6	-6.231649	-0.650263	3.960403
1	-5.827828	-0.479867	4.965387
6	-7.016643	0.584900	3.498819
1	-7.588653	0.995671	4.337277
1	-7.750160	0.314804	2.730308
1	-6.665431	2.650538	3.022885
1	-5.203623	1.806235	3.519778
1	-6.916151	-1.503610	4.034117
1	-4.700524	-1.989629	3.223639
1	-5.111221	-0.508628	-0.868912

[**12-13**]‡ **P2** *endo-re*

Number of imaginary frequencies= 1
The smallest frequencies are=-318.6077 13.9405 17.0332cm(-1)
Electronic energy= -3467.3649174
Zero-point correction= 1.217795
(Hartree/Particle)
Thermal correction to Energy= 1.283606
Thermal correction to Enthalpy= 1.284550
Thermal correction to Gibbs Free Energy= 1.116649
Sum of electronic and zero-point Energies= -3466.147122
Sum of electronic and thermal Energies= -3466.081312
Sum of electronic and thermal Enthalpies= -3466.080368
Sum of electronic and thermal Free Energies= -3466.248269

.....

Cartesian Coordinates

.....

77	0.123998	-1.192235	-1.414125
15	-1.467843	0.239623	-0.514578
8	-1.995500	0.388896	1.056733
8	-2.925134	-0.129891	-1.251601
7	-1.029235	1.829155	-0.817833
6	-2.742115	-0.637339	1.631039
6	-2.096088	-1.402701	2.625567
1	-1.086630	-1.127724	2.903704
6	-2.757875	-2.449674	3.216774
1	-2.274346	-3.037647	3.991951
6	-4.071421	-2.797455	2.800890
6	-4.734362	-3.933272	3.340078
1	-4.224940	-4.516637	4.102703
6	-5.985518	-4.298602	2.897802
1	-6.480297	-5.172157	3.312060
6	-6.621179	-3.541319	1.885354
1	-7.596465	-3.847244	1.517676
6	-6.013826	-2.423164	1.356048
1	-6.513464	-1.863601	0.574607
6	-4.731598	-1.999961	1.806065
6	-4.064125	-0.841108	1.265388
6	-4.744534	0.077490	0.312144
6	-5.995726	0.718170	0.629390
6	-6.580340	0.659772	1.925701
1	-6.068223	0.123100	2.715619
6	-7.776856	1.288169	2.196398
1	-8.196077	1.235542	3.197115
6	-8.461371	2.006397	1.187315
1	-9.406884	2.490532	1.413501
6	-7.914945	2.101861	-0.072603
1	-8.418772	2.665834	-0.853337
6	-6.673705	1.481333	-0.379956
6	-6.083381	1.621370	-1.665476
1	-6.612129	2.181039	-2.431860
6	-4.844854	1.090741	-1.923566
1	-4.353830	1.221053	-2.882281
6	-4.172323	0.358735	-0.918630
6	0.226456	1.929007	-1.615918
1	1.066409	2.022795	-0.918893
6	0.246227	3.137021	-2.537124
6	-0.822466	3.409776	-3.404258
1	-1.707400	2.779848	-3.369770
6	-0.762710	4.489736	-4.284354
1	-1.600854	4.695632	-4.944369
6	0.371486	5.308475	-4.317624
1	0.417214	6.149228	-5.003901
6	1.441554	5.041750	-3.461523
1	2.324413	5.674997	-3.477705
6	1.374747	3.963989	-2.573787
1	2.202821	3.765343	-1.896804
6	0.396243	0.660849	-2.461386
1	-0.330579	0.701703	-3.280123
1	1.386024	0.681293	-2.924731
6	-1.483422	3.092736	-0.153533
1	-1.263796	3.859980	-0.897865
6	-0.692759	3.496296	1.091421
6	0.308987	4.470391	0.966807
1	0.563234	4.845910	-0.021046
6	0.951452	4.992324	2.092926
1	1.713882	5.757893	1.974142
6	0.596566	4.546119	3.366798
1	1.082033	4.958253	4.247257
6	-0.384334	3.559634	3.501496
1	-0.660065	3.199303	4.488649
6	-1.020564	3.036673	2.375556
1	-1.786617	2.280817	2.497011
6	-2.992554	3.179151	0.076923
1	-3.529474	3.047925	-0.863499
1	-3.362357	2.447805	0.794583
1	-3.223967	4.176244	0.463231
6	-1.305803	-1.773006	-3.015450
1	-1.731846	-0.857049	-3.413670
6	-0.002803	-2.105762	-3.467952
1	0.461227	-1.421906	-4.177521
6	0.512899	-3.531673	-3.556625
1	0.047347	-4.027539	-4.421840
1	1.584608	-3.500187	-3.768597
6	0.265098	-4.364061	-2.279891
1	-0.661551	-4.937664	-2.376821
1	1.067862	-5.099929	-2.171657
6	0.198058	-3.543652	-0.994635
1	1.031296	-3.689041	-0.315313
6	-0.980688	-3.051170	-0.449656
1	-0.998903	-2.853342	0.619198
6	-2.337878	-3.190033	-1.109851
1	-3.039033	-2.549038	-0.576952
1	-2.692592	-4.222048	-0.973561
6	-2.352305	-2.815364	-2.610045
1	-2.216805	-3.710208	-3.226859
1	-3.341741	-2.420950	-2.856658
6	2.791428	-1.893315	-1.921336
1	2.615357	-2.934701	-1.707791
1	2.938886	-1.625522	-2.959653
6	2.322445	-0.886308	-1.035044
1	2.601424	0.133327	-1.276933
6	1.728904	-1.137707	0.233955
1	1.730649	-2.171084	0.566555
6	1.806811	-0.217989	1.390004
6	2.330617	1.084365	1.324308
6	1.447580	-0.719440	2.654774
6	2.476637	1.853575	2.476586
1	2.660733	1.486906	0.373732
6	1.581570	0.052718	3.807590
1	1.081850	-1.740278	2.728809
6	2.099605	1.346998	3.723406
1	2.873221	2.859880	2.401394
1	1.295778	-0.361186	4.770521
1	2.208635	1.955102	4.615775
8	4.383369	-4.106832	-0.801221
6	5.075835	-3.128065	-1.067046
8	4.709926	-2.022340	-1.649260
8	6.405784	-3.076332	-0.751672
6	6.917109	-4.235379	-0.077466
1	6.796823	-5.134003	-0.689495
1	7.977710	-4.038730	0.091239
1	6.410912	-4.392127	0.880362
6	5.234318	1.586816	-1.310025
6	6.035585	2.716948	-0.682848
1	4.189468	1.886592	-1.464635
1	5.642308	1.287973	-2.278894

6	5.639725	2.858005	0.782262
1	5.842385	3.656577	-1.206628
1	7.106858	2.503649	-0.754502
1	6.268143	3.598563	1.278072
1	4.597628	3.185379	0.875529
7	5.265896	0.420587	-0.429674
6	5.531519	0.434680	0.871984
7	5.794952	1.577254	1.508280
6	5.482668	-0.933298	1.529008
1	4.743386	-1.492573	0.952832
1	6.443979	-1.429797	1.353133
6	5.087559	-0.989744	3.008123
1	4.241108	-0.319197	3.176080
6	6.133101	1.702786	2.947773
6	6.236711	-0.651509	3.962130
1	5.827091	-0.480382	4.964628
6	7.020430	0.584775	3.501836
1	7.592290	0.995220	4.340472
1	7.754142	0.315882	2.733085
1	6.666390	2.650967	3.028994
1	5.205441	1.803318	3.523189
1	6.923409	-1.502507	4.041644
1	4.718028	-1.999336	3.214722
1	5.105147	-0.500670	-0.866590

[12-13]‡ P2 *endo-re* conf2

Number of imaginary frequencies : 1
The smallest frequency is : -322.0638 cm(-1)
Electronic energy=-3467.3655764
Zero-point correction= 1.217927
(Hartree/Particle)
Thermal correction to Energy= 1.283721
Thermal correction to Enthalpy= 1.284666
Thermal correction to Gibbs Free Energy= 1.116036
Sum of electronic and zero-point Energies= -3466.147649
Sum of electronic and thermal Energies= -3466.081855
Sum of electronic and thermal Enthalpies= -3466.080911
Sum of electronic and thermal Free Energies= -3466.249541

.....

Cartesian Coordinates

.....

77	0.123998	-1.192235	-1.414125
15	-1.467843	0.239623	-0.514578
8	-1.995500	0.388896	1.056733
8	-2.925134	-0.129891	-1.251601
7	-1.029235	1.829155	-0.817833
6	-2.742115	-0.637339	1.631039
6	-2.096088	-1.402701	2.625567
1	-1.086630	-1.127724	2.903704
6	-2.757875	-2.449674	3.216774
1	-2.274346	-3.037647	3.991951
6	-4.071421	-2.797455	2.800890
6	-4.734362	-3.933272	3.340078
1	-4.224940	-4.516637	4.102703
6	-5.985518	-4.298602	2.897802
1	-6.480297	-5.172157	3.312060
6	-6.621179	-3.541319	1.885354
1	-7.596465	-3.847244	1.517676
6	-6.013826	-2.423164	1.356048
1	-6.513464	-1.863601	0.574607
6	-4.731598	-1.999961	1.806065
6	-4.064125	-0.841108	1.265388
6	-4.744534	0.077490	0.312144
6	-5.995726	0.718170	0.629390
6	-6.580340	0.659772	1.925701
1	-6.068223	0.123100	2.715619
6	-7.776856	1.288169	2.196398
1	-8.196077	1.235542	3.197115
6	-8.461371	2.006397	1.187315
1	-9.406884	2.490532	1.413501
6	-7.914945	2.101861	-0.072603
1	-8.418772	2.665834	-0.853337
6	-6.673705	1.481333	-0.379956
6	-6.083381	1.621370	-1.665476
1	-6.612129	2.181039	-2.431860
6	-4.844854	1.090741	-1.923566
1	-4.353830	1.221053	-2.882281
6	-4.172323	0.358735	-0.918630
6	0.226456	1.929007	-1.615918
1	1.066409	2.022795	-0.918893
6	0.246227	3.137021	-2.537124
6	-0.822466	3.409776	-3.404258
1	-1.707400	2.779848	-3.369770
6	-0.762710	4.489736	-4.284354
1	-1.600854	4.695632	-4.944369
6	0.371486	5.308475	-4.317624
1	0.417214	6.149228	-5.003901
6	1.441554	5.041750	-3.461523
1	2.324413	5.674997	-3.477705
6	1.374747	3.963989	-2.573787
1	2.202821	3.765343	-1.896804
6	0.396243	0.660849	-2.461386
1	-0.330579	0.701703	-3.280123
1	1.386024	0.681293	-2.924731
6	-1.483422	3.092736	-0.153533
1	-1.263796	3.859980	-0.897865
6	-0.692759	3.496296	1.091421
6	0.308987	4.470391	0.966807
1	0.563234	4.845910	-0.021046
6	0.951452	4.992324	2.092926
1	1.713882	5.757893	1.974142
6	0.596566	4.546119	3.366798
1	1.082033	4.958253	4.247257
6	-0.384334	3.559634	3.501496
1	-0.660065	3.199303	4.488649
6	-1.020564	3.036673	2.375556
1	-1.786617	2.280817	2.497011
6	-2.992554	3.179151	0.076923
1	-3.529474	3.047925	-0.863499
1	-3.362357	2.447805	0.794583
1	-3.223967	4.176244	0.463231
6	-1.305803	-1.773006	-3.015450
1	-1.731846	-0.857049	-3.413670
6	-0.002803	-2.105762	-3.467952
1	0.461227	-1.421906	-4.177521
6	0.512899	-3.531673	-3.556625
1	0.047347	-4.027539	-4.421840
1	1.584608	-3.500187	-3.768597
6	0.265098	-4.364061	-2.279891
1	-0.661551	-4.937664	-2.376821
1	1.067862	-5.099929	-2.171657
6	0.198058	-3.543652	-0.994635
1	1.031296	-3.689041	-0.315313
6	-0.980688	-3.051170	-0.449656
1	-0.998903	-2.853342	0.619198
6	-2.337878	-3.190033	-1.109851
1	-3.039033	-2.549038	-0.576952
1	-2.692592	-4.222048	-0.973561
6	-2.352305	-2.815364	-2.610045
1	-2.216805	-3.710208	-3.226859
1	-3.341741	-2.420950	-2.856658
6	2.791428	-1.893315	-1.921336
1	2.615357	-2.934701	-1.707791
1	2.938886	-1.625522	-2.959653
6	2.322445	-0.886308	-1.035044
1	2.601424	0.133327	-1.276933
6	1.728904	-1.137707	0.233955
1	1.730649	-2.171084	0.566555
6	1.806811	-0.217989	1.390004
6	2.330617	1.084365	1.324308
6	1.447580	-0.719440	2.654774

6	2.476637	1.853575	2.476586
1	2.660733	1.486906	0.373732
6	1.581570	0.052718	3.807590
1	1.081850	-1.740278	2.728809
6	2.099605	1.346998	3.723406
1	2.873221	2.859880	2.401394
1	1.295778	-0.361186	4.770521
1	2.208635	1.955102	4.615775
8	4.383369	-4.106832	-0.801221
6	5.075835	-3.128065	-1.067046
8	4.709926	-2.022340	-1.649260
8	6.405784	-3.076332	-0.751672
6	6.917109	-4.235379	-0.077466
1	6.796823	-5.134003	-0.689495
1	7.977710	-4.038730	0.091239
1	6.410912	-4.392127	0.880362
6	5.234318	1.586816	-1.310025
6	6.035585	2.716948	-0.682848
1	4.189468	1.886592	-1.464635
1	5.642308	1.287973	-2.278894
6	5.639725	2.858005	0.782262
1	5.842385	3.656577	-1.206628
1	7.106858	2.503649	-0.754502
1	6.268143	3.598563	1.278072
1	4.597628	3.185379	0.875529
7	5.265896	0.420587	-0.429674
6	5.531519	0.434680	0.871984
7	5.794952	1.577254	1.508280
6	5.482668	-0.933298	1.529008
1	4.743386	-1.492573	0.952832
1	6.443979	-1.429797	1.353133
6	5.087559	-0.989744	3.008123
1	4.241108	-0.319197	3.176080
6	6.133101	1.702786	2.947773
6	6.236711	-0.651509	3.962130
1	5.827091	-0.480382	4.964628
6	7.020430	0.584775	3.501836
1	7.592290	0.995220	4.340472
1	7.754142	0.315882	2.733085
1	6.666390	2.650967	3.028994
1	5.205441	1.803318	3.523189
1	6.923409	-1.502507	4.041644
1	4.718028	-1.999336	3.214722
1	5.105147	-0.500670	-0.866590

[12-13]‡ P2 *endo-re* conf2

Number of imaginary frequencies : 1
The smallest frequency is : -322.0722 cm(-1)
Electronic energy=-3467.3655765
Zero-point correction= 1.217923
(Hartree/Particle)
Thermal correction to Energy= 1.283719
Thermal correction to Enthalpy= 1.284663
Thermal correction to Gibbs Free Energy= 1.116010
Sum of electronic and zero-point Energies= -3466.147654
Sum of electronic and thermal Energies= -3466.081857
Sum of electronic and thermal Enthalpies= -3466.080913
Sum of electronic and thermal Free Energies= -3466.249567

Cartesian Coordinates

77	0.123979	-1.192426	-1.414026
15	-1.467863	0.239514	-0.514582
8	-1.995528	0.388905	1.056716
8	-2.925159	-0.130038	-1.251579
7	-1.029211	1.829015	-0.817923
6	-2.742193	-0.637262	1.631077
6	-2.096197	-1.402615	2.625631
1	-1.086717	-1.127685	2.903741
6	-2.758039	-2.449516	3.216902
1	-2.274534	-3.037480	3.992100
6	-4.071615	-2.797235	2.801060
6	-4.734619	-3.932978	3.340326
1	-4.225222	-4.516329	4.102979
6	-5.985804	-4.298257	2.898089
1	-6.480632	-5.171755	3.312407
6	-6.621431	-3.540995	1.885605
1	-7.596741	-3.846881	1.517959
6	-6.014015	-2.422909	1.356223
1	-6.513630	-1.863364	0.574756
6	-4.731756	-1.999758	1.806197
6	-4.064217	-0.840978	1.265444
6	-4.744567	0.077580	0.312119
6	-5.995727	0.718357	0.629293
6	-6.580358	0.660107	1.925603
1	-6.068278	0.123476	2.715574
6	-7.776843	1.288594	2.196231
1	-8.196078	1.236080	3.196947
6	-8.461307	2.006768	1.187075
1	-9.406796	2.490975	1.413206
6	-7.914864	2.102087	-0.072847
1	-8.418653	2.666016	-0.853637
6	-6.673655	1.481463	-0.380131
6	-6.083314	1.621344	-1.665659
1	-6.612026	2.180967	-2.432102
6	-4.844813	1.090624	-1.923689
1	-4.353776	1.220813	-2.882414
6	-4.172330	0.358680	-0.918675
6	0.226446	1.928795	-1.616068
1	1.066427	2.022631	-0.919084
6	0.246207	3.136734	-2.537372
6	-0.822534	3.409483	-3.404447
1	-1.707499	2.779604	-3.369850
6	-0.762785	4.489381	-4.284621
1	-1.600966	4.695276	-4.944588
6	0.371451	5.308058	-4.318027
1	0.417173	6.148763	-5.004364
6	1.441568	5.041335	-3.461987
1	2.324459	5.674534	-3.478276
6	1.374768	3.963640	-2.574171
1	2.202879	3.764993	-1.897233
6	0.396193	0.660571	-2.461443
1	-0.330654	0.701373	-3.280162
1	1.385957	0.680967	-2.924825
6	-1.483383	3.092657	-0.153734
1	-1.263757	3.859835	-0.898134
6	-0.692700	3.496316	1.091173
6	0.309041	4.470404	0.966463
1	0.563279	4.845833	-0.021427
6	0.951514	4.992439	2.092530
1	1.713940	5.758000	1.973673
6	0.596639	4.546345	3.366444
1	1.082110	4.958560	4.246863
6	-0.384253	3.559865	3.501238
1	-0.659973	3.199620	4.488426
6	-1.020490	3.036801	2.375350
1	-1.786537	2.280950	2.496875
6	-2.992510	3.179117	0.076737
1	-3.529448	3.047810	-0.863663
1	-3.362314	2.447845	0.794473
1	-3.223900	4.176250	0.462952
6	-1.305909	-1.773383	-3.015211
1	-1.732020	-0.857472	-3.413462
6	-0.002932	-2.106112	-3.467792
1	0.460999	-1.422279	-4.177447
6	0.512895	-3.531982	-3.556370
1	0.047444	-4.027945	-4.421584
1	1.584612	-3.500408	-3.768281
6	0.265105	-4.364304	-2.279596

1	-0.661589	-4.937843	-2.376455
1	1.067823	-5.100226	-2.171373
6	0.198185	-3.543816	-0.994385
1	1.031495	-3.689138	-0.315142
6	-0.980525	-3.051327	-0.449323
1	-0.998642	-2.853432	0.619520
6	-2.337775	-3.190259	-1.109383
1	-3.038881	-2.549208	-0.576486
1	-2.692486	-4.222258	-0.972962
6	-2.352345	-2.815733	-2.609613
1	-2.216880	-3.710630	-3.226356
1	-3.341813	-2.421367	-2.856173
6	2.791432	-1.893481	-1.921190
1	2.615410	-2.934855	-1.707541
1	2.938836	-1.625784	-2.959540
6	2.322411	-0.886412	-1.034989
1	2.601360	0.133210	-1.276968
6	1.728878	-1.137721	0.234034
1	1.730651	-2.171070	0.566724
6	1.806791	-0.217915	1.390015
6	2.330630	1.084421	1.324227
6	1.447542	-0.719263	2.654822
6	2.476670	1.853710	2.476450
1	2.660757	1.486885	0.373623
6	1.581552	0.052974	3.807582
1	1.081795	-1.740089	2.728932
6	2.099623	1.347233	3.723305
1	2.873280	2.860000	2.401184
1	1.295749	-0.360854	4.770542
1	2.208672	1.955397	4.615631
8	4.383741	-4.106935	-0.801323
6	5.076031	-3.128021	-1.067058
8	4.709925	-2.022308	-1.649172
8	6.405967	-3.076066	-0.751671
6	6.917476	-4.235025	-0.077455
1	6.797385	-5.133666	-0.689497
1	7.978033	-4.038185	0.091301
1	6.411265	-4.391875	0.880348
6	5.234177	1.586779	-1.310020
6	6.035510	2.716954	-0.683001
1	4.189315	1.886551	-1.464565
1	5.642082	1.287859	-2.278901
6	5.639807	2.858125	0.782139
1	5.842264	3.656546	-1.206829
1	7.106774	2.503642	-0.754751
1	6.268308	3.598695	1.277829
1	4.597733	3.185546	0.875501
7	5.265836	0.420614	-0.429586
6	5.531603	0.434801	0.872038
7	5.795073	1.577424	1.508234
6	5.482953	-0.933131	1.529169
1	4.743946	-1.492671	0.952904
1	6.444436	-1.429392	1.353561
6	5.087578	-0.989483	3.008224
1	4.241063	-0.318969	3.175983
6	6.133121	1.703088	2.947738
6	6.236558	-0.651080	3.962386
1	5.826755	-0.479752	4.964776
6	7.020367	0.585108	3.501998
1	7.592187	0.995629	4.340623
1	7.754118	0.316086	2.733330
1	6.666430	2.651263	3.028906
1	5.205413	1.803700	3.523065
1	6.923236	-1.502066	4.042191
1	4.718075	-1.999079	3.214853
1	5.105109	-0.500675	-0.866445

[12-13]‡ P2 *exo-si* conf2

Number of imaginary frequencies : 1

The smallest frequency is : -259.0647 cm(-1)
Electronic energy=-3467.3737764
Zero-point correction= 1.217210
(Hartree/Particle)
Thermal correction to Energy= 1.283171
Thermal correction to Enthalpy= 1.284115
Thermal correction to Gibbs Free Energy= 1.117493
Sum of electronic and zero-point Energies= -3466.156566
Sum of electronic and thermal Energies= -3466.090605
Sum of electronic and thermal Enthalpies= -3466.089661
Sum of electronic and thermal Free Energies= -3466.256283

.....

Cartesian Coordinates

.....

77	0.071396	-1.323578	-1.357272
15	-1.262961	0.363673	-0.545280
8	-1.955104	0.448766	0.956521
8	-2.631730	0.500377	-1.488270
7	-0.398777	1.799304	-0.526791
6	-2.998884	-0.412128	1.291052
6	-2.698848	-1.438646	2.211167
1	-1.697475	-1.489821	2.615978
6	-3.672202	-2.341509	2.558038
1	-3.453490	-3.132846	3.269359
6	-4.959474	-2.280308	1.958421
6	-5.943206	-3.269078	2.232267
1	-5.701121	-4.057630	2.940041
6	-7.167660	-3.242505	1.603892
1	-7.909245	-4.007331	1.814830
6	-7.452923	-2.223914	0.663781
1	-8.408827	-2.220433	0.148018
6	-6.528209	-1.239374	0.390038
1	-6.762510	-0.475039	-0.341082
6	-5.261019	-1.220582	1.037312
6	-4.263668	-0.216460	0.759848
6	-4.553034	0.963443	-0.100789
6	-5.640339	1.864733	0.189854
6	-6.403455	1.783581	1.388504
1	-6.160842	1.023924	2.121769
6	-7.432890	2.665043	1.638901
1	-7.993254	2.585604	2.566077
6	-7.762685	3.676206	0.705426
1	-8.581383	4.358838	0.913407
6	-7.031722	3.798832	-0.454531
1	-7.259198	4.582861	-1.172132
6	-5.953026	2.916956	-0.735451
6	-5.164960	3.074834	-1.907441
1	-5.420457	3.859606	-2.613766
6	-4.073202	2.273057	-2.124469
1	-3.431934	2.400564	-2.990270
6	-3.758066	1.251875	-1.200068
6	0.968566	1.656763	-1.082182
1	1.665988	1.503284	-0.248152
6	1.427679	2.890907	-1.838497
6	0.593357	3.532298	-2.764683
1	-0.426865	3.179674	-2.889892
6	1.061420	4.618690	-3.503974
1	0.402963	5.112827	-4.213017
6	2.374611	5.071585	-3.336031
1	2.738180	5.916125	-3.914207
6	3.212647	4.436209	-2.417378
1	4.232640	4.784480	-2.278561
6	2.736854	3.356364	-1.668493
1	3.384261	2.868610	-0.943978
6	1.038847	0.448398	-2.029324
1	0.576518	0.733790	-2.981536
1	2.096615	0.287259	-2.240963
6	-0.614604	3.013491	0.329804
1	-0.025510	3.780988	-0.177156
6	-0.015701	2.888741	1.729370

6	1.320721	3.267756	1.928325
1	1.901550	3.624567	1.081507
6	1.898924	3.226988	3.200167
1	2.928933	3.541825	3.338639
6	1.144053	2.809058	4.297730
1	1.587115	2.782901	5.289190
6	-0.191914	2.442909	4.112998
1	-0.792312	2.130638	4.962750
6	-0.765214	2.479069	2.841213
1	-1.801855	2.190414	2.718647
6	-2.050776	3.531048	0.326714
1	-2.377580	3.729559	-0.695291
1	-2.758674	2.842414	0.786277
1	-2.083403	4.471252	0.885332
6	-1.178316	-1.344574	-3.262683
1	-1.222193	-0.311422	-3.597073
6	0.027825	-2.028960	-3.505814
1	0.815047	-1.471234	-4.012043
6	0.166643	-3.535105	-3.641290
1	-0.148255	-3.832832	-4.652622
1	1.228805	-3.784975	-3.568728
6	-0.617677	-4.366286	-2.599534
1	-1.621350	-4.585269	-2.975899
1	-0.120181	-5.333668	-2.479872
6	-0.745510	-3.721343	-1.230595
1	-0.127223	-4.131871	-0.442513
6	-1.792304	-2.920623	-0.852600
1	-1.944792	-2.765227	0.210565
6	-2.944323	-2.543756	-1.760519
1	-3.537319	-1.781950	-1.259091
1	-3.597513	-3.422028	-1.863778
6	-2.541663	-2.030034	-3.164952
1	-2.564533	-2.853537	-3.886853
1	-3.302475	-1.316852	-3.492530
6	2.762095	-2.178552	-1.666111
6	1.923740	-2.369968	-0.555147
1	1.765553	-3.407444	-0.298067
6	1.462151	-1.358882	0.363868
1	1.996984	-0.413285	0.345906
6	1.002871	-1.712548	1.734944
6	0.698985	-3.025855	2.139093
6	0.884455	-0.690011	2.693744
6	0.303287	-3.304568	3.447755
1	0.784825	-3.848124	1.438538
6	0.501287	-0.969168	4.006019
1	1.091748	0.335735	2.407156
6	0.207794	-2.279332	4.392680
1	0.077621	-4.329351	3.730162
1	0.428188	-0.157244	4.721988
1	-0.092712	-2.498118	5.413233
8	4.223860	-4.302933	-0.054038
6	4.912914	-3.308837	-0.264478
8	4.710884	-2.368590	-1.132940
8	6.058490	-3.059600	0.454534
6	6.350959	-4.011921	1.483603
1	6.476558	-5.018405	1.072722
1	7.285059	-3.680703	1.942751
1	5.557193	-4.036476	2.237484
6	5.768512	0.959196	-2.008943
6	6.842786	1.975943	-1.651546
1	4.890664	1.455238	-2.440441
1	6.128511	0.219501	-2.727484
6	6.366252	2.828187	-0.482909
1	7.061900	2.623387	-2.504289
1	7.764294	1.452455	-1.375998
1	7.194069	3.426530	-0.095989
1	5.573775	3.518789	-0.791016
7	5.371580	0.245016	-0.795815
6	5.430437	0.755004	0.428004
7	5.864741	2.001096	0.641086
6	4.985523	-0.191452	1.528878
1	4.374980	-0.950408	1.038974
1	5.873131	-0.717030	1.898709
6	4.192736	0.418812	2.692342
1	3.473401	1.145326	2.301375
6	5.792213	2.719203	1.938509
6	5.073316	1.068419	3.764193
1	4.443886	1.700774	4.401314
6	6.213154	1.902558	3.163061
1	6.598341	2.598698	3.915553
1	7.056348	1.263439	2.876655
1	6.463799	3.571189	1.829165
1	4.782003	3.125738	2.060751
1	5.500407	0.294958	4.413100
1	3.590708	-0.374708	3.142090
1	5.159298	-0.771408	-0.879950
1	2.860248	-2.989804	-2.373016
1	3.024469	-1.198240	-2.025899

[12-13]‡ P2 *endo-si* conf2

Number of imaginary frequencies : 1
The smallest frequency is : -282.1375 cm(-1)
Electronic energy=-3467.3779014
Zero-point correction= 1.217317
(Hartree/Particle)
Thermal correction to Energy= 1.283551
Thermal correction to Enthalpy= 1.284495
Thermal correction to Gibbs Free Energy= 1.114537
Sum of electronic and zero-point Energies= -3466.160585
Sum of electronic and thermal Energies= -3466.094351
Sum of electronic and thermal Enthalpies= -3466.093406
Sum of electronic and thermal Free Energies= -3466.263365

.....

Cartesian Coordinates

.....

77	0.096730	-0.842829	-1.277449
15	-1.656629	0.293603	-0.305434
8	-2.361265	-0.059379	1.155221
8	-3.008541	0.266324	-1.284579
7	-1.160973	1.864901	-0.012206
6	-3.290416	-1.089531	1.269521
6	-2.879248	-2.232135	1.989339
1	-1.883265	-2.243878	2.419507
6	-3.740229	-3.293158	2.123652
1	-3.440206	-4.176581	2.679930
6	-5.021901	-3.263988	1.510455
6	-5.888890	-4.388895	1.572041
1	-5.561841	-5.265654	2.124897
6	-7.109037	-4.376732	0.935070
1	-7.761610	-5.243473	0.983404
6	-7.507349	-3.235031	0.199263
1	-8.459576	-3.237821	-0.323258
6	-6.697652	-2.121956	0.133296
1	-7.016207	-1.261324	-0.442744
6	-5.439088	-2.089652	0.796777
6	-4.563815	-0.947591	0.739490
6	-4.972412	0.334316	0.099421
6	-6.134827	1.071021	0.521165
6	-6.912730	0.697090	1.653018
1	-6.625526	-0.173547	2.230773
6	-8.014307	1.432576	2.033469
1	-8.586771	1.130070	2.905654
6	-8.403905	2.581725	1.304631
1	-9.278310	3.147426	1.612600
6	-7.662806	2.984985	0.217269
1	-7.938914	3.875695	-0.340911
6	-6.512034	2.258560	-0.193321
6	-5.719835	2.702045	-1.286986
1	-6.022788	3.590868	-1.833053

6	-4.569472	2.035300	-1.629418
1	-3.931573	2.369131	-2.440511
6	-4.196921	0.878229	-0.911795
6	0.116567	2.209508	-0.696945
1	0.912265	2.190722	0.057598
6	0.082636	3.607111	-1.293458
6	-1.018822	4.048939	-2.039946
1	-1.884540	3.400853	-2.139003
6	-1.015890	5.314727	-2.625640
1	-1.879030	5.647512	-3.195775
6	0.092399	6.155482	-2.478081
1	0.093732	7.141726	-2.933361
6	1.193445	5.723124	-1.735938
1	2.055332	6.372723	-1.610065
6	1.184750	4.456944	-1.144127
1	2.038573	4.127590	-0.556247
6	0.444323	1.187115	-1.797038
1	-0.167153	1.420363	-2.676529
1	1.483977	1.324555	-2.095509
6	-1.506484	2.807356	1.101362
1	-1.345644	3.794738	0.660179
6	-0.516084	2.679872	2.256871
6	0.445429	3.680597	2.449644
1	0.472903	4.528521	1.769808
6	1.359211	3.604961	3.504991
1	2.088219	4.398467	3.645497
6	1.331565	2.514156	4.376499
1	2.040866	2.450499	5.196640
6	0.381806	1.505116	4.187943
1	0.353139	0.653055	4.861534
6	-0.537866	1.590364	3.141291
1	-1.278758	0.810115	3.013311
6	-2.963138	2.803036	1.569510
1	-3.640695	2.949417	0.726850
1	-3.245525	1.893034	2.095909
1	-3.092172	3.645802	2.255985
6	0.955445	-1.299969	1.271515
1	0.700695	-2.336716	1.133239
1	0.402288	-0.739150	2.013065
6	1.683647	-0.586322	0.298730
1	1.890084	0.453726	0.525276
6	2.317675	-1.200831	-0.833114
1	2.435569	-2.277764	-0.787135
6	-1.044585	-1.069815	-3.160018
1	-1.428136	-0.087382	-3.421018
6	0.334910	-1.294706	-3.419174
1	0.890606	-0.471487	-3.867955
6	0.943573	-2.653740	-3.706692
1	0.730933	-2.929033	-4.750846
1	2.026953	-2.547124	-3.637779
6	0.481862	-3.791056	-2.767184
1	-0.378688	-4.309911	-3.199494
1	1.280894	-4.536112	-2.698357
6	0.122885	-3.348359	-1.357275
1	0.834860	-3.600149	-0.575239
6	-1.142890	-2.990444	-0.957591
1	-1.348094	-2.998503	0.108723
6	-2.359677	-2.874286	-1.848474
1	-3.117255	-2.310573	-1.301996
1	-2.777215	-3.877937	-2.014371
6	-2.101813	-2.176700	-3.200626
1	-1.810178	-2.912215	-3.957364
1	-3.044121	-1.741926	-3.546030
6	3.385989	-0.539793	-1.612590
6	3.741817	0.815762	-1.462395
6	4.110144	-1.299280	-2.553401
6	4.733216	1.394202	-2.256401
1	3.244783	1.428869	-0.719170
6	5.100478	-0.723297	-3.347950
1	3.897155	-2.360067	-2.648713
6	5.412224	0.632996	-3.212206
1	4.974125	2.445808	-2.126348
1	5.636610	-1.336726	-4.066656
1	6.181103	1.086243	-3.830820
8	2.416858	-3.841851	1.438866
6	2.857511	-3.003013	2.230656
8	2.339109	-1.919582	2.662710
8	4.132837	-3.181500	2.779266
6	4.807373	-4.391838	2.407680
1	4.233901	-5.268409	2.722557
1	5.768157	-4.374686	2.926603
1	4.966697	-4.447248	1.326298
6	4.012317	0.663857	3.120533
6	4.743232	1.995920	3.143282
1	3.072681	0.726950	2.565093
1	3.771768	0.308126	4.124155
6	5.325093	2.269159	1.762450
1	4.054006	2.797181	3.414185
1	5.551078	1.974731	3.882768
1	5.917425	3.184960	1.766601
1	4.528058	2.386666	1.017936
7	4.871905	-0.336295	2.485961
6	5.895407	-0.086625	1.678459
7	6.211505	1.163346	1.333226
6	6.643670	-1.309264	1.191295
1	5.982856	-2.158374	1.368094
1	7.518299	-1.460862	1.834943
6	7.047402	-1.262852	-0.290059
1	6.256990	-0.761566	-0.855581
6	7.292685	1.576747	0.401500
6	8.389468	-0.557811	-0.516166
1	8.475670	-0.285110	-1.574499
6	8.540292	0.694977	0.357209
1	9.355957	1.315205	-0.029539
1	8.822623	0.429692	1.382136
1	7.583811	2.574354	0.736714
1	6.858253	1.683565	-0.599424
1	9.215989	-1.243679	-0.296376
1	7.092167	-2.287209	-0.672629
1	4.645974	-1.313990	2.668477

[12-13]‡ P2 *exo-re* conf2

Number of imaginary frequencies : 1
The smallest frequency is : -254.3128 cm(-1)
Electronic energy=-3467.3768167
Zero-point correction= 1.217893
(Hartree/Particle)
Thermal correction to Energy= 1.283844
Thermal correction to Enthalpy= 1.284789
Thermal correction to Gibbs Free Energy= 1.117015
Sum of electronic and zero-point Energies= -3466.158924
Sum of electronic and thermal Energies= -3466.092972
Sum of electronic and thermal Enthalpies= -3466.092028
Sum of electronic and thermal Free Energies= -3466.259802

.....

Cartesian Coordinates

.....

77	0.266500	-0.791632	-1.277111
15	-1.495907	0.505635	-0.514856
8	-2.159044	0.367545	1.004782
8	-2.856635	0.285316	-1.447120
7	-1.038381	2.113320	-0.489027
6	-2.828568	-0.807739	1.333993
6	-2.194745	-1.670688	2.256593
1	-1.260767	-1.363557	2.718808
6	-2.788729	-2.871514	2.560949
1	-2.324831	-3.545550	3.275480
6	-3.996977	-3.265818	1.923191
6	-4.565746	-4.547459	2.156878

1	-4.067472	-5.216980	2.853123
6	-5.713362	-4.941383	1.506542
1	-6.135517	-5.925534	1.687289
6	-6.337806	-4.065169	0.586823
1	-7.229742	-4.387780	0.057555
6	-5.823446	-2.808407	0.352024
1	-6.310167	-2.153118	-0.360881
6	-4.649376	-2.360676	1.019151
6	-4.075265	-1.060786	0.785606
6	-4.774140	-0.009552	-0.007307
6	-6.096768	0.442233	0.349794
6	-6.762668	0.011237	1.531687
1	-6.261502	-0.672898	2.205604
6	-8.027276	0.462499	1.842404
1	-8.508523	0.121989	2.754720
6	-8.701897	1.369186	0.990918
1	-9.701273	1.709676	1.245414
6	-8.078762	1.827739	-0.147460
1	-8.574798	2.540379	-0.801288
6	-6.768680	1.394691	-0.488767
6	-6.105395	1.908951	-1.635456
1	-6.625122	2.618602	-2.272988
6	-4.813980	1.540626	-1.915846
1	-4.273549	1.946701	-2.764384
6	-4.154733	0.608622	-1.083277
6	0.306149	2.373300	-1.062086
1	0.988016	2.553128	-0.224256
6	0.320449	3.620510	-1.931380
6	-0.687974	3.851364	-2.877807
1	-1.521022	3.156411	-2.943608
6	-0.633593	4.967924	-3.711892
1	-1.424659	5.139535	-4.436748
6	0.434103	5.866801	-3.614734
1	0.474991	6.737183	-4.263339
6	1.442312	5.643842	-2.674598
1	2.270270	6.342086	-2.587417
6	1.382377	4.527577	-1.835422
1	2.159863	4.363188	-1.092666
6	0.831422	1.181240	-1.885705
1	0.467384	1.299377	-2.911030
1	1.920166	1.278773	-1.934942
6	-1.528979	3.228979	0.393456
1	-1.333972	4.126516	-0.200073
6	-0.671395	3.345259	1.652946
6	0.356691	4.299196	1.688980
1	0.493902	4.962795	0.839183
6	1.208599	4.400077	2.792790
1	1.999570	5.145514	2.798425
6	1.039212	3.545320	3.884256
1	1.706701	3.606503	4.738960
6	0.002999	2.608456	3.869062
1	-0.132998	1.930064	4.704859
6	-0.844418	2.509052	2.764978
1	-1.630216	1.764936	2.764090
6	-3.032847	3.228727	0.662220
1	-3.587877	3.214437	-0.278114
1	-3.364904	2.391443	1.274574
1	-3.283450	4.154843	1.188511
6	1.073720	0.002636	1.211322
6	1.543717	-1.136886	0.534592
1	1.324399	-2.096949	0.991372
6	2.429421	-1.043464	-0.586125
1	2.832626	-0.051087	-0.764995
6	-0.698323	-1.007347	-3.258160
1	-0.978964	-0.011734	-3.592170
6	0.677588	-1.344118	-3.386048
1	1.329046	-0.585001	-3.817705
6	1.202327	-2.756327	-3.561316
1	1.047159	-3.070864	-4.604293
1	2.282386	-2.733140	-3.406180
6	0.578789	-3.788604	-2.600386
1	-0.283604	-4.273855	-3.067801
1	1.310737	-4.578650	-2.409438
6	0.146519	-3.209694	-1.260745
1	0.750067	-3.491947	-0.407506
6	-1.129443	-2.754997	-0.989865
1	-1.439842	-2.723020	0.049096
6	-2.242346	-2.681483	-2.013793
1	-3.065578	-2.117206	-1.577653
1	-2.620537	-3.699046	-2.188025
6	-1.831439	-2.032404	-3.355003
1	-1.538321	-2.803865	-4.075077
1	-2.707862	-1.535211	-3.779236
6	3.370975	-2.092926	-1.021953
6	3.423421	-3.389309	-0.478387
6	4.321939	-1.752524	-2.004701
6	4.372904	-4.312211	-0.919148
1	2.743421	-3.674858	0.316711
6	5.273232	-2.672288	-2.442949
1	4.305611	-0.750197	-2.425874
6	5.300606	-3.962686	-1.903878
1	4.396070	-5.305361	-0.479295
1	5.992906	-2.382457	-3.203509
1	6.040518	-4.682541	-2.240947
8	0.649156	-0.639936	4.111391
6	1.744223	-0.091197	3.957950
8	2.310985	0.236781	2.847663
8	2.527594	0.241074	5.031295
6	1.986804	-0.099046	6.313469
1	1.040218	0.418548	6.499349
1	2.730643	0.221300	7.046368
1	1.818277	-1.176898	6.403297
6	3.917848	2.469188	0.573913
6	5.133359	2.993195	-0.172280
1	3.133905	2.171031	-0.130790
1	3.491516	3.214771	1.249912
6	5.836768	1.825114	-0.853270
1	4.831323	3.727385	-0.923408
1	5.823526	3.481660	0.523357
1	6.763477	2.158443	-1.322681
1	5.203394	1.387571	-1.635262
7	4.303811	1.307487	1.372091
6	5.363080	0.538373	1.153739
7	6.182875	0.766132	0.123403
6	5.547719	-0.584476	2.155711
1	4.573500	-0.724839	2.630117
1	6.221377	-0.225097	2.943258
6	6.051224	-1.916017	1.578168
1	5.582572	-2.084653	0.605057
6	7.350860	-0.066829	-0.262037
6	7.576737	-1.973650	1.443671
1	7.843369	-2.807033	0.783101
6	8.158822	-0.665948	0.891080
1	9.173873	-0.843196	0.520004
1	8.252330	0.087179	1.681836
1	7.997172	0.603051	-0.831611
1	7.007443	-0.848569	-0.950515
1	8.033640	-2.182072	2.418295
1	5.701732	-2.726397	2.225477
1	3.646766	1.004222	2.109662
1	0.239437	-0.070804	1.889193
1	1.358288	0.989268	0.882203

[12-13]‡ P2 *exo-re* conf2 [BF_4^-]

Number of imaginary frequencies : 1
The smallest frequency is : -271.3676 cm(-1)
Electronic energy=-3892.0061101
Zero-point correction= 1.233671
(Hartree/Particle)

Thermal correction to Energy= 1.305756
Thermal correction to Enthalpy= 1.306700
Thermal correction to Gibbs Free Energy= 1.124792
Sum of electronic and zero-point Energies= -3890.772439
Sum of electronic and thermal Energies= -3890.700355
Sum of electronic and thermal Enthalpies= -3890.699410
Sum of electronic and thermal Free Energies= -3890.881318

Cartesian Coordinates

77	-0.213677	-1.186275	-1.202814
15	-1.784741	0.384507	-0.543188
8	-2.413816	0.510582	0.996290
8	-3.204994	0.195754	-1.403410
7	-1.167057	1.925662	-0.728283
6	-3.230464	-0.504940	1.477669
6	-2.686488	-1.344398	2.476825
1	-1.689461	-1.138683	2.856488
6	-3.439175	-2.390735	2.951621
1	-3.042935	-3.042284	3.725442
6	-4.728689	-2.659324	2.415709
6	-5.475628	-3.794152	2.834106
1	-5.049273	-4.443294	3.594510
6	-6.704190	-4.076862	2.280935
1	-7.262637	-4.950841	2.603292
6	-7.234201	-3.232938	1.275822
1	-8.192160	-3.471768	0.822847
6	-6.544438	-2.114267	0.861098
1	-6.961548	-1.484304	0.084202
6	-5.281326	-1.779545	1.424249
6	-4.527334	-0.626634	1.003944
6	-5.089844	0.406095	0.087368
6	-6.311894	1.105294	0.396919
6	-6.990492	0.952541	1.639039
1	-6.574767	0.296788	2.394441
6	-8.157572	1.636392	1.903298
1	-8.650280	1.505738	2.862639
6	-8.716513	2.512030	0.942364
1	-9.640167	3.039586	1.162046
6	-8.074752	2.703830	-0.260135
1	-8.479881	3.388768	-1.000572
6	-6.861510	2.025958	-0.558189
6	-6.172208	2.264378	-1.777845
1	-6.601761	2.950854	-2.502022
6	-4.964198	1.661894	-2.023103
1	-4.400863	1.854352	-2.930275
6	-4.422859	0.763110	-1.075928
6	0.166521	1.953638	-1.391089
1	0.921190	2.125808	-0.619908
6	0.286680	3.083879	-2.400908
6	-0.787780	3.450839	-3.222824
1	-1.747729	2.959092	-3.088871
6	-0.634199	4.446965	-4.188453
1	-1.477913	4.727988	-4.813464
6	0.600341	5.083260	-4.350462
1	0.720380	5.858871	-5.101870
6	1.677632	4.715432	-3.539997
1	2.642236	5.201056	-3.661524
6	1.522399	3.723572	-2.568580
1	2.363709	3.430510	-1.948096
6	0.477857	0.628525	-2.107219
1	0.015266	0.675270	-3.099499
1	1.552451	0.590764	-2.262163
6	-1.482936	3.180762	0.031070
1	-1.225218	3.976207	-0.673085
6	-0.561792	3.360897	1.237067
6	0.519826	4.247685	1.140187
1	0.687335	4.783302	0.209051
6	1.385811	4.446311	2.218657
1	2.216685	5.139749	2.121640
6	1.186359	3.749574	3.412172
1	1.861820	3.893038	4.251114
6	0.114852	2.859428	3.517903
1	-0.041774	2.297098	4.433311
6	-0.754769	2.671694	2.443315
1	-1.577702	1.975541	2.539895
6	-2.959837	3.394624	0.366955
1	-3.572487	3.343571	-0.535403
1	-3.347370	2.680115	1.091802
1	-3.067374	4.398562	0.789429
6	0.825690	-0.150043	1.140208
6	1.129105	-1.414473	0.591604
1	0.837719	-2.281844	1.175866
6	1.965055	-1.539749	-0.561434
1	2.433920	-0.618972	-0.883614
6	-1.299169	-1.562156	-3.079814
1	-1.502635	-0.600897	-3.544427
6	0.031355	-2.052680	-3.221801
1	0.725145	-1.430091	-3.785785
6	0.403067	-3.523812	-3.229784
1	0.163311	-3.954620	-4.213879
1	1.486530	-3.593533	-3.119801
6	-0.269788	-4.347201	-2.112947
1	-1.205841	-4.786722	-2.471742
1	0.382184	-5.185647	-1.849831
6	-0.553470	-3.551098	-0.846532
1	0.076745	-3.783278	0.002256
6	-1.756127	-2.923901	-0.578918
1	-1.995021	-2.718020	0.459128
6	-2.920195	-2.883041	-1.547191
1	-3.659125	-2.183661	-1.158144
1	-3.401062	-3.872074	-1.557468
6	-2.532576	-2.465294	-2.984438
1	-2.366332	-3.351447	-3.606684
1	-3.379923	-1.935987	-3.429254
6	2.759164	-2.724549	-0.931040
6	2.720593	-3.952572	-0.246891
6	3.660495	-2.592358	-2.006975
6	3.526325	-5.020137	-0.646555
1	2.081455	-4.071767	0.621861
6	4.467508	-3.657272	-2.402054
1	3.731091	-1.634693	-2.514114
6	4.399262	-4.882166	-1.729287
1	3.480123	-5.959174	-0.101251
1	5.156889	-3.529376	-3.232338
1	5.028307	-5.713185	-2.035599
8	0.344562	-0.564620	4.055200
6	1.481276	-0.127089	3.859332
8	2.065857	0.091566	2.730360
8	2.309002	0.191864	4.905754
6	1.760135	-0.029732	6.209278
1	0.852178	0.560628	6.368047
1	2.531159	0.282796	6.917178
1	1.521379	-1.086678	6.367076
6	4.478701	2.691374	1.903595
6	5.914057	3.190027	1.852564
1	3.956698	2.880196	0.961012
1	3.912091	3.162543	2.709099
6	6.719795	2.295766	0.919222
1	5.945748	4.219903	1.487264
1	6.354585	3.172268	2.855749
1	7.777983	2.565022	0.954330
1	6.369926	2.395459	-0.113305
7	4.481851	1.251141	2.148123
6	5.469804	0.424953	1.842724
7	6.613806	0.873470	1.314033
6	5.212291	-1.031310	2.176216
1	4.144814	-1.109267	2.390226
1	5.733426	-1.266380	3.112368
6	5.598848	-2.027001	1.070130

1	5.360857	-1.579552	0.102688
6	7.662879	0.022176	0.704502
6	7.073802	-2.443235	1.125428
1	7.354524	-2.882035	0.160518
6	8.005945	-1.267774	1.451750
1	9.036109	-1.535147	1.191686
1	8.009586	-1.057097	2.527468
1	8.552779	0.654176	0.671366
1	7.367835	-0.182709	-0.330671
1	7.215178	-3.226639	1.880519
1	4.961517	-2.910874	1.159473
1	3.598883	0.833184	2.487621
5	4.255145	1.272504	-1.681636
9	5.189511	0.361984	-1.150322
9	4.877662	2.502301	-1.942749
9	3.709305	0.734881	-2.863378
9	3.217816	1.483957	-0.734641
1	-0.009563	-0.036380	1.811541
1	1.233702	0.739161	0.683293

[12-13]‡ P2 *endo-re* conf2 [BF_4^-]

Number of imaginary frequencies : 1
The smallest frequency is : -292.7258 cm(-1)
Electronic energy=-3891.9940773
Zero-point correction= 1.233050
(Hartree/Particle)
Thermal correction to Energy= 1.305225
Thermal correction to Enthalpy= 1.306169
Thermal correction to Gibbs Free Energy= 1.123094
Sum of electronic and zero-point Energies= -3890.761027
Sum of electronic and thermal Energies= -3890.688853
Sum of electronic and thermal Enthalpies= -3890.687909
Sum of electronic and thermal Free Energies= -3890.870983

Cartesian Coordinates

77	-0.267105	-0.840835	-1.558150
15	-1.695286	0.514853	-0.369206
8	-2.238515	0.314352	1.193875
8	-3.181583	0.526864	-1.155245
7	-1.089988	2.058047	-0.266244
6	-2.968017	-0.835005	1.479623
6	-2.307248	-1.836711	2.222266
1	-1.300197	-1.634757	2.563895
6	-2.946382	-3.022997	2.482362
1	-2.450326	-3.799947	3.057406
6	-4.248795	-3.266119	1.966848
6	-4.882011	-4.527041	2.139497
1	-4.358574	-5.296366	2.701266
6	-6.120664	-4.777931	1.593822
1	-6.592246	-5.747465	1.725329
6	-6.774313	-3.771712	0.843444
1	-7.739655	-3.979867	0.390855
6	-6.196230	-2.531999	0.674617
1	-6.708471	-1.779047	0.087809
6	-4.926346	-2.228911	1.241298
6	-4.284563	-0.949736	1.063608
6	-4.981445	0.200615	0.426466
6	-6.241746	0.689874	0.930082
6	-6.814458	0.224029	2.147172
1	-6.286556	-0.518597	2.733357
6	-8.019850	0.713794	2.602669
1	-8.427971	0.345982	3.539905
6	-8.726017	1.695327	1.868084
1	-9.678103	2.067000	2.235618
6	-8.191245	2.186351	0.698277
1	-8.710311	2.955770	0.132383
6	-6.942851	1.714428	0.210251
6	-6.365422	2.256990	-0.969872
1	-6.909228	3.017942	-1.522730
6	-5.122176	1.854110	-1.383531
1	-4.641624	2.284901	-2.255788
6	-4.422310	0.858368	-0.660853
6	0.149001	2.300911	-1.049905
1	0.970054	2.430769	-0.342586
6	0.031939	3.576699	-1.874122
6	-1.118536	3.830411	-2.638166
1	-1.948099	3.129117	-2.592983
6	-1.206548	4.973267	-3.431616
1	-2.105927	5.161167	-4.012447
6	-0.139802	5.878223	-3.478838
1	-0.207192	6.769349	-4.096956
6	1.007059	5.631996	-2.721873
1	1.836783	6.333579	-2.746794
6	1.091956	4.489626	-1.918926
1	1.974808	4.308129	-1.314323
6	0.460061	1.129411	-2.010474
1	0.018620	1.378775	-2.980013
1	1.539926	1.110050	-2.152124
6	-1.495138	3.183507	0.631424
1	-1.153573	4.070044	0.092056
6	-0.769638	3.214670	1.974457
6	0.357983	4.035528	2.111971
1	0.753947	4.549439	1.241500
6	0.978019	4.204921	3.352213
1	1.850686	4.847091	3.433840
6	0.477023	3.549588	4.478014
1	0.951973	3.682797	5.446311
6	-0.632714	2.709304	4.347938
1	-1.022245	2.184511	5.216169
6	-1.250096	2.542869	3.107966
1	-2.115073	1.895917	3.025226
6	-3.006864	3.352963	0.776609
1	-3.467039	3.493947	-0.202803
1	-3.488239	2.507436	1.267766
1	-3.202949	4.246582	1.376588
6	-1.569802	-0.638444	-3.366711
1	-1.758708	0.422769	-3.502832
6	-0.303777	-1.112505	-3.793821
1	0.380426	-0.383572	-4.225656
6	-0.056964	-2.536002	-4.264486
1	-0.490544	-2.662925	-5.268286
1	1.020595	-2.672415	-4.382859
6	-0.611427	-3.626279	-3.318610
1	-1.600781	-3.948777	-3.658326
1	0.031000	-4.510848	-3.379411
6	-0.714672	-3.212195	-1.854160
1	-0.018229	-3.696360	-1.176447
6	-1.851674	-2.649808	-1.305199
1	-1.985875	-2.731605	-0.231258
6	-3.095358	-2.327039	-2.107523
1	-3.788283	-1.788258	-1.464357
1	-3.591225	-3.274235	-2.366318
6	-2.835415	-1.500198	-3.389283
1	-2.789835	-2.162739	-4.261173
1	-3.693057	-0.841573	-3.551212
6	2.226152	-2.176863	-2.001601
1	1.703167	-3.106178	-2.122938
1	2.748144	-1.796739	-2.872089
6	1.881470	-1.256807	-0.985457
1	2.478317	-0.352043	-0.945374
6	1.040601	-1.552212	0.138563
1	0.763691	-2.594583	0.263463
6	1.282661	-0.891151	1.444368
6	1.743474	0.428939	1.556166
6	1.150268	-1.648570	2.622365
6	2.057128	0.975353	2.796294
1	1.890150	1.023024	0.666433
6	1.447910	-1.096296	3.871033

1	0.826840	-2.684845	2.554581
6	1.901575	0.221075	3.963085
1	2.423903	1.993046	2.837218
1	1.332881	-1.699933	4.767620
1	2.137174	0.655145	4.930454
8	2.339729	-4.590281	-0.400346
6	3.453326	-4.081384	-0.529701
8	3.819060	-3.154737	-1.359798
8	4.509778	-4.469050	0.253278
6	4.198579	-5.425983	1.273713
1	3.811266	-6.355124	0.845081
1	5.137432	-5.620612	1.796567
1	3.460185	-5.025633	1.976189
6	5.846818	-0.320968	-2.050294
6	7.233682	0.296406	-1.950952
1	5.081869	0.452574	-2.169073
1	5.772947	-1.021629	-2.885630
6	7.351421	1.051279	-0.633187
1	7.404293	0.988703	-2.779424
1	7.995712	-0.489185	-2.001757
1	8.382510	1.378095	-0.477042
1	6.706959	1.936107	-0.627527
7	5.571458	-1.062032	-0.819648
6	6.083857	-0.775758	0.369244
7	6.983165	0.199839	0.521013
6	5.591397	-1.643604	1.508710
1	4.744945	-2.209187	1.122776
1	6.363945	-2.382499	1.749867
6	5.166177	-0.859579	2.761308
1	4.704337	0.077629	2.444164
6	7.416917	0.774790	1.818180
6	6.335548	-0.587560	3.715384
1	6.055519	0.219557	4.402859
6	7.623995	-0.209657	2.970907
1	8.325900	0.255905	3.671623
1	8.130516	-1.101811	2.585260
1	8.370458	1.261259	1.602634
1	6.702149	1.559609	2.086990
1	6.532211	-1.473412	4.331895
1	4.383237	-1.424302	3.275693
1	4.941977	-1.875045	-0.897099
5	4.020924	2.593823	-0.057317
9	4.675230	1.860310	0.950410
9	4.929669	3.458345	-0.682076
9	2.963751	3.329849	0.514463
9	3.494389	1.696057	-1.022530

[12-13]‡ P2 *exo-si* conf2 [BF_4^-]

Number of imaginary frequencies : 1
The smallest frequency is : -280.8071 cm(-1)
Electronic energy=-3892.0000815
Zero-point correction= 1.232644
(Hartree/Particle)
Thermal correction to Energy= 1.304981
Thermal correction to Enthalpy= 1.305925
Thermal correction to Gibbs Free Energy= 1.122976
Sum of electronic and zero-point Energies= -3890.767438
Sum of electronic and thermal Energies= -3890.695101
Sum of electronic and thermal Enthalpies= -3890.694156
Sum of electronic and thermal Free Energies= -3890.877105

Cartesian Coordinates

77	-0.258071	-1.003377	-1.600391
15	-1.707836	0.377278	-0.476987
8	-2.262255	0.229991	1.079327
8	-3.183476	0.401724	-1.278653
7	-1.049992	1.897111	-0.366015
6	-3.151057	-0.782980	1.414697
6	-2.638345	-1.828819	2.211178
1	-1.606871	-1.769631	2.530039
6	-3.450798	-2.878935	2.556829
1	-3.067716	-3.686104	3.174913
6	-4.787966	-2.942696	2.078977
6	-5.609913	-4.070127	2.350037
1	-5.201760	-4.872131	2.959742
6	-6.885928	-4.155912	1.840727
1	-7.502363	-5.025575	2.049082
6	-7.388376	-3.112835	1.026929
1	-8.385320	-3.193813	0.603101
6	-6.623890	-1.997242	0.760940
1	-7.023257	-1.214624	0.127085
6	-5.309198	-1.862433	1.289128
6	-4.478153	-0.715166	1.019073
6	-4.996353	0.486911	0.309243
6	-6.151497	1.208602	0.782310
6	-6.779081	0.921417	2.027266
1	-6.373715	0.138862	2.657454
6	-7.880675	1.632790	2.451685
1	-8.334273	1.397705	3.410366
6	-8.422244	2.670416	1.656340
1	-9.295025	3.217727	2.000208
6	-7.826806	2.992028	0.457570
1	-8.217457	3.800376	-0.155060
6	-6.679211	2.290133	-0.000845
6	-6.031598	2.657627	-1.211565
1	-6.445618	3.465771	-1.808108
6	-4.876920	2.028261	-1.600672
1	-4.338589	2.320506	-2.496269
6	-4.351757	0.973608	-0.819142
6	0.148715	2.111636	-1.216443
1	1.013752	2.197582	-0.554054
6	0.003358	3.394741	-2.024843
6	-1.196505	3.669834	-2.700619
1	-2.029870	2.979858	-2.600902
6	-1.327482	4.820402	-3.476607
1	-2.264254	5.023488	-3.989327
6	-0.256115	5.713473	-3.592663
1	-0.357448	6.612150	-4.195031
6	0.939453	5.445438	-2.923715
1	1.773705	6.137752	-3.001833
6	1.069379	4.293448	-2.140547
1	1.992248	4.097566	-1.605067
6	0.385362	0.937047	-2.192850
1	-0.151538	1.149210	-3.123466
1	1.447847	0.960839	-2.435547
6	-1.319415	2.989134	0.628295
1	-0.824707	3.853583	0.178570
6	-0.631801	2.767644	1.973628
6	0.697288	3.183746	2.124832
1	1.225599	3.628895	1.290361
6	1.369749	3.016134	3.337605
1	2.407487	3.326857	3.419967
6	0.707788	2.458640	4.432371
1	1.223445	2.334770	5.381016
6	-0.625817	2.058541	4.298887
1	-1.150618	1.623112	5.145093
6	-1.286642	2.204711	3.078905
1	-2.315056	1.874635	2.990234
6	-2.794144	3.368336	0.742819
1	-3.187034	3.645031	-0.237275
1	-3.410783	2.565625	1.146723
1	-2.887815	4.233159	1.406957
6	-1.659274	-1.027587	-3.360454
1	-1.864472	0.013251	-3.595992
6	-0.402726	-1.519124	-3.783974
1	0.243541	-0.817878	-4.310766
6	-0.089499	-2.969539	-4.104269
1	-0.426090	-3.192836	-5.128224

1	0.997821	-3.085545	-4.112838
6	-0.698168	-4.005865	-3.133657
1	-1.700989	-4.286726	-3.467986
1	-0.096093	-4.919288	-3.175281
6	-0.774941	-3.549673	-1.689308
1	-0.015955	-3.939180	-1.022725
6	-1.866518	-2.947400	-1.127459
1	-1.923835	-2.908311	-0.043543
6	-3.132024	-2.602437	-1.882432
1	-3.746158	-1.971559	-1.242308
1	-3.703309	-3.528884	-2.040309
6	-2.919187	-1.888935	-3.240142
1	-2.912613	-2.623708	-4.052707
1	-3.785481	-1.246041	-3.417969
6	2.473743	-1.457032	-2.147051
6	1.743489	-1.872574	-1.018431
1	1.708243	-2.945209	-0.882047
6	1.268279	-1.014737	0.032620
1	1.681072	-0.011618	0.065209
6	0.968938	-1.554735	1.384945
6	0.752489	-2.921384	1.646169
6	0.945998	-0.668038	2.477353
6	0.536619	-3.384707	2.943869
1	0.760334	-3.639444	0.834686
6	0.731509	-1.131818	3.776665
1	1.123608	0.387923	2.304445
6	0.527713	-2.492557	4.020305
1	0.376179	-4.446237	3.113459
1	0.728852	-0.422516	4.597601
1	0.362494	-2.852171	5.032014
8	3.912581	-4.000331	-1.718042
6	4.644770	-3.036837	-1.499204
8	4.428938	-1.788918	-1.764651
8	5.871589	-3.191043	-0.895237
6	6.203466	-4.528622	-0.511756
1	6.229265	-5.198778	-1.377068
1	7.196099	-4.473151	-0.059001
1	5.486964	-4.924460	0.215611
6	6.882241	0.850621	-1.444893
6	8.197830	1.238138	-0.787840
1	6.260192	1.726895	-1.651079
1	7.040470	0.311449	-2.382773
6	7.926456	1.717959	0.632285
1	8.689091	2.035635	-1.351786
1	8.872555	0.375362	-0.766084
1	8.867448	1.873247	1.165817
1	7.371315	2.662050	0.625028
7	6.142550	-0.028821	-0.546298
6	6.238183	-0.031463	0.770220
7	7.137441	0.733903	1.404077
6	5.285695	-0.975465	1.478968
1	4.540867	-1.261923	0.735952
1	5.831148	-1.890605	1.737295
6	4.579175	-0.386556	2.710887
1	4.327106	0.655457	2.502551
6	7.121836	1.021595	2.855844
6	5.406639	-0.511041	3.995042
1	4.990199	0.162009	4.754405
6	6.889812	-0.183654	3.770837
1	7.369788	0.028905	4.732372
1	7.421261	-1.044847	3.349150
1	8.105839	1.443171	3.070901
1	6.383489	1.811831	3.040345
1	5.323687	-1.528208	4.397681
1	3.623788	-0.902810	2.835064
1	5.467076	-0.681404	-0.980262
5	3.772115	2.497690	0.197305
9	4.997736	2.526873	0.891520
9	3.967959	2.081085	-1.132828
9	3.210958	3.792464	0.209081
9	2.896910	1.596639	0.841500
1	2.542142	-2.126307	-2.991405
1	2.681757	-0.413068	-2.325166

[12-13]‡ P2 *endo-si* conf2 [BF_4^-]

Number of imaginary frequencies : 1
The smallest frequency is : -253.4738 cm(-1)
Electronic energy=-3892.0090717
Zero-point correction= 1.233359
(Hartree/Particle)
Thermal correction to Energy= 1.305517
Thermal correction to Enthalpy= 1.306461
Thermal correction to Gibbs Free Energy= 1.124599
Sum of electronic and zero-point Energies= -3890.775712
Sum of electronic and thermal Energies= -3890.703555
Sum of electronic and thermal Enthalpies= -3890.702611
Sum of electronic and thermal Free Energies= -3890.884473

.....

Cartesian Coordinates

.....

77	-0.340824	-0.762008	-1.656276
15	-1.861696	0.404244	-0.375316
8	-2.361907	0.054162	1.170997
8	-3.360287	0.456400	-1.133758
7	-1.245725	1.929722	-0.111420
6	-3.205184	-1.026925	1.389104
6	-2.640669	-2.162813	2.010790
1	-1.597903	-2.127917	2.305638
6	-3.417469	-3.275337	2.220572
1	-2.998281	-4.155360	2.700069
6	-4.768727	-3.304866	1.780818
6	-5.556170	-4.480700	1.913588
1	-5.107923	-5.352821	2.382475
6	-6.850318	-4.522555	1.446556
1	-7.440418	-5.428753	1.547565
6	-7.408133	-3.383681	0.817791
1	-8.421442	-3.426450	0.428782
6	-6.676959	-2.222869	0.687249
1	-7.117589	-1.364624	0.193827
6	-5.343080	-2.135809	1.175962
6	-4.545300	-0.944132	1.042917
6	-5.103159	0.335787	0.523894
6	-6.235832	0.978053	1.139653
6	-6.823323	0.506655	2.347675
1	-6.404670	-0.364081	2.837874
6	-7.905684	1.146836	2.911320
1	-8.329804	0.768865	3.837286
6	-8.465653	2.294432	2.301040
1	-9.322951	2.784475	2.753305
6	-7.909025	2.792736	1.144868
1	-8.315550	3.684447	0.674396
6	-6.782944	2.165304	0.545721
6	-6.178586	2.705329	-0.621348
1	-6.607729	3.594203	-1.075160
6	-5.048722	2.133330	-1.149973
1	-4.551282	2.548244	-2.020099
6	-4.504947	0.973097	-0.554115
6	-0.096392	2.281063	-0.991611
1	0.812638	2.273828	-0.383416
6	-0.275429	3.672148	-1.585838
6	-1.523049	4.078486	-2.083501
1	-2.371925	3.408199	-1.988392
6	-1.678632	5.330607	-2.677373
1	-2.652857	5.633903	-3.052048
6	-0.584737	6.195797	-2.786361
1	-0.704378	7.172482	-3.247299
6	0.659839	5.797764	-2.294169
1	1.513652	6.466114	-2.368421
6	0.814544	4.544705	-1.693148

1	1.779022	4.244976	-1.297670
6	0.060609	1.262176	-2.135849
1	-0.629914	1.543731	-2.938816
1	1.067475	1.359056	-2.542628
6	-1.427790	2.828136	1.075748
1	-0.977757	3.768029	0.745268
6	-0.613899	2.370302	2.285269
6	0.739860	2.727245	2.366134
1	1.196133	3.317329	1.578493
6	1.524669	2.337790	3.454180
1	2.569264	2.628718	3.474774
6	0.961815	1.586819	4.487657
1	1.565908	1.286308	5.339609
6	-0.389569	1.234047	4.425381
1	-0.840531	0.658601	5.229766
6	-1.169922	1.624979	3.335741
1	-2.216143	1.345225	3.305964
6	-2.889805	3.149265	1.381306
1	-3.366250	3.586752	0.501546
1	-3.465379	2.273692	1.680667
1	-2.931900	3.879626	2.195401
6	0.848779	-1.530863	0.765685
1	0.447988	-2.508333	0.560545
1	0.488596	-1.026888	1.654553
6	1.431457	-0.741515	-0.251342
1	1.765059	0.245034	0.050079
6	1.859012	-1.276554	-1.518040
1	1.909834	-2.358391	-1.580273
6	-1.701715	-0.823055	-3.382465
1	-2.046496	0.191061	-3.568690
6	-0.374798	-1.116880	-3.815312
1	0.169836	-0.305748	-4.299158
6	0.123415	-2.487533	-4.234285
1	-0.172390	-2.680395	-5.277000
1	1.215428	-2.452238	-4.230255
6	-0.345034	-3.657660	-3.340585
1	-1.292967	-4.059336	-3.710445
1	0.382064	-4.472436	-3.421746
6	-0.500840	-3.303809	-1.871956
1	0.292361	-3.634715	-1.207461
6	-1.671395	-2.878313	-1.297346
1	-1.745207	-2.931529	-0.215784
6	-2.975018	-2.631133	-2.025175
1	-3.625738	-2.069198	-1.354956
1	-3.471741	-3.595769	-2.205454
6	-2.837187	-1.850763	-3.350356
1	-2.707238	-2.543282	-4.188705
1	-3.779676	-1.326692	-3.534248
6	2.899076	-0.616472	-2.339310
6	3.329824	0.707646	-2.130745
6	3.541355	-1.361023	-3.348588
6	4.342321	1.266271	-2.909689
1	2.907834	1.302583	-1.333484
6	4.548142	-0.800130	-4.134948
1	3.260402	-2.400238	-3.499120
6	4.953042	0.521343	-3.921810
1	4.671279	2.278269	-2.693195
1	5.026459	-1.400246	-4.904567
1	5.744984	0.957221	-4.524367
8	2.019129	-4.194053	0.334965
6	2.633765	-3.590248	1.217747
8	2.335989	-2.466175	1.781828
8	3.802920	-4.092214	1.734942
6	4.278924	-5.297198	1.124240
1	3.544343	-6.103857	1.207299
1	5.189259	-5.568450	1.663315
1	4.510411	-5.139135	0.065711
6	4.164140	-0.360174	4.040203
6	5.436628	0.196428	4.657157
1	3.449427	0.439514	3.823679
1	3.675648	-1.085333	4.696838
6	6.197856	0.986698	3.600086
1	5.198162	0.851455	5.499473
1	6.061063	-0.622410	5.031097
1	7.176987	1.283241	3.981831
1	5.650520	1.889602	3.312927
7	4.492961	-1.033949	2.789828
6	5.513493	-0.722033	2.004201
7	6.424966	0.179928	2.377805
6	5.560106	-1.491288	0.697487
1	4.534829	-1.812862	0.515428
1	6.143211	-2.406113	0.859098
6	6.067392	-0.720353	-0.527136
1	5.667233	0.293764	-0.492338
6	7.543284	0.672019	1.535621
6	7.594380	-0.691119	-0.636726
1	7.880693	0.073666	-1.368702
6	8.265596	-0.397027	0.712262
1	9.293251	-0.054942	0.547944
1	8.341616	-1.308093	1.318108
1	8.252230	1.110569	2.240419
1	7.165690	1.483044	0.903600
1	7.965623	-1.649638	-1.020840
1	5.639797	-1.182311	-1.421232
1	3.755325	-1.639615	2.399368
5	4.091115	2.519146	0.827401
9	5.262154	2.537939	0.046007
9	4.322473	3.188423	2.046120
9	3.049384	3.167253	0.122835
9	3.704241	1.191047	1.085427

P1 *endo-re* [BF_4^-]

Number of imaginary frequencies : 0
The smallest frequency is : 12.8582 cm(-1)
Electronic energy=-3125.4962645
Zero-point correction= 0.914550
(Hartree/Particle)
Thermal correction to Energy= 0.969328
Thermal correction to Enthalpy= 0.970272
Thermal correction to Gibbs Free Energy= 0.825821
Sum of electronic and zero-point Energies= -3124.581715
Sum of electronic and thermal Energies= -3124.526937
Sum of electronic and thermal Enthalpies= -3124.525992
Sum of electronic and thermal Free Energies= -3124.670443

.....

Cartesian Coordinates

.....

77	-1.143406	-1.367048	-0.238216
15	0.592702	0.095956	-0.137958
8	1.640024	0.205066	1.122888
8	1.656429	-0.181158	-1.389421
7	-0.010229	1.640208	-0.135852
6	2.710553	-0.662991	1.298692
6	2.649576	-1.504939	2.430322
1	1.803104	-1.404964	3.101529
6	3.654405	-2.414019	2.650767
1	3.624957	-3.065077	3.519806
6	4.729562	-2.537922	1.729272
6	5.727925	-3.535636	1.897440
1	5.665549	-4.190241	2.762757
6	6.743294	-3.682207	0.979527
1	7.497265	-4.452239	1.114117
6	6.795451	-2.835000	-0.152940
1	7.583765	-2.968191	-0.888294
6	5.853002	-1.846438	-0.336447
1	5.904764	-1.214106	-1.214821
6	4.800355	-1.652645	0.601224
6	3.791706	-0.638219	0.431518
6	3.874576	0.388027	-0.644230
6	5.010146	1.265829	-0.771956
6	6.063035	1.303712	0.184742
1	6.016499	0.655882	1.051763

6	7.129281	2.163814	0.035320
1	7.915619	2.178648	0.784603
6	7.207109	3.032894	-1.078979
1	8.057010	3.700418	-1.186349
6	6.194854	3.040466	-2.011463
1	6.229551	3.716952	-2.861430
6	5.072453	2.178609	-1.878527
6	4.001733	2.223850	-2.811408
1	4.064760	2.904807	-3.655308
6	2.885841	1.445619	-2.630138
1	2.044281	1.486475	-3.312160
6	2.824829	0.561694	-1.531820
6	-1.422806	1.723442	-0.608625
1	-2.058174	1.905488	0.258410
6	-1.584402	2.884713	-1.580040
6	-2.547015	3.876372	-1.354980
1	-3.175415	3.820868	-0.473412
6	-2.684972	4.939893	-2.253010
1	-3.433181	5.705369	-2.065242
6	-1.863306	5.025988	-3.378003
1	-1.969961	5.855755	-4.071438
6	-0.894966	4.041449	-3.603861
1	-0.245000	4.104260	-4.472714
6	-0.758639	2.980494	-2.710074
1	0.001388	2.224137	-2.876975
6	-1.845481	0.394193	-1.251427
1	-1.479506	0.352166	-2.282386
1	-2.935751	0.358775	-1.294089
6	0.479346	2.828685	0.650017
1	-0.193978	3.625722	0.323355
6	0.250778	2.649123	2.150128
6	-1.046325	2.804976	2.659307
1	-1.854307	3.128278	2.014144
6	-1.325805	2.558796	4.005405
1	-2.349326	2.652126	4.353498
6	-0.299999	2.185772	4.875660
1	-0.511476	1.995687	5.924555
6	1.006040	2.071336	4.388800
1	1.816194	1.798307	5.060119
6	1.277231	2.298542	3.038378
1	2.292887	2.184446	2.677120
6	1.887350	3.262425	0.253282
1	1.928429	3.446655	-0.822401
1	2.644945	2.518700	0.499929
1	2.139193	4.190316	0.776166
6	-1.568277	-0.844508	1.838847
1	-1.288653	-1.697142	2.456207
1	-1.203245	0.106353	2.216910
6	-2.862544	-0.820405	1.219203
1	-3.300571	0.144262	0.995674
6	-3.513452	-1.977838	0.789035
1	-3.190436	-2.927945	1.198949
6	-0.395876	-2.135319	-2.251574
1	-0.199188	-1.241114	-2.833938
6	-1.737120	-2.518689	-2.114060
1	-2.490592	-1.900936	-2.600754
6	-2.202931	-3.921825	-1.777671
1	-2.151491	-4.536090	-2.688692
1	-3.259595	-3.863037	-1.511942
6	-1.429968	-4.626582	-0.636242
1	-0.609666	-5.223318	-1.047303
1	-2.105788	-5.336642	-0.149830
6	-0.862587	-3.701035	0.431413
1	-1.338868	-3.734999	1.407015
6	0.393948	-3.137661	0.377410
1	0.818466	-2.789486	1.313577
6	1.376645	-3.304376	-0.761925
1	2.182499	-2.584479	-0.620799
1	1.834151	-4.300714	-0.682620
6	0.773521	-3.114737	-2.172080
1	0.445781	-4.077626	-2.576059
1	1.563804	-2.755747	-2.836747
6	-4.761883	-2.038592	0.026956
6	-5.399234	-0.904694	-0.517642
6	-5.358231	-3.301254	-0.171231
6	-6.577667	-1.042709	-1.247879
1	-4.996882	0.085964	-0.347097
6	-6.537502	-3.433866	-0.901620
1	-4.888481	-4.182400	0.258963
6	-7.149365	-2.303485	-1.449600
1	-7.057283	-0.157180	-1.655470
1	-6.979074	-4.416643	-1.040634
1	-8.068452	-2.401647	-2.020256
5	-4.625540	2.553491	1.657912
9	-4.394765	1.975914	0.374436
9	-5.997009	2.685133	1.868376
9	-4.051506	1.722915	2.638004
9	-3.997421	3.815990	1.686558

P1 *exo-si* [BF_4^-]

Number of imaginary frequencies : 0
The smallest frequency is : 13.3872 cm(-1)
Electronic energy=-3125.4910399
Zero-point correction= 0.914402
(Hartree/Particle)
Thermal correction to Energy= 0.969248
Thermal correction to Enthalpy= 0.970192
Thermal correction to Gibbs Free Energy= 0.825039
Sum of electronic and zero-point Energies= -3124.576637
Sum of electronic and thermal Energies= -3124.521792
Sum of electronic and thermal Enthalpies= -3124.520848
Sum of electronic and thermal Free Energies= -3124.666001

Cartesian Coordinates

77	-1.255554	-1.046700	-0.340122
15	0.607243	0.237829	-0.139153
8	1.624092	0.193146	1.154207
8	1.683399	-0.076388	-1.371409
7	0.151698	1.834617	-0.082783
6	2.552362	-0.829340	1.316434
6	2.317362	-1.727555	2.379469
1	1.453394	-1.561149	3.014056
6	3.183937	-2.772873	2.583121
1	3.022778	-3.468400	3.401733
6	4.284330	-2.978158	1.707122
6	5.138539	-4.104473	1.856834
1	4.947237	-4.793871	2.675055
6	6.175119	-4.327779	0.979186
1	6.818104	-5.194733	1.099212
6	6.393561	-3.431317	-0.094060
1	7.196681	-3.623194	-0.799755
6	5.594782	-2.320394	-0.257274
1	5.772423	-1.651062	-1.090417
6	4.527677	-2.044920	0.642825
6	3.667077	-0.898883	0.496393
6	3.923750	0.161771	-0.516833
6	5.166955	0.888141	-0.561609
6	6.174098	0.746978	0.434057
1	6.007258	0.075790	1.268124
6	7.349502	1.462881	0.363539
1	8.098320	1.342646	1.141216
6	7.588154	2.358606	-0.705902
1	8.522176	2.910863	-0.751279
6	6.626524	2.537993	-1.674195
1	6.786332	3.237472	-2.490597
6	5.396087	1.828288	-1.622341
6	4.382180	2.049173	-2.593018
1	4.570904	2.744701	-3.405775
6	3.167626	1.418400	-2.488425
1	2.370795	1.591749	-3.202895
6	2.942413	0.509854	-1.431864
6	-1.242003	2.080790	-0.535795
1	-1.847879	2.326429	0.338245
6	-1.308310	3.248551	-1.510985
6	-2.386001	4.141925	-1.464008
1	-3.141550	4.023570	-0.695604
6	-2.479317	5.181189	-2.393962
1	-3.319008	5.869455	-2.345394

6	-1.498216	5.342903	-3.374844
1	-1.570803	6.155022	-4.093138
6	-0.417162	4.457019	-3.421848
1	0.355958	4.578808	-4.176160
6	-0.325674	3.416777	-2.496903
1	0.518712	2.736472	-2.522320
6	-1.833144	0.826938	-1.192831
1	-1.514383	0.799464	-2.240298
1	-2.916970	0.924984	-1.183406
6	0.740812	2.942985	0.750535
1	0.217015	3.826887	0.376310
6	0.361647	2.797294	2.223519
6	-0.914515	3.205241	2.640475
1	-1.600227	3.667932	1.939504
6	-1.337257	3.012719	3.957412
1	-2.341992	3.311897	4.241111
6	-0.475084	2.437264	4.892145
1	-0.798229	2.289505	5.919079
6	0.814275	2.065479	4.499037
1	1.501437	1.634579	5.222705
6	1.226978	2.242002	3.177082
1	2.225979	1.935505	2.890271
6	2.224657	3.179805	0.482264
1	2.387493	3.353668	-0.583647
1	2.852933	2.344447	0.790049
1	2.547785	4.069188	1.031999
6	-1.616578	-0.321375	1.728000
1	-0.858593	-0.560792	2.469023
1	-1.889101	0.726198	1.688920
6	-2.640522	-1.290627	1.511440
1	-2.540478	-2.258725	1.991221
6	-3.661638	-1.071967	0.586403
1	-3.866706	-0.044663	0.311373
6	-0.582521	-1.659501	-2.405807
1	-0.329805	-0.731267	-2.908663
6	-1.953607	-1.956260	-2.297842
1	-2.649207	-1.230715	-2.717672
6	-2.538998	-3.346165	-2.160992
1	-2.591592	-3.802096	-3.160827
1	-3.570673	-3.247278	-1.820413
6	-1.781198	-4.293303	-1.204829
1	-1.002185	-4.836677	-1.747278
1	-2.485647	-5.046225	-0.838552
6	-1.150294	-3.614607	-0.003450
1	-1.674676	-3.728033	0.938191
6	0.136525	-3.147481	0.042484
1	0.568033	-2.944504	1.018273
6	1.106515	-3.172336	-1.117790
1	1.950053	-2.531262	-0.864812
1	1.509788	-4.190358	-1.214866
6	0.521224	-2.715463	-2.474835
1	0.134892	-3.576328	-3.029917
1	1.340190	-2.306999	-3.072477
6	-4.687049	-2.035151	0.184115
6	-4.716235	-3.377980	0.610643
6	-5.683235	-1.593118	-0.708339
6	-5.698747	-4.247789	0.143983
1	-3.969436	-3.747341	1.305587
6	-6.663384	-2.466638	-1.176480
1	-5.680098	-0.552430	-1.021937
6	-6.671714	-3.799504	-0.756547
1	-5.706825	-5.280129	0.482517
1	-7.422028	-2.106538	-1.865526
1	-7.433594	-4.482781	-1.120592
5	-4.582637	2.544256	1.343808
9	-3.851638	3.754182	1.390241
9	-3.973220	1.609828	2.202485
9	-5.905690	2.768378	1.726946
9	-4.550366	2.042617	0.015410

P1 *exo-re* [BF_4^-]

Number of imaginary frequencies : 0
The smallest frequency is : 17.8007 cm(-1)
Electronic energy=-3125.4892174
Zero-point correction= 0.915265
(Hartree/Particle)
Thermal correction to Energy= 0.969867
Thermal correction to Enthalpy= 0.970811
Thermal correction to Gibbs Free Energy= 0.828279
Sum of electronic and zero-point Energies= -3124.573952
Sum of electronic and thermal Energies= -3124.519351
Sum of electronic and thermal Enthalpies= -3124.518407
Sum of electronic and thermal Free Energies= -3124.660938

Cartesian Coordinates

77	-1.181172	-1.486648	-1.252955
15	0.155142	0.229926	-0.396493
8	1.030573	0.254436	1.002055
8	1.372813	0.544092	-1.494701
7	-0.800702	1.554276	-0.120061
6	2.214055	-0.470110	1.122365
6	2.176766	-1.571634	2.001097
1	1.260611	-1.762303	2.542180
6	3.291391	-2.357105	2.151881
1	3.275179	-3.204023	2.832081
6	4.466604	-2.090666	1.398429
6	5.598385	-2.946631	1.479265
1	5.555106	-3.798874	2.152364
6	6.718953	-2.712769	0.714779
1	7.576262	-3.376307	0.780565
6	6.745456	-1.611829	-0.173977
1	7.619823	-1.443907	-0.796213
6	5.671671	-0.752435	-0.262757
1	5.709227	0.078904	-0.956497
6	4.505880	-0.947382	0.530055
6	3.361767	-0.072528	0.453825
6	3.384464	1.188747	-0.337003
6	4.373810	2.212537	-0.112587
6	5.302757	2.159880	0.964483
1	5.269098	1.326203	1.655554
6	6.233646	3.158674	1.151960
1	6.925159	3.097260	1.987462
6	6.293053	4.266387	0.273324
1	7.036833	5.042265	0.429343
6	5.394437	4.362976	-0.764836
1	5.413089	5.218180	-1.435507
6	4.410254	3.359346	-0.975807
6	3.448008	3.486010	-2.013932
1	3.491926	4.348533	-2.672831
6	2.452626	2.552539	-2.157906
1	1.681263	2.647960	-2.914748
6	2.414258	1.434046	-1.296547
6	-2.164821	1.457662	-0.694716
1	-2.869299	1.279905	0.118694
6	-2.557106	2.742748	-1.411002
6	-3.848071	3.262937	-1.261834
1	-4.542261	2.774442	-0.585271
6	-4.228879	4.410183	-1.964737
1	-5.232607	4.807517	-1.839682
6	-3.324516	5.049701	-2.815105
1	-3.620912	5.944512	-3.355590
6	-2.031069	4.536701	-2.962261
1	-1.318982	5.032734	-3.616684
6	-1.652150	3.388808	-2.267329
1	-0.645391	2.993280	-2.371395
6	-2.262273	0.302058	-1.698011
1	-1.868365	0.645708	-2.659671
1	-3.321401	0.096373	-1.836273
6	-0.601994	2.685236	0.850548
1	-1.356696	3.407212	0.530387
6	-0.956816	2.327107	2.291237
6	-2.299431	2.386317	2.690939
1	-3.075028	2.624178	1.970955
6	-2.666418	2.135110	4.015018
1	-3.715709	2.171137	4.292335
6	-1.689557	1.839185	4.967204
1	-1.969348	1.654879	6.000876
6	-0.347930	1.775516	4.579049

1	0.419612	1.538914	5.311023
6	0.014107	2.010621	3.252054
1	1.058834	1.951876	2.969028
6	0.740373	3.396387	0.700736
1	0.867491	3.743327	-0.326054
1	1.590260	2.765121	0.957752
1	0.753717	4.267734	1.362541
6	-3.267377	-2.452801	-1.308640
1	-3.935615	-1.608142	-1.411310
1	-3.456239	-3.286841	-1.976321
6	-2.675075	-2.742627	-0.066638
1	-2.380813	-3.768839	0.123561
6	-2.235737	-1.743516	0.835658
1	-2.809285	-0.826978	0.900658
6	-0.098613	-1.200136	-3.219460
1	-0.151983	-0.135847	-3.426586
6	-1.272986	-1.936210	-3.466207
1	-2.131717	-1.380388	-3.838581
6	-1.316397	-3.415318	-3.796005
1	-1.074435	-3.535447	-4.861986
1	-2.346884	-3.759969	-3.680512
6	-0.379578	-4.307313	-2.951297
1	0.600601	-4.382560	-3.430475
1	-0.788637	-5.321987	-2.933227
6	-0.186413	-3.846296	-1.517255
1	-0.724258	-4.406791	-0.762105
6	0.829315	-3.026059	-1.099398
1	1.046458	-2.983784	-0.035230
6	1.868494	-2.427445	-2.021943
1	2.426066	-1.677890	-1.464264
1	2.587401	-3.215960	-2.285707
6	1.311095	-1.784087	-3.313625
1	1.321679	-2.509883	-4.133092
1	1.987828	-0.978237	-3.606767
6	-1.521939	-2.133423	2.076089
6	-0.821903	-3.349297	2.205882
6	-1.596146	-1.286443	3.193255
6	-0.243915	-3.717050	3.419383
1	-0.712448	-4.015070	1.357104
6	-1.007060	-1.651307	4.405184
1	-2.145241	-0.355789	3.114677
6	-0.333552	-2.868237	4.527519
1	0.288061	-4.661392	3.496337
1	-1.083656	-0.980178	5.254315
1	0.120349	-3.151880	5.472807
5	-5.313314	0.484511	1.298851
9	-4.872086	0.058579	0.017412
9	-6.637685	0.088805	1.492278
9	-4.482097	-0.085402	2.281156
9	-5.212647	1.893892	1.363578

P1 *endo-si* [BF_4^-]

Number of imaginary frequencies : 0
The smallest frequency is : 14.5966 cm(-1)
Electronic energy=-3125.4843546
Zero-point correction= 0.914562
(Hartree/Particle)
Thermal correction to Energy= 0.969392
Thermal correction to Enthalpy= 0.970337
Thermal correction to Gibbs Free Energy= 0.825586
Sum of electronic and zero-point Energies= -3124.569793
Sum of electronic and thermal Energies= -3124.514962
Sum of electronic and thermal Enthalpies= -3124.514018
Sum of electronic and thermal Free Energies= -3124.658769

Cartesian Coordinates

77	1.000990	-1.587439	-1.276688
15	-0.178764	0.300072	-0.437323
8	-1.012170	0.450911	0.990685
8	-1.399511	0.690108	-1.512200
7	0.912374	1.530843	-0.240434
6	-2.165137	-0.310488	1.161110
6	-2.072186	-1.398999	2.053246
1	-1.140347	-1.549109	2.582314
6	-3.153330	-2.225635	2.229081
1	-3.095929	-3.062903	2.918954
6	-4.347102	-2.016078	1.485839
6	-5.440594	-2.918380	1.586624
1	-5.355807	-3.759898	2.269296
6	-6.575785	-2.742907	0.827909
1	-7.402756	-3.442390	0.908142
6	-6.656822	-1.655397	-0.073981
1	-7.542095	-1.533845	-0.691581
6	-5.621877	-0.751626	-0.181799
1	-5.698905	0.068938	-0.885140
6	-4.442770	-0.887090	0.603292
6	-3.334686	0.029869	0.500333
6	-3.409369	1.277704	-0.308973
6	-4.433373	2.267422	-0.082823
6	-5.345297	2.192867	1.007468
1	-5.268833	1.371050	1.709281
6	-6.313125	3.156175	1.194826
1	-6.990965	3.077955	2.040096
6	-6.428054	4.249032	0.303387
1	-7.200111	4.996787	0.459420
6	-5.547473	4.366874	-0.748074
1	-5.609032	5.211454	-1.429586
6	-4.528176	3.399441	-0.960412
6	-3.587897	3.547103	-2.015902
1	-3.674746	4.397706	-2.686023
6	-2.562529	2.648582	-2.164860
1	-1.808855	2.761903	-2.937031
6	-2.464899	1.542847	-1.290326
6	2.275715	1.269990	-0.778472
1	2.942202	1.088723	0.065762
6	2.779918	2.473703	-1.566401
6	4.090762	2.934632	-1.401112
1	4.735153	2.455116	-0.673120
6	4.558133	4.012557	-2.160094
1	5.576867	4.364173	-2.019727
6	3.723128	4.640789	-3.085796
1	4.087443	5.481855	-3.669377
6	2.410818	4.184720	-3.253548
1	1.751518	4.670925	-3.967904
6	1.945318	3.107265	-2.501306
1	0.923213	2.758075	-2.622459
6	2.309592	0.042272	-1.703586
1	2.058624	0.373987	-2.715634
1	3.343048	-0.304120	-1.723455
6	0.793980	2.761057	0.610335
1	1.601711	3.394846	0.237684
6	1.108281	2.522537	2.085413
6	2.450189	2.467371	2.490964
1	3.248726	2.526455	1.759018
6	2.787597	2.352002	3.841023
1	3.834948	2.304012	4.124931
6	1.784474	2.315769	4.811888
1	2.043062	2.248980	5.865335
6	0.443631	2.351948	4.417814
1	-0.344563	2.309509	5.164907
6	0.109181	2.446622	3.065935
1	-0.935950	2.474160	2.778171
6	-0.493043	3.544429	0.363807
1	-0.574883	3.801195	-0.694112
1	-1.390455	2.999270	0.656422
1	-0.460287	4.473391	0.940919
6	2.810653	-2.793300	-1.123627
1	3.645330	-2.429675	-1.717573
1	2.609594	-3.851752	-1.268798
6	2.678345	-2.263186	0.215775
1	3.284905	-1.423765	0.539919
6	1.735719	-2.831414	1.067744
1	1.289497	-3.760636	0.729718
6	0.042225	-1.199155	-3.220914
1	0.182805	-0.147713	-3.454677
6	1.179502	-2.030177	-3.423461
1	2.079077	-1.539531	-3.791253
6	1.131447	-3.505261	-3.766075

1	0.935804	-3.607199	-4.843576
1	2.128015	-3.922331	-3.596598
6	0.092423	-4.313297	-2.962142
1	-0.872641	-4.307965	-3.475992
1	0.411413	-5.359282	-2.923010
6	-0.101084	-3.819589	-1.538189
1	0.379874	-4.415190	-0.770256
6	-1.075857	-2.930316	-1.149243
1	-1.330760	-2.878083	-0.093849
6	-2.050140	-2.275042	-2.105163
1	-2.572266	-1.487136	-1.565872
1	-2.811323	-3.015056	-2.390015
6	-1.405851	-1.671781	-3.375540
1	-1.442646	-2.391001	-4.200416
1	-2.007688	-0.814406	-3.685728
6	1.378466	-2.500830	2.437674
6	1.803911	-1.340231	3.112040
6	0.568262	-3.432316	3.123761
6	1.433300	-1.136738	4.438287
1	2.428202	-0.612943	2.608866
6	0.197409	-3.219300	4.448284
1	0.231886	-4.326396	2.604817
6	0.630605	-2.066492	5.108598
1	1.770482	-0.243603	4.949616
1	-0.425016	-3.946135	4.961962
1	0.345698	-1.891176	6.142144
5	5.438129	0.365646	1.181763
9	5.436338	1.770298	1.328331
9	4.457229	-0.183137	2.037559
9	6.695371	-0.150613	1.496868
9	5.103289	0.035548	-0.153602

P2 *endo-si* [BF_4^-]

Number of imaginary frequencies : 0
The smallest frequency is : 12.9605 cm(-1)
Electronic energy=-3125.4962636
Zero-point correction= 0.914550
(Hartree/Particle)
Thermal correction to Energy= 0.969328
Thermal correction to Enthalpy= 0.970273
Thermal correction to Gibbs Free Energy= 0.825831
Sum of electronic and zero-point Energies= -3124.581713
Sum of electronic and thermal Energies= -3124.526935
Sum of electronic and thermal Enthalpies= -3124.525991
Sum of electronic and thermal Free Energies= -3124.670432

Cartesian Coordinates

77	1.143753	-1.367025	-0.238186
15	-0.592515	0.095860	-0.137981
8	-1.639828	0.204811	1.122880
8	-1.656212	-0.181415	-1.389414
7	0.010195	1.640202	-0.135972
6	-2.710391	-0.663213	1.298616
6	-2.649453	-1.505158	2.430252
1	-1.802996	-1.405183	3.101477
6	-3.654307	-2.414207	2.650702
1	-3.624891	-3.065246	3.519755
6	-4.729454	-2.538093	1.729193
6	-5.727848	-3.535774	1.897372
1	-5.665505	-4.190354	2.762710
6	-6.743205	-3.682342	0.979446
1	-7.497202	-4.452347	1.114045
6	-6.795310	-2.835170	-0.153049
1	-7.583607	-2.968363	-0.888419
6	-5.852828	-1.846639	-0.336564
1	-5.904556	-1.214338	-1.214962
6	-4.800200	-1.652837	0.601126
6	-3.791533	-0.638424	0.431422
6	-3.874376	0.387808	-0.644346
6	-5.009955	1.265581	-0.772180
6	-6.062914	1.303469	0.184440
1	-6.016415	0.655682	1.051496
6	-7.129194	2.163507	0.034889
1	-7.915591	2.178340	0.784110
6	-7.206980	3.032520	-1.079464
1	-8.056910	3.699989	-1.186941
6	-6.194648	3.040102	-2.011865
1	-6.229313	3.716542	-2.861870
6	-5.072212	2.178310	-1.878797
6	-4.001415	2.223575	-2.811590
1	-4.064396	2.904518	-3.655505
6	-2.885510	1.445386	-2.630210
1	-2.043865	1.486277	-3.312129
6	-2.824587	0.561463	-1.531888
6	1.422830	1.723561	-0.608565
1	2.058060	1.905755	0.258528
6	1.584374	2.884763	-1.580074
6	2.546691	3.876680	-1.354934
1	3.174844	3.821485	-0.473174
6	2.684659	4.940064	-2.253126
1	3.432646	5.705743	-2.065297
6	1.863289	5.025758	-3.378366
1	1.969956	5.855413	-4.071933
6	0.895230	4.040957	-3.604306
1	0.245495	4.103450	-4.473355
6	0.758899	2.980143	-2.710353
1	-0.000912	2.223575	-2.877325
6	1.845808	0.394335	-1.251204
1	1.480138	0.352198	-2.282263
1	2.936094	0.359107	-1.293574
6	-0.479517	2.828576	0.649977
1	0.193962	3.625625	0.323654
6	-0.251476	2.648792	2.150147
6	1.045508	2.804088	2.659778
1	1.853921	3.126983	2.014958
6	1.324442	2.557754	4.005974
1	2.347929	2.650604	4.354352
6	0.298189	2.185163	4.875884
1	0.509227	1.994969	5.924847
6	-1.007724	2.071237	4.388555
1	-1.818224	1.798509	5.059579
6	-1.278356	2.298566	3.038042
1	-2.293932	2.184845	2.676440
6	-1.887394	3.262417	0.252885
1	-1.928154	3.446835	-0.822773
1	-2.645054	2.518633	0.499160
1	-2.139414	4.190211	0.775855
6	1.568350	-0.844465	1.839002
1	1.288474	-1.697124	2.456209
1	1.203290	0.106416	2.216984
6	2.862666	-0.820336	1.219535
1	3.300652	0.144375	0.996049
6	3.513615	-1.977727	0.789261
1	3.190687	-2.927867	1.199154
6	0.396198	-2.135021	-2.251670
1	0.199360	-1.240742	-2.833863
6	1.737492	-2.518222	-2.114263
1	2.490883	-1.900320	-2.600889
6	2.203391	-3.921397	-1.778132
1	2.151666	-4.535568	-2.689198
1	3.260136	-3.862630	-1.512736
6	1.430737	-4.626258	-0.636545
1	0.610588	-5.223295	-1.047481
1	2.106810	-5.336065	-0.150118
6	0.863152	-3.700821	0.431121
1	1.339276	-3.734982	1.406797
6	-0.393481	-3.137621	0.377170
1	-0.818106	-2.789695	1.313388
6	-1.376159	-3.304438	-0.762162
1	-2.182148	-2.584699	-0.621003
1	-1.833471	-4.300870	-0.682905
6	-0.773046	-3.114622	-2.172290
1	-0.445157	-4.077439	-2.576314
1	-1.563359	-2.755703	-2.836958
6	4.762073	-2.038334	0.027214
6	5.399473	-0.904309	-0.517047
6	5.358415	-3.300954	-0.171258
6	6.577940	-1.042152	-1.247263

1	4.997108	0.086313	-0.346306
6	6.537723	-3.433397	-0.901615
1	4.888638	-4.182199	0.258705
6	7.149630	-2.302884	-1.449279
1	7.057587	-0.156527	-1.654608
1	6.979294	-4.416144	-1.040847
1	8.068746	-2.400914	-2.019910
5	4.624460	2.554117	1.658511
9	4.394401	1.976084	0.375118
9	5.995781	2.686632	1.869339
9	4.050647	1.723439	2.638662
9	3.995538	3.816234	1.686703

P2 *exo-re* [BF_4^-]

Number of imaginary frequencies : 0
The smallest frequency is : 8.5256 cm(-1)
Electronic energy=-3125.4910832
Zero-point correction= 0.914283
(Hartree/Particle)
Thermal correction to Energy= 0.969111
Thermal correction to Enthalpy= 0.970055
Thermal correction to Gibbs Free Energy= 0.824645
Sum of electronic and zero-point Energies= -3124.576800
Sum of electronic and thermal Energies= -3124.521973
Sum of electronic and thermal Enthalpies= -3124.521029
Sum of electronic and thermal Free Energies= -3124.666439

Cartesian Coordinates

77	1.254169	-1.042307	-0.327675
15	-0.621314	0.214944	-0.100960
8	-1.637232	0.129418	1.190687
8	-1.691112	-0.080325	-1.342798
7	-0.187471	1.816123	-0.012046
6	-2.583829	-0.881489	1.316792
6	-2.368811	-1.813412	2.354893
1	-1.504240	-1.680946	2.996778
6	-3.252910	-2.849975	2.524765
1	-3.106323	-3.571191	3.323684
6	-4.352792	-3.011955	1.639418
6	-5.226017	-4.127849	1.753937
1	-5.050224	-4.842961	2.553317
6	-6.261641	-4.309749	0.865693
1	-6.919237	-5.169065	0.958477
6	-6.459783	-3.380464	-0.183262
1	-7.261926	-3.539578	-0.898172
6	-5.642334	-2.278592	-0.311571
1	-5.805131	-1.584535	-1.127275
6	-4.575604	-2.045269	0.600918
6	-3.695981	-0.909639	0.490125
6	-3.930392	0.179860	-0.498011
6	-5.160760	0.927726	-0.534487
6	-6.176056	0.782181	0.452040
1	-6.025563	0.089957	1.271981
6	-7.338551	1.519674	0.390385
1	-8.094122	1.395723	1.160907
6	-7.555332	2.442001	-0.660984
1	-8.479458	3.011156	-0.699660
6	-6.585385	2.624983	-1.620293
1	-6.728736	3.343914	-2.422758
6	-5.367587	1.893254	-1.576947
6	-4.344952	2.116202	-2.538232
1	-4.517698	2.830624	-3.338064
6	-3.142073	1.461832	-2.441104
1	-2.338006	1.634640	-3.147785
6	-2.939095	0.529235	-1.400951
6	1.186464	2.091843	-0.500280
1	1.806560	2.358973	0.358193
6	1.214328	3.249677	-1.490285
6	2.388290	4.002258	-1.636481
1	3.237475	3.788444	-0.997911
6	2.457210	5.020438	-2.589731
1	3.372547	5.597448	-2.691748
6	1.355956	5.306114	-3.401772
1	1.410869	6.103469	-4.137962
6	0.180923	4.564740	-3.253392
1	-0.685529	4.784745	-3.871845
6	0.113065	3.541717	-2.305496
1	-0.802576	2.975380	-2.178609
6	1.799971	0.847723	-1.164398
1	1.484724	0.822400	-2.213059
1	2.881988	0.965028	-1.151249
6	-0.762896	2.895365	0.868626
1	-0.292710	3.800325	0.474526
6	-0.284506	2.742079	2.311196
6	0.978700	3.241176	2.662972
1	1.579317	3.773680	1.933864
6	1.499014	3.045723	3.943907
1	2.492853	3.416514	4.176537
6	0.747807	2.373186	4.908878
1	1.147243	2.221458	5.907965
6	-0.529723	1.907456	4.582886
1	-1.131923	1.400353	5.332425
6	-1.039767	2.088224	3.295933
1	-2.027120	1.709662	3.061066
6	-2.268236	3.092354	0.703496
1	-2.513836	3.254295	-0.348319
1	-2.853920	2.247509	1.063297
1	-2.569788	3.979923	1.268368
6	1.635117	-0.323395	1.737355
1	0.886795	-0.567747	2.486396
1	1.901579	0.725960	1.697189
6	2.660878	-1.287481	1.505398
1	2.570689	-2.258119	1.982155
6	3.671357	-1.060735	0.570725
1	3.868273	-0.032255	0.296431
6	0.569498	-1.646297	-2.394667
1	0.306132	-0.715441	-2.886927
6	1.942869	-1.934217	-2.300984
1	2.629896	-1.199568	-2.719272
6	2.539930	-3.320271	-2.178056
1	2.589729	-3.768233	-3.181630
1	3.572891	-3.215633	-1.843251
6	1.795991	-4.281145	-1.224474
1	1.015956	-4.824210	-1.765793
1	2.508417	-5.032858	-0.871414
6	1.170900	-3.617954	-0.011717
1	1.704950	-3.733650	0.924270
6	-0.117823	-3.158963	0.048856
1	-0.542278	-2.966991	1.029916
6	-1.097493	-3.181517	-1.103309
1	-1.943950	-2.549211	-0.837991
1	-1.493993	-4.201680	-1.205424
6	-0.527770	-2.709064	-2.461836
1	-0.141059	-3.562702	-3.027679
1	-1.355002	-2.301052	-3.048242
6	4.699705	-2.016048	0.157814
6	4.737920	-3.361502	0.575258
6	5.690793	-1.561591	-0.734131
6	5.723845	-4.222406	0.099350
1	3.995713	-3.739466	1.270576
6	6.674490	-2.426246	-1.211160
1	5.681716	-0.518013	-1.037551
6	6.691345	-3.762110	-0.801053
1	5.739033	-5.257033	0.430603
1	7.429462	-2.056864	-1.899343
1	7.455950	-4.438445	-1.172308
5	4.604286	2.562936	1.225220
9	3.802510	3.725451	1.204889
9	4.023283	1.620200	2.094850
9	5.898611	2.877546	1.641989
9	4.647851	2.017130	-0.087553

P2 *exo-si* [BF_4^-]

Number of imaginary frequencies : 0
The smallest frequency is : 17.8206 cm(-1)
Electronic energy=-3125.4892183

Zero-point correction= 0.915272
(Hartree/Particle)
Thermal correction to Energy= 0.969872
Thermal correction to Enthalpy= 0.970816
Thermal correction to Gibbs Free Energy= 0.828300
Sum of electronic and zero-point Energies= -3124.573946
Sum of electronic and thermal Energies= -3124.519347
Sum of electronic and thermal Enthalpies= -3124.518402
Sum of electronic and thermal Free Energies= -3124.660918

Cartesian Coordinates

77	1.181272	-1.486198	-1.253366
15	-0.155265	0.230082	-0.396632
8	-1.030592	0.254278	1.002014
8	-1.372997	0.544219	-1.494727
7	0.800353	1.554605	-0.120083
6	-2.214054	-0.470292	1.122247
6	-2.176667	-1.571974	2.000792
1	-1.260462	-1.762702	2.541797
6	-3.291242	-2.357542	2.151447
1	-3.274966	-3.204593	2.831479
6	-4.466491	-2.091027	1.398075
6	-5.598218	-2.947076	1.478782
1	-5.554867	-3.799442	2.151720
6	-6.718828	-2.713136	0.714381
1	-7.576094	-3.376739	0.780069
6	-6.745434	-1.612020	-0.174153
1	-7.619837	-1.444023	-0.796321
6	-5.671703	-0.752547	-0.262808
1	-5.709337	0.078924	-0.956384
6	-4.505867	-0.947580	0.529917
6	-3.361803	-0.072654	0.453795
6	-3.384573	1.188731	-0.336878
6	-4.373916	2.212488	-0.112304
6	-5.302865	2.159665	0.964756
1	-5.269214	1.325874	1.655689
6	-6.233760	3.158427	1.152379
1	-6.925279	3.096882	1.987865
6	-6.293166	4.266272	0.273909
1	-7.036949	5.042124	0.430042
6	-5.394552	4.363018	-0.764236
1	-5.413209	5.218320	-1.434782
6	-4.410365	3.359424	-0.975359
6	-3.448125	3.486257	-2.013471
1	-3.492040	4.348896	-2.672218
6	-2.452753	2.552800	-2.157610
1	-1.681365	2.648334	-2.914417
6	-2.414412	1.434175	-1.296429
6	2.164608	1.458038	-0.694329
1	2.868845	1.279861	0.119218
6	2.557143	2.743418	-1.409935
6	3.848010	3.263619	-1.260004
1	4.541910	2.774895	-0.583324
6	4.229030	4.411173	-1.962285
1	5.232673	4.808537	-1.836641
6	3.324978	5.050965	-2.812781
1	3.621545	5.946010	-3.352785
6	2.031618	4.537957	-2.960677
1	1.319776	5.034231	-3.615182
6	1.652468	3.389765	-2.266362
1	0.645755	2.994236	-2.370925
6	2.262133	0.302835	-1.698027
1	1.868068	0.646744	-2.659541
1	3.321242	0.097333	-1.836482
6	0.601548	2.685132	0.851012
1	1.356425	3.407164	0.531397
6	0.955986	2.326244	2.291604
6	2.298509	2.385476	2.691634
1	3.074257	2.623783	1.971946
6	2.665245	2.133716	4.015679
1	3.714476	2.169728	4.293244
6	1.688215	1.837196	4.967495
1	1.967803	1.652382	6.001135
6	0.346687	1.773522	4.578990
1	-0.420984	1.536503	5.310683
6	-0.015110	2.009143	3.252022
1	-1.059747	1.950247	2.968676
6	-0.740726	3.396445	0.701213
1	-0.867666	3.743694	-0.325491
1	-1.590702	2.765176	0.957929
1	-0.754094	4.267597	1.363277
6	3.267612	-2.452089	-1.309120
1	3.935896	-1.607453	-1.411650
1	3.456521	-3.286052	-1.976885
6	2.675342	-2.742083	-0.067161
1	2.381226	-3.768351	0.122971
6	2.235762	-1.743217	0.835285
1	2.808977	-0.826509	0.900633
6	0.098832	-1.199620	-3.219845
1	0.152101	-0.135317	-3.426908
6	1.273303	-1.935556	-3.466611
1	2.132019	-1.379609	-3.838829
6	1.316902	-3.414625	-3.796540
1	1.075166	-3.534692	-4.862580
1	2.347390	-3.759214	-3.680870
6	0.379988	-4.306731	-2.952083
1	-0.600153	-4.381847	-3.431351
1	0.788998	-5.321428	-2.934166
6	0.186757	-3.845954	-1.517974
1	0.724665	-4.406548	-0.762943
6	-0.829092	-3.025918	-1.100025
1	-1.046306	-2.983781	-0.035866
6	-1.868258	-2.427266	-2.022564
1	-2.425933	-1.677841	-1.464807
1	-2.587080	-3.215804	-2.286488
6	-1.310844	-1.783663	-3.314125
1	-1.321373	-2.509316	-4.133719
1	-1.987624	-0.977810	-3.607146
6	1.522118	-2.133807	2.075606
6	0.821992	-3.349689	2.204684
6	1.596769	-1.287736	3.193422
6	0.244284	-3.718344	3.418037
1	0.712277	-4.014734	1.355392
6	1.008122	-1.653572	4.405276
1	2.145938	-0.357067	3.115473
6	0.334435	-2.870475	4.526849
1	-0.287824	-4.662663	3.494360
1	1.085194	-0.983185	5.254947
1	-0.119158	-3.154842	5.472067
5	5.313307	0.484656	1.298841
9	4.873084	0.060778	0.016378
9	6.637301	0.088013	1.492989
9	4.480902	-0.086281	2.279560
9	5.213201	1.893969	1.365504

P2 *endo-re* [BF_4^-]

Number of imaginary frequencies : 0
The smallest frequency is : 14.5966 cm(-1)
Electronic energy=-3125.4843546
Zero-point correction= 0.914562
(Hartree/Particle)
Thermal correction to Energy= 0.969392
Thermal correction to Enthalpy= 0.970337
Thermal correction to Gibbs Free Energy= 0.825586
Sum of electronic and zero-point Energies= -3124.569793
Sum of electronic and thermal Energies= -3124.514962
Sum of electronic and thermal Enthalpies= -3124.514018
Sum of electronic and thermal Free Energies= -3124.658769

Cartesian Coordinates

77	1.000990	-1.587439	-1.276688
15	-0.178764	0.300072	-0.437323
8	-1.012170	0.450911	0.990685
8	-1.399511	0.690108	-1.512200
7	0.912374	1.530843	-0.240434
6	-2.165137	-0.310488	1.161110
6	-2.072186	-1.398999	2.053246

1	-1.140347	-1.549109	2.582314
6	-3.153330	-2.225635	2.229081
1	-3.095929	-3.062903	2.918954
6	-4.347102	-2.016078	1.485839
6	-5.440594	-2.918380	1.586624
1	-5.355807	-3.759898	2.269296
6	-6.575785	-2.742907	0.827909
1	-7.402756	-3.442390	0.908142
6	-6.656822	-1.655397	-0.073981
1	-7.542095	-1.533845	-0.691581
6	-5.621877	-0.751626	-0.181799
1	-5.698905	0.068938	-0.885140
6	-4.442770	-0.887090	0.603292
6	-3.334686	0.029869	0.500333
6	-3.409369	1.277704	-0.308973
6	-4.433373	2.267422	-0.082823
6	-5.345297	2.192867	1.007468
1	-5.268833	1.371050	1.709281
6	-6.313125	3.156175	1.194826
1	-6.990965	3.077955	2.040096
6	-6.428054	4.249032	0.303387
1	-7.200111	4.996787	0.459420
6	-5.547473	4.366874	-0.748074
1	-5.609032	5.211454	-1.429586
6	-4.528176	3.399441	-0.960412
6	-3.587897	3.547103	-2.015902
1	-3.674746	4.397706	-2.686023
6	-2.562529	2.648582	-2.164860
1	-1.808855	2.761903	-2.937031
6	-2.464899	1.542847	-1.290326
6	2.275715	1.269990	-0.778472
1	2.942202	1.088723	0.065762
6	2.779918	2.473703	-1.566401
6	4.090762	2.934632	-1.401112
1	4.735153	2.455116	-0.673120
6	4.558133	4.012557	-2.160094
1	5.576867	4.364173	-2.019727
6	3.723128	4.640789	-3.085796
1	4.087443	5.481855	-3.669377
6	2.410818	4.184720	-3.253548
1	1.751518	4.670925	-3.967904
6	1.945318	3.107265	-2.501306
1	0.923213	2.758075	-2.622459
6	2.309592	0.042272	-1.703586
1	2.058624	0.373987	-2.715634
1	3.343048	-0.304120	-1.723455
6	0.793980	2.761057	0.610335
1	1.601711	3.394846	0.237684
6	1.108281	2.522537	2.085413
6	2.450189	2.467371	2.490964
1	3.248726	2.526455	1.759018
6	2.787597	2.352002	3.841023
1	3.834948	2.304012	4.124931
6	1.784474	2.315769	4.811888
1	2.043062	2.248980	5.865335
6	0.443631	2.351948	4.417814
1	-0.344563	2.309509	5.164907
6	0.109181	2.446622	3.065935
1	-0.935950	2.474160	2.778171
6	-0.493043	3.544429	0.363807
1	-0.574883	3.801195	-0.694112
1	-1.390455	2.999270	0.656422
1	-0.460287	4.473391	0.940919
6	2.810653	-2.793300	-1.123627
1	3.645330	-2.429675	-1.717573
1	2.609594	-3.851752	-1.268798
6	2.678345	-2.263186	0.215775
1	3.284905	-1.423765	0.539919
6	1.735719	-2.831414	1.067744
1	1.289497	-3.760636	0.729718
6	0.042225	-1.199155	-3.220914
1	0.182805	-0.147713	-3.454677
6	1.179502	-2.030177	-3.423461
1	2.079077	-1.539531	-3.791253
6	1.131447	-3.505261	-3.766075
1	0.935804	-3.607199	-4.843576
1	2.128015	-3.922331	-3.596598
6	0.092423	-4.313297	-2.962142
1	-0.872641	-4.307965	-3.475992
1	0.411413	-5.359282	-2.923010
6	-0.101084	-3.819589	-1.538189
1	0.379874	-4.415190	-0.770256
6	-1.075857	-2.930316	-1.149243
1	-1.330760	-2.878083	-0.093849
6	-2.050140	-2.275042	-2.105163
1	-2.572266	-1.487136	-1.565872
1	-2.811323	-3.015056	-2.390015
6	-1.405851	-1.671781	-3.375540
1	-1.442646	-2.391001	-4.200416
1	-2.007688	-0.814406	-3.685728
6	1.378466	-2.500830	2.437674
6	1.803911	-1.340231	3.112040
6	0.568262	-3.432316	3.123761
6	1.433300	-1.136738	4.438287
1	2.428202	-0.612943	2.608866
6	0.197409	-3.219300	4.448284
1	0.231886	-4.326396	2.604817
6	0.630605	-2.066492	5.108598
1	1.770482	-0.243603	4.949616
1	-0.425016	-3.946135	4.961962
1	0.345698	-1.891176	6.142144
5	5.438129	0.365646	1.181763
9	5.436338	1.770298	1.328331
9	4.457229	-0.183137	2.037559
9	6.695371	-0.150613	1.496868
9	5.103289	0.035548	-0.153602

P1 *endo-re*

Number of imaginary frequencies : 0
The smallest frequency is : 19.0304 cm(-1)
Electronic energy=-2700.877626
Zero-point correction= 0.898344
(Hartree/Particle)
Thermal correction to Energy= 0.946899
Thermal correction to Enthalpy= 0.947843
Thermal correction to Gibbs Free Energy= 0.817642
Sum of electronic and zero-point Energies= -2699.979282
Sum of electronic and thermal Energies= -2699.930727
Sum of electronic and thermal Enthalpies= -2699.929783
Sum of electronic and thermal Free Energies= -2700.059984

.....

Cartesian Coordinates

.....

77	-1.558666	-1.024203	-0.170337
15	0.323955	0.213928	-0.022867
8	1.416958	0.044447	1.188513
8	1.284709	-0.021635	-1.351950
7	-0.093947	1.816913	0.177910
6	2.396796	-0.947401	1.180553
6	2.289353	-1.933277	2.184055
1	1.479535	-1.855752	2.901752
6	3.208922	-2.951572	2.229635
1	3.145948	-3.713957	3.000701
6	4.237910	-3.037578	1.253339
6	5.148664	-4.128718	1.244941
1	5.056025	-4.886030	2.018970
6	6.117360	-4.233604	0.272871
1	6.805198	-5.073984	0.272806
6	6.207218	-3.248958	-0.739873
1	6.956830	-3.347032	-1.519769
6	5.350773	-2.169398	-0.750585
1	5.429827	-1.430678	-1.539298
6	4.351570	-2.015968	0.250564
6	3.437845	-0.902175	0.267210
6	3.575572	0.250901	-0.665966
6	4.778720	1.039418	-0.735859
6	5.868364	0.858284	0.161344
1	5.801386	0.102776	0.935084
6	6.998394	1.642026	0.073922

1	7.812173	1.490204	0.777127
6	7.106968	2.647293	-0.916364
1	8.006993	3.251999	-0.976460
6	6.063380	2.865232	-1.786809
1	6.123749	3.647815	-2.538517
6	4.875620	2.087840	-1.712420
6	3.774987	2.351390	-2.572107
1	3.864605	3.134747	-3.319308
6	2.601358	1.651260	-2.438176
1	1.736690	1.856401	-3.059890
6	2.512171	0.632401	-1.466560
6	-1.526352	2.072561	-0.127668
1	-2.062940	2.150309	0.824255
6	-1.725573	3.370642	-0.889350
6	-2.823100	4.186222	-0.589602
1	-3.491547	3.906575	0.221565
6	-3.062314	5.352486	-1.320887
1	-3.917116	5.977162	-1.077029
6	-2.197994	5.718703	-2.354964
1	-2.377960	6.628859	-2.919952
6	-1.095050	4.912373	-2.654460
1	-0.415002	5.196042	-3.453047
6	-0.861756	3.744479	-1.927931
1	0.001504	3.124006	-2.148673
6	-2.109254	0.897961	-0.920284
1	-1.786461	0.975944	-1.964587
1	-3.200188	0.960431	-0.913594
6	0.540972	2.850550	1.073423
1	0.106626	3.784086	0.705892
6	0.069948	2.686570	2.516659
6	-1.106593	3.336132	2.922183
1	-1.619196	3.992534	2.223396
6	-1.621278	3.160898	4.209184
1	-2.535070	3.672046	4.499576
6	-0.954020	2.340912	5.121244
1	-1.348494	2.202672	6.123980
6	0.236532	1.714980	4.740501
1	0.774224	1.092517	5.450650
6	0.744966	1.887267	3.451597
1	1.666971	1.391238	3.175681
6	2.051405	2.996177	0.903549
1	2.298482	3.164127	-0.146648
1	2.613311	2.132606	1.255398
1	2.377873	3.869133	1.477061
6	-1.734601	-0.732360	1.985759
1	-1.538821	-1.685764	2.473742
1	-1.193436	0.096466	2.435225
6	-3.069422	-0.448659	1.535364
1	-3.353861	0.595409	1.450113
6	-3.960318	-1.417008	1.088059
1	-3.769634	-2.455152	1.335979
6	-1.035861	-1.647580	-2.319354
1	-0.719090	-0.727251	-2.800262
6	-2.413558	-1.823776	-2.151109
1	-3.068178	-1.036128	-2.521380
6	-3.112933	-3.144482	-1.895557
1	-3.279385	-3.651714	-2.857244
1	-4.103230	-2.914660	-1.494674
6	-2.385944	-4.103231	-0.923879
1	-1.693797	-4.747171	-1.474031
1	-3.130226	-4.770077	-0.478013
6	-1.621993	-3.421051	0.204592
1	-2.045235	-3.517666	1.199490
6	-0.293689	-3.047982	0.136767
1	0.221289	-2.892988	1.079860
6	0.607947	-3.208172	-1.068081
1	1.505206	-2.611169	-0.899378
1	0.938347	-4.255151	-1.119612
6	-0.029924	-2.792529	-2.411204
1	-0.520980	-3.650358	-2.879431
1	0.769464	-2.487474	-3.091859
6	-5.248730	-1.154990	0.449524
6	-5.693793	0.137181	0.097902
6	-6.082448	-2.251219	0.148529
6	-6.918481	0.316301	-0.539297
1	-5.084592	1.005482	0.325595
6	-7.308563	-2.068947	-0.488434
1	-5.757260	-3.252285	0.419581
6	-7.729819	-0.783971	-0.839187
1	-7.243712	1.318565	-0.803327
1	-7.933503	-2.928724	-0.711854
1	-8.683228	-0.638160	-1.338408

P1 *exo-si*

Number of imaginary frequencies : 0
The smallest frequency is : 10.9775 cm(-1)
Electronic energy=-2700.871334
Zero-point correction= 0.897960
(Hartree/Particle)
Thermal correction to Energy= 0.946703
Thermal correction to Enthalpy= 0.947647
Thermal correction to Gibbs Free Energy= 0.816297
Sum of electronic and zero-point Energies= -2699.973374
Sum of electronic and thermal Energies= -2699.924631
Sum of electronic and thermal Enthalpies= -2699.923687
Sum of electronic and thermal Free Energies= -2700.055037

Cartesian Coordinates

77	-1.721212	-0.612148	-0.215835
15	0.338494	0.299110	-0.039200
8	1.357153	-0.053155	1.199999
8	1.287281	-0.070975	-1.344971
7	0.183532	1.949763	0.154884
6	2.166914	-1.187639	1.202910
6	1.872038	-2.159149	2.182916
1	1.063147	-1.963741	2.879010
6	2.613645	-3.313458	2.232641
1	2.404711	-4.068232	2.985228
6	3.643539	-3.549950	1.282549
6	4.363416	-4.775650	1.273881
1	4.125352	-5.521415	2.027689
6	5.330788	-5.020426	0.325873
1	5.872041	-5.961888	0.325171
6	5.610418	-4.046309	-0.662002
1	6.356994	-4.252008	-1.423559
6	4.942287	-2.841135	-0.671760
1	5.164449	-2.112206	-1.441777
6	3.951589	-2.543894	0.305339
6	3.228980	-1.297520	0.319679
6	3.572405	-0.172276	-0.593966
6	4.886730	0.415609	-0.623314
6	5.908098	0.055790	0.299831
1	5.699976	-0.687864	1.059590
6	7.150513	0.649846	0.251832
1	7.910510	0.363484	0.973022
6	7.444752	1.633670	-0.722111
1	8.430782	2.087813	-0.751029
6	6.474312	2.021486	-1.617718
1	6.679695	2.789626	-2.358575
6	5.177078	1.440840	-1.585825
6	4.159020	1.875971	-2.477055
1	4.393806	2.636753	-3.215868
6	2.886566	1.368504	-2.383424
1	2.085320	1.704916	-3.031715
6	2.606643	0.376464	-1.420544
6	-1.177275	2.446631	-0.176403
1	-1.704285	2.647311	0.762206
6	-1.134375	3.744866	-0.964085
6	-2.040240	4.768696	-0.661434
1	-2.736970	4.639555	0.163729
6	-2.050670	5.951181	-1.405910
1	-2.757138	6.738734	-1.158983
6	-1.146215	6.124316	-2.455846
1	-1.147071	7.046104	-3.030564
6	-0.233945	5.108395	-2.759022
1	0.477146	5.240047	-3.570091
6	-0.230071	3.925603	-2.019562
1	0.485986	3.141510	-2.244013

6	-1.959458	1.378435	-0.948157
1	-1.632226	1.388701	-1.994091
1	-3.016533	1.651202	-0.948540
6	0.962901	2.869337	1.062344
1	0.717363	3.858552	0.666438
6	0.417474	2.816329	2.487746
6	-0.619519	3.689892	2.850035
1	-0.967531	4.428645	2.132320
6	-1.205609	3.628452	4.117100
1	-2.010569	4.311632	4.373615
6	-0.749464	2.696960	5.051707
1	-1.200183	2.645161	6.038839
6	0.305249	1.843737	4.713939
1	0.682103	1.130918	5.442604
6	0.884482	1.903958	3.445439
1	1.698788	1.233112	3.203153
6	2.481550	2.743809	0.958535
1	2.801444	2.844223	-0.080253
1	2.867902	1.803837	1.348435
1	2.929827	3.558673	1.535253
6	-1.863714	-0.001862	1.901892
1	-1.173019	-0.490943	2.583444
1	-1.847653	1.080739	1.983746
6	-3.123664	-0.656588	1.697806
1	-3.243070	-1.659546	2.094521
6	-4.120821	-0.129821	0.889266
1	-4.058832	0.920211	0.622637
6	-1.256574	-1.261469	-2.359852
1	-0.850405	-0.371777	-2.831319
6	-2.648469	-1.291740	-2.198089
1	-3.201597	-0.421446	-2.549352
6	-3.509202	-2.523746	-2.017158
1	-3.773481	-2.918277	-3.009344
1	-4.448857	-2.208237	-1.557297
6	-2.887288	-3.649370	-1.164552
1	-2.253008	-4.288517	-1.784578
1	-3.697354	-4.284668	-0.793784
6	-2.081292	-3.163760	0.025926
1	-2.568707	-3.226541	0.992951
6	-0.729994	-2.936306	0.019727
1	-0.231500	-2.858466	0.981400
6	0.177274	-3.090494	-1.179590
1	1.132602	-2.619577	-0.945576
1	0.388969	-4.159786	-1.319523
6	-0.366818	-2.495992	-2.498840
1	-0.922157	-3.256840	-3.055403
1	0.488481	-2.223248	-3.122318
6	-5.344303	-0.812175	0.471363
6	-5.681489	-2.116304	0.887175
6	-6.199189	-0.156672	-0.436296
6	-6.825304	-2.741945	0.399170
1	-5.047889	-2.642410	1.593848
6	-7.342047	-0.786476	-0.926177
1	-5.952679	0.850928	-0.761863
6	-7.657698	-2.083455	-0.513265
1	-7.070426	-3.747221	0.729659
1	-7.985495	-0.266145	-1.629737
1	-8.546739	-2.577116	-0.894454

P1 *exo-re*

Number of imaginary frequencies : 0
The smallest frequency is : 18.4795 cm(-1)
Electronic energy=-2700.8703735
Zero-point correction= 0.899973
(Hartree/Particle)
Thermal correction to Energy= 0.948165
Thermal correction to Enthalpy= 0.949110
Thermal correction to Gibbs Free Energy= 0.821341
Sum of electronic and zero-point Energies= -2699.970401
Sum of electronic and thermal Energies= -2699.922208
Sum of electronic and thermal Enthalpies= -2699.921264
Sum of electronic and thermal Free Energies= -2700.049033

.....

Cartesian Coordinates

.....

77	-1.857936	-1.344757	-0.888315
15	-0.274482	0.273993	-0.274676
8	0.778709	0.227528	0.992651
8	0.789283	0.484918	-1.531431
7	-1.081536	1.677005	0.107191
6	1.916646	-0.579676	0.955284
6	1.925722	-1.673985	1.843835
1	1.083551	-1.800085	2.510533
6	2.993479	-2.535888	1.844997
1	3.015677	-3.378289	2.530647
6	4.065632	-2.355838	0.929686
6	5.133181	-3.291581	0.858418
1	5.126725	-4.136898	1.541476
6	6.144462	-3.142405	-0.063312
1	6.952577	-3.866278	-0.113103
6	6.121374	-2.048641	-0.960887
1	6.906177	-1.946948	-1.704935
6	5.110895	-1.113143	-0.905181
1	5.108161	-0.289118	-1.608474
6	4.061150	-1.221055	0.049544
6	2.982424	-0.266638	0.125913
6	2.985178	0.985715	-0.679244
6	4.066824	1.935667	-0.610325
6	5.124543	1.826733	0.335302
1	5.124685	1.005032	1.041423
6	6.138789	2.758776	0.378876
1	6.929461	2.657020	1.116701
6	6.157717	3.850157	-0.521732
1	6.967887	4.572212	-0.480179
6	5.139047	3.999815	-1.435155
1	5.128638	4.844039	-2.119484
6	4.068081	3.067119	-1.494504
6	2.987160	3.252263	-2.398531
1	3.005488	4.100408	-3.076930
6	1.914972	2.395812	-2.386164
1	1.056881	2.540622	-3.034037
6	1.914721	1.295403	-1.501852
6	-2.532426	1.650828	-0.194638
1	-3.071553	1.496437	0.748041
6	-3.005088	2.962800	-0.801819
6	-4.195446	3.551818	-0.362995
1	-4.755447	3.088061	0.445702
6	-4.665141	4.728420	-0.954293
1	-5.590425	5.176785	-0.603464
6	-3.941539	5.329960	-1.985494
1	-4.301665	6.247633	-2.441670
6	-2.746800	4.749219	-2.425463
1	-2.176719	5.216680	-3.223610
6	-2.283826	3.571673	-1.840154
1	-1.350551	3.123656	-2.171260
6	-2.870717	0.511519	-1.165233
1	-2.628209	0.841896	-2.180906
1	-3.953468	0.379782	-1.133041
6	-0.648315	2.809310	0.999146
1	-1.344378	3.605611	0.727325
6	-0.887475	2.535054	2.480481
6	-2.148614	2.821839	3.025084
1	-2.930528	3.212549	2.379145
6	-2.400477	2.649523	4.388585
1	-3.383073	2.880491	4.790677
6	-1.381013	2.206977	5.234397
1	-1.566252	2.085914	6.298003
6	-0.118832	1.927255	4.703638
1	0.680377	1.584473	5.354716
6	0.123372	2.080235	3.338145
1	1.106614	1.852031	2.944058
6	0.741260	3.361247	0.693626
1	0.804916	3.665791	-0.352041
1	1.543161	2.652829	0.896574
1	0.905696	4.244401	1.318060
6	-3.980664	-2.177938	-0.673163
1	-4.610969	-1.303335	-0.775932
1	-4.289302	-3.034782	-1.262547
6	-3.284529	-2.447490	0.521222

1	-3.038833	-3.484130	0.724468
6	-2.659861	-1.463302	1.325634
1	-3.128103	-0.488188	1.417468
6	-1.021186	-1.142314	-2.986275
1	-1.014857	-0.077562	-3.196665
6	-2.271078	-1.779800	-3.073690
1	-3.124084	-1.155119	-3.332367
6	-2.468194	-3.249420	-3.386731
1	-2.338549	-3.382486	-4.470375
1	-3.507496	-3.510829	-3.175275
6	-1.527311	-4.218352	-2.634386
1	-0.623852	-4.397885	-3.224078
1	-2.027481	-5.186894	-2.543041
6	-1.117385	-3.763553	-1.244307
1	-1.604853	-4.268981	-0.419316
6	0.009226	-3.030123	-0.971504
1	0.367077	-3.004591	0.054455
6	0.970172	-2.539416	-2.033851
1	1.674120	-1.852702	-1.568016
1	1.561734	-3.398015	-2.380682
6	0.311064	-1.844067	-3.250328
1	0.156692	-2.564599	-4.059727
1	1.011499	-1.098326	-3.632406
6	-1.821841	-1.870591	2.480797
6	-1.208524	-3.137106	2.565233
6	-1.669900	-0.988056	3.561808
6	-0.503941	-3.517246	3.705135
1	-1.265173	-3.835233	1.737839
6	-0.958407	-1.368534	4.701330
1	-2.119053	-0.000836	3.516958
6	-0.377708	-2.634792	4.782764
1	-0.042650	-4.499912	3.747006
1	-0.863426	-0.669994	5.525449
1	0.173158	-2.929639	5.671145

P1 *endo-si*

Number of imaginary frequencies : 0
The smallest frequency is : 18.7378 cm(-1)
Electronic energy=-2700.8687245
Zero-point correction= 0.898446
(Hartree/Particle)
Thermal correction to Energy= 0.947129
Thermal correction to Enthalpy= 0.948073
Thermal correction to Gibbs Free Energy= 0.817839
Sum of electronic and zero-point Energies= -2699.970278
Sum of electronic and thermal Energies= -2699.921595
Sum of electronic and thermal Enthalpies= -2699.920651
Sum of electronic and thermal Free Energies= -2700.050886

Cartesian Coordinates

77	-1.401000	-1.871831	-0.598444
15	-0.187747	0.144016	-0.442284
8	0.710631	0.665208	0.847613
8	0.967343	0.195534	-1.634461
7	-1.279151	1.398079	-0.573958
6	1.881597	-0.017103	1.176994
6	1.842437	-0.794383	2.353258
1	0.934409	-0.783409	2.943801
6	2.944906	-1.526023	2.718111
1	2.933856	-2.120112	3.627700
6	4.102270	-1.543079	1.892920
6	5.214435	-2.369670	2.209289
1	5.173969	-2.967175	3.116228
6	6.312041	-2.426653	1.380658
1	7.154030	-3.066078	1.628837
6	6.334669	-1.660492	0.191247
1	7.189548	-1.727408	-0.475464
6	5.281140	-0.833778	-0.134240
1	5.315249	-0.262882	-1.054253
6	4.140599	-0.729383	0.710245
6	3.015460	0.116089	0.392562
6	3.044247	1.068642	-0.751590
6	4.078938	2.066394	-0.877171
6	5.031785	2.316648	0.149995
1	4.982186	1.750071	1.072053
6	6.007083	3.278755	-0.001651
1	6.716526	3.454036	0.802001
6	6.089500	4.045150	-1.188132
1	6.867942	4.794756	-1.295912
6	5.169548	3.847672	-2.192786
1	5.205288	4.442259	-3.101860
6	4.141952	2.874788	-2.061571
6	3.162363	2.705333	-3.077059
1	3.227229	3.305760	-3.979955
6	2.126132	1.824079	-2.903106
1	1.341066	1.709285	-3.643096
6	2.058351	1.045176	-1.726399
6	-2.692738	0.952394	-0.749354
1	-3.164134	0.914919	0.240029
6	-3.493068	1.904604	-1.624183
6	-4.776468	2.300931	-1.232561
1	-5.169399	1.970194	-0.274066
6	-5.550814	3.121376	-2.058073
1	-6.544952	3.422585	-1.739777
6	-5.043768	3.559022	-3.282824
1	-5.641048	4.202325	-3.922600
6	-3.760390	3.168886	-3.680629
1	-3.358516	3.509583	-4.630868
6	-2.992992	2.343494	-2.859627
1	-1.991751	2.048028	-3.162904
6	-2.743977	-0.439694	-1.396403
1	-2.518238	-0.325557	-2.462567
1	-3.771857	-0.808037	-1.331449
6	-1.100226	2.832864	-0.170926
1	-1.862558	3.352547	-0.753173
6	-1.424693	3.131478	1.292532
6	-2.705450	3.606594	1.611548
1	-3.455389	3.677178	0.828165
6	-3.016003	4.029098	2.906681
1	-4.010467	4.407435	3.127518
6	-2.043157	3.982984	3.906748
1	-2.275587	4.319489	4.913320
6	-0.769720	3.491981	3.606169
1	-0.008811	3.444686	4.380314
6	-0.462860	3.070293	2.312036
1	0.534638	2.709490	2.093572
6	0.231621	3.434597	-0.614650
1	0.356723	3.324730	-1.693224
1	1.093588	2.990228	-0.117482
1	0.223342	4.502828	-0.379673
6	-3.145845	-3.117454	-0.100093
1	-3.974293	-3.056677	-0.801911
1	-2.849322	-4.134435	0.137997
6	-3.111242	-2.134166	0.945024
1	-3.824031	-1.315945	0.926400
6	-2.107257	-2.139698	1.910997
1	-1.506063	-3.038753	2.005474
6	-0.495987	-2.092016	-2.624186
1	-0.656192	-1.152334	-3.143501
6	-1.622612	-2.944322	-2.530532
1	-2.544411	-2.586691	-2.985706
6	-1.559705	-4.453708	-2.411988
1	-1.367572	-4.865609	-3.413064
1	-2.550606	-4.811618	-2.121327
6	-0.504461	-4.991082	-1.418135
1	0.442660	-5.165263	-1.936488
1	-0.835497	-5.967057	-1.051445
6	-0.240632	-4.094008	-0.219743
1	-0.679521	-4.408465	0.722539
6	0.745930	-3.142643	-0.177890
1	1.049197	-2.761512	0.793347
6	1.658274	-2.809756	-1.338441
1	2.213919	-1.909018	-1.085087
1	2.401491	-3.613674	-1.434224
6	0.945539	-2.598128	-2.694866
1	0.946450	-3.527834	-3.273268
1	1.526227	-1.875537	-3.272569
6	-1.993568	-1.217634	3.041734

6	-2.770787	-0.051024	3.177313
6	-1.129609	-1.576369	4.094946
6	-2.697403	0.711149	4.337930
1	-3.439618	0.261684	2.382621
6	-1.043635	-0.798982	5.248899
1	-0.535080	-2.482175	4.007948
6	-1.831552	0.346470	5.374644
1	-3.306522	1.602362	4.429086
1	-0.371403	-1.092753	6.049643
1	-1.774420	0.953679	6.273211

P2 *endo-si*

Number of imaginary frequencies : 0
The smallest frequency is : 19.0197 cm(-1)
Electronic energy=-2700.8776262
Zero-point correction= 0.898342
(Hartree/Particle)
Thermal correction to Energy= 0.946897
Thermal correction to Enthalpy= 0.947841
Thermal correction to Gibbs Free Energy= 0.817638
Sum of electronic and zero-point Energies= -2699.979284
Sum of electronic and thermal Energies= -2699.930729
Sum of electronic and thermal Enthalpies= -2699.929785
Sum of electronic and thermal Free Energies= -2700.059989

Cartesian Coordinates

77	1.558698	-1.024312	-0.170316
15	-0.323936	0.213843	-0.022874
8	-1.416933	0.044379	1.188517
8	-1.284674	-0.021749	-1.351960
7	0.093935	1.816852	0.177841
6	-2.396838	-0.947404	1.180532
6	-2.289457	-1.933297	2.184024
1	-1.479641	-1.855823	2.901728
6	-3.209080	-2.951542	2.229590
1	-3.146151	-3.713937	3.000651
6	-4.238067	-3.037485	1.253288
6	-5.148884	-4.128572	1.244880
1	-5.056294	-4.885891	2.018908
6	-6.117579	-4.233398	0.272803
1	-6.805466	-5.073738	0.272731
6	-6.207371	-3.248745	-0.739940
1	-6.956981	-3.346774	-1.519842
6	-5.350862	-2.169236	-0.750642
1	-5.429865	-1.430511	-1.539357
6	-4.351659	-2.015864	0.250516
6	-3.437873	-0.902120	0.267175
6	-3.575523	0.250951	-0.666020
6	-4.778616	1.039546	-0.735941
6	-5.868287	0.858492	0.161247
1	-5.801370	0.102985	0.934993
6	-6.998263	1.642308	0.073798
1	-7.812064	1.490545	0.776991
6	-7.106752	2.647574	-0.916497
1	-8.006736	3.252341	-0.976611
6	-6.063137	2.865436	-1.786928
1	-6.123442	3.648018	-2.538642
6	-4.875430	2.087965	-1.712515
6	-3.774768	2.351429	-2.572193
1	-3.864323	3.134785	-3.319402
6	-2.601190	1.651217	-2.438241
1	-1.736498	1.856282	-3.059947
6	-2.512091	0.632365	-1.466612
6	1.526363	2.072464	-0.127656
1	2.062900	2.150189	0.824296
6	1.725671	3.370544	-0.889317
6	2.823292	4.186002	-0.589573
1	3.491734	3.906262	0.221567
6	3.062612	5.352256	-1.320836
1	3.917488	5.976835	-1.076987
6	2.198305	5.718591	-2.354883
1	2.378356	6.628742	-2.919853
6	1.095267	4.912388	-2.654370
1	0.415228	5.196152	-3.452930
6	0.861866	3.744499	-1.927866
1	-0.001469	3.124127	-2.148608
6	2.109277	0.897863	-0.920262
1	1.786496	0.975847	-1.964569
1	3.200211	0.960339	-0.913562
6	-0.540998	2.850485	1.073363
1	-0.106582	3.784009	0.705885
6	-0.070093	2.686473	2.516640
6	1.106529	3.335850	2.922231
1	1.619328	3.992105	2.223451
6	1.621058	3.160616	4.209295
1	2.534924	3.671604	4.499733
6	0.953545	2.340842	5.121358
1	1.347891	2.202610	6.124147
6	-0.237101	1.715126	4.740556
1	-0.774997	1.092844	5.450708
6	-0.745367	1.887397	3.451584
1	-1.667475	1.391570	3.175637
6	-2.051409	2.996181	0.903351
1	-2.298374	3.164183	-0.146862
1	-2.613389	2.132619	1.255099
1	-2.377904	3.869123	1.476869
6	1.734540	-0.732549	1.985808
1	1.538830	-1.685997	2.473731
1	1.193300	0.096211	2.435297
6	3.069321	-0.448730	1.535413
1	3.353694	0.595358	1.450229
6	3.960286	-1.416994	1.088052
1	3.769680	-2.455170	1.335901
6	1.035903	-1.647660	-2.319368
1	0.719143	-0.727324	-2.800266
6	2.413595	-1.823863	-2.151112
1	3.068226	-1.036216	-2.521367
6	3.112954	-3.144575	-1.895560
1	3.279404	-3.651814	-2.857244
1	4.103252	-2.914756	-1.494676
6	2.385947	-4.103305	-0.923875
1	1.693790	-4.747236	-1.474024
1	3.130215	-4.770160	-0.478000
6	1.622006	-3.421093	0.204587
1	2.045233	-3.517728	1.199488
6	0.293702	-3.048000	0.136751
1	-0.221283	-2.893008	1.079842
6	-0.607927	-3.208224	-1.068099
1	-1.505194	-2.611226	-0.899417
1	-0.938315	-4.255208	-1.119610
6	0.029956	-2.792600	-2.411221
1	0.521011	-3.650440	-2.879431
1	-0.769421	-2.487545	-3.091889
6	5.248709	-1.154847	0.449583
6	5.693741	0.137388	0.098161
6	6.082482	-2.251003	0.148480
6	6.918445	0.316638	-0.538975
1	5.084517	1.005641	0.325974
6	7.308610	-2.068602	-0.488421
1	5.757326	-3.252116	0.419400
6	7.729828	-0.783564	-0.838993
1	7.243652	1.318950	-0.802852
1	7.933590	-2.928326	-0.711931
1	8.683248	-0.637651	-1.338164

P2 *exo-re*

Number of imaginary frequencies : 0
The smallest frequency is : 17.5090 cm(-1)
Electronic energy=-2700.8715565
Zero-point correction= 0.897923
(Hartree/Particle)
Thermal correction to Energy= 0.946654
Thermal correction to Enthalpy= 0.947599
Thermal correction to Gibbs Free Energy= 0.816615
Sum of electronic and zero-point Energies= -2699.973633
Sum of electronic and thermal Energies= -2699.924902
Sum of electronic and thermal Enthalpies= -2699.923958

Sum of electronic and thermal Free Energies= -2700.054942

	Cartesian Coordinates		
77	1.762335	-0.535043	-0.194108
15	-0.333375	0.326232	-0.026426
8	-1.346982	-0.042721	1.213206
8	-1.269453	-0.078068	-1.329979
7	-0.218333	1.979073	0.155548
6	-2.122520	-1.201226	1.226005
6	-1.801437	-2.150256	2.219973
1	-1.003592	-1.919771	2.917951
6	-2.501980	-3.329268	2.279189
1	-2.272059	-4.066893	3.042520
6	-3.514496	-3.614027	1.323941
6	-4.186905	-4.866395	1.322936
1	-3.927890	-5.593620	2.087870
6	-5.134113	-5.159137	0.368261
1	-5.638444	-6.120862	0.372932
6	-5.440248	-4.207806	-0.633789
1	-6.169424	-4.451078	-1.401086
6	-4.819147	-2.977771	-0.650677
1	-5.060870	-2.267238	-1.431783
6	-3.851007	-2.631024	0.332794
6	-3.175051	-1.358038	0.337911
6	-3.553947	-0.258155	-0.592948
6	-4.891167	0.274707	-0.645399
6	-5.908534	-0.114534	0.270185
1	-5.678876	-0.836384	1.044533
6	-7.175097	0.423194	0.196041
1	-7.931724	0.114470	0.911527
6	-7.498981	1.377255	-0.797843
1	-8.503875	1.785890	-0.848259
6	-6.533763	1.793863	-1.686088
1	-6.762249	2.539818	-2.442664
6	-5.212879	1.271730	-1.627438
6	-4.203355	1.737468	-2.512783
1	-4.461266	2.476570	-3.265752
6	-2.912147	1.285425	-2.397178
1	-2.117453	1.645806	-3.040784
6	-2.603146	0.318217	-1.418073
6	1.129309	2.514960	-0.168656
1	1.630637	2.753924	0.774898
6	1.048925	3.796755	-0.980615
6	1.899236	4.865987	-0.674470
1	2.580232	4.782573	0.169434
6	1.874378	6.035415	-1.439112
1	2.537960	6.858450	-1.188933
6	0.989774	6.149312	-2.513632
1	0.963389	7.060366	-3.104630
6	0.132432	5.087629	-2.820710
1	-0.563415	5.173115	-3.650953
6	0.163304	3.918627	-2.060402
1	-0.512403	3.100265	-2.288356
6	1.967987	1.465565	-0.910636
1	1.674738	1.464049	-1.966263
1	3.013802	1.778545	-0.877508
6	-1.036345	2.891696	1.035228
1	-0.815961	3.880388	0.623661
6	-0.508407	2.881633	2.468287
6	0.483025	3.805427	2.833249
1	0.812530	4.545929	2.108813
6	1.045152	3.793285	4.112597
1	1.814164	4.515839	4.371459
6	0.610163	2.861086	5.056406
1	1.041385	2.848680	6.053482
6	-0.398796	1.955682	4.714597
1	-0.759488	1.241037	5.449608
6	-0.954004	1.966713	3.433981
1	-1.733977	1.257171	3.189247
6	-2.549331	2.719438	0.916326
1	-2.859877	2.795956	-0.127339
1	-2.912132	1.774146	1.315789
1	-3.027777	3.528930	1.476066
6	1.905817	0.122558	1.917191
1	1.204647	-0.324112	2.616579
1	1.921656	1.207078	1.954477
6	3.128553	-0.582952	1.696441
1	3.225378	-1.572168	2.130892
6	4.110677	-0.132892	0.815471
1	4.107030	0.916205	0.540323
6	1.290830	-1.170473	-2.327229
1	0.877895	-0.283201	-2.797315
6	2.685791	-1.196217	-2.172031
1	3.234521	-0.324261	-2.525686
6	3.538519	-2.439935	-2.043448
1	3.741478	-2.827545	-3.052583
1	4.505409	-2.144177	-1.633333
6	2.944490	-3.566674	-1.170486
1	2.306657	-4.217367	-1.774927
1	3.768748	-4.188659	-0.809271
6	2.152723	-3.086219	0.031129
1	2.659322	-3.140953	0.988343
6	0.799666	-2.869526	0.038176
1	0.306533	-2.795440	1.002711
6	-0.108023	-3.037927	-1.159728
1	-1.075442	-2.597949	-0.918725
1	-0.288124	-4.111533	-1.309682
6	0.414281	-2.414191	-2.475363
1	0.974080	-3.158594	-3.049905
1	-0.451203	-2.143441	-3.085115
6	5.311707	-0.875068	0.427443
6	5.574099	-2.195210	0.846205
6	6.227648	-0.254679	-0.443652
6	6.707753	-2.867977	0.398423
1	4.887050	-2.702665	1.515617
6	7.360301	-0.931509	-0.893309
1	6.038666	0.764443	-0.771822
6	7.603251	-2.242720	-0.476606
1	6.893899	-3.885549	0.729848
1	8.052536	-0.436274	-1.568062
1	8.484032	-2.773161	-0.826279

P2 *exo-si*

Number of imaginary frequencies : 0
The smallest frequency is : 18.4507 cm(-1)
Electronic energy=-2700.8703732
Zero-point correction= 0.899968
(Hartree/Particle)
Thermal correction to Energy= 0.948162
Thermal correction to Enthalpy= 0.949106
Thermal correction to Gibbs Free Energy= 0.821325
Sum of electronic and zero-point Energies= -2699.970405
Sum of electronic and thermal Energies= -2699.922211
Sum of electronic and thermal Enthalpies= -2699.921267
Sum of electronic and thermal Free Energies= -2700.049048

	Cartesian Coordinates		
77	1.857988	-1.344926	-0.888166
15	0.274404	0.273864	-0.274770
8	-0.778808	0.227469	0.992545
8	-0.789369	0.484628	-1.531566
7	1.081495	1.676892	0.107010
6	-1.916732	-0.579766	0.955167
6	-1.925791	-1.674116	1.843671
1	-1.083598	-1.800291	2.510327
6	-2.993552	-2.536014	1.844819
1	-3.015725	-3.378452	2.530424
6	-4.065740	-2.355907	0.929561
6	-5.133316	-3.291621	0.858313
1	-5.126844	-4.136963	1.541340
6	-6.144647	-3.142378	-0.063351
1	-6.952786	-3.866226	-0.113124
6	-6.121584	-2.048572	-0.960876
1	-6.906435	-1.946818	-1.704864
6	-5.111072	-1.113109	-0.905194
1	-5.108365	-0.289049	-1.608445
6	-4.061269	-1.221093	0.049458

6	-2.982512	-0.266714	0.125809
6	-2.985218	0.985607	-0.679393
6	-4.066794	1.935628	-0.610459
6	-5.124440	1.826823	0.335263
1	-5.124590	1.005155	1.041423
6	-6.138602	2.758955	0.378882
1	-6.929217	2.657304	1.116783
6	-6.157515	3.850293	-0.521780
1	-6.967617	4.572422	-0.480186
6	-5.138918	3.999815	-1.435309
1	-5.128506	4.843999	-2.119687
6	-4.068036	3.067024	-1.494708
6	-2.987188	3.251999	-2.398857
1	-3.005525	4.100075	-3.077343
6	-1.915047	2.395484	-2.386504
1	-1.057029	2.540180	-3.034503
6	-1.914779	1.295167	-1.502074
6	2.532344	1.650727	-0.195100
1	3.071687	1.496327	0.747452
6	3.004926	2.962667	-0.802400
6	4.195627	3.551394	-0.364106
1	4.755935	3.087439	0.444261
6	4.665257	4.727962	-0.955512
1	5.590809	5.176106	-0.605103
6	3.941256	5.329762	-1.986287
1	4.301334	6.247416	-2.442540
6	2.746187	4.749305	-2.425722
1	2.175798	5.216964	-3.223533
6	2.283273	3.571781	-1.840311
1	1.349763	3.123964	-2.171013
6	2.870412	0.511425	-1.165753
1	2.627349	0.841644	-2.181352
1	3.953188	0.379847	-1.134063
6	0.648316	2.809353	0.998794
1	1.344302	3.605640	0.726744
6	0.887673	2.535490	2.480174
6	2.148905	2.822422	3.024491
1	2.930698	3.212943	2.378295
6	2.400990	2.650507	4.387999
1	3.383657	2.881579	4.789858
6	1.381662	2.208219	5.234112
1	1.567082	2.087450	6.297720
6	0.119390	1.928361	4.703643
1	-0.679710	1.585740	5.354941
6	-0.123036	2.080951	3.338145
1	-1.106350	1.852656	2.944305
6	-0.741319	3.361161	0.693317
1	-0.805124	3.665433	-0.352419
1	-1.543171	2.652773	0.896559
1	-0.905704	4.244471	1.317545
6	3.980729	-2.177746	-0.672474
1	4.611014	-1.303125	-0.775292
1	4.289515	-3.034686	-1.261648
6	3.284490	-2.447152	0.521896
1	3.038895	-3.483786	0.725293
6	2.659538	-1.462899	1.326009
1	3.127577	-0.487676	1.417680
6	1.021178	-1.142992	-2.986042
1	1.014691	-0.078279	-3.196630
6	2.271183	-1.780305	-3.073375
1	3.124062	-1.155524	-3.332238
6	2.468578	-3.249958	-3.386111
1	2.339154	-3.383270	-4.469753
1	3.507883	-3.511149	-3.174409
6	1.527729	-4.218895	-2.633737
1	0.624282	-4.398493	-3.223424
1	2.027938	-5.187413	-2.542342
6	1.117800	-3.764021	-1.243690
1	1.605440	-4.269236	-0.418669
6	-0.008811	-3.030611	-0.970888
1	-0.366538	-3.004919	0.055112
6	-0.969919	-2.540127	-2.033209
1	-1.673822	-1.853349	-1.567391
1	-1.561512	-3.398789	-2.379824
6	-0.311003	-1.844947	-3.249883
1	-0.156614	-2.565605	-4.059165
1	-1.011556	-1.099359	-3.632043
6	1.821495	-1.870072	2.481198
6	1.208474	-3.136711	2.565978
6	1.669297	-0.987268	3.561957
6	0.503849	-3.516653	3.705921
1	1.265417	-3.835140	1.738864
6	0.957759	-1.367550	4.701515
1	2.118316	0.000005	3.516905
6	0.377287	-2.633892	4.783258
1	0.042810	-4.499426	3.748056
1	0.862560	-0.668791	5.525422
1	-0.173614	-2.928586	5.671667

P2 *endo-re*

Number of imaginary frequencies : 0
The smallest frequency is : 18.7759 cm(-1)
Electronic energy=-2700.8687246
Zero-point correction= 0.898443
(Hartree/Particle)
Thermal correction to Energy= 0.947125
Thermal correction to Enthalpy= 0.948069
Thermal correction to Gibbs Free Energy= 0.817844
Sum of electronic and zero-point Energies= -2699.970282
Sum of electronic and thermal Energies= -2699.921599
Sum of electronic and thermal Enthalpies= -2699.920655
Sum of electronic and thermal Free Energies= -2700.050881

Cartesian Coordinates

77	1.400767	-1.871898	-0.598513
15	0.187698	0.144026	-0.442390
8	-0.710527	0.665341	0.847560
8	-0.967475	0.195651	-1.634498
7	1.279268	1.397944	-0.574139
6	-1.881479	-0.016937	1.177065
6	-1.842229	-0.794230	2.353316
1	-0.934137	-0.783279	2.943764
6	-2.944681	-1.525855	2.718253
1	-2.933564	-2.119965	3.627829
6	-4.102114	-1.542885	1.893157
6	-5.214256	-2.369483	2.209593
1	-5.173719	-2.967014	3.116512
6	-6.311925	-2.426444	1.381043
1	-7.153893	-3.065879	1.629266
6	-6.334649	-1.660250	0.191654
1	-7.189581	-1.727150	-0.474991
6	-5.281144	-0.833528	-0.133895
1	-5.315319	-0.262610	-1.053893
6	-4.140536	-0.729166	0.710502
6	-3.015406	0.116283	0.392733
6	-3.044253	1.068852	-0.751402
6	-4.078908	2.066659	-0.876852
6	-5.031659	2.316914	0.150402
1	-4.982015	1.750293	1.072430
6	-6.006923	3.279075	-0.001123
1	-6.716292	3.454352	0.802595
6	-6.089395	4.045530	-1.187560
1	-6.867808	4.795181	-1.295241
6	-5.169533	3.848055	-2.192297
1	-5.205312	4.442689	-3.101337
6	-4.141977	2.875112	-2.061210
6	-3.162476	2.705655	-3.076782
1	-3.227378	3.306133	-3.979642
6	-2.126280	1.824336	-2.902959
1	-1.341277	1.709541	-3.643016
6	-2.058442	1.045369	-1.726299
6	2.692790	0.952092	-0.749778
1	3.164366	0.914523	0.239520
6	3.493034	1.904270	-1.624715
6	4.776431	2.300692	-1.233188
1	5.169460	1.969979	-0.274724
6	5.550655	3.121207	-2.058745
1	6.544790	3.422490	-1.740512

6	5.043484	3.558831	-3.283450
1	5.640664	4.202191	-3.923261
6	3.760107	3.168597	-3.681165
1	3.358135	3.509273	-4.631370
6	2.992835	2.343134	-2.860117
1	1.991604	2.047583	-3.163338
6	2.743748	-0.440011	-1.396835
1	2.517782	-0.325892	-2.462951
1	3.771589	-0.808505	-1.332057
6	1.100544	2.832748	-0.171083
1	1.863009	3.352315	-0.753254
6	1.424947	3.131281	1.292394
6	2.705754	3.606222	1.611470
1	3.455698	3.676822	0.828092
6	3.016357	4.028528	2.906653
1	4.010868	4.406713	3.127543
6	2.043517	3.982363	3.906721
1	2.275996	4.318663	4.913351
6	0.770015	3.491569	3.606072
1	0.009107	3.444239	4.380217
6	0.463096	3.070102	2.311881
1	-0.534450	2.709470	2.093372
6	-0.231165	3.434672	-0.614950
1	-0.356157	3.324790	-1.693538
1	-1.093247	2.990415	-0.117876
1	-0.222777	4.502905	-0.379986
6	3.145446	-3.117711	-0.100216
1	3.973823	-3.057217	-0.802142
1	2.848670	-4.134589	0.138027
6	3.111191	-2.134308	0.944801
1	3.824164	-1.316248	0.926011
6	2.107321	-2.139479	1.910886
1	1.505781	-3.038294	2.005425
6	0.495461	-2.092349	-2.624019
1	0.655772	-1.152810	-3.143561
6	1.621956	-2.944842	-2.530335
1	2.543754	-2.587473	-2.985723
6	1.558826	-4.454210	-2.411562
1	1.366621	-4.866202	-3.412587
1	2.549686	-4.812223	-2.120892
6	0.503532	-4.991431	-1.417653
1	-0.443616	-5.165504	-1.935993
1	0.834470	-5.967450	-1.050987
6	0.239789	-4.094350	-0.219261
1	0.678793	-4.408691	0.723013
6	-0.746518	-3.142755	-0.177519
1	-1.049608	-2.761381	0.793677
6	-1.658823	-2.809705	-1.338050
1	-2.214228	-1.908825	-1.084679
1	-2.402247	-3.613438	-1.433779
6	-0.946146	-2.598258	-2.694528
1	-0.947237	-3.527994	-3.272881
1	-1.526784	-1.875625	-3.272229
6	1.994115	-1.217251	3.041541
6	2.771946	-0.051027	3.176958
6	1.130086	-1.575454	4.094876
6	2.699097	0.711252	4.337536
1	3.440887	0.261261	2.382197
6	1.044586	-0.797901	5.248755
1	0.535157	-2.481015	4.008054
6	1.833112	0.347147	5.374338
1	3.308748	1.602108	4.428595
1	0.372265	-1.091248	6.049579
1	1.776387	0.954463	6.272859

13' P1 *endo-re* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 18.3229 20.5963 24.1703 cm(-1)
Electronic energy= -3892.0338464
Zero-point correction= 1.233643
(Hartree/Particle)
Thermal correction to Energy= 1.306605
Thermal correction to Enthalpy= 1.307549
Thermal correction to Gibbs Free Energy= 1.123538
Sum of electronic and zero-point Energies= -3890.800203
Sum of electronic and thermal Energies= -3890.727241
Sum of electronic and thermal Enthalpies= -3890.726297
Sum of electronic and thermal Free Energies= -3890.910309

.....

Cartesian Coordinates

.....

77	-0.153630	-0.520289	-1.401376
15	1.676133	0.362977	-0.392687
8	2.356939	-0.272956	0.959420
8	2.983135	0.374961	-1.422496
7	1.296273	1.885730	0.165015
6	3.241984	-1.349769	0.913035
6	2.778813	-2.562510	1.464864
1	1.769548	-2.625033	1.858887
6	3.601645	-3.661567	1.444172
1	3.257575	-4.604471	1.859199
6	4.887481	-3.596218	0.843968
6	5.714289	-4.749526	0.757593
1	5.352039	-5.678436	1.190160
6	6.937760	-4.698233	0.129273
1	7.559451	-5.586554	0.065698
6	7.379212	-3.485212	-0.451438
1	8.333185	-3.453196	-0.970010
6	6.608362	-2.345632	-0.373069
1	6.960367	-1.430325	-0.833610
6	5.349625	-2.353806	0.291699
6	4.516046	-1.182936	0.391627
6	4.973124	0.153366	-0.083984
6	6.175196	0.774508	0.409296
6	6.932275	0.230944	1.484799
1	6.597608	-0.683237	1.960397
6	8.072099	0.857216	1.940230
1	8.626551	0.425989	2.768789
6	8.523716	2.059523	1.345360
1	9.427789	2.537830	1.710591
6	7.804592	2.625560	0.317321
1	8.127802	3.558636	-0.136827
6	6.614770	2.015345	-0.164722
6	5.843684	2.625743	-1.190644
1	6.194786	3.552259	-1.635866
6	4.652997	2.071138	-1.589916
1	4.029583	2.533773	-2.347153
6	4.218850	0.862055	-1.005218
6	0.072247	2.452609	-0.459475
1	-0.724946	2.444938	0.289367
6	0.274217	3.885822	-0.932184
6	1.530214	4.361645	-1.331105
1	2.397292	3.717741	-1.230955
6	1.672932	5.656833	-1.833038
1	2.655450	6.013436	-2.131443
6	0.558531	6.491980	-1.947077
1	0.667923	7.500809	-2.335593
6	-0.696913	6.022146	-1.551495
1	-1.569436	6.665285	-1.629319
6	-0.839808	4.729464	-1.043286
1	-1.819796	4.376099	-0.742779
6	-0.366682	1.594344	-1.656424
1	0.220383	1.884025	-2.535215
1	-1.413070	1.812893	-1.881975
6	1.697729	2.548745	1.455766
1	1.420735	3.592364	1.285231
6	0.850516	2.066890	2.632360
6	-0.347170	2.736684	2.919747
1	-0.659030	3.582575	2.317256
6	-1.168278	2.325040	3.972403
1	-2.095730	2.857470	4.161501
6	-0.795045	1.240680	4.767145
1	-1.427226	0.920318	5.590826
6	0.404681	0.572563	4.500254
1	0.708915	-0.267775	5.118553
6	1.220413	0.982170	3.443781
1	2.145782	0.452609	3.254754
6	3.202122	2.552820	1.722242
1	3.737628	2.974070	0.868831

1	3.606012	1.562259	1.924795
1	3.396871	3.183681	2.595051
6	-0.867042	-0.833241	0.644903
1	-0.795880	-1.898059	0.807401
1	-0.432286	-0.231489	1.437911
6	-1.974640	-0.248608	-0.036248
1	-2.185865	0.787885	0.188113
6	-2.698826	-0.863738	-1.063177
1	-2.685275	-1.943869	-1.148167
6	0.914100	-0.566891	-3.403893
1	1.378031	0.410362	-3.494334
6	-0.468807	-0.636805	-3.642513
1	-0.980656	0.284970	-3.914257
6	-1.212305	-1.898436	-4.036605
1	-1.054927	-2.078429	-5.110550
1	-2.277824	-1.698732	-3.916554
6	-0.837648	-3.170983	-3.239351
1	-0.048493	-3.721385	-3.760950
1	-1.707933	-3.834902	-3.221831
6	-0.393457	-2.937830	-1.801187
1	-1.071287	-3.273445	-1.018740
6	0.909202	-2.710251	-1.413877
1	1.128667	-2.908991	-0.370025
6	2.103963	-2.601399	-2.335865
1	2.934084	-2.179078	-1.767820
1	2.413445	-3.616027	-2.625563
6	1.868713	-1.744320	-3.597631
1	1.490599	-2.368443	-4.413090
1	2.832237	-1.350823	-3.933689
6	-3.748466	-0.172922	-1.823719
6	-4.068506	1.186258	-1.620700
6	-4.510419	-0.899016	-2.762019
6	-5.111331	1.786026	-2.322742
1	-3.535925	1.782991	-0.892877
6	-5.549629	-0.294034	-3.469078
1	-4.291507	-1.950743	-2.924015
6	-5.855905	1.052760	-3.252187
1	-5.339932	2.828667	-2.123324
1	-6.123516	-0.876782	-4.184138
1	-6.669722	1.523047	-3.796604
8	-2.229309	-4.176975	0.831440
6	-1.336855	-3.896347	1.656464
8	-0.094872	-3.949442	1.576837
8	-1.878532	-3.399409	2.890592
6	-0.930947	-2.876557	3.823831
1	-0.423229	-1.990058	3.428988
1	-1.496246	-2.599932	4.719009
1	-0.175652	-3.624169	4.083645
6	-3.554519	-0.266387	3.075718
6	-4.773289	0.635737	3.167797
1	-2.767894	0.221178	2.495188
1	-3.143500	-0.503632	4.060048
6	-5.464912	0.670580	1.812537
1	-4.477226	1.652200	3.426895
1	-5.466311	0.262803	3.930150
1	-6.394513	1.238449	1.870834
1	-4.823136	1.150822	1.072192
7	-3.935573	-1.527585	2.436147
6	-4.998637	-1.712455	1.660689
7	-5.803134	-0.694318	1.345343
6	-5.215494	-3.141753	1.210087
1	-4.255650	-3.651991	1.334514
1	-5.929908	-3.603076	1.903808
6	-5.676803	-3.322604	-0.242410
1	-5.144516	-2.602157	-0.868778
6	-6.905813	-0.742721	0.354236
6	-7.189757	-3.168939	-0.436945
1	-7.398764	-3.011497	-1.502216
6	-7.769563	-2.005553	0.379253
1	-8.756722	-1.738802	-0.013540
1	-7.925687	-2.299908	1.423381
1	-7.531514	0.119446	0.589754
1	-6.487473	-0.569060	-0.644648
1	-7.700820	-4.095414	-0.148298
1	-5.356156	-4.313503	-0.580396
1	-3.295466	-2.321539	2.569985
5	-3.555729	3.683729	1.254510
9	-2.902673	2.417191	1.249348
9	-4.669543	3.612716	2.102675
9	-3.964885	3.973214	-0.064520
9	-2.653694	4.656422	1.703596

[**13'-14'**]‡ **P1**-*endo-re* [BF_4^-]

Number of imaginary frequencies= 1
The smallest frequencies are=-262.8389 15.5912 18.2300cm(-1)
Electronic energy= -3892.0074697
Zero-point correction= 1.228298
(Hartree/Particle)
Thermal correction to Energy= 1.301187
Thermal correction to Enthalpy= 1.302131
Thermal correction to Gibbs Free Energy= 1.118458
Sum of electronic and zero-point Energies= -3890.779171
Sum of electronic and thermal Energies= -3890.706283
Sum of electronic and thermal Enthalpies= -3890.705338
Sum of electronic and thermal Free Energies= -3890.889012

.....

Cartesian Coordinates

.....

77	-0.137435	-0.452292	-1.431226
15	1.675298	0.433438	-0.384319
8	2.343272	-0.213309	0.970660
8	2.994167	0.457579	-1.397355
7	1.275646	1.939538	0.194505
6	3.187186	-1.320076	0.916386
6	2.683530	-2.517825	1.465342
1	1.687167	-2.524705	1.892089
6	3.455062	-3.652506	1.421185
1	3.078826	-4.583537	1.834529
6	4.732595	-3.634093	0.799247
6	5.505577	-4.821276	0.680869
1	5.108441	-5.741018	1.102176
6	6.721516	-4.812677	0.036000
1	7.301405	-5.726656	-0.052875
6	7.210273	-3.609883	-0.527756
1	8.158357	-3.611017	-1.057876
6	6.492984	-2.438384	-0.417806
1	6.879806	-1.530131	-0.864457
6	5.242837	-2.403872	0.261507
6	4.462412	-1.199737	0.387204
6	4.971466	0.127443	-0.059851
6	6.197659	0.686755	0.448648
6	6.937498	0.081382	1.503023
1	6.571285	-0.833821	1.952588
6	8.101885	0.649458	1.972486
1	8.642523	0.171409	2.784308
6	8.596349	1.852272	1.414044
1	9.519002	2.284454	1.790090
6	7.895303	2.477486	0.408078
1	8.251785	3.412156	-0.017034
6	6.681649	1.927965	-0.087524
6	5.929921	2.599858	-1.088808
1	6.312607	3.527920	-1.503624
6	4.719228	2.102555	-1.502797
1	4.112092	2.613440	-2.241934
6	4.242881	0.890740	-0.958224
6	0.053911	2.510426	-0.430262
1	-0.748995	2.488318	0.311960
6	0.260371	3.950735	-0.879060
6	1.513368	4.412986	-1.303731
1	2.370135	3.750126	-1.245435
6	1.666549	5.717508	-1.776407
1	2.646567	6.064004	-2.094241
6	0.565011	6.575559	-1.836308
1	0.682549	7.592150	-2.201479
6	-0.687251	6.118647	-1.417117
1	-1.549236	6.779397	-1.453428
6	-0.840407	4.815951	-0.937307
1	-1.817646	4.472734	-0.617219
6	-0.370718	1.667861	-1.642706

1	0.217174	1.977899	-2.513474
1	-1.418632	1.876049	-1.869532
6	1.678533	2.590126	1.491665
1	1.375480	3.629668	1.342460
6	0.856629	2.066316	2.667818
6	-0.368606	2.682511	2.959328
1	-0.714954	3.520945	2.365702
6	-1.172247	2.227042	4.006996
1	-2.122989	2.715653	4.198022
6	-0.752990	1.154152	4.794359
1	-1.373292	0.798138	5.612194
6	0.475670	0.541934	4.525393
1	0.815406	-0.288855	5.138369
6	1.273738	0.994209	3.472802
1	2.222869	0.508760	3.282261
6	3.186664	2.623459	1.732501
1	3.694140	3.083922	0.882088
1	3.619019	1.637426	1.896309
1	3.383217	3.231977	2.620563
6	-0.860600	-0.843910	0.597771
1	-0.815745	-1.915372	0.739053
1	-0.430767	-0.277238	1.419053
6	-1.966960	-0.233170	-0.064648
1	-2.182051	0.793386	0.199342
6	-2.683459	-0.812548	-1.116610
1	-2.663002	-1.887362	-1.245348
6	0.931834	-0.436964	-3.430521
1	1.388265	0.545577	-3.498188
6	-0.450388	-0.511080	-3.675991
1	-0.967267	0.414000	-3.925713
6	-1.185261	-1.765910	-4.105020
1	-1.026916	-1.915555	-5.183270
1	-2.252437	-1.578570	-3.977959
6	-0.798111	-3.053752	-3.341248
1	0.002162	-3.580505	-3.869492
1	-1.658712	-3.729989	-3.343399
6	-0.366369	-2.843571	-1.895959
1	-1.059761	-3.195416	-1.137902
6	0.933887	-2.619735	-1.493070
1	1.163186	-2.833101	-0.454202
6	2.130577	-2.492252	-2.411116
1	2.959129	-2.085404	-1.830141
1	2.437853	-3.499802	-2.725958
6	1.897348	-1.601156	-3.650304
1	1.531481	-2.204233	-4.486909
1	2.860410	-1.190592	-3.966068
6	-3.738823	-0.108714	-1.853815
6	-4.061290	1.243768	-1.616495
6	-4.505696	-0.819273	-2.799753
6	-5.109654	1.855469	-2.299292
1	-3.528992	1.822900	-0.874575
6	-5.549817	-0.201533	-3.487831
1	-4.290043	-1.869035	-2.978904
6	-5.856307	1.140058	-3.240780
1	-5.341798	2.891907	-2.073929
1	-6.129265	-0.770389	-4.209483
1	-6.674794	1.619659	-3.769878
8	-2.212068	-4.451180	0.733471
6	-1.288357	-4.185535	1.448610
8	-0.108438	-4.210350	1.657333
8	-2.061391	-3.354015	2.926778
6	-1.140620	-2.710906	3.803597
1	-0.737240	-1.785704	3.375626
1	-1.638914	-2.473886	4.751573
1	-0.310577	-3.392605	4.004561
6	-3.557559	-0.341080	3.079149
6	-4.777184	0.561870	3.191025
1	-2.793571	0.154344	2.471190
1	-3.106699	-0.518131	4.060929
6	-5.488655	0.575830	1.847550
1	-4.487832	1.582510	3.445813
1	-5.456193	0.185687	3.965908
1	-6.427389	1.132871	1.913269
1	-4.863133	1.072543	1.099980
7	-3.889438	-1.644344	2.497329
6	-4.947956	-1.803348	1.743149
7	-5.806434	-0.795883	1.409077
6	-5.211390	-3.230354	1.289338
1	-4.331451	-3.805993	1.570238
1	-6.051627	-3.630498	1.870415
6	-5.475001	-3.408097	-0.215078
1	-4.860987	-2.688668	-0.765040
6	-6.797712	-0.833988	0.312900
6	-6.951405	-3.234464	-0.598326
1	-7.022849	-3.027220	-1.673472
6	-7.637034	-2.107810	0.187419
1	-8.574123	-1.838666	-0.313090
1	-7.914194	-2.444143	1.192908
1	-7.472184	0.002078	0.513895
1	-6.300534	-0.608490	-0.640320
1	-7.495262	-4.170989	-0.422559
1	-5.126193	-4.400317	-0.520364
1	-2.887731	-2.661229	2.693787
5	-3.579226	3.662154	1.305852
9	-2.921716	2.399324	1.281814
9	-4.704668	3.575753	2.133932
9	-3.966454	3.983638	-0.013612
9	-2.683206	4.627609	1.787732

14' P1-*endo*-*re* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 16.4291 22.7816 23.7797 cm(-1)
Electronic energy= -3892.0133451
Zero-point correction= 1.229876
(Hartree/Particle)
Thermal correction to Energy= 1.304178
Thermal correction to Enthalpy= 1.305122
Thermal correction to Gibbs Free Energy= 1.118060
Sum of electronic and zero-point Energies= -3890.783469
Sum of electronic and thermal Energies= -3890.709168
Sum of electronic and thermal Enthalpies= -3890.708223
Sum of electronic and thermal Free Energies= -3890.895286

.....

Cartesian Coordinates

.....

77	-0.181320	-0.446533	-1.413549
15	1.619610	0.484387	-0.375173
8	2.302905	-0.127847	0.989656
8	2.934853	0.498729	-1.394287
7	1.207884	1.996972	0.174786
6	3.150998	-1.231468	0.947815
6	2.655579	-2.421724	1.520443
1	1.666667	-2.413152	1.963925
6	3.429407	-3.555106	1.493367
1	3.057534	-4.479123	1.924656
6	4.702404	-3.543677	0.862242
6	5.478322	-4.730519	0.761188
1	5.087317	-5.643127	1.203251
6	6.689655	-4.730487	0.107715
1	7.272177	-5.644009	0.032611
6	7.170158	-3.537173	-0.482581
1	8.114370	-3.545363	-1.019480
6	6.449960	-2.365951	-0.389714
1	6.830956	-1.465366	-0.856263
6	5.204926	-2.321919	0.298307
6	4.422196	-1.117399	0.407456
6	4.923887	0.202653	-0.068436
6	6.153865	0.774845	0.415869
6	6.907522	0.191808	1.473020
1	6.548756	-0.715327	1.944437
6	8.076154	0.771366	1.917254
1	8.627629	0.310279	2.731581
6	8.561219	1.964140	1.329751
1	9.487321	2.405414	1.686224
6	7.846771	2.568204	0.320305
1	8.195806	3.495023	-0.127524
6	6.628762	2.006433	-0.150071
6	5.864434	2.656883	-1.155989
1	6.240305	3.577524	-1.592994

6	4.650912	2.148408	-1.547295
1	4.034162	2.643142	-2.289563
6	4.184159	0.945972	-0.974342
6	-0.024814	2.539959	-0.452966
1	-0.824074	2.518776	0.293025
6	0.157609	3.974989	-0.927928
6	1.398109	4.444153	-1.381381
1	2.264209	3.792949	-1.324562
6	1.527256	5.741235	-1.880740
1	2.497449	6.093682	-2.221332
6	0.414254	6.584696	-1.938386
1	0.513346	7.595407	-2.324740
6	-0.825179	6.121147	-1.489646
1	-1.695729	6.770660	-1.524118
6	-0.954420	4.825926	-0.983026
1	-1.922440	4.476579	-0.641650
6	-0.438571	1.671960	-1.650144
1	0.143703	1.977049	-2.526391
1	-1.489376	1.861673	-1.878926
6	1.620068	2.687539	1.447581
1	1.315197	3.721852	1.268729
6	0.808218	2.201615	2.646032
6	-0.410121	2.832962	2.933590
1	-0.761882	3.652059	2.316407
6	-1.200616	2.417024	4.007270
1	-2.146131	2.917016	4.194769
6	-0.774355	1.369732	4.824584
1	-1.383979	1.045359	5.663274
6	0.446278	0.741222	4.557524
1	0.790632	-0.070552	5.192791
6	1.230544	1.152888	3.478163
1	2.173450	0.654918	3.288498
6	3.129929	2.730980	1.676945
1	3.630861	3.164947	0.808917
1	3.566082	1.751979	1.870542
1	3.330288	3.368789	2.543308
6	-0.907679	-0.861911	0.615992
1	-0.904485	-1.936592	0.771999
1	-0.470428	-0.302312	1.437801
6	-2.003875	-0.229550	-0.041943
1	-2.215889	0.796132	0.227983
6	-2.720720	-0.805937	-1.096828
1	-2.697888	-1.880842	-1.224157
6	0.886758	-0.436600	-3.412303
1	1.337662	0.547696	-3.488985
6	-0.495603	-0.520775	-3.656431
1	-1.017629	0.398495	-3.916204
6	-1.221857	-1.784530	-4.074380
1	-1.058517	-1.947660	-5.149847
1	-2.290721	-1.602752	-3.952709
6	-0.826900	-3.056372	-3.289455
1	-0.023281	-3.588047	-3.807308
1	-1.682781	-3.738513	-3.276991
6	-0.397365	-2.810616	-1.848812
1	-1.092920	-3.144708	-1.086573
6	0.904853	-2.581296	-1.446435
1	1.140522	-2.779595	-0.406128
6	2.099869	-2.469536	-2.369012
1	2.928340	-2.051083	-1.796294
1	2.408261	-3.481379	-2.668790
6	1.859384	-1.597407	-3.620294
1	1.495957	-2.214220	-4.447855
1	2.819138	-1.184987	-3.943477
6	-3.784520	-0.110926	-1.828564
6	-4.115312	1.239206	-1.590633
6	-4.555185	-0.830665	-2.764514
6	-5.174126	1.841297	-2.265776
1	-3.582010	1.822087	-0.852697
6	-5.610826	-0.223030	-3.443651
1	-4.333824	-1.879682	-2.941788
6	-5.924087	1.117361	-3.198051
1	-5.412053	2.876339	-2.040365
1	-6.193909	-0.798356	-4.157242
1	-6.751285	1.589187	-3.720595
8	-1.755123	-5.120403	0.426435
6	-0.715275	-4.961725	0.940901
8	0.370806	-4.887938	1.372083
8	-1.599183	-3.291514	2.643583
6	-0.705665	-2.775168	3.607652
1	-0.334679	-1.770375	3.354515
1	-1.157516	-2.717057	4.611496
1	0.158133	-3.446480	3.672405
6	-3.481119	-0.323785	3.167058
6	-4.738806	0.528776	3.277615
1	-2.739567	0.204082	2.556819
1	-3.016421	-0.470916	4.149020
6	-5.464670	0.486773	1.940802
1	-4.494879	1.565981	3.515342
1	-5.394541	0.135570	4.064406
1	-6.423193	1.010130	2.004965
1	-4.864904	0.994625	1.178197
7	-3.739574	-1.643633	2.592423
6	-4.791652	-1.856667	1.854563
7	-5.732264	-0.904888	1.537565
6	-4.962159	-3.297868	1.387490
1	-4.022763	-3.797213	1.629231
1	-5.732774	-3.779427	2.003620
6	-5.290136	-3.494063	-0.102000
1	-4.767791	-2.728353	-0.683155
6	-6.736836	-1.013202	0.463003
6	-6.793340	-3.433688	-0.405902
1	-6.936155	-3.262622	-1.480379
6	-7.510629	-2.333313	0.389833
1	-8.482255	-2.128631	-0.074081
1	-7.724233	-2.666972	1.411764
1	-7.450815	-0.208747	0.659020
1	-6.277633	-0.786004	-0.509837
1	-7.259115	-4.400502	-0.177405
1	-4.886242	-4.457584	-0.432379
1	-2.419194	-2.707264	2.627092
5	-3.676162	3.666521	1.299164
9	-2.976343	2.427251	1.266092
9	-4.808726	3.531961	2.110381
9	-4.057470	3.993958	-0.021233
9	-2.818172	4.654406	1.804741

[13'-14'] P1-*endo-re* [BF_4^-] conf2

Number of imaginary frequencies= 1
The smallest frequencies are=-854.3408 11.9374 17.3799cm(-1)
Electronic energy= -3892.0000937
Zero-point correction= 1.226904
(Hartree/Particle)
Thermal correction to Energy= 1.300235
Thermal correction to Enthalpy= 1.301179
Thermal correction to Gibbs Free Energy= 1.115254
Sum of electronic and zero-point Energies= -3890.773190
Sum of electronic and thermal Energies= -3890.699859
Sum of electronic and thermal Enthalpies= -3890.698915
Sum of electronic and thermal Free Energies= -3890.884840

.....

Cartesian Coordinates

.....

77	0.135427	-0.708930	1.820428
15	1.666294	-0.678064	0.128314
8	1.914555	0.612670	-0.858768
8	3.201072	-0.885413	0.735623
7	1.252412	-1.812919	-1.012209
6	2.572785	1.748508	-0.395881
6	1.778641	2.901532	-0.223943
1	0.720527	2.843628	-0.461012
6	2.362563	4.049659	0.252436
1	1.764024	4.945267	0.388756
6	3.739032	4.064351	0.608550
6	4.333290	5.222513	1.179581
1	3.716173	6.107203	1.313040
6	5.653795	5.222936	1.568645
1	6.095390	6.112212	2.008858
6	6.434716	4.053429	1.408792
1	7.469499	4.048445	1.739121

6	5.894290	2.918297	0.844144
1	6.505012	2.029422	0.738368
6	4.539809	2.887941	0.409497
6	3.940131	1.716096	-0.176162
6	4.726619	0.497241	-0.520807
6	5.864074	0.548257	-1.404460
6	6.242263	1.730207	-2.101642
1	5.655642	2.632275	-1.976425
6	7.330579	1.741206	-2.946952
1	7.591361	2.654915	-3.473386
6	8.106551	0.574097	-3.143016
1	8.965492	0.599941	-3.807170
6	7.756694	-0.593379	-2.503630
1	8.329168	-1.503860	-2.660761
6	6.629507	-0.644198	-1.639201
6	6.233476	-1.864504	-1.028109
1	6.825022	-2.758828	-1.201971
6	5.096718	-1.921694	-0.261293
1	4.748722	-2.848454	0.182669
6	4.345691	-0.747015	-0.041133
6	0.219806	-2.775243	-0.548009
1	-0.727699	-2.516792	-1.028931
6	0.573298	-4.207928	-0.917415
6	1.898995	-4.663586	-0.873338
1	2.694218	-3.963268	-0.632393
6	2.199179	-5.996512	-1.156323
1	3.231422	-6.335560	-1.127076
6	1.175742	-6.892893	-1.480189
1	1.408831	-7.930469	-1.703084
6	-0.146830	-6.445220	-1.519658
1	-0.948551	-7.133407	-1.773584
6	-0.448525	-5.108953	-1.243392
1	-1.479935	-4.770629	-1.272222
6	0.055841	-2.681247	0.974765
1	0.846078	-3.273766	1.447955
1	-0.897619	-3.132127	1.257346
6	1.438009	-1.760603	-2.504881
1	1.268614	-2.798227	-2.803869
6	0.354586	-0.935419	-3.195511
6	-0.835300	-1.572000	-3.573302
1	-0.981964	-2.625461	-3.363564
6	-1.858564	-0.869124	-4.212024
1	-2.772933	-1.393880	-4.467144
6	-1.698346	0.486387	-4.500549
1	-2.489345	1.038056	-5.001344
6	-0.512599	1.132678	-4.136258
1	-0.377177	2.187268	-4.357482
6	0.504126	0.429460	-3.488032
1	1.415152	0.947532	-3.214528
6	2.861637	-1.428420	-2.947338
1	3.570227	-2.124168	-2.493618
1	3.167768	-0.414183	-2.694139
1	2.920811	-1.538481	-4.034457
6	-1.079597	0.537576	0.474133
1	-1.168798	1.516523	0.929054
1	-0.806826	0.575396	-0.575459
6	-1.936107	-0.529511	0.866441
1	-2.134132	-1.297630	0.132136
6	-2.420514	-0.706636	2.168992
1	-2.445690	0.139438	2.846327
6	1.665766	-1.515691	3.276171
1	2.174939	-2.315379	2.747056
6	0.384086	-1.807481	3.778871
1	0.000007	-2.813138	3.616409
6	-0.287136	-1.069699	4.920195
1	0.123551	-1.437280	5.872306
1	-1.341944	-1.350580	4.914258
6	-0.169221	0.469315	4.858512
1	0.711506	0.805784	5.413814
1	-1.034075	0.906799	5.366894
6	-0.103345	1.045594	3.449790
1	-0.973136	1.605112	3.117807
6	1.072380	1.277980	2.759067
1	1.031108	2.007248	1.956996
6	2.461492	0.945245	3.259330
1	3.150497	1.034140	2.419064
1	2.762281	1.708724	3.991023
6	2.596844	-0.463190	3.877507
1	2.425522	-0.423088	4.957802
1	3.627434	-0.802963	3.742983
6	-3.203603	-1.876329	2.584633
6	-3.480581	-2.953900	1.716833
6	-3.729835	-1.921548	3.891242
6	-4.233895	-4.040855	2.152485
1	-3.147496	-2.940848	0.687805
6	-4.476847	-3.015303	4.326584
1	-3.558061	-1.083904	4.562568
6	-4.726856	-4.084020	3.460490
1	-4.442516	-4.844460	1.452603
1	-4.870312	-3.029920	5.339192
1	-5.312850	-4.934502	3.797274
8	-1.634933	3.617990	1.637192
6	-1.226930	4.383406	0.820042
8	-0.758910	5.417468	0.464586
8	-1.456066	3.344332	-0.871569
6	-1.167208	4.046392	-2.064076
1	-0.139493	3.848050	-2.398038
1	-1.851501	3.734904	-2.865998
1	-1.268821	5.131945	-1.927282
6	-3.741828	0.884598	-1.543630
6	-4.883815	0.582378	-2.500075
1	-3.871204	0.301545	-0.625459
1	-2.779153	0.600084	-1.969186
6	-6.167411	1.141863	-1.905647
1	-4.985232	-0.495196	-2.645456
1	-4.688453	1.048152	-3.473115
1	-6.985055	1.084134	-2.630465
1	-6.466901	0.557954	-1.024277
7	-3.694586	2.310279	-1.214157
6	-4.782365	3.040916	-1.202116
7	-6.013730	2.560958	-1.524277
6	-4.579211	4.507904	-0.855542
1	-3.553519	4.593198	-0.501362
1	-4.633824	5.095964	-1.779848
6	-5.541659	5.085814	0.196964
1	-5.764397	4.313404	0.942499
6	-7.300253	3.222746	-1.219498
6	-6.841935	5.624107	-0.415858
1	-7.595135	5.732842	0.374000
6	-7.387396	4.719801	-1.531257
1	-8.440970	4.961602	-1.710460
1	-6.866930	4.907188	-2.477276
1	-8.039254	2.700415	-1.831283
1	-7.571970	3.031840	-0.171378
1	-6.670410	6.627093	-0.825577
1	-5.029673	5.888471	0.738190
1	-2.525170	2.845943	-0.983308
5	-3.767455	-3.230183	-2.075601
9	-3.045470	-2.140615	-1.521355
9	-5.093778	-2.834585	-2.295773
9	-3.723311	-4.304783	-1.159353
9	-3.165115	-3.616097	-3.283483

13' P1-*exo*-*si* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 19.9193 24.3672 25.2023 cm(-1)
Electronic energy= -3892.0316167
Zero-point correction= 1.234459
(Hartree/Particle)
Thermal correction to Energy= 1.307014
Thermal correction to Enthalpy= 1.307958
Thermal correction to Gibbs Free Energy= 1.126722
Sum of electronic and zero-point Energies= -3890.797158
Sum of electronic and thermal Energies= -3890.724602
Sum of electronic and thermal Enthalpies= -3890.723658
Sum of electronic and thermal Free Energies= -3890.904895
.....
Cartesian Coordinates
.....

77	-0.169447	-0.227210	-1.387304
15	1.739889	0.333474	-0.332972
8	2.341964	-0.442908	0.981636
8	3.039794	0.231701	-1.371662
7	1.578771	1.873510	0.284774
6	3.110651	-1.602955	0.879778
6	2.522127	-2.783511	1.377605
1	1.514014	-2.748721	1.776610
6	3.219930	-3.963158	1.295216
1	2.777928	-4.882721	1.668569
6	4.502556	-4.009573	0.686313
6	5.196133	-5.240758	0.529258
1	4.735496	-6.146309	0.915462
6	6.413899	-5.291198	-0.110185
1	6.932081	-6.238265	-0.229679
6	6.984025	-4.104618	-0.630307
1	7.932319	-4.150004	-1.158249
6	6.345378	-2.892711	-0.480861
1	6.793971	-1.998390	-0.896382
6	5.096494	-2.797861	0.195938
6	4.396159	-1.549578	0.362177
6	4.995616	-0.252357	-0.056443
6	6.259815	0.212422	0.452175
6	6.955176	-0.454203	1.499591
1	6.523513	-1.345696	1.938914
6	8.157280	0.025156	1.973044
1	8.663476	-0.497405	2.779659
6	8.735565	1.194598	1.424103
1	9.687047	1.556660	1.802499
6	8.080926	1.876433	0.423499
1	8.504310	2.786075	0.005559
6	6.830870	1.419404	-0.075680
6	6.130091	2.147695	-1.074887
1	6.580245	3.045831	-1.488163
6	4.886093	1.740863	-1.489834
1	4.318414	2.296309	-2.228030
6	4.320199	0.567727	-0.945393
6	0.478029	2.647068	-0.342880
1	-0.328446	2.748717	0.388433
6	0.925922	4.039432	-0.772581
6	2.266929	4.329953	-1.054351
1	3.017341	3.564086	-0.899603
6	2.642509	5.595586	-1.510058
1	3.689432	5.804069	-1.715544
6	1.678488	6.589265	-1.694741
1	1.968220	7.575516	-2.047076
6	0.338408	6.306212	-1.414840
1	-0.419194	7.074026	-1.548339
6	-0.036928	5.043143	-0.953339
1	-1.076263	4.831501	-0.733128
6	-0.079770	1.896614	-1.564688
1	0.552606	2.121224	-2.431509
1	-1.071030	2.294850	-1.782733
6	2.028686	2.405532	1.618614
1	1.875514	3.482426	1.509256
6	1.114276	1.952201	2.755820
6	-0.040043	2.695944	3.041988
1	-0.274752	3.585250	2.465960
6	-0.918345	2.299626	4.053647
1	-1.813471	2.885124	4.241346
6	-0.645702	1.160799	4.812171
1	-1.322983	0.852949	5.604236
6	0.511945	0.421307	4.549080
1	0.740538	-0.461564	5.140136
6	1.381188	0.812013	3.529634
1	2.269195	0.222034	3.339377
6	3.520046	2.219504	1.895228
1	4.111952	2.620837	1.069979
1	3.802871	1.178451	2.041133
1	3.777725	2.771671	2.804471
6	-0.991858	-0.191225	0.647148
1	-0.950941	0.815753	1.046393
1	-0.598284	-0.957413	1.308093
6	-2.151554	-0.558465	-0.122410
1	-2.469572	-1.595124	-0.102543
6	-2.806709	0.354300	-0.934669
1	-2.600255	1.404074	-0.773380
6	0.950641	-0.378101	-3.356717
1	1.540914	0.531551	-3.411790
6	-0.417930	-0.242655	-3.639978
1	-0.768695	0.755614	-3.899487
6	-1.349770	-1.346585	-4.094208
1	-1.280758	-1.444250	-5.188331
1	-2.372345	-1.022630	-3.885975
6	-1.121215	-2.725804	-3.438293
1	-0.362613	-3.284868	-3.993806
1	-2.048410	-3.301988	-3.523282
6	-0.724141	-2.679223	-1.972330
1	-1.487855	-2.937343	-1.243711
6	0.566288	-2.665710	-1.510121
1	0.692649	-2.916324	-0.460957
6	1.812524	-2.626748	-2.363996
1	2.652934	-2.353286	-1.724236
1	2.022521	-3.644764	-2.722949
6	1.761646	-1.657097	-3.566546
1	1.368432	-2.170893	-4.449057
1	2.787408	-1.368032	-3.811894
6	-3.936373	0.077602	-1.815965
6	-4.287203	-1.216965	-2.249341
6	-4.720098	1.168760	-2.245229
6	-5.391656	-1.410828	-3.076608
1	-3.688379	-2.068994	-1.944356
6	-5.828045	0.968891	-3.067726
1	-4.455935	2.166755	-1.906028
6	-6.168359	-0.320758	-3.486818
1	-5.647551	-2.414999	-3.402531
1	-6.426280	1.819721	-3.381286
1	-7.028567	-0.477130	-4.131321
8	-2.652804	-3.656480	0.769433
6	-1.741480	-3.445206	1.597322
8	-0.502931	-3.449680	1.477185
8	-2.256244	-3.137851	2.899192
6	-1.290979	-2.735769	3.873839
1	-1.845007	-2.546826	4.798371
1	-0.549365	-3.522115	4.046244
1	-0.767865	-1.824099	3.569993
6	-3.745501	0.085274	3.041625
6	-4.847522	1.127319	2.950142
1	-2.878760	0.402781	2.460479
1	-3.420357	-0.076926	4.073206
6	-5.486335	1.045482	1.570044
1	-4.433520	2.126799	3.079821
1	-5.608354	0.953606	3.719277
1	-6.320595	1.742135	1.488309
1	-4.756016	1.302827	0.799905
7	-4.238719	-1.192920	2.523324
6	-5.314634	-1.366306	1.763290
7	-6.006932	-0.318201	1.311415
6	-5.662182	-2.818356	1.497721
1	-4.714374	-3.359715	1.568788
1	-6.301914	-3.156737	2.323203
6	-6.302048	-3.148615	0.144740
1	-5.773740	-2.595919	-0.635729
6	-7.183790	-0.389185	0.412798
6	-7.804790	-2.857282	0.073199
1	-8.116516	-2.855743	-0.978467
6	-8.172765	-1.515992	0.722261
1	-9.161884	-1.198190	0.375032
1	-8.249157	-1.618642	1.810997
1	-7.689581	0.569935	0.533364
1	-6.836236	-0.437001	-0.626083
1	-8.367178	-3.658862	0.567428
1	-6.120351	-4.208662	-0.061895
1	-3.645652	-2.014126	2.698366
5	-3.068906	3.671204	0.869984
9	-2.589203	2.423027	1.327122
9	-4.371926	3.874075	1.346050
9	-3.077438	3.653361	-0.550606
9	-2.214013	4.686535	1.324202

[**13'-14'**] **P1**-*exo-si* [BF_4^-]

Number of imaginary frequencies= 1
The smallest frequencies are=-717.0067 18.7547 20.4633cm(-1)
Electronic energy= -3892.0043517
Zero-point correction= 1.226309
(Hartree/Particle)
Thermal correction to Energy= 1.299755
Thermal correction to Enthalpy= 1.300700
Thermal correction to Gibbs Free Energy= 1.116160
Sum of electronic and zero-point Energies= -3890.778043
Sum of electronic and thermal Energies= -3890.704596
Sum of electronic and thermal Enthalpies= -3890.703652
Sum of electronic and thermal Free Energies= -3890.888191

.....

Cartesian Coordinates

.....

77	-0.273723	0.148656	-1.506230
15	1.591792	0.637457	-0.346531
8	2.150735	-0.225131	0.936995
8	2.922443	0.575770	-1.344915
7	1.404121	2.117745	0.382090
6	2.743375	-1.471222	0.757825
6	2.010980	-2.586787	1.216531
1	1.056536	-2.418651	1.704881
6	2.524349	-3.847018	1.031351
1	1.969207	-4.713908	1.374875
6	3.757513	-4.030523	0.348537
6	4.250035	-5.334010	0.067643
1	3.674556	-6.189139	0.412450
6	5.418051	-5.512776	-0.638549
1	5.781093	-6.513570	-0.853543
6	6.140025	-4.386451	-1.100657
1	7.047994	-4.530187	-1.679417
6	5.699967	-3.108818	-0.829715
1	6.260198	-2.258722	-1.200813
6	4.508160	-2.885510	-0.085305
6	4.008255	-1.564638	0.198841
6	4.786141	-0.332960	-0.115151
6	6.113494	-0.117814	0.403923
6	6.721697	-0.996546	1.344018
1	6.170823	-1.859213	1.698963
6	7.992579	-0.759872	1.821546
1	8.429775	-1.443199	2.543946
6	8.730705	0.366696	1.387080
1	9.734134	0.535958	1.766550
6	8.164841	1.251949	0.497949
1	8.710678	2.133184	0.171066
6	6.850121	1.046273	-0.001782
6	6.246565	1.987277	-0.878795
1	6.815210	2.857919	-1.192689
6	4.950565	1.817919	-1.296532
1	4.456737	2.539323	-1.938370
6	4.229144	0.675730	-0.886515
6	0.260020	2.913599	-0.133193
1	-0.518376	2.926341	0.632589
6	0.686843	4.343169	-0.434373
6	1.894330	4.598110	-1.102403
1	2.544935	3.766037	-1.354988
6	2.266565	5.902933	-1.423774
1	3.207369	6.086299	-1.936369
6	1.432663	6.973470	-1.082980
1	1.721551	7.991147	-1.331139
6	0.230933	6.726089	-0.416729
1	-0.419528	7.552385	-0.142357
6	-0.140986	5.418089	-0.090137
1	-1.071218	5.233005	0.437233
6	-0.321825	2.273255	-1.401510
1	0.246999	2.637237	-2.263826
1	-1.346351	2.628077	-1.518182
6	1.941117	2.586552	1.705056
1	1.706464	3.654524	1.693944
6	1.178270	1.989037	2.887103
6	-0.043982	2.561226	3.273126
1	-0.440230	3.418374	2.738584
6	-0.774625	2.039132	4.342229
1	-1.724213	2.492082	4.611990
6	-0.284922	0.946630	5.059617
1	-0.847788	0.543187	5.896769
6	0.938989	0.378471	4.695523
1	1.336043	-0.465466	5.253180
6	1.661341	0.894249	3.618166
1	2.606291	0.437656	3.348616
6	3.461523	2.490215	1.811210
1	3.926975	3.032306	0.985343
1	3.827041	1.463632	1.793300
1	3.782715	2.948691	2.751488
6	-1.101262	-0.123670	0.503287
1	-1.121837	0.833919	1.010890
1	-0.690410	-0.932489	1.099174
6	-2.244084	-0.469657	-0.299245
1	-2.487598	-1.521442	-0.397526
6	-2.981545	0.478156	-0.986194
1	-2.842011	1.514833	-0.708312
6	0.884031	0.341473	-3.463857
1	1.435044	1.271843	-3.365615
6	-0.482236	0.463264	-3.753808
1	-0.872669	1.474244	-3.863398
6	-1.366330	-0.590081	-4.391134
1	-1.289774	-0.507206	-5.485693
1	-2.404055	-0.348757	-4.141682
6	-1.075875	-2.044152	-3.963215
1	-0.271848	-2.463665	-4.573625
1	-1.965249	-2.648521	-4.169492
6	-0.720333	-2.205711	-2.497687
1	-1.502059	-2.568213	-1.842161
6	0.553074	-2.209339	-1.993804
1	0.687511	-2.598081	-0.988916
6	1.813264	-2.004328	-2.803093
1	2.629675	-1.810519	-2.108208
1	2.059579	-2.946583	-3.313147
6	1.754492	-0.857396	-3.839702
1	1.412635	-1.238525	-4.806932
1	2.774058	-0.495212	-3.996757
6	-4.132578	0.209860	-1.841380
6	-4.360474	-1.028342	-2.475360
6	-5.089063	1.234173	-1.995063
6	-5.523554	-1.243365	-3.211312
1	-3.620267	-1.817058	-2.399229
6	-6.255548	1.011677	-2.725874
1	-4.912045	2.190500	-1.509933
6	-6.479450	-0.227624	-3.332661
1	-5.684201	-2.202643	-3.695279
1	-6.990783	1.805705	-2.820620
1	-7.387559	-0.400561	-3.902971
8	-1.503001	-3.660252	0.279112
6	-1.013634	-4.158780	1.248460
8	-0.462057	-5.057511	1.803716
8	-1.226080	-2.774714	2.581044
6	-0.859723	-3.088331	3.913780
1	-0.252521	-2.282104	4.346483
1	-1.747871	-3.235825	4.546188
1	-0.273821	-4.013908	3.926001
6	-3.227108	-0.247337	3.267267
6	-4.527146	0.542887	3.324328
1	-2.489281	0.305509	2.682315
1	-2.798156	-0.380480	4.266519
6	-5.234320	0.407516	1.983351
1	-4.326335	1.598841	3.516881
1	-5.176933	0.160962	4.120770
1	-6.208143	0.901630	2.004266
1	-4.639031	0.882813	1.198931
7	-3.411369	-1.578016	2.685955
6	-4.471736	-1.898041	1.983904
7	-5.452937	-1.015363	1.659006
6	-4.551892	-3.359791	1.577965
1	-3.577127	-3.784955	1.808133
1	-5.266471	-3.864258	2.239990
6	-4.910515	-3.620009	0.107918
1	-4.459773	-2.835288	-0.506450

6	-6.557717	-1.241031	0.702205
6	-6.425301	-3.669672	-0.137549
1	-6.623986	-3.502130	-1.203269
6	-7.192735	-2.632689	0.694641
1	-8.206131	-2.526655	0.291331
1	-7.311957	-2.970544	1.730289
1	-7.326410	-0.514913	0.979481
1	-6.222393	-0.971365	-0.308024
1	-6.809392	-4.669046	0.101873
1	-4.447504	-4.558942	-0.212217
1	-2.267554	-2.274406	2.597145
5	-3.363386	3.539167	1.141663
9	-2.648983	2.386424	1.539755
9	-4.697341	3.425353	1.550806
9	-3.304224	3.644938	-0.271256
9	-2.761722	4.668781	1.726142

14' P1-*exo-si* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 16.5970 21.3308 24.2483 cm(-1)
Electronic energy= -3892.0103178
Zero-point correction= 1.229271 (Hartree/Particle)
Thermal correction to Energy= 1.303960
Thermal correction to Enthalpy= 1.304904
Thermal correction to Gibbs Free Energy= 1.116339
Sum of electronic and zero-point Energies= -3890.781047
Sum of electronic and thermal Energies= -3890.706358
Sum of electronic and thermal Enthalpies= -3890.705414
Sum of electronic and thermal Free Energies= -3890.893979

.....

Cartesian Coordinates

.....

77	-0.299340	0.181699	-1.493650
15	1.577225	0.649564	-0.344934
8	2.134101	-0.239018	0.920710
8	2.902964	0.594215	-1.350631
7	1.401718	2.120693	0.404008
6	2.739270	-1.476329	0.726338
6	2.015114	-2.604908	1.169006
1	1.049935	-2.453560	1.644479
6	2.551386	-3.855806	0.981904
1	2.017366	-4.736920	1.324243
6	3.792600	-4.019389	0.308417
6	4.307809	-5.314047	0.027712
1	3.744705	-6.179650	0.366942
6	5.483052	-5.472065	-0.671457
1	5.863918	-6.466263	-0.886131
6	6.189254	-4.333117	-1.126744
1	7.102709	-4.460589	-1.700591
6	5.727254	-3.063524	-0.854647
1	6.276390	-2.203619	-1.219507
6	4.528127	-2.861359	-0.115977
6	4.008866	-1.549230	0.174787
6	4.774586	-0.306798	-0.127253
6	6.098456	-0.081382	0.396534
6	6.710968	-0.956489	1.337105
1	6.166530	-1.824878	1.688043
6	7.977457	-0.708715	1.820707
1	8.417859	-1.389105	2.543908
6	8.706923	0.425490	1.391563
1	9.707001	0.603522	1.775807
6	8.136714	1.307060	0.501574
1	8.675510	2.194065	0.178627
6	6.825975	1.090267	-0.003730
6	6.217426	2.027602	-0.881159
1	6.779977	2.903065	-1.192571
6	4.923579	1.849053	-1.301606
1	4.426180	2.567796	-1.943571
6	4.210112	0.700712	-0.894695
6	0.254567	2.926295	-0.090396
1	-0.512888	2.937452	0.686493
6	0.681769	4.356588	-0.386741
6	1.889313	4.615658	-1.052610
1	2.542116	3.785535	-1.305177
6	2.258068	5.921893	-1.372809
1	3.199093	6.108338	-1.883916
6	1.420218	6.989632	-1.033317
1	1.706070	8.008312	-1.280897
6	0.217694	6.738002	-0.369912
1	-0.436769	7.561872	-0.097751
6	-0.150519	5.428810	-0.044340
1	-1.084171	5.241239	0.476362
6	-0.353630	2.301921	-1.355919
1	0.191895	2.682115	-2.226031
1	-1.382153	2.653888	-1.439961
6	1.943676	2.568138	1.733233
1	1.719731	3.638466	1.734367
6	1.174272	1.962995	2.906918
6	-0.027634	2.560247	3.317882
1	-0.398264	3.444336	2.808784
6	-0.766308	2.031404	4.378049
1	-1.700179	2.504134	4.667969
6	-0.306365	0.902956	5.058484
1	-0.877258	0.491690	5.886298
6	0.896421	0.308261	4.668989
1	1.266525	-0.568020	5.193970
6	1.629262	0.834561	3.604178
1	2.558881	0.358713	3.316226
6	3.462664	2.455099	1.840910
1	3.935910	2.998261	1.020245
1	3.817527	1.425027	1.816868
1	3.786032	2.903347	2.785367
6	-1.121113	-0.078295	0.523744
1	-1.167099	0.889121	1.010877
1	-0.685613	-0.858960	1.138933
6	-2.252687	-0.460320	-0.276138
1	-2.479131	-1.517177	-0.367007
6	-3.005670	0.464610	-0.979112
1	-2.884674	1.506455	-0.712841
6	0.849760	0.396867	-3.455840
1	1.395759	1.329734	-3.352710
6	-0.517793	0.512463	-3.740317
1	-0.915222	1.521978	-3.838013
6	-1.398143	-0.540935	-4.382246
1	-1.326412	-0.449822	-5.476394
1	-2.436094	-0.308759	-4.126053
6	-1.097000	-1.996296	-3.966341
1	-0.291872	-2.406336	-4.581650
1	-1.983170	-2.604743	-4.174173
6	-0.736018	-2.165411	-2.503136
1	-1.516458	-2.535093	-1.850951
6	0.538905	-2.167421	-2.003869
1	0.683711	-2.564120	-1.003606
6	1.792190	-1.953976	-2.822217
1	2.615958	-1.771187	-2.133209
1	2.030607	-2.890188	-3.346943
6	1.725811	-0.794117	-3.844723
1	1.384834	-1.165829	-4.815935
1	2.743316	-0.425157	-3.998389
6	-4.151465	0.167052	-1.832174
6	-4.360787	-1.081348	-2.452228
6	-5.123187	1.174966	-1.998235
6	-5.518355	-1.321261	-3.189081
1	-3.611477	-1.859534	-2.365233
6	-6.284700	0.927152	-2.728701
1	-4.962008	2.138673	-1.522606
6	-6.488629	-0.321192	-3.323659
1	-5.664162	-2.288373	-3.662138
1	-7.031849	1.708826	-2.832404
1	-7.392837	-0.513603	-3.893960
8	-1.382800	-3.971608	0.100605
6	-0.926555	-4.605158	0.973726
8	-0.469711	-5.340939	1.760713
8	-1.001009	-2.650896	2.625964
6	-0.630964	-3.014031	3.944041
1	-0.752510	-2.180500	4.649903

1	-1.212982	-3.869002	4.321922
1	0.426246	-3.302086	3.943498
6	-3.348029	-0.109134	3.321416
6	-4.683858	0.626373	3.281912
1	-2.606468	0.456661	2.750748
1	-2.964871	-0.165087	4.347273
6	-5.323323	0.387260	1.921844
1	-4.542308	1.699853	3.429254
1	-5.352021	0.253662	4.068060
1	-6.319987	0.833958	1.876644
1	-4.718527	0.858983	1.140539
7	-3.417233	-1.473263	2.799069
6	-4.421027	-1.865558	2.066298
7	-5.456917	-1.057335	1.667575
6	-4.392458	-3.342662	1.694028
1	-3.382981	-3.673913	1.938079
1	-5.063254	-3.891140	2.367937
6	-4.726379	-3.679885	0.232992
1	-4.333138	-2.887365	-0.411381
6	-6.512001	-1.391855	0.692948
6	-6.231698	-3.848251	-0.013985
1	-6.433667	-3.759984	-1.088812
6	-7.070851	-2.815848	0.752219
1	-8.083626	-2.793144	0.334066
1	-7.181557	-3.104961	1.803618
1	-7.329131	-0.696134	0.904707
1	-6.169132	-1.164500	-0.325900
1	-6.548209	-4.855912	0.283789
1	-4.196938	-4.594421	-0.055187
1	-1.916807	-2.227314	2.675430
5	-3.436662	3.580946	1.042914
9	-2.672208	2.486648	1.508962
9	-4.774846	3.414136	1.419314
9	-3.345652	3.629825	-0.372444
9	-2.914616	4.766555	1.589002

13' P1-*endo-re*

Number of imaginary frequencies= 0
The smallest frequencies = 10.1488 20.2479 23.6708 cm(-1)
Electronic energy= -3467.4038844
Zero-point correction= 1.217471
(Hartree/Particle)
Thermal correction to Energy= 1.284354
Thermal correction to Enthalpy= 1.285298
Thermal correction to Gibbs Free Energy= 1.113934
Sum of electronic and zero-point Energies= -3466.186414
Sum of electronic and thermal Energies= -3466.119531
Sum of electronic and thermal Enthalpies= -3466.118587
Sum of electronic and thermal Free Energies= -3466.289950

.....

Cartesian Coordinates

.....

77	-0.447445	-0.024230	-1.344821
15	1.498812	0.491171	-0.316612
8	2.139399	-0.406906	0.895279
8	2.760743	0.534027	-1.390018
7	1.309158	1.958447	0.464038
6	2.940335	-1.527681	0.660492
6	2.400032	-2.768088	1.057156
1	1.406738	-2.805767	1.492409
6	3.129316	-3.911429	0.841845
1	2.726343	-4.876015	1.136914
6	4.394264	-3.856714	0.197565
6	5.120265	-5.044102	-0.092297
1	4.696969	-5.996518	0.215782
6	6.323407	-4.993301	-0.758694
1	6.867586	-5.907054	-0.978942
6	6.844545	-3.744690	-1.174497
1	7.781157	-3.708959	-1.723471
6	6.173039	-2.573838	-0.897146
1	6.584447	-1.629907	-1.234091
6	4.938975	-2.585153	-0.187758
6	4.207592	-1.381771	0.116635
6	4.760819	-0.029086	-0.174540
6	6.019357	0.419781	0.362551
6	6.759982	-0.337377	1.312811
1	6.370598	-1.289843	1.652041
6	7.954071	0.129145	1.818283
1	8.495885	-0.464187	2.549192
6	8.478340	1.375658	1.400575
1	9.424201	1.726724	1.802505
6	7.778590	2.144408	0.498551
1	8.159803	3.112210	0.183363
6	6.535260	1.701342	-0.029350
6	5.786220	2.518364	-0.919104
1	6.193766	3.477388	-1.225979
6	4.548015	2.117637	-1.356978
1	3.940390	2.736059	-2.008528
6	4.043186	0.864535	-0.951332
6	0.090327	2.686061	0.020907
1	-0.681384	2.537908	0.785438
6	0.323439	4.180497	-0.110667
6	1.500578	4.691000	-0.674142
1	2.289825	4.005130	-0.965788
6	1.668141	6.066785	-0.834560
1	2.588365	6.451284	-1.265811
6	0.658448	6.949766	-0.438799
1	0.790885	8.020785	-0.562661
6	-0.517266	6.448350	0.124320
1	-1.303106	7.128025	0.442047
6	-0.679958	5.070837	0.291417
1	-1.590879	4.681756	0.741401
6	-0.418523	2.107456	-1.305786
1	0.214371	2.470932	-2.124059
1	-1.430484	2.475391	-1.493184
6	1.807178	2.373468	1.823178
1	1.685034	3.459621	1.801850
6	0.897094	1.856551	2.936736
6	-0.177080	2.655358	3.359223
1	-0.317439	3.635952	2.911165
6	-1.051553	2.219856	4.358753
1	-1.870487	2.859310	4.676935
6	-0.858217	0.974697	4.960408
1	-1.531440	0.633582	5.741566
6	0.216078	0.175221	4.558639
1	0.382795	-0.788847	5.030858
6	1.086401	0.612423	3.557918
1	1.913843	-0.020527	3.263234
6	3.295751	2.130106	2.066621
1	3.887929	2.575728	1.265328
1	3.557976	1.076538	2.143339
1	3.570668	2.617028	3.007361
6	-1.172177	-0.467757	0.665777
1	-1.231566	-1.545620	0.722990
1	-0.655687	-0.006175	1.502966
6	-2.231845	0.295597	0.083145
1	-2.323076	1.329945	0.395967
6	-3.042891	-0.147688	-0.961460
1	-3.110498	-1.213118	-1.144506
6	0.581265	0.034093	-3.372378
1	1.152319	0.957643	-3.363322
6	-0.799415	0.153927	-3.591129
1	-1.197720	1.156687	-3.740844
6	-1.700240	-0.951663	-4.102752
1	-1.589812	-1.012132	-5.195699
1	-2.731253	-0.644085	-3.921283
6	-1.467539	-2.351852	-3.485281
1	-0.748092	-2.912090	-4.090411
1	-2.407635	-2.910099	-3.539828
6	-0.993811	-2.363916	-2.038932
1	-1.702209	-2.700200	-1.283577
6	0.327074	-2.339594	-1.654425
1	0.524626	-2.681151	-0.642820
6	1.519330	-2.254009	-2.582744
1	2.401099	-2.021208	-1.983681
1	1.696612	-3.250409	-3.011974
6	1.391457	-1.214228	-3.718722
1	0.946965	-1.676828	-4.605173
1	2.396761	-0.896924	-4.009057

6	-4.038137	0.680964	-1.647362
6	-4.234454	2.050255	-1.369648
6	-4.876114	0.074783	-2.605814
6	-5.231272	2.774380	-2.020755
1	-3.619350	2.552909	-0.631221
6	-5.873156	0.800487	-3.255964
1	-4.745690	-0.980085	-2.829082
6	-6.056159	2.155020	-2.965512
1	-5.368034	3.826452	-1.787350
1	-6.507574	0.307467	-3.986776
1	-6.833934	2.722588	-3.467657
8	-2.799322	-3.591244	0.499032
6	-1.890627	-3.637703	1.354420
8	-0.653559	-3.716794	1.238195
8	-2.407816	-3.549938	2.688168
6	-1.436692	-3.416835	3.727986
1	-0.855570	-2.493362	3.622003
1	-1.992157	-3.393225	4.670192
1	-0.742781	-4.262623	3.732513
6	-3.595467	-0.363493	3.381726
6	-4.564501	0.798393	3.527501
1	-2.663650	-0.040825	2.909257
1	-3.336776	-0.798017	4.351011
6	-5.163141	1.123924	2.164158
1	-4.043242	1.674333	3.921626
1	-5.368404	0.538877	4.224114
1	-5.923378	1.901103	2.255127
1	-4.394630	1.488216	1.472981
7	-4.209108	-1.411398	2.568533
6	-5.255248	-1.267978	1.764059
7	-5.809870	-0.067376	1.569865
6	-5.735582	-2.551815	1.121116
1	-4.871215	-3.221652	1.127931
1	-6.502101	-2.987803	1.773923
6	-6.245191	-2.427135	-0.319516
1	-5.595835	-1.730211	-0.855629
6	-6.953963	0.230237	0.670545
6	-7.704038	-1.969036	-0.419927
1	-7.901887	-1.620726	-1.440872
6	-8.030859	-0.852038	0.579258
1	-8.964776	-0.359764	0.287546
1	-8.201681	-1.261760	1.581276
1	-7.402635	1.137866	1.078027
1	-6.563048	0.482127	-0.322096
1	-8.376319	-2.816054	-0.238562
1	-6.121872	-3.397399	-0.811307
1	-3.722737	-2.317507	2.573305

[**13'-14'**]‡ **P1** *endo-re*

Number of imaginary frequencies= 1
The smallest frequencies are= -265.8285 13.5242 16.5706 cm(-1)
Electronic energy= -3467.3792646
Zero-point correction= 1.211686 (Hartree/Particle)
Thermal correction to Energy= 1.278715
Thermal correction to Enthalpy= 1.279659
Thermal correction to Gibbs Free Energy= 1.107396
Sum of electronic and zero-point Energies= -3466.167579
Sum of electronic and thermal Energies= -3466.100549
Sum of electronic and thermal Enthalpies= -3466.099605
Sum of electronic and thermal Free Energies= -3466.271869

.....

Cartesian Coordinates

.....

77	-0.426616	-0.040167	-1.322550
15	1.519042	0.501711	-0.305683
8	2.153968	-0.366977	0.931694
8	2.777530	0.503339	-1.381725
7	1.334800	1.987705	0.434764
6	2.929348	-1.509000	0.722634
6	2.369693	-2.725870	1.164292
1	1.392470	-2.717485	1.633810
6	3.065361	-3.893412	0.969865
1	2.647544	-4.839335	1.301975
6	4.319518	-3.885176	0.302211
6	5.011809	-5.096994	0.032190
1	4.570962	-6.030731	0.371012
6	6.205333	-5.092253	-0.653124
1	6.723955	-6.024237	-0.857841
6	6.750279	-3.867710	-1.107874
1	7.679188	-3.868824	-1.670803
6	6.112000	-2.673961	-0.850375
1	6.541597	-1.749015	-1.215938
6	4.888924	-2.637361	-0.123390
6	4.192091	-1.408423	0.159018
6	4.774294	-0.076128	-0.169297
6	6.048537	0.354646	0.345530
6	6.785226	-0.401530	1.299606
1	6.381274	-1.339996	1.659856
6	7.995268	0.048157	1.781880
1	8.533864	-0.544092	2.516019
6	8.540136	1.275953	1.336308
1	9.498030	1.613869	1.720560
6	7.845431	2.043521	0.429442
1	8.242858	2.997380	0.092682
6	6.586696	1.617761	-0.075640
6	5.845006	2.435108	-0.971192
1	6.268983	3.380241	-1.298174
6	4.594283	2.053050	-1.389698
1	3.991644	2.673854	-2.043740
6	4.069129	0.817633	-0.957176
6	0.115766	2.705601	-0.022984
1	-0.652513	2.581069	0.748908
6	0.353673	4.194222	-0.201056
6	1.535748	4.682945	-0.773643
1	2.324999	3.985878	-1.038575
6	1.708006	6.052501	-0.976759
1	2.631909	6.420835	-1.414184
6	0.698137	6.950066	-0.615808
1	0.834210	8.016230	-0.773076
6	-0.482439	6.469998	-0.044265
1	-1.268400	7.161383	0.246564
6	-0.650075	5.099025	0.165905
1	-1.564702	4.727090	0.622838
6	-0.397200	2.091188	-1.331299
1	0.232834	2.432959	-2.160758
1	-1.410139	2.451239	-1.526485
6	1.844277	2.437526	1.779520
1	1.711106	3.521651	1.735564
6	0.951706	1.935890	2.913198
6	-0.144831	2.718106	3.309270
1	-0.312181	3.679211	2.829323
6	-1.007445	2.291847	4.322734
1	-1.847567	2.915634	4.615639
6	-0.777617	1.075357	4.968445
1	-1.442563	0.740872	5.759251
6	0.322119	0.296566	4.597341
1	0.517321	-0.644465	5.104160
6	1.178517	0.722191	3.579674
1	2.025429	0.104290	3.308763
6	3.338031	2.211741	2.005586
1	3.914542	2.651647	1.189853
1	3.611384	1.161620	2.091804
1	3.621924	2.713143	2.935906
6	-1.165355	-0.438114	0.687060
1	-1.252009	-1.512272	0.788612
1	-0.656034	0.034491	1.522472
6	-2.226776	0.315835	0.088515
1	-2.314746	1.356999	0.378440
6	-3.042606	-0.151291	-0.939268
1	-3.104800	-1.219850	-1.103102
6	0.595695	-0.015000	-3.359198
1	1.164758	0.909615	-3.364957
6	-0.784704	0.099063	-3.579366
1	-1.184489	1.099126	-3.741793
6	-1.687883	-1.014281	-4.068146
1	-1.586711	-1.089680	-5.160883

1	-2.718385	-0.707900	-3.881146
6	-1.443507	-2.403493	-3.433115
1	-0.716828	-2.966091	-4.026510
1	-2.377633	-2.971924	-3.478741
6	-0.972688	-2.383193	-1.986878
1	-1.696988	-2.688737	-1.238571
6	0.347038	-2.352794	-1.597922
1	0.561060	-2.666592	-0.581015
6	1.537036	-2.289177	-2.531217
1	2.419953	-2.049198	-1.937067
1	1.708383	-3.293338	-2.943831
6	1.409493	-1.266857	-3.683438
1	0.969517	-1.743805	-4.564312
1	2.415197	-0.951992	-3.974228
6	-4.034500	0.652824	-1.655004
6	-4.215333	2.035648	-1.442310
6	-4.879666	0.008220	-2.581323
6	-5.206540	2.736925	-2.125700
1	-3.591655	2.568028	-0.732499
6	-5.869241	0.712243	-3.265518
1	-4.761790	-1.057818	-2.752184
6	-6.038123	2.080663	-3.039093
1	-5.333403	3.800000	-1.942311
1	-6.510280	0.191760	-3.970994
1	-6.811221	2.631183	-3.566800
8	-2.908693	-3.907689	0.525954
6	-1.942228	-3.803752	1.229478
8	-0.755279	-3.929681	1.358007
8	-2.582172	-3.162905	2.824370
6	-1.571341	-2.711308	3.725223
1	-1.045731	-1.829409	3.342197
1	-2.029813	-2.465357	4.689898
1	-0.845304	-3.513901	3.872275
6	-3.693266	-0.037218	3.302510
6	-4.724433	1.079345	3.392098
1	-2.801528	0.314695	2.771518
1	-3.354117	-0.333931	4.300622
6	-5.382952	1.242680	2.029436
1	-4.253708	2.018248	3.699963
1	-5.490716	0.828711	4.134268
1	-6.190016	1.978342	2.075486
1	-4.656701	1.599970	1.286061
7	-4.215973	-1.228491	2.632094
6	-5.281851	-1.183637	1.872443
7	-5.958639	-0.034553	1.579258
6	-5.757418	-2.528580	1.349693
1	-4.954317	-3.233683	1.555880
1	-6.619562	-2.848225	1.947946
6	-6.101499	-2.569340	-0.147609
1	-5.418943	-1.900417	-0.681008
6	-7.025638	0.128551	0.566903
6	-7.555024	-2.175481	-0.443153
1	-7.648427	-1.900096	-1.500998
6	-8.035902	-1.013029	0.435900
1	-8.951893	-0.590192	0.008124
1	-8.302814	-1.364116	1.439030
1	-7.566917	1.029635	0.867384
1	-6.571499	0.345782	-0.408966
1	-8.214850	-3.036991	-0.283229
1	-5.902314	-3.575604	-0.529966
1	-3.336156	-2.370926	2.699991

14' P1 *endo-re*

Number of imaginary frequencies= 0
The smallest frequencies are= 17.4672 19.2288 23.7868 cm(-1)
Electronic energy= -3467.3869162
Zero-point correction= 1.213967
(Hartree/Particle)
Thermal correction to Energy= 1.282193
Thermal correction to Enthalpy= 1.283137
Thermal correction to Gibbs Free Energy= 1.109033
Sum of electronic and zero-point Energies= -3466.172949
Sum of electronic and thermal Energies= -3466.104723
Sum of electronic and thermal Enthalpies= -3466.103779
Sum of electronic and thermal Free Energies= -3466.277883

.....

Cartesian Coordinates

.....

77	-0.526735	0.207519	-1.203815
15	1.483319	0.591405	-0.241960
8	2.086353	-0.340366	0.964934
8	2.705075	0.500215	-1.359177
7	1.443374	2.078045	0.516011
6	2.761845	-1.537421	0.724534
6	2.123144	-2.709506	1.178445
1	1.175486	-2.617516	1.694683
6	2.712675	-3.928329	0.954380
1	2.229584	-4.839391	1.292958
6	3.939424	-4.015242	0.243197
6	4.520482	-5.276848	-0.058773
1	4.015522	-6.174820	0.287381
6	5.687267	-5.362641	-0.783598
1	6.120912	-6.331652	-1.012474
6	6.316123	-4.181965	-1.246039
1	7.223744	-4.253047	-1.838430
6	5.786936	-2.942544	-0.958210
1	6.279337	-2.051763	-1.329301
6	4.594773	-2.813610	-0.191850
6	4.009205	-1.534732	0.121195
6	4.685324	-0.250471	-0.213842
6	6.006357	0.067844	0.262759
6	6.705311	-0.754503	1.190294
1	6.233516	-1.656793	1.560508
6	7.963896	-0.412595	1.634988
1	8.472773	-1.052910	2.349740
6	8.597729	0.766618	1.175825
1	9.593029	1.018591	1.529747
6	7.942685	1.596581	0.294686
1	8.409104	2.514943	-0.051976
6	6.636468	1.283167	-0.170290
6	5.938633	2.165002	-1.039268
1	6.432084	3.070876	-1.379537
6	4.646904	1.893354	-1.417971
1	4.084026	2.563811	-2.057854
6	4.030907	0.704945	-0.972781
6	0.292640	2.909237	0.075426
1	-0.466727	2.866179	0.862865
6	0.680209	4.364416	-0.118833
6	1.893977	4.720599	-0.722045
1	2.595959	3.940578	-0.998719
6	2.208158	6.062105	-0.940504
1	3.155448	6.325904	-1.402895
6	1.310541	7.065394	-0.561615
1	1.556634	8.109960	-0.729866
6	0.099736	6.718033	0.041754
1	-0.599136	7.491815	0.347042
6	-0.210335	5.374186	0.265726
1	-1.149112	5.106927	0.745920
6	-0.312736	2.337477	-1.213169
1	0.309809	2.627622	-2.067133
1	-1.302900	2.773404	-1.369825
6	1.999068	2.458224	1.864934
1	1.940488	3.550058	1.848292
6	1.077911	1.985206	2.988437
6	0.018536	2.814355	3.391020
1	-0.079957	3.803519	2.950715
6	-0.899938	2.395563	4.357502
1	-1.713745	3.053234	4.650604
6	-0.761008	1.140912	4.954187
1	-1.471025	0.810061	5.706497
6	0.310123	0.320271	4.588376
1	0.438612	-0.648511	5.062871
6	1.221457	0.738603	3.616591
1	2.041087	0.085634	3.344919
6	3.475994	2.120298	2.057679
1	4.066390	2.532509	1.236746
1	3.672372	1.051182	2.117641
1	3.815591	2.580280	2.990742
6	-1.221907	-0.164473	0.828235

1	-1.430334	-1.226683	0.934365
1	-0.625807	0.240384	1.641074
6	-2.233142	0.713120	0.313324
1	-2.193667	1.750138	0.628171
6	-3.167560	0.356578	-0.652802
1	-3.344756	-0.694347	-0.843483
6	0.440364	0.156030	-3.285110
1	1.107246	1.012648	-3.296134
6	-0.922673	0.420015	-3.461971
1	-1.218567	1.457975	-3.606030
6	-1.964292	-0.592714	-3.891922
1	-1.930796	-0.695542	-4.986558
1	-2.944047	-0.172421	-3.654917
6	-1.835021	-1.986593	-3.236233
1	-1.199170	-2.634085	-3.846836
1	-2.822843	-2.457465	-3.222496
6	-1.294950	-1.980016	-1.810936
1	-2.005551	-2.230555	-1.030259
6	0.040930	-2.098179	-1.476855
1	0.261991	-2.442551	-0.471951
6	1.188559	-2.180346	-2.458313
1	2.116121	-2.012116	-1.909820
1	1.242114	-3.206637	-2.848187
6	1.104605	-1.176014	-3.628829
1	0.572523	-1.623438	-4.473537
1	2.119518	-0.968990	-3.978973
6	-4.098168	1.275297	-1.307129
6	-4.133020	2.662072	-1.048441
6	-5.020934	0.750181	-2.235715
6	-5.056228	3.482198	-1.692705
1	-3.444686	3.102763	-0.335067
6	-5.943202	1.573322	-2.879742
1	-5.011653	-0.315550	-2.445466
6	-5.965113	2.944097	-2.610158
1	-5.069424	4.546664	-1.476616
1	-6.645409	1.144315	-3.588580
1	-6.684150	3.588181	-3.107578
8	-2.686121	-4.698655	-0.435044
6	-1.614408	-4.832686	0.017343
8	-0.525623	-5.042182	0.391361
8	-1.993885	-3.121745	1.926307
6	-1.159700	-3.178007	3.066843
1	-0.646727	-2.221942	3.262537
1	-1.717601	-3.448519	3.976946
1	-0.396669	-3.946638	2.903934
6	-3.697850	-0.379050	3.395608
6	-4.856204	0.590188	3.610839
1	-2.849641	0.146006	2.939660
1	-3.331176	-0.762993	4.355521
6	-5.540758	0.836367	2.271468
1	-4.502615	1.535995	4.034839
1	-5.584025	0.161976	4.309770
1	-6.430184	1.458572	2.401668
1	-4.867292	1.368770	1.584050
7	-4.052374	-1.523415	2.559973
6	-5.114400	-1.511121	1.804429
7	-5.960835	-0.437935	1.669744
6	-5.382256	-2.819906	1.070302
1	-4.460519	-3.397013	1.154068
1	-6.144392	-3.384610	1.622319
6	-5.790876	-2.695683	-0.405247
1	-5.250820	-1.853588	-0.851028
6	-7.084247	-0.306843	0.721125
6	-7.301910	-2.504337	-0.595055
1	-7.495842	-2.105420	-1.598648
6	-7.909792	-1.568166	0.458595
1	-8.904508	-1.249236	0.127352
1	-8.058875	-2.093041	1.408884
1	-7.744921	0.446856	1.159743
1	-6.723734	0.112364	-0.229366
1	-7.808188	-3.475922	-0.540891
1	-5.458731	-3.589835	-0.943199
1	-2.797418	-2.564071	2.170247

Number of imaginary frequencies= 0
The smallest frequencies are= 14.8061 19.2664 21.2452 cm(-1)
Electronic energy= -3467.4003726
Zero-point correction= 1.217318
(Hartree/Particle)
Thermal correction to Energy= 1.284245
Thermal correction to Enthalpy= 1.285189
Thermal correction to Gibbs Free Energy= 1.113582
Sum of electronic and zero-point Energies= -3466.183055
Sum of electronic and thermal Energies= -3466.116128
Sum of electronic and thermal Enthalpies= -3466.115184
Sum of electronic and thermal Free Energies= -3466.286790

.....

Cartesian Coordinates

.....

77	-0.346039	0.113595	-1.361658
15	1.615997	0.485052	-0.312435
8	2.138774	-0.416177	0.952664
8	2.892866	0.340858	-1.361555
7	1.571644	2.002506	0.389916
6	2.821431	-1.625840	0.794146
6	2.149378	-2.777964	1.250448
1	1.151394	-2.685071	1.664687
6	2.754851	-4.002293	1.110774
1	2.248590	-4.900718	1.452308
6	4.023421	-4.119180	0.482556
6	4.619536	-5.391517	0.265792
1	4.095248	-6.275284	0.619919
6	5.823533	-5.506289	-0.390968
1	6.267496	-6.483725	-0.555690
6	6.476828	-4.345262	-0.869201
1	7.413673	-4.440075	-1.410704
6	5.934010	-3.095804	-0.661278
1	6.445199	-2.220967	-1.044696
6	4.703185	-2.936218	0.035457
6	4.102647	-1.646258	0.265260
6	4.804214	-0.380849	-0.086662
6	6.102703	-0.052961	0.442717
6	6.740345	-0.836156	1.445239
1	6.236337	-1.713012	1.833597
6	7.979143	-0.487955	1.937920
1	8.441073	-1.097897	2.708909
6	8.653460	0.658771	1.454607
1	9.633097	0.915555	1.846805
6	8.056870	1.452014	0.501063
1	8.553986	2.346211	0.134302
6	6.771767	1.131725	-0.015312
6	6.132016	1.976516	-0.962283
1	6.654834	2.858209	-1.321714
6	4.857336	1.701264	-1.392501
1	4.339305	2.345190	-2.094039
6	4.200902	0.544537	-0.921408
6	0.459394	2.844423	-0.120198
1	-0.335195	2.853064	0.634956
6	0.889556	4.282643	-0.352694
6	2.111997	4.584620	-0.967908
1	2.785817	3.775022	-1.227582
6	2.469186	5.908845	-1.221373
1	3.422717	6.129622	-1.693439
6	1.605827	6.950317	-0.865998
1	1.885161	7.981673	-1.061631
6	0.386304	6.657792	-0.251582
1	-0.286550	7.461457	0.034487
6	0.033576	5.330536	0.007233
1	-0.912366	5.106012	0.494947
6	-0.104874	2.239444	-1.408217
1	0.567687	2.485599	-2.238582
1	-1.060006	2.717147	-1.633786
6	2.092301	2.433497	1.734443
1	2.097768	3.523701	1.650129
6	1.102477	2.087236	2.845046
6	0.115880	3.024508	3.188745
1	0.106565	3.991394	2.691834
6	-0.843132	2.739314	4.164786

13' P1 *exo-si*

1	-1.596593	3.481244	4.415228
6	-0.817491	1.511015	4.828371
1	-1.551670	1.288025	5.597348
6	0.174554	0.578167	4.510891
1	0.214388	-0.371711	5.036307
6	1.123029	0.861276	3.526271
1	1.878475	0.122897	3.289061
6	3.537744	2.034535	2.026136
1	4.190050	2.357582	1.212532
1	3.673804	0.964404	2.172219
1	3.853479	2.543932	2.941816
6	-1.125452	0.058719	0.677590
1	-0.979264	1.015643	1.172137
1	-0.797085	-0.793732	1.264473
6	-2.334234	-0.139825	-0.081844
1	-2.747074	-1.141788	-0.113855
6	-2.923785	0.863317	-0.830418
1	-2.616655	1.889286	-0.651570
6	0.722322	0.011470	-3.376817
1	1.368973	0.883771	-3.389556
6	-0.638567	0.244229	-3.620557
1	-0.934301	1.275079	-3.812550
6	-1.645063	-0.783961	-4.093562
1	-1.584114	-0.861518	-5.189404
1	-2.644069	-0.398158	-3.875372
6	-1.501930	-2.188244	-3.466120
1	-0.802747	-2.791729	-4.052448
1	-2.470810	-2.693061	-3.532277
6	-1.059856	-2.201565	-2.009997
1	-1.811381	-2.467792	-1.272031
6	0.245966	-2.274886	-1.586547
1	0.384997	-2.593265	-0.558312
6	1.461929	-2.311500	-2.483982
1	2.345202	-2.123234	-1.872672
1	1.571633	-3.333435	-2.873944
6	1.438917	-1.307825	-3.658637
1	0.980901	-1.767840	-4.539256
1	2.472114	-1.078876	-3.933541
6	-4.085718	0.700358	-1.701120
6	-4.546618	-0.561075	-2.133547
6	-4.784422	1.849619	-2.121259
6	-5.675068	-0.661728	-2.943774
1	-4.016133	-1.461880	-1.841798
6	-5.917566	1.744578	-2.927380
1	-4.435644	2.828152	-1.800147
6	-6.368602	0.488051	-3.340338
1	-6.015215	-1.640842	-3.268201
1	-6.446685	2.642109	-3.234355
1	-7.247956	0.403411	-3.971867
8	-3.100615	-3.175589	0.616626
6	-2.166646	-3.129545	1.445700
8	-0.934678	-3.225862	1.304253
8	-2.643228	-2.905826	2.778717
6	-1.640198	-2.724238	3.780884
1	-1.012772	-1.853246	3.567456
1	-2.170811	-2.571055	4.725359
1	-0.996425	-3.605421	3.860700
6	-3.837170	0.430275	3.094768
6	-4.861468	1.554192	3.098345
1	-2.965454	0.694070	2.490058
1	-3.480040	0.205373	4.103356
6	-5.595488	1.570283	1.761760
1	-4.365642	2.514749	3.260393
1	-5.585863	1.406909	3.906239
1	-6.387887	2.320051	1.770535
1	-4.913710	1.811205	0.937942
7	-4.445715	-0.783680	2.551820
6	-5.574863	-0.853195	1.855548
7	-6.221810	0.256941	1.489612
6	-6.030722	-2.264484	1.545221
1	-5.120474	-2.870089	1.555942
1	-6.662057	-2.596984	2.379101
6	-6.738861	-2.482733	0.203525
1	-6.211697	-1.915319	-0.567834
6	-7.461175	0.305245	0.673675
6	-8.224012	-2.104361	0.216851
1	-8.579162	-2.014639	-0.816911
6	-8.485391	-0.792646	0.968643
1	-9.473163	-0.404262	0.698444
1	-8.509804	-0.961986	2.051435
1	-7.909722	1.274313	0.898334
1	-7.186032	0.317989	-0.388074
1	-8.811172	-2.903997	0.684077
1	-6.625717	-3.537207	-0.068196
1	-3.910575	-1.654221	2.676211

[13'-14'] P1 *exo-si*

Number of imaginary frequencies= 1
The smallest frequencies are=-782.8364 14.2660 19.3358cm(-1)
Electronic energy= -3467.375979
Zero-point correction= 1.210341
(Hartree/Particle)
Thermal correction to Energy= 1.277556
Thermal correction to Enthalpy= 1.278500
Thermal correction to Gibbs Free Energy= 1.106963
Sum of electronic and zero-point Energies= -3466.165638
Sum of electronic and thermal Energies= -3466.098423
Sum of electronic and thermal Enthalpies= -3466.097479
Sum of electronic and thermal Free Energies= -3466.269016

.....

Cartesian Coordinates

.....

77	-0.534337	0.437757	-1.434134
15	1.396161	0.738134	-0.324585
8	1.888787	-0.221071	0.914068
8	2.684615	0.597036	-1.354812
7	1.359479	2.210965	0.452066
6	2.383590	-1.505235	0.685396
6	1.573978	-2.569478	1.133169
1	0.643823	-2.339110	1.642308
6	1.979838	-3.861742	0.906404
1	1.364064	-4.689684	1.242816
6	3.178043	-4.125308	0.188988
6	3.556846	-5.456321	-0.135359
1	2.923253	-6.271273	0.204475
6	4.689073	-5.709407	-0.876054
1	4.965354	-6.730035	-1.123929
6	5.487146	-4.632625	-1.330496
1	6.366040	-4.833443	-1.936383
6	5.157891	-3.331209	-1.018422
1	5.775657	-2.520136	-1.385264
6	4.007175	-3.032616	-0.236776
6	3.623708	-1.682440	0.093108
6	4.496190	-0.513500	-0.212523
6	5.853747	-0.431651	0.265956
6	6.407834	-1.381257	1.169461
1	5.791392	-2.196191	1.529085
6	7.710342	-1.272672	1.606343
1	8.105540	-2.007623	2.301712
6	8.535977	-0.211731	1.164454
1	9.563059	-0.144597	1.510780
6	8.025810	0.740109	0.311297
1	8.640173	1.573013	-0.020346
6	6.681358	0.668051	-0.144081
6	6.139178	1.681866	-0.979319
1	6.776609	2.502498	-1.295852
6	4.818822	1.644059	-1.351515
1	4.369561	2.424441	-1.956723
6	4.011644	0.561907	-0.939694
6	0.207403	3.063706	0.070740
1	-0.524462	3.025563	0.885879
6	0.619968	4.513094	-0.125604
6	1.784885	4.838514	-0.835840
1	2.425680	4.038888	-1.198104
6	2.128678	6.171811	-1.056695
1	3.037162	6.412242	-1.602202
6	1.308545	7.198133	-0.575733
1	1.577343	8.236563	-0.747149
6	0.147394	6.881734	0.132239

1	-0.490432	7.673367	0.515524
6	-0.191645	5.544803	0.359550
1	-1.090122	5.299354	0.921311
6	-0.447446	2.540948	-1.216391
1	0.120252	2.925297	-2.070645
1	-1.451757	2.965319	-1.288296
6	2.017487	2.609848	1.744688
1	2.009061	3.701764	1.693355
6	1.175970	2.232554	2.962626
6	0.252144	3.164734	3.459687
1	0.152655	4.128451	2.966418
6	-0.515957	2.886056	4.593729
1	-1.217332	3.627171	4.967319
6	-0.362901	1.666927	5.255956
1	-0.949881	1.448289	6.143332
6	0.553192	0.729308	4.770140
1	0.681062	-0.220792	5.281544
6	1.315220	1.008445	3.634655
1	2.026587	0.272942	3.280197
6	3.488078	2.214640	1.862061
1	4.054422	2.605954	1.015001
1	3.645274	1.138402	1.914687
1	3.890074	2.660242	2.776899
6	-1.392637	0.184970	0.546176
1	-1.378303	1.134643	1.075687
1	-1.027009	-0.643155	1.146786
6	-2.550176	-0.110345	-0.259438
1	-2.820059	-1.154259	-0.360818
6	-3.254083	0.844355	-0.971394
1	-3.073615	1.890683	-0.741899
6	0.606186	0.618937	-3.429626
1	1.214776	1.509936	-3.304901
6	-0.752447	0.832056	-3.680747
1	-1.085101	1.867975	-3.738801
6	-1.716675	-0.145729	-4.321307
1	-1.666992	-0.023135	-5.413375
1	-2.729888	0.145415	-4.031288
6	-1.506629	-1.634686	-3.965834
1	-0.741600	-2.071653	-4.612802
1	-2.437048	-2.168879	-4.182752
6	-1.136203	-1.892182	-2.519004
1	-1.928414	-2.222456	-1.858315
6	0.140626	-1.980511	-2.040371
1	0.272408	-2.400656	-1.047406
6	1.392926	-1.813791	-2.870131
1	2.236446	-1.709647	-2.190322
1	1.563576	-2.744341	-3.429520
6	1.390834	-0.620700	-3.856965
1	1.011334	-0.940948	-4.832179
1	2.429186	-0.318793	-4.016270
6	-4.376617	0.589163	-1.870769
6	-4.666679	-0.684546	-2.404560
6	-5.225190	1.662547	-2.208860
6	-5.781368	-0.877795	-3.216195
1	-4.013265	-1.522953	-2.194191
6	-6.340848	1.466422	-3.021659
1	-5.010087	2.652123	-1.813242
6	-6.626671	0.194411	-3.524103
1	-5.988024	-1.866290	-3.615987
1	-6.986907	2.305714	-3.262226
1	-7.495549	0.039248	-4.156748
8	-2.051132	-3.272339	0.311499
6	-1.558320	-3.906410	1.196802
8	-1.104491	-4.913082	1.642831
8	-1.434378	-2.597983	2.620042
6	-0.971114	-3.048275	3.880590
1	-0.616072	-4.081984	3.800331
1	-0.140435	-2.422923	4.237326
1	-1.775108	-3.020651	4.631030
6	-2.910339	0.107614	3.667597
6	-4.011613	1.150719	3.803248
1	-2.063646	0.514333	3.106574
1	-2.515871	-0.175071	4.649064
6	-4.777455	1.224761	2.488133
1	-3.585140	2.127519	4.050121
1	-4.704921	0.873611	4.605136
1	-5.617609	1.918088	2.566311
1	-4.124005	1.579575	1.679194
7	-3.379136	-1.110867	3.010039
6	-4.518743	-1.180060	2.362960
7	-5.313233	-0.102122	2.136676
6	-4.907000	-2.574079	1.904556
1	-4.005580	-3.177181	1.997348
1	-5.621156	-2.983587	2.629696
6	-5.468622	-2.678587	0.480458
1	-4.949165	-1.955931	-0.153800
6	-6.534898	-0.062235	1.302235
6	-6.981214	-2.433154	0.410566
1	-7.258404	-2.192746	-0.623247
6	-7.433113	-1.299992	1.341541
1	-8.441878	-0.979400	1.058583
1	-7.504626	-1.648169	2.378041
1	-7.108812	0.789526	1.676755
1	-6.257809	0.175180	0.265694
1	-7.522557	-3.348561	0.678775
1	-5.228593	-3.666270	0.074083
1	-2.406757	-1.957961	2.782141

14' P1 *exo-si*

Number of imaginary frequencies= 0
The smallest frequencies are= 18.6275 20.8049 24.3040 cm(-1)
Electronic energy= -3467.3838156
Zero-point correction= 1.214032
(Hartree/Particle)
Thermal correction to Energy= 1.282318
Thermal correction to Enthalpy= 1.283262
Thermal correction to Gibbs Free Energy= 1.109278
Sum of electronic and zero-point Energies= -3466.169783
Sum of electronic and thermal Energies= -3466.101498
Sum of electronic and thermal Enthalpies= -3466.100554
Sum of electronic and thermal Free Energies= -3466.274538

.....

Cartesian Coordinates

.....

77	-0.456590	0.464939	-1.442831
15	1.471454	0.732479	-0.321811
8	1.907294	-0.220572	0.944002
8	2.768899	0.519370	-1.325448
7	1.474780	2.222557	0.418478
6	2.337152	-1.532577	0.757964
6	1.479413	-2.541823	1.246477
1	0.566808	-2.248851	1.757769
6	1.827983	-3.857708	1.063693
1	1.192366	-4.652027	1.444427
6	3.007323	-4.201057	0.347580
6	3.323295	-5.557716	0.065270
1	2.654621	-6.331695	0.432993
6	4.440510	-5.885958	-0.668990
1	4.668615	-6.925664	-0.884418
6	5.287028	-4.862613	-1.157844
1	6.154279	-5.123029	-1.757732
6	5.019644	-3.538284	-0.885648
1	5.673948	-2.767892	-1.276192
6	3.885598	-3.162438	-0.113464
6	3.569061	-1.786410	0.176925
6	4.503775	-0.668381	-0.139566
6	5.857779	-0.648253	0.357785
6	6.353895	-1.615495	1.276256
1	5.694876	-2.396788	1.634559
6	7.654175	-1.565858	1.730324
1	8.004207	-2.313320	2.436410
6	8.535675	-0.549166	1.292756
1	9.559932	-0.528169	1.652946
6	8.082990	0.419327	0.426212
1	8.740515	1.219986	0.097876
6	6.743128	0.407512	-0.047940
6	6.262934	1.440587	-0.897259
1	6.943541	2.227746	-1.208616
6	4.948568	1.462424	-1.290385

1	4.546244	2.258675	-1.907828
6	4.084600	0.422537	-0.884609
6	0.350103	3.102520	0.014120
1	-0.368943	3.119842	0.840597
6	0.813188	4.527884	-0.238179
6	1.984980	4.784486	-0.964727
1	2.596281	3.948907	-1.295383
6	2.372454	6.095377	-1.241167
1	3.286002	6.282747	-1.798923
6	1.589644	7.167586	-0.799712
1	1.892116	8.188526	-1.014555
6	0.422264	6.919506	-0.074903
1	-0.186866	7.747107	0.277918
6	0.039319	5.605198	0.207683
1	-0.863950	5.413295	0.782071
6	-0.349837	2.566227	-1.245274
1	0.187638	2.937777	-2.123848
1	-1.354848	2.994368	-1.283253
6	2.121144	2.638708	1.712574
1	2.226314	3.720788	1.596486
6	1.187762	2.416324	2.901229
6	0.438433	3.497922	3.387458
1	0.538860	4.469888	2.910659
6	-0.425374	3.345176	4.475525
1	-0.994188	4.197241	4.837667
6	-0.546428	2.102320	5.099482
1	-1.210317	1.979502	5.950458
6	0.194431	1.016538	4.623135
1	0.109238	0.046483	5.103236
6	1.052661	1.171602	3.534100
1	1.617094	0.320082	3.177719
6	3.536554	2.107816	1.936522
1	4.178412	2.358352	1.089641
1	3.575742	1.031717	2.098449
1	3.942310	2.598352	2.826455
6	-1.310583	0.287675	0.557891
1	-1.307240	1.265798	1.031493
1	-0.928433	-0.496393	1.202729
6	-2.454041	-0.060980	-0.240055
1	-2.706754	-1.112333	-0.305078
6	-3.174579	0.850846	-0.992628
1	-3.010016	1.908870	-0.810513
6	0.688272	0.616380	-3.430184
1	1.301139	1.506039	-3.314630
6	-0.669645	0.835401	-3.689191
1	-0.995290	1.872716	-3.758404
6	-1.638490	-0.140246	-4.326883
1	-1.588582	-0.022737	-5.419456
1	-2.650587	0.155150	-4.036243
6	-1.432814	-1.627730	-3.964594
1	-0.665220	-2.069082	-4.605366
1	-2.363241	-2.161684	-4.182094
6	-1.070590	-1.874183	-2.514693
1	-1.875608	-2.180066	-1.858473
6	0.202377	-1.969200	-2.029250
1	0.330610	-2.376248	-1.030706
6	1.454955	-1.823976	-2.862688
1	2.302559	-1.737199	-2.185867
1	1.605544	-2.756418	-3.424638
6	1.469273	-0.629338	-3.848518
1	1.096834	-0.946945	-4.827428
1	2.510856	-0.334048	-3.998119
6	-4.300531	0.530418	-1.865839
6	-4.581949	-0.778025	-2.313004
6	-5.168000	1.569493	-2.256592
6	-5.703580	-1.035710	-3.096378
1	-3.918105	-1.593533	-2.053144
6	-6.291949	1.308676	-3.039419
1	-4.962219	2.584099	-1.924818
6	-6.567217	0.004661	-3.458396
1	-5.903610	-2.050091	-3.429266
1	-6.953529	2.122862	-3.320569
1	-7.442950	-0.200887	-4.066799
8	-1.828869	-3.309506	0.285893
6	-1.651857	-4.020906	1.199026
8	-1.484338	-4.818351	2.037447
8	-1.380685	-2.032413	2.893842
6	-1.114946	-2.525666	4.195031
1	-0.046233	-2.757031	4.275225
1	-1.363456	-1.790031	4.972753
1	-1.673981	-3.448325	4.411832
6	-3.444748	0.839681	3.365486
6	-4.734230	1.652394	3.308069
1	-2.687236	1.285516	2.708424
1	-3.015538	0.866060	4.372959
6	-5.448690	1.342232	1.999393
1	-4.526532	2.724990	3.381128
1	-5.387985	1.380958	4.145203
1	-6.422640	1.838368	1.964378
1	-4.862965	1.709564	1.143809
7	-3.634001	-0.560305	2.994560
6	-4.686711	-0.945410	2.329253
7	-5.671756	-0.105322	1.868502
6	-4.789079	-2.450311	2.119713
1	-3.813464	-2.842057	2.408159
1	-5.503368	-2.859069	2.845651
6	-5.159970	-2.912788	0.701721
1	-4.708975	-2.228637	-0.023563
6	-6.746707	-0.452337	0.917050
6	-6.675486	-2.984198	0.472304
1	-6.876364	-2.997268	-0.606088
6	-7.423442	-1.810462	1.120272
1	-8.431266	-1.746448	0.695009
1	-7.555890	-1.976468	2.195376
1	-7.502795	0.327647	1.043310
1	-6.377965	-0.364017	-0.115015
1	-7.070067	-3.924142	0.877492
1	-4.710292	-3.894098	0.513959
1	-2.231124	-1.492923	2.936473

P1 *endo-re* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 12.8582 21.9550 26.3544 cm(-1)
Electronic energy= -3125.4962645
Zero-point correction= 0.914550
(Hartree/Particle)
Thermal correction to Energy= 0.969328
Thermal correction to Enthalpy= 0.970272
Thermal correction to Gibbs Free Energy= 0.825821
Sum of electronic and zero-point Energies= -3124.581715
Sum of electronic and thermal Energies= -3124.526937
Sum of electronic and thermal Enthalpies= -3124.525992
Sum of electronic and thermal Free Energies= -3124.670443

.....

Cartesian Coordinates

.....

77	-1.143406	-1.367048	-0.238216
15	0.592702	0.095956	-0.137958
8	1.640024	0.205066	1.122888
8	1.656429	-0.181158	-1.389421
7	-0.010229	1.640208	-0.135852
6	2.710553	-0.662991	1.298692
6	2.649576	-1.504939	2.430322
1	1.803104	-1.404964	3.101529
6	3.654405	-2.414019	2.650767
1	3.624957	-3.065077	3.519806
6	4.729562	-2.537922	1.729272
6	5.727925	-3.535636	1.897440
1	5.665549	-4.190241	2.762757
6	6.743294	-3.682207	0.979527
1	7.497265	-4.452239	1.114117
6	6.795451	-2.835000	-0.152940
1	7.583765	-2.968191	-0.888294
6	5.853002	-1.846438	-0.336447
1	5.904764	-1.214106	-1.214821
6	4.800355	-1.652645	0.601224
6	3.791706	-0.638219	0.431518
6	3.874576	0.388027	-0.644230
6	5.010146	1.265829	-0.771956

6	6.063035	1.303712	0.184742
1	6.016499	0.655882	1.051763
6	7.129281	2.163814	0.035320
1	7.915619	2.178648	0.784603
6	7.207109	3.032894	-1.078979
1	8.057010	3.700418	-1.186349
6	6.194854	3.040466	-2.011463
1	6.229551	3.716952	-2.861430
6	5.072453	2.178609	-1.878527
6	4.001733	2.223850	-2.811408
1	4.064760	2.904807	-3.655308
6	2.885841	1.445619	-2.630138
1	2.044281	1.486475	-3.312160
6	2.824829	0.561694	-1.531820
6	-1.422806	1.723442	-0.608625
1	-2.058174	1.905488	0.258410
6	-1.584402	2.884713	-1.580040
6	-2.547015	3.876372	-1.354980
1	-3.175415	3.820868	-0.473412
6	-2.684972	4.939893	-2.253010
1	-3.433181	5.705369	-2.065242
6	-1.863306	5.025988	-3.378003
1	-1.969961	5.855755	-4.071438
6	-0.894966	4.041449	-3.603861
1	-0.245000	4.104260	-4.472714
6	-0.758639	2.980494	-2.710074
1	0.001388	2.224137	-2.876975
6	-1.845481	0.394193	-1.251427
1	-1.479506	0.352166	-2.282386
1	-2.935751	0.358775	-1.294089
6	0.479346	2.828685	0.650017
1	-0.193978	3.625722	0.323355
6	0.250778	2.649123	2.150128
6	-1.046325	2.804976	2.659307
1	-1.854307	3.128278	2.014144
6	-1.325805	2.558796	4.005405
1	-2.349326	2.652126	4.353498
6	-0.299999	2.185772	4.875660
1	-0.511476	1.995687	5.924555
6	1.006040	2.071336	4.388800
1	1.816194	1.798307	5.060119
6	1.277231	2.298542	3.038378
1	2.292887	2.184446	2.677120
6	1.887350	3.262425	0.253282
1	1.928429	3.446655	-0.822401
1	2.644945	2.518700	0.499929
1	2.139193	4.190316	0.776166
6	-1.568277	-0.844508	1.838847
1	-1.288653	-1.697142	2.456207
1	-1.203245	0.106353	2.216910
6	-2.862544	-0.820405	1.219203
1	-3.300571	0.144262	0.995674
6	-3.513452	-1.977838	0.789035
1	-3.190436	-2.927945	1.198949
6	-0.395876	-2.135319	-2.251574
1	-0.199188	-1.241114	-2.833938
6	-1.737120	-2.518689	-2.114060
1	-2.490592	-1.900936	-2.600754
6	-2.202931	-3.921825	-1.777671
1	-2.151491	-4.536090	-2.688692
1	-3.259595	-3.863037	-1.511942
6	-1.429968	-4.626582	-0.636242
1	-0.609666	-5.223318	-1.047303
1	-2.105788	-5.336642	-0.149830
6	-0.862587	-3.701035	0.431413
1	-1.338868	-3.734999	1.407015
6	0.393948	-3.137661	0.377410
1	0.818466	-2.789486	1.313577
6	1.376645	-3.304376	-0.761925
1	2.182499	-2.584479	-0.620799
1	1.834151	-4.300714	-0.682620
6	0.773521	-3.114737	-2.172080
1	0.445781	-4.077626	-2.576059
1	1.563804	-2.755747	-2.836747
6	-4.761883	-2.038592	0.026956
6	-5.399234	-0.904694	-0.517642
6	-5.358231	-3.301254	-0.171231
6	-6.577667	-1.042709	-1.247879
1	-4.996882	0.085964	-0.347097
6	-6.537502	-3.433866	-0.901620
1	-4.888481	-4.182400	0.258963
6	-7.149365	-2.303485	-1.449600
1	-7.057283	-0.157180	-1.655470
1	-6.979074	-4.416643	-1.040634
1	-8.068452	-2.401647	-2.020256
5	-4.625540	2.553491	1.657912
9	-4.394765	1.975914	0.374436
9	-5.997009	2.685133	1.868376
9	-4.051506	1.722915	2.638004
9	-3.997421	3.815990	1.686558

P1 *exo-si* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 13.3872 19.2537 24.8597 cm(-1)
Electronic energy= -3125.4910399
Zero-point correction= 0.914402
(Hartree/Particle)
Thermal correction to Energy= 0.969248
Thermal correction to Enthalpy= 0.970192
Thermal correction to Gibbs Free Energy= 0.825039
Sum of electronic and zero-point Energies= -3124.576637
Sum of electronic and thermal Energies= -3124.521792
Sum of electronic and thermal Enthalpies= -3124.520848
Sum of electronic and thermal Free Energies= -3124.666001

.....

Cartesian Coordinates

.....

77	-1.255554	-1.046700	-0.340122
15	0.607243	0.237829	-0.139153
8	1.624092	0.193146	1.154207
8	1.683399	-0.076388	-1.371409
7	0.151698	1.834617	-0.082783
6	2.552362	-0.829340	1.316434
6	2.317362	-1.727555	2.379469
1	1.453394	-1.561149	3.014056
6	3.183937	-2.772873	2.583121
1	3.022778	-3.468400	3.401733
6	4.284330	-2.978158	1.707122
6	5.138539	-4.104473	1.856834
1	4.947237	-4.793871	2.675055
6	6.175119	-4.327779	0.979186
1	6.818104	-5.194733	1.099212
6	6.393561	-3.431317	-0.094060
1	7.196681	-3.623194	-0.799755
6	5.594782	-2.320394	-0.257274
1	5.772423	-1.651062	-1.090417
6	4.527677	-2.044920	0.642825
6	3.667077	-0.898883	0.496393
6	3.923750	0.161771	-0.516833
6	5.166955	0.888141	-0.561609
6	6.174098	0.746978	0.434057
1	6.007258	0.075790	1.268124
6	7.349502	1.462881	0.363539
1	8.098320	1.342646	1.141216
6	7.588154	2.358606	-0.705902
1	8.522176	2.910863	-0.751279
6	6.626524	2.537993	-1.674195
1	6.786332	3.237472	-2.490597
6	5.396087	1.828288	-1.622341
6	4.382180	2.049173	-2.593018
1	4.570904	2.744701	-3.405775
6	3.167626	1.418400	-2.488425
1	2.370795	1.591749	-3.202895
6	2.942413	0.509854	-1.431864
6	-1.242003	2.080790	-0.535795
1	-1.847879	2.326429	0.338245
6	-1.308310	3.248551	-1.510985
6	-2.386001	4.141925	-1.464008
1	-3.141550	4.023570	-0.695604

6	-2.479317	5.181189	-2.393962
1	-3.319008	5.869455	-2.345394
6	-1.498216	5.342903	-3.374844
1	-1.570803	6.155022	-4.093138
6	-0.417162	4.457019	-3.421848
1	0.355958	4.578808	-4.176160
6	-0.325674	3.416777	-2.496903
1	0.518712	2.736472	-2.522320
6	-1.833144	0.826938	-1.192831
1	-1.514383	0.799464	-2.240298
1	-2.916970	0.924984	-1.183406
6	0.740812	2.942985	0.750535
1	0.217015	3.826887	0.376310
6	0.361647	2.797294	2.223519
6	-0.914515	3.205241	2.640475
1	-1.600227	3.667932	1.939504
6	-1.337257	3.012719	3.957412
1	-2.341992	3.311897	4.241111
6	-0.475084	2.437264	4.892145
1	-0.798229	2.289505	5.919079
6	0.814275	2.065479	4.499037
1	1.501437	1.634579	5.222705
6	1.226978	2.242002	3.177082
1	2.225979	1.935505	2.890271
6	2.224657	3.179805	0.482264
1	2.387493	3.353668	-0.583647
1	2.852933	2.344447	0.790049
1	2.547785	4.069188	1.031999
6	-1.616578	-0.321375	1.728000
1	-0.858593	-0.560792	2.469023
1	-1.889101	0.726198	1.688920
6	-2.640522	-1.290627	1.511440
1	-2.540478	-2.258725	1.991221
6	-3.661638	-1.071967	0.586403
1	-3.866706	-0.044663	0.311373
6	-0.582521	-1.659501	-2.405807
1	-0.329805	-0.731267	-2.908663
6	-1.953607	-1.956260	-2.297842
1	-2.649207	-1.230715	-2.717672
6	-2.538998	-3.346165	-2.160992
1	-2.591592	-3.802096	-3.160827
1	-3.570673	-3.247278	-1.820413
6	-1.781198	-4.293303	-1.204829
1	-1.002185	-4.836677	-1.747278
1	-2.485647	-5.046225	-0.838552
6	-1.150294	-3.614607	-0.003450
1	-1.674676	-3.728033	0.938191
6	0.136525	-3.147481	0.042484
1	0.568033	-2.944504	1.018273
6	1.106515	-3.172336	-1.117790
1	1.950053	-2.531262	-0.864812
1	1.509788	-4.190358	-1.214866
6	0.521224	-2.715463	-2.474835
1	0.134892	-3.576328	-3.029917
1	1.340190	-2.306999	-3.072477
6	-4.687049	-2.035151	0.184115
6	-4.716235	-3.377980	0.610643
6	-5.683235	-1.593118	-0.708339
6	-5.698747	-4.247789	0.143983
1	-3.969436	-3.747341	1.305587
6	-6.663384	-2.466638	-1.176480
1	-5.680098	-0.552430	-1.021937
6	-6.671714	-3.799504	-0.756547
1	-5.706825	-5.280129	0.482517
1	-7.422028	-2.106538	-1.865526
1	-7.433594	-4.482781	-1.120592
5	-4.582637	2.544256	1.343808
9	-3.851638	3.754182	1.390241
9	-3.973220	1.609828	2.202485
9	-5.905690	2.768378	1.726946
9	-4.550366	2.042617	0.015410

P1 *endo-re*

Number of imaginary frequencies= 0

The smallest frequencies are= 19.0304 22.0844 26.5184 cm(-1)
Electronic energy= -2700.877626
Zero-point correction= 0.898344
(Hartree/Particle)
Thermal correction to Energy= 0.946899
Thermal correction to Enthalpy= 0.947843
Thermal correction to Gibbs Free Energy= 0.817642
Sum of electronic and zero-point Energies= -2699.979282
Sum of electronic and thermal Energies= -2699.930727
Sum of electronic and thermal Enthalpies= -2699.929783
Sum of electronic and thermal Free Energies= -2700.059984

.....

Cartesian Coordinates

.....

77	-1.558666	-1.024203	-0.170337
15	0.323955	0.213928	-0.022867
8	1.416958	0.044447	1.188513
8	1.284709	-0.021635	-1.351950
7	-0.093947	1.816913	0.177910
6	2.396796	-0.947401	1.180553
6	2.289353	-1.933277	2.184055
1	1.479535	-1.855752	2.901752
6	3.208922	-2.951572	2.229635
1	3.145948	-3.713957	3.000701
6	4.237910	-3.037578	1.253339
6	5.148664	-4.128718	1.244941
1	5.056025	-4.886030	2.018970
6	6.117360	-4.233604	0.272871
1	6.805198	-5.073984	0.272806
6	6.207218	-3.248958	-0.739873
1	6.956830	-3.347032	-1.519769
6	5.350773	-2.169398	-0.750585
1	5.429827	-1.430678	-1.539298
6	4.351570	-2.015968	0.250564
6	3.437845	-0.902175	0.267210
6	3.575572	0.250901	-0.665966
6	4.778720	1.039418	-0.735859
6	5.868364	0.858284	0.161344
1	5.801386	0.102776	0.935084
6	6.998394	1.642026	0.073922
1	7.812173	1.490204	0.777127
6	7.106968	2.647293	-0.916364
1	8.006993	3.251999	-0.976460
6	6.063380	2.865232	-1.786809
1	6.123749	3.647815	-2.538517
6	4.875620	2.087840	-1.712420
6	3.774987	2.351390	-2.572107
1	3.864605	3.134747	-3.319308
6	2.601358	1.651260	-2.438176
1	1.736690	1.856401	-3.059890
6	2.512171	0.632401	-1.466560
6	-1.526352	2.072561	-0.127668
1	-2.062940	2.150309	0.824255
6	-1.725573	3.370642	-0.889350
6	-2.823100	4.186222	-0.589602
1	-3.491547	3.906575	0.221565
6	-3.062314	5.352486	-1.320887
1	-3.917116	5.977162	-1.077029
6	-2.197994	5.718703	-2.354964
1	-2.377960	6.628859	-2.919952
6	-1.095050	4.912373	-2.654460
1	-0.415002	5.196042	-3.453047
6	-0.861756	3.744479	-1.927931
1	0.001504	3.124006	-2.148673
6	-2.109254	0.897961	-0.920284
1	-1.786461	0.975944	-1.964587
1	-3.200188	0.960431	-0.913594
6	0.540972	2.850550	1.073423
1	0.106626	3.784086	0.705892
6	0.069948	2.686570	2.516659
6	-1.106593	3.336132	2.922183
1	-1.619196	3.992534	2.223396
6	-1.621278	3.160898	4.209184
1	-2.535070	3.672046	4.499576
6	-0.954020	2.340912	5.121244

1	-1.348494	2.202672	6.123980
6	0.236532	1.714980	4.740501
1	0.774224	1.092517	5.450650
6	0.744966	1.887267	3.451597
1	1.666971	1.391238	3.175681
6	2.051405	2.996177	0.903549
1	2.298482	3.164127	-0.146648
1	2.613311	2.132606	1.255398
1	2.377873	3.869133	1.477061
6	-1.734601	-0.732360	1.985759
1	-1.538821	-1.685764	2.473742
1	-1.193436	0.096466	2.435225
6	-3.069422	-0.448659	1.535364
1	-3.353861	0.595409	1.450113
6	-3.960318	-1.417008	1.088059
1	-3.769634	-2.455152	1.335979
6	-1.035861	-1.647580	-2.319354
1	-0.719090	-0.727251	-2.800262
6	-2.413558	-1.823776	-2.151109
1	-3.068178	-1.036128	-2.521380
6	-3.112933	-3.144482	-1.895557
1	-3.279385	-3.651714	-2.857244
1	-4.103230	-2.914660	-1.494674
6	-2.385944	-4.103231	-0.923879
1	-1.693797	-4.747171	-1.474031
1	-3.130226	-4.770077	-0.478013
6	-1.621993	-3.421051	0.204592
1	-2.045235	-3.517666	1.199490
6	-0.293689	-3.047982	0.136767
1	0.221289	-2.892988	1.079860
6	0.607947	-3.208172	-1.068081
1	1.505206	-2.611169	-0.899378
1	0.938347	-4.255151	-1.119612
6	-0.029924	-2.792529	-2.411204
1	-0.520980	-3.650358	-2.879431
1	0.769464	-2.487474	-3.091859
6	-5.248730	-1.154990	0.449524
6	-5.693793	0.137181	0.097902
6	-6.082448	-2.251219	0.148529
6	-6.918481	0.316301	-0.539297
1	-5.084592	1.005482	0.325595
6	-7.308563	-2.068947	-0.488434
1	-5.757260	-3.252285	0.419581
6	-7.729819	-0.783971	-0.839187
1	-7.243712	1.318565	-0.803327
1	-7.933503	-2.928724	-0.711854
1	-8.683228	-0.638160	-1.338408

P1 *exo-si*

Number of imaginary frequencies= 0
The smallest frequencies are= 10.9775 23.2155 26.7037 cm(-1)
Electronic energy= -2700.871334
Zero-point correction= 0.897960
(Hartree/Particle)
Thermal correction to Energy= 0.946703
Thermal correction to Enthalpy= 0.947647
Thermal correction to Gibbs Free Energy= 0.816297
Sum of electronic and zero-point Energies= -2699.973374
Sum of electronic and thermal Energies= -2699.924631
Sum of electronic and thermal Enthalpies= -2699.923687
Sum of electronic and thermal Free Energies= -2700.055037

.....

Cartesian Coordinates

.....

77	-1.721212	-0.612148	-0.215835
15	0.338494	0.299110	-0.039200
8	1.357153	-0.053155	1.199999
8	1.287281	-0.070975	-1.344971
7	0.183532	1.949763	0.154884
6	2.166914	-1.187639	1.202910
6	1.872038	-2.159149	2.182916
1	1.063147	-1.963741	2.879010
6	2.613645	-3.313458	2.232641
1	2.404711	-4.068232	2.985228
6	3.643539	-3.549950	1.282549
6	4.363416	-4.775650	1.273881
1	4.125352	-5.521415	2.027689
6	5.330788	-5.020426	0.325873
1	5.872041	-5.961888	0.325171
6	5.610418	-4.046309	-0.662002
1	6.356994	-4.252008	-1.423559
6	4.942287	-2.841135	-0.671760
1	5.164449	-2.112206	-1.441777
6	3.951589	-2.543894	0.305339
6	3.228980	-1.297520	0.319679
6	3.572405	-0.172276	-0.593966
6	4.886730	0.415609	-0.623314
6	5.908098	0.055790	0.299831
1	5.699976	-0.687864	1.059590
6	7.150513	0.649846	0.251832
1	7.910510	0.363484	0.973022
6	7.444752	1.633670	-0.722111
1	8.430782	2.087813	-0.751029
6	6.474312	2.021486	-1.617718
1	6.679695	2.789626	-2.358575
6	5.177078	1.440840	-1.585825
6	4.159020	1.875971	-2.477055
1	4.393806	2.636753	-3.215868
6	2.886566	1.368504	-2.383424
1	2.085320	1.704916	-3.031715
6	2.606643	0.376464	-1.420544
6	-1.177275	2.446631	-0.176403
1	-1.704285	2.647311	0.762206
6	-1.134375	3.744866	-0.964085
6	-2.040240	4.768696	-0.661434
1	-2.736970	4.639555	0.163729
6	-2.050670	5.951181	-1.405910
1	-2.757138	6.738734	-1.158983
6	-1.146215	6.124316	-2.455846
1	-1.147071	7.046104	-3.030564
6	-0.233945	5.108395	-2.759022
1	0.477146	5.240047	-3.570091
6	-0.230071	3.925603	-2.019562
1	0.485986	3.141510	-2.244013
6	-1.959458	1.378435	-0.948157
1	-1.632226	1.388701	-1.994091
1	-3.016533	1.651202	-0.948540
6	0.962901	2.869337	1.062344
1	0.717363	3.858552	0.666438
6	0.417474	2.816329	2.487746
6	-0.619519	3.689892	2.850035
1	-0.967531	4.428645	2.132320
6	-1.205609	3.628452	4.117100
1	-2.010569	4.311632	4.373615
6	-0.749464	2.696960	5.051707
1	-1.200183	2.645161	6.038839
6	0.305249	1.843737	4.713939
1	0.682103	1.130918	5.442604
6	0.884482	1.903958	3.445439
1	1.698788	1.233112	3.203153
6	2.481550	2.743809	0.958535
1	2.801444	2.844223	-0.080253
1	2.867902	1.803837	1.348435
1	2.929827	3.558673	1.535253
6	-1.863714	-0.001862	1.901892
1	-1.173019	-0.490943	2.583444
1	-1.847653	1.080739	1.983746
6	-3.123664	-0.656588	1.697806
1	-3.243070	-1.659546	2.094521
6	-4.120821	-0.129821	0.889266
1	-4.058832	0.920211	0.622637
6	-1.256574	-1.261469	-2.359852
1	-0.850405	-0.371777	-2.831319
6	-2.648469	-1.291740	-2.198089
1	-3.201597	-0.421446	-2.549352
6	-3.509202	-2.523746	-2.017158
1	-3.773481	-2.918277	-3.009344
1	-4.448857	-2.208237	-1.557297
6	-2.887288	-3.649370	-1.164552

1	-2.253008	-4.288517	-1.784578
1	-3.697354	-4.284668	-0.793784
6	-2.081292	-3.163760	0.025926
1	-2.568707	-3.226541	0.992951
6	-0.729994	-2.936306	0.019727
1	-0.231500	-2.858466	0.981400
6	0.177274	-3.090494	-1.179590
1	1.132602	-2.619577	-0.945576
1	0.388969	-4.159786	-1.319523
6	-0.366818	-2.495992	-2.498840
1	-0.922157	-3.256840	-3.055403
1	0.488481	-2.223248	-3.122318
6	-5.344303	-0.812175	0.471363
6	-5.681489	-2.116304	0.887175
6	-6.199189	-0.156672	-0.436296
6	-6.825304	-2.741945	0.399170
1	-5.047889	-2.642410	1.593848
6	-7.342047	-0.786476	-0.926177
1	-5.952679	0.850928	-0.761863
6	-7.657698	-2.083455	-0.513265
1	-7.070426	-3.747221	0.729659
1	-7.985495	-0.266145	-1.629737
1	-8.546739	-2.577116	-0.894454

1

Number of imaginary frequencies= 0
The smallest frequencies are= 10.0716 12.6371 17.3733 cm(-1)
Electronic energy= -5180.7406719
Zero-point correction= 0.789537
(Hartree/Particle)
Thermal correction to Energy= 0.862696
Thermal correction to Enthalpy= 0.863640
Thermal correction to Gibbs Free Energy= 0.672323
Sum of electronic and zero-point Energies= -5179.951135
Sum of electronic and thermal Energies= -5179.877976
Sum of electronic and thermal Enthalpies= -5179.877031
Sum of electronic and thermal Free Energies= -5180.068349

.....

Cartesian Coordinates

.....

26	0.660887	-3.063994	-3.570398
15	-1.420290	-1.656033	0.986016
15	1.300945	0.514837	-0.487597
6	0.188687	-2.516170	-1.609163
6	0.732123	-1.399507	-2.348797
6	-0.126403	-1.158092	-3.464738
1	0.019164	-0.394903	-4.216422
6	-1.172981	-2.125289	-3.444084
1	-1.954709	-2.233165	-4.184043
6	-0.977984	-2.962977	-2.308856
1	-1.590017	-3.807326	-2.032099
6	2.578410	-3.704751	-4.033883
1	3.477672	-3.347602	-3.549471
6	1.957401	-3.126033	-5.183433
1	2.300198	-2.251405	-5.719930
6	0.776510	-3.876392	-5.472076
1	0.067551	-3.666348	-6.262152
6	0.667665	-4.919752	-4.502689
1	-0.138010	-5.638311	-4.428367
6	1.780507	-4.815139	-3.615814
1	1.965712	-5.447420	-2.758137
6	0.735895	-2.998111	-0.308961
6	1.989044	-3.628930	-0.286552
1	2.487571	-3.809688	-1.230872
6	2.609232	-3.993576	0.908257
1	3.593385	-4.450944	0.891503
6	1.967347	-3.739810	2.117848
1	2.439382	-4.002908	3.059876
6	0.718592	-3.117610	2.121766
1	0.253916	-2.894576	3.074064
6	0.088321	-2.730683	0.928363
6	1.916525	-0.573256	-1.924503
1	2.660718	-1.244733	-1.489976
6	2.559950	0.210371	-3.071851
1	3.461108	0.732109	-2.740216
1	1.877779	0.956809	-3.490065
1	2.836107	-0.482873	-3.872676
6	-1.880430	-1.562543	2.766537
6	-1.807499	-0.319616	3.408990
1	-1.496722	0.555369	2.849661
6	-2.148365	-0.197940	4.758343
1	-2.080989	0.770572	5.244847
6	-2.570291	-1.317274	5.475231
1	-2.835393	-1.224469	6.524702
6	-2.660723	-2.559734	4.838340
1	-2.998902	-3.432075	5.390577
6	-2.323872	-2.682264	3.491429
1	-2.408500	-3.649334	3.005728
6	-2.782891	-2.659686	0.280115
6	-2.800435	-4.062132	0.303007
1	-1.963513	-4.612102	0.724089
6	-3.882979	-4.755450	-0.241931
1	-3.889689	-5.841932	-0.227463
6	-4.954870	-4.054583	-0.805449
1	-5.795013	-4.597686	-1.229343
6	-4.944111	-2.657598	-0.818861
1	-5.774355	-2.101402	-1.244476
6	-3.860387	-1.961501	-0.281740
1	-3.857927	-0.879329	-0.293879
6	2.350172	0.047378	0.953384
6	3.648353	-0.466636	0.861162
1	4.137016	-0.576891	-0.100223
6	4.332540	-0.852959	2.015390
6	3.744010	-0.730989	3.273374
1	4.277722	-1.042375	4.163898
6	2.455624	-0.206310	3.364497
6	1.760405	0.174036	2.217741
1	0.748550	0.554523	2.301532
6	1.835588	2.239597	-0.852701
6	0.832297	3.118586	-1.278895
1	-0.183629	2.758542	-1.399212
6	1.127062	4.460170	-1.520813
6	2.423900	4.944745	-1.358169
1	2.649579	5.988499	-1.541117
6	3.424462	4.064915	-0.942760
6	3.137853	2.723286	-0.682038
1	3.928879	2.067466	-0.333653
29	-0.970035	0.353149	-0.015858
6	4.844817	4.543484	-0.807316
6	-0.001060	5.397866	-1.848697
6	5.678299	-1.509984	1.886493
6	1.756590	-0.159926	4.694910
9	2.622849	-0.031357	5.723488
9	0.879454	0.866171	4.769708
9	1.050238	-1.297278	4.919258
9	5.556530	-2.856659	1.759656
9	6.460045	-1.289476	2.965000
9	6.353428	-1.077963	0.797550
9	5.587708	4.206036	-1.889852
9	5.456288	3.993187	0.266815
9	4.924035	5.884772	-0.677039
9	0.420829	6.513093	-2.479295
9	-0.935723	4.811650	-2.630870
9	-0.643199	5.802234	-0.719859
6	-1.881516	3.171368	1.239552
6	-2.933969	1.177681	-2.377993
7	-2.113199	0.817166	-1.646209
15	-5.428473	1.801018	0.402681
9	-4.324726	2.764765	-0.351780
9	-6.628932	2.627541	-0.332146
9	-5.465529	2.848318	1.664488
9	-4.205516	0.979634	1.126482
9	-6.516166	0.843824	1.146379
9	-5.373661	0.758622	-0.869766
7	-1.336702	2.175226	1.009176
6	-2.585562	4.410402	1.514877
1	-2.564606	5.042568	0.623614
1	-3.620762	4.172389	1.769177
1	-2.104113	4.936727	2.343834

6	-3.968306	1.635969	-3.287319
1	-3.514834	2.054555	-4.190093
1	-4.616708	0.797915	-3.555662
1	-4.561934	2.396273	-2.775685

3

Number of imaginary frequencies= 0
The smallest frequencies are= 8.4238 14.3206 21.2311 cm(-1)
Electronic energy= -5462.9553639
Zero-point correction= 0.888922
(Hartree/Particle)
Thermal correction to Energy= 0.966353
Thermal correction to Enthalpy= 0.967298
Thermal correction to Gibbs Free Energy= 0.768962
Sum of electronic and zero-point Energies= -5462.066442
Sum of electronic and thermal Energies= -5461.989011
Sum of electronic and thermal Enthalpies= -5461.988066
Sum of electronic and thermal Free Energies= -5462.186402

.....

Cartesian Coordinates

.....

26	-1.545863	-2.987153	-3.549717
15	-1.289912	-1.622405	1.514704
15	1.158662	-0.078718	-0.902259
6	-1.116474	-2.575109	-1.538954
6	-0.584069	-1.555711	-2.413338
6	-1.677458	-0.975875	-3.128306
1	-1.602857	-0.195898	-3.873487
6	-2.874695	-1.644574	-2.730965
1	-3.865052	-1.463791	-3.125325
6	-2.529483	-2.630817	-1.761450
1	-3.213063	-3.317504	-1.286487
6	-0.184769	-4.078595	-4.675850
1	0.886491	-4.066016	-4.524284
6	-0.924226	-3.191047	-5.515994
1	-0.512399	-2.384687	-6.108210
6	-2.308381	-3.523755	-5.400285
1	-3.128222	-3.010747	-5.885793
6	-2.425183	-4.617845	-4.489796
1	-3.348067	-5.080158	-4.165403
6	-1.114475	-4.961894	-4.043364
1	-0.875446	-5.733051	-3.323780
6	-0.280954	-3.325331	-0.554504
6	0.631710	-4.278700	-1.031864
1	0.631115	-4.497961	-2.091721
6	1.546630	-4.912948	-0.192056
1	2.258082	-5.622687	-0.602017
6	1.556048	-4.603806	1.165539
1	2.272160	-5.071864	1.834493
6	0.650492	-3.668928	1.667626
1	0.693605	-3.419924	2.721020
6	-0.271554	-3.015895	0.833532
6	0.859841	-1.138078	-2.454856
1	1.464545	-2.032917	-2.293538
6	1.289532	-0.494979	-3.775417
1	2.354160	-0.245535	-3.765660
1	0.734161	0.421889	-3.991202
1	1.105529	-1.197372	-4.593986
6	-1.000358	-1.673690	3.329848
6	-0.304941	-0.604394	3.910578
1	0.004344	0.237386	3.303271
6	-0.050230	-0.592722	5.283069
1	0.484189	0.245207	5.720399
6	-0.488686	-1.645512	6.086018
1	-0.293541	-1.634551	7.154799
6	-1.193969	-2.709996	5.515233
1	-1.547915	-3.526747	6.138223
6	-1.451114	-2.724627	4.144891
1	-2.005013	-3.552892	3.715696
6	-3.022401	-2.192473	1.290537
6	-3.381096	-3.546713	1.379477
1	-2.627302	-4.298394	1.594347
6	-4.700343	-3.940726	1.150837
1	-4.969089	-4.991182	1.219294
6	-5.670286	-2.987355	0.824812
1	-6.695336	-3.296305	0.640164
6	-5.319280	-1.637826	0.738793
1	-6.069221	-0.892413	0.489541
6	-4.001296	-1.241006	0.970636
1	-3.732076	-0.192847	0.910497
6	2.510762	-0.953777	-0.004736
6	3.453080	-1.789701	-0.615598
1	3.468448	-1.922644	-1.691284
6	4.388950	-2.475126	0.162066
6	4.417469	-2.327386	1.548468
1	5.146138	-2.864721	2.144728
6	3.492032	-1.477772	2.150914
6	2.538223	-0.807114	1.388397
1	1.820763	-0.158520	1.873193
6	1.952839	1.474438	-1.478692
6	1.130679	2.432595	-2.093273
1	0.083045	2.218767	-2.273850
6	1.652401	3.672305	-2.459221
6	2.981559	3.997538	-2.186865
1	3.372456	4.976043	-2.443095
6	3.788855	3.052745	-1.557261
6	3.290093	1.794352	-1.218754
1	3.941000	1.079780	-0.729682
29	-0.647890	0.318319	0.552784
6	5.211588	3.418905	-1.233650
6	0.764774	4.726954	-3.058045
6	5.313016	-3.467390	-0.486740
6	3.441248	-1.360785	3.648582
9	4.654748	-1.539318	4.214899
9	2.980666	-0.150787	4.046378
9	2.615188	-2.290361	4.190297
9	4.789742	-4.719962	-0.451488
9	6.510098	-3.530282	0.136432
9	5.544683	-3.178867	-1.786629
9	6.000694	3.423808	-2.330960
9	5.769132	2.565569	-0.344545
9	5.287262	4.661538	-0.694726
9	1.393268	5.425221	-4.027642
9	-0.362920	4.210617	-3.592165
9	0.380219	5.634863	-2.118957
6	0.756128	2.918869	1.465384
6	-0.532466	3.687903	1.224465
6	-1.403440	3.274633	0.060281
7	1.927692	3.586285	1.513164
6	3.104464	2.952794	2.110186
1	3.525753	3.630870	2.859815
1	2.823306	2.018631	2.591455
1	3.869314	2.753685	1.355227
6	2.114189	4.973405	1.082184
1	1.467898	5.217164	0.239838
1	1.936133	5.677844	1.903074
1	3.145836	5.084481	0.742488
8	0.698291	1.695603	1.717606
6	-1.967843	4.268861	-0.746950
6	-2.852030	3.933846	-1.766945
1	-1.706433	5.306932	-0.581723
6	-3.155263	2.587893	-1.930712
6	-2.574810	1.635145	-1.106577
1	-2.797365	0.581275	-1.214944
7	-1.702428	1.972601	-0.138164
1	-3.283152	4.698221	-2.403502
35	-4.397366	2.009358	-3.320961
15	-3.149612	2.058034	3.898785
9	-1.514625	2.242758	3.862387
9	-3.272801	2.947787	2.517597
9	-3.275955	3.424109	4.784703
9	-3.013496	1.164022	5.256016
9	-4.771576	1.875807	3.919746
9	-3.008260	0.703188	2.983662
1	-1.112118	3.490594	2.131301
1	-0.370765	4.762461	1.174334

5

Number of imaginary frequencies= 0
The smallest frequencies are= 12.1948 15.0782 16.8789 cm(-1)
Electronic energy= -5925.1252622
Zero-point correction= 1.137580
(Hartree/Particle)
Thermal correction to Energy= 1.226509
Thermal correction to Enthalpy= 1.227453
Thermal correction to Gibbs Free Energy= 1.004486
Sum of electronic and zero-point Energies= -5923.987682
Sum of electronic and thermal Energies= -5923.898753
Sum of electronic and thermal Enthalpies= -5923.897809
Sum of electronic and thermal Free Energies= -5924.120776
.....
Cartesian Coordinates
.....

26	-4.537812	-3.104264	0.805549
15	-0.664536	-1.201265	-2.169769
15	-1.861760	0.827211	0.837238
6	-3.203889	-2.033928	-0.398979
6	-3.182313	-1.556765	0.966007
6	-2.793497	-2.646663	1.805074
1	-2.699955	-2.614138	2.881951
6	-2.606442	-3.798687	0.983179
1	-2.350284	-4.791011	1.327560
6	-2.861234	-3.423951	-0.368093
1	-2.830292	-4.082174	-1.222061
6	-6.471456	-2.400725	1.064043
1	-6.750438	-1.355376	1.076849
6	-6.070529	-3.176019	2.195528
1	-5.983590	-2.819392	3.213195
6	-5.758189	-4.493400	1.739575
1	-5.389036	-5.306438	2.350790
6	-5.966339	-4.533201	0.326929
1	-5.782131	-5.380574	-0.320210
6	-6.408029	-3.242149	-0.090202
1	-6.618732	-2.944565	-1.108567
6	-3.465907	-1.156200	-1.577956
6	-4.744337	-0.597675	-1.734128
1	-5.518329	-0.890959	-1.035903
6	-5.028899	0.333506	-2.733131
1	-6.019736	0.772432	-2.799189
6	-4.026345	0.707129	-3.624188
1	-4.222090	1.435026	-4.406116
6	-2.750389	0.157020	-3.498022
1	-1.976119	0.483657	-4.181117
6	-2.440471	-0.759327	-2.480105
6	-3.415671	-0.128210	1.374392
1	-4.210333	0.271996	0.741313
6	-3.827218	0.046525	2.837891
1	-4.020724	1.097492	3.069950
1	-3.060846	-0.312182	3.530160
1	-4.741473	-0.526032	3.024332
6	0.237227	-0.449388	-3.589750
6	0.980656	0.717192	-3.360165
1	1.073642	1.110441	-2.354096
6	1.629159	1.358770	-4.417262
1	2.187281	2.269524	-4.229561
6	1.562537	0.829058	-5.706276
1	2.073507	1.325556	-6.526554
6	0.843808	-0.347498	-5.938447
1	0.797158	-0.770607	-6.938066
6	0.181719	-0.982490	-4.887880
1	-0.376480	-1.892250	-5.082773
6	-0.551049	-3.004883	-2.490648
6	-1.409474	-3.666632	-3.383339
1	-2.191168	-3.114814	-3.897598
6	-1.280965	-5.040879	-3.590896
1	-1.951258	-5.547048	-4.280151
6	-0.293630	-5.763474	-2.912368
1	-0.195395	-6.833171	-3.075191
6	0.568021	-5.106621	-2.030802
1	1.347223	-5.656264	-1.510568
6	0.438868	-3.733084	-1.816566
1	1.114557	-3.230215	-1.138033
6	-2.490383	2.172916	-0.248797
6	-3.765173	2.742506	-0.155491
1	-4.447691	2.455827	0.637297
6	-4.179222	3.685509	-1.099392
6	-3.329783	4.096830	-2.126306
1	-3.661099	4.827326	-2.854680
6	-2.050623	3.548099	-2.198770
6	-1.639746	2.581943	-1.283057
1	-0.654850	2.141008	-1.368301
6	-1.216136	1.693936	2.320750
6	-0.579661	0.896232	3.284949
1	-0.576577	-0.182384	3.182954
6	0.087883	1.484443	4.355311
6	0.151116	2.873288	4.479179
1	0.689574	3.329723	5.303104
6	-0.470888	3.663615	3.513670
6	-1.157756	3.086380	2.444087
1	-1.622593	3.724220	1.702208
29	-0.117498	-0.354763	-0.150150
6	-0.335201	5.157789	3.621680
6	0.847252	0.635385	5.336543
6	-5.598594	4.178722	-1.058498
6	-1.129604	3.903602	-3.332433
9	-1.393058	5.124494	-3.844930
9	0.169209	3.897166	-2.943398
9	-1.234242	3.016656	-4.352843
9	-6.438112	3.300345	-1.665339
9	-5.750150	5.364047	-1.685905
9	-6.047327	4.327646	0.208804
9	-0.807553	5.624946	4.798853
9	-0.986374	5.810275	2.634523
9	0.967423	5.534861	3.551444
9	0.601478	0.995669	6.614910
9	0.557167	-0.677374	5.217219
9	2.189264	0.762887	5.153866
6	1.890108	1.757651	0.884097
6	2.598730	0.767452	1.781852
6	2.129852	-0.660053	1.955840
7	2.122492	3.063234	1.154552
6	1.539035	4.107058	0.314673
1	2.333662	4.689946	-0.163698
1	0.918610	3.660042	-0.456762
1	0.931688	4.780120	0.927235
6	3.022013	3.515615	2.225947
1	2.585921	3.343407	3.213937
1	3.994022	3.019563	2.154257
1	3.171104	4.589032	2.109324
8	1.186231	1.417738	-0.092000
6	2.857091	-1.416855	2.891021
6	2.495450	-2.722310	3.184055
1	3.704549	-0.964722	3.394551
6	1.392667	-3.241465	2.512832
6	0.716701	-2.471285	1.586187
1	-0.129301	-2.862104	1.036677
7	1.077343	-1.198614	1.316790
1	3.051293	-3.307742	3.907896
35	0.790489	-5.069230	2.848368
15	3.981097	-2.220880	-1.246433
9	4.274791	-0.938685	-0.261771
9	3.163033	-2.956101	-0.027682
9	5.373329	-2.918582	-0.738670
9	4.789146	-1.483399	-2.465697
9	3.673957	-3.499526	-2.214793
9	2.598847	-1.496498	-1.752931
1	3.638117	0.748867	1.413928
1	2.670300	1.180259	2.789453
6	6.422191	0.455642	1.881719
6	7.787816	0.104342	1.298678
1	5.803562	-0.453268	1.933813
1	6.523019	0.824627	2.910785
6	7.608824	-0.213920	-0.179219
1	8.235877	-0.752200	1.814063
1	8.470428	0.955937	1.410305
1	8.582303	-0.350157	-0.663086
1	7.043001	-1.146297	-0.307345
7	5.706603	1.459707	1.099925

6	5.947446	1.576857	-0.172609
7	6.910422	0.880658	-0.870904
6	5.062279	2.573799	-0.903108
1	4.386264	2.964858	-0.144373
1	5.651072	3.424007	-1.266920
6	4.251768	1.940820	-2.049888
1	3.984558	0.919333	-1.770068
6	7.046194	0.745055	-2.335781
6	5.009123	1.937575	-3.391637
1	4.669494	1.087707	-3.994350
6	6.534406	1.872255	-3.231654
1	6.983312	1.707980	-4.218887
1	6.933606	2.829813	-2.878475
1	8.122568	0.638190	-2.518690
1	6.578364	-0.197936	-2.641789
1	4.765464	2.842997	-3.962872
1	3.306130	2.482252	-2.156760

[5-6]‡

Number of imaginary frequencies= 1
The smallest frequencies are=-1562.3364 7.6852 16.5731cm(-1)
Electronic energy= -5925.110299
Zero-point correction= 1.133303
(Hartree/Particle)
Thermal correction to Energy= 1.221451
Thermal correction to Enthalpy= 1.222396
Thermal correction to Gibbs Free Energy= 1.002049
Sum of electronic and zero-point Energies= -5923.976996
Sum of electronic and thermal Energies= -5923.888848
Sum of electronic and thermal Enthalpies= -5923.887903
Sum of electronic and thermal Free Energies= -5924.108250

.....

Cartesian Coordinates

.....

26	-3.872270	-3.503252	1.401645
15	-0.579582	-1.408034	-2.047029
15	-1.794517	0.738875	0.790199
6	-2.833946	-2.408074	-0.048164
6	-2.781662	-1.756563	1.240353
6	-2.149435	-2.651490	2.157495
1	-1.971403	-2.461183	3.207004
6	-1.842337	-3.858806	1.462852
1	-1.395866	-4.743064	1.895539
6	-2.266727	-3.713375	0.110322
1	-2.193164	-4.465476	-0.659852
6	-5.873639	-3.093024	1.771747
1	-6.330013	-2.115654	1.686619
6	-5.251802	-3.629798	2.940866
1	-5.145291	-3.126498	3.892781
6	-4.752911	-4.929047	2.618848
1	-4.198713	-5.579451	3.282755
6	-5.064745	-5.195532	1.250685
1	-4.789925	-6.082921	0.695896
6	-5.758733	-4.063579	0.728168
1	-6.103376	-3.950220	-0.290720
6	-3.311566	-1.719366	-1.282885
6	-4.680104	-1.440048	-1.418940
1	-5.356360	-1.820004	-0.663365
6	-5.174005	-0.667939	-2.469739
1	-6.234939	-0.446802	-2.529615
6	-4.290749	-0.158456	-3.418507
1	-4.653218	0.463502	-4.231526
6	-2.926745	-0.432481	-3.311604
1	-2.251793	-0.005391	-4.043562
6	-2.413999	-1.204902	-2.257588
6	-3.201600	-0.334293	1.490537
1	-4.061642	-0.125303	0.851335
6	-3.598613	-0.046179	2.940630
1	-3.920976	0.991370	3.063889
1	-2.778098	-0.226447	3.640280
1	-4.427325	-0.704128	3.220953
6	0.151326	-0.672515	-3.571149
6	0.951745	0.471192	-3.442110
1	1.143631	0.893794	-2.461683
6	1.523740	1.059806	-4.572562
1	2.134176	1.949776	-4.463775
6	1.312002	0.509070	-5.836079
1	1.760905	0.967631	-6.712886
6	0.526944	-0.639983	-5.971238
1	0.365683	-1.079927	-6.951518
6	-0.047661	-1.229089	-4.845980
1	-0.647748	-2.125370	-4.963628
6	-0.352924	-3.217718	-2.307443
6	-1.227623	-3.973018	-3.105806
1	-2.076986	-3.498161	-3.587589
6	-1.030574	-5.346422	-3.258709
1	-1.715103	-5.923066	-3.874844
6	0.040808	-5.978455	-2.618575
1	0.190586	-7.048052	-2.736997
6	0.917174	-5.229422	-1.830273
1	1.758833	-5.705836	-1.335607
6	0.719521	-3.856518	-1.673007
1	1.402646	-3.286186	-1.061638
6	-2.587395	1.796813	-0.495154
6	-3.944282	2.136087	-0.522902
1	-4.615451	1.818563	0.266741
6	-4.454421	2.895272	-1.578911
6	-3.626138	3.340615	-2.607849
1	-4.029471	3.926921	-3.425642
6	-2.270335	3.018138	-2.566523
6	-1.753278	2.246096	-1.528587
1	-0.700071	1.992452	-1.510538
6	-1.361234	1.952056	2.101101
6	-0.634156	1.476629	3.204239
1	-0.406074	0.420398	3.293048
6	-0.167202	2.362588	4.171413
6	-0.382315	3.736237	4.047567
1	0.013328	4.424999	4.785656
6	-1.079571	4.208253	2.938406
6	-1.580958	3.328015	1.977837
1	-2.111656	3.727267	1.121913
29	0.078522	-0.360573	-0.137400
6	-1.287741	5.688317	2.775486
6	0.692385	1.870873	5.301209
6	-5.932259	3.157380	-1.663504
6	-1.381352	3.404480	-3.714852
9	-1.762416	4.569084	-4.285076
9	-0.088239	3.543850	-3.336843
9	-1.405598	2.465420	-4.693515
9	-6.557861	2.216384	-2.417058
9	-6.204436	4.351694	-2.234245
9	-6.525683	3.141433	-0.449304
9	-2.365275	6.133666	3.461632
9	-1.479295	6.032280	1.479176
9	-0.221135	6.393641	3.221674
9	0.379632	2.466807	6.472693
9	0.599501	0.537503	5.482649
9	2.007655	2.148385	5.073055
6	1.689325	2.115165	0.767121
6	2.439504	1.364843	1.779181
6	2.162861	-0.041689	2.120584
7	1.676183	3.483712	0.872545
6	1.177116	4.301338	-0.228411
1	1.975580	4.952760	-0.605107
1	0.833712	3.665046	-1.038156
1	0.348549	4.932325	0.111381
6	2.344773	4.230920	1.935810
1	2.181783	3.778877	2.913656
1	3.425024	4.313239	1.758985
1	1.918394	5.235624	1.971323
8	1.139093	1.576676	-0.231980
6	2.739214	-0.528969	3.320131
6	2.580544	-1.845235	3.712931
1	3.302733	0.151964	3.947386
6	1.836058	-2.679634	2.879012
6	1.278109	-2.174628	1.721544
1	0.692074	-2.799766	1.060629
7	1.420501	-0.882808	1.355811
1	3.021490	-2.208589	4.634962

35	1.572367	-4.565392	3.333795
15	4.143633	-2.099297	-1.407326
9	4.273226	-0.827171	-0.382250
9	3.409681	-2.961234	-0.215988
9	5.602931	-2.650823	-0.903787
9	4.882039	-1.231869	-2.588346
9	3.992257	-3.369600	-2.418884
9	2.692361	-1.520271	-1.909302
1	3.745621	1.453618	1.345946
1	2.592773	1.922226	2.698135
6	5.757749	0.506127	1.951757
6	7.234209	0.410527	1.593088
1	5.278260	-0.474323	1.845502
1	5.621427	0.827678	2.990370
6	7.351596	0.146635	0.098793
1	7.720147	-0.396598	2.149764
1	7.743459	1.348020	1.846260
1	8.397069	0.200332	-0.220687
1	6.973051	-0.850967	-0.150816
7	5.067550	1.462969	1.087673
6	5.480297	1.693892	-0.138924
7	6.596649	1.148353	-0.677808
6	4.613248	2.639129	-0.943661
1	3.828599	2.982195	-0.273091
1	5.190292	3.529210	-1.212588
6	3.988294	1.983911	-2.187481
1	3.701362	0.962283	-1.934698
6	6.979829	1.104549	-2.108180
6	4.921961	1.983220	-3.417268
1	4.778548	1.050250	-3.972268
6	6.409393	2.141230	-3.074914
1	6.991559	2.031642	-3.997993
1	6.624400	3.150968	-2.707903
1	8.071875	1.195460	-2.121186
1	6.732622	0.101641	-2.474260
1	4.647550	2.799347	-4.097265
1	3.060011	2.514188	-2.418005

6

Number of imaginary frequencies= 0
The smallest frequencies are= 14.7007 16.4833 19.9006 cm(-1)
Electronic energy= -5925.1275433
Zero-point correction= 1.138909
(Hartree/Particle)
Thermal correction to Energy= 1.227390
Thermal correction to Enthalpy= 1.228334
Thermal correction to Gibbs Free Energy= 1.008422
Sum of electronic and zero-point Energies= -5923.988634
Sum of electronic and thermal Energies= -5923.900153
Sum of electronic and thermal Enthalpies= -5923.899209
Sum of electronic and thermal Free Energies= -5924.119121

.....

Cartesian Coordinates

.....

26	-3.767409	-3.661952	1.332446
15	-0.543458	-1.356390	-2.040361
15	-1.863378	0.673844	0.829153
6	-2.765384	-2.494504	-0.085137
6	-2.742822	-1.872373	1.218523
6	-2.080865	-2.764022	2.116965
1	-1.913774	-2.591758	3.171391
6	-1.724556	-3.941760	1.395524
1	-1.246504	-4.818819	1.809385
6	-2.149030	-3.780533	0.044763
1	-2.044563	-4.510743	-0.742825
6	-5.783796	-3.327905	1.690992
1	-6.270891	-2.365012	1.612565
6	-5.151898	-3.855844	2.858794
1	-5.068163	-3.359181	3.816305
6	-4.605573	-5.133245	2.526044
1	-4.033496	-5.771274	3.186811
6	-4.898468	-5.395237	1.152808
1	-4.590238	-6.266910	0.590601
6	-5.627974	-4.282380	0.637656
1	-5.969207	-4.169489	-0.382466
6	-3.264847	-1.796198	-1.305858
6	-4.643092	-1.574363	-1.448633
1	-5.307747	-2.001711	-0.708483
6	-5.161536	-0.799495	-2.485393
1	-6.230529	-0.622932	-2.550472
6	-4.293570	-0.227874	-3.412730
1	-4.676756	0.399866	-4.211427
6	-2.919890	-0.444544	-3.299673
1	-2.257954	0.028337	-4.015905
6	-2.382927	-1.220183	-2.259907
6	-3.226581	-0.475836	1.498689
1	-4.093200	-0.296094	0.859652
6	-3.644279	-0.237003	2.951829
1	-4.007571	0.784446	3.095322
1	-2.821835	-0.400416	3.653250
1	-4.448509	-0.932352	3.212536
6	0.155627	-0.548186	-3.544672
6	0.831750	0.669660	-3.385403
1	0.960288	1.091596	-2.394237
6	1.362307	1.329849	-4.496284
1	1.869223	2.279623	-4.363795
6	1.238129	0.775484	-5.769889
1	1.655799	1.288987	-6.631611
6	0.580369	-0.447355	-5.934282
1	0.487702	-0.889397	-6.922540
6	0.041965	-1.105675	-4.829327
1	-0.462636	-2.055630	-4.971094
6	-0.247456	-3.147106	-2.356791
6	-1.089038	-3.913660	-3.179733
1	-1.954863	-3.458653	-3.651441
6	-0.836202	-5.273070	-3.371965
1	-1.495572	-5.858828	-4.006738
6	0.259170	-5.879579	-2.747816
1	0.452432	-6.938341	-2.896980
6	1.102944	-5.118943	-1.935352
1	1.962570	-5.574582	-1.452040
6	0.848717	-3.760610	-1.738416
1	1.504554	-3.180937	-1.106490
6	-2.697855	1.731171	-0.430956
6	-4.075842	1.962237	-0.500935
1	-4.749343	1.559024	0.245683
6	-4.606589	2.716888	-1.549241
6	-3.779208	3.267987	-2.525896
1	-4.198487	3.848808	-3.340188
6	-2.403427	3.057184	-2.440014
6	-1.862998	2.289392	-1.410437
1	-0.793896	2.118676	-1.349794
6	-1.488176	1.875442	2.170350
6	-0.757300	1.402215	3.271761
1	-0.491948	0.353317	3.338858
6	-0.325883	2.282533	4.259783
6	-0.571283	3.652662	4.154401
1	-0.194739	4.339436	4.904113
6	-1.265569	4.125551	3.043849
6	-1.738220	3.247594	2.065806
1	-2.266135	3.648083	1.208561
29	0.077213	-0.332520	-0.109589
6	-1.489608	5.603176	2.887926
6	0.559098	1.796773	5.371516
6	-6.094446	2.869452	-1.696616
6	-1.519892	3.565655	-3.543550
9	-1.938636	4.760487	-4.019696
9	-0.234013	3.719008	-3.148955
9	-1.509879	2.710880	-4.596823
9	-6.582345	2.043577	-2.659030
9	-6.440239	4.125462	-2.060351
9	-6.759560	2.578927	-0.557391
9	-2.600540	6.029021	3.533681
9	-1.633836	5.957785	1.588079
9	-0.452195	6.320669	3.382822
9	0.240934	2.363068	6.557924
9	0.507888	0.458321	5.531524
9	1.863613	2.116374	5.137221
6	1.573113	2.129910	0.869324

6	2.178035	1.383606	1.917358
6	2.108711	-0.019269	2.152085
7	1.570951	3.517780	0.969098
6	1.149933	4.340749	-0.153717
1	1.979081	4.967913	-0.510923
1	0.817070	3.706210	-0.968793
1	0.326572	5.003099	0.142210
6	2.176651	4.247453	2.072612
1	1.975914	3.768225	3.030750
1	3.265885	4.356766	1.954827
1	1.736601	5.247118	2.116068
8	1.045639	1.620183	-0.175408
6	2.796859	-0.541817	3.294003
6	2.768401	-1.883055	3.604706
1	3.339675	0.145619	3.934250
6	2.038404	-2.732156	2.762500
6	1.373661	-2.207673	1.674671
1	0.794845	-2.839778	1.013661
7	1.388842	-0.893538	1.374701
1	3.294164	-2.264499	4.474021
35	1.955068	-4.661603	3.114553
15	4.257562	-1.937053	-1.399302
9	4.285203	-0.739456	-0.278209
9	3.543724	-2.926761	-0.304113
9	5.731584	-2.447580	-0.888589
9	4.988039	-0.938448	-2.478685
9	4.210648	-3.126311	-2.512641
9	2.793442	-1.396467	-1.901611
1	4.224408	1.698494	1.346877
1	2.605447	1.932888	2.743882
6	5.941686	0.580024	1.883800
6	7.385281	0.553500	1.405881
1	5.475659	-0.405381	1.789330
1	5.866671	0.901015	2.926224
6	7.408491	0.347567	-0.102495
1	7.929647	-0.260460	1.891389
1	7.883861	1.494872	1.662425
1	8.424366	0.459079	-0.488553
1	7.044255	-0.647620	-0.371107
7	5.196779	1.535095	1.064269
6	5.481298	1.830430	-0.203323
7	6.561417	1.342688	-0.802035
6	4.492649	2.743205	-0.887646
1	3.727865	2.990799	-0.152863
1	4.988359	3.684723	-1.140301
6	3.828406	2.104435	-2.118008
1	3.540009	1.084719	-1.862762
6	6.945879	1.474102	-2.229285
6	4.714454	2.114768	-3.386146
1	4.648069	1.138119	-3.874568
6	6.188641	2.448161	-3.128135
1	6.725156	2.422388	-4.084227
1	6.303027	3.471020	-2.754024
1	8.005447	1.751837	-2.226446
1	6.869199	0.465415	-2.648298
1	4.329913	2.850804	-4.101780
1	2.897200	2.646575	-2.297944

Cu-enolate

Number of imaginary frequencies= 0
The smallest frequencies are= 6.6441 13.0346 15.6166 cm(-1)
Electronic energy= -4521.7141033
Zero-point correction= 0.854615
(Hartree/Particle)
Thermal correction to Energy= 0.924057
Thermal correction to Enthalpy= 0.925001
Thermal correction to Gibbs Free Energy= 0.743664
Sum of electronic and zero-point Energies= -4520.859488
Sum of electronic and thermal Energies= -4520.790046
Sum of electronic and thermal Enthalpies= -4520.789102
Sum of electronic and thermal Free Energies= -4520.970439

.....

Cartesian Coordinates

.....

26	3.417990	-1.167671	2.826815
15	1.016548	-1.727956	-1.778626
15	-0.692451	0.242166	0.870878
6	2.190953	-1.557160	1.174025
6	1.759359	-0.371609	1.879704
6	2.839444	0.562983	1.862549
1	2.834313	1.543642	2.318227
6	3.942148	-0.038402	1.186604
1	4.917955	0.405395	1.045631
6	3.545872	-1.340806	0.764598
1	4.166059	-2.055112	0.245209
6	2.915750	-1.946343	4.686339
1	1.904536	-2.126609	5.026628
6	3.648698	-0.729327	4.838278
1	3.285748	0.177301	5.303871
6	4.925567	-0.902604	4.221999
1	5.696076	-0.147978	4.134238
6	4.982872	-2.226711	3.689338
1	5.806556	-2.654360	3.133032
6	3.743239	-2.871931	3.977193
1	3.470041	-3.875414	3.680260
6	1.293354	-2.713628	0.885035
6	0.903725	-3.549103	1.943184
1	1.341472	-3.373763	2.917751
6	-0.043411	-4.558525	1.776150
1	-0.344696	-5.166908	2.623127
6	-0.622855	-4.752958	0.524685
1	-1.383001	-5.514876	0.382193
6	-0.243585	-3.943609	-0.546354
1	-0.731253	-4.086471	-1.503161
6	0.708814	-2.922496	-0.394263
6	0.365459	-0.148052	2.403044
1	-0.004805	-1.106633	2.771826
6	0.276273	0.878214	3.535204
1	-0.749874	0.970548	3.901938
1	0.607572	1.871029	3.218962
1	0.915125	0.560038	4.365056
6	0.095337	-2.411041	-3.223597
6	-0.943262	-1.641175	-3.768487
1	-1.186486	-0.674922	-3.336465
6	-1.661088	-2.109688	-4.872797
1	-2.470355	-1.509441	-5.278303
6	-1.347461	-3.343327	-5.442303
1	-1.907405	-3.707512	-6.299286
6	-0.305616	-4.111504	-4.910516
1	-0.053213	-5.070237	-5.355192
6	0.415300	-3.647563	-3.811425
1	1.226243	-4.248507	-3.411172
6	2.764200	-2.021295	-2.271880
6	3.436354	-3.231532	-2.043716
1	2.931198	-4.046532	-1.533898
6	4.764711	-3.382893	-2.445773
1	5.280395	-4.321133	-2.260323
6	5.430938	-2.330203	-3.081343
1	6.466583	-2.448364	-3.387337
6	4.762337	-1.127169	-3.322982
1	5.274010	-0.306894	-3.818617
6	3.434631	-0.973307	-2.919393
1	2.915818	-0.035556	-3.098337
6	-2.015366	-1.041684	0.841316
6	-2.397487	-1.822584	1.938027
1	-1.982184	-1.646863	2.922916
6	-3.317234	-2.859690	1.772360
6	-3.882139	-3.125293	0.526188
1	-4.584325	-3.942403	0.401777
6	-3.520264	-2.329254	-0.559657
6	-2.592721	-1.299342	-0.411698
1	-2.304723	-0.691109	-1.262976
6	-1.602071	1.801196	1.207144
6	-0.859299	2.990193	1.129801
1	0.209073	2.951389	0.950305
6	-1.495820	4.223250	1.227675
6	-2.883508	4.301313	1.358506
1	-3.381268	5.263930	1.389398
6	-3.622274	3.121465	1.398943

6	-2.991319	1.875971	1.343978
1	-3.592381	0.974286	1.367653
29	0.381394	0.354306	-1.187174
6	-5.120743	3.192372	1.486329
6	-0.715877	5.494806	1.047151
6	-3.641312	-3.779505	2.915882
6	-4.028262	-2.684209	-1.928934
9	-5.280438	-3.193675	-1.892219
9	-4.048972	-1.621779	-2.765810
9	-3.242931	-3.627172	-2.509902
9	-3.050149	-4.992206	2.752945
9	-4.969761	-4.013814	3.016169
9	-3.223832	-3.295823	4.105518
9	-5.559076	3.281370	2.764197
9	-5.709471	2.098530	0.946008
9	-5.609525	4.272795	0.830818
9	-1.082891	6.440377	1.943139
9	0.614972	5.309877	1.172744
9	-0.924872	6.034171	-0.183448
6	-1.624779	2.370267	-2.177475
6	-0.634328	3.389007	-2.212775
6	0.745985	3.284518	-1.929376
1	-0.964455	4.397788	-2.417077
7	-2.957467	2.742467	-2.159758
6	-4.010209	1.754270	-2.329037
1	-4.688325	2.057880	-3.137770
1	-3.578108	0.789111	-2.577902
1	-4.603920	1.650956	-1.410498
6	-3.416486	4.118752	-2.056865
1	-2.721812	4.722470	-1.473895
1	-3.554592	4.588044	-3.042370
1	-4.378211	4.133037	-1.534482
8	-1.373187	1.113819	-2.158762
6	1.543084	4.480202	-1.994210
6	2.885864	4.474426	-1.704348
1	1.056579	5.411376	-2.267110
6	3.471959	3.249998	-1.338643
6	2.693494	2.116212	-1.267942
1	3.118147	1.162417	-0.980854
7	1.371498	2.116656	-1.540930
1	3.471121	5.386969	-1.754256
35	5.390550	3.141423	-0.923165

---

8 P1-C1 *endo re-re* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 10.1931 11.0876 15.2988 cm(-1)
Electronic energy= -7647.26473
Zero-point correction= 1.771428
(Hartree/Particle)
Thermal correction to Energy= 1.897342
Thermal correction to Enthalpy= 1.898286
Thermal correction to Gibbs Free Energy= 1.598970
Sum of electronic and zero-point Energies= -7645.493302
Sum of electronic and thermal Energies= -7645.367388
Sum of electronic and thermal Enthalpies= -7645.366444
Sum of electronic and thermal Free Energies= -7645.665760

.....

Cartesian Coordinates

.....

26	4.686491	4.728347	1.989701
15	2.744773	1.766480	-1.832938
15	4.687906	0.096269	0.868121
6	4.268027	3.451490	0.384665
6	4.454545	2.707676	1.608561
6	3.472011	3.154668	2.543881
1	3.357542	2.799769	3.558775
6	2.701368	4.185209	1.927496
1	1.905627	4.747074	2.396658
6	3.190291	4.369834	0.601323
1	2.827436	5.090179	-0.116406
6	6.658163	5.162192	2.475356
1	7.489719	4.484730	2.332775
6	5.829867	5.241729	3.636928
1	5.917357	4.629447	4.524504
6	4.832324	6.236478	3.401403
1	4.031058	6.504547	4.077310
6	5.043444	6.772734	2.094460
1	4.433973	7.522925	1.607914
6	6.171192	6.111042	1.523203
1	6.566415	6.281622	0.531174
6	5.024565	3.191929	-0.874111
6	6.370960	3.576109	-0.960520
1	6.807067	4.102363	-0.120695
6	7.152072	3.277991	-2.077041
1	8.198451	3.565867	-2.099869
6	6.586489	2.585544	-3.145012
1	7.184824	2.329396	-4.013383
6	5.249159	2.192591	-3.082820
1	4.829168	1.636907	-3.913686
6	4.454034	2.474867	-1.960779
6	5.439396	1.582370	1.783249
1	6.340841	1.847091	1.227790
6	5.836681	1.317968	3.238126
1	6.578597	0.517241	3.301312
1	4.981788	1.031840	3.856495
1	6.268621	2.228887	3.664164
6	2.474861	0.941572	-3.464089
6	2.568668	-0.459079	-3.512024
1	2.783326	-1.018710	-2.607979
6	2.342566	-1.139880	-4.711898
1	2.420664	-2.221844	-4.736563
6	2.008929	-0.434242	-5.869222
1	1.820929	-0.966576	-6.797365
6	1.912632	0.959987	-5.828415
1	1.651470	1.515271	-6.724959
6	2.146943	1.644648	-4.635632
1	2.060042	2.725715	-4.619860
6	1.643484	3.236742	-1.948352
6	2.004873	4.409380	-2.631645
1	2.989716	4.493667	-3.081839
6	1.108601	5.476091	-2.722818
1	1.398748	6.379520	-3.251971
6	-0.159410	5.379919	-2.139738
1	-0.861217	6.205750	-2.215811
6	-0.522891	4.218040	-1.455463
1	-1.504351	4.137550	-1.001473
6	0.378805	3.156783	-1.351040
1	0.102978	2.264490	-0.801171
6	5.917099	-0.416753	-0.405143
6	5.474475	-1.401230	-1.302317
1	4.477779	-1.815844	-1.177169
6	6.301119	-1.831859	-2.340350
6	7.556990	-1.259792	-2.535823
1	8.186696	-1.575595	-3.359977
6	7.982495	-0.262425	-1.658309
6	7.186945	0.142089	-0.586260
1	7.565695	0.905193	0.080055
6	4.685104	-1.325127	2.037429
6	3.723196	-1.300046	3.060311
1	3.083087	-0.434121	3.182117
6	3.543702	-2.405930	3.885428
6	4.282642	-3.573833	3.687480
1	4.103797	-4.450846	4.299020
6	5.218672	-3.606308	2.657855
6	5.439266	-2.487205	1.851131
1	6.171345	-2.552669	1.055501
29	2.553176	0.330766	-0.099941
6	5.997077	-4.863633	2.389298
6	2.445999	-2.418610	4.912270
6	5.838871	-2.964937	-3.213723
6	9.311346	0.391829	-1.915549
9	9.343532	0.981268	-3.137710
9	9.604733	1.349051	-1.007793
9	10.326539	-0.503688	-1.898848
9	5.992614	-4.161925	-2.594451
9	6.517776	-3.032314	-4.378432
9	4.521702	-2.864082	-3.523045
9	7.185087	-4.883659	3.039956
9	6.277583	-5.005664	1.069956

9	5.319349	-5.969146	2.773813
9	2.862608	-2.960753	6.081679
9	1.977440	-1.181701	5.185270
9	1.390616	-3.162717	4.499017
6	1.976427	-2.600537	0.343102
6	1.034092	-2.282433	1.357794
6	0.606537	-1.019252	1.803723
1	0.554143	-3.108525	1.859147
77	-3.252178	-0.982788	-1.538013
15	-5.124022	-0.252149	-0.478483
8	-5.147174	0.824998	0.765662
8	-6.118051	0.534600	-1.561193
7	-5.847114	-1.536081	0.283044
6	-4.873006	2.169015	0.561740
6	-3.665323	2.654287	1.108472
1	-3.041595	1.974180	1.678475
6	-3.315761	3.965356	0.902457
1	-2.396089	4.356436	1.324832
6	-4.126750	4.810904	0.096933
6	-3.707807	6.129455	-0.229203
1	-2.766760	6.489089	0.178965
6	-4.466109	6.927422	-1.056457
1	-4.133063	7.930294	-1.307241
6	-5.680230	6.433511	-1.590823
1	-6.266542	7.057857	-2.258895
6	-6.124443	5.166790	-1.277335
1	-7.052246	4.802493	-1.702954
6	-5.371875	4.317075	-0.419739
6	-5.785345	2.973900	-0.102000
6	-7.125218	2.437231	-0.472897
6	-8.341504	3.087966	-0.053042
6	-8.349924	4.208659	0.824505
1	-7.411868	4.589610	1.209495
6	-9.531691	4.806670	1.205285
1	-9.508963	5.656237	1.881826
6	-10.773655	4.321939	0.730802
1	-11.696275	4.808570	1.033291
6	-10.805792	3.224037	-0.098548
1	-11.752703	2.826748	-0.454420
6	-9.606574	2.573082	-0.496929
6	-9.643612	1.405914	-1.306728
1	-10.604056	1.028394	-1.645701
6	-8.485528	0.745045	-1.629165
1	-8.489844	-0.166999	-2.216577
6	-7.244807	1.255037	-1.188642
6	-5.321800	-2.860944	-0.148189
1	-4.658313	-3.229167	0.635100
6	-6.444430	-3.867268	-0.334475
6	-6.325525	-5.153533	0.205968
1	-5.441710	-5.405726	0.785001
6	-7.334940	-6.099536	0.003892
1	-7.232636	-7.094152	0.429430
6	-8.473841	-5.766364	-0.732179
1	-9.260821	-6.500141	-0.883222
6	-8.600153	-4.480792	-1.270141
1	-9.486389	-4.213585	-1.839755
6	-7.590808	-3.538788	-1.073426
1	-7.690252	-2.536757	-1.481753
6	-4.516522	-2.709349	-1.444934
1	-5.207501	-2.666529	-2.294576
1	-3.894273	-3.597849	-1.579966
6	-6.625861	-1.522205	1.566334
1	-6.858239	-2.579953	1.719370
6	-5.792735	-1.085067	2.773054
6	-4.722771	-1.886513	3.199517
1	-4.478451	-2.809130	2.683298
6	-3.942361	-1.515866	4.296889
1	-3.122995	-2.159193	4.596094
6	-4.224824	-0.339785	4.995246
1	-3.624437	-0.055236	5.855399
6	-5.290834	0.463557	4.582997
1	-5.522032	1.381250	5.117670
6	-6.066898	0.091426	3.483376
1	-6.880932	0.738183	3.174420
6	-7.962958	-0.800802	1.414068
1	-8.521036	-1.234176	0.581569
1	-7.840702	0.266782	1.225082
1	-8.554210	-0.919789	2.327124
6	-2.343522	-0.952803	0.446430
1	-1.613305	-0.149137	0.454599
1	-2.997765	-0.952774	1.312385
6	-1.970098	-2.236696	-0.063070
1	-2.507779	-3.098688	0.307743
6	-1.015767	-2.413573	-1.062697
1	-0.324438	-1.605643	-1.265270
6	-4.152740	-0.511146	-3.564658
1	-5.164231	-0.904838	-3.530402
6	-3.122123	-1.444439	-3.766049
1	-3.406915	-2.489411	-3.878652
6	-1.741049	-1.115353	-4.297258
1	-1.782352	-1.040458	-5.394471
1	-1.091483	-1.965472	-4.074238
6	-1.112185	0.166289	-3.711446
1	-1.365145	1.034098	-4.327483
1	-0.027664	0.069486	-3.757653
6	-1.501051	0.461093	-2.269397
1	-0.720221	0.319353	-1.529740
6	-2.566283	1.264188	-1.904433
1	-2.537214	1.708203	-0.914926
6	-3.533041	1.907900	-2.875797
1	-4.377479	2.292482	-2.304571
1	-3.040995	2.778897	-3.332477
6	-4.060465	0.958824	-3.975080
1	-3.436676	1.031804	-4.871161
1	-5.059528	1.292894	-4.268911
6	-0.689029	-3.681161	-1.707224
6	-1.362408	-4.890377	-1.432808
6	0.368681	-3.693709	-2.638332
6	-0.992574	-6.061613	-2.089707
1	-2.139467	-4.925085	-0.678877
6	0.733378	-4.867979	-3.293167
1	0.914307	-2.774271	-2.823370
6	0.048984	-6.056821	-3.025034
1	-1.512943	-6.987838	-1.862530
1	1.558304	-4.858703	-4.000357
1	0.331761	-6.976144	-3.530153
7	2.446893	-3.895160	0.275941
6	3.268809	-4.340236	-0.836413
1	2.902563	-5.305531	-1.204274
1	3.215361	-3.623264	-1.649375
1	4.316858	-4.463558	-0.533883
6	2.148007	-4.922790	1.266207
1	1.983263	-4.484607	2.249802
1	1.261509	-5.507193	0.996054
1	3.009150	-5.594150	1.344131
8	2.418521	-1.768119	-0.531539
6	-0.365263	-0.980848	2.866059
6	-0.805837	0.203493	3.400169
1	-0.763892	-1.920741	3.229772
6	-0.287114	1.397307	2.863658
6	0.622270	1.347012	1.830918
1	1.032890	2.251113	1.399539
7	1.064753	0.184937	1.301098
1	-1.546996	0.214911	4.191265
35	-0.809050	3.136363	3.621772
5	-2.179135	-4.879906	2.385696
9	-2.301549	-6.031392	3.160293
9	-2.153369	-3.733420	3.206475
9	-3.303286	-4.780507	1.505964
9	-1.010147	-4.920101	1.609635

[8-9]‡ P1-C1 *endo re-re* [BF_4^-]

Number of imaginary frequencies= 1
The smallest frequencies are=-221.7513 11.3144 12.4751cm(-1)
Electronic energy= -7647.2600588
Zero-point correction= 1.771281
(Hartree/Particle)
Thermal correction to Energy= 1.896114
Thermal correction to Enthalpy= 1.897058

Thermal correction to Gibbs Free Energy= 1.601868
Sum of electronic and zero-point Energies= -7645.488778
Sum of electronic and thermal Energies= -7645.363945
Sum of electronic and thermal Enthalpies= -7645.363001
Sum of electronic and thermal Free Energies= -7645.658190
.....
Cartesian Coordinates
.....

26	4.527102	4.680237	2.206900
15	2.726247	1.866186	-1.799305
15	4.655960	0.105492	0.898054
6	4.166454	3.457332	0.546751
6	4.337096	2.673630	1.748082
6	3.325154	3.071265	2.675171
1	3.194206	2.678905	3.674215
6	2.552482	4.111758	2.077363
1	1.738233	4.645726	2.546989
6	3.069559	4.350986	0.770844
1	2.712500	5.091400	0.070872
6	6.481988	5.123825	2.747443
1	7.325398	4.463637	2.593799
6	5.631355	5.145897	3.895184
1	5.710635	4.499452	4.759008
6	4.623331	6.134529	3.679280
1	3.806199	6.365340	4.349989
6	4.850319	6.724348	2.398444
1	4.238474	7.484031	1.929967
6	5.998094	6.101743	1.823547
1	6.408336	6.314161	0.845588
6	4.957241	3.269347	-0.704298
6	6.300274	3.672756	-0.738007
1	6.713540	4.148291	0.142307
6	7.106560	3.459010	-1.855809
1	8.149460	3.758972	-1.837542
6	6.570330	2.837136	-2.980782
1	7.186763	2.653110	-3.854824
6	5.237808	2.423797	-2.971240
1	4.837339	1.927005	-3.848011
6	4.420265	2.615511	-1.846299
6	5.336892	1.559481	1.911280
1	6.255406	1.865841	1.407361
6	5.676347	1.228988	3.367280
1	6.436337	0.444855	3.423031
1	4.802108	0.889077	3.928922
1	6.064565	2.126210	3.859442
6	2.507967	1.107887	-3.467296
6	2.727825	-0.273893	-3.585921
1	3.013503	-0.851644	-2.714364
6	2.540702	-0.916967	-4.811702
1	2.715674	-1.985102	-4.888382
6	2.120296	-0.190575	-5.927620
1	1.959915	-0.693836	-6.876826
6	1.901801	1.185613	-5.817938
1	1.573713	1.756220	-6.682192
6	2.097728	1.833403	-4.597496
1	1.914471	2.900149	-4.528337
6	1.593306	3.312643	-1.857759
6	1.941543	4.518325	-2.489006
1	2.927928	4.636305	-2.928034
6	1.028341	5.572718	-2.545361
1	1.307747	6.501698	-3.034435
6	-0.243463	5.430425	-1.980567
1	-0.960005	6.245454	-2.030770
6	-0.593923	4.234911	-1.349908
1	-1.579378	4.118006	-0.914386
6	0.324430	3.185458	-1.278164
1	0.055663	2.266737	-0.769672
6	5.945718	-0.317891	-0.347678
6	5.571657	-1.286314	-1.291010
1	4.591229	-1.745404	-1.211799
6	6.441567	-1.647100	-2.319155
6	7.679774	-1.022739	-2.456779
1	8.344814	-1.284563	-3.271975
6	8.038876	-0.041423	-1.532191
6	7.196218	0.297249	-0.472893
1	7.522651	1.055522	0.225418
6	4.613993	-1.375007	1.991113
6	3.582612	-1.430434	2.942756
1	2.913839	-0.586933	3.068479
6	3.380833	-2.584148	3.696445
6	4.172523	-3.715665	3.495780
1	3.983641	-4.626841	4.052260
6	5.184217	-3.664580	2.540189
6	5.421988	-2.501513	1.805366
1	6.215035	-2.499979	1.067834
29	2.557752	0.343939	-0.138988
6	6.027146	-4.885672	2.298147
6	2.219496	-2.678919	4.647160
6	6.037409	-2.760733	-3.244774
6	9.347349	0.673219	-1.727389
9	9.378752	1.331298	-2.913844
9	9.590336	1.587692	-0.762500
9	10.393068	-0.186105	-1.741046
9	6.202219	-3.974080	-2.661025
9	6.751066	-2.769578	-4.388876
9	4.725670	-2.682669	-3.588615
9	7.033533	-4.999894	3.196080
9	6.596321	-4.872275	1.069744
9	5.295508	-6.022048	2.387493
9	2.561855	-3.307672	5.794582
9	1.727058	-1.466090	4.980309
9	1.195897	-3.390200	4.108637
6	2.034251	-2.660873	0.136045
6	0.871426	-2.404637	0.951344
6	0.524196	-1.167832	1.584190
1	0.400273	-3.261406	1.408141
77	-3.297397	-0.941917	-1.649865
15	-5.167937	-0.258277	-0.540221
8	-5.216634	0.789709	0.741456
8	-6.205607	0.542435	-1.583991
7	-5.870750	-1.571715	0.207437
6	-4.916066	2.127274	0.563831
6	-3.706747	2.585786	1.131198
1	-3.098172	1.882384	1.688322
6	-3.342420	3.898559	0.967725
1	-2.424304	4.270097	1.411492
6	-4.136390	4.773753	0.175917
6	-3.704393	6.098078	-0.107016
1	-2.765625	6.438686	0.322251
6	-4.446828	6.925562	-0.919857
1	-4.103675	7.932931	-1.136894
6	-5.657561	6.456361	-1.483502
1	-6.231060	7.104151	-2.140325
6	-6.114366	5.184414	-1.212117
1	-7.039929	4.838634	-1.658037
6	-5.378708	4.304677	-0.370269
6	-5.811350	2.960055	-0.088560
6	-7.162328	2.451245	-0.459164
6	-8.362729	3.114505	-0.012361
6	-8.342453	4.220079	0.884437
1	-7.393752	4.580864	1.262493
6	-9.509308	4.828028	1.294809
1	-9.463279	5.664819	1.986053
6	-10.765539	4.369477	0.832449
1	-11.676424	4.862870	1.158755
6	-10.825604	3.286874	-0.015379
1	-11.783505	2.908277	-0.362477
6	-9.642341	2.626303	-0.444209
6	-9.708892	1.472721	-1.271554
1	-10.679918	1.116050	-1.603371
6	-8.566037	0.798432	-1.618258
1	-8.593499	-0.104974	-2.218392
6	-7.308578	1.278082	-1.186956
6	-5.288329	-2.875176	-0.218934
1	-4.591764	-3.206215	0.554510
6	-6.363543	-3.937827	-0.373749
6	-6.157526	-5.220990	0.148235
1	-5.240421	-5.431287	0.691288
6	-7.120057	-6.219197	-0.029714
1	-6.948797	-7.210444	0.381639

6	-8.300163	-5.943149	-0.723542
1	-9.050828	-6.717625	-0.855598
6	-8.513191	-4.662034	-1.244262
1	-9.430774	-4.438790	-1.782498
6	-7.550219	-3.667845	-1.071899
1	-7.716193	-2.670224	-1.469082
6	-4.512361	-2.704020	-1.531704
1	-5.224351	-2.690027	-2.366534
1	-3.873857	-3.581328	-1.668825
6	-6.646703	-1.587260	1.490071
1	-6.874741	-2.648215	1.626528
6	-5.821776	-1.167779	2.710152
6	-4.763897	-1.981022	3.144080
1	-4.519729	-2.899983	2.621622
6	-3.995909	-1.628515	4.256558
1	-3.186300	-2.281914	4.560738
6	-4.277541	-0.457075	4.962665
1	-3.687510	-0.186510	5.834573
6	-5.331523	0.358940	4.543475
1	-5.563293	1.272876	5.084359
6	-6.095279	0.003502	3.430258
1	-6.899737	0.659858	3.116935
6	-7.988502	-0.870761	1.352123
1	-8.544918	-1.292479	0.512320
1	-7.872388	0.200395	1.181171
1	-8.579046	-1.008481	2.263189
6	-2.418581	-0.951509	0.352361
1	-1.765359	-0.089288	0.453134
1	-3.112599	-1.058023	1.180988
6	-1.907131	-2.161617	-0.213287
1	-2.415539	-3.077728	0.059087
6	-0.659081	-2.299048	-0.867268
1	-0.111711	-1.405730	-1.135439
6	-4.104012	-0.582967	-3.674100
1	-5.106004	-1.004529	-3.712426
6	-3.027839	-1.505470	-3.789809
1	-3.289259	-2.555610	-3.919671
6	-1.648090	-1.147770	-4.314244
1	-1.666723	-1.082365	-5.413832
1	-0.978780	-1.976654	-4.070130
6	-1.069238	0.152350	-3.720711
1	-1.298019	1.006163	-4.366104
1	0.019482	0.076156	-3.699715
6	-1.554007	0.459835	-2.307643
1	-0.800466	0.380673	-1.531216
6	-2.654983	1.260521	-2.015720
1	-2.663517	1.754289	-1.049062
6	-3.585617	1.864153	-3.048377
1	-4.472003	2.224355	-2.522760
1	-3.103980	2.746478	-3.496360
6	-4.023482	0.871970	-4.148295
1	-3.346951	0.932793	-5.007270
1	-5.008823	1.173586	-4.517257
6	-0.278172	-3.506007	-1.605827
6	-0.823351	-4.775890	-1.328348
6	0.678404	-3.392332	-2.633159
6	-0.427674	-5.885953	-2.072121
1	-1.522874	-4.901636	-0.511155
6	1.067160	-4.504443	-3.377112
1	1.119807	-2.423306	-2.833704
6	0.514637	-5.757647	-3.099761
1	-0.849972	-6.860137	-1.841725
1	1.807784	-4.394198	-4.164736
1	0.817888	-6.628842	-3.673703
7	2.540092	-3.929413	0.111614
6	3.529114	-4.313766	-0.886985
1	3.283570	-5.309774	-1.268426
1	3.511089	-3.616405	-1.718618
1	4.538133	-4.345239	-0.458891
6	2.131529	-5.000449	1.018535
1	1.784159	-4.604220	1.969891
1	1.333746	-5.611273	0.584218
1	3.001638	-5.632102	1.216622
8	2.561514	-1.780602	-0.619703
6	-0.431494	-1.217799	2.639289
6	-0.855307	-0.069814	3.276835
1	-0.830737	-2.178241	2.939963
6	-0.325650	1.147240	2.838212
6	0.589937	1.171987	1.803161
1	1.012602	2.103071	1.447808
7	1.013152	0.049503	1.186891
1	-1.590357	-0.116863	4.071678
35	-0.852423	2.828886	3.697588
5	-2.137057	-5.001210	2.366384
9	-2.439002	-6.151828	3.092114
9	-2.209239	-3.863181	3.198255
9	-3.076601	-4.846089	1.306123
9	-0.843303	-5.090770	1.819860

---

9 P1-C1 *endo re-re* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 11.7503 13.7028 15.4507 cm(-1)
Electronic energy= -7647.2862608
Zero-point correction= 1.775206
(Hartree/Particle)
Thermal correction to Energy= 1.899380
Thermal correction to Enthalpy= 1.900324
Thermal correction to Gibbs Free Energy= 1.606315
Sum of electronic and zero-point Energies= -7645.511055
Sum of electronic and thermal Energies= -7645.386881
Sum of electronic and thermal Enthalpies= -7645.385937
Sum of electronic and thermal Free Energies= -7645.679945

.....

Cartesian Coordinates

.....

26	4.062655	4.819043	2.026582
15	2.651588	1.789896	-1.991157
15	4.398536	0.173199	0.954522
6	3.853617	3.517189	0.397651
6	3.931638	2.789262	1.642609
6	2.846112	3.218705	2.467753
1	2.636728	2.875028	3.470982
6	2.112225	4.218508	1.759606
1	1.258292	4.765104	2.135918
6	2.735472	4.407721	0.491923
1	2.431219	5.112144	-0.267459
6	5.960564	5.319275	2.703005
1	6.821575	4.665999	2.650475
6	5.018928	5.380415	3.775737
1	5.037310	4.778495	4.674515
6	4.019295	6.340601	3.431846
1	3.147904	6.589747	4.023068
6	4.342649	6.874357	2.147160
1	3.761670	7.601094	1.594822
6	5.542120	6.246213	1.698256
1	6.027076	6.419829	0.747269
6	4.751505	3.292104	-0.772705
6	6.083246	3.728405	-0.713930
1	6.412921	4.245062	0.178037
6	6.981438	3.497104	-1.755356
1	8.011976	3.825190	-1.665170
6	6.551968	2.824002	-2.896530
1	7.240427	2.629247	-3.712591
6	5.233979	2.373771	-2.976779
1	4.915829	1.836319	-3.863167
6	4.325841	2.581656	-1.926984
6	4.935445	1.708092	1.940033
1	5.882362	2.015446	1.493805
6	5.170421	1.465966	3.433589
1	5.942386	0.708126	3.591909
1	4.265035	1.134800	3.948901
1	5.498562	2.399758	3.900145
6	2.590539	0.989979	-3.649908
6	3.005459	-0.348661	-3.736124
1	3.331264	-0.872054	-2.845079
6	2.972698	-1.023232	-4.957964
1	3.301317	-2.055970	-5.007483
6	2.503735	-0.375015	-6.102613
1	2.461005	-0.905041	-7.049737

6	2.084380	0.955496	-6.023951
1	1.714834	1.464142	-6.909781
6	2.133138	1.638545	-4.807634
1	1.796087	2.668186	-4.765570
6	1.497788	3.207588	-2.133225
6	1.835450	4.374677	-2.838674
1	2.814263	4.465916	-3.300415
6	0.922745	5.425981	-2.934103
1	1.192267	6.326281	-3.479017
6	-0.336028	5.317612	-2.332661
1	-1.051580	6.131407	-2.408303
6	-0.674204	4.160303	-1.628910
1	-1.648511	4.070933	-1.165157
6	0.244066	3.114596	-1.517806
1	-0.012039	2.227501	-0.949498
6	5.805844	-0.232524	-0.168933
6	5.564471	-1.253509	-1.099373
1	4.603910	-1.756592	-1.099265
6	6.544574	-1.622451	-2.019442
6	7.767518	-0.957155	-2.064475
1	8.520393	-1.229194	-2.795643
6	7.997418	0.075059	-1.154125
6	7.040803	0.425149	-0.200353
1	7.272911	1.222460	0.492243
6	4.371959	-1.256070	2.118498
6	3.326810	-1.322236	3.055520
1	2.617316	-0.506536	3.143500
6	3.185227	-2.444193	3.871952
6	4.036818	-3.540491	3.735826
1	3.895833	-4.428078	4.342936
6	5.059382	-3.481227	2.792645
6	5.246855	-2.343661	2.008392
1	6.059970	-2.331325	1.294463
29	2.411534	0.295462	-0.308297
6	5.952463	-4.679270	2.619839
6	2.052471	-2.544441	4.856638
6	6.272138	-2.793274	-2.922162
6	9.294183	0.832089	-1.247892
9	9.401360	1.484912	-2.432379
9	9.426703	1.758726	-0.273240
9	10.363561	0.006858	-1.168850
9	6.443530	-3.969841	-2.268854
9	7.079051	-2.815317	-4.001201
9	4.990421	-2.795887	-3.372575
9	6.785574	-4.850423	3.670800
9	6.720185	-4.590714	1.510424
9	5.224732	-5.818771	2.512016
9	2.453857	-3.096260	6.023046
9	1.512223	-1.339401	5.145115
9	1.053383	-3.329644	4.381765
6	1.968146	-2.760739	-0.059127
6	0.532048	-2.515352	0.386260
6	0.358614	-1.346965	1.327151
1	0.119757	-3.396566	0.872693
77	-3.285850	-0.959771	-1.809311
15	-5.108378	-0.238812	-0.603136
8	-5.070692	0.749109	0.738215
8	-6.179359	0.657499	-1.542715
7	-5.833060	-1.561948	0.121169
6	-4.703056	2.072152	0.614395
6	-3.447046	2.437869	1.150444
1	-2.854601	1.671426	1.637372
6	-3.021546	3.738373	1.048685
1	-2.065531	4.038786	1.467283
6	-3.804380	4.698673	0.348779
6	-3.319763	6.016936	0.129034
1	-2.349161	6.285909	0.537718
6	-4.049571	6.926837	-0.603158
1	-3.665846	7.928860	-0.771779
6	-5.300084	6.549019	-1.148352
1	-5.864091	7.261233	-1.743843
6	-5.806818	5.284672	-0.936977
1	-6.762439	5.009182	-1.368111
6	-5.086572	4.321700	-0.176378
6	-5.577230	2.985656	0.045930
6	-6.968258	2.567864	-0.290105
6	-8.109975	3.274013	0.239497
6	-7.991229	4.330203	1.187405
1	-7.009673	4.617660	1.543786
6	-9.103381	4.982549	1.674778
1	-8.980706	5.779564	2.402805
6	-10.401651	4.620248	1.244558
1	-11.268659	5.147487	1.631873
6	-10.557593	3.585698	0.350101
1	-11.548790	3.278819	0.025842
6	-9.432627	2.882092	-0.159266
6	-9.599820	1.777001	-1.036718
1	-10.602738	1.493035	-1.343268
6	-8.513461	1.056628	-1.461515
1	-8.618078	0.186074	-2.100414
6	-7.211236	1.438823	-1.063426
6	-5.255341	-2.864974	-0.324954
1	-4.526832	-3.187034	0.420825
6	-6.328347	-3.935606	-0.429496
6	-6.090783	-5.213916	0.092250
1	-5.153138	-5.410462	0.604808
6	-7.048510	-6.223185	-0.043730
1	-6.851658	-7.209958	0.367216
6	-8.256442	-5.963999	-0.695090
1	-9.003267	-6.747054	-0.795005
6	-8.501930	-4.688024	-1.214226
1	-9.441228	-4.477485	-1.719297
6	-7.543621	-3.682842	-1.083806
1	-7.734575	-2.689456	-1.480686
6	-4.523463	-2.707421	-1.664824
1	-5.266648	-2.679080	-2.473334
1	-3.917982	-3.604619	-1.820036
6	-6.563275	-1.594999	1.430261
1	-6.850405	-2.645526	1.528289
6	-5.679176	-1.284256	2.643321
6	-4.698325	-2.205376	3.042066
1	-4.558750	-3.132225	2.496364
6	-3.878107	-1.952878	4.145129
1	-3.124727	-2.684606	4.414344
6	-4.034526	-0.776675	4.881205
1	-3.407094	-0.583098	5.747729
6	-5.013621	0.145389	4.500620
1	-5.148862	1.063530	5.066740
6	-5.826097	-0.109534	3.394708
1	-6.569313	0.626357	3.109397
6	-7.865512	-0.798587	1.374429
1	-8.472227	-1.147305	0.535489
1	-7.696372	0.271691	1.249775
1	-8.432415	-0.947984	2.298759
6	-2.369024	-1.128314	0.167435
1	-1.798524	-0.229152	0.383168
1	-3.065466	-1.383896	0.961644
6	-1.798979	-2.181471	-0.603920
1	-2.242276	-3.155804	-0.423241
6	-0.319934	-2.292542	-0.944029
1	0.066523	-1.370578	-1.377739
6	-4.101562	-0.585430	-3.789802
1	-5.105774	-0.999720	-3.864079
6	-3.018512	-1.519405	-3.910929
1	-3.286175	-2.562943	-4.078698
6	-1.666187	-1.141341	-4.494284
1	-1.748214	-0.986888	-5.582603
1	-0.999600	-1.995099	-4.357298
6	-1.034444	0.101795	-3.831347
1	-1.192363	0.992800	-4.449455
1	0.049215	-0.032759	-3.778932
6	-1.548580	0.386048	-2.420969
1	-0.802072	0.304499	-1.637988
6	-2.637733	1.213309	-2.131537
1	-2.627582	1.716512	-1.169826
6	-3.542913	1.849484	-3.169523
1	-4.425668	2.227419	-2.647506
1	-3.037010	2.723578	-3.608848
6	-3.994213	0.868140	-4.273114
1	-3.310612	0.920176	-5.128575

1	-4.970443	1.190108	-4.651206
6	-0.025485	-3.434112	-1.903897
6	-0.470563	-4.740378	-1.646091
6	0.767496	-3.208399	-3.035763
6	-0.140466	-5.785588	-2.512409
1	-1.045829	-4.951181	-0.750664
6	1.096563	-4.250758	-3.904935
1	1.136724	-2.208089	-3.228960
6	0.640985	-5.545634	-3.646680
1	-0.491248	-6.791038	-2.295402
1	1.706376	-4.047269	-4.781385
1	0.895564	-6.361032	-4.318340
7	2.544805	-3.950498	0.185940
6	3.712521	-4.355344	-0.599254
1	3.641110	-5.429075	-0.790409
1	3.713625	-3.830298	-1.551807
1	4.649244	-4.156514	-0.072476
6	2.040319	-4.948033	1.134229
1	1.500931	-4.482101	1.955816
1	1.380393	-5.665661	0.639963
1	2.901727	-5.472329	1.552605
8	2.551041	-1.895028	-0.758631
6	-0.391276	-1.525037	2.495417
6	-0.705212	-0.434937	3.298935
1	-0.759100	-2.509666	2.756515
6	-0.261922	0.814689	2.882904
6	0.487499	0.944416	1.722931
1	0.849057	1.906783	1.385301
7	0.808506	-0.123294	0.966159
1	-1.299788	-0.561274	4.194801
35	-0.678025	2.410223	3.929378
5	-2.098674	-5.162304	2.250988
9	-2.516765	-6.387444	2.763966
9	-1.886748	-4.240439	3.301757
9	-3.081802	-4.647557	1.369826
9	-0.889458	-5.316756	1.537279

---

8 P1-C1 *endo si-re* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 9.3115 9.8052 14.1056 cm(-1)
Electronic energy= -7647.2565111
Zero-point correction= 1.772082
(Hartree/Particle)
Thermal correction to Energy= 1.897640
Thermal correction to Enthalpy= 1.898584
Thermal correction to Gibbs Free Energy= 1.600752
Sum of electronic and zero-point Energies= -7645.484430
Sum of electronic and thermal Energies= -7645.358871
Sum of electronic and thermal Enthalpies= -7645.357927
Sum of electronic and thermal Free Energies= -7645.655759

.....

Cartesian Coordinates

.....

26	4.193871	5.079880	2.032509
15	2.465492	2.051622	-1.814141
15	4.789256	0.509462	0.844492
6	3.828546	3.893206	0.344841
6	4.379327	3.109911	1.420386
6	3.484377	3.207010	2.531124
1	3.619643	2.729638	3.492016
6	2.403870	4.059714	2.161757
1	1.584435	4.358796	2.801473
6	2.617283	4.489482	0.819548
1	1.985891	5.159115	0.253324
6	6.046633	6.002972	2.222089
1	6.972567	5.616031	1.817981
6	5.506035	5.703752	3.510163
1	5.942863	5.041502	4.245511
6	4.259655	6.389852	3.635517
1	3.589511	6.339714	4.483694
6	4.028735	7.112196	2.425198
1	3.153038	7.704433	2.194109
6	5.132589	6.874670	1.552436
1	5.238642	7.262171	0.548345
6	4.416465	3.965958	-1.020636
6	5.572391	4.729692	-1.238774
1	5.988782	5.275825	-0.402322
6	6.188824	4.789098	-2.488862
1	7.088861	5.382636	-2.621391
6	5.641133	4.084003	-3.557741
1	6.103876	4.118924	-4.539351
6	4.497112	3.309654	-3.360942
1	4.097715	2.753291	-4.200089
6	3.881450	3.218606	-2.101872
6	5.560795	2.193303	1.281088
1	6.119628	2.485557	0.387318
6	6.515956	2.197606	2.476811
1	7.340555	1.493469	2.330437
1	6.006058	1.935135	3.407620
1	6.935144	3.201304	2.595191
6	2.275297	1.252492	-3.465210
6	3.224322	0.276198	-3.814456
1	4.038646	0.053335	-3.132884
6	3.154915	-0.381706	-5.040737
1	3.904183	-1.125594	-5.294711
6	2.120509	-0.086284	-5.934410
1	2.057146	-0.605275	-6.886355
6	1.170558	0.880216	-5.597138
1	0.365350	1.117880	-6.286649
6	1.250676	1.551987	-4.372941
1	0.517847	2.313977	-4.133932
6	1.014809	3.171646	-1.658450
6	0.847299	4.312310	-2.460289
1	1.586197	4.559064	-3.217551
6	-0.264569	5.138292	-2.282199
1	-0.389936	6.016646	-2.909173
6	-1.210373	4.839900	-1.294195
1	-2.074901	5.483527	-1.155807
6	-1.035686	3.716316	-0.483819
1	-1.760914	3.482515	0.287880
6	0.070097	2.882159	-0.662799
1	0.229066	2.030357	-0.006220
6	5.987146	-0.303160	-0.287239
6	6.347749	-1.655259	-0.186905
1	6.029974	-2.253436	0.658278
6	7.104120	-2.259172	-1.192238
6	7.487390	-1.550576	-2.330448
1	8.061753	-2.030116	-3.113688
6	7.099308	-0.216568	-2.446387
6	6.361814	0.406636	-1.439501
1	6.057015	1.439439	-1.577639
6	4.845451	-0.397357	2.441468
6	3.654346	-0.377657	3.178721
1	2.780472	0.107691	2.760498
6	3.599078	-0.964530	4.443955
6	4.716770	-1.596674	4.984505
1	4.668808	-2.063759	5.961098
6	5.902164	-1.617047	4.247408
6	5.977549	-1.011433	2.992372
1	6.918812	-1.024961	2.455084
29	2.701171	0.535956	-0.143783
6	7.141786	-2.227651	4.840291
6	2.297441	-0.951925	5.198589
6	7.568036	-3.679698	-1.012204
6	7.395729	0.561311	-3.698563
9	6.280371	0.709403	-4.461225
9	7.838317	1.810097	-3.422900
9	8.325117	-0.036768	-4.472497
9	6.715099	-4.403304	-0.257383
9	8.773849	-3.724100	-0.389849
9	7.721332	-4.319356	-2.193485
9	7.892007	-1.300588	5.487965
9	7.937089	-2.773232	3.891874
9	6.856716	-3.195425	5.738172
9	2.484205	-1.060887	6.533988
9	1.610385	0.196284	4.981036
9	1.483689	-1.969137	4.833144
6	3.079536	-2.199934	-1.229624
6	1.648915	-2.239481	0.642441

6	3.170254	-3.573330	-1.267672
1	3.597730	-1.589546	-1.956394
6	1.752140	-3.671108	0.642311
6	2.501258	-4.337996	-0.298333
1	1.195757	-4.236432	1.380436
6	0.797513	-1.634317	1.601203
6	0.540486	-0.259393	1.792534
8	1.201514	0.701212	1.247658
7	2.359574	-1.535696	-0.303625
1	0.286610	-2.336912	2.241577
7	-0.492734	0.122274	2.633465
6	-0.566908	1.485120	3.129401
1	-0.359219	1.522255	4.208035
1	-1.570990	1.900671	2.968811
1	0.162248	2.102236	2.607943
6	-1.336772	-0.834925	3.328806
1	-0.858500	-1.231574	4.233668
1	-1.595716	-1.678545	2.691452
1	-2.261910	-0.334403	3.622347
77	-3.568920	-0.562246	-1.627269
15	-5.383073	-0.488273	-0.241052
8	-5.489353	0.479723	1.096682
8	-6.720151	0.028070	-1.079738
7	-5.605948	-1.974099	0.465456
6	-5.507917	1.861719	0.944766
6	-4.362148	2.562594	1.381315
1	-3.554065	2.002676	1.837315
6	-4.304909	3.925127	1.223740
1	-3.441948	4.483030	1.575086
6	-5.353325	4.618194	0.559935
6	-5.250568	6.008329	0.281698
1	-4.363699	6.539608	0.617432
6	-6.242792	6.666022	-0.409797
1	-6.150809	7.726552	-0.624871
6	-7.381436	5.952598	-0.854336
1	-8.151915	6.468482	-1.420043
6	-7.521798	4.608912	-0.581127
1	-8.397502	4.078138	-0.935763
6	-6.524622	3.899579	0.144450
6	-6.630868	2.490671	0.431471
6	-7.885941	1.723326	0.194213
6	-9.138934	2.141878	0.776878
6	-9.232696	3.211760	1.710754
1	-8.333232	3.731870	2.016375
6	-10.445734	3.586769	2.247181
1	-10.485412	4.402217	2.963775
6	-11.636864	2.916604	1.881709
1	-12.586437	3.227840	2.307042
6	-11.581253	1.859699	1.001755
1	-12.483497	1.318996	0.728065
6	-10.344371	1.436902	0.443924
6	-10.280577	0.309191	-0.418282
1	-11.198404	-0.211400	-0.676492
6	-9.072930	-0.139678	-0.887201
1	-8.992616	-1.022731	-1.512183
6	-7.888497	0.553337	-0.551255
6	-4.646388	-3.014431	-0.004549
1	-3.837571	-3.092427	0.725049
6	-5.319944	-4.371579	-0.137347
6	-4.682481	-5.519740	0.346344
1	-3.737310	-5.425328	0.869078
6	-5.270773	-6.776553	0.174616
1	-4.767980	-7.659595	0.559612
6	-6.500298	-6.896641	-0.475675
1	-6.958509	-7.873570	-0.603416
6	-7.144216	-5.750872	-0.956379
1	-8.104546	-5.835874	-1.458178
6	-6.556034	-4.497607	-0.789881
1	-7.058616	-3.604599	-1.152907
6	-4.068511	-2.618597	-1.366590
1	-4.804324	-2.869796	-2.136684
1	-3.180651	-3.220380	-1.566260
6	-6.308980	-2.284319	1.755877
1	-6.462545	-3.364442	1.696960
6	-5.441700	-2.048583	2.991920
6	-4.536838	-3.045837	3.384631
1	-4.435240	-3.953980	2.801330
6	-3.756525	-2.900702	4.533789
1	-3.041534	-3.675482	4.786395
6	-3.889255	-1.759359	5.325875
1	-3.290022	-1.644520	6.224977
6	-4.787621	-0.757246	4.946479
1	-4.896410	0.136177	5.556038
6	-5.551187	-0.897261	3.785656
1	-6.241853	-0.109575	3.506867
6	-7.703777	-1.668909	1.841517
1	-8.299233	-1.969357	0.976796
1	-7.693521	-0.579674	1.889152
1	-8.197952	-2.039222	2.744531
6	-2.366757	-0.056189	0.135586
1	-1.969681	0.941592	-0.024562
1	-2.815455	-0.199202	1.111274
6	-1.691140	-1.186167	-0.415655
1	-1.821525	-2.137346	0.084297
6	-1.011591	-1.140183	-1.637108
1	-0.671834	-0.179061	-2.006841
6	-4.945728	-0.571883	-3.431750
1	-5.706527	-1.316461	-3.215494
6	-3.692636	-1.063198	-3.839135
1	-3.577758	-2.143468	-3.911509
6	-2.674275	-0.285905	-4.647767
1	-2.954443	-0.332208	-5.711002
1	-1.717905	-0.805435	-4.562484
6	-2.496009	1.183498	-4.218107
1	-3.201987	1.825602	-4.752580
1	-1.499600	1.514271	-4.517868
6	-2.649276	1.423589	-2.723634
1	-1.735861	1.610745	-2.170064
6	-3.837840	1.796942	-2.132632
1	-3.787260	2.273314	-1.158454
6	-5.144013	1.963991	-2.879963
1	-5.938879	2.086430	-2.146101
1	-5.099696	2.903920	-3.448663
6	-5.506392	0.795043	-3.827182
1	-5.181061	1.018304	-4.848250
1	-6.595865	0.712970	-3.864379
6	-0.463499	-2.308833	-2.327478
6	-0.644227	-3.632692	-1.874423
6	0.285515	-2.101620	-3.503491
6	-0.131510	-4.703115	-2.604882
1	-1.145251	-3.831986	-0.934147
6	0.795754	-3.174900	-4.229083
1	0.473148	-1.086985	-3.837582
6	0.578096	-4.482877	-3.789049
1	-0.272886	-5.714450	-2.234513
1	1.374607	-2.986167	-5.128075
1	0.979469	-5.322176	-4.349115
1	2.552733	-5.421697	-0.300750
35	4.216194	-4.431791	-2.686511
5	-1.430451	-4.769122	2.395753
9	-2.568673	-5.453204	2.861472
9	-0.463010	-5.684584	1.957772
9	-0.906350	-3.963711	3.418869
9	-1.816835	-3.940817	1.300328

[**8-9**]‡ **P1-C1** *endo si-re* [BF_4^-]

Number of imaginary frequencies= 1
The smallest frequencies are= -209.2380 7.6161 10.0335 cm(-1)
Electronic energy= -7647.2448607
Zero-point correction= 1.771051
(Hartree/Particle)
Thermal correction to Energy= 1.896066
Thermal correction to Enthalpy= 1.897010
Thermal correction to Gibbs Free Energy= 1.598936
Sum of electronic and zero-point Energies= -7645.473809
Sum of electronic and thermal Energies= -7645.348795
Sum of electronic and thermal Enthalpies= -7645.347850
Sum of electronic and thermal Free Energies= -7645.645925
.....

Cartesian Coordinates

26	3.702977	4.996167	2.532092
15	2.510671	2.127947	-1.614685
15	4.896006	0.613927	1.041874
6	3.561194	3.912290	0.744713
6	4.114130	3.101347	1.798887
6	3.147003	3.033742	2.850019
1	3.271597	2.508718	3.787545
6	2.014514	3.810581	2.465271
1	1.133398	3.990318	3.066674
6	2.271203	4.358550	1.174901
1	1.615684	5.008332	0.613190
6	5.437124	6.075192	2.918652
1	6.421337	5.810865	2.555300
6	4.846345	5.631423	4.141078
1	5.299406	4.962161	4.860116
6	3.531315	6.182859	4.220630
1	2.813466	6.002745	5.010147
6	3.309618	6.968289	3.048363
1	2.396281	7.490691	2.795568
6	4.486413	6.902501	2.244443
1	4.619505	7.371498	1.279100
6	4.209357	4.152509	-0.573908
6	5.288939	5.042110	-0.671709
1	5.622918	5.543175	0.227713
6	5.931895	5.284149	-1.886101
1	6.771817	5.971709	-1.926251
6	5.487016	4.642280	-3.039284
1	5.971259	4.821895	-3.994189
6	4.426363	3.739268	-2.961799
1	4.109840	3.230022	-3.864042
6	3.791308	3.461987	-1.740948
6	5.397713	2.328194	1.690596
1	5.984453	2.760967	0.874830
6	6.252218	2.333740	2.960665
1	7.186337	1.784004	2.815450
1	5.724778	1.893105	3.811093
1	6.500542	3.367512	3.216764
6	2.461823	1.415709	-3.312033
6	3.554157	0.624343	-3.709537
1	4.415059	0.529801	-3.056213
6	3.558205	-0.016183	-4.946614
1	4.414548	-0.617238	-5.238616
6	2.458120	0.109188	-5.801662
1	2.451744	-0.401210	-6.760278
6	1.368772	0.892420	-5.416638
1	0.510486	0.994696	-6.074479
6	1.371345	1.549162	-4.182221
1	0.518496	2.157307	-3.902277
6	0.936636	3.054954	-1.444248
6	0.666121	4.211221	-2.193451
1	1.393189	4.575848	-2.913678
6	-0.534308	4.898974	-2.010594
1	-0.742119	5.789353	-2.597292
6	-1.465899	4.444494	-1.070761
1	-2.402089	4.976977	-0.933435
6	-1.191771	3.303736	-0.313585
1	-1.910787	2.950637	0.416660
6	0.003159	2.605450	-0.499713
1	0.230731	1.728441	0.100035
6	6.275810	0.124712	-0.075605
6	6.880171	-1.140935	-0.050696
1	6.638875	-1.856624	0.725295
6	7.785427	-1.509507	-1.046066
6	8.091445	-0.646664	-2.097477
1	8.782618	-0.946652	-2.875382
6	7.472200	0.601230	-2.137185
6	6.575228	0.989242	-1.140483
1	6.091316	1.958421	-1.215917
6	5.009794	-0.519480	2.485978
6	3.795124	-1.003700	2.982820
1	2.866238	-0.687906	2.520422
6	3.776526	-1.886259	4.065373
6	4.960763	-2.298755	4.668430
1	4.945793	-2.996349	5.497278
6	6.172902	-1.805579	4.179117
6	6.204716	-0.920241	3.102698
1	7.160853	-0.562792	2.738509
29	2.889036	0.484217	-0.096798
6	7.462738	-2.189741	4.851278
6	2.446185	-2.422780	4.517323
6	8.481495	-2.840876	-0.952318
6	7.699016	1.532099	-3.297001
9	6.588819	1.623367	-4.075646
9	7.984046	2.788471	-2.884502
9	8.709020	1.129779	-4.095612
9	7.722179	-3.767908	-0.330298
9	9.635888	-2.743301	-0.246653
9	8.811151	-3.328592	-2.169116
9	7.819901	-1.284175	5.795182
9	8.487736	-2.256324	3.971029
9	7.378263	-3.387324	5.469067
9	2.533545	-3.137469	5.657868
9	1.556809	-1.421364	4.736551
9	1.896579	-3.227960	3.577434
6	3.866174	-1.953076	-1.503814
6	1.954472	-2.460632	-0.251446
6	4.006801	-3.264630	-1.915076
1	4.561651	-1.190245	-1.824895
6	2.093682	-3.829353	-0.623370
6	3.108326	-4.237108	-1.465759
1	1.379377	-4.548185	-0.238022
6	0.801769	-2.102614	0.518970
6	0.632348	-0.941457	1.342448
8	1.286177	0.147217	1.191701
7	2.865070	-1.547292	-0.702630
1	0.175329	-2.950814	0.745013
7	-0.319203	-0.972335	2.325060
6	-0.659151	0.246358	3.044270
1	-0.146116	0.286398	4.014171
1	-1.738639	0.264947	3.226960
1	-0.370577	1.120728	2.463682
6	-0.947353	-2.179015	2.857287
1	-0.437496	-3.082742	2.537717
1	-1.997017	-2.245137	2.560043
1	-0.902053	-2.137834	3.949735
77	-3.852960	-0.741685	-1.501797
15	-5.640651	-0.378733	-0.138440
8	-5.708252	0.751355	1.077479
8	-6.964620	0.100862	-1.037928
7	-5.960420	-1.746322	0.765176
6	-5.745146	2.102173	0.775058
6	-4.598030	2.851287	1.114901
1	-3.781554	2.336043	1.609201
6	-4.552462	4.191213	0.821804
1	-3.683260	4.783655	1.090987
6	-5.625641	4.809271	0.123205
6	-5.547646	6.168592	-0.284811
1	-4.656946	6.735986	-0.027126
6	-6.567894	6.752103	-1.001782
1	-6.494254	7.789259	-1.315501
6	-7.711892	5.991804	-1.343227
1	-8.505120	6.447663	-1.928759
6	-7.828072	4.677562	-0.944769
1	-8.707475	4.107637	-1.221188
6	-6.801347	4.045628	-0.189471
6	-6.886651	2.670197	0.231140
6	-8.137341	1.868906	0.108853
6	-9.377895	2.316018	0.693384
6	-9.468942	3.476604	1.512974
1	-8.574300	4.048473	1.726995
6	-10.672007	3.876694	2.053513
1	-10.709335	4.762819	2.680832
6	-11.855817	3.141759	1.807624
1	-12.798235	3.473195	2.233722
6	-11.801014	1.997822	1.044084
1	-12.696806	1.409019	0.864154
6	-10.573703	1.548844	0.485188
6	-10.509019	0.338152	-0.256255

1	-11.420330	-0.230048	-0.420284
6	-9.307534	-0.124228	-0.730172
1	-9.226306	-1.062545	-1.268746
6	-8.132256	0.631775	-0.519661
6	-5.142981	-2.922063	0.345151
1	-4.298789	-3.017502	1.033750
6	-5.953587	-4.208975	0.397120
6	-5.384319	-5.382777	0.908324
1	-4.372356	-5.366217	1.297913
6	-6.110320	-6.577518	0.905901
1	-5.653322	-7.479812	1.303567
6	-7.411691	-6.613128	0.400840
1	-7.975821	-7.541827	0.404814
6	-7.986168	-5.443498	-0.108139
1	-8.999952	-5.460135	-0.499910
6	-7.260335	-4.252309	-0.112136
1	-7.708498	-3.340212	-0.497673
6	-4.606960	-2.708376	-1.076704
1	-5.416131	-2.920280	-1.785929
1	-3.823038	-3.445968	-1.257964
6	-6.539139	-1.848475	2.144266
1	-6.856673	-2.892643	2.203419
6	-5.481533	-1.666925	3.233099
6	-4.806488	-2.800731	3.711406
1	-5.044512	-3.776379	3.296349
6	-3.841998	-2.696873	4.716321
1	-3.329544	-3.589091	5.064744
6	-3.536023	-1.449937	5.263733
1	-2.785553	-1.363567	6.044596
6	-4.203681	-0.312757	4.799700
1	-3.980558	0.661198	5.227637
6	-5.169477	-0.420162	3.796119
1	-5.684080	0.470167	3.456769
6	-7.807172	-1.022613	2.361734
1	-8.552204	-1.270442	1.602675
1	-7.634996	0.052590	2.334021
1	-8.221158	-1.275909	3.342656
6	-2.629457	-0.468448	0.294839
1	-2.153036	0.510637	0.289693
1	-3.127349	-0.699917	1.232713
6	-1.989277	-1.546714	-0.393006
1	-2.249574	-2.552609	-0.099911
6	-0.835750	-1.409889	-1.201178
1	-0.417136	-0.414181	-1.315869
6	-5.068133	-0.765905	-3.358022
1	-5.936763	-1.390040	-3.163390
6	-3.846063	-1.441661	-3.615674
1	-3.868803	-2.530981	-3.617916
6	-2.708749	-0.850816	-4.429926
1	-2.964972	-0.882737	-5.500685
1	-1.837607	-1.498466	-4.307121
6	-2.325533	0.589514	-4.025216
1	-2.831252	1.316334	-4.670170
1	-1.254992	0.723078	-4.196923
6	-2.618280	0.942216	-2.569009
1	-1.747441	1.126325	-1.950871
6	-3.809304	1.509550	-2.126159
1	-3.761555	2.097103	-1.214136
6	-5.018421	1.785625	-2.999057
1	-5.860439	2.011373	-2.341817
1	-4.832159	2.695009	-3.590416
6	-5.403115	0.613880	-3.928497
1	-4.916366	0.727354	-4.903087
1	-6.479470	0.660208	-4.120945
6	-0.379137	-2.389301	-2.178654
6	-0.854244	-3.715480	-2.200934
6	0.579218	-1.998891	-3.134840
6	-0.399769	-4.610248	-3.165624
1	-1.551891	-4.058508	-1.448844
6	1.024946	-2.896025	-4.104061
1	0.970415	-0.987115	-3.114454
6	0.532404	-4.204079	-4.127501
1	-0.764788	-5.632914	-3.150709
1	1.759119	-2.571363	-4.834622
1	0.882327	-4.905666	-4.879709
1	3.198318	-5.275103	-1.766776
35	5.459826	-3.726259	-3.143189
5	-1.551904	-5.560627	0.886094
9	-2.158303	-6.437534	1.791920
9	-1.430938	-6.158904	-0.375762
9	-0.274402	-5.173751	1.356105
9	-2.358195	-4.394425	0.773606

---

9 P1-C1 *endo si-re* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 9.4782 10.2667 12.2814 cm(-1)
Electronic energy= -7647.2756488
Zero-point correction= 1.774025
(Hartree/Particle)
Thermal correction to Energy= 1.898786
Thermal correction to Enthalpy= 1.899730
Thermal correction to Gibbs Free Energy= 1.602157
Sum of electronic and zero-point Energies= -7645.501624
Sum of electronic and thermal Energies= -7645.376863
Sum of electronic and thermal Enthalpies= -7645.375918
Sum of electronic and thermal Free Energies= -7645.673492
.....
Cartesian Coordinates
.....

26	3.361765	4.411832	3.458842
15	2.139323	2.475885	-1.207461
15	4.803569	0.570812	0.980305
6	3.194791	3.747351	1.476705
6	3.865135	2.767170	2.292814
6	2.972490	2.386566	3.342663
1	3.191494	1.674707	4.127313
6	1.765965	3.132521	3.194049
1	0.910561	3.096579	3.855502
6	1.905567	3.977487	2.054633
1	1.171360	4.679575	1.686987
6	5.022691	5.533315	4.013466
1	6.003075	5.444873	3.564911
6	4.538786	4.778982	5.125830
1	5.084726	4.013655	5.661086
6	3.190017	5.176912	5.374943
1	2.534334	4.762832	6.129632
6	2.839382	6.175887	4.416047
1	1.872343	6.650924	4.316150
6	3.971548	6.397670	3.576496
1	4.009658	7.074245	2.733701
6	3.749779	4.332444	0.223307
6	4.753466	5.309214	0.293498
1	5.091772	5.626745	1.271530
6	5.318435	5.865455	-0.855004
1	6.099415	6.614991	-0.764544
6	4.874176	5.455096	-2.109360
1	5.301101	5.878125	-3.013290
6	3.887735	4.472658	-2.204792
1	3.570339	4.144046	-3.187240
6	3.329080	3.888069	-1.058016
6	5.193147	2.152813	1.960212
1	5.679323	2.791070	1.215742
6	6.137294	1.996586	3.154461
1	7.116042	1.621935	2.842979
1	5.732339	1.321860	3.913711
1	6.281526	2.976047	3.617977
6	2.045488	2.175986	-3.017826
6	3.099130	1.440111	-3.589131
1	3.921797	1.107727	-2.964430
6	3.103850	1.143903	-4.950171
1	3.928295	0.580076	-5.377004
6	2.042278	1.564772	-5.758100
1	2.035574	1.324807	-6.817271
6	0.988633	2.289033	-5.197911
1	0.158113	2.611357	-5.818921
6	0.988156	2.598230	-3.834114
1	0.158050	3.156053	-3.414562
6	0.547895	3.240312	-0.712534
6	0.188404	4.536638	-1.115351

1	0.815699	5.084924	-1.812261
6	-0.958196	5.137692	-0.594326
1	-1.229217	6.143163	-0.903372
6	-1.743864	4.455379	0.341372
1	-2.617827	4.936642	0.769190
6	-1.395260	3.161688	0.734484
1	-1.995452	2.629315	1.466646
6	-0.254505	2.553722	0.207528
1	0.049046	1.570272	0.548203
6	6.185025	0.483060	-0.244168
6	7.073361	-0.594466	-0.372764
1	7.043351	-1.427429	0.317256
6	8.002961	-0.618875	-1.411565
6	8.059301	0.408414	-2.353614
1	8.774765	0.374134	-3.166622
6	7.164512	1.469407	-2.238590
6	6.235302	1.512168	-1.197030
1	5.536201	2.341770	-1.145543
6	5.083157	-0.861900	2.104314
6	3.989025	-1.703438	2.341246
1	3.032315	-1.471851	1.892674
6	4.127228	-2.842429	3.137257
6	5.353502	-3.162682	3.714990
1	5.463303	-4.053526	4.320749
6	6.442686	-2.322800	3.485513
6	6.314975	-1.181073	2.694217
1	7.187204	-0.561051	2.525029
29	2.764112	0.578058	-0.136511
6	7.792802	-2.624551	4.078025
6	2.922060	-3.716041	3.360880
6	8.999722	-1.742897	-1.510632
6	7.161744	2.586280	-3.247891
9	5.951441	2.703951	-3.850019
9	7.422090	3.781428	-2.668201
9	8.075532	2.404501	-4.222728
9	8.657673	-2.805239	-0.752788
9	10.229651	-1.344690	-1.104796
9	9.137592	-2.177600	-2.785745
9	8.169426	-1.668733	4.961269
9	8.750854	-2.661525	3.121188
9	7.821778	-3.805996	4.726307
9	3.238565	-4.898825	3.923532
9	2.018509	-3.115855	4.177227
9	2.280561	-3.976767	2.197587
6	3.913219	-1.685402	-1.707365
6	1.953084	-2.404596	-0.692809
6	4.264901	-2.987730	-2.028509
1	4.543561	-0.849404	-1.981587
6	2.283048	-3.741285	-0.955339
6	3.456317	-4.048526	-1.635329
1	1.611766	-4.530429	-0.636092
6	0.584041	-2.099030	-0.116300
6	0.654937	-1.273418	1.157581
8	1.220363	-0.148221	1.141356
7	2.780978	-1.398257	-1.041357
1	0.115349	-3.060606	0.075799
7	0.122872	-1.719285	2.305643
6	0.181271	-0.808383	3.452619
1	-0.062699	-1.363735	4.355193
1	-0.536223	0.009846	3.332973
1	1.181471	-0.382341	3.541241
6	-0.649189	-2.957891	2.454941
1	-0.245465	-3.757491	1.840905
1	-1.699369	-2.797313	2.198723
1	-0.583231	-3.272229	3.496368
77	-3.657865	-0.631366	-1.510848
15	-5.480593	-0.272220	-0.135864
8	-5.699714	0.976013	0.957951
8	-6.894505	-0.079977	-1.030705
7	-5.658142	-1.590271	0.893368
6	-6.130746	2.221808	0.520750
6	-5.182961	3.267739	0.551746
1	-4.187025	3.045807	0.913054
6	-5.534363	4.521365	0.118818
1	-4.811693	5.331847	0.134495
6	-6.836970	4.770308	-0.389971
6	-7.192259	6.046828	-0.904544
1	-6.450411	6.840906	-0.876398
6	-8.440210	6.272009	-1.439791
1	-8.699729	7.249956	-1.834743
6	-9.383068	5.217477	-1.490918
1	-10.358488	5.389380	-1.937115
6	-9.074539	3.972241	-0.987776
1	-9.805769	3.175188	-1.047549
6	-7.803059	3.708471	-0.404292
6	-7.446457	2.417635	0.125775
6	-8.424330	1.297421	0.196535
6	-9.666289	1.393955	0.914799
6	-10.000432	2.516717	1.723252
1	-9.295119	3.335043	1.809799
6	-11.196306	2.572000	2.405715
1	-11.424181	3.437375	3.021690
6	-12.128036	1.509796	2.317969
1	-13.069337	1.569549	2.856550
6	-11.828971	0.398800	1.562091
1	-12.527180	-0.432044	1.499946
6	-10.598088	0.302739	0.857469
6	-10.267571	-0.861658	0.111867
1	-10.986870	-1.673986	0.055641
6	-9.045026	-0.972644	-0.503708
1	-8.760184	-1.861315	-1.056130
6	-8.123203	0.095577	-0.424862
6	-4.840413	-2.755496	0.447022
1	-3.930488	-2.787127	1.059662
6	-5.563246	-4.082156	0.623538
6	-4.820408	-5.226402	0.945090
1	-3.751888	-5.146217	1.105521
6	-5.438518	-6.476324	1.019061
1	-4.837412	-7.351451	1.251087
6	-6.811461	-6.598356	0.789645
1	-7.294067	-7.569984	0.852451
6	-7.560583	-5.459302	0.478360
1	-8.630222	-5.542095	0.302547
6	-6.939468	-4.211872	0.390654
1	-7.522521	-3.326169	0.158486
6	-4.435783	-2.584328	-1.025831
1	-5.311748	-2.794778	-1.654334
1	-3.689216	-3.346030	-1.256550
6	-6.079872	-1.664247	2.324203
1	-6.409308	-2.699911	2.440444
6	-4.904709	-1.484529	3.282615
6	-4.373657	-2.608332	3.929457
1	-4.779160	-3.591746	3.704789
6	-3.338145	-2.480645	4.859844
1	-2.945250	-3.364498	5.354752
6	-2.816005	-1.220176	5.152352
1	-2.020919	-1.113619	5.884690
6	-3.319610	-0.094033	4.492670
1	-2.912340	0.890067	4.710180
6	-4.353727	-0.224613	3.564611
1	-4.742184	0.653374	3.061821
6	-7.290256	-0.811634	2.714993
1	-8.134613	-1.019313	2.055727
1	-7.087992	0.257800	2.698263
1	-7.580514	-1.087921	3.733924
6	-2.355391	-0.516394	0.249235
1	-1.882610	0.456532	0.346975
1	-2.847269	-0.845964	1.161490
6	-1.776131	-1.479925	-0.628739
1	-2.008146	-2.510988	-0.401095
6	-0.355448	-1.364518	-1.170099
1	-0.029433	-0.321511	-1.219792
6	-4.918727	-0.598655	-3.296770
1	-5.807152	-1.196238	-3.105791
6	-3.722172	-1.312741	-3.609178
1	-3.789332	-2.399632	-3.651469
6	-2.637221	-0.729902	-4.496487
1	-2.995967	-0.674654	-5.537119
1	-1.797982	-1.423811	-4.498412
6	-2.145929	0.658307	-4.035134

1	-2.621530	1.450203	-4.625659
1	-1.074831	0.736036	-4.233390
6	-2.377436	0.950342	-2.551020
1	-1.475877	1.072328	-1.957507
6	-3.526415	1.582052	-2.058336
1	-3.416513	2.159927	-1.144654
6	-4.738361	1.944076	-2.902336
1	-5.551876	2.202747	-2.219406
1	-4.524247	2.852756	-3.486726
6	-5.214471	0.806294	-3.836236
1	-4.763352	0.919052	-4.828874
1	-6.294643	0.906785	-3.984119
6	-0.142236	-2.012066	-2.524265
6	-0.648315	-3.290222	-2.800404
6	0.644261	-1.374861	-3.491900
6	-0.380032	-3.909707	-4.021696
1	-1.231639	-3.816526	-2.055261
6	0.908216	-1.989576	-4.718780
1	1.051368	-0.390812	-3.285461
6	0.395177	-3.261090	-4.988637
1	-0.770075	-4.906545	-4.208385
1	1.511143	-1.469920	-5.458199
1	0.600628	-3.743843	-5.940320
1	3.715960	-5.077188	-1.859543
35	5.909820	-3.301773	-3.029314
5	-1.164972	-5.806859	-0.028714
9	-1.865394	-6.770977	0.704612
9	-1.038710	-6.187085	-1.368527
9	0.121047	-5.608405	0.537584
9	-1.865635	-4.573217	0.043214

---

8 P1-C1 *exo si-si* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 12.0758 14.9164 15.9028 cm(-1)
Electronic energy= -7647.2549713
Zero-point correction= 1.772157
(Hartree/Particle)
Thermal correction to Energy= 1.897848
Thermal correction to Enthalpy= 1.898792
Thermal correction to Gibbs Free Energy= 1.600907
Sum of electronic and zero-point Energies= -7645.482815
Sum of electronic and thermal Energies= -7645.357124
Sum of electronic and thermal Enthalpies= -7645.356180
Sum of electronic and thermal Free Energies= -7645.654064

.....

Cartesian Coordinates

.....

26	3.938183	4.988352	2.700517
15	1.487585	2.183596	-0.956735
15	4.727675	0.762615	0.645435
6	3.204858	3.966530	1.021410
6	4.168707	3.167356	1.734845
6	3.679355	2.972775	3.063379
1	4.181454	2.418521	3.844838
6	2.435923	3.659305	3.184292
1	1.835295	3.732926	4.081028
6	2.146775	4.278748	1.933339
1	1.285604	4.891287	1.710900
6	5.604903	6.217547	2.490331
1	6.394050	6.070020	1.765001
6	5.560082	5.660591	3.804727
1	6.303116	5.008276	4.243861
6	4.337648	6.073398	4.417270
1	3.991737	5.786061	5.401548
6	3.626153	6.884940	3.481708
1	2.648297	7.322852	3.633213
6	4.408535	6.974576	2.291599
1	4.128555	7.500631	1.388823
6	3.333476	4.293077	-0.427226
6	4.261551	5.263545	-0.831811
1	4.808363	5.795518	-0.064516
6	4.504101	5.536855	-2.178431
1	5.237274	6.289240	-2.454599
6	3.807106	4.833281	-3.156564
1	3.989147	5.020302	-4.210307
6	2.876573	3.864214	-2.778708
1	2.357744	3.316889	-3.555289
6	2.629698	3.571322	-1.427792
6	5.349808	2.499726	1.092233
1	5.517052	2.971438	0.118821
6	6.647155	2.573585	1.899257
1	7.470206	2.076433	1.377341
1	6.541900	2.117661	2.887381
1	6.916917	3.624053	2.042700
6	0.840858	1.659439	-2.604419
6	1.510711	0.600034	-3.236388
1	2.296709	0.078538	-2.703834
6	1.194132	0.232416	-4.545738
1	1.735850	-0.578947	-5.023098
6	0.184474	0.909884	-5.233924
1	-0.068135	0.625662	-6.251277
6	-0.511452	1.944843	-4.602139
1	-1.309544	2.463748	-5.125382
6	-0.185251	2.320821	-3.297788
1	-0.719335	3.141430	-2.832841
6	0.094558	3.081986	-0.155035
6	-0.279599	4.381337	-0.537521
1	0.231950	4.875872	-1.357814
6	-1.287086	5.054606	0.154230
1	-1.571673	6.058251	-0.148610
6	-1.929648	4.438200	1.233156
1	-2.713206	4.964412	1.770926
6	-1.560826	3.147932	1.618573
1	-2.048645	2.669911	2.462170
6	-0.549195	2.471206	0.931756
1	-0.210890	1.496621	1.268361
6	5.687854	0.323356	-0.864685
6	6.449343	-0.843174	-1.021394
1	6.613292	-1.516436	-0.189862
6	6.980419	-1.174151	-2.268750
6	6.746694	-0.375656	-3.387787
1	7.144189	-0.652520	-4.356598
6	5.969642	0.771355	-3.237413
6	5.448874	1.125137	-1.992316
1	4.822804	2.009530	-1.914848
6	5.344994	-0.321799	1.996332
6	4.369218	-0.815251	2.872640
1	3.327838	-0.557377	2.710548
6	4.735937	-1.616329	3.955658
6	6.070038	-1.951985	4.175905
1	6.351312	-2.582676	5.010745
6	7.040512	-1.460195	3.302279
6	6.689924	-0.642600	2.227250
1	7.470104	-0.266289	1.575878
29	2.443505	0.509396	0.242613
6	8.495961	-1.751525	3.542288
6	3.658417	-2.154334	4.857381
6	7.861172	-2.386834	-2.403947
6	5.621994	1.629611	-4.422454
9	4.278524	1.665876	-4.623594
9	6.018279	2.912573	-4.248681
9	6.181854	1.187289	-5.567354
9	7.739341	-2.968691	-3.619282
9	7.590655	-3.324175	-1.471661
9	9.170721	-2.059899	-2.262250
9	9.160336	-1.961161	2.381805
9	8.681855	-2.839446	4.319356
9	9.115881	-0.714234	4.158487
9	4.141514	-2.522705	6.065311
9	2.689672	-1.231931	5.075682
9	3.047678	-3.240065	4.329119
6	3.141742	-1.986090	-1.227328
6	1.807124	-2.489705	0.648091
6	3.296661	-3.313713	-1.556967
1	3.618780	-1.212833	-1.816807
6	1.921260	-3.879303	0.299419
6	2.657925	-4.296418	-0.783009
1	1.388372	-4.607192	0.900497
6	1.060339	-2.163285	1.808338

6	0.854195	-0.894057	2.389706
8	1.393390	0.199461	1.982191
7	2.413744	-1.563593	-0.172122
1	0.576881	-3.012999	2.265645
7	0.017461	-0.775331	3.497388
6	0.073313	0.457560	4.274082
1	0.865978	0.427861	5.037119
1	-0.884623	0.607476	4.780769
1	0.266395	1.303706	3.618161
6	-0.417840	-1.954278	4.240149
1	-0.940473	-2.659780	3.594057
1	-1.113223	-1.637132	5.021014
1	0.424554	-2.472265	4.718810
77	-3.272084	-1.675436	-1.435085
15	-4.614385	-0.289422	-0.260718
8	-4.232945	1.290460	0.033493
8	-6.108160	-0.110113	-0.974888
7	-4.756719	-0.851270	1.300706
6	-4.507304	2.303548	-0.879018
6	-3.389282	2.919497	-1.477627
1	-2.400881	2.592903	-1.180658
6	-3.578787	3.919738	-2.396794
1	-2.725583	4.413675	-2.852624
6	-4.890156	4.310055	-2.778216
6	-5.096201	5.291554	-3.785472
1	-4.225069	5.757587	-4.238671
6	-6.365980	5.634888	-4.190396
1	-6.512121	6.382132	-4.964890
6	-7.485226	4.996237	-3.605528
1	-8.486040	5.247883	-3.944576
6	-7.320317	4.052307	-2.614925
1	-8.191816	3.568909	-2.190901
6	-6.024115	3.689785	-2.151521
6	-5.812400	2.701535	-1.122557
6	-6.950045	2.069182	-0.398520
6	-7.942870	2.838673	0.304614
6	-7.799219	4.233640	0.545046
1	-6.909398	4.742367	0.192387
6	-8.762724	4.938339	1.233301
1	-8.624866	6.000456	1.414483
6	-9.926898	4.291534	1.713536
1	-10.679778	4.861536	2.249951
6	-10.092653	2.940139	1.510882
1	-10.973619	2.427008	1.887724
6	-9.110734	2.179579	0.818816
6	-9.252974	0.775903	0.650235
1	-10.149173	0.286741	1.020329
6	-8.249904	0.038337	0.071857
1	-8.323329	-1.037713	-0.036208
6	-7.093949	0.690142	-0.408293
6	-4.334063	-2.268566	1.454610
1	-3.392264	-2.287733	2.003168
6	-5.342209	-3.117725	2.212632
6	-4.886077	-4.120991	3.075084
1	-3.821174	-4.271862	3.208163
6	-5.797234	-4.930886	3.757950
1	-5.427987	-5.704831	4.425615
6	-7.170950	-4.745838	3.587377
1	-7.878848	-5.367431	4.129001
6	-7.629893	-3.754382	2.713662
1	-8.696763	-3.596713	2.578712
6	-6.719822	-2.954345	2.024865
1	-7.072988	-2.162718	1.374918
6	-4.089720	-2.925198	0.078518
1	-5.047205	-3.292364	-0.307747
1	-3.451483	-3.791377	0.240953
6	-4.710862	0.056365	2.499045
1	-4.898094	1.053674	2.105643
6	-5.829201	-0.221137	3.494829
6	-7.055291	0.431435	3.320786
1	-7.170553	1.130132	2.499091
6	-8.126767	0.192749	4.182538
1	-9.069823	0.709264	4.024910
6	-7.979766	-0.703384	5.243778
1	-8.811442	-0.898911	5.915210
6	-6.752050	-1.341311	5.442395
1	-6.626844	-2.038241	6.266307
6	-5.682793	-1.094040	4.580351
1	-4.743191	-1.610428	4.741983
6	-3.313289	0.077563	3.127327
1	-2.566505	0.347925	2.379196
1	-3.021786	-0.882069	3.557322
1	-3.291352	0.820566	3.930247
6	-1.704222	-0.967857	-0.043673
1	-1.523370	0.101864	-0.007352
1	-1.864189	-1.425712	0.925654
6	-0.969195	-1.700920	-1.022989
1	-0.392511	-1.134132	-1.746171
6	-1.093736	-3.080488	-1.167902
1	-1.489947	-3.647064	-0.334199
6	-5.035410	-2.220459	-2.752456
1	-5.823332	-2.493816	-2.057342
6	-4.031110	-3.181350	-2.959231
1	-4.115746	-4.111238	-2.397547
6	-3.162765	-3.299949	-4.195230
1	-3.722291	-3.860283	-4.959136
1	-2.300227	-3.916405	-3.939059
6	-2.663090	-1.969872	-4.806746
1	-3.399660	-1.582487	-5.516915
1	-1.756165	-2.180724	-5.381998
6	-2.341936	-0.887568	-3.798702
1	-1.296978	-0.736219	-3.563220
6	-3.228824	0.050571	-3.356482
1	-2.826018	0.909334	-2.830160
6	-4.673619	0.151166	-3.791000
1	-5.177451	0.859295	-3.133360
1	-4.705144	0.591910	-4.797782
6	-5.459750	-1.182305	-3.791836
1	-5.401700	-1.650342	-4.779855
1	-6.514293	-0.949540	-3.623094
6	-0.459190	-3.872354	-2.223281
6	0.272778	-3.303310	-3.285014
6	-0.588768	-5.273995	-2.171918
6	0.838628	-4.110025	-4.267647
1	0.412269	-2.229915	-3.342398
6	-0.020872	-6.078178	-3.159322
1	-1.125515	-5.719948	-1.340694
6	0.690042	-5.500204	-4.214692
1	1.408642	-3.655828	-5.072688
1	-0.130474	-7.157615	-3.102190
1	1.133259	-6.125799	-4.984393
1	2.722935	-5.348034	-1.040080
35	4.393620	-3.801246	-3.106686
5	-1.641388	-5.379413	1.833331
9	-2.301624	-6.006572	2.894163
9	-2.254652	-5.730044	0.604783
9	-0.288954	-5.748603	1.813692
9	-1.739169	-3.968781	1.986808

[8-9]‡ P1-C1 *exo si-si* [BF_4^-]

Number of imaginary frequencies= 1
The smallest frequencies are=-240.7042 10.3511 12.6986cm(-1)
Electronic energy= -7647.2386579
Zero-point correction= 1.771235
(Hartree/Particle)
Thermal correction to Energy= 1.896165
Thermal correction to Enthalpy= 1.897109
Thermal correction to Gibbs Free Energy= 1.600918
Sum of electronic and zero-point Energies= -7645.467423
Sum of electronic and thermal Energies= -7645.342493
Sum of electronic and thermal Enthalpies= -7645.341549
Sum of electronic and thermal Free Energies= -7645.637740

.....

Cartesian Coordinates

.....

26	3.610104	4.144078	3.958280
15	1.475687	2.497411	-0.519294
15	4.644297	0.610644	0.908990
6	3.035836	3.628550	2.005252

6	3.916291	2.634891	2.567684
6	3.295001	2.112916	3.745168
1	3.714325	1.358338	4.397281
6	2.053815	2.790280	3.929424
1	1.368045	2.648286	4.754078
6	1.901427	3.732641	2.871715
1	1.076551	4.417825	2.748612
6	5.302015	5.323018	4.240113
1	6.160717	5.337550	3.582291
6	5.112946	4.450701	5.355165
1	5.798356	3.681424	5.684361
6	3.836938	4.738474	5.928602
1	3.385998	4.222962	6.766406
6	3.236951	5.788267	5.168219
1	2.252680	6.208094	5.329005
6	4.141486	6.149734	4.125645
1	3.962635	6.896907	3.364335
6	3.290735	4.323074	0.709750
6	4.260171	5.334564	0.653032
1	4.756390	5.615907	1.572850
6	4.604608	5.960797	-0.545808
1	5.367434	6.734111	-0.552580
6	3.970320	5.581534	-1.725356
1	4.232028	6.047982	-2.669905
6	3.001592	4.576997	-1.695679
1	2.529697	4.282406	-2.625296
6	2.653644	3.930981	-0.499558
6	5.165600	2.138898	1.902219
1	5.437505	2.855344	1.120485
6	6.365556	1.964292	2.835199
1	7.252499	1.638385	2.283860
1	6.166598	1.240192	3.629980
1	6.591948	2.925079	3.305355
6	0.884333	2.450600	-2.265991
6	1.479853	1.496799	-3.107273
1	2.193194	0.794774	-2.689471
6	1.160428	1.443389	-4.465410
1	1.632780	0.701040	-5.102312
6	0.229888	2.339383	-4.997169
1	-0.023318	2.300066	-6.052402
6	-0.388953	3.274961	-4.162980
1	-1.125856	3.962104	-4.568740
6	-0.065685	3.332288	-2.805893
1	-0.552758	4.067657	-2.175668
6	0.063123	3.155147	0.462583
6	-0.331382	4.502766	0.396370
1	0.160822	5.183721	-0.291584
6	-1.320485	4.988437	1.253205
1	-1.617185	6.031863	1.197920
6	-1.919034	4.137067	2.188511
1	-2.683022	4.519166	2.859378
6	-1.531643	2.797444	2.256721
1	-1.985400	2.135344	2.987761
6	-0.544517	2.306785	1.398346
1	-0.199553	1.281826	1.480589
6	5.821207	0.660016	-0.510273
6	6.764462	-0.322164	-0.835730
1	6.905450	-1.192167	-0.207728
6	7.522276	-0.207297	-2.002374
6	7.339330	0.859737	-2.880408
1	7.915748	0.926347	-3.795007
6	6.376374	1.819409	-2.573146
6	5.629788	1.729884	-1.398640
1	4.871202	2.479719	-1.192489
6	5.110239	-0.852907	1.926150
6	4.046771	-1.648392	2.369579
1	3.031940	-1.364148	2.120665
6	4.284491	-2.793434	3.132376
6	5.583126	-3.169014	3.464542
1	5.767976	-4.065846	4.043727
6	6.644501	-2.370037	3.034820
6	6.417862	-1.218480	2.281005
1	7.266431	-0.622726	1.968497
29	2.440416	0.532694	0.126120
6	8.054102	-2.716506	3.430637
6	3.109499	-3.642231	3.538425
6	8.586696	-1.229113	-2.299405
6	6.094853	2.961030	-3.511245
9	4.769364	3.045751	-3.794975
9	6.449780	4.153214	-2.975971
9	6.746845	2.839587	-4.685763
9	8.748476	-1.419958	-3.628892
9	8.313608	-2.428991	-1.744415
9	9.791746	-0.838976	-1.813982
9	8.943026	-2.366098	2.472616
9	8.208501	-4.037089	3.664762
9	8.427133	-2.069317	4.562000
9	3.425225	-4.527949	4.506179
9	2.087711	-2.880772	4.003296
9	2.617166	-4.349506	2.494102
6	3.602468	-1.376230	-1.906529
6	2.136572	-2.516615	-0.484410
6	4.103290	-2.556617	-2.419944
1	3.964371	-0.417947	-2.259170
6	2.667017	-3.751713	-0.953941
6	3.645246	-3.782041	-1.926422
1	2.257817	-4.674452	-0.557476
6	0.992245	-2.587089	0.384978
6	0.638352	-1.597743	1.375863
8	1.129333	-0.424797	1.422856
7	2.646928	-1.340125	-0.955588
1	0.717156	-3.604175	0.622911
7	-0.256077	-1.919294	2.359663
6	-0.357785	-0.992454	3.486945
1	0.625821	-0.791496	3.924119
1	-0.999618	-1.436128	4.247891
1	-0.791278	-0.037748	3.181289
6	-0.787567	-3.272021	2.517472
1	-1.224693	-3.629045	1.589345
1	-1.575801	-3.254561	3.270811
1	-0.018400	-3.983243	2.832112
77	-3.304414	-0.925406	-1.905174
15	-4.838077	-0.173505	-0.421136
8	-4.673415	1.262188	0.406892
8	-6.343269	0.066418	-1.108098
7	-4.958518	-1.219112	0.884183
6	-4.998053	2.473580	-0.185218
6	-3.923780	3.340638	-0.483646
1	-2.918738	3.028107	-0.227059
6	-4.176342	4.552304	-1.076205
1	-3.359723	5.233698	-1.296485
6	-5.502073	4.919794	-1.431864
6	-5.764944	6.137435	-2.116216
1	-4.929302	6.795626	-2.339806
6	-7.043354	6.471385	-2.502193
1	-7.232193	7.401783	-3.029818
6	-8.113815	5.588324	-2.223985
1	-9.118223	5.840770	-2.551754
6	-7.895276	4.407468	-1.547808
1	-8.727152	3.740859	-1.355129
6	-6.591323	4.039471	-1.111746
6	-6.324689	2.810631	-0.407786
6	-7.416049	1.894310	0.029776
6	-8.498196	2.330247	0.873091
6	-8.521069	3.613078	1.489322
1	-7.691696	4.291995	1.328773
6	-9.570471	3.996321	2.295935
1	-9.559467	4.977737	2.761487
6	-10.659032	3.122134	2.530546
1	-11.481369	3.440044	3.164798
6	-10.662155	1.867148	1.965402
1	-11.482241	1.178362	2.151046
6	-9.589009	1.434285	1.139361
6	-9.566820	0.121888	0.594538
1	-10.402584	-0.544728	0.787328
6	-8.481650	-0.315717	-0.123879
1	-8.421621	-1.325939	-0.513354
6	-7.407537	0.566105	-0.372006
6	-4.267203	-2.516245	0.657220
1	-3.338064	-2.515432	1.236650

6	-5.095968	-3.721580	1.076223
6	-4.460624	-4.846365	1.614070
1	-3.386522	-4.852780	1.755644
6	-5.201287	-5.978693	1.961261
1	-4.688669	-6.841230	2.378985
6	-6.585331	-5.998502	1.777713
1	-7.163876	-6.873991	2.060092
6	-7.222464	-4.881602	1.226046
1	-8.300012	-4.883929	1.083585
6	-6.480442	-3.756957	0.868396
1	-6.976468	-2.878983	0.467978
6	-3.913686	-2.683502	-0.837583
1	-4.804980	-3.069917	-1.345770
1	-3.162381	-3.470373	-0.908586
6	-5.137216	-0.707739	2.286287
1	-5.636412	0.254135	2.173372
6	-6.070329	-1.568784	3.127038
6	-7.438717	-1.273422	3.129665
1	-7.798729	-0.428169	2.553306
6	-8.343176	-2.055563	3.849415
1	-9.401990	-1.810872	3.830449
6	-7.884192	-3.147014	4.590218
1	-8.583389	-3.765725	5.146052
6	-6.516974	-3.434714	4.617448
1	-6.149541	-4.280840	5.191215
6	-5.617247	-2.644981	3.900194
1	-4.562252	-2.894499	3.922038
6	-3.780620	-0.447175	2.951303
1	-3.210752	0.266080	2.353670
1	-3.186505	-1.357080	3.054854
1	-3.927366	-0.028303	3.951993
6	-1.859650	-0.334870	-0.381287
1	-1.727850	0.740541	-0.314567
1	-2.048420	-0.804021	0.580363
6	-1.028973	-1.025392	-1.319315
1	-0.451921	-0.410859	-1.997986
6	-0.687305	-2.400767	-1.264074
1	-1.259834	-3.044211	-0.613967
6	-4.824125	-1.401070	-3.449276
1	-5.616708	-1.964743	-2.964032
6	-3.637416	-2.121202	-3.745880
1	-3.622477	-3.177105	-3.475380
6	-2.647350	-1.764713	-4.840356
1	-3.005947	-2.137647	-5.812745
1	-1.719644	-2.301798	-4.625587
6	-2.333942	-0.257036	-4.941574
1	-3.028414	0.232965	-5.630928
1	-1.336657	-0.130128	-5.374088
6	-2.363805	0.476229	-3.606050
1	-1.399593	0.780154	-3.217563
6	-3.465894	1.136358	-3.094740
1	-3.277018	1.915523	-2.364336
6	-4.837997	1.170866	-3.735942
1	-5.545925	1.541333	-2.991418
1	-4.831045	1.905576	-4.555111
6	-5.326577	-0.200377	-4.257379
1	-5.039983	-0.330590	-5.305842
1	-6.420730	-0.205509	-4.240136
6	-0.038670	-3.068320	-2.399750
6	0.660177	-2.355050	-3.395534
6	-0.114924	-4.469313	-2.513500
6	1.250024	-3.018998	-4.466982
1	0.752210	-1.277612	-3.332462
6	0.471030	-5.131016	-3.592883
1	-0.641069	-5.028953	-1.750674
6	1.157122	-4.411226	-4.573477
1	1.788109	-2.451076	-5.220708
1	0.394936	-6.212533	-3.662029
1	1.618216	-4.926582	-5.411430
1	4.027177	-4.723890	-2.304285
35	5.423949	-2.499014	-3.862360
5	-0.989522	-6.178731	0.786866
9	-1.426315	-6.144197	2.123116
9	-1.172111	-7.448402	0.241739
9	0.371680	-5.807810	0.718698
9	-1.750207	-5.229293	0.039821

---

9 P1-C1 *exo si-si* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 9.0914 11.8318 15.1039 cm(-1)
Electronic energy= -7647.2677172
Zero-point correction= 1.774346
(Hartree/Particle)
Thermal correction to Energy= 1.898710
Thermal correction to Enthalpy= 1.899654
Thermal correction to Gibbs Free Energy= 1.605238
Sum of electronic and zero-point Energies= -7645.493371
Sum of electronic and thermal Energies= -7645.369008
Sum of electronic and thermal Enthalpies= -7645.368064
Sum of electronic and thermal Free Energies= -7645.662479

.....

Cartesian Coordinates

.....

26	-3.688441	-3.258115	4.559529
15	-1.247057	-2.696323	0.001790
15	-4.498341	-0.557435	0.690498
6	-2.961475	-3.232731	2.593200
6	-3.873920	-2.141137	2.820540
6	-3.343329	-1.338732	3.878620
1	-3.806594	-0.451246	4.288462
6	-2.123840	-1.934643	4.318837
1	-1.504298	-1.585782	5.134141
6	-1.893781	-3.105175	3.537884
1	-1.063194	-3.787804	3.642328
6	-5.394842	-4.372568	4.971779
1	-6.180258	-4.578562	4.257004
6	-5.323022	-3.237541	5.835692
1	-6.040524	-2.429679	5.885107
6	-4.111386	-3.330483	6.585811
1	-3.748918	-2.602474	7.299667
6	-3.434032	-4.522589	6.186155
1	-2.470358	-4.857868	6.546359
6	-4.227067	-5.167467	5.190483
1	-3.968973	-6.079875	4.669979
6	-3.124206	-4.228679	1.497355
6	-4.063459	-5.261027	1.629485
1	-4.618135	-5.332257	2.556077
6	-4.301306	-6.173823	0.600764
1	-5.041119	-6.957945	0.733921
6	-3.589983	-6.067446	-0.591183
1	-3.765925	-6.763889	-1.404982
6	-2.653268	-5.044729	-0.748060
1	-2.120243	-4.966847	-1.687363
6	-2.415585	-4.111935	0.272969
6	-5.065853	-1.851851	1.956509
1	-5.254579	-2.736659	1.340522
6	-6.348723	-1.513198	2.718245
1	-7.178388	-1.319638	2.031983
1	-6.223545	-0.641122	3.365439
1	-6.619979	-2.363803	3.348790
6	-0.639992	-3.008193	-1.704949
6	-1.392202	-2.445574	-2.749968
1	-2.237616	-1.807214	-2.511847
6	-1.073964	-2.716060	-4.080426
1	-1.670918	-2.283767	-4.878123
6	0.017100	-3.536506	-4.381392
1	0.274703	-3.740526	-5.416424
6	0.785940	-4.078628	-3.349024
1	1.647834	-4.698430	-3.578764
6	0.458984	-3.821840	-2.016139
1	1.068049	-4.250730	-1.228434
6	0.137671	-3.136775	1.127918
6	0.519620	-4.473237	1.335104
1	0.032870	-5.271485	0.783032
6	1.502932	-4.785395	2.274473
1	1.795251	-5.820454	2.425617
6	2.103796	-3.769060	3.024037
1	2.863154	-4.013815	3.760942
6	1.723893	-2.440028	2.826021

1	2.180351	-1.651502	3.415440
6	0.747484	-2.122584	1.879205
1	0.423860	-1.097334	1.744833
6	-5.532325	-0.972781	-0.777655
6	-6.515606	-0.164060	-1.362099
1	-6.759556	0.806028	-0.950967
6	-7.183858	-0.594081	-2.508768
6	-6.870033	-1.810093	-3.115492
1	-7.382385	-2.126990	-4.016463
6	-5.868318	-2.598394	-2.553739
6	-5.208657	-2.191843	-1.393714
1	-4.427644	-2.822426	-0.977669
6	-5.076960	1.051346	1.368192
6	-4.068779	1.881976	1.870108
1	-3.036759	1.560612	1.811244
6	-4.380678	3.108038	2.459357
6	-5.700645	3.539463	2.544291
1	-5.942383	4.499873	2.983469
6	-6.709647	2.708994	2.051717
6	-6.411213	1.470629	1.483081
1	-7.225133	0.842927	1.142814
29	-2.215248	-0.638697	0.215954
6	-8.152884	3.112477	2.190556
6	-3.243662	3.965074	2.945223
6	-8.284009	0.239216	-3.111191
6	-5.475945	-3.908829	-3.181294
9	-4.130681	-3.998877	-3.332533
9	-5.849581	-4.962152	-2.416806
9	-6.028890	-4.082592	-4.398902
9	-8.120389	0.391890	-4.447707
9	-8.357727	1.471456	-2.568145
9	-9.492432	-0.348408	-2.939135
9	-8.886574	2.714588	1.125265
9	-8.300582	4.448062	2.311047
9	-8.721205	2.549643	3.284756
9	-3.662288	5.031970	3.650673
9	-2.398127	3.256251	3.739434
9	-2.499608	4.422566	1.913830
6	-3.203892	1.061247	-2.163551
6	-1.917141	2.397440	-0.773197
6	-3.880610	2.169339	-2.656800
1	-3.435847	0.061612	-2.512192
6	-2.626721	3.538776	-1.177948
6	-3.627218	3.433739	-2.136714
1	-2.351775	4.506963	-0.775175
6	-0.659778	2.620906	0.032277
6	-0.510381	1.772305	1.287830
8	-1.055964	0.647718	1.416490
7	-2.245152	1.167666	-1.225880
1	-0.701421	3.662761	0.344473
7	0.231540	2.246211	2.308302
6	0.260221	1.450968	3.540809
1	-0.730824	1.419108	4.003087
1	0.964513	1.909874	4.234238
1	0.575983	0.428208	3.335196
6	0.749086	3.613295	2.412344
1	0.899753	4.069156	1.441638
1	1.715013	3.587185	2.920709
1	0.064314	4.246286	2.981060
77	3.065882	0.653165	-2.068993
15	4.672149	0.072873	-0.542065
8	4.580544	-1.233544	0.499332
8	6.160193	-0.252206	-1.248485
7	4.857351	1.295419	0.607847
6	4.877646	-2.510403	0.052114
6	3.795035	-3.409395	-0.071059
1	2.804117	-3.063617	0.195910
6	4.021706	-4.688061	-0.513933
1	3.199116	-5.392916	-0.597227
6	5.328571	-5.100110	-0.890899
6	5.562950	-6.397040	-1.422961
1	4.721620	-7.079759	-1.511602
6	6.820718	-6.778769	-1.832100
1	6.986638	-7.770407	-2.242994
6	7.898496	-5.866996	-1.731713
1	8.885176	-6.160291	-2.078864
6	7.708646	-4.607990	-1.203987
1	8.544603	-3.921178	-1.145448
6	6.427728	-4.185910	-0.748980
6	6.192467	-2.875921	-0.197146
6	7.298126	-1.911005	0.065982
6	8.419893	-2.231755	0.908802
6	8.487997	-3.430518	1.673386
1	7.662618	-4.131763	1.633074
6	9.576242	-3.704615	2.473003
1	9.599045	-4.623214	3.052508
6	10.660892	-2.798327	2.553787
1	11.514199	-3.030205	3.184467
6	10.620734	-1.619903	1.843705
1	11.437599	-0.905726	1.909684
6	9.507559	-1.299508	1.019321
6	9.442853	-0.061557	0.324285
1	10.273757	0.633653	0.404605
6	8.324672	0.274140	-0.398357
1	8.231849	1.231904	-0.899181
6	7.255391	-0.643407	-0.498504
6	4.133048	2.535326	0.223647
1	3.194942	2.572083	0.790698
6	4.904552	3.812943	0.503714
6	4.204102	4.955242	0.906170
1	3.133160	4.908289	1.072299
6	4.869618	6.167664	1.100600
1	4.302746	7.041229	1.411125
6	6.249167	6.247964	0.899489
1	6.773405	7.185723	1.062638
6	6.953147	5.111297	0.484944
1	8.027830	5.163545	0.330930
6	6.283564	3.906173	0.276984
1	6.832197	3.018025	-0.020789
6	3.793067	2.509070	-1.281154
1	4.704934	2.770823	-1.833339
1	3.085775	3.314981	-1.477682
6	5.048038	0.985851	2.064627
1	5.515535	0.002452	2.083870
6	6.023965	1.927146	2.760076
6	7.389392	1.618459	2.733205
1	7.717581	0.711821	2.236799
6	8.330692	2.461182	3.325978
1	9.385754	2.202860	3.286600
6	7.913977	3.629188	3.969025
1	8.642214	4.293364	4.426392
6	6.551413	3.933897	4.026157
1	6.215259	4.838306	4.525445
6	5.615090	3.083808	3.435782
1	4.564347	3.348112	3.477821
6	3.702213	0.860850	2.791115
1	3.094549	0.097189	2.304004
1	3.139585	1.795740	2.795213
1	3.866062	0.566551	3.832615
6	1.611050	0.214535	-0.483964
1	1.343145	-0.837861	-0.516169
1	1.898290	0.556116	0.506978
6	0.963797	1.129595	-1.358179
1	0.251178	0.711938	-2.060590
6	0.633166	2.534260	-0.905488
1	1.438812	2.881318	-0.259322
6	4.403483	0.924692	-3.764404
1	5.244446	1.552361	-3.473788
6	3.172119	1.608404	-4.039916
1	3.183040	2.694363	-3.945840
6	2.144534	1.100229	-5.038435
1	2.503921	1.256717	-6.068360
1	1.249901	1.717048	-4.931192
6	1.768109	-0.381146	-4.828484
1	2.351030	-1.025056	-5.495904
1	0.720427	-0.535175	-5.106477
6	1.953403	-0.866870	-3.392477
1	1.035672	-1.111843	-2.868315
6	3.112279	-1.483722	-2.922763
1	2.994916	-2.182234	-2.101144

6	4.391487	-1.650705	-3.722923
1	5.183723	-1.933988	-3.024655
1	4.276537	-2.490903	-4.425694
6	4.820680	-0.370515	-4.474745
1	4.416927	-0.375446	-5.493716
1	5.910102	-0.378292	-4.584892
6	0.490566	3.530398	-2.047192
6	-0.117764	3.178079	-3.260132
6	0.934426	4.849877	-1.883896
6	-0.266138	4.111343	-4.288074
1	-0.488217	2.169209	-3.406403
6	0.793008	5.785102	-2.911709
1	1.369903	5.162744	-0.941757
6	0.194626	5.419653	-4.119738
1	-0.740484	3.813790	-5.219744
1	1.144044	6.802093	-2.759605
1	0.082097	6.147315	-4.918845
1	-4.159935	4.311453	-2.485377
35	-5.174349	1.938088	-4.096526
5	-0.026034	6.711295	1.192165
9	-0.385722	6.559348	2.540610
9	-0.188406	8.037781	0.788541
9	-0.830189	5.867421	0.387030
9	1.332303	6.326856	1.028811

---

8 P1-C1 *exo re-si* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 11.0338 14.4408 15.9896 cm(-1)
Electronic energy= -7647.2628012
Zero-point correction= 1.772049
(Hartree/Particle)
Thermal correction to Energy= 1.897722
Thermal correction to Enthalpy= 1.898667
Thermal correction to Gibbs Free Energy= 1.600983
Sum of electronic and zero-point Energies= -7645.490752
Sum of electronic and thermal Energies= -7645.365079
Sum of electronic and thermal Enthalpies= -7645.364135
Sum of electronic and thermal Free Energies= -7645.661818

.....

Cartesian Coordinates

.....

26	-4.166826	-4.448765	3.168931
15	-1.612583	-2.209045	-0.832637
15	-4.487269	-0.378365	0.706234
6	-3.467738	-3.541662	1.413839
6	-4.128380	-2.582765	2.267290
6	-3.429382	-2.553738	3.512496
1	-3.687278	-1.944119	4.367440
6	-2.363645	-3.501359	3.451377
1	-1.675484	-3.733975	4.251895
6	-2.386691	-4.109243	2.162302
1	-1.718379	-4.880693	1.809758
6	-6.096965	-5.213353	3.222871
1	-6.931828	-4.816174	2.660545
6	-5.691903	-4.796463	4.527872
1	-6.159468	-4.022940	5.122276
6	-4.529736	-5.543745	4.889708
1	-3.961813	-5.431898	5.803984
6	-4.216475	-6.423742	3.809234
1	-3.371425	-7.098031	3.761731
6	-5.184210	-6.221140	2.780579
1	-5.200849	-6.722659	1.822568
6	-3.844135	-3.805740	-0.004701
6	-5.041570	-4.486753	-0.274495
1	-5.633479	-4.826714	0.565219
6	-5.487629	-4.713655	-1.575587
1	-6.433042	-5.219127	-1.745375
6	-4.720289	-4.266911	-2.648136
1	-5.052831	-4.426590	-3.668782
6	-3.529540	-3.582444	-2.406015
1	-2.957123	-3.228083	-3.254427
6	-3.079057	-3.322797	-1.100568
6	-5.266055	-1.697615	1.833972
1	-5.913487	-2.290911	1.186355
6	-6.112263	-1.154334	2.988254
1	-6.942659	-0.549190	2.613960
1	-5.527849	-0.533539	3.672469
1	-6.522448	-1.992157	3.561254
6	-1.063865	-1.878516	-2.564461
6	-1.631349	-0.770192	-3.217389
1	-2.265394	-0.087833	-2.660639
6	-1.386188	-0.551443	-4.575344
1	-1.855539	0.286668	-5.077311
6	-0.538340	-1.407334	-5.283628
1	-0.341175	-1.228590	-6.336751
6	0.063986	-2.485051	-4.630738
1	0.735375	-3.146054	-5.171435
6	-0.206920	-2.727368	-3.282295
1	0.237719	-3.589826	-2.799296
6	-0.314721	-3.324057	-0.158082
6	-0.226228	-4.684128	-0.497919
1	-0.945766	-5.120330	-1.184808
6	0.771469	-5.484329	0.061287
1	0.834043	-6.534933	-0.207914
6	1.685158	-4.937514	0.968826
1	2.458748	-5.563319	1.404371
6	1.602648	-3.586788	1.312083
1	2.310240	-3.153908	2.012016
6	0.606844	-2.785003	0.750525
1	0.535418	-1.738417	1.023054
6	-5.396080	-0.454234	-0.895097
6	-4.923949	0.406894	-1.898633
1	-4.107030	1.085105	-1.665642
6	-5.476669	0.370201	-3.179073
6	-6.477959	-0.544726	-3.499459
1	-6.890832	-0.586104	-4.500885
6	-6.929698	-1.414474	-2.506358
6	-6.412456	-1.363488	-1.211900
1	-6.798102	-2.055404	-0.475799
6	-4.958563	1.262479	1.394667
6	-4.255078	1.677238	2.537084
1	-3.528054	1.016908	2.994408
6	-4.445153	2.953101	3.057352
6	-5.307075	3.857252	2.434230
1	-5.429461	4.861729	2.823417
6	-5.992825	3.450669	1.292770
6	-5.835913	2.160129	0.779259
1	-6.387901	1.876728	-0.109221
29	-2.148010	-0.359208	0.334135
6	-6.833735	4.441564	0.539646
6	-3.642060	3.420125	4.239292
6	-5.002108	1.367508	-4.198896
6	-7.969233	-2.436101	-2.874868
9	-7.508296	-3.296590	-3.817919
9	-8.364979	-3.182025	-1.819611
9	-9.076937	-1.858857	-3.397305
9	-3.647409	1.498204	-4.191989
9	-5.497649	2.604794	-3.955806
9	-5.359574	1.034935	-5.456620
9	-6.104756	5.086955	-0.410917
9	-7.349399	5.395714	1.344558
9	-7.865812	3.850876	-0.104768
9	-4.417830	4.068455	5.142008
9	-3.037530	2.400149	4.886504
9	-2.672491	4.292001	3.871731
6	-2.121193	2.618144	0.009048
6	-1.365515	2.756325	1.201865
6	-0.897518	1.768042	2.085775
1	-1.124172	3.758461	1.514326
77	2.944869	1.550340	-1.866242
15	4.282859	0.204458	-0.665730
8	3.855184	-1.354388	-0.321133
8	5.775343	-0.039137	-1.361933
7	4.456807	0.815493	0.876251
6	4.139751	-2.415472	-1.173384
6	3.030617	-3.042513	-1.778348
1	2.040622	-2.681052	-1.535553
6	3.229623	-4.096400	-2.632943
1	2.382491	-4.594995	-3.094764

6	4.545307	-4.533451	-2.943746
6	4.765868	-5.576202	-3.883953
1	3.901537	-6.054025	-4.337946
6	6.041645	-5.963629	-4.225688
1	6.198858	-6.757901	-4.949552
6	7.153031	-5.310006	-3.642537
1	8.159475	-5.597943	-3.932559
6	6.973520	-4.306384	-2.715097
1	7.839266	-3.813180	-2.290376
6	5.669914	-3.896049	-2.317358
6	5.444025	-2.846629	-1.354559
6	6.567050	-2.190022	-0.629052
6	7.518635	-2.929011	0.158068
6	7.348707	-4.307658	0.466620
1	6.469804	-4.827214	0.102499
6	8.273410	-4.982276	1.233666
1	8.116412	-6.031959	1.464827
6	9.422405	-4.320475	1.729947
1	10.144489	-4.867197	2.329245
6	9.611564	-2.983507	1.463190
1	10.480084	-2.458102	1.851721
6	8.670003	-2.253287	0.687621
6	8.837192	-0.862443	0.448586
1	9.721380	-0.362143	0.832688
6	7.871087	-0.148532	-0.216640
1	7.961081	0.919178	-0.380897
6	6.731396	-0.815910	-0.712964
6	4.008459	2.226568	1.008616
1	3.076354	2.239537	1.579600
6	5.013805	3.126824	1.714608
6	4.543197	4.236502	2.426872
1	3.478090	4.419522	2.489569
6	5.438590	5.112911	3.043159
1	5.052783	5.969459	3.589693
6	6.814842	4.889387	2.958880
1	7.511635	5.563671	3.449560
6	7.289169	3.788828	2.238330
1	8.357361	3.598518	2.173021
6	6.394070	2.921022	1.612305
1	6.760454	2.050128	1.082929
6	3.732645	2.846874	-0.381919
1	4.678135	3.230102	-0.781238
1	3.069520	3.697122	-0.231943
6	4.416125	-0.087986	2.081262
1	4.793231	-1.046876	1.727150
6	5.363672	0.356333	3.183875
6	6.668622	-0.149786	3.193042
1	6.967703	-0.856127	2.425872
6	7.586850	0.248908	4.165084
1	8.596531	-0.153194	4.150612
6	7.203804	1.160432	5.151937
1	7.915297	1.480011	5.908411
6	5.896432	1.654352	5.165380
1	5.589543	2.363424	5.929019
6	4.980790	1.249232	4.192715
1	3.974707	1.654980	4.207615
6	2.977606	-0.298572	2.560926
1	2.381772	-0.737219	1.760868
1	2.496461	0.630399	2.869464
1	2.964103	-0.977160	3.418165
6	1.377456	0.836615	-0.493639
1	1.202911	-0.235038	-0.473176
1	1.525328	1.277463	0.486183
6	0.623312	1.570119	-1.461579
1	0.061069	0.999718	-2.189743
6	0.686860	2.952070	-1.579555
1	1.065236	3.524676	-0.739467
6	4.718144	2.071361	-3.201494
1	5.503079	2.358063	-2.507656
6	3.722007	3.032429	-3.431946
1	3.810341	3.971132	-2.886122
6	2.828339	3.126807	-4.651565
1	3.354812	3.703456	-5.426892
1	1.951677	3.718525	-4.378458
6	2.356533	1.783153	-5.252717
1	3.110070	1.395508	-5.944155
1	1.457785	1.975125	-5.847701
6	2.028125	0.715829	-4.231240
1	0.982218	0.576138	-3.994243
6	2.907300	-0.217977	-3.765811
1	2.498745	-1.063940	-3.222333
6	4.357112	-0.330475	-4.179475
1	4.852525	-1.019234	-3.494461
1	4.402693	-0.799627	-5.172680
6	5.144233	1.002680	-4.209412
1	5.094193	1.443714	-5.209991
1	6.197175	0.772578	-4.027442
6	0.028214	3.724596	-2.632830
6	-0.628081	3.130281	-3.730351
6	0.047919	5.130247	-2.546080
6	-1.230110	3.914052	-4.710084
1	-0.684291	2.051555	-3.810786
6	-0.555958	5.912990	-3.530282
1	0.515169	5.597831	-1.685313
6	-1.191403	5.310152	-4.619665
1	-1.743744	3.435722	-5.539478
1	-0.534436	6.995673	-3.442674
1	-1.662229	5.920288	-5.385285
8	-2.300860	1.520276	-0.638668
6	-0.159346	2.206924	3.244457
6	0.227818	1.329801	4.225289
1	0.059400	3.264372	3.335306
6	-0.097203	-0.030411	4.054658
6	-0.755582	-0.439250	2.918438
1	-0.992686	-1.481892	2.754237
7	-1.146071	0.416048	1.947125
6	-3.362568	3.736405	-1.800917
1	-3.027192	2.876757	-2.370434
1	-4.454076	3.695349	-1.695318
1	-3.105430	4.638330	-2.364999
6	-2.668807	5.042523	0.182962
1	-2.858129	4.917939	1.251437
1	-1.706910	5.555875	0.061285
1	-3.462979	5.673103	-0.222918
7	-2.699124	3.758472	-0.509009
1	0.768739	1.674456	5.100666
35	0.434343	-1.357561	5.405057
5	1.057932	5.574609	1.651446
9	2.097705	6.299589	2.248395
9	0.641011	6.214480	0.465419
9	-0.027993	5.469926	2.540764
9	1.523028	4.271495	1.331173

[8-9]‡ P1-C1 *exo re-si* [BF_4^-]

Number of imaginary frequencies= 1
The smallest frequencies are=-180.1786 11.7290 13.0385cm(-1)
Electronic energy= -7647.2560876
Zero-point correction= 1.770967
(Hartree/Particle)
Thermal correction to Energy= 1.895815
Thermal correction to Enthalpy= 1.896759
Thermal correction to Gibbs Free Energy= 1.602136
Sum of electronic and zero-point Energies= -7645.485121
Sum of electronic and thermal Energies= -7645.360273
Sum of electronic and thermal Enthalpies= -7645.359329
Sum of electronic and thermal Free Energies= -7645.653951

.....

Cartesian Coordinates

.....

26	-3.792829	-4.024702	3.805116
15	-1.560703	-2.332699	-0.619115
15	-4.493679	-0.410255	0.784259
6	-3.245774	-3.370065	1.892410
6	-3.900806	-2.320531	2.638273
6	-3.126749	-2.072616	3.813820
1	-3.360617	-1.351113	4.584335
6	-2.021447	-2.976629	3.821570
1	-1.278120	-3.063409	4.601934
6	-2.097302	-3.777125	2.644691

1	-1.417456	-4.570353	2.372260
6	-5.677524	-4.848318	4.094313
1	-6.562706	-4.573716	3.536008
6	-5.218925	-4.227029	5.296150
1	-5.689557	-3.395197	5.802743
6	-4.002593	-4.865274	5.686917
1	-3.389390	-4.597136	6.537207
6	-3.709129	-5.882263	4.727898
1	-2.835911	-6.521342	4.724431
6	-4.743652	-5.873175	3.745132
1	-4.788665	-6.506322	2.869443
6	-3.689760	-3.847674	0.550270
6	-4.874915	-4.593078	0.450415
1	-5.403792	-4.835779	1.363418
6	-5.388976	-5.003443	-0.779031
1	-6.324032	-5.552869	-0.820344
6	-4.704549	-4.682950	-1.948499
1	-5.092615	-4.987235	-2.915398
6	-3.523543	-3.943677	-1.876563
1	-3.011721	-3.692957	-2.798298
6	-3.006409	-3.501769	-0.647818
6	-5.110386	-1.562790	2.162881
1	-5.771366	-2.277667	1.670443
6	-5.897361	-0.871656	3.279272
1	-6.785876	-0.374532	2.880197
1	-5.299985	-0.119664	3.801762
1	-6.215182	-1.619068	4.013003
6	-1.080296	-2.224165	-2.397563
6	-1.703481	-1.223691	-3.165363
1	-2.352271	-0.500126	-2.682126
6	-1.486051	-1.152403	-4.543155
1	-1.986993	-0.387119	-5.125989
6	-0.623414	-2.059005	-5.165126
1	-0.448543	-1.998187	-6.235306
6	0.029622	-3.030712	-4.402886
1	0.717101	-3.725472	-4.876785
6	-0.200791	-3.117953	-3.028083
1	0.301356	-3.889199	-2.454985
6	-0.228257	-3.320545	0.176665
6	-0.099051	-4.703636	-0.036365
1	-0.774617	-5.214079	-0.716378
6	0.872438	-5.434668	0.649098
1	0.965103	-6.502999	0.475951
6	1.715858	-4.795711	1.563865
1	2.466705	-5.366997	2.101792
6	1.592560	-3.422469	1.782463
1	2.244568	-2.921560	2.490482
6	0.628367	-2.687839	1.089066
1	0.529531	-1.624043	1.269128
6	-5.522208	-0.774807	-0.701426
6	-5.144758	-0.103897	-1.874341
1	-4.329598	0.611702	-1.829304
6	-5.781010	-0.378064	-3.084261
6	-6.778245	-1.348713	-3.162470
1	-7.254485	-1.580753	-4.108682
6	-7.138649	-2.028722	-1.998326
6	-6.536146	-1.737264	-0.773870
1	-6.853089	-2.287851	0.101194
6	-4.979378	1.297249	1.267314
6	-4.157054	1.913782	2.223676
1	-3.343124	1.358438	2.672085
6	-4.346475	3.248667	2.565269
6	-5.348511	4.003054	1.952053
1	-5.482434	5.049481	2.201836
6	-6.164957	3.390439	1.004278
6	-5.992209	2.045562	0.661476
1	-6.637553	1.599493	-0.086686
29	-2.194616	-0.340403	0.236741
6	-7.184109	4.215268	0.269498
6	-3.399365	3.922993	3.520405
6	-5.391649	0.420398	-4.297473
6	-8.159077	-3.128150	-2.102968
9	-7.718545	-4.135669	-2.899035
9	-8.459675	-3.676635	-0.904837
9	-9.317724	-2.690584	-2.648592
9	-4.045840	0.611598	-4.368570
9	-5.943809	1.658512	-4.279956
9	-5.770762	-0.169140	-5.449059
9	-6.645869	4.792385	-0.839677
9	-7.672835	5.219825	1.027474
9	-8.232321	3.474794	-0.153384
9	-4.050539	4.741552	4.378288
9	-2.700297	3.032498	4.260252
9	-2.494545	4.688810	2.864194
6	-2.380860	2.549283	-0.661942
6	-1.294192	2.913541	0.211112
6	-0.810614	2.159544	1.324376
1	-1.063519	3.964950	0.285983
77	2.916766	1.070068	-2.115110
15	4.391995	0.083606	-0.714379
8	4.134204	-1.436304	-0.085408
8	5.909421	-0.140324	-1.377063
7	4.519194	0.954361	0.714704
6	4.468184	-2.589247	-0.779736
6	3.395611	-3.402383	-1.209867
1	2.385119	-3.095598	-0.969308
6	3.655822	-4.557147	-1.903600
1	2.839408	-5.196833	-2.226659
6	4.991004	-4.919367	-2.228314
6	5.267771	-6.074444	-3.008683
1	4.433544	-6.690703	-3.334240
6	6.558765	-6.400416	-3.358246
1	6.758553	-7.283023	-3.958867
6	7.628830	-5.570868	-2.946116
1	8.644401	-5.815158	-3.244233
6	7.395868	-4.452107	-2.175555
1	8.227766	-3.824469	-1.878840
6	6.077442	-4.097156	-1.773977
6	5.797506	-2.935673	-0.968473
6	6.880309	-2.099767	-0.377314
6	7.893855	-2.648446	0.485358
6	7.854047	-3.989400	0.960884
1	7.029282	-4.630099	0.671934
6	8.835414	-4.477645	1.795846
1	8.776383	-5.502064	2.152385
6	9.915216	-3.656390	2.200565
1	10.683700	-4.056827	2.855299
6	9.976932	-2.349063	1.774734
1	10.789978	-1.701103	2.091829
6	8.973451	-1.808669	0.924752
6	9.007304	-0.444776	0.527191
1	9.834178	0.179864	0.852707
6	7.984365	0.090618	-0.216000
1	7.966916	1.138062	-0.495398
6	6.920672	-0.737236	-0.634683
6	3.878026	2.293460	0.631768
1	2.926415	2.256529	1.175164
6	4.714831	3.420647	1.219050
6	4.058499	4.531544	1.761863
1	2.975766	4.561428	1.782521
6	4.785192	5.620499	2.245818
1	4.249744	6.476285	2.647003
6	6.181163	5.606816	2.203361
1	6.750546	6.446819	2.592233
6	6.841782	4.504646	1.650512
1	7.927995	4.482011	1.615405
6	6.112883	3.425856	1.149240
1	6.626571	2.561870	0.742059
6	3.586875	2.657372	-0.842360
1	4.515942	3.042240	-1.279491
1	2.884748	3.491419	-0.838885
6	4.608229	0.247906	2.040691
1	5.130229	-0.684309	1.826502
6	5.462088	0.986322	3.061333
6	6.823967	0.677243	3.156209
1	7.240149	-0.089921	2.512035
6	7.652387	1.347685	4.057551
1	8.708263	1.095245	4.110076
6	7.122529	2.337244	4.888503
1	7.763684	2.867500	5.587324

6	5.759122	2.636479	4.820487
1	5.336481	3.404787	5.461766
6	4.935194	1.959911	3.920037
1	3.883297	2.219026	3.867590
6	3.216396	-0.105591	2.574048
1	2.681962	-0.714282	1.844566
1	2.616962	0.780334	2.781819
1	3.304810	-0.669285	3.507140
6	1.407301	0.422298	-0.669900
1	1.223287	-0.648262	-0.671875
1	1.597493	0.820936	0.321898
6	0.623125	1.202194	-1.578505
1	0.036615	0.656271	-2.304365
6	0.387428	2.590647	-1.486314
1	0.957508	3.168492	-0.778392
6	4.462825	1.687951	-3.607473
1	5.258181	2.182374	-3.055007
6	3.293463	2.452379	-3.836378
1	3.284430	3.468670	-3.443939
6	2.304787	2.223381	-4.964710
1	2.690312	2.668397	-5.895269
1	1.393962	2.772254	-4.715215
6	1.940866	0.741579	-5.206537
1	2.608866	0.302209	-5.954241
1	0.933258	0.690501	-5.631519
6	1.967531	-0.127487	-3.955297
1	1.004356	-0.462603	-3.594584
6	3.062941	-0.852254	-3.525458
1	2.864832	-1.705486	-2.886107
6	4.435199	-0.836792	-4.165658
1	5.135442	-1.294548	-3.464290
1	4.418066	-1.480905	-5.057677
6	4.945954	0.573035	-4.538511
1	4.660302	0.819581	-5.566402
1	6.040083	0.558828	-4.523912
6	-0.240778	3.345321	-2.574347
6	-1.003200	2.720971	-3.583112
6	-0.070602	4.742320	-2.628046
6	-1.561141	3.467105	-4.617599
1	-1.179273	1.652684	-3.546593
6	-0.625446	5.484503	-3.669949
1	0.487328	5.242683	-1.845395
6	-1.371337	4.852474	-4.669718
1	-2.157975	2.967598	-5.376052
1	-0.479944	6.560890	-3.693902
1	-1.806430	5.433412	-5.478116
8	-2.596728	1.355606	-1.053004
6	0.008755	2.837140	2.277823
6	0.423814	2.213917	3.434341
1	0.257262	3.873543	2.096323
6	0.030828	0.882903	3.632963
6	-0.714448	0.234974	2.670204
1	-1.015413	-0.797264	2.792947
7	-1.118521	0.841577	1.533940
6	-4.078930	3.294924	-2.263129
1	-3.731445	2.444788	-2.841110
1	-5.097357	3.103595	-1.908438
1	-4.099784	4.168981	-2.920270
6	-3.150157	4.924903	-0.653806
1	-2.859854	4.958267	0.394642
1	-2.465098	5.559480	-1.228051
1	-4.161832	5.329617	-0.736652
7	-3.163818	3.552755	-1.158510
1	1.020520	2.745077	4.168166
35	0.533922	-0.074128	5.265265
5	0.778183	6.212854	0.750891
9	1.632081	6.741513	1.727686
9	0.669921	7.080264	-0.343444
9	-0.495355	5.963918	1.303233
9	1.315223	4.971296	0.298214

---

9 P1-C1 *exo re-si* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 10.7106 12.0987 13.7119 cm(-1)

Electronic energy= -7647.2813729
Zero-point correction= 1.774143
(Hartree/Particle)
Thermal correction to Energy= 1.898584
Thermal correction to Enthalpy= 1.899528
Thermal correction to Gibbs Free Energy= 1.604842
Sum of electronic and zero-point Energies= -7645.507230
Sum of electronic and thermal Energies= -7645.382789
Sum of electronic and thermal Enthalpies= -7645.381845
Sum of electronic and thermal Free Energies= -7645.676530

.....

Cartesian Coordinates

.....

26	-3.620112	-3.997170	3.849908
15	-1.498508	-2.441869	-0.679269
15	-4.370650	-0.434357	0.756306
6	-3.109295	-3.414563	1.902990
6	-3.720715	-2.328156	2.632014
6	-2.913220	-2.063379	3.781666
1	-3.115128	-1.316435	4.536706
6	-1.826632	-2.990293	3.788053
1	-1.065032	-3.070963	4.551272
6	-1.952048	-3.825150	2.639655
1	-1.295479	-4.639776	2.373477
6	-5.510650	-4.779587	4.211998
1	-6.404657	-4.513002	3.663915
6	-5.015043	-4.120189	5.378168
1	-5.461506	-3.262977	5.863914
6	-3.799941	-4.762747	5.765861
1	-3.163170	-4.472097	6.591041
6	-3.543811	-5.819675	4.840007
1	-2.679766	-6.471067	4.840279
6	-4.600517	-5.831493	3.881243
1	-4.675604	-6.496933	3.032100
6	-3.593705	-3.924106	0.586765
6	-4.780610	-4.671204	0.537344
1	-5.285762	-4.890584	1.469558
6	-5.324253	-5.114632	-0.667871
1	-6.259438	-5.665301	-0.671223
6	-4.668521	-4.827803	-1.862335
1	-5.079188	-5.160226	-2.810318
6	-3.487121	-4.086023	-1.840511
1	-2.997022	-3.860262	-2.780479
6	-2.941717	-3.610550	-0.637174
6	-4.934288	-1.567028	2.174287
1	-5.612852	-2.285353	1.711709
6	-5.687912	-0.857702	3.302910
1	-6.582121	-0.355630	2.924085
1	-5.070933	-0.109289	3.807379
1	-5.992035	-1.599387	4.047613
6	-1.051425	-2.373153	-2.463943
6	-1.702847	-1.403114	-3.246455
1	-2.366810	-0.687423	-2.774655
6	-1.497466	-1.353676	-4.626071
1	-2.019635	-0.610859	-5.219530
6	-0.614847	-2.250277	-5.234121
1	-0.444470	-2.204103	-6.305708
6	0.063514	-3.193029	-4.458045
1	0.765536	-3.879148	-4.922943
6	-0.158160	-3.261625	-3.080884
1	0.366334	-4.007865	-2.494943
6	-0.148772	-3.380922	0.138560
6	0.008394	-4.766273	-0.035914
1	-0.652276	-5.309041	-0.705497
6	0.988528	-5.457333	0.677730
1	1.104658	-6.527879	0.535774
6	1.811459	-4.775417	1.580208
1	2.569589	-5.316021	2.139148
6	1.662061	-3.398775	1.757244
1	2.302169	-2.865004	2.451911
6	0.689139	-2.704414	1.035877
1	0.566039	-1.637228	1.178058
6	-5.419273	-0.859996	-0.698835
6	-5.066753	-0.224609	-1.897785

1	-4.251611	0.490584	-1.897988
6	-5.732413	-0.527625	-3.084022
6	-6.734195	-1.495749	-3.111837
1	-7.234214	-1.750242	-4.039949
6	-7.069304	-2.142497	-1.921582
6	-6.438289	-1.819204	-0.719628
1	-6.738594	-2.342034	0.177956
6	-4.895056	1.269644	1.207605
6	-4.112488	1.930725	2.167990
1	-3.288403	1.415634	2.646275
6	-4.374957	3.256710	2.501173
6	-5.393771	3.963603	1.860727
1	-5.578481	5.004459	2.102297
6	-6.162186	3.309612	0.900559
6	-5.930567	1.969360	0.581043
1	-6.549493	1.488091	-0.166791
29	-2.109534	-0.419219	0.127322
6	-7.187254	4.094176	0.129699
6	-3.488160	3.977238	3.479669
6	-5.373927	0.244015	-4.323307
6	-8.097814	-3.238988	-1.972534
9	-7.676899	-4.274184	-2.742118
9	-8.380363	-3.744598	-0.751732
9	-9.262121	-2.810783	-2.512418
9	-4.036405	0.478269	-4.403052
9	-5.968690	1.462524	-4.338199
9	-5.737503	-0.392835	-5.453546
9	-6.608140	4.774045	-0.897052
9	-7.809996	5.012352	0.898168
9	-8.135967	3.303428	-0.416088
9	-4.189222	4.822896	4.265546
9	-2.825187	3.121234	4.291759
9	-2.553362	4.720042	2.839813
6	-2.268366	2.489713	-0.897098
6	-0.985434	2.872862	-0.187346
6	-0.729040	2.180462	1.136090
1	-0.996770	3.933996	0.046913
77	2.837314	1.016966	-2.192086
15	4.299375	0.042811	-0.730902
8	4.085779	-1.475289	-0.054588
8	5.852785	-0.161186	-1.344673
7	4.383455	0.947243	0.689316
6	4.474308	-2.624566	-0.722728
6	3.443384	-3.471075	-1.190407
1	2.416022	-3.185972	-1.002262
6	3.760907	-4.630153	-1.851999
1	2.974987	-5.293615	-2.202130
6	5.117249	-4.967371	-2.108389
6	5.455296	-6.129675	-2.853160
1	4.650958	-6.772638	-3.201677
6	6.767330	-6.429676	-3.142370
1	7.013764	-7.317828	-3.717036
6	7.797666	-5.564586	-2.703353
1	8.830717	-5.787020	-2.955181
6	7.504496	-4.437884	-1.965533
1	8.307848	-3.783306	-1.649551
6	6.162088	-4.109169	-1.624216
6	5.818838	-2.940174	-0.854082
6	6.858867	-2.053585	-0.260202
6	7.873970	-2.541149	0.635591
6	7.857651	-3.861438	1.167027
1	7.049154	-4.530359	0.895568
6	8.840240	-4.293088	2.031304
1	8.799332	-5.302733	2.430218
6	9.898534	-3.432415	2.410683
1	10.668435	-3.788137	3.089202
6	9.938125	-2.143678	1.928539
1	10.735105	-1.466072	2.223899
6	8.932805	-1.661429	1.046452
6	8.942952	-0.316720	0.586294
1	9.755647	0.338388	0.886876
6	7.913330	0.163662	-0.184516
1	7.878379	1.196430	-0.513129
6	6.865975	-0.701234	-0.572492
6	3.747440	2.286330	0.552556
1	2.771943	2.258012	1.053172
6	4.563769	3.409765	1.174509
6	3.900567	4.481238	1.782971
1	2.818718	4.482774	1.835068
6	4.615359	5.563637	2.299585
1	4.072174	6.390474	2.749530
6	6.009996	5.579661	2.228202
1	6.571539	6.413790	2.640440
6	6.679678	4.511762	1.620467
1	7.765411	4.510036	1.567017
6	5.960921	3.442368	1.086744
1	6.481676	2.603627	0.637734
6	3.510935	2.624270	-0.940150
1	4.460700	2.988252	-1.353067
1	2.829219	3.476193	-0.974280
6	4.431255	0.287734	2.036847
1	4.904606	-0.677241	1.860081
6	5.317726	1.009018	3.043424
6	6.669875	0.656028	3.121687
1	7.050126	-0.127458	2.475566
6	7.532601	1.300276	4.009493
1	8.579973	1.012192	4.047842
6	7.046611	2.308050	4.845551
1	7.714061	2.818601	5.534438
6	5.692542	2.650869	4.795612
1	5.303932	3.433139	5.441642
6	4.834236	1.999290	3.908572
1	3.790681	2.292082	3.871527
6	3.021532	0.012514	2.572079
1	2.477727	-0.608953	1.860750
1	2.450053	0.927895	2.732681
1	3.078510	-0.514839	3.528975
6	1.258312	0.417877	-0.791595
1	0.993609	-0.628185	-0.922427
1	1.472905	0.680394	0.238844
6	0.655573	1.380393	-1.647490
1	0.028033	0.974580	-2.431660
6	0.242244	2.768218	-1.217489
1	1.042362	3.229752	-0.646011
6	4.306881	1.627669	-3.689434
1	5.121621	2.158066	-3.199477
6	3.098931	2.371208	-3.891421
1	3.097596	3.407792	-3.554788
6	2.130998	2.110819	-5.033710
1	2.543371	2.493532	-5.981402
1	1.229066	2.690429	-4.831159
6	1.742919	0.623923	-5.193209
1	2.364757	0.145091	-5.957504
1	0.712943	0.558173	-5.559542
6	1.836265	-0.188863	-3.904086
1	0.891380	-0.535337	-3.502095
6	2.962219	-0.899858	-3.505319
1	2.795330	-1.754964	-2.859079
6	4.302419	-0.892470	-4.217137
1	5.040764	-1.320809	-3.534736
1	4.254689	-1.561516	-5.090550
6	4.772690	0.517103	-4.639614
1	4.433545	0.740483	-5.657278
1	5.867060	0.521697	-4.681182
6	-0.060428	3.658631	-2.420351
6	-0.894584	3.221693	-3.464007
6	0.454956	4.960033	-2.487688
6	-1.206970	4.058877	-4.535923
1	-1.313536	2.221197	-3.441445
6	0.154762	5.796020	-3.567424
1	1.076112	5.329227	-1.682421
6	-0.679056	5.351927	-4.595297
1	-1.859927	3.697238	-5.326143
1	0.567319	6.801087	-3.592014
1	-0.918215	6.004426	-5.430666
8	-2.451479	1.305515	-1.276706
6	-0.148950	2.946894	2.160565
6	0.126790	2.383428	3.399768
1	0.061174	3.990690	1.980338
6	-0.187957	1.040491	3.574458

6	-0.755845	0.318830	2.537779
1	-1.015730	-0.725058	2.653776
7	-1.027886	0.879784	1.341329
6	-4.129496	3.201151	-2.280575
1	-3.770612	2.417771	-2.943699
1	-5.092022	2.907006	-1.856939
1	-4.269123	4.114884	-2.862145
6	-3.063695	4.852287	-0.764705
1	-2.679461	4.915574	0.250461
1	-2.432433	5.458696	-1.423311
1	-4.078043	5.254806	-0.766600
7	-3.135137	3.464181	-1.237391
1	0.563898	2.977690	4.194404
35	0.167680	0.147477	5.271633
5	0.556463	6.381343	0.873624
9	1.215263	6.937988	1.975650
9	0.554447	7.263137	-0.209583
9	-0.769722	6.034443	1.223325
9	1.227009	5.180658	0.499562

[8-9]‡ P1-C1 *endo re-re* [BF_4^-] conf2

Number of imaginary frequencies= 1
The smallest frequencies are= -215.7510 7.3507 11.2519 cm(-1)
Electronic energy= -7647.2545687
Zero-point correction= 1.770463
(Hartree/Particle)
Thermal correction to Energy= 1.895450
Thermal correction to Enthalpy= 1.896395
Thermal correction to Gibbs Free Energy= 1.599331
Sum of electronic and zero-point Energies= -7645.484106
Sum of electronic and thermal Energies= -7645.359118
Sum of electronic and thermal Enthalpies= -7645.358174
Sum of electronic and thermal Free Energies= -7645.655238

.....

Cartesian Coordinates

.....

26	5.019122	4.481424	2.165110
15	2.964252	1.739319	-1.765180
15	4.828715	-0.109281	0.914472
6	4.551459	3.269858	0.523645
6	4.692987	2.486985	1.729561
6	3.725524	2.956194	2.670341
1	3.586065	2.581588	3.675176
6	3.010166	4.038785	2.075749
1	2.241675	4.629265	2.555034
6	3.518317	4.233809	0.758232
1	3.198174	4.991010	0.058420
6	7.008291	4.814255	2.658437
1	7.810534	4.107358	2.492861
6	6.186423	4.894336	3.824369
1	6.248318	4.251247	4.692050
6	5.232291	5.937703	3.621377
1	4.444558	6.220080	4.307261
6	5.463978	6.503091	2.330347
1	4.885808	7.292227	1.867919
6	6.560709	5.810463	1.735941
1	6.959510	5.991113	0.747163
6	5.303062	3.015111	-0.739165
6	6.667314	3.334701	-0.806274
1	7.125785	3.803939	0.055239
6	7.436293	3.047882	-1.934148
1	8.495742	3.283483	-1.942374
6	6.840384	2.436596	-3.034740
1	7.427331	2.195283	-3.915156
6	5.484796	2.108648	-2.992419
1	5.036992	1.619488	-3.850361
6	4.702860	2.375355	-1.857475
6	5.624990	1.314792	1.884095
1	6.544277	1.554599	1.347010
6	5.989622	0.988294	3.334905
1	6.699309	0.157751	3.382250
1	5.115173	0.715458	3.931498
1	6.450722	1.866885	3.796879
6	2.668117	0.973698	-3.416748
6	2.817119	-0.418622	-3.523901
1	3.089187	-1.001352	-2.650703
6	2.579622	-1.062983	-4.740310
1	2.700931	-2.138921	-4.809228
6	2.177284	-0.327327	-5.856906
1	1.977692	-0.831227	-6.798315
6	2.027817	1.058775	-5.757973
1	1.714085	1.636489	-6.622834
6	2.275566	1.707699	-4.547571
1	2.147496	2.782885	-4.486013
6	1.921413	3.250824	-1.823417
6	2.331047	4.429182	-2.468740
1	3.317659	4.486973	-2.919212
6	1.478637	5.533473	-2.524102
1	1.805306	6.441483	-3.023140
6	0.206671	5.467670	-1.945779
1	-0.462757	6.321831	-1.994139
6	-0.204983	4.298436	-1.302839
1	-1.191278	4.241065	-0.858168
6	0.653039	3.199314	-1.230899
1	0.338874	2.300496	-0.712009
6	6.064694	-0.651444	-0.340252
6	5.611921	-1.616410	-1.251843
1	4.606825	-2.011175	-1.141060
6	6.434676	-2.050363	-2.290572
6	7.703113	-1.502798	-2.471200
1	8.331540	-1.820670	-3.295526
6	8.142208	-0.525636	-1.576982
6	7.347000	-0.115757	-0.506448
1	7.736366	0.633678	0.168970
6	4.698249	-1.552680	2.046487
6	3.687262	-1.498083	3.019089
1	3.084221	-0.603745	3.124944
6	3.421307	-2.605455	3.820169
6	4.122553	-3.799142	3.644296
1	3.881770	-4.672857	4.239703
6	5.109035	-3.858451	2.662851
6	5.414404	-2.742539	1.881660
1	6.185677	-2.825030	1.125926
29	2.725231	0.250556	-0.083723
6	5.848289	-5.149922	2.447568
6	2.283778	-2.579085	4.802728
6	5.940102	-3.156037	-3.181128
6	9.486877	0.103630	-1.815981
9	9.537994	0.712404	-3.027423
9	9.795983	1.038609	-0.890233
9	10.481571	-0.814253	-1.808689
9	6.020097	-4.361364	-2.564217
9	6.638289	-3.250294	-4.330900
9	4.633899	-2.989876	-3.515457
9	6.835377	-5.330814	3.355588
9	6.423395	-5.208849	1.223612
9	5.022900	-6.219449	2.553071
9	2.616878	-3.176185	5.969801
9	1.879451	-1.323115	5.090855
9	1.203738	-3.246073	4.322326
6	2.023163	-2.709299	0.244205
6	0.875612	-2.365711	1.045213
6	0.608684	-1.107924	1.670847
1	0.345543	-3.183612	1.506113
77	-3.245499	-0.714164	-1.536451
15	-5.077268	0.088534	-0.460704
8	-5.002260	1.101089	0.863716
8	-6.022166	1.026653	-1.467788
7	-5.968141	-1.160274	0.213787
6	-4.584658	2.411861	0.712634
6	-3.325804	2.745689	1.260745
1	-2.764374	1.975110	1.777564
6	-2.850851	4.026406	1.127485
1	-1.894378	4.303028	1.558684
6	-3.581840	4.993381	0.384361
6	-3.042674	6.285618	0.138476
1	-2.071567	6.529759	0.561086
6	-3.723403	7.200398	-0.633417
1	-3.299328	8.182312	-0.822246

6	-4.976465	6.853495	-1.193168
1	-5.501257	7.568606	-1.820167
6	-5.535853	5.616192	-0.956013
1	-6.492678	5.365632	-1.399151
6	-4.867701	4.649991	-0.153010
6	-5.412501	3.340602	0.100224
6	-6.806958	2.967491	-0.269492
6	-7.941057	3.731155	0.187893
6	-7.823216	4.802648	1.117854
1	-6.849024	5.053738	1.519659
6	-8.928857	5.515484	1.528730
1	-8.809801	6.323550	2.244944
6	-10.217478	5.200831	1.035533
1	-11.078645	5.775614	1.363608
6	-10.373561	4.154349	0.155374
1	-11.358911	3.885559	-0.216645
6	-9.256103	3.389439	-0.276968
6	-9.424976	2.278372	-1.145950
1	-10.421223	2.033369	-1.503277
6	-8.349943	1.502457	-1.501432
1	-8.458430	0.627357	-2.132991
6	-7.058574	1.839435	-1.038150
6	-5.386114	-2.503915	-0.089518
1	-4.744978	-2.803030	0.744545
6	-6.440886	-3.576637	-0.305844
6	-6.266783	-4.845372	0.257916
1	-5.394351	-5.037075	0.874817
6	-7.205144	-5.856306	0.028959
1	-7.061733	-6.834894	0.479808
6	-8.326708	-5.607925	-0.763960
1	-9.063898	-6.388771	-0.930578
6	-8.497555	-4.344706	-1.342272
1	-9.370855	-4.140469	-1.956049
6	-7.555723	-3.341981	-1.122653
1	-7.700526	-2.353979	-1.549076
6	-4.531738	-2.416693	-1.369184
1	-5.205176	-2.414972	-2.234787
1	-3.928348	-3.325813	-1.437615
6	-6.743093	-0.952592	1.488020
1	-6.971896	0.113892	1.503876
6	-8.093947	-1.661976	1.488196
6	-9.176463	-1.052280	0.841895
1	-9.033978	-0.087825	0.365530
6	-10.428072	-1.667188	0.796743
1	-11.252658	-1.176456	0.285978
6	-10.618768	-2.907391	1.411030
1	-11.589436	-3.394453	1.374502
6	-9.552847	-3.513165	2.080608
1	-9.689579	-4.475974	2.565005
6	-8.303979	-2.890595	2.126071
1	-7.486287	-3.383249	2.639942
6	-5.888652	-1.253743	2.724702
1	-5.016433	-0.596966	2.738513
1	-5.528724	-2.282808	2.756564
1	-6.476246	-1.068413	3.629686
6	-2.330896	-0.744575	0.442289
1	-1.638952	0.089084	0.527860
1	-3.008657	-0.827827	1.284631
6	-1.880133	-1.980191	-0.121175
1	-2.433815	-2.866385	0.155070
6	-0.646593	-2.182598	-0.782448
1	-0.056496	-1.319402	-1.061589
6	-4.059879	-0.353081	-3.567831
1	-5.081443	-0.726309	-3.583155
6	-3.032512	-1.327613	-3.673675
1	-3.343896	-2.367090	-3.774158
6	-1.641215	-1.049711	-4.214598
1	-1.665939	-1.005982	-5.315044
1	-1.013239	-1.906175	-3.957253
6	-0.991288	0.231188	-3.652477
1	-1.177935	1.081181	-4.316376
1	0.092347	0.097200	-3.635247
6	-1.450762	0.595903	-2.244002
1	-0.696090	0.495659	-1.470950
6	-2.506380	1.457313	-1.962633
1	-2.481076	1.974333	-1.008681
6	-3.412185	2.082460	-3.003821
1	-4.270925	2.509514	-2.482621
1	-2.883050	2.920955	-3.481301
6	-3.913235	1.086141	-4.073071
1	-3.244228	1.092966	-4.940004
1	-4.886673	1.427391	-4.438901
6	-0.318136	-3.417331	-1.499725
6	-0.897550	-4.663265	-1.184807
6	0.630497	-3.358319	-2.538581
6	-0.541154	-5.803579	-1.902552
1	-1.601996	-4.746405	-0.364763
6	0.980840	-4.500339	-3.255784
1	1.095254	-2.407525	-2.769347
6	0.396000	-5.729564	-2.940228
1	-0.991278	-6.758292	-1.644931
1	1.717769	-4.432428	-4.051562
1	0.669479	-6.623896	-3.493115
7	2.443726	-4.009539	0.261079
6	3.401275	-4.493690	-0.724458
1	3.084311	-5.479383	-1.079093
1	3.431236	-3.820159	-1.574997
1	4.406462	-4.584259	-0.296198
6	1.958878	-5.011341	1.208697
1	1.704668	-4.560029	2.166692
1	1.080134	-5.540752	0.822048
1	2.759829	-5.733511	1.385018
8	2.610091	-1.884494	-0.529169
6	-0.347555	-1.093373	2.727497
6	-0.670545	0.077046	3.381987
1	-0.820504	-2.024163	3.012427
6	-0.047781	1.253515	2.950564
6	0.850282	1.217660	1.900239
1	1.333592	2.117044	1.540969
7	1.182002	0.070977	1.272461
1	-1.388937	0.078104	4.194596
35	-0.405363	2.958234	3.849630
5	-2.719139	-4.237432	2.498572
9	-1.307237	-4.242693	2.498373
9	-3.182245	-2.917269	2.679835
9	-3.204822	-5.062013	3.512066
9	-3.176264	-4.710477	1.237290

[**8-9**]‡ **P1-C1** *endo si-re* [BF_4^-] conf2

Number of imaginary frequencies= 1
The smallest frequencies are= -205.0956 8.4014 11.8927 cm(-1)

Electronic energy= -7647.2404677
Zero-point correction= 1.770207
(Hartree/Particle)
Thermal correction to Energy= 1.895472
Thermal correction to Enthalpy= 1.896416
Thermal correction to Gibbs Free Energy= 1.596963
Sum of electronic and zero-point Energies= -7645.470260
Sum of electronic and thermal Energies= -7645.344996
Sum of electronic and thermal Enthalpies= -7645.344052
Sum of electronic and thermal Free Energies= -7645.643505

.....

Cartesian Coordinates

.....

26	4.119151	4.767577	2.750452
15	2.801268	2.091587	-1.497466
15	5.150260	0.405310	1.084500
6	3.924701	3.753129	0.928526
6	4.469271	2.887706	1.943010
6	3.516356	2.808642	3.006132
1	3.638787	2.244637	3.920954
6	2.400727	3.630186	2.667769
1	1.533517	3.811130	3.288572
6	2.653184	4.217263	1.393465
1	2.007184	4.904367	0.865981
6	5.884926	5.787824	3.150630
1	6.856518	5.509836	2.764424
6	5.297982	5.317503	4.364945

1	5.742461	4.613689	5.055560
6	3.998748	5.899366	4.480696
1	3.286279	5.710517	5.273059
6	3.782707	6.729499	3.338613
1	2.879019	7.280830	3.114071
6	4.947612	6.661786	2.517643
1	5.080445	7.159945	1.566928
6	4.569546	4.023276	-0.385825
6	5.677587	4.880141	-0.458261
1	6.031712	5.337894	0.456236
6	6.325686	5.141406	-1.665846
1	7.187216	5.802635	-1.685575
6	5.858685	4.551750	-2.838068
1	6.346988	4.746000	-3.788055
6	4.768677	3.682595	-2.786795
1	4.434108	3.213657	-3.704211
6	4.125844	3.387533	-1.573688
6	5.724226	2.079681	1.779228
1	6.305110	2.521033	0.963905
6	6.608642	2.017481	3.026724
1	7.521341	1.444518	2.839709
1	6.088323	1.566931	3.876233
1	6.894423	3.035040	3.308556
6	2.760755	1.455333	-3.223070
6	3.794632	0.577645	-3.595497
1	4.586500	0.350614	-2.889171
6	3.830917	0.022038	-4.872474
1	4.644405	-0.643210	-5.147204
6	2.815857	0.314732	-5.789709
1	2.831550	-0.130725	-6.780112
6	1.782685	1.180845	-5.427488
1	0.991057	1.412084	-6.134425
6	1.759980	1.759321	-4.154574
1	0.958810	2.441133	-3.893113
6	1.261575	3.069385	-1.269518
6	1.021750	4.270613	-1.956048
1	1.737935	4.631955	-2.688639
6	-0.129333	5.013852	-1.686824
1	-0.312108	5.939350	-2.225547
6	-1.038667	4.575179	-0.717668
1	-1.932433	5.155377	-0.506762
6	-0.795715	3.388463	-0.023575
1	-1.492888	3.046641	0.734958
6	0.344731	2.632737	-0.302028
1	0.550304	1.722529	0.252214
6	6.501155	-0.111138	-0.055324
6	7.069841	-1.393747	-0.059195
1	6.823405	-2.113476	0.711413
6	7.943995	-1.772807	-1.078054
6	8.257240	-0.901653	-2.121246
1	8.925763	-1.209117	-2.916269
6	7.678821	0.365970	-2.127764
6	6.809989	0.762790	-1.109936
1	6.354075	1.746807	-1.162122
6	5.214424	-0.760086	2.504438
6	3.977111	-1.183229	3.001188
1	3.065387	-0.816075	2.543052
6	3.913910	-2.066835	4.080579
6	5.076056	-2.545139	4.678384
1	5.025628	-3.242033	5.506281
6	6.311426	-2.115365	4.187308
6	6.387775	-1.226467	3.115611
1	7.360496	-0.912805	2.754507
29	3.129974	0.372716	-0.045592
6	7.582300	-2.566942	4.853904
6	2.555990	-2.523623	4.537559
6	8.602685	-3.125616	-1.030636
6	7.917598	1.312131	-3.272917
9	6.802225	1.449729	-4.036235
9	8.242399	2.551923	-2.839685
9	8.907175	0.897105	-4.090431
9	7.881116	-4.021184	-0.324446
9	9.824727	-3.057296	-0.446958
9	8.794300	-3.636425	-2.268637
9	8.000262	-1.672925	5.783599
9	8.593512	-2.702371	3.965430
9	7.434347	-3.750742	5.485920
9	2.604038	-3.238425	5.679716
9	1.728019	-1.470429	4.753677
9	1.957421	-3.298052	3.600629
6	3.916027	-2.164103	-1.377549
6	1.943857	-2.503088	-0.163569
6	3.952923	-3.482990	-1.786472
1	4.679952	-1.464226	-1.687599
6	1.956430	-3.871630	-0.559175
6	2.951268	-4.368562	-1.376481
1	1.149077	-4.513819	-0.224586
6	0.818257	-2.050237	0.600998
6	0.769503	-0.870747	1.423930
8	1.524935	0.144921	1.257943
7	2.937799	-1.670499	-0.596298
1	0.128102	-2.841846	0.848522
7	-0.165907	-0.795497	2.417953
6	-0.366039	0.463212	3.121824
1	0.199082	0.483057	4.063156
1	-1.430301	0.574875	3.355281
1	-0.039713	1.300141	2.507205
6	-0.858201	-1.939645	3.007354
1	-0.357080	-2.875921	2.783446
1	-1.891775	-2.010931	2.664968
1	-0.851434	-1.821263	4.095577
77	-3.669512	-0.426399	-1.572724
15	-5.475025	0.008226	-0.269581
8	-5.489934	1.093232	0.993705
8	-6.746591	0.603184	-1.175207
7	-5.928156	-1.370717	0.566685
6	-5.650721	2.453339	0.784486
6	-4.535212	3.267386	1.080373
1	-3.640416	2.789343	1.463156
6	-4.611306	4.623555	0.886230
1	-3.764445	5.261605	1.122247
6	-5.791413	5.207758	0.350872
6	-5.854630	6.599011	0.067383
1	-4.985681	7.212416	0.291818
6	-6.982106	7.157216	-0.491224
1	-7.017719	8.220617	-0.709135
6	-8.093611	6.336538	-0.797554
1	-8.972935	6.773889	-1.261734
6	-8.070548	4.986668	-0.520409
1	-8.927775	4.374595	-0.773654
6	-6.931443	4.377538	0.077014
6	-6.870927	2.967900	0.372821
6	-8.051543	2.072763	0.206946
6	-9.309586	2.325043	0.860274
6	-9.473027	3.339415	1.844938
1	-8.620359	3.945960	2.127115
6	-10.690183	3.547955	2.456406
1	-10.785691	4.322261	3.212336
6	-11.815221	2.759036	2.115982
1	-12.769121	2.938203	2.603395
6	-11.690049	1.757783	1.179891
1	-12.540355	1.132131	0.921018
6	-10.445587	1.505896	0.540214
6	-10.302374	0.440482	-0.389334
1	-11.170078	-0.163713	-0.638161
6	-9.073928	0.145275	-0.926181
1	-8.929784	-0.690432	-1.601909
6	-7.959186	0.946644	-0.597435
6	-5.263497	-2.597831	0.040826
1	-4.457936	-2.869041	0.722279
6	-6.205882	-3.782206	-0.089218
6	-5.758348	-5.062057	0.259633
1	-4.762804	-5.192152	0.672468
6	-6.597338	-6.169097	0.102152
1	-6.240545	-7.156155	0.384831
6	-7.890876	-6.007247	-0.397799
1	-8.548238	-6.865930	-0.505237
6	-8.337966	-4.730518	-0.756027
1	-9.346274	-4.593844	-1.138181
6	-7.496652	-3.629118	-0.612861

1	-7.850741	-2.634205	-0.863363
6	-4.647400	-2.316768	-1.343983
1	-5.439309	-2.385750	-2.099373
1	-3.934878	-3.117010	-1.561894
6	-6.375278	-1.341319	2.001801
1	-6.705160	-0.317624	2.172277
6	-7.594606	-2.217720	2.262868
6	-8.866369	-1.675603	2.042325
1	-8.951941	-0.645247	1.715120
6	-10.018152	-2.440384	2.231581
1	-10.994515	-1.998434	2.050396
6	-9.910602	-3.766060	2.658801
1	-10.802612	-4.369770	2.802831
6	-8.647171	-4.308993	2.909271
1	-8.552788	-5.337993	3.244635
6	-7.499110	-3.537025	2.722998
1	-6.526491	-3.978918	2.907584
6	-5.211262	-1.607609	2.966103
1	-4.447635	-0.833643	2.849350
1	-4.735127	-2.578280	2.813019
1	-5.576729	-1.570147	3.997208
6	-2.542231	-0.466168	0.300211
1	-1.995008	0.464012	0.444771
1	-3.117149	-0.766491	1.169568
6	-1.930732	-1.510182	-0.463578
1	-2.261825	-2.525150	-0.283198
6	-0.709245	-1.354060	-1.165618
1	-0.263209	-0.364784	-1.178599
6	-4.772180	-0.151931	-3.480489
1	-5.702972	-0.707102	-3.398454
6	-3.604325	-0.913277	-3.747385
1	-3.732095	-1.989302	-3.866202
6	-2.359570	-0.367362	-4.421584
1	-2.520389	-0.302158	-5.509333
1	-1.557761	-1.094656	-4.273290
6	-1.895316	0.999693	-3.875969
1	-2.313811	1.816066	-4.474021
1	-0.811295	1.064744	-3.989518
6	-2.232089	1.240488	-2.407657
1	-1.385399	1.269600	-1.733269
6	-3.389639	1.862877	-1.958028
1	-3.340574	2.341702	-0.985265
6	-4.524900	2.336121	-2.844059
1	-5.379267	2.561803	-2.201413
1	-4.234442	3.283210	-3.323288
6	-4.954847	1.305970	-3.912691
1	-4.406670	1.475639	-4.845391
1	-6.010958	1.469206	-4.148600
6	-0.239731	-2.254498	-2.212000
6	-0.788995	-3.536637	-2.418174
6	0.794736	-1.820608	-3.064737
6	-0.329465	-4.342083	-3.456727
1	-1.552921	-3.910973	-1.748711
6	1.255011	-2.632020	-4.099534
1	1.234169	-0.840415	-2.912956
6	0.691200	-3.894368	-4.303141
1	-0.762971	-5.327729	-3.601119
1	2.051672	-2.275107	-4.743638
1	1.047018	-4.527237	-5.111426
1	2.947556	-5.406490	-1.690629
35	5.405457	-4.073723	-2.957116
5	-2.018802	-4.963720	1.572141
9	-1.247568	-4.612507	0.433744
9	-2.959109	-3.929945	1.818856
9	-2.707152	-6.156945	1.320772
9	-1.176009	-5.098105	2.681141

[**8-9**]‡ **P1-C1** *exo si-si* [BF_4^-] conf2

Number of imaginary frequencies= 1
The smallest frequencies are= -272.5272 7.8080 10.7684 cm(-1)

Electronic energy= -7647.2324557

Zero-point correction= 1.771941
(Hartree/Particle)
Thermal correction to Energy= 1.896556
Thermal correction to Enthalpy= 1.897500
Thermal correction to Gibbs Free Energy= 1.601958
Sum of electronic and zero-point Energies= -7645.460515
Sum of electronic and thermal Energies= -7645.335900
Sum of electronic and thermal Enthalpies= -7645.334956
Sum of electronic and thermal Free Energies= -7645.630498

.....

Cartesian Coordinates

.....

26	-3.767637	-1.273569	5.332092
15	-1.316393	-2.290113	0.810585
15	-4.651295	-0.161150	0.761243
6	-3.040347	-1.897656	3.463517
6	-3.989283	-0.820636	3.320622
6	-3.484076	0.310687	4.033318
1	-3.975255	1.270375	4.121438
6	-2.247977	-0.062282	4.638117
1	-1.639119	0.561138	5.278991
6	-1.983357	-1.421743	4.303504
1	-1.132595	-1.998537	4.632048
6	-5.448347	-2.203502	6.131974
1	-6.250890	-2.634325	5.547939
6	-5.370583	-0.849782	6.580361
1	-6.101371	-0.074353	6.393544
6	-4.138033	-0.688077	7.283446
1	-3.766787	0.233924	7.711292
6	-3.453106	-1.941480	7.269588
1	-2.474117	-2.136069	7.687337
6	-4.262218	-2.877925	6.559071
1	-4.004197	-3.907963	6.353461
6	-3.172448	-3.213819	2.770841
6	-4.128593	-4.132544	3.228888
1	-4.698225	-3.874364	4.112530
6	-4.371658	-5.338469	2.569607
1	-5.130207	-6.018064	2.947126
6	-3.642332	-5.655848	1.426948
1	-3.823638	-6.584035	0.894027
6	-2.683569	-4.760318	0.950828
1	-2.135078	-5.013065	0.050412
6	-2.440094	-3.536898	1.594632
6	-5.195808	-0.870707	2.433550
1	-5.398616	-1.921351	2.206288
6	-6.463206	-0.258541	3.033446
1	-7.305259	-0.336684	2.339119
1	-6.328003	0.794258	3.294546
1	-6.720242	-0.800676	3.947373
6	-0.530011	-3.206031	-0.585640
6	-1.090030	-3.029652	-1.860638
1	-1.918450	-2.342008	-1.983351
6	-0.586165	-3.719763	-2.965015
1	-1.035192	-3.573604	-3.943333
6	0.498817	-4.586299	-2.809746
1	0.900394	-5.116909	-3.668001
6	1.077927	-4.753243	-1.548419
1	1.934040	-5.410111	-1.423454
6	0.565765	-4.071117	-0.443269
1	1.025998	-4.213603	0.525985
6	0.015356	-2.079921	2.060802
6	0.471734	-0.779886	2.318993
1	0.069645	0.049090	1.746989
6	1.398154	-0.548645	3.337690
1	1.742014	0.461654	3.532207
6	1.874492	-1.612642	4.106179
1	2.594914	-1.430075	4.898103
6	1.428890	-2.914336	3.849368
1	1.798869	-3.744818	4.443846
6	0.500184	-3.148664	2.833689
1	0.125418	-4.155007	2.671018
6	-5.761491	-1.055605	-0.404259
6	-6.635164	-0.458176	-1.320841
1	-6.756098	0.617149	-1.355081

6	-7.347278	-1.245257	-2.227903
6	-7.186588	-2.629431	-2.263943
1	-7.728132	-3.230377	-2.983912
6	-6.286637	-3.219091	-1.378151
6	-5.583004	-2.447568	-0.454168
1	-4.870666	-2.934927	0.206453
6	-5.187808	1.599948	0.792962
6	-4.152954	2.538462	0.890451
1	-3.125081	2.196186	0.922714
6	-4.433997	3.904075	0.956047
6	-5.748525	4.360770	0.925127
1	-5.967027	5.420902	0.969324
6	-6.782152	3.425794	0.839327
6	-6.513903	2.057519	0.780568
1	-7.342373	1.361425	0.726034
29	-2.428893	-0.429226	0.137511
6	-8.215828	3.879690	0.877663
6	-3.276030	4.865589	1.006316
6	-8.332480	-0.586377	-3.155866
6	-6.016065	-4.698019	-1.416232
9	-4.698076	-4.948720	-1.629047
9	-6.335055	-5.297797	-0.245172
9	-6.704096	-5.326782	-2.391171
9	-8.490970	-1.279017	-4.306160
9	-7.957188	0.669841	-3.483521
9	-9.559366	-0.490492	-2.586280
9	-8.740082	3.761369	2.122233
9	-8.996773	3.136874	0.058788
9	-8.355313	5.171419	0.511436
9	-3.654585	6.113185	1.348206
9	-2.338458	4.461292	1.889727
9	-2.662437	4.952036	-0.203456
6	-3.461073	-0.331180	-2.688011
6	-2.224788	1.599534	-2.219563
6	-3.960200	0.206697	-3.859608
1	-3.737773	-1.330350	-2.372752
6	-2.773989	2.207115	-3.382812
6	-3.633078	1.517248	-4.215161
1	-2.483436	3.221515	-3.632327
6	-1.173238	2.305608	-1.533400
6	-0.825060	2.161735	-0.135294
8	-1.240533	1.206044	0.594032
7	-2.615685	0.335875	-1.879334
1	-1.008747	3.292087	-1.946257
7	-0.000390	3.079754	0.430565
6	0.303213	3.000228	1.860150
1	-0.460503	2.416755	2.370900
1	0.334644	4.010063	2.267349
1	1.278251	2.527435	2.023417
6	0.515296	4.256908	-0.266159
1	0.895411	4.011488	-1.258106
1	1.335283	4.655127	0.320842
1	-0.245896	5.036438	-0.349182
77	3.528278	0.240722	-2.035894
15	5.149019	0.409897	-0.452873
8	5.136308	-0.377110	1.015317
8	6.619465	-0.129799	-1.038522
7	5.273037	1.988755	0.071408
6	5.147693	-1.765291	1.010452
6	3.946102	-2.417628	1.364386
1	3.098229	-1.815651	1.663969
6	3.885365	-3.788111	1.324890
1	2.978206	-4.302508	1.623548
6	4.991964	-4.545798	0.855711
6	4.896351	-5.953925	0.686321
1	3.965623	-6.445763	0.958014
6	5.948791	-6.677668	0.172613
1	5.862134	-7.751866	0.037588
6	7.143607	-6.014537	-0.196503
1	7.963503	-6.583270	-0.625722
6	7.275986	-4.653482	-0.023246
1	8.194648	-4.161799	-0.320811
6	6.215856	-3.875337	0.520057
6	6.311307	-2.447059	0.691299
6	7.595302	-1.712001	0.519330
6	8.769686	-2.083701	1.273021
6	8.737378	-3.053293	2.314834
1	7.797855	-3.527760	2.570652
6	9.875954	-3.385832	3.017317
1	9.818282	-4.122910	3.813323
6	11.115152	-2.771915	2.719373
1	12.005618	-3.048711	3.276230
6	11.179623	-1.811671	1.734944
1	12.118852	-1.313920	1.507589
6	10.020841	-1.434339	1.004145
6	10.076158	-0.404581	0.026150
1	11.028840	0.072471	-0.186246
6	8.936104	0.008199	-0.612538
1	8.944914	0.821135	-1.330837
6	7.700182	-0.623109	-0.336524
6	4.306922	2.912600	-0.587633
1	3.435240	3.021306	0.068747
6	4.910533	4.292965	-0.800089
6	4.205751	5.438509	-0.415436
1	3.257876	5.355654	0.101162
6	4.721785	6.712875	-0.666165
1	4.145207	7.579715	-0.357654
6	5.960356	6.854657	-1.293296
1	6.368424	7.843553	-1.484008
6	6.680742	5.713663	-1.667616
1	7.650359	5.816282	-2.148007
6	6.157877	4.443318	-1.426645
1	6.720118	3.557325	-1.710828
6	3.851779	2.339573	-1.943954
1	4.626346	2.569944	-2.684429
1	2.962878	2.898622	-2.245522
6	5.872034	2.480143	1.353920
1	5.985120	3.553239	1.182391
6	4.945893	2.344518	2.563536
6	4.009072	3.356899	2.813247
1	3.930322	4.204964	2.142325
6	3.177865	3.313405	3.935997
1	2.463392	4.115321	4.087666
6	3.286647	2.258216	4.842946
1	2.652583	2.224504	5.724882
6	4.222635	1.244899	4.609348
1	4.320969	0.422267	5.312825
6	5.038924	1.284176	3.478204
1	5.754106	0.486564	3.314707
6	7.280614	1.942443	1.594975
1	7.919474	2.165082	0.737621
1	7.303069	0.866729	1.769993
1	7.703088	2.433995	2.476426
6	2.004615	0.410441	-0.490138
1	1.965952	-0.432216	0.192228
1	2.050007	1.367515	0.022482
6	1.209765	0.300861	-1.680425
1	0.781376	-0.672014	-1.888534
6	0.734468	1.380014	-2.476098
1	1.195877	2.341088	-2.314340
6	5.089536	0.084242	-3.656144
1	5.777196	0.910992	-3.495899
6	3.855882	0.402036	-4.265043
1	3.681773	1.446289	-4.522699
6	3.010875	-0.567597	-5.068231
1	3.439531	-0.676731	-6.076969
1	2.029252	-0.112474	-5.202535
6	2.828742	-1.970192	-4.440318
1	3.592193	-2.654039	-4.826062
1	1.864397	-2.373466	-4.766078
6	2.869738	-2.018555	-2.920504
1	1.927453	-2.192353	-2.415626
6	4.013176	-2.227138	-2.190782
1	3.899610	-2.568040	-1.167856
6	5.399068	-2.355227	-2.783817
1	6.119428	-2.328234	-1.968515
1	5.488603	-3.353444	-3.237895
6	5.772987	-1.275072	-3.826790
1	5.558620	-1.642284	-4.836756
1	6.855405	-1.123346	-3.782634

6	0.207363	1.172131	-3.829986
6	-0.363158	-0.047259	-4.241888
6	0.270803	2.227118	-4.757587
6	-0.837295	-0.206955	-5.541330
1	-0.439728	-0.872481	-3.544669
6	-0.194514	2.063062	-6.062470
1	0.694919	3.179213	-4.448365
6	-0.749715	0.843995	-6.460573
1	-1.278001	-1.153888	-5.839878
1	-0.126179	2.887405	-6.766703
1	-1.115429	0.714697	-7.475164
1	-4.022782	1.975156	-5.117533
35	-5.091309	-0.886378	-5.019036
5	1.307926	6.801656	1.865493
9	-0.049199	6.426134	1.867199
9	2.088722	5.687014	2.278570
9	1.703631	7.158416	0.558730
9	1.517848	7.868994	2.742817

[8-9]‡ P1-C1 *exo re-si* [BF_4^-] conf2

Number of imaginary frequencies= 1
The smallest frequencies are=-231.1139 11.5066 14.2666cm(-1)
Electronic energy= -7647.2535997
Zero-point correction= 1.771838
(Hartree/Particle)
Thermal correction to Energy= 1.896472
Thermal correction to Enthalpy= 1.897416
Thermal correction to Gibbs Free Energy= 1.603623
Sum of electronic and zero-point Energies= -7645.481762
Sum of electronic and thermal Energies= -7645.357128
Sum of electronic and thermal Enthalpies= -7645.356184
Sum of electronic and thermal Free Energies= -7645.649977

.....

Cartesian Coordinates

.....

26	-4.440802	-3.727251	3.687582
15	-1.500216	-2.263432	-0.433365
15	-4.602446	-0.289147	0.378386
6	-3.565407	-3.172867	1.861684
6	-4.342778	-2.091082	2.419037
6	-3.793229	-1.773329	3.699156
1	-4.158797	-1.011825	4.373590
6	-2.703035	-2.660335	3.951587
1	-2.106060	-2.691289	4.852238
6	-2.566553	-3.523238	2.825755
1	-1.845158	-4.319314	2.718102
6	-6.338699	-4.579886	3.697045
1	-7.116612	-4.368901	2.974825
6	-6.108797	-3.866289	4.912874
1	-6.674046	-3.014137	5.266790
6	-4.972523	-4.444328	5.556373
1	-4.523239	-4.103245	6.479802
6	-4.499987	-5.516153	4.738981
1	-3.632222	-6.131729	4.936190
6	-5.343282	-5.600352	3.591224
1	-5.227210	-6.295711	2.770904
6	-3.771364	-3.748965	0.501122
6	-4.916495	-4.525494	0.264676
1	-5.592255	-4.697532	1.092180
6	-5.208117	-5.053051	-0.992176
1	-6.118152	-5.624583	-1.144249
6	-4.332062	-4.821390	-2.049208
1	-4.541117	-5.219508	-3.036991
6	-3.190334	-4.047630	-1.841932
1	-2.532254	-3.865353	-2.682625
6	-2.896951	-3.484682	-0.588306
6	-5.447007	-1.368911	1.694850
1	-6.012455	-2.116428	1.136135
6	-6.416358	-0.619668	2.613489
1	-7.223293	-0.158124	2.037704
1	-5.918406	0.170048	3.182748
1	-6.857030	-1.322529	3.327477
6	-0.756385	-2.302651	-2.117816
6	-1.306846	-1.430234	-3.073650
1	-2.045744	-0.696840	-2.768200
6	-0.914049	-1.509503	-4.411095
1	-1.364996	-0.847832	-5.142206
6	0.059219	-2.433420	-4.801566
1	0.371719	-2.488416	-5.840237
6	0.644843	-3.269974	-3.848778
1	1.420410	-3.972576	-4.140095
6	0.234419	-3.211821	-2.515333
1	0.685536	-3.880947	-1.792729
6	-0.286927	-3.103703	0.662169
6	-0.073613	-4.491511	0.622299
1	-0.612423	-5.104002	-0.094835
6	0.807002	-5.093925	1.522286
1	0.967603	-6.167495	1.483307
6	1.476670	-4.318787	2.474570
1	2.158511	-4.789874	3.176439
6	1.269342	-2.938503	2.521218
1	1.790921	-2.335853	3.257368
6	0.392007	-2.332763	1.618302
1	0.222187	-1.262719	1.661289
6	-5.348827	-0.763055	-1.239253
6	-4.788689	-0.134366	-2.361302
1	-4.016582	0.613897	-2.210894
6	-5.189695	-0.490315	-3.648038
6	-6.128783	-1.500116	-3.848752
1	-6.421273	-1.794219	-4.850455
6	-6.673214	-2.135432	-2.731964
6	-6.305248	-1.766020	-1.437458
1	-6.758318	-2.286337	-0.604819
6	-5.184441	1.436626	0.648631
6	-4.571536	2.143867	1.694588
1	-3.845790	1.653875	2.331962
6	-4.865044	3.488673	1.905835
6	-5.749212	4.165409	1.065912
1	-5.960997	5.217864	1.218830
6	-6.348965	3.465268	0.020948
6	-6.082551	2.109952	-0.186548
1	-6.565516	1.595811	-1.008882
29	-2.242871	-0.233683	0.173052
6	-7.224200	4.217734	-0.941569
6	-4.150604	4.253103	2.985844
6	-4.611745	0.263096	-4.813480
6	-7.641570	-3.263004	-2.959857
9	-7.060076	-4.287711	-3.633157
9	-8.128055	-3.773699	-1.807166
9	-8.700882	-2.870409	-3.705616
9	-3.278635	0.495081	-4.653989
9	-5.186417	1.481813	-4.956025
9	-4.763473	-0.390789	-5.982103
9	-6.477481	4.923184	-1.833344
9	-8.016873	5.113366	-0.312857
9	-8.022160	3.400783	-1.661992
9	-4.957189	5.165082	3.573237
9	-3.677084	3.442228	3.957701
9	-3.088548	4.937937	2.490038
6	-2.211093	2.614495	-0.855843
6	-1.234259	3.005400	0.138002
6	-1.074722	2.329793	1.398775
1	-1.013681	4.061246	0.204294
77	3.273710	1.075017	-1.667063
15	4.811824	0.149028	-0.275108
8	4.572767	-1.287662	0.538964
8	6.220753	-0.231294	-1.098957
7	5.127461	1.174172	0.995060
6	4.673688	-2.502882	-0.127031
6	3.472923	-3.223713	-0.313774
1	2.551915	-2.804038	0.070794
6	3.499101	-4.429873	-0.968289
1	2.585580	-5.002016	-1.096905
6	4.711992	-4.931907	-1.510067
6	4.735006	-6.136003	-2.264970
1	3.804149	-6.682028	-2.396192
6	5.902944	-6.594173	-2.831251
1	5.908299	-7.512180	-3.411676
6	7.098838	-5.854185	-2.670340

1	8.014156	-6.202946	-3.139940
6	7.113377	-4.691843	-1.929914
1	8.036795	-4.134543	-1.826580
6	5.930571	-4.200252	-1.309146
6	5.909766	-2.987665	-0.530999
6	7.158209	-2.248932	-0.193823
6	8.250401	-2.868441	0.510272
6	8.170934	-4.184325	1.047156
1	7.253087	-4.748920	0.933684
6	9.234555	-4.744417	1.720893
1	9.144370	-5.748083	2.126695
6	10.440054	-4.023671	1.896049
1	11.272466	-4.480638	2.423192
6	10.544528	-2.739733	1.410976
1	11.456587	-2.166203	1.554973
6	9.460901	-2.126156	0.725319
6	9.549240	-0.782214	0.270585
1	10.473682	-0.232724	0.424575
6	8.470588	-0.174560	-0.322427
1	8.499562	0.860867	-0.644749
6	7.278467	-0.906946	-0.520148
6	4.529584	2.533121	0.826499
1	3.687446	2.608646	1.517879
6	5.528632	3.626632	1.173405
6	5.101715	4.767199	1.863223
1	4.069099	4.843599	2.181062
6	5.993114	5.812261	2.120724
1	5.641571	6.695335	2.647744
6	7.322849	5.725237	1.702402
1	8.016347	6.536326	1.907632
6	7.756817	4.585425	1.017098
1	8.790857	4.506293	0.691002
6	6.864028	3.546889	0.750732
1	7.200498	2.656001	0.226811
6	4.010801	2.769723	-0.604369
1	4.835912	3.175704	-1.200792
1	3.256677	3.551540	-0.542920
6	5.603091	0.925615	2.390171
1	6.301569	1.743220	2.591571
6	4.447745	1.072041	3.371966
6	4.502577	2.053553	4.366703
1	5.361961	2.717328	4.414298
6	3.458277	2.199125	5.283191
1	3.512137	2.969131	6.047947
6	2.343172	1.365485	5.204207
1	1.525366	1.479728	5.907629
6	2.275808	0.388377	4.205371
1	1.398120	-0.245639	4.132013
6	3.322078	0.239530	3.295726
1	3.266585	-0.513463	2.515755
6	6.383264	-0.365373	2.654383
1	7.257951	-0.442859	2.009165
1	5.772844	-1.260178	2.540244
1	6.736074	-0.322513	3.689712
6	1.834417	0.685066	-0.034541
1	1.701090	-0.369837	0.185973
1	2.072747	1.287778	0.838061
6	1.002343	1.240410	-1.051988
1	0.428897	0.540403	-1.646243
6	0.680602	2.614117	-1.200080
1	1.191421	3.316796	-0.556839
6	4.822163	1.464370	-3.209670
1	5.649050	1.963304	-2.710806
6	3.691688	2.268427	-3.508489
1	3.735622	3.315664	-3.209740
6	2.740568	2.008263	-4.659427
1	3.212567	2.321216	-5.604387
1	1.871882	2.654024	-4.525898
6	2.267254	0.542475	-4.781724
1	2.903744	-0.002706	-5.486783
1	1.259678	0.531448	-5.208553
6	2.228993	-0.230569	-3.471473
1	1.245542	-0.451727	-3.081275
6	3.270541	-0.989721	-2.987416
1	3.027570	-1.772190	-2.277300
6	4.632334	-1.092937	-3.638994
1	5.304348	-1.589727	-2.939156
1	4.551199	-1.752673	-4.516155
6	5.248845	0.263209	-4.058907
1	5.011833	0.474255	-5.107852
1	6.337758	0.173209	-4.005708
6	0.151072	3.155399	-2.460062
6	-0.462068	2.344154	-3.436113
6	0.277051	4.533237	-2.718084
6	-0.922170	2.891481	-4.630572
1	-0.593019	1.285342	-3.255486
6	-0.177876	5.076971	-3.919707
1	0.745237	5.166869	-1.972551
6	-0.778910	4.260119	-4.882080
1	-1.410679	2.250962	-5.359182
1	-0.062867	6.141694	-4.103828
1	-1.135620	4.685001	-5.816251
8	-2.407868	1.405833	-1.202527
6	-0.611416	3.089608	2.511161
6	-0.618476	2.564276	3.785691
1	-0.304298	4.112393	2.343197
6	-1.059517	1.244015	3.939042
6	-1.401038	0.498050	2.831686
1	-1.695626	-0.538954	2.920411
7	-1.408985	1.017574	1.584514
6	-3.662000	3.299424	-2.709926
1	-3.280197	2.393499	-3.167279
1	-4.730057	3.182319	-2.498168
1	-3.537010	4.119715	-3.422681
6	-2.947985	4.987824	-1.050440
1	-2.890812	5.048788	0.036119
1	-2.136940	5.583685	-1.485510
1	-3.904695	5.416890	-1.359026
7	-2.903018	3.598791	-1.501676
1	-0.310935	3.163679	4.634865
35	-1.238045	0.443558	5.720399
5	1.703422	5.560664	0.934216
9	2.182463	5.650636	-0.391822
9	0.315303	5.822300	0.946961
9	2.374551	6.474401	1.752374
9	1.924949	4.244762	1.408607

---

8 P1-C2 *endo si-re* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 11.9132 14.0811 15.6683 cm(-1)
Electronic energy= -7647.2667522
Zero-point correction= 1.771747
(Hartree/Particle)
Thermal correction to Energy= 1.897448
Thermal correction to Enthalpy= 1.898392
Thermal correction to Gibbs Free Energy= 1.601068
Sum of electronic and zero-point Energies= -7645.495005
Sum of electronic and thermal Energies= -7645.369304
Sum of electronic and thermal Enthalpies= -7645.368360
Sum of electronic and thermal Free Energies= -7645.665684

.....

Cartesian Coordinates

.....

26	7.920044	-0.029804	-1.234545
15	2.921525	1.387491	-2.050180
15	4.092551	0.790777	1.466934
6	6.003907	0.814471	-1.344478
6	6.211234	0.145267	-0.082932
6	6.487956	-1.229212	-0.359243
1	6.693932	-1.992945	0.377967
6	6.493104	-1.409439	-1.773879
1	6.705010	-2.332298	-2.295008
6	6.193475	-0.154352	-2.381307
1	6.141289	0.043947	-3.441479
6	9.485035	1.056902	-0.405838
1	9.376476	1.785706	0.386540
6	9.704480	-0.343997	-0.230866
1	9.783711	-0.862359	0.715467
6	9.754222	-0.948190	-1.524192

1	9.872479	-2.004331	-1.727896
6	9.564680	0.078341	-2.498959
1	9.517634	-0.062668	-3.570756
6	9.399962	1.316629	-1.809144
1	9.209947	2.275905	-2.271101
6	5.600697	2.242246	-1.480478
6	6.527114	3.243534	-1.147571
1	7.515628	2.936690	-0.830753
6	6.203827	4.598304	-1.202153
1	6.938608	5.343813	-0.914606
6	4.931385	4.981029	-1.619308
1	4.659028	6.030176	-1.670186
6	3.990930	4.004443	-1.945485
1	3.000263	4.322269	-2.246483
6	4.289271	2.633154	-1.862248
6	5.981063	0.780303	1.261189
1	6.276721	1.828561	1.189867
6	6.761987	0.136759	2.409532
1	6.566405	0.654217	3.353126
1	6.501998	-0.916333	2.545871
1	7.834119	0.194830	2.195690
6	1.456865	2.463879	-2.363784
6	0.740372	2.920712	-1.246377
1	1.011617	2.568425	-0.257405
6	-0.314351	3.819059	-1.405212
1	-0.846072	4.178854	-0.534843
6	-0.696364	4.237260	-2.682319
1	-1.529384	4.924617	-2.801069
6	-0.011784	3.758643	-3.801855
1	-0.308756	4.071129	-4.799116
6	1.067283	2.885095	-3.644244
1	1.605582	2.539563	-4.520674
6	3.177018	0.597275	-3.688773
6	3.992544	1.136514	-4.693941
1	4.539094	2.057557	-4.514172
6	4.111799	0.485999	-5.924432
1	4.751063	0.906137	-6.695862
6	3.410845	-0.699605	-6.164426
1	3.507902	-1.204558	-7.121232
6	2.586762	-1.235311	-5.170707
1	2.042754	-2.158399	-5.349983
6	2.473702	-0.591212	-3.937818
1	1.852175	-1.015554	-3.154897
6	3.596820	2.510713	1.899225
6	2.221835	2.707899	2.102317
1	1.556544	1.849471	2.062512
6	1.709765	3.992833	2.281570
6	2.543830	5.108437	2.239499
1	2.140043	6.107710	2.357684
6	3.908523	4.911270	2.020925
6	4.438218	3.630005	1.862526
1	5.500833	3.527181	1.687377
6	3.728797	-0.181923	2.984586
6	3.807298	-1.576776	2.847552
1	4.114751	-2.008996	1.902292
6	3.447943	-2.409612	3.902243
6	2.961080	-1.877148	5.097201
1	2.646344	-2.528687	5.904525
6	2.864515	-0.493734	5.224518
6	3.261023	0.354806	4.186615
1	3.177297	1.427030	4.321150
29	2.711715	0.015328	-0.274347
6	2.221244	0.101152	6.443864
6	3.466696	-3.903488	3.731527
6	0.233964	4.143930	2.524483
6	4.793185	6.123744	1.924219
9	4.441073	6.911930	0.877603
9	6.097159	5.809262	1.762950
9	4.701080	6.898432	3.031334
9	-0.494356	3.360466	1.677683
9	-0.119218	3.770395	3.775308
9	-0.198343	5.410785	2.344268
9	2.745188	1.307550	6.760177
9	0.888697	0.300743	6.248424
9	2.338349	-0.691000	7.530726
9	4.020548	-4.518755	4.804589
9	4.164571	-4.288651	2.641059
9	2.216466	-4.408831	3.602948
6	0.717095	-1.019649	1.723135
6	1.004665	-2.359676	1.361311
6	1.860244	-2.839681	0.348957
1	0.496826	-3.140061	1.906378
77	-3.060097	-0.826585	-1.717200
15	-4.917394	-0.179210	-0.540863
8	-4.918732	0.971937	0.641579
8	-6.041055	0.463615	-1.582553
7	-5.504892	-1.468152	0.332332
6	-4.746192	2.317694	0.343065
6	-3.557964	2.917670	0.815273
1	-2.862561	2.315535	1.389149
6	-3.326128	4.245464	0.554647
1	-2.442815	4.735727	0.949168
6	-4.223930	4.986356	-0.260184
6	-3.926452	6.320649	-0.649640
1	-3.008555	6.773976	-0.284293
6	-4.770176	7.018136	-1.484764
1	-4.528963	8.033901	-1.783985
6	-5.950965	6.403024	-1.965419
1	-6.603508	6.947541	-2.641859
6	-6.279340	5.118624	-1.588271
1	-7.184086	4.660437	-1.970491
6	-5.438054	4.372303	-0.716999
6	-5.742941	3.022541	-0.314882
6	-7.071192	2.397924	-0.573539
6	-8.294111	3.020974	-0.127194
6	-8.311211	4.192261	0.681713
1	-7.374753	4.637666	0.994182
6	-9.498646	4.760207	1.090249
1	-9.480496	5.649452	1.713891
6	-10.739324	4.193841	0.713851
1	-11.666952	4.657138	1.036883
6	-10.761846	3.045455	-0.044392
1	-11.705770	2.584205	-0.322736
6	-9.555324	2.424720	-0.467835
6	-9.580796	1.208089	-1.201550
1	-10.539144	0.769817	-1.465082
6	-8.411768	0.576119	-1.541126
1	-8.404217	-0.372201	-2.067906
6	-7.174788	1.164773	-1.199065
6	-4.789823	-2.743491	0.041806
1	-4.033121	-2.892055	0.813719
6	-5.725393	-3.940238	0.052118
6	-5.292555	-5.146004	0.618634
1	-4.317106	-5.201411	1.090896
6	-6.113485	-6.276337	0.576657
1	-5.765868	-7.204605	1.022055
6	-7.373046	-6.211782	-0.023414
1	-8.012672	-7.089805	-0.048855
6	-7.810389	-5.008271	-0.586941
1	-8.791452	-4.949054	-1.051005
6	-6.989465	-3.880766	-0.552795
1	-7.329710	-2.941555	-0.981357
6	-4.106704	-2.653863	-1.324858
1	-4.868309	-2.775611	-2.102943
1	-3.405636	-3.483130	-1.428198
6	-6.247024	-1.436383	1.639753
1	-6.620625	-2.459159	1.730629
6	-5.328742	-1.212128	2.840313
6	-4.644604	-2.310408	3.382654
1	-4.765095	-3.293422	2.938688
6	-3.807967	-2.164989	4.490885
1	-3.268887	-3.029882	4.862136
6	-3.655594	-0.912420	5.087888
1	-3.007630	-0.793214	5.951894
6	-4.338820	0.189389	4.564374
1	-4.229480	1.167470	5.025727
6	-5.165715	0.041028	3.448974
1	-5.686377	0.907071	3.057291
6	-7.484058	-0.541779	1.612675
1	-8.143238	-0.838358	0.794091

1	-7.248498	0.515791	1.495522
1	-8.027732	-0.664553	2.554200
6	-1.893600	-0.410936	0.108749
1	-1.223189	0.412520	-0.113582
1	-2.424815	-0.308120	1.049941
6	-1.533064	-1.735316	-0.261993
1	-1.921078	-2.541527	0.345048
6	-0.871939	-2.040761	-1.462661
1	-0.235068	-1.289955	-1.914442
6	-4.231189	-0.682505	-3.650526
1	-5.179295	-1.176068	-3.460536
6	-3.119099	-1.514821	-3.873792
1	-3.282161	-2.590588	-3.845412
6	-1.875843	-1.096173	-4.634177
1	-2.095193	-1.118151	-5.711985
1	-1.115781	-1.859112	-4.462398
6	-1.309962	0.284433	-4.238286
1	-1.701977	1.064714	-4.898010
1	-0.227057	0.279525	-4.391727
6	-1.582218	0.688380	-2.795300
1	-0.713834	0.728749	-2.147337
6	-2.686725	1.419215	-2.391429
1	-2.598238	1.977913	-1.465618
6	-3.812441	1.851465	-3.305096
1	-4.623728	2.231456	-2.684782
1	-3.460186	2.697326	-3.912882
6	-4.355235	0.731092	-4.220757
1	-3.850622	0.756824	-5.191812
1	-5.412707	0.926862	-4.418061
6	-0.624626	-3.419662	-1.906851
6	-1.112636	-4.548856	-1.214400
6	0.177875	-3.636415	-3.042693
6	-0.823061	-5.835347	-1.662608
1	-1.677849	-4.432897	-0.298435
6	0.463643	-4.924342	-3.491730
1	0.600317	-2.782739	-3.560704
6	-0.041150	-6.031956	-2.805413
1	-1.196771	-6.686358	-1.100348
1	1.092410	-5.062890	-4.366475
1	0.185371	-7.037730	-3.147727
6	1.958093	-4.264737	0.178631
6	2.768490	-4.822192	-0.777504
1	1.352140	-4.897001	0.816953
6	3.507449	-3.948849	-1.597590
6	3.408919	-2.589441	-1.416435
1	3.968188	-1.898725	-2.032916
7	2.619994	-2.031750	-0.470189
8	1.058059	0.025207	1.055005
7	-0.009324	-0.811051	2.879389
6	-0.594436	0.487303	3.169204
1	-1.647470	0.369411	3.449829
1	-0.078230	0.988560	3.998339
1	-0.537309	1.118235	2.287938
6	-0.364343	-1.888077	3.796298
1	-1.251222	-2.436247	3.467781
1	0.457821	-2.596174	3.903521
1	-0.561273	-1.453900	4.779853
1	2.822292	-5.897801	-0.905184
35	4.663727	-4.660584	-3.021564
5	-1.843833	-5.078996	2.576569
9	-0.499595	-5.261391	2.210208
9	-2.592213	-6.219716	2.252439
9	-2.372108	-3.970446	1.848145
9	-1.939345	-4.800528	3.949042

[8-9]‡ P1-C2 *endo si-re* [BF_4^-]

Number of imaginary frequencies= 1
The smallest frequencies are=-200.2306 12.6332 15.8549cm(-1)

Electronic energy= -7647.2593186
Zero-point correction= 1.772212
(Hartree/Particle)
Thermal correction to Energy= 1.896726
Thermal correction to Enthalpy= 1.897670
Thermal correction to Gibbs Free Energy= 1.603398
Sum of electronic and zero-point Energies= -7645.487107
Sum of electronic and thermal Energies= -7645.362593
Sum of electronic and thermal Enthalpies= -7645.361649
Sum of electronic and thermal Free Energies= -7645.655921

.....

Cartesian Coordinates

.....

26	8.216916	0.349719	-0.767204
15	3.256633	1.430368	-2.098114
15	4.055078	0.709317	1.520691
6	6.259398	1.041268	-1.052938
6	6.369270	0.261700	0.158069
6	6.810321	-1.048145	-0.204870
1	7.000315	-1.863232	0.480028
6	7.007105	-1.079515	-1.618008
1	7.371059	-1.921979	-2.189003
6	6.667018	0.202654	-2.139922
1	6.728315	0.504679	-3.174715
6	9.544373	1.495567	0.343908
1	9.258981	2.143241	1.162493
6	9.876014	0.109900	0.448943
1	9.879514	-0.476834	1.357839
6	10.153388	-0.378971	-0.864238
1	10.399705	-1.400467	-1.122566
6	9.993595	0.704017	-1.781501
1	10.099816	0.648180	-2.856867
6	9.618874	1.861644	-1.036276
1	9.396297	2.834887	-1.451927
6	5.750454	2.441688	-1.119746
6	6.535244	3.478876	-0.591975
1	7.502567	3.226053	-0.177375
6	6.098474	4.803082	-0.578600
1	6.719771	5.575285	-0.136051
6	4.856379	5.119621	-1.123010
1	4.499220	6.144444	-1.123819
6	4.054963	4.105680	-1.647196
1	3.083318	4.367730	-2.048952
6	4.466197	2.762256	-1.637404
6	5.952595	0.740620	1.522619
1	6.223921	1.795225	1.595204
6	6.615371	-0.006990	2.682602
1	6.303263	0.407011	3.645472
1	6.369868	-1.072351	2.680287
1	7.702674	0.087978	2.598948
6	1.746627	2.383295	-2.558322
6	0.862304	2.732329	-1.523991
1	1.041025	2.364011	-0.520057
6	-0.245764	3.538035	-1.786261
1	-0.917676	3.807952	-0.981129
6	-0.506475	3.972653	-3.088089
1	-1.378177	4.589307	-3.288863
6	0.347927	3.599652	-4.128286
1	0.145836	3.924959	-5.144950
6	1.474990	2.816810	-3.865066
1	2.142032	2.552996	-4.679070
6	3.843545	0.760866	-3.702034
6	4.626186	1.501377	-4.600736
1	4.921989	2.516875	-4.353665
6	5.036923	0.930195	-5.806697
1	5.646907	1.506956	-6.496263
6	4.666433	-0.380254	-6.126047
1	4.992099	-0.823465	-7.062790
6	3.878150	-1.118571	-5.239573
1	3.588609	-2.136983	-5.482582
6	3.470081	-0.550099	-4.031722
1	2.874487	-1.127112	-3.311450
6	3.495801	2.404324	1.975188
6	2.107117	2.599682	1.963785
1	1.460194	1.758110	1.738551
6	1.566397	3.862930	2.201226
6	2.392273	4.966000	2.408905
1	1.970598	5.951986	2.569262
6	3.774692	4.774545	2.392035
6	4.327547	3.508063	2.199349

1	5.404418	3.409976	2.207640
6	3.514513	-0.336397	2.937156
6	3.635456	-1.723741	2.755111
1	4.095071	-2.113772	1.854510
6	3.131734	-2.607378	3.704990
6	2.469530	-2.133376	4.838764
1	2.053023	-2.824314	5.563123
6	2.338182	-0.757747	5.012816
6	2.865746	0.140628	4.080711
1	2.748237	1.204563	4.248817
29	2.944271	-0.021386	-0.405327
6	1.535546	-0.239632	6.173736
6	3.199727	-4.092291	3.470077
6	0.070814	3.996841	2.267441
6	4.663632	5.977235	2.552904
9	4.496102	6.856935	1.534033
9	5.975504	5.653598	2.584308
9	4.388254	6.655795	3.691238
9	-0.541623	3.279226	1.283023
9	-0.426384	3.525469	3.434874
9	-0.348004	5.273087	2.137522
9	1.888609	1.017621	6.520437
9	0.206135	-0.199815	5.878343
9	1.661569	-1.017169	7.269885
9	3.529714	-4.760643	4.599276
9	4.108100	-4.420214	2.524823
9	2.005718	-4.588563	3.062323
6	0.661408	-1.101223	1.211266
6	0.902014	-2.432625	0.715784
6	2.034101	-2.906010	-0.004512
1	0.319858	-3.226435	1.158053
77	-3.359084	-0.846837	-1.773469
15	-5.166432	-0.134518	-0.584035
8	-5.122364	1.026389	0.600537
8	-6.310801	0.542448	-1.595150
7	-5.791248	-1.406023	0.307420
6	-4.916255	2.357202	0.265349
6	-3.678049	2.924052	0.641615
1	-2.964949	2.307294	1.177325
6	-3.410266	4.232508	0.321993
1	-2.476088	4.691676	0.627316
6	-4.338995	4.992179	-0.439751
6	-4.025152	6.308961	-0.872972
1	-3.066130	6.732824	-0.586156
6	-4.905784	7.026805	-1.650506
1	-4.652979	8.029640	-1.982196
6	-6.140696	6.448700	-2.030677
1	-6.824357	7.008564	-2.662460
6	-6.482938	5.180744	-1.612531
1	-7.429347	4.750665	-1.919208
6	-5.604745	4.415382	-0.795575
6	-5.923860	3.082789	-0.352649
6	-7.274456	2.479361	-0.536783
6	-8.463399	3.114413	-0.025172
6	-8.424273	4.293376	0.771677
1	-7.467335	4.736464	1.019182
6	-9.581128	4.870977	1.248625
1	-9.520481	5.766186	1.861014
6	-10.845447	4.306659	0.956548
1	-11.748952	4.776662	1.333837
6	-10.920770	3.152768	0.210038
1	-11.882610	2.694451	-0.005097
6	-9.746239	2.522555	-0.283809
6	-9.821969	1.301118	-1.006298
1	-10.796975	0.865941	-1.206869
6	-8.678833	0.661608	-1.414475
1	-8.708395	-0.289755	-1.935123
6	-7.419420	1.244903	-1.152414
6	-5.140275	-2.705889	-0.032141
1	-4.347545	-2.889842	0.697629
6	-6.116306	-3.868070	0.022940
6	-5.691583	-5.103837	0.530713
1	-4.686483	-5.203477	0.930622
6	-6.554842	-6.202911	0.520120
1	-6.214237	-7.155171	0.917926
6	-7.849455	-6.078682	0.010462
1	-8.520962	-6.932977	0.008776
6	-8.279021	-4.846425	-0.493096
1	-9.286613	-4.740412	-0.886819
6	-7.416491	-3.749708	-0.489182
1	-7.749109	-2.787898	-0.870752
6	-4.512864	-2.623856	-1.428476
1	-5.309482	-2.686798	-2.179980
1	-3.866898	-3.494353	-1.572734
6	-6.429946	-1.355992	1.666643
1	-6.848614	-2.359692	1.777144
6	-5.407275	-1.196987	2.791872
6	-4.734998	-2.336456	3.260644
1	-4.955588	-3.307368	2.828461
6	-3.781087	-2.248535	4.276344
1	-3.246704	-3.142983	4.579996
6	-3.497485	-1.012204	4.859745
1	-2.749382	-0.933753	5.644207
6	-4.172414	0.128992	4.415786
1	-3.962858	1.095090	4.867815
6	-5.115438	0.038027	3.389266
1	-5.622323	0.935135	3.054158
6	-7.616778	-0.397856	1.747699
1	-8.353659	-0.648926	0.981821
1	-7.335585	0.647073	1.619634
1	-8.090248	-0.504911	2.728579
6	-2.323092	-0.716570	0.146756
1	-1.652986	0.138133	0.137402
1	-2.947252	-0.770045	1.034965
6	-1.862991	-1.959530	-0.389866
1	-2.347492	-2.858492	-0.037617
6	-0.682788	-2.130891	-1.139754
1	-0.108312	-1.253473	-1.409340
6	-4.331824	-0.665584	-3.764457
1	-5.324665	-1.099761	-3.676201
6	-3.250099	-1.575387	-3.884133
1	-3.491839	-2.637475	-3.897377
6	-1.919652	-1.241324	-4.537506
1	-2.030658	-1.247992	-5.633345
1	-1.228501	-2.051644	-4.295312
6	-1.302355	0.097139	-4.076932
1	-1.565008	0.903663	-4.769460
1	-0.210781	0.017832	-4.112551
6	-1.701063	0.518977	-2.665328
1	-0.891544	0.548144	-1.943874
6	-2.801014	1.319397	-2.365689
1	-2.740162	1.900645	-1.452088
6	-3.823130	1.823205	-3.363990
1	-4.680106	2.196038	-2.798876
1	-3.402780	2.683593	-3.906278
6	-4.308070	0.745522	-4.356518
1	-3.682011	0.747528	-5.255128
1	-5.318319	1.003297	-4.689628
6	-0.351725	-3.355491	-1.861553
6	-0.898007	-4.610779	-1.526145
6	0.572087	-3.283292	-2.921972
6	-0.542979	-5.746572	-2.250782
1	-1.563209	-4.701771	-0.675427
6	0.921514	-4.421013	-3.646887
1	1.003779	-2.320311	-3.178144
6	0.361297	-5.657917	-3.315414
1	-0.964402	-6.708838	-1.974208
1	1.630719	-4.344271	-4.466290
1	0.634449	-6.548399	-3.874435
6	2.192696	-4.320507	-0.122315
6	3.227230	-4.862447	-0.851533
1	1.475301	-4.961923	0.375625
6	4.124002	-3.976242	-1.463827
6	3.957907	-2.614092	-1.320602
1	4.637883	-1.911018	-1.782094
7	2.942065	-2.079274	-0.611356
8	1.061462	-0.039789	0.623731
7	-0.110831	-0.975573	2.328791
6	-0.597026	0.331381	2.751152
1	-1.625135	0.236597	3.109803

1	0.012592	0.741391	3.563428
1	-0.580185	1.021598	1.913719
6	-0.562789	-2.113303	3.130394
1	-1.492908	-2.530744	2.743390
1	0.188978	-2.898455	3.161008
1	-0.728381	-1.768301	4.151467
1	3.338107	-5.937086	-0.946424
35	5.610953	-4.657593	-2.548101
5	-1.878126	-5.247618	2.242608
9	-0.593755	-5.269740	1.656681
9	-2.497156	-6.492890	2.105932
9	-2.665925	-4.271068	1.565150
9	-1.779320	-4.889825	3.597844

---

9 P1-C2 *endo si-re* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 13.8756 16.7659 19.3367 cm(-1)
Electronic energy= -7647.2886223
Zero-point correction= 1.775812
(Hartree/Particle)
Thermal correction to Energy= 1.899770
Thermal correction to Enthalpy= 1.900714
Thermal correction to Gibbs Free Energy= 1.608276
Sum of electronic and zero-point Energies= -7645.512810
Sum of electronic and thermal Energies= -7645.388853
Sum of electronic and thermal Enthalpies= -7645.387908
Sum of electronic and thermal Free Energies= -7645.680347

.....

Cartesian Coordinates

.....

26	8.140027	0.607998	-0.933262
15	3.114780	1.630891	-2.078579
15	4.006327	0.593714	1.463921
6	6.151422	1.247738	-1.127682
6	6.308284	0.352705	-0.005651
6	6.800646	-0.892433	-0.507863
1	7.038482	-1.764462	0.085251
6	6.974993	-0.769423	-1.919995
1	7.370893	-1.529078	-2.579299
6	6.578913	0.545807	-2.300348
1	6.612153	0.957293	-3.298106
6	9.446766	1.684136	0.273296
1	9.157446	2.241001	1.154882
6	9.823118	0.306602	0.238060
1	9.857446	-0.365037	1.085606
6	10.097819	-0.041620	-1.119451
1	10.373037	-1.024021	-1.480071
6	9.891865	1.120482	-1.923831
1	9.986947	1.174571	-3.000319
6	9.491746	2.186437	-1.064238
1	9.234641	3.188957	-1.378147
6	5.593021	2.627349	-1.048847
6	6.353203	3.635293	-0.436483
1	7.330163	3.371882	-0.052966
6	5.879487	4.939412	-0.302112
1	6.483168	5.687382	0.201821
6	4.623697	5.266449	-0.807652
1	4.239010	6.277184	-0.717118
6	3.844302	4.279242	-1.410115
1	2.862052	4.547579	-1.780343
6	4.293184	2.952407	-1.520023
6	5.904255	0.669582	1.408721
1	6.153177	1.715266	1.595646
6	6.612486	-0.182422	2.466169
1	6.314699	0.115632	3.475129
1	6.396541	-1.248206	2.354147
1	7.693998	-0.046565	2.368806
6	1.578193	2.573029	-2.444768
6	0.725695	2.854848	-1.363740
1	0.938407	2.437441	-0.386217
6	-0.396463	3.661558	-1.543603
1	-1.042415	3.876872	-0.701977
6	-0.705115	4.163544	-2.810331
1	-1.589194	4.779655	-2.947649
6	0.114560	3.853584	-3.897664
1	-0.127792	4.227343	-4.888429
6	1.257652	3.070289	-3.716450
1	1.894979	2.854455	-4.567269
6	3.727584	1.074048	-3.712399
6	4.387430	1.929086	-4.608602
1	4.554637	2.969329	-4.344177
6	4.844816	1.439120	-5.832979
1	5.357566	2.103974	-6.522243
6	4.647312	0.095814	-6.170855
1	5.009333	-0.282734	-7.122432
6	3.987776	-0.758432	-5.283603
1	3.835905	-1.803219	-5.539361
6	3.532387	-0.270639	-4.057449
1	3.040601	-0.935933	-3.355496
6	3.434061	2.240598	2.065955
6	2.043820	2.416867	2.094027
1	1.401676	1.593125	1.803794
6	1.488928	3.644826	2.451195
6	2.303427	4.735799	2.746036
1	1.872156	5.697377	3.001484
6	3.687799	4.567300	2.688637
6	4.255537	3.332280	2.371181
1	5.333690	3.252823	2.344492
6	3.550543	-0.566236	2.821932
6	3.710493	-1.938035	2.563631
1	4.156423	-2.270994	1.633736
6	3.282400	-2.884408	3.492352
6	2.646285	-2.491665	4.670248
1	2.284051	-3.232862	5.374147
6	2.473551	-1.132291	4.918511
6	2.937974	-0.172136	4.017008
1	2.795707	0.877269	4.244626
29	2.851961	0.048322	-0.499550
6	1.679792	-0.714881	6.126323
6	3.407234	-4.354904	3.200228
6	-0.007959	3.750065	2.547343
6	4.560702	5.767634	2.935710
9	4.371249	6.719727	1.988407
9	5.876912	5.462255	2.932135
9	4.284351	6.352382	4.124206
9	-0.623332	3.076060	1.535414
9	-0.477799	3.209122	3.696142
9	-0.445765	5.025305	2.493809
9	1.834033	0.593458	6.418964
9	0.347894	-0.916593	5.926475
9	2.013177	-1.424565	7.225358
9	3.765876	-5.053727	4.299288
9	4.323967	-4.611547	2.239994
9	2.228491	-4.876193	2.776789
6	0.511596	-1.141301	1.059426
6	0.526347	-2.374878	0.167358
6	1.897661	-2.875013	-0.220935
1	0.011930	-3.203187	0.649082
77	-3.350840	-0.762691	-1.853825
15	-5.166875	-0.125446	-0.582006
8	-5.143661	0.965516	0.683480
8	-6.369669	0.588394	-1.516580
7	-5.752232	-1.460720	0.253884
6	-4.945557	2.309234	0.417913
6	-3.709058	2.865211	0.816120
1	-2.988819	2.224287	1.311521
6	-3.454224	4.192452	0.574497
1	-2.525050	4.642164	0.908561
6	-4.391927	4.987216	-0.139023
6	-4.092538	6.329709	-0.497230
1	-3.135455	6.745341	-0.192040
6	-4.984229	7.083407	-1.227080
1	-4.742027	8.105948	-1.501866
6	-6.216575	6.517197	-1.632870
1	-6.909000	7.106331	-2.227463
6	-6.544760	5.224108	-1.286485
1	-7.489229	4.803021	-1.611472
6	-5.654916	4.420611	-0.520258
6	-5.962429	3.063938	-0.149008

6	-7.313966	2.465686	-0.341090
6	-8.494129	3.070554	0.224841
6	-8.442622	4.207167	1.080937
1	-7.482120	4.639625	1.333450
6	-9.591034	4.756971	1.608741
1	-9.519776	5.619736	2.265139
6	-10.859883	4.205331	1.312308
1	-11.756950	4.652988	1.730137
6	-10.946871	3.090873	0.509092
1	-11.911882	2.641329	0.289154
6	-9.780955	2.489691	-0.038364
6	-9.867737	1.306082	-0.820315
1	-10.845647	0.879006	-1.024721
6	-8.731185	0.692018	-1.282020
1	-8.769347	-0.231055	-1.850949
6	-7.465041	1.262017	-1.015822
6	-5.074016	-2.726724	-0.156240
1	-4.265794	-2.926448	0.552764
6	-6.022217	-3.913871	-0.141754
6	-5.556682	-5.166407	0.283420
1	-4.538269	-5.266165	0.647105
6	-6.393842	-6.284348	0.233170
1	-6.019222	-7.248206	0.567868
6	-7.704264	-6.164990	-0.235937
1	-8.355720	-7.034163	-0.268559
6	-8.173931	-4.917820	-0.660863
1	-9.192916	-4.815086	-1.025414
6	-7.337289	-3.801878	-0.616402
1	-7.701273	-2.829444	-0.937561
6	-4.464504	-2.577070	-1.555269
1	-5.273027	-2.625789	-2.296375
1	-3.816866	-3.439117	-1.734143
6	-6.368915	-1.504504	1.620775
1	-6.794716	-2.510090	1.670547
6	-5.327544	-1.437598	2.739876
6	-4.690679	-2.622456	3.142304
1	-4.952105	-3.560691	2.662350
6	-3.725115	-2.621522	4.151198
1	-3.219630	-3.548344	4.402313
6	-3.395356	-1.427674	4.796187
1	-2.641203	-1.416743	5.579038
6	-4.033279	-0.241982	4.417987
1	-3.787132	0.691279	4.918231
6	-4.986244	-0.246161	3.396903
1	-5.463428	0.683679	3.112012
6	-7.549335	-0.549870	1.797561
1	-8.299442	-0.735678	1.025494
1	-7.266488	0.500964	1.748795
1	-8.008967	-0.734850	2.773658
6	-2.275925	-0.768209	0.061037
1	-1.678676	0.134243	0.168702
1	-2.906241	-0.976239	0.922926
6	-1.776118	-1.864036	-0.697559
1	-2.196856	-2.822413	-0.422247
6	-0.329671	-2.022016	-1.131125
1	0.082218	-1.092857	-1.528258
6	-4.313910	-0.555213	-3.794293
1	-5.295370	-1.025732	-3.768526
6	-3.189196	-1.435237	-3.936429
1	-3.405070	-2.500591	-4.020819
6	-1.906172	-1.021010	-4.639455
1	-2.079047	-0.931877	-5.724537
1	-1.187516	-1.831056	-4.508773
6	-1.298189	0.286435	-4.088989
1	-1.549877	1.134524	-4.735911
1	-0.204921	0.215196	-4.107841
6	-1.728281	0.617908	-2.659401
1	-0.919361	0.640749	-1.935531
6	-2.843468	1.402786	-2.339146
1	-2.787925	1.969850	-1.415703
6	-3.859031	1.929699	-3.336502
1	-4.727980	2.269694	-2.766866
1	-3.448945	2.814685	-3.848289
6	-4.320018	0.870810	-4.360716
1	-3.691642	0.912083	-5.258123
1	-5.333910	1.118789	-4.692733
6	-0.140729	-3.127062	-2.153570
6	-0.685321	-4.405753	-1.956604
6	0.665718	-2.909195	-3.277379
6	-0.435852	-5.431378	-2.870516
1	-1.278156	-4.611846	-1.071105
6	0.919274	-3.933518	-4.193047
1	1.087458	-1.921808	-3.438515
6	0.367342	-5.200836	-3.991722
1	-0.862535	-6.415923	-2.699186
1	1.541250	-3.739039	-5.062969
1	0.561921	-6.001840	-4.699565
6	2.148181	-4.252286	-0.158097
6	3.332845	-4.772630	-0.663510
1	1.404103	-4.906855	0.276747
6	4.233059	-3.877125	-1.230216
6	3.952423	-2.520053	-1.254174
1	4.640210	-1.805554	-1.684696
7	2.806897	-2.025225	-0.744771
8	0.910856	-0.040513	0.598795
7	-0.036326	-1.217717	2.281598
6	-0.435180	0.019811	2.955863
1	-1.329111	-0.182249	3.545985
1	0.347504	0.394363	3.618387
1	-0.667977	0.780918	2.214777
6	-0.440942	-2.471414	2.929145
1	-1.454666	-2.748419	2.644081
1	0.234861	-3.284954	2.677732
1	-0.395319	-2.319775	4.007517
1	3.534827	-5.836993	-0.621655
35	5.906552	-4.514543	-2.010732
5	-1.813832	-5.374023	1.849609
9	-0.475690	-5.386392	1.383565
9	-2.451996	-6.572040	1.519771
9	-2.494508	-4.298857	1.220000
9	-1.821713	-5.172248	3.240489

---

8 P1-C2 *endo re-re* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 13.3274 13.8659 16.4012 cm(-1)
Electronic energy= -7647.2606003
Zero-point correction= 1.771808
(Hartree/Particle)
Thermal correction to Energy= 1.897604
Thermal correction to Enthalpy= 1.898549
Thermal correction to Gibbs Free Energy= 1.601354
Sum of electronic and zero-point Energies= -7645.488792
Sum of electronic and thermal Energies= -7645.362996
Sum of electronic and thermal Enthalpies= -7645.362052
Sum of electronic and thermal Free Energies= -7645.659246

Cartesian Coordinates

26	7.607984	-1.768224	-1.645119
15	3.005969	0.607669	-2.335866
15	4.385803	0.405589	1.136393
6	5.930109	-0.524559	-1.795444
6	6.058125	-1.068170	-0.464605
6	5.997338	-2.489334	-0.566951
1	6.072702	-3.184928	0.256978
6	5.870188	-2.834333	-1.943266
1	5.843145	-3.837098	-2.346634
6	5.831127	-1.628699	-2.700301
1	5.754461	-1.550938	-3.774986
6	9.424725	-0.959951	-1.045890
1	9.532553	-0.118688	-0.373916
6	9.340888	-2.333677	-0.661579
1	9.365955	-2.714470	0.350673
6	9.169882	-3.113840	-1.845956
1	9.038512	-4.187238	-1.885841
6	9.148507	-2.223445	-2.962626
1	9.001023	-2.502960	-3.997519
6	9.307484	-0.894127	-2.469390
1	9.306750	0.005676	-3.069313

6	5.837717	0.927961	-2.117644
6	6.989290	1.725427	-2.038988
1	7.921078	1.248732	-1.763056
6	6.956585	3.096294	-2.291099
1	7.861640	3.687474	-2.196319
6	5.752606	3.698114	-2.648543
1	5.707413	4.763904	-2.849204
6	4.591712	2.928232	-2.724236
1	3.660721	3.416630	-2.987503
6	4.602832	1.551657	-2.444579
6	6.141181	-0.233420	0.783858
1	6.709703	0.659556	0.522933
6	6.852765	-0.911281	1.958418
1	6.887219	-0.251675	2.830262
1	6.365087	-1.841073	2.260003
1	7.878935	-1.152352	1.664682
6	1.743559	1.875213	-2.785103
6	1.325389	2.738948	-1.758312
1	1.754563	2.637143	-0.766892
6	0.383794	3.736402	-2.004404
1	0.085373	4.402916	-1.205529
6	-0.175886	3.871499	-3.277731
1	-0.923864	4.637508	-3.461081
6	0.226601	3.013561	-4.303135
1	-0.203888	3.110690	-5.295961
6	1.185276	2.025118	-4.062208
1	1.485422	1.369613	-4.871750
6	3.049234	-0.537054	-3.770543
6	3.570826	-0.167663	-5.020115
1	3.979102	0.828525	-5.165708
6	3.578973	-1.083219	-6.074032
1	3.982963	-0.791903	-7.039547
6	3.071629	-2.373636	-5.886287
1	3.081157	-3.084564	-6.707824
6	2.565031	-2.749923	-4.639841
1	2.185263	-3.756312	-4.486303
6	2.557611	-1.837772	-3.582066
1	2.220899	-2.138519	-2.593979
6	4.545434	2.238723	1.309375
6	3.355362	2.960965	1.485835
1	2.433695	2.432146	1.687195
6	3.332071	4.351087	1.372352
6	4.497329	5.061655	1.095607
1	4.475608	6.139404	0.979800
6	5.689111	4.351849	0.951633
6	5.720808	2.961667	1.057351
1	6.668442	2.462091	0.913176
6	3.908042	-0.233068	2.791292
6	3.745586	-1.625782	2.874374
1	3.977603	-2.251351	2.020912
6	3.227350	-2.206178	4.026590
6	2.808659	-1.413440	5.095837
1	2.365485	-1.865719	5.976753
6	2.948069	-0.029577	5.002453
6	3.509863	0.563469	3.869704
1	3.606845	1.641630	3.831383
29	2.660853	-0.337656	-0.302858
6	2.401263	0.817769	6.117126
6	3.028981	-3.694432	4.113739
6	2.022728	5.074078	1.531511
6	6.938093	5.127236	0.630255
9	6.810758	5.809662	-0.535036
9	8.027650	4.337609	0.511257
9	7.210993	6.048744	1.583346
9	0.998424	4.353172	0.995750
9	1.706779	5.287809	2.827371
9	2.019226	6.274989	0.916886
9	2.717820	2.124444	5.980677
9	1.048650	0.738338	6.173062
9	2.858543	0.416995	7.327537
9	3.648973	-4.210660	5.204340
9	3.515485	-4.348095	3.034511
9	1.721226	-4.021152	4.229392
6	0.601568	0.744018	1.544646
6	0.713662	-1.605208	1.685315
6	-0.102364	0.840832	2.725302
1	0.830765	1.627649	0.962661
6	-0.114245	-1.532518	2.860749
6	-0.489272	-0.330043	3.402542
6	1.118832	-2.886515	1.264886
6	2.008821	-3.230856	0.218993
8	2.704622	-2.392979	-0.458484
7	1.037451	-0.430076	1.035027
1	0.682294	-3.688353	1.837014
77	-3.183331	-1.155262	-1.563686
15	-4.920382	-0.027117	-0.627406
8	-4.761580	1.157156	0.500201
8	-5.776710	0.796060	-1.793218
7	-5.841557	-1.092697	0.254827
6	-4.209517	2.385849	0.174138
6	-2.939728	2.666608	0.720498
1	-2.479992	1.929418	1.367601
6	-2.330098	3.859455	0.424134
1	-1.363276	4.098806	0.852303
6	-2.940871	4.771888	-0.479248
6	-2.271106	5.960521	-0.878146
1	-1.300552	6.178638	-0.439918
6	-2.831505	6.811102	-1.805152
1	-2.307060	7.712030	-2.109781
6	-4.093261	6.504308	-2.369287
1	-4.522881	7.165694	-3.116218
6	-4.782859	5.375725	-1.980229
1	-5.748011	5.155167	-2.421959
6	-4.240565	4.480599	-1.017052
6	-4.925530	3.283139	-0.600226
6	-6.345843	2.992850	-0.949909
6	-7.400907	3.922808	-0.624777
6	-7.174212	5.110475	0.126954
1	-6.176694	5.332084	0.485365
6	-8.205842	5.974143	0.425824
1	-8.003660	6.868082	1.008940
6	-9.524749	5.705067	-0.009965
1	-10.326297	6.398535	0.226953
6	-9.786963	4.553115	-0.715847
1	-10.798307	4.319191	-1.038084
6	-8.749120	3.632328	-1.025151
6	-9.033639	2.413588	-1.697573
1	-10.054417	2.205777	-2.005566
6	-8.039947	1.495476	-1.922015
1	-8.238096	0.541262	-2.398593
6	-6.715857	1.783588	-1.523862
6	-5.500722	-2.520715	0.012397
1	-4.885468	-2.867500	0.843764
6	-6.744190	-3.390351	-0.051629
6	-6.773338	-4.610662	0.634717
1	-5.918650	-4.899712	1.239988
6	-7.892388	-5.443550	0.544901
1	-7.904958	-6.387132	1.083668
6	-8.993666	-5.061042	-0.223993
1	-9.865767	-5.705961	-0.287914
6	-8.972026	-3.840001	-0.906869
1	-9.828187	-3.534267	-1.502488
6	-7.853193	-3.011417	-0.822429
1	-7.836404	-2.058789	-1.344906
6	-4.693186	-2.649603	-1.282698
1	-5.377067	-2.601404	-2.137180
1	-4.212850	-3.630408	-1.307221
6	-6.599692	-0.803103	1.519298
1	-7.027084	-1.776800	1.774862
6	-5.692382	-0.404837	2.686148
6	-4.803150	-1.346868	3.226462
1	-4.763249	-2.359697	2.838450
6	-3.941897	-1.003349	4.271356
1	-3.259170	-1.753439	4.652831
6	-3.966174	0.286014	4.806063
1	-3.297824	0.555146	5.619526
6	-4.860065	1.226915	4.289519
1	-4.891455	2.233069	4.699536
6	-5.714092	0.882039	3.240807
1	-6.385185	1.634632	2.841906

6	-7.775980	0.137155	1.266742
1	-8.408483	-0.270912	0.475197
1	-7.454758	1.135791	0.966168
1	-8.376648	0.232714	2.176379
6	-2.292533	-0.996239	0.432002
1	-1.455636	-0.313301	0.349526
1	-2.944081	-0.789989	1.275540
6	-2.128073	-2.372148	0.089108
1	-2.781796	-3.085507	0.570673
6	-1.243252	-2.823017	-0.891671
1	-0.430625	-2.175086	-1.193279
6	-4.001258	-0.862768	-3.645943
1	-5.056836	-1.112004	-3.584903
6	-3.100522	-1.945301	-3.681547
1	-3.519717	-2.950066	-3.652725
6	-1.693381	-1.873663	-4.241490
1	-1.741816	-1.937581	-5.339271
1	-1.160551	-2.767439	-3.910579
6	-0.892226	-0.619080	-3.832652
1	-1.026170	0.175295	-4.571269
1	0.171364	-0.864983	-3.850498
6	-1.226696	-0.054616	-2.457185
1	-0.468450	-0.176492	-1.687995
6	-2.180054	0.921798	-2.240444
1	-2.097880	1.498983	-1.325648
6	-3.067792	1.526337	-3.308944
1	-3.854518	2.091365	-2.809434
1	-2.474884	2.253665	-3.878389
6	-3.711797	0.502460	-4.268141
1	-3.079339	0.357489	-5.149647
1	-4.655296	0.917751	-4.633768
6	-1.156807	-4.202002	-1.369884
6	-2.019726	-5.229629	-0.933304
6	-0.146868	-4.525715	-2.297660
6	-1.880389	-6.524080	-1.429323
1	-2.764859	-5.031659	-0.173054
6	-0.013080	-5.820865	-2.794137
1	0.544171	-3.751747	-2.614589
6	-0.883542	-6.826106	-2.363808
1	-2.546642	-7.305318	-1.074514
1	0.772925	-6.046985	-3.509293
1	-0.780755	-7.838504	-2.744164
7	2.153132	-4.567299	-0.104633
6	3.183840	-4.984810	-1.036941
1	4.042624	-5.438756	-0.518324
1	2.776485	-5.727584	-1.732861
1	3.533729	-4.121386	-1.596498
6	1.479726	-5.629186	0.632004
1	1.572508	-6.558117	0.065025
1	1.921499	-5.783289	1.625845
1	0.416382	-5.419233	0.754865
1	-1.084845	-0.284333	4.305852
1	-0.441196	-2.456651	3.323587
35	-0.498173	2.598089	3.498033
5	-2.596648	-4.729279	2.818636
9	-1.449563	-4.702927	2.004694
9	-2.747934	-5.980731	3.412228
9	-2.492674	-3.725319	3.798074
9	-3.738601	-4.457882	1.998339

[8-9]‡ P1-C2 *endo re-re* [BF_4^-]

Number of imaginary frequencies= 1
The smallest frequencies are=-249.3050 13.4193 15.5271cm(-1)
Electronic energy= -7647.2526318
Zero-point correction= 1.772247
(Hartree/Particle)
Thermal correction to Energy= 1.896862
Thermal correction to Enthalpy= 1.897806
Thermal correction to Gibbs Free Energy= 1.604410
Sum of electronic and zero-point Energies= -7645.480385
Sum of electronic and thermal Energies= -7645.355770
Sum of electronic and thermal Enthalpies= -7645.354826
Sum of electronic and thermal Free Energies= -7645.648221
.....

Cartesian Coordinates
.....

26	7.611726	-1.586968	-1.728655
15	2.986467	0.740081	-2.364246
15	4.328100	0.390446	1.138366
6	5.915759	-0.366522	-1.834847
6	6.028085	-0.989833	-0.537017
6	5.997998	-2.402323	-0.726755
1	6.073469	-3.145396	0.054457
6	5.901720	-2.663846	-2.124815
1	5.900611	-3.640026	-2.590212
6	5.855853	-1.414174	-2.807801
1	5.798026	-1.273622	-3.877110
6	9.399457	-0.796227	-1.032063
1	9.480148	-0.008511	-0.294711
6	9.337884	-2.197585	-0.759882
1	9.351752	-2.657163	0.219341
6	9.203742	-2.883786	-2.005418
1	9.095424	-3.952841	-2.133694
6	9.184527	-1.907884	-3.048088
1	9.062240	-2.106938	-4.104652
6	9.307901	-0.619397	-2.447995
1	9.301532	0.324752	-2.975347
6	5.799770	1.103553	-2.052847
6	6.926525	1.917349	-1.859903
1	7.860837	1.438964	-1.595282
6	6.863584	3.305072	-1.976905
1	7.746201	3.906874	-1.786313
6	5.656235	3.908778	-2.320257
1	5.588053	4.988001	-2.417863
6	4.521437	3.121321	-2.518065
1	3.587732	3.610268	-2.771009
6	4.560993	1.725246	-2.366804
6	6.085247	-0.227709	0.757741
1	6.643586	0.684262	0.545250
6	6.797871	-0.957013	1.900078
1	6.819211	-0.343605	2.805469
1	6.320432	-1.907310	2.149991
1	7.828386	-1.169443	1.600081
6	1.688661	1.977452	-2.787752
6	1.266516	2.833014	-1.755133
1	1.728000	2.759295	-0.775640
6	0.281287	3.791413	-1.981579
1	-0.016613	4.454866	-1.179980
6	-0.322022	3.891407	-3.238266
1	-1.104182	4.625988	-3.406016
6	0.083079	3.040068	-4.267473
1	-0.381634	3.109322	-5.246894
6	1.087412	2.092621	-4.048633
1	1.385072	1.440210	-4.861240
6	3.097747	-0.350828	-3.831921
6	3.599090	0.083616	-5.068304
1	3.942670	1.107401	-5.187053
6	3.670387	-0.804201	-6.143207
1	4.058684	-0.464565	-7.099221
6	3.245800	-2.128954	-5.989735
1	3.304001	-2.816875	-6.828537
6	2.756947	-2.568213	-4.756948
1	2.438168	-3.599005	-4.629560
6	2.688568	-1.682993	-3.679603
1	2.363250	-2.024993	-2.702109
6	4.510013	2.204288	1.446435
6	3.326424	2.949904	1.544423
1	2.378024	2.438004	1.611121
6	3.346292	4.343964	1.523863
6	4.551633	5.033545	1.415273
1	4.567565	6.116650	1.365377
6	5.734794	4.298329	1.351091
6	5.723323	2.903740	1.374211
1	6.669473	2.384119	1.312529
6	3.829942	-0.371114	2.732694
6	3.694005	-1.769887	2.717116
1	3.961441	-2.327440	1.827291
6	3.173272	-2.439077	3.819048
6	2.733190	-1.730784	4.939116

1	2.300136	-2.251170	5.786299
6	2.849034	-0.342382	4.943700
6	3.403431	0.341079	3.857302
1	3.482255	1.421650	3.892781
29	2.624261	-0.270999	-0.376123
6	2.277302	0.429258	6.100872
6	2.986875	-3.931382	3.781604
6	2.048062	5.101540	1.597761
6	7.027364	5.049555	1.179846
9	7.036801	5.749369	0.016941
9	8.103832	4.234411	1.160264
9	7.219129	5.951123	2.169691
9	1.040953	4.416193	0.988794
9	1.652042	5.319099	2.871364
9	2.126146	6.305650	0.995192
9	2.810900	1.666848	6.207093
9	0.936415	0.589871	5.969274
9	2.477003	-0.202101	7.279651
9	3.413544	-4.516021	4.924708
9	3.662566	-4.505556	2.758198
9	1.683857	-4.271278	3.637056
6	0.566952	0.786383	1.455995
6	0.562486	-1.550874	1.516763
6	-0.123567	0.870289	2.651185
1	0.819132	1.676092	0.894469
6	-0.214172	-1.500596	2.707074
6	-0.532928	-0.296515	3.301236
6	0.801485	-2.848345	0.946875
6	1.953157	-3.207332	0.162669
8	2.702485	-2.350992	-0.410829
7	0.947738	-0.386274	0.911936
1	0.326817	-3.632349	1.510969
77	-3.225896	-1.129652	-1.655556
15	-4.957064	-0.045806	-0.643766
8	-4.817798	1.140950	0.502115
8	-5.889863	0.777600	-1.767185
7	-5.831545	-1.143078	0.259618
6	-4.281279	2.369735	0.165162
6	-2.998649	2.664883	0.676775
1	-2.516156	1.929751	1.309432
6	-2.409853	3.865904	0.370300
1	-1.433288	4.116158	0.772158
6	-3.055837	4.776478	-0.511113
6	-2.416025	5.978661	-0.918124
1	-1.438042	6.209972	-0.504212
6	-3.013134	6.828481	-1.822770
1	-2.510328	7.739907	-2.132787
6	-4.284088	6.506806	-2.356836
1	-4.743280	7.167211	-3.086887
6	-4.945321	5.364569	-1.958945
1	-5.918424	5.132157	-2.376503
6	-4.364849	4.470262	-1.017208
6	-5.024119	3.263674	-0.588128
6	-6.451718	2.962367	-0.894746
6	-7.504103	3.879949	-0.529095
6	-7.264947	5.064053	0.224883
1	-6.258382	5.292368	0.552758
6	-8.294477	5.915139	0.564796
1	-8.081927	6.806136	1.148881
6	-9.624322	5.636666	0.170003
1	-10.424594	6.319820	0.439251
6	-9.897744	4.488092	-0.537427
1	-10.916767	4.246754	-0.828839
6	-8.861726	3.580413	-0.888416
6	-9.155077	2.364752	-1.562896
1	-10.182799	2.150154	-1.842212
6	-8.160415	1.458034	-1.825054
1	-8.365276	0.506661	-2.304568
6	-6.825426	1.751268	-1.464081
6	-5.432502	-2.559105	0.024626
1	-4.779640	-2.869051	0.842711
6	-6.640133	-3.481028	0.008096
6	-6.586784	-4.710200	0.677518
1	-5.693458	-4.969671	1.238512
6	-7.670920	-5.591040	0.624936
1	-7.617810	-6.540900	1.150334
6	-8.821166	-5.249498	-0.089815
1	-9.666187	-5.931778	-0.124472
6	-8.882234	-4.020960	-0.756549
1	-9.775868	-3.746306	-1.311054
6	-7.797864	-3.144713	-0.709310
1	-7.844813	-2.186567	-1.219528
6	-4.650598	-2.685476	-1.290055
1	-5.362577	-2.707674	-2.124228
1	-4.130622	-3.647211	-1.286234
6	-6.570071	-0.877108	1.538043
1	-6.971332	-1.859877	1.801317
6	-5.656551	-0.461485	2.695713
6	-4.747551	-1.387255	3.231480
1	-4.688377	-2.397182	2.838809
6	-3.893041	-1.031649	4.278211
1	-3.198061	-1.770987	4.658585
6	-3.941034	0.254592	4.818649
1	-3.280206	0.531853	5.635771
6	-4.850948	1.181169	4.303641
1	-4.901107	2.185306	4.716873
6	-5.698934	0.823546	3.254493
1	-6.383890	1.564966	2.858624
6	-7.773099	0.037025	1.314054
1	-8.410749	-0.380801	0.531734
1	-7.480280	1.044021	1.013079
1	-8.359452	0.114062	2.234950
6	-2.311139	-0.959841	0.328847
1	-1.555216	-0.184653	0.288940
1	-2.991688	-0.851739	1.168192
6	-2.000582	-2.295620	-0.063701
1	-2.618802	-3.067723	0.373588
6	-0.828277	-2.738443	-0.736343
1	-0.178013	-1.995734	-1.177566
6	-4.006149	-0.993522	-3.712393
1	-5.051571	-1.295237	-3.697946
6	-3.046717	-2.045836	-3.667097
1	-3.432495	-3.064924	-3.639429
6	-1.639355	-1.943244	-4.228930
1	-1.659379	-2.061345	-5.324343
1	-1.073789	-2.793690	-3.841410
6	-0.905529	-0.640334	-3.854706
1	-1.046067	0.118113	-4.629967
1	0.170050	-0.833848	-3.823790
6	-1.324913	-0.048164	-2.511743
1	-0.574171	-0.081647	-1.726378
6	-2.322391	0.910210	-2.363747
1	-2.263385	1.548597	-1.488468
6	-3.200689	1.440000	-3.479623
1	-4.036223	1.966902	-3.015313
1	-2.635595	2.186920	-4.054470
6	-3.757007	0.345211	-4.413716
1	-3.081303	0.188144	-5.261319
1	-4.701036	0.697649	-4.841586
6	-0.731378	-4.088452	-1.303406
6	-1.584272	-5.143684	-0.917901
6	0.245305	-4.347434	-2.284320
6	-1.467721	-6.398210	-1.511934
1	-2.315536	-4.997241	-0.133477
6	0.359548	-5.602908	-2.878181
1	0.913077	-3.548171	-2.583476
6	-0.499718	-6.636195	-2.494529
1	-2.131111	-7.199416	-1.198464
1	1.117502	-5.773737	-3.637857
1	-0.415200	-7.617608	-2.952680
7	2.252157	-4.530482	-0.023443
6	3.393977	-4.898950	-0.846293
1	4.241228	-5.213592	-0.220944
1	3.116991	-5.737083	-1.495123
1	3.701140	-4.051739	-1.452551
6	1.600227	-5.666770	0.617084
1	1.307372	-6.389125	-0.152022
1	2.296710	-6.154055	1.309736
1	0.706581	-5.389180	1.164120
1	-1.096048	-0.260613	4.224653

1	-0.559060	-2.427135	3.149781
35	-0.470260	2.619206	3.446516
5	-2.497515	-4.782187	2.849892
9	-1.272130	-4.984560	2.180995
9	-2.845180	-5.920219	3.573885
9	-2.375170	-3.670951	3.706875
9	-3.507072	-4.507338	1.881972

---

9 P1-C2 *endo re-re* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 11.8619 14.0247 16.9918 cm(-1)
Electronic energy= -7647.2794543
Zero-point correction= 1.775431
(Hartree/Particle)
Thermal correction to Energy= 1.899614
Thermal correction to Enthalpy= 1.900559
Thermal correction to Gibbs Free Energy= 1.607571
Sum of electronic and zero-point Energies= -7645.504023
Sum of electronic and thermal Energies= -7645.379840
Sum of electronic and thermal Enthalpies= -7645.378896
Sum of electronic and thermal Free Energies= -7645.671884

.....

Cartesian Coordinates

.....

26	7.578807	-1.642230	-1.537315
15	2.989710	0.654340	-2.447610
15	4.171059	0.422766	1.131911
6	5.890055	-0.425481	-1.755560
6	5.942113	-1.010177	-0.436289
6	5.923330	-2.428140	-0.586507
1	5.966561	-3.147871	0.218092
6	5.886342	-2.730876	-1.979400
1	5.904350	-3.720378	-2.415681
6	5.873666	-1.501437	-2.699120
1	5.862090	-1.390187	-3.773363
6	9.339506	-0.819033	-0.807130
1	9.393324	0.002992	-0.105642
6	9.263748	-2.205539	-0.470535
1	9.240823	-2.617557	0.529465
6	9.178477	-2.950781	-1.685758
1	9.072330	-4.024645	-1.766685
6	9.203635	-2.026233	-2.774097
1	9.122040	-2.275358	-3.823896
6	9.305897	-0.710565	-2.232279
1	9.321018	0.207089	-2.804212
6	5.785978	1.035579	-2.033210
6	6.911173	1.854068	-1.855329
1	7.836903	1.387520	-1.544189
6	6.857626	3.233348	-2.051391
1	7.739724	3.840663	-1.877355
6	5.660867	3.823624	-2.450495
1	5.601112	4.896289	-2.606982
6	4.526072	3.031771	-2.630038
1	3.599622	3.508549	-2.928971
6	4.558609	1.645414	-2.409504
6	5.940089	-0.219688	0.842114
1	6.519935	0.681848	0.646851
6	6.584765	-0.935469	2.032594
1	6.571893	-0.305070	2.926119
1	6.084177	-1.875346	2.276869
1	7.625250	-1.165511	1.784934
6	1.695965	1.874041	-2.920564
6	1.233275	2.736559	-1.911384
1	1.663670	2.681117	-0.916428
6	0.240856	3.676239	-2.179157
1	-0.094754	4.341065	-1.394331
6	-0.325725	3.752370	-3.454448
1	-1.113959	4.472457	-3.653802
6	0.121050	2.894636	-4.460522
1	-0.316753	2.943527	-5.453377
6	1.131195	1.964132	-4.200138
1	1.459944	1.303897	-4.994322
6	3.179203	-0.455465	-3.889119
6	3.704874	-0.026935	-5.117378
1	4.003527	1.008988	-5.250695
6	3.859944	-0.937213	-6.164124
1	4.266363	-0.602880	-7.114370
6	3.497348	-2.277736	-5.989412
1	3.622044	-2.983274	-6.805925
6	2.985438	-2.710121	-4.763745
1	2.716961	-3.752392	-4.617374
6	2.832819	-1.801440	-3.715406
1	2.486921	-2.133757	-2.741814
6	4.357832	2.254692	1.321618
6	3.182740	3.013321	1.405544
1	2.229930	2.517986	1.508938
6	3.212687	4.405890	1.336587
6	4.420908	5.083562	1.200430
1	4.444879	6.164810	1.120451
6	5.597429	4.336496	1.151218
6	5.574643	2.943575	1.211451
1	6.516572	2.417504	1.147866
6	3.649542	-0.212014	2.773214
6	3.457074	-1.600350	2.844569
1	3.671303	-2.218454	1.979469
6	2.976175	-2.185941	4.012820
6	2.615827	-1.399237	5.105652
1	2.207900	-1.854969	6.001210
6	2.775883	-0.015788	5.019959
6	3.305853	0.580487	3.874639
1	3.432277	1.656112	3.843694
29	2.561950	-0.327872	-0.451923
6	2.294250	0.826814	6.169500
6	2.729338	-3.668653	4.045780
6	1.916513	5.166991	1.395461
6	6.897856	5.073646	0.975065
9	6.911795	5.776425	-0.184717
9	7.964839	4.245938	0.951378
9	7.101933	5.968989	1.968012
9	0.915541	4.471151	0.786640
9	1.510077	5.394254	2.664313
9	1.995845	6.363700	0.781647
9	2.621972	2.129105	6.031388
9	0.942994	0.763252	6.282421
9	2.798642	0.404014	7.350861
9	2.857176	-4.178687	5.287392
9	3.583743	-4.341998	3.237365
9	1.476196	-3.971803	3.622624
6	0.499137	0.742053	1.366656
6	0.379425	-1.572321	1.395885
6	-0.048468	0.822264	2.638791
1	0.726806	1.629598	0.792053
6	-0.190289	-1.547147	2.674569
6	-0.382501	-0.336316	3.330714
6	0.418409	-2.878699	0.635212
6	1.832601	-3.289984	0.243616
8	2.600890	-2.451756	-0.296655
7	0.765831	-0.435380	0.776385
1	-0.049252	-3.624803	1.270515
77	-3.233500	-1.211518	-1.728583
15	-4.937248	-0.065731	-0.690200
8	-4.767943	1.123481	0.460309
8	-5.894226	0.785143	-1.785301
7	-5.816555	-1.142405	0.241838
6	-4.220870	2.343392	0.127776
6	-2.936021	2.625087	0.643959
1	-2.462962	1.880131	1.273282
6	-2.338986	3.825570	0.353835
1	-1.366654	4.069397	0.766196
6	-2.972528	4.747838	-0.524119
6	-2.318229	5.945884	-0.920622
1	-1.338514	6.162860	-0.501792
6	-2.902705	6.806079	-1.823842
1	-2.389252	7.713586	-2.127972
6	-4.174905	6.499852	-2.364314
1	-4.624297	7.168431	-3.093097
6	-4.849621	5.362303	-1.975013
1	-5.823485	5.141846	-2.397484
6	-4.281993	4.456366	-1.036573

6	-4.955579	3.255013	-0.613923
6	-6.392198	2.982228	-0.905199
6	-7.420405	3.922991	-0.527430
6	-7.148428	5.100952	0.225551
1	-6.134367	5.305957	0.545443
6	-8.154758	5.975871	0.574798
1	-7.916132	6.861191	1.157557
6	-9.494089	5.729174	0.191504
1	-10.275946	6.430855	0.467278
6	-9.799781	4.586769	-0.512830
1	-10.826628	4.368715	-0.795241
6	-8.788366	3.655319	-0.872637
6	-9.116647	2.446074	-1.542593
1	-10.151895	2.254882	-1.811242
6	-8.145656	1.517158	-1.813441
1	-8.377238	0.570425	-2.289988
6	-6.798568	1.777767	-1.468403
6	-5.422163	-2.565963	0.030240
1	-4.743704	-2.854378	0.834622
6	-6.631003	-3.485354	0.079601
6	-6.565152	-4.686012	0.798376
1	-5.660432	-4.921640	1.351786
6	-7.650457	-5.567041	0.805937
1	-7.586318	-6.494420	1.369153
6	-8.815996	-5.253926	0.102980
1	-9.661923	-5.935984	0.114545
6	-8.890766	-4.053239	-0.611603
1	-9.796206	-3.800274	-1.157407
6	-7.805010	-3.177586	-0.624529
1	-7.862327	-2.241495	-1.173212
6	-4.676185	-2.736450	-1.302135
1	-5.412789	-2.762368	-2.116240
1	-4.188021	-3.714745	-1.284836
6	-6.527427	-0.852154	1.530156
1	-6.928378	-1.827689	1.819352
6	-5.594496	-0.419796	2.667845
6	-4.681416	-1.339773	3.205752
1	-4.638502	-2.357813	2.833519
6	-3.798870	-0.967304	4.223610
1	-3.102256	-1.704678	4.605528
6	-3.823400	0.331559	4.734398
1	-3.140654	0.623626	5.528170
6	-4.741909	1.251725	4.222134
1	-4.776175	2.265199	4.613861
6	-5.617560	0.876321	3.202270
1	-6.305758	1.614280	2.805496
6	-7.730850	0.063646	1.313264
1	-8.382401	-0.362708	0.546906
1	-7.438603	1.064522	0.992348
1	-8.302637	0.157247	2.242008
6	-2.322363	-1.168225	0.261486
1	-1.655957	-0.317010	0.330551
1	-3.037488	-1.212683	1.077933
6	-1.906067	-2.393816	-0.331685
1	-2.474984	-3.250730	0.012508
6	-0.472603	-2.785304	-0.682320
1	0.003574	-2.029585	-1.307303
6	-4.003249	-1.112794	-3.757318
1	-5.046469	-1.425657	-3.777857
6	-3.025639	-2.163666	-3.682662
1	-3.404916	-3.186337	-3.670965
6	-1.642608	-2.041738	-4.302989
1	-1.712289	-2.082865	-5.402574
1	-1.070014	-2.919917	-4.001946
6	-0.882199	-0.768940	-3.873746
1	-0.963518	0.004693	-4.643613
1	0.186429	-0.994259	-3.798067
6	-1.342296	-0.175867	-2.541636
1	-0.605246	-0.193206	-1.742714
6	-2.336164	0.798100	-2.427356
1	-2.277473	1.460247	-1.569112
6	-3.187139	1.318145	-3.571987
1	-4.027428	1.860112	-3.131764
1	-2.606774	2.050355	-4.151581
6	-3.738738	0.208343	-4.491493
1	-3.052154	0.033526	-5.328500
1	-4.673816	0.559435	-4.941316
6	-0.418895	-4.124914	-1.406619
6	-1.111881	-5.248289	-0.927803
6	0.384903	-4.279406	-2.542761
6	-1.016102	-6.477402	-1.584273
1	-1.697377	-5.179778	-0.018181
6	0.490911	-5.508344	-3.197771
1	0.923303	-3.421650	-2.924267
6	-0.215288	-6.614942	-2.721679
1	-1.561769	-7.333128	-1.195814
1	1.116297	-5.595894	-4.082570
1	-0.141264	-7.573484	-3.227923
7	2.244863	-4.560826	0.404833
6	3.536612	-4.962727	-0.150884
1	4.288747	-5.027516	0.643852
1	3.427011	-5.949007	-0.610702
1	3.861139	-4.243003	-0.896866
6	1.543747	-5.648190	1.087802
1	1.250718	-6.410097	0.359941
1	2.230281	-6.092449	1.814245
1	0.661037	-5.313803	1.617644
1	-0.802368	-0.301644	4.328040
1	-0.510501	-2.469295	3.141777
35	-0.298237	2.573876	3.449634
5	-2.545680	-4.741513	2.969434
9	-1.370089	-5.132088	2.283957
9	-3.040214	-5.810594	3.712303
9	-2.235871	-3.656912	3.815458
9	-3.506436	-4.332420	2.012291

---

8 P1-C2 *exo si-si* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 12.7735 14.9945 17.4871 cm(-1)
Electronic energy= -7647.262549
Zero-point correction= 1.773198
(Hartree/Particle)
Thermal correction to Energy= 1.898486
Thermal correction to Enthalpy= 1.899431
Thermal correction to Gibbs Free Energy= 1.603479
Sum of electronic and zero-point Energies= -7645.489351
Sum of electronic and thermal Energies= -7645.364063
Sum of electronic and thermal Enthalpies= -7645.363118
Sum of electronic and thermal Free Energies= -7645.659070

.....

Cartesian Coordinates

.....

26	8.347620	0.804018	-0.498234
15	3.406058	1.378363	-2.055140
15	4.069760	0.666804	1.566473
6	6.350822	1.309189	-0.858159
6	6.478669	0.487593	0.323294
6	7.061274	-0.755484	-0.069603
1	7.296552	-1.579029	0.590438
6	7.327388	-0.702603	-1.470191
1	7.806978	-1.475669	-2.054956
6	6.895225	0.565926	-1.955071
1	6.983524	0.918683	-2.971148
6	9.490804	2.016803	0.737052
1	9.103923	2.581513	1.574915
6	9.969326	0.671265	0.782226
1	9.997810	0.034986	1.656787
6	10.355994	0.295074	-0.540322
1	10.725727	-0.676030	-0.842217
6	10.116800	1.407367	-1.403842
1	10.275787	1.428079	-2.473950
6	9.583696	2.470883	-0.615693
1	9.274058	3.438282	-0.987042
6	5.677436	2.640304	-0.874833
6	6.296281	3.728269	-0.240281
1	7.275566	3.574181	0.195405
6	5.675025	4.972230	-0.134578
1	6.169354	5.783167	0.391121
6	4.409061	5.155113	-0.685989

1	3.905970	6.113346	-0.602866
6	3.773679	4.089693	-1.324574
1	2.781673	4.242590	-1.734919
6	4.377132	2.825305	-1.419980
6	5.955501	0.862667	1.683428
1	6.134679	1.930067	1.822131
6	6.617380	0.109423	2.840176
1	6.228830	0.451748	3.803415
1	6.451839	-0.969610	2.778228
1	7.697470	0.286703	2.817864
6	1.813532	2.121338	-2.619614
6	0.715868	2.033123	-1.748075
1	0.815408	1.496513	-0.810648
6	-0.509509	2.602820	-2.099803
1	-1.351394	2.528129	-1.422164
6	-0.659853	3.251954	-3.327130
1	-1.617686	3.687371	-3.597705
6	0.422200	3.325548	-4.208088
1	0.311539	3.821144	-5.168602
6	1.652778	2.766397	-3.856633
1	2.484272	2.836455	-4.549945
6	4.239490	0.936560	-3.632724
6	4.942071	1.870284	-4.411305
1	5.013197	2.904655	-4.087467
6	5.573926	1.468186	-5.589389
1	6.120197	2.195581	-6.183482
6	5.508280	0.132732	-6.001380
1	6.007048	-0.179046	-6.914741
6	4.802299	-0.798346	-5.235663
1	4.745398	-1.836969	-5.548991
6	4.172709	-0.397793	-4.055357
1	3.632454	-1.122652	-3.457400
6	3.345031	2.289788	2.055962
6	1.961081	2.407936	1.859268
1	1.415776	1.548166	1.482259
6	1.308390	3.612970	2.119322
6	2.021546	4.735510	2.536852
1	1.518323	5.680068	2.711481
6	3.401961	4.622512	2.706493
6	4.060742	3.411028	2.491040
1	5.130586	3.370019	2.644749
6	3.575200	-0.462813	2.930514
6	3.756386	-1.831547	2.677107
1	4.186859	-2.151627	1.735585
6	3.337838	-2.781990	3.601648
6	2.697879	-2.393844	4.780444
1	2.343258	-3.135926	5.486553
6	2.497945	-1.036077	5.020667
6	2.940594	-0.069481	4.111320
1	2.768808	0.979950	4.324353
29	3.133599	-0.168459	-0.424854
6	1.706154	-0.595731	6.219006
6	3.466664	-4.246657	3.283214
6	-0.185236	3.673445	1.959942
6	4.178963	5.858568	3.064659
9	4.120809	6.783143	2.071516
9	5.487050	5.605162	3.288566
9	3.688123	6.460693	4.173001
9	-0.598434	2.958984	0.877683
9	-0.837866	3.147396	3.026160
9	-0.643396	4.932910	1.796831
9	2.166161	0.565438	6.736829
9	0.399466	-0.376274	5.893446
9	1.708665	-1.512872	7.208113
9	3.890497	-4.954059	4.357805
9	4.337941	-4.477525	2.276874
9	2.281394	-4.788292	2.909423
6	0.853602	-1.384573	1.123069
6	1.193436	-2.687458	0.671656
6	2.239223	-3.067380	-0.192785
1	0.588723	-3.506926	1.028340
77	-3.714420	-1.126396	-1.568170
15	-5.303728	-0.272093	-0.212846
8	-5.091975	1.099167	0.689984
8	-6.653257	0.155672	-1.079585
7	-5.644338	-1.352567	1.003247
6	-4.921635	2.324301	0.060223
6	-3.646562	2.918111	0.175197
1	-2.898792	2.430991	0.787596
6	-3.391687	4.102077	-0.470790
1	-2.421705	4.578892	-0.371977
6	-4.381811	4.689900	-1.304651
6	-4.091462	5.841396	-2.085542
1	-3.098903	6.278231	-2.012285
6	-5.036312	6.380026	-2.929812
1	-4.800672	7.254123	-3.529740
6	-6.316069	5.783095	-3.026069
1	-7.051872	6.196622	-3.709784
6	-6.637058	4.678849	-2.266044
1	-7.619028	4.229467	-2.358555
6	-5.690559	4.101963	-1.374691
6	-5.985156	2.930295	-0.588382
6	-7.364279	2.381291	-0.448657
6	-8.451434	3.211081	0.015800
6	-8.259847	4.544509	0.475417
1	-7.260671	4.961456	0.499494
6	-9.320742	5.310434	0.908942
1	-9.141906	6.322502	1.260712
6	-10.636598	4.791074	0.908766
1	-11.463933	5.408894	1.245376
6	-10.856497	3.495607	0.499204
1	-11.857469	3.072342	0.514585
6	-9.782231	2.673931	0.062548
6	-10.004192	1.318927	-0.303046
1	-11.015325	0.922858	-0.276547
6	-8.951651	0.512345	-0.651156
1	-9.089169	-0.534379	-0.900977
6	-7.643319	1.044309	-0.694412
6	-4.953951	-2.661947	0.860618
1	-4.108474	-2.675879	1.552590
6	-5.868141	-3.826329	1.205686
6	-5.328219	-4.961230	1.822974
1	-4.273930	-4.982973	2.073025
6	-6.133556	-6.073080	2.081570
1	-5.697539	-6.950476	2.551626
6	-7.486825	-6.059489	1.735591
1	-8.113359	-6.922804	1.942529
6	-8.031122	-4.927596	1.120134
1	-9.083580	-4.907890	0.849285
6	-7.224962	-3.820410	0.851808
1	-7.646234	-2.937629	0.378153
6	-4.420607	-2.861136	-0.566742
1	-5.231807	-3.263954	-1.182220
1	-3.633298	-3.611644	-0.525239
6	-6.146085	-1.054092	2.386991
1	-6.530879	-2.019751	2.724479
6	-5.017813	-0.685139	3.351695
6	-4.355295	-1.713802	4.039758
1	-4.656255	-2.745312	3.874969
6	-3.324993	-1.432863	4.940983
1	-2.823719	-2.247105	5.456234
6	-2.942992	-0.111166	5.176898
1	-2.129978	0.108335	5.862623
6	-3.599742	0.923374	4.503654
1	-3.304194	1.955581	4.672627
6	-4.629177	0.639537	3.603645
1	-5.130104	1.455864	3.097798
6	-7.338596	-0.099248	2.413704
1	-8.143595	-0.486255	1.784383
1	-7.094090	0.907782	2.076136
1	-7.710203	-0.031205	3.440528
6	-2.412080	-0.715623	0.149035
1	-2.429990	0.293562	0.541676
1	-2.567977	-1.480047	0.902536
6	-1.466511	-0.976739	-0.888590
1	-0.956116	-0.126332	-1.321461
6	-1.224642	-2.248505	-1.394168
1	-1.604114	-3.100496	-0.844898
6	-5.270106	-1.506282	-3.186062
1	-6.077230	-2.024896	-2.675923

6	-4.139526	-2.281919	-3.494579
1	-4.156986	-3.325080	-3.181389
6	-3.126794	-2.002446	-4.585815
1	-3.498224	-2.422339	-5.532747
1	-2.215947	-2.554846	-4.343235
6	-2.766546	-0.515071	-4.793086
1	-3.483718	-0.043394	-5.470973
1	-1.790425	-0.465033	-5.285302
6	-2.690612	0.293277	-3.514748
1	-1.699709	0.482684	-3.127215
6	-3.726927	1.008956	-2.981936
1	-3.493762	1.752190	-2.224710
6	-5.114187	1.075771	-3.579302
1	-5.770784	1.558403	-2.858014
1	-5.081853	1.738234	-4.456238
6	-5.726228	-0.286732	-3.988504
1	-5.525703	-0.484274	-5.046760
1	-6.812427	-0.208531	-3.892312
6	-0.344074	-2.552912	-2.517181
6	0.323950	-1.565103	-3.271967
6	-0.161268	-3.904661	-2.872484
6	1.111147	-1.919347	-4.363511
1	0.242514	-0.517774	-3.005079
6	0.645558	-4.255194	-3.954269
1	-0.653343	-4.670654	-2.281850
6	1.277764	-3.265274	-4.710688
1	1.607337	-1.143596	-4.937980
1	0.780606	-5.303360	-4.205886
1	1.900045	-3.536632	-5.558907
6	2.332591	-4.455102	-0.561840
6	3.369040	-4.928663	-1.326894
1	1.554562	-5.126527	-0.215433
6	4.348957	-4.009289	-1.744609
6	4.235600	-2.682184	-1.398143
1	4.975286	-1.954717	-1.709649
7	3.211215	-2.203541	-0.659398
8	1.216446	-0.297636	0.541648
7	0.049083	-1.262226	2.234826
6	-0.505440	0.024800	2.614373
1	-1.546961	-0.099691	2.917526
1	0.040477	0.468024	3.457290
1	-0.470558	0.705783	1.771369
6	-0.303177	-2.366601	3.118956
1	-1.283542	-2.787560	2.878593
1	0.437414	-3.161757	3.057738
1	-0.319156	-1.996298	4.147642
1	3.426385	-5.977060	-1.600709
35	5.876902	-4.599218	-2.836771
5	-1.792152	-5.381195	0.739823
9	-0.417817	-5.591004	0.948880
9	-2.076357	-5.401956	-0.648042
9	-2.533022	-6.370573	1.395485
9	-2.155623	-4.106346	1.247248

[8-9]‡ P1-C2 *exo si-si* [BF_4^-]

Number of imaginary frequencies= 1
The smallest frequencies are=-162.4656 10.6070 12.7531cm(-1)
Electronic energy= -7647.2559268
Zero-point correction= 1.771823
(Hartree/Particle)
Thermal correction to Energy= 1.896472
Thermal correction to Enthalpy= 1.897416
Thermal correction to Gibbs Free Energy= 1.602470
Sum of electronic and zero-point Energies= -7645.484104
Sum of electronic and thermal Energies= -7645.359455
Sum of electronic and thermal Enthalpies= -7645.358510
Sum of electronic and thermal Free Energies= -7645.653457

.....

Cartesian Coordinates

.....

26	8.187235	0.694637	-0.695070
15	3.196836	1.523967	-2.041619
15	3.988762	0.691339	1.546762
6	6.197312	1.283858	-0.971458
6	6.338900	0.443481	0.194554
6	6.859621	-0.815714	-0.235252
1	7.091546	-1.655785	0.404975
6	7.073911	-0.754263	-1.644740
1	7.498349	-1.538242	-2.256359
6	6.669113	0.535256	-2.097850
1	6.728319	0.898629	-3.112524
6	9.432098	1.843932	0.504263
1	9.106272	2.421783	1.358994
6	9.846589	0.476942	0.524920
1	9.875586	-0.165746	1.394783
6	10.165352	0.091789	-0.813029
1	10.476378	-0.893901	-1.133290
6	9.949088	1.220491	-1.661118
1	10.070047	1.241162	-2.736196
6	9.498064	2.302856	-0.848251
1	9.223664	3.287251	-1.202240
6	5.591845	2.647136	-0.953041
6	6.294826	3.699448	-0.345910
1	7.278033	3.490830	0.055902
6	5.754986	4.979906	-0.231112
1	6.314734	5.762230	0.271791
6	4.487639	5.237631	-0.747584
1	4.048658	6.226564	-0.663320
6	3.767357	4.207993	-1.352922
1	2.775694	4.422167	-1.734010
6	4.286316	2.906525	-1.451578
6	5.882568	0.820001	1.577979
1	6.098464	1.880196	1.719047
6	6.570615	0.038313	2.700608
1	6.232936	0.382548	3.682138
1	6.374997	-1.035511	2.637184
1	7.652834	0.188134	2.632722
6	1.635130	2.387167	-2.498416
6	0.645192	2.490770	-1.507218
1	0.779922	1.981263	-0.559186
6	-0.512285	3.232812	-1.745417
1	-1.271152	3.305353	-0.977899
6	-0.710994	3.851006	-2.982080
1	-1.620377	4.416707	-3.164780
6	0.251726	3.719845	-3.985767
1	0.098143	4.186435	-4.954793
6	1.422860	2.997366	-3.744718
1	2.171711	2.920816	-4.526063
6	3.911758	1.028075	-3.657951
6	4.633902	1.912248	-4.475036
1	4.790313	2.939819	-4.159960
6	5.172888	1.467926	-5.683756
1	5.734406	2.156457	-6.308947
6	4.996248	0.139989	-6.086367
1	5.424788	-0.205313	-7.022883
6	4.269843	-0.741371	-5.281649
1	4.131653	-1.774786	-5.586667
6	3.729195	-0.297949	-4.073172
1	3.175429	-0.984814	-3.442746
6	3.339830	2.330829	2.083751
6	1.945929	2.473317	2.016774
1	1.347932	1.623129	1.706276
6	1.342656	3.694782	2.314235
6	2.112342	4.809020	2.644277
1	1.644118	5.765042	2.850839
6	3.500162	4.671065	2.687027
6	4.113975	3.444618	2.428378
1	5.192926	3.387759	2.475580
6	3.508069	-0.444336	2.912390
6	3.678293	-1.813822	2.654177
1	4.116445	-2.137087	1.717559
6	3.250806	-2.765069	3.574394
6	2.619571	-2.377143	4.757823
1	2.263311	-3.119828	5.462413
6	2.438075	-1.018998	5.007549
6	2.884147	-0.052468	4.100294
1	2.726462	0.996623	4.323147
29	2.931674	-0.027596	-0.422410
6	1.666317	-0.583807	6.222283

6	3.363026	-4.230012	3.250462
6	-0.158715	3.777002	2.308282
6	4.329392	5.893613	2.969712
9	4.191941	6.823104	1.990492
9	5.648460	5.616443	3.067326
9	3.956583	6.497282	4.122091
9	-0.696543	3.044223	1.294127
9	-0.698709	3.286214	3.449123
9	-0.611649	5.040222	2.162106
9	2.091769	0.607692	6.697005
9	0.341384	-0.432693	5.938626
9	1.745262	-1.477483	7.229617
9	3.738805	-4.953322	4.330238
9	4.260843	-4.469851	2.268460
9	2.177922	-4.739322	2.835066
6	0.677969	-1.270567	1.177577
6	0.917451	-2.569293	0.594411
6	2.068477	-2.962543	-0.158578
1	0.401173	-3.403180	1.042831
77	-3.455070	-0.845779	-1.773057
15	-5.152038	-0.274979	-0.373986
8	-5.103258	0.977913	0.723397
8	-6.511378	0.166886	-1.240667
7	-5.478535	-1.522390	0.679468
6	-4.982487	2.279268	0.266646
6	-3.764266	2.939177	0.542556
1	-3.017786	2.423006	1.133344
6	-3.559997	4.210561	0.066761
1	-2.640349	4.739585	0.297018
6	-4.533804	4.829949	-0.763739
6	-4.282972	6.086848	-1.378311
1	-3.334012	6.579124	-1.181327
6	-5.210292	6.661182	-2.218847
1	-5.003686	7.616954	-2.691570
6	-6.432642	5.996196	-2.478376
1	-7.152865	6.441056	-3.159028
6	-6.716031	4.787015	-1.880621
1	-7.653252	4.286263	-2.094800
6	-5.786642	4.168523	-0.999090
6	-6.044267	2.894135	-0.378574
6	-7.390633	2.254535	-0.391172
6	-8.549856	2.958615	0.106226
6	-8.466384	4.233380	0.734882
1	-7.497939	4.699824	0.866687
6	-9.593536	4.878291	1.197494
1	-9.495995	5.846561	1.680312
6	-10.872564	4.290161	1.058545
1	-11.752938	4.813270	1.420371
6	-10.989454	3.045903	0.481498
1	-11.961281	2.568097	0.387366
6	-9.845194	2.347005	0.010490
6	-9.962250	1.037666	-0.529227
1	-10.946573	0.585105	-0.609709
6	-8.844794	0.340985	-0.909590
1	-8.904126	-0.673962	-1.288201
6	-7.568830	0.943354	-0.811789
6	-4.688655	-2.758181	0.413115
1	-3.868470	-2.799478	1.134627
6	-5.553733	-3.998839	0.590178
6	-5.075513	-5.100293	1.308630
1	-4.097410	-5.056494	1.769836
6	-5.849039	-6.258667	1.427660
1	-5.455772	-7.105641	1.983611
6	-7.112441	-6.326521	0.837912
1	-7.715084	-7.225673	0.933785
6	-7.599735	-5.226124	0.123352
1	-8.584252	-5.267746	-0.335592
6	-6.824441	-4.073465	-0.001403
1	-7.204642	-3.215657	-0.550155
6	-4.098039	-2.741130	-1.008027
1	-4.869632	-3.097677	-1.699926
1	-3.293460	-3.476966	-1.035094
6	-6.093957	-1.451687	2.042815
1	-6.424105	-2.478272	2.222550
6	-5.074180	-1.139223	3.140576
6	-4.401815	-2.203140	3.761162
1	-4.608270	-3.221994	3.445277
6	-3.480712	-1.976508	4.787211
1	-2.970035	-2.818235	5.245967
6	-3.218392	-0.674926	5.217317
1	-2.489237	-0.493354	6.002138
6	-3.887403	0.394015	4.612675
1	-3.692134	1.412076	4.939564
6	-4.806163	0.164269	3.586363
1	-5.316323	1.005621	3.133791
6	-7.358678	-0.595863	2.107796
1	-8.085157	-0.943936	1.370109
1	-7.174538	0.464175	1.933813
1	-7.803475	-0.702915	3.101927
6	-2.122793	-0.430775	-0.106784
1	-2.001373	0.630646	0.089702
1	-2.370429	-1.004123	0.783463
6	-1.225164	-1.017665	-1.059909
1	-0.617277	-0.345212	-1.650650
6	-0.854964	-2.383825	-1.070468
1	-1.401070	-3.051295	-0.418343
6	-4.800575	-1.163012	-3.522799
1	-5.614555	-1.806495	-3.195735
6	-3.563427	-1.808932	-3.779114
1	-3.533373	-2.888391	-3.632036
6	-2.488294	-1.301972	-4.722688
1	-2.747464	-1.559427	-5.761902
1	-1.569055	-1.845685	-4.490727
6	-2.212016	0.211876	-4.612421
1	-2.849455	0.766843	-5.308004
1	-1.180214	0.409859	-4.921582
6	-2.403853	0.780013	-3.211971
1	-1.497713	1.051311	-2.687118
6	-3.574266	1.358478	-2.762647
1	-3.500153	2.051160	-1.929849
6	-4.856543	1.431744	-3.565241
1	-5.656032	1.752912	-2.897460
1	-4.749810	2.224124	-4.321429
6	-5.264786	0.104424	-4.246032
1	-4.890564	0.078095	-5.275415
1	-6.356180	0.079093	-4.320462
6	-0.161582	-3.013753	-2.188666
6	0.622143	-2.287560	-3.109824
6	-0.283358	-4.406300	-2.361685
6	1.232636	-2.931438	-4.182596
1	0.755095	-1.218195	-2.982738
6	0.327320	-5.046170	-3.440620
1	-0.858279	-4.981974	-1.643094
6	1.084260	-4.312904	-4.356964
1	1.821161	-2.355452	-4.890058
1	0.215406	-6.120152	-3.560565
1	1.558834	-4.809960	-5.198426
6	2.256502	-4.357732	-0.385367
6	3.316609	-4.824139	-1.132972
1	1.546605	-5.051274	0.049046
6	4.209800	-3.879352	-1.649771
6	4.017152	-2.535850	-1.398721
1	4.702999	-1.790058	-1.778191
7	2.971413	-2.076170	-0.682067
8	1.060425	-0.181368	0.641162
7	-0.074454	-1.205164	2.314990
6	-0.588994	0.074654	2.783076
1	-1.613008	-0.058446	3.138648
1	0.011529	0.469559	3.610156
1	-0.594615	0.788997	1.967627
6	-0.417888	-2.353322	3.153058
1	-1.407236	-2.747180	2.911794
1	0.312269	-3.152187	3.043420
1	-0.408217	-2.027380	4.195259
1	3.447746	-5.886020	-1.310372
35	5.739176	-4.440601	-2.740875
5	-1.524003	-5.572301	1.262093
9	-0.137276	-5.569175	1.517887
9	-1.782006	-6.153421	0.009164
9	-2.194153	-6.270788	2.274195

9	-1.990186	-4.227770	1.244632

---

9 P1-C2 *exo si-si* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 11.3488 13.4780 14.7365 cm(-1)
Electronic energy= -7647.2823841
Zero-point correction= 1.774828
(Hartree/Particle)
Thermal correction to Energy= 1.898964
Thermal correction to Enthalpy= 1.899908
Thermal correction to Gibbs Free Energy= 1.606673
Sum of electronic and zero-point Energies= -7645.507556
Sum of electronic and thermal Energies= -7645.383420
Sum of electronic and thermal Enthalpies= -7645.382476
Sum of electronic and thermal Free Energies= -7645.675712

.....

Cartesian Coordinates

.....

26	7.809167	0.523151	-1.410503
15	2.737231	1.862724	-1.897025
15	3.973813	0.595449	1.437647
6	5.853603	1.277276	-1.357709
6	6.088644	0.362088	-0.267855
6	6.441353	-0.904161	-0.829109
1	6.695101	-1.795510	-0.271609
6	6.457515	-0.772249	-2.250773
1	6.730350	-1.543284	-2.955660
6	6.091744	0.566163	-2.576717
1	6.030334	0.985831	-3.569877
6	9.321613	1.514625	-0.385075
1	9.181660	2.083129	0.524718
6	9.607100	0.117218	-0.463274
1	9.709951	-0.559682	0.374409
6	9.685308	-0.241010	-1.843539
1	9.852303	-1.236712	-2.232846
6	9.446152	0.934068	-2.618962
1	9.402209	0.985375	-3.698885
6	9.222348	2.018624	-1.719129
1	8.984200	3.034939	-2.001936
6	5.396966	2.684774	-1.191722
6	6.292859	3.633723	-0.673786
1	7.297306	3.309622	-0.435272
6	5.921134	4.959063	-0.455300
1	6.633539	5.660643	-0.032507
6	4.630479	5.368049	-0.780801
1	4.320874	6.396240	-0.625760
6	3.719672	4.440438	-1.284108
1	2.716030	4.777612	-1.510262
6	4.066779	3.091183	-1.474821
6	5.852409	0.695078	1.179265
1	6.102537	1.748237	1.317606
6	6.690025	-0.130116	2.159941
1	6.495118	0.168336	3.193723
1	6.488947	-1.201461	2.076333
1	7.750836	0.030763	1.944808
6	1.253311	2.943222	-2.005470
6	0.541707	3.174701	-0.818429
1	0.820739	2.645373	0.085026
6	-0.519136	4.078623	-0.796249
1	-1.050404	4.254605	0.129029
6	-0.906790	4.733467	-1.967651
1	-1.746579	5.422500	-1.951598
6	-0.221649	4.486084	-3.159650
1	-0.525041	4.983255	-4.076545
6	0.861358	3.603705	-3.178791
1	1.395807	3.435244	-4.107780
6	3.024923	1.343413	-3.630603
6	3.742338	2.109393	-4.561081
1	4.187965	3.053308	-4.260677
6	3.893740	1.652695	-5.872202
1	4.454226	2.247056	-6.588213
6	3.325881	0.436229	-6.264175
1	3.447888	0.084148	-7.284436
6	2.602861	-0.326853	-5.343196
1	2.160188	-1.272694	-5.642084
6	2.456558	0.124038	-4.030279
1	1.909934	-0.472548	-3.306423
6	3.441488	2.200068	2.171098
6	2.062041	2.326950	2.389931
1	1.414714	1.482314	2.180331
6	1.515897	3.536653	2.814832
6	2.325110	4.654390	3.006536
1	1.898282	5.602973	3.312632
6	3.696820	4.530890	2.775962
6	4.259987	3.318026	2.374510
1	5.327712	3.276161	2.202190
6	3.705343	-0.635881	2.773595
6	3.851935	-1.984849	2.409914
1	4.147338	-2.245644	1.399606
6	3.608954	-2.993069	3.338763
6	3.172944	-2.684563	4.628427
1	2.959067	-3.472761	5.341034
6	3.010505	-1.347516	4.980468
6	3.287756	-0.323882	4.070417
1	3.164987	0.707722	4.378674
29	2.561818	0.163241	-0.400475
6	2.444727	-1.007084	6.330951
6	3.726618	-4.439335	2.942540
6	0.034046	3.595636	3.067533
6	4.554499	5.757846	2.928343
9	4.212711	6.714124	2.029640
9	5.868574	5.498878	2.752687
9	4.413828	6.317165	4.152810
9	-0.663353	2.913101	2.115644
9	-0.300034	3.031851	4.251043
9	-0.443449	4.858532	3.071069
9	2.849669	0.206434	6.764535
9	1.084641	-0.973888	6.296798
9	2.786052	-1.913186	7.270720
9	4.275655	-5.184412	3.927277
9	4.485874	-4.606725	1.835886
9	2.511540	-4.977585	2.677829
6	0.529160	-1.303316	1.451053
6	0.491645	-2.512552	0.535818
6	1.774088	-2.836049	-0.193475
1	0.245106	-3.401883	1.107448
77	-3.067192	-0.452141	-1.861412
15	-4.944706	-0.200371	-0.556083
8	-5.069482	0.766573	0.803361
8	-6.219674	0.436536	-1.446711
7	-5.376813	-1.661944	0.139572
6	-4.927091	2.134554	0.670208
6	-3.764767	2.712958	1.228457
1	-3.066121	2.069292	1.749745
6	-3.558547	4.064557	1.112179
1	-2.695888	4.528939	1.579098
6	-4.454634	4.864708	0.352153
6	-4.179678	6.236088	0.098758
1	-3.278746	6.670502	0.524859
6	-5.022472	6.994554	-0.683056
1	-4.797288	8.038902	-0.878910
6	-6.181593	6.405964	-1.243508
1	-6.833653	7.000465	-1.877094
6	-6.488558	5.084880	-0.997822
1	-7.376258	4.646739	-1.439631
6	-5.646077	4.273121	-0.188268
6	-5.929089	2.884990	0.072441
6	-7.246985	2.263253	-0.241674
6	-8.473843	2.826329	0.272800
6	-8.497609	3.915910	1.189229
1	-7.563438	4.340965	1.534685
6	-9.686705	4.428538	1.662260
1	-9.670679	5.255301	2.366937
6	-10.925269	3.885395	1.247415
1	-11.854766	4.304017	1.622211
6	-10.941543	2.813070	0.384465
1	-11.882770	2.366849	0.073486
6	-9.732860	2.250226	-0.107479
6	-9.751542	1.104997	-0.948578

1	-10.707447	0.680975	-1.243258
6	-8.578945	0.521799	-1.352872
1	-8.566703	-0.375038	-1.963470
6	-7.337777	1.086119	-0.973882
6	-4.490015	-2.786182	-0.276726
1	-3.738426	-2.935106	0.505316
6	-5.267006	-4.083035	-0.444410
6	-4.708150	-5.291782	-0.010737
1	-3.754148	-5.289201	0.502748
6	-5.373884	-6.500287	-0.233256
1	-4.921878	-7.426409	0.112255
6	-6.609287	-6.515182	-0.884289
1	-7.129924	-7.454190	-1.052255
6	-7.175523	-5.310283	-1.315477
1	-8.138626	-5.311637	-1.819700
6	-6.507458	-4.104476	-1.099951
1	-6.947841	-3.166642	-1.429191
6	-3.778917	-2.458793	-1.598183
1	-4.488591	-2.648576	-2.413249
1	-2.971166	-3.177244	-1.725410
6	-6.132991	-1.898680	1.410968
1	-6.453759	-2.940247	1.324562
6	-5.235408	-1.838718	2.648364
6	-4.566838	-3.004736	3.049848
1	-4.703152	-3.920580	2.483465
6	-3.723656	-3.011804	4.162712
1	-3.197626	-3.924881	4.423137
6	-3.546298	-1.843970	4.907038
1	-2.891838	-1.841622	5.774712
6	-4.218012	-0.676864	4.528280
1	-4.093386	0.234748	5.107266
6	-5.053629	-0.673972	3.409247
1	-5.563324	0.239781	3.128946
6	-7.418210	-1.079829	1.523887
1	-8.056112	-1.262976	0.656083
1	-7.242054	-0.007053	1.596835
1	-7.960734	-1.397159	2.419924
6	-1.897152	-0.192854	-0.027378
1	-1.677096	0.862166	0.115747
1	-2.303314	-0.670183	0.863502
6	-1.083974	-0.974413	-0.897089
1	-0.281297	-0.461429	-1.419320
6	-0.763794	-2.394519	-0.491535
1	-1.591683	-2.762097	0.111032
6	-4.104434	-0.435110	-3.777362
1	-4.946481	-1.124974	-3.748837
6	-2.810751	-1.031526	-3.961387
1	-2.780037	-2.116683	-4.059004
6	-1.666615	-0.332670	-4.677717
1	-1.847022	-0.315288	-5.764872
1	-0.764377	-0.932771	-4.531394
6	-1.410246	1.095634	-4.158996
1	-1.916014	1.833269	-4.791299
1	-0.342536	1.322350	-4.234393
6	-1.842061	1.308231	-2.709487
1	-1.030017	1.464734	-2.009094
6	-3.086115	1.814722	-2.334479
1	-3.140676	2.347448	-1.389347
6	-4.214962	2.101741	-3.307423
1	-5.121252	2.274465	-2.723605
1	-4.002209	3.041430	-3.840858
6	-4.472244	0.955965	-4.313104
1	-3.929494	1.142463	-5.247314
1	-5.534328	0.959244	-4.579828
6	-0.543788	-3.372535	-1.632488
6	0.050465	-2.969383	-2.834635
6	-0.884491	-4.724709	-1.476360
6	0.310235	-3.888182	-3.853153
1	0.310824	-1.928141	-2.974124
6	-0.631853	-5.646154	-2.494654
1	-1.346724	-5.055334	-0.554012
6	-0.028304	-5.234207	-3.686017
1	0.773480	-3.552127	-4.777431
1	-0.906643	-6.687959	-2.353109
1	0.171221	-5.951697	-4.477277
6	2.127499	-4.191683	-0.275767
6	3.148817	-4.601596	-1.120768
1	1.569378	-4.919444	0.299182
6	3.796925	-3.618187	-1.858959
6	3.463206	-2.282297	-1.695571
1	3.976449	-1.498633	-2.236398
7	2.472542	-1.894941	-0.865455
8	0.918664	-0.188183	1.027578
7	0.023959	-1.416273	2.696438
6	-0.324970	-0.201477	3.433940
1	-1.192247	-0.419764	4.060925
1	0.495730	0.134324	4.073791
1	-0.587181	0.589007	2.734620
6	-0.167576	-2.674658	3.427275
1	-1.194931	-3.024333	3.347420
1	0.501336	-3.451332	3.064814
1	0.073932	-2.486575	4.475720
1	3.408641	-5.650228	-1.211364
35	5.169165	-4.124038	-3.154642
5	-1.443388	-5.546525	2.095143
9	-0.050147	-5.512520	1.847705
9	-2.017197	-6.626240	1.411755
9	-1.677148	-5.637292	3.474485
9	-2.019026	-4.342926	1.606013

---

8 P1-C2 *exo re-si* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are=9.4809 13.0403 16.2326 cm(-1)
Electronic energy= -7647.2412462
Zero-point correction= 1.770572
(Hartree/Particle)
Thermal correction to Energy= 1.896360
Thermal correction to Enthalpy= 1.897304
Thermal correction to Gibbs Free Energy= 1.599230
Sum of electronic and zero-point Energies= -7645.470674
Sum of electronic and thermal Energies= -7645.344886
Sum of electronic and thermal Enthalpies= -7645.343942
Sum of electronic and thermal Free Energies= -7645.642016

.....

Cartesian Coordinates

.....

77	-4.141716	0.269213	1.775798
15	-5.896433	0.711160	0.437980
8	-6.270248	-0.134354	-0.920838
8	-7.321327	0.551700	1.284219
7	-5.734748	2.245503	-0.211171
6	-6.923900	-1.362609	-0.891686
6	-6.172041	-2.463641	-1.345137
1	-5.167802	-2.287622	-1.703182
6	-6.735463	-3.713884	-1.333537
1	-6.161656	-4.562909	-1.691673
6	-8.051048	-3.903291	-0.828754
6	-8.618320	-5.202826	-0.731700
1	-8.027132	-6.050134	-1.069022
6	-9.879210	-5.389539	-0.211407
1	-10.299209	-6.388488	-0.137642
6	-10.625036	-4.275655	0.242709
1	-11.610630	-4.427519	0.673672
6	-10.111359	-3.000093	0.149006
1	-10.693564	-2.159609	0.508741
6	-8.820080	-2.766511	-0.401274
6	-8.252701	-1.446484	-0.508288
6	-9.032194	-0.207558	-0.229465
6	-10.258471	0.095661	-0.922688
6	-10.758619	-0.708181	-1.985688
1	-10.200158	-1.581320	-2.300131
6	-11.930921	-0.384214	-2.633322
1	-12.284867	-1.011076	-3.446786
6	-12.673389	0.760143	-2.256279
1	-13.599353	0.998788	-2.771392
6	-12.206969	1.575601	-1.250486
1	-12.754409	2.470115	-0.964982
6	-10.992235	1.280080	-0.573474
6	-10.480403	2.154963	0.422644

1	-11.047122	3.042983	0.687882
6	-9.269100	1.900890	1.016535
1	-8.839997	2.570871	1.753886
6	-8.552228	0.736739	0.664254
6	-4.666073	3.028543	0.463979
1	-3.768059	2.987636	-0.165481
6	-5.050879	4.486998	0.637547
6	-4.111467	5.490975	0.375028
1	-3.129544	5.216754	-0.003899
6	-4.428864	6.835362	0.587693
1	-3.690250	7.604495	0.378894
6	-5.695852	7.189144	1.056632
1	-5.947285	8.234018	1.215598
6	-6.642826	6.191677	1.312691
1	-7.633250	6.461181	1.669674
6	-6.321291	4.850125	1.107235
1	-7.059285	4.073740	1.289091
6	-4.351129	2.398969	1.825522
1	-5.156473	2.654770	2.525508
1	-3.439172	2.845749	2.225591
6	-6.079863	2.757149	-1.580648
1	-6.207587	3.831628	-1.421736
6	-4.909838	2.591359	-2.548378
6	-4.207257	3.723000	-2.984425
1	-4.510848	4.706948	-2.634677
6	-3.117706	3.599475	-3.852680
1	-2.584712	4.488645	-4.178759
6	-2.703888	2.336358	-4.282004
1	-1.839601	2.232568	-4.931537
6	-3.398208	1.201393	-3.853766
1	-3.077264	0.210371	-4.152396
6	-4.495436	1.330657	-3.003264
1	-5.014091	0.439878	-2.675593
6	-7.408703	2.266440	-2.160089
1	-8.222824	2.422031	-1.449311
1	-7.388417	1.217463	-2.450756
1	-7.621010	2.860967	-3.054285
6	-3.001061	0.081161	-0.053545
1	-3.111750	-0.888476	-0.525390
1	-3.138924	0.903864	-0.752453
6	-1.908139	0.212289	0.885237
1	-1.448014	-0.684310	1.273998
6	-1.368270	1.432499	1.241842
1	-1.773644	2.314289	0.753180
6	-5.358103	0.135314	3.687371
1	-6.013812	1.002279	3.681913
6	-4.011191	0.375440	4.019032
1	-3.741784	1.400811	4.272600
6	-3.008320	-0.655751	4.508159
1	-3.100380	-0.770858	5.599058
1	-2.008289	-0.245535	4.330118
6	-3.111309	-2.037638	3.826578
1	-3.837070	-2.666138	4.350358
1	-2.146228	-2.546097	3.919719
6	-3.477812	-1.983022	2.348574
1	-2.685651	-2.228066	1.648112
6	-4.760676	-2.051684	1.840825
1	-4.847788	-2.347986	0.800294
6	-6.036241	-2.132056	2.650055
1	-6.867793	-1.882583	1.988182
1	-6.189428	-3.175125	2.962774
6	-6.076286	-1.199607	3.880077
1	-5.655681	-1.705023	4.754358
1	-7.123494	-0.994050	4.121562
6	-0.340865	1.689114	2.229690
6	0.302667	0.666816	2.961754
6	0.034311	3.028279	2.474805
6	1.287432	0.976550	3.894627
1	0.043029	-0.370574	2.787873
6	1.009936	3.334865	3.418507
1	-0.444617	3.822534	1.908238
6	1.642563	2.309645	4.128375
1	1.790609	0.179664	4.434383
1	1.292004	4.368809	3.591394
1	2.418670	2.543748	4.849733
26	7.177306	3.404227	-2.216491
15	5.161368	1.148804	2.011169
15	4.736900	-0.607663	-1.314567
6	6.602436	2.210473	-0.597654
6	5.909589	1.820966	-1.803841
6	5.159889	2.946245	-2.258744
1	4.540522	2.973072	-3.144875
6	5.403333	4.034985	-1.372796
1	5.008929	5.036906	-1.473538
6	6.294908	3.587754	-0.356199
1	6.686128	4.182705	0.455537
6	8.774708	2.797737	-3.396402
1	9.048500	1.767459	-3.581114
6	7.854650	3.572031	-4.167669
1	7.303865	3.229926	-5.033601
6	7.753423	4.864550	-3.567794
1	7.108389	5.668656	-3.897033
6	8.611342	4.890490	-2.426049
1	8.730218	5.716581	-1.737424
6	9.242936	3.615210	-2.320379
1	9.928200	3.313684	-1.539996
6	7.403323	1.288105	0.259398
6	8.659000	0.847028	-0.184226
1	9.026714	1.219381	-1.132409
6	9.423430	-0.060154	0.549558
1	10.378424	-0.401434	0.163223
6	8.942767	-0.535960	1.767159
1	9.522963	-1.245668	2.348658
6	7.695836	-0.113265	2.229773
1	7.328975	-0.502171	3.173105
6	6.903536	0.777777	1.489743
6	5.922352	0.431579	-2.378725
1	6.910189	0.020548	-2.171276
6	5.704153	0.365935	-3.893099
1	5.729938	-0.667501	-4.249851
1	4.750855	0.803058	-4.198193
1	6.501198	0.926753	-4.390813
6	4.937219	0.267595	3.615544
6	4.733906	-1.122673	3.572693
1	4.798548	-1.645532	2.624918
6	4.456903	-1.841982	4.734627
1	4.315274	-2.916159	4.678128
6	4.355386	-1.176167	5.960280
1	4.125164	-1.731443	6.865120
6	4.551563	0.204953	6.014286
1	4.476116	0.729931	6.962562
6	4.847870	0.923140	4.852046
1	4.996938	1.995143	4.915424
6	5.213467	2.920925	2.484912
6	6.318849	3.485198	3.141478
1	7.171826	2.864481	3.401753
6	6.332343	4.847327	3.444466
1	7.190990	5.280841	3.949657
6	5.243097	5.653377	3.093275
1	5.258246	6.715086	3.324008
6	4.141171	5.093060	2.442796
1	3.297655	5.717834	2.161605
6	4.123743	3.730047	2.136193
1	3.290980	3.294541	1.593780
6	5.752100	-2.032678	-0.716601
6	5.162290	-2.872391	0.239744
1	4.123279	-2.732966	0.512572
6	5.902113	-3.878709	0.862159
6	7.250496	-4.060127	0.564272
1	7.832151	-4.820629	1.073134
6	7.838713	-3.229381	-0.388334
6	7.100876	-2.239239	-1.035216
1	7.605310	-1.624840	-1.767148
6	3.482029	-1.362222	-2.433794
6	2.613992	-0.474753	-3.095444
1	2.774286	0.593914	-3.029486
6	1.505073	-0.955455	-3.781864
6	1.198265	-2.318825	-3.789974
1	0.281528	-2.680283	-4.239592
6	2.062571	-3.196293	-3.145544

6	3.204273	-2.731447	-2.483341
1	3.847425	-3.448738	-1.986121
29	3.662128	0.519851	0.437594
6	1.717127	-4.655047	-3.039790
6	0.529525	-0.009282	-4.420887
6	5.224090	-4.780163	1.856698
6	9.305570	-3.401788	-0.674721
9	10.049613	-3.243232	0.448381
9	9.767301	-2.515143	-1.583937
9	9.581928	-4.640566	-1.144573
9	4.291128	-4.111356	2.579839
9	4.582943	-5.805371	1.250213
9	6.097444	-5.321238	2.733114
9	2.813514	-5.438899	-3.200986
9	1.210715	-4.956791	-1.819427
9	0.807025	-5.040692	-3.955995
9	0.335657	-0.285439	-5.731431
9	0.919541	1.285181	-4.341917
9	-0.689679	-0.092499	-3.830264
6	1.874585	-1.789367	1.191959
6	0.907024	-0.338292	-0.388054
6	0.977811	-2.795576	0.889656
1	2.616393	-1.913452	1.973061
6	0.032940	-1.400789	-0.784025
6	0.060809	-2.624650	-0.155763
1	-0.674470	-1.231693	-1.585849
6	0.684815	0.945378	-0.945098
6	1.431993	2.131726	-0.722503
8	2.574363	2.173371	-0.157539
7	1.876185	-0.601501	0.554092
1	-0.161002	0.993937	-1.613735
7	0.891450	3.345345	-1.126835
6	1.751863	4.516693	-1.211156
1	2.072683	4.709165	-2.247087
1	1.213303	5.402347	-0.854509
1	2.635365	4.361635	-0.596486
6	-0.348116	3.421908	-1.885994
1	-1.141917	2.844549	-1.407850
1	-0.673388	4.464574	-1.928358
1	-0.233799	3.055416	-2.914012
1	-0.620298	-3.405540	-0.461675
35	0.982782	-4.467808	1.918132
5	-2.835452	-3.105356	-2.258942
9	-3.784591	-3.982221	-2.803202
9	-1.538565	-3.464082	-2.662857
9	-2.924079	-3.150083	-0.843303
9	-3.114385	-1.782955	-2.684941

[8-9]‡ P1-C2 *exo re-si* [BF_4^-]

Number of imaginary frequencies= 1
The smallest frequencies are : -36.1005 8.4397 11.3461 cm(-1)
Electronic energy= -7647.2408933
Zero-point correction= 1.769999
(Hartree/Particle)
Thermal correction to Energy= 1.895171
Thermal correction to Enthalpy= 1.896115
Thermal correction to Gibbs Free Energy= 1.599819
Sum of electronic and zero-point Energies= -7645.470895
Sum of electronic and thermal Energies= -7645.345723
Sum of electronic and thermal Enthalpies= -7645.344778
Sum of electronic and thermal Free Energies= -7645.641074

.....

Cartesian Coordinates

.....

77	-4.138918	0.209671	1.785793
15	-5.846176	0.797364	0.424896
8	-6.258386	0.011679	-0.966521
8	-7.299465	0.706495	1.238304
7	-5.571567	2.332004	-0.193111
6	-6.876697	-1.232643	-0.946152
6	-6.105527	-2.313913	-1.418234
1	-5.110165	-2.115469	-1.793979
6	-6.636168	-3.578579	-1.392857
1	-6.045133	-4.411987	-1.758632
6	-7.933167	-3.801194	-0.853811
6	-8.459351	-5.115932	-0.732792
1	-7.852718	-5.948023	-1.080431
6	-9.698891	-5.335961	-0.175283
1	-10.086469	-6.346353	-0.082209
6	-10.464429	-4.241142	0.292173
1	-11.432140	-4.418811	0.752875
6	-9.991827	-2.951640	0.174715
1	-10.588032	-2.125656	0.545231
6	-8.723559	-2.684439	-0.412139
6	-8.195179	-1.349953	-0.537068
6	-9.000665	-0.127510	-0.254306
6	-10.250046	0.129195	-0.926781
6	-10.748825	-0.705401	-1.966723
1	-10.169993	-1.564443	-2.282941
6	-11.946521	-0.430255	-2.590313
1	-12.298285	-1.081002	-3.385816
6	-12.717916	0.694176	-2.211919
1	-13.663632	0.894179	-2.707236
6	-12.254220	1.539425	-1.229742
1	-12.823588	2.419892	-0.943198
6	-11.014813	1.293996	-0.578154
6	-10.509695	2.200356	0.392729
1	-11.098814	3.074034	0.657108
6	-9.279490	1.992331	0.964119
1	-8.855167	2.686475	1.682118
6	-8.532110	0.844961	0.616981
6	-4.406620	2.999043	0.451295
1	-3.535264	2.858968	-0.201382
6	-4.620932	4.492116	0.622766
6	-3.579805	5.380347	0.327863
1	-2.646084	4.992895	-0.073628
6	-3.733959	6.753056	0.540105
1	-2.917676	7.431035	0.305694
6	-4.938128	7.252479	1.041356
1	-5.063088	8.319925	1.200191
6	-5.985765	6.371706	1.331256
1	-6.927593	6.754727	1.714916
6	-5.826554	5.001064	1.126570
1	-6.642749	4.314934	1.337408
6	-4.121559	2.350633	1.811573
1	-4.882138	2.692294	2.525887
1	-3.162333	2.716405	2.182974
6	-5.923759	2.904145	-1.534256
1	-5.973244	3.980489	-1.347864
6	-4.806410	2.690704	-2.554913
6	-4.101052	3.797679	-3.045494
1	-4.352918	4.792772	-2.686713
6	-3.073052	3.637082	-3.980559
1	-2.537390	4.508703	-4.347204
6	-2.723166	2.360295	-4.424863
1	-1.906247	2.226788	-5.128424
6	-3.419883	1.249271	-3.941274
1	-3.146964	0.247451	-4.253224
6	-4.454602	1.414869	-3.021921
1	-4.979922	0.543081	-2.657409
6	-7.301819	2.519234	-2.080098
1	-8.080990	2.712777	-1.339470
1	-7.362232	1.478036	-2.392258
1	-7.501689	3.147748	-2.953621
6	-2.969313	-0.094161	-0.004338
1	-3.119356	-1.077021	-0.435260
1	-3.044990	0.703353	-0.741107
6	-1.931653	0.034606	0.991935
1	-1.530367	-0.860526	1.446983
6	-1.253996	1.233655	1.219876
1	-1.593933	2.104422	0.670103
6	-5.371269	0.215089	3.674504
1	-5.946525	1.137964	3.664991
6	-4.008345	0.335378	4.023921
1	-3.652862	1.333691	4.279784
6	-3.115907	-0.780063	4.543169
1	-3.247156	-0.890766	5.630949
1	-2.078611	-0.461283	4.391752
6	-3.324966	-2.143590	3.848962

1	-4.105096	-2.714746	4.360970
1	-2.406502	-2.731893	3.945620
6	-3.673729	-2.044405	2.366822
1	-2.899770	-2.360050	1.672996
6	-4.961578	-2.018014	1.858859
1	-5.078330	-2.319362	0.823023
6	-6.235168	-2.004664	2.676729
1	-7.050967	-1.713356	2.013681
1	-6.453869	-3.030355	3.008207
6	-6.206764	-1.048244	3.888272
1	-5.838517	-1.570596	4.776665
1	-7.234246	-0.748628	4.116596
6	-0.297213	1.499410	2.273134
6	0.282825	0.480811	3.061866
6	0.074003	2.838268	2.525735
6	1.202793	0.794640	4.057919
1	0.026584	-0.556224	2.880618
6	0.976719	3.149145	3.538087
1	-0.355000	3.628687	1.915898
6	1.550615	2.127874	4.301737
1	1.661258	0.000797	4.640409
1	1.250859	4.183437	3.721104
1	2.274360	2.365471	5.074822
26	6.958836	3.500910	-2.218676
15	5.105058	1.147570	2.035187
15	4.654419	-0.587653	-1.304054
6	6.451843	2.280096	-0.596960
6	5.740069	1.885194	-1.790663
6	4.952474	2.995440	-2.217489
1	4.315492	3.016630	-3.091274
6	5.191303	4.082183	-1.327402
1	4.771029	5.075278	-1.409692
6	6.116786	3.647403	-0.335442
1	6.512018	4.244831	0.472515
6	8.537814	2.937790	-3.443822
1	8.826814	1.914832	-3.644653
6	7.583744	3.700083	-4.184972
1	7.019097	3.354862	-5.040675
6	7.471928	4.985070	-3.571285
1	6.804931	5.779684	-3.879010
6	8.357265	5.018503	-2.451007
1	8.477408	5.841258	-1.758635
6	9.016405	3.755359	-2.372445
1	9.727585	3.461449	-1.612677
6	7.295321	1.365250	0.227865
6	8.547600	0.957385	-0.255492
1	8.881484	1.352906	-1.206391
6	9.348639	0.052141	0.440581
1	10.299027	-0.263573	0.022545
6	8.909740	-0.455023	1.661245
1	9.518560	-1.163679	2.214214
6	7.668152	-0.064524	2.164519
1	7.334656	-0.476941	3.110221
6	6.839283	0.823527	1.461882
6	5.780091	0.503298	-2.380282
1	6.783634	0.121494	-2.194932
6	5.535388	0.445121	-3.890663
1	5.585055	-0.583572	-4.258395
1	4.564127	0.856576	-4.174229
1	6.306058	1.034327	-4.396745
6	4.937504	0.240799	3.630957
6	4.783471	-1.155611	3.577101
1	4.855220	-1.667987	2.623872
6	4.548659	-1.894501	4.735866
1	4.445035	-2.972623	4.671318
6	4.440930	-1.243367	5.968967
1	4.243983	-1.814420	6.871795
6	4.587728	0.143450	6.033322
1	4.506576	0.656767	6.987473
6	4.841102	0.882437	4.874003
1	4.949517	1.958919	4.944298
6	5.127266	2.914822	2.525822
6	6.238528	3.501521	3.151868
1	7.113961	2.900560	3.381663
6	6.228526	4.862044	3.462077
1	7.091796	5.313616	3.942914
6	5.110074	5.643603	3.149410
1	5.107415	6.704258	3.385214
6	4.001412	5.060244	2.531479
1	3.134295	5.665721	2.281721
6	4.007810	3.698897	2.217676
1	3.168013	3.244726	1.702928
6	5.727055	-1.995028	-0.768366
6	5.203799	-2.861451	0.202539
1	4.173781	-2.757068	0.520122
6	6.000179	-3.848678	0.784602
6	7.339194	-3.986443	0.426934
1	7.966259	-4.730151	0.905928
6	7.859389	-3.133335	-0.545204
6	7.065101	-2.160803	-1.150332
1	7.518268	-1.528852	-1.901017
6	3.388776	-1.345629	-2.404326
6	2.488119	-0.461315	-3.023945
1	2.627618	0.608690	-2.930705
6	1.381978	-0.949636	-3.709491
6	1.110439	-2.319792	-3.754224
1	0.199798	-2.693072	-4.205897
6	2.004426	-3.193220	-3.144871
6	3.144108	-2.719336	-2.485686
1	3.814116	-3.433017	-2.019571
29	3.592168	0.489857	0.488194
6	1.700684	-4.664747	-3.084319
6	0.372018	-0.006056	-4.296542
6	5.396980	-4.777094	1.802720
6	9.317717	-3.255797	-0.894226
9	10.100594	-3.087603	0.200546
9	9.712998	-2.342409	-1.808188
9	9.613718	-4.478232	-1.393033
9	4.454193	-4.151236	2.550964
9	4.790488	-5.836368	1.220247
9	6.322275	-5.269153	2.654499
9	2.821141	-5.409846	-3.264324
9	1.200134	-5.018319	-1.875974
9	0.807065	-5.048614	-4.016431
9	0.085243	-0.298116	-5.585337
9	0.780494	1.286036	-4.262770
9	-0.802355	-0.067633	-3.621260
6	1.913791	-1.902400	1.207493
6	0.828406	-0.445491	-0.277713
6	1.057618	-2.940544	0.887495
1	2.684276	-2.018161	1.961411
6	-0.014706	-1.522540	-0.684399
6	0.092124	-2.770546	-0.109775
1	-0.757418	-1.354096	-1.453086
6	0.511265	0.856949	-0.758488
6	1.261696	2.060018	-0.588549
8	2.408959	2.115419	-0.045789
7	1.834344	-0.690847	0.623074
1	-0.325435	0.879103	-1.438411
7	0.697988	3.253602	-1.005667
6	1.526380	4.451622	-1.049133
1	1.899111	4.646083	-2.066253
1	0.936896	5.318996	-0.732171
1	2.378182	4.330525	-0.384637
6	-0.509378	3.305031	-1.822666
1	-1.307059	2.689624	-1.404735
1	-0.869482	4.335708	-1.855307
1	-0.327962	2.971855	-2.850805
1	-0.566953	-3.567534	-0.423599
35	1.189766	-4.653730	1.831457
5	-2.780039	-3.230597	-2.259127
9	-3.780242	-4.036149	-2.823726
9	-1.505662	-3.656518	-2.674348
9	-2.866462	-3.305113	-0.846759
9	-2.974932	-1.884901	-2.658534

---

9 P1-C2 *exo re-si* [BF_4^-]

Number of imaginary frequencies= 0
The smallest frequencies are= 5.7186 8.1984 12.4651 cm(-1)

Electronic energy= -7647.2701262
Zero-point correction= 1.773081
(Hartree/Particle)
Thermal correction to Energy= 1.897970
Thermal correction to Enthalpy= 1.898914
Thermal correction to Gibbs Free Energy= 1.600729
Sum of electronic and zero-point Energies= -7645.497045
Sum of electronic and thermal Energies= -7645.372156
Sum of electronic and thermal Enthalpies= -7645.371212
Sum of electronic and thermal Free Energies= -7645.669398
.....
Cartesian Coordinates
.....

77	-3.995098	0.333145	1.761801
15	-5.763899	0.799999	0.370302
8	-6.214703	-0.092475	-0.962086
8	-7.235918	0.795504	1.183392
7	-5.486396	2.271402	-0.394256
6	-6.747038	-1.360780	-0.793652
6	-5.928385	-2.444155	-1.176705
1	-4.956307	-2.233532	-1.603791
6	-6.386493	-3.726084	-1.006241
1	-5.764324	-4.561335	-1.311672
6	-7.651831	-3.961018	-0.400291
6	-8.099871	-5.282268	-0.128499
1	-7.458459	-6.112750	-0.411976
6	-9.307778	-5.509037	0.492432
1	-9.635125	-6.523685	0.700373
6	-10.119087	-4.413923	0.874651
1	-11.060898	-4.594364	1.385346
6	-9.723159	-3.120344	0.610535
1	-10.351828	-2.291739	0.916216
6	-8.490290	-2.848409	-0.045322
6	-8.043468	-1.508715	-0.327474
6	-8.910808	-0.307059	-0.160659
6	-10.188054	-0.201619	-0.822713
6	-10.658135	-1.177312	-1.747285
1	-10.034499	-2.031440	-1.980541
6	-11.883674	-1.045908	-2.364118
1	-12.211671	-1.803162	-3.070652
6	-12.714315	0.067429	-2.094163
1	-13.680780	0.154259	-2.582213
6	-12.281368	1.045117	-1.227452
1	-12.896716	1.918392	-1.025979
6	-11.015720	0.948375	-0.587548
6	-10.545618	1.987511	0.260068
1	-11.181913	2.849111	0.442707
6	-9.292426	1.918138	0.813863
1	-8.897300	2.713148	1.437922
6	-8.478199	0.786038	0.578787
6	-4.306448	2.999695	0.146086
1	-3.480586	2.861630	-0.564524
6	-4.581168	4.490724	0.275586
6	-3.578769	5.420986	-0.022582
1	-2.622467	5.071387	-0.401670
6	-3.791076	6.789251	0.167674
1	-3.000603	7.496355	-0.069769
6	-5.017937	7.246287	0.653176
1	-5.188722	8.309691	0.795886
6	-6.027791	6.324859	0.949974
1	-6.987368	6.671768	1.324267
6	-5.809416	4.959564	0.765908
1	-6.596275	4.243506	0.986928
6	-3.876169	2.449181	1.518133
1	-4.523066	2.903233	2.280054
1	-2.867845	2.814273	1.724312
6	-5.889461	2.745533	-1.754530
1	-5.919883	3.834530	-1.655725
6	-4.826218	2.440274	-2.811822
6	-4.194084	3.497709	-3.480230
1	-4.456435	4.522398	-3.226585
6	-3.228324	3.252747	-4.462904
1	-2.749986	4.088143	-4.967633
6	-2.866340	1.941338	-4.778572
1	-2.095906	1.743875	-5.519046
6	-3.488443	0.879305	-4.115936
1	-3.203248	-0.145798	-4.325473
6	-4.460232	1.127595	-3.147457
1	-4.927747	0.294792	-2.641379
6	-7.294656	2.338853	-2.209298
1	-8.038216	2.609354	-1.455856
1	-7.380869	1.274617	-2.421814
1	-7.525059	2.890936	-3.126031
6	-2.910835	-0.219864	-0.050551
1	-3.110559	-1.249160	-0.320626
1	-3.019447	0.469824	-0.886365
6	-1.939210	0.085844	0.947641
1	-1.479704	-0.752053	1.460525
6	-0.968875	1.225750	0.696271
1	-1.519373	2.052136	0.242447
6	-4.984176	0.661862	3.677361
1	-5.488729	1.627103	3.675726
6	-3.559801	0.696787	3.862551
1	-3.109636	1.680521	4.001709
6	-2.762823	-0.416771	4.525801
1	-2.903115	-0.394426	5.618739
1	-1.704811	-0.205989	4.349168
6	-3.092478	-1.824201	3.982560
1	-3.843470	-2.310807	4.613540
1	-2.197667	-2.453291	4.043826
6	-3.583427	-1.832094	2.536397
1	-2.904469	-2.275937	1.811787
6	-4.922605	-1.780849	2.166611
1	-5.180256	-2.210105	1.204174
6	-6.088451	-1.594950	3.119648
1	-6.961256	-1.332065	2.518512
1	-6.317668	-2.556790	3.603710
6	-5.863154	-0.492791	4.176274
1	-5.425261	-0.920064	5.085669
1	-6.838058	-0.092664	4.475114
6	-0.275476	1.767011	1.929635
6	0.249334	0.931642	2.927466
6	-0.154228	3.155127	2.097737
6	0.881831	1.465974	4.051568
1	0.162480	-0.143405	2.832946
6	0.461272	3.694981	3.229583
1	-0.556197	3.819339	1.336618
6	0.988409	2.850336	4.208666
1	1.290807	0.799506	4.805312
1	0.535826	4.772716	3.341709
1	1.478461	3.265215	5.084771
26	6.760541	3.437716	-2.279128
15	4.829607	1.344279	2.062250
15	4.590684	-0.693777	-1.163678
6	6.229412	2.322296	-0.593033
6	5.566682	1.822560	-1.775131
6	4.769542	2.877413	-2.308813
1	4.163923	2.819122	-3.202333
6	4.949862	4.031266	-1.491828
1	4.507479	5.003971	-1.658624
6	5.851199	3.694488	-0.441496
1	6.202810	4.359042	0.333258
6	8.386555	2.838295	-3.423090
1	8.701569	1.811983	-3.558108
6	7.442278	3.539808	-4.233968
1	6.910554	3.136623	-5.085488
6	7.288700	4.854031	-3.696046
1	6.616278	5.617142	-4.065583
6	8.138124	4.966183	-2.553184
1	8.221798	5.827866	-1.904173
6	8.817278	3.722622	-2.385225
1	9.509980	3.484505	-1.589631
6	7.069813	1.491044	0.316315
6	8.335056	1.061174	-0.111596
1	8.683463	1.384210	-1.084761
6	9.129950	0.219704	0.666592
1	10.087381	-0.124243	0.288711
6	8.677592	-0.185277	1.920306
1	9.286680	-0.834244	2.542571
6	7.424044	0.231912	2.370760

1	7.081369	-0.102702	3.343306
6	6.595059	1.042400	1.579078
6	5.681335	0.408352	-2.267109
1	6.693747	0.088916	-2.023755
6	5.485432	0.238366	-3.775727
1	5.606100	-0.806856	-4.074453
1	4.499291	0.569972	-4.109757
1	6.235237	0.839653	-4.298074
6	4.619922	0.549345	3.708661
6	4.594298	-0.855866	3.761655
1	4.787965	-1.431972	2.862591
6	4.340092	-1.519120	4.960881
1	4.338440	-2.604036	4.983772
6	4.085689	-0.784810	6.123897
1	3.874913	-1.299163	7.057110
6	4.103856	0.610140	6.079997
1	3.906733	1.186471	6.979594
6	4.373957	1.276766	4.881195
1	4.377767	2.360801	4.864597
6	4.723987	3.140385	2.394613
6	5.758533	3.844189	3.031456
1	6.647773	3.318413	3.367753
6	5.654341	5.223218	3.214934
1	6.457994	5.765676	3.704786
6	4.518069	5.905918	2.765050
1	4.441866	6.980730	2.903996
6	3.483594	5.206098	2.140275
1	2.599074	5.732417	1.793267
6	3.584768	3.825797	1.954059
1	2.794434	3.281517	1.448315
6	5.719734	-2.044989	-0.599542
6	5.293007	-2.843568	0.471080
1	4.278576	-2.759572	0.836233
6	6.173072	-3.723567	1.102958
6	7.499538	-3.820508	0.689919
1	8.194845	-4.468839	1.211186
6	7.921157	-3.046111	-0.389365
6	7.042695	-2.184658	-1.043599
1	7.420641	-1.608772	-1.877028
6	3.348727	-1.467239	-2.269311
6	2.436947	-0.575657	-2.861820
1	2.556623	0.491288	-2.710466
6	1.362241	-1.056911	-3.598467
6	1.138309	-2.431164	-3.725891
1	0.255735	-2.806486	-4.228554
6	2.041697	-3.310106	-3.137170
6	3.149465	-2.840827	-2.419715
1	3.833652	-3.551939	-1.968516
29	3.442286	0.461645	0.518318
6	1.794390	-4.794181	-3.188371
6	0.345009	-0.105984	-4.160544
6	5.690288	-4.564718	2.253836
6	9.369910	-3.111722	-0.791383
9	10.178575	-2.870489	0.270196
9	9.684670	-2.207036	-1.744245
9	9.708936	-4.331633	-1.265833
9	4.728483	-3.927295	2.968026
9	5.155317	-5.734336	1.835973
9	6.688067	-4.870059	3.109983
9	2.943091	-5.476970	-3.421887
9	1.310333	-5.259142	-2.010769
9	0.915762	-5.139518	-4.147628
9	0.098118	-0.324744	-5.470278
9	0.721645	1.190250	-4.034466
9	-0.842149	-0.235876	-3.519162
6	1.941105	-1.940444	1.251011
6	0.645210	-0.593495	-0.124866
6	1.294648	-3.082202	0.799179
1	2.703393	-1.982906	2.019358
6	-0.007802	-1.722468	-0.637967
6	0.322958	-2.994593	-0.190048
1	-0.783018	-1.607772	-1.382360
6	0.050572	0.758155	-0.452586
6	1.010453	1.881312	-0.802802
8	2.218607	1.864896	-0.479097
7	1.651682	-0.718129	0.765627
1	-0.586444	0.583790	-1.317243
7	0.512984	2.965971	-1.439679
6	1.398213	4.107135	-1.669437
1	1.907378	4.017479	-2.636275
1	0.797131	5.020157	-1.671710
1	2.148499	4.161874	-0.883495
6	-0.772550	3.058599	-2.130709
1	-1.365833	2.155001	-2.035490
1	-1.348274	3.899551	-1.736824
1	-0.595953	3.229361	-3.195596
1	-0.180608	-3.858343	-0.598690
35	1.794534	-4.817749	1.533214
5	-2.632873	-3.437126	-2.155269
9	-3.649599	-4.263465	-2.650176
9	-1.373083	-3.852876	-2.637641
9	-2.629239	-3.487633	-0.743626
9	-2.862365	-2.100384	-2.568740

[**8-9**]‡ **P1-C2** *endo si-re* [BF_4^-] conf2

Number of imaginary frequencies= 1
The smallest frequencies are=-191.0325 11.8768 13.7626cm(-1)
Electronic energy= -7647.2550994
Zero-point correction= 1.771637
(Hartree/Particle)
Thermal correction to Energy= 1.896247
Thermal correction to Enthalpy= 1.897191
Thermal correction to Gibbs Free Energy= 1.602906
Sum of electronic and zero-point Energies= -7645.483463
Sum of electronic and thermal Energies= -7645.358852
Sum of electronic and thermal Enthalpies= -7645.357908
Sum of electronic and thermal Free Energies= -7645.652193

.....

Cartesian Coordinates

.....

26	8.463431	0.029180	-0.575056
15	3.558421	1.029441	-2.129554
15	4.260951	0.715919	1.562992
6	6.526149	0.719231	-0.979293
6	6.589651	0.056988	0.302681
6	7.019970	-1.286944	0.079230
1	7.175293	-2.037139	0.842306
6	7.251474	-1.456274	-1.319710
1	7.621259	-2.352829	-1.797311
6	6.949761	-0.224177	-1.969949
1	7.044129	-0.022780	-3.026627
6	9.784715	1.252223	0.460276
1	9.491028	1.976406	1.208606
6	10.088356	-0.123081	0.700361
1	10.060439	-0.623767	1.658943
6	10.389225	-0.734711	-0.554715
1	10.624150	-1.779175	-0.712249
6	10.271020	0.261424	-1.571276
1	10.401379	0.105000	-2.633972
6	9.899377	1.488607	-0.945166
1	9.703883	2.422720	-1.453905
6	6.034843	2.111990	-1.186223
6	6.819950	3.185295	-0.737330
1	7.774929	2.961353	-0.279491
6	6.396346	4.508809	-0.848934
1	7.016344	5.311912	-0.463343
6	5.167382	4.785574	-1.442399
1	4.819555	5.809076	-1.539034
6	4.365246	3.735812	-1.889738
1	3.404341	3.969901	-2.332173
6	4.762998	2.395522	-1.753663
6	6.158698	0.678816	1.603746
1	6.470100	1.724316	1.581755
6	6.769374	0.022597	2.845005
1	6.459757	0.541436	3.756519
1	6.478871	-1.027129	2.941539
1	7.860689	0.065037	2.773188
6	2.081188	1.945029	-2.743085
6	1.201827	2.462891	-1.775473

1	1.361851	2.232579	-0.728113
6	0.126935	3.265683	-2.155898
1	-0.537987	3.669109	-1.401210
6	-0.109175	3.527319	-3.507999
1	-0.955123	4.142002	-3.802091
6	0.734724	2.982348	-4.477687
1	0.549282	3.170661	-5.531439
6	1.831550	2.203322	-4.098980
1	2.490910	1.807551	-4.863734
6	4.246484	0.213193	-3.623166
6	4.971483	0.916406	-4.598623
1	5.136459	1.984349	-4.488741
6	5.498893	0.243048	-5.701625
1	6.061265	0.793135	-6.450847
6	5.308973	-1.136132	-5.840129
1	5.727072	-1.658470	-6.695868
6	4.586146	-1.840501	-4.874381
1	4.442186	-2.912866	-4.971657
6	4.058586	-1.167923	-3.770590
1	3.519048	-1.719076	-3.009725
6	3.758304	2.464521	1.850721
6	2.379778	2.713155	1.777042
1	1.703123	1.881341	1.607322
6	1.886947	4.013641	1.880651
6	2.752939	5.096259	2.021235
1	2.370093	6.109154	2.075523
6	4.125377	4.848757	2.075333
6	4.629126	3.548912	2.010736
1	5.699821	3.408316	2.065098
6	3.667405	-0.169150	3.062003
6	3.722519	-1.571107	3.007634
1	4.157642	-2.061817	2.145665
6	3.184538	-2.338921	4.034837
6	2.559112	-1.732860	5.126358
1	2.119158	-2.333365	5.914213
6	2.498856	-0.342721	5.175734
6	3.054386	0.440776	4.159634
1	2.989891	1.520450	4.230137
29	3.148684	-0.207007	-0.284262
6	1.744119	0.333534	6.285500
6	3.172979	-3.838610	3.923811
6	0.397481	4.215656	1.868916
6	5.060642	6.025026	2.151559
9	5.005882	6.774000	1.021076
9	6.349633	5.653841	2.315622
9	4.744485	6.853591	3.173500
9	-0.205224	3.442261	0.920614
9	-0.170241	3.868623	3.047336
9	0.043941	5.492586	1.613374
9	2.276282	1.534686	6.603557
9	0.451376	0.568599	5.929093
9	1.706900	-0.408856	7.411442
9	3.439710	-4.432139	5.109051
9	4.077378	-4.291970	3.028107
9	1.958898	-4.297024	3.526476
6	0.734024	-0.969403	1.356788
6	0.875771	-2.352270	0.970827
6	2.016763	-2.971448	0.385016
1	0.197292	-3.051749	1.435025
77	-3.305158	-0.854540	-1.733786
15	-5.013561	0.098633	-0.603344
8	-4.787765	1.312701	0.515780
8	-6.122620	0.838501	-1.608889
7	-5.765050	-1.029705	0.380556
6	-4.610569	2.632542	0.133541
6	-3.337120	3.196459	0.375261
1	-2.579404	2.585195	0.852549
6	-3.089088	4.495277	0.006351
1	-2.122290	4.946254	0.204561
6	-4.087192	5.257498	-0.659144
6	-3.813078	6.571686	-1.125599
1	-2.826688	6.989917	-0.941920
6	-4.766659	7.294838	-1.805983
1	-4.544897	8.296361	-2.162924
6	-6.037318	6.722829	-2.053653
1	-6.780785	7.285425	-2.611147
6	-6.340525	5.456934	-1.600639
1	-7.315795	5.033419	-1.809290
6	-5.387223	4.687385	-0.876551
6	-5.667315	3.358731	-0.395309
6	-7.028048	2.754782	-0.473584
6	-8.182631	3.386679	0.110854
6	-8.091635	4.550987	0.924467
1	-7.118267	4.982147	1.126348
6	-9.217524	5.126496	1.472129
1	-9.119164	6.009734	2.096829
6	-10.499662	4.574807	1.236452
1	-11.378297	5.042523	1.671006
6	-10.624081	3.438037	0.470685
1	-11.599758	2.991644	0.296671
6	-9.481947	2.810406	-0.097764
6	-9.604176	1.609307	-0.847367
1	-10.591472	1.186810	-1.011250
6	-8.487005	0.965422	-1.319023
1	-8.551348	0.027043	-1.858704
6	-7.212410	1.532488	-1.102700
6	-5.351306	-2.430057	0.078357
1	-4.668288	-2.764987	0.860948
6	-6.519743	-3.400821	0.001118
6	-6.353986	-4.716150	0.451742
1	-5.405285	-5.016383	0.885322
6	-7.400316	-5.636446	0.348675
1	-7.260301	-6.651493	0.711447
6	-8.623882	-5.253291	-0.205067
1	-9.442555	-5.964806	-0.271681
6	-8.788859	-3.944507	-0.671085
1	-9.739057	-3.633510	-1.097585
6	-7.740434	-3.030305	-0.577265
1	-7.875875	-2.006478	-0.910568
6	-4.608822	-2.489575	-1.275766
1	-5.356714	-2.553174	-2.074910
1	-4.043612	-3.423538	-1.293810
6	-6.248191	-0.676902	1.760825
1	-6.476787	0.387572	1.714940
6	-7.554317	-1.367304	2.129371
6	-8.764154	-0.735230	1.818759
1	-8.746178	0.236615	1.336912
6	-9.987622	-1.339515	2.110983
1	-10.914612	-0.832392	1.855996
6	-10.015495	-2.590733	2.731298
1	-10.964328	-3.070388	2.955975
6	-8.813838	-3.219806	3.067881
1	-8.825130	-4.192435	3.551743
6	-7.593357	-2.608258	2.777642
1	-6.669992	-3.117071	3.032824
6	-5.146076	-0.864729	2.813410
1	-4.319503	-0.180448	2.606811
1	-4.748088	-1.881179	2.837449
1	-5.542155	-0.630424	3.806735
6	-2.306360	-0.806565	0.194948
1	-1.640425	0.049970	0.255597
1	-2.950109	-0.917066	1.060537
6	-1.804472	-2.017687	-0.383831
1	-2.297402	-2.944107	-0.128136
6	-0.542643	-2.101140	-1.009060
1	0.001490	-1.179051	-1.167234
6	-4.263908	-0.714934	-3.745872
1	-5.282785	-1.077575	-3.635404
6	-3.244269	-1.696623	-3.807030
1	-3.551703	-2.740701	-3.757042
6	-1.885328	-1.483518	-4.452514
1	-1.977870	-1.550676	-5.548127
1	-1.245375	-2.315371	-4.147985
6	-1.191475	-0.156350	-4.067734
1	-1.397669	0.617282	-4.814781
1	-0.107545	-0.306583	-4.086844
6	-1.569888	0.384682	-2.690916
1	-0.764913	0.421978	-1.966965
6	-2.623084	1.258062	-2.449269
1	-2.535960	1.884234	-1.568015

6	-3.606603	1.761291	-3.485049
1	-4.441668	2.227891	-2.957234
1	-3.122911	2.554462	-4.075195
6	-4.148409	0.656122	-4.416454
1	-3.513647	0.567385	-5.304079
1	-5.137388	0.954209	-4.778701
6	-0.066722	-3.234332	-1.789173
6	-0.588444	-4.537373	-1.664745
6	0.982395	-3.009014	-2.701830
6	-0.076884	-5.570945	-2.447682
1	-1.372726	-4.742204	-0.944432
6	1.491027	-4.044391	-3.481209
1	1.382899	-2.004731	-2.797915
6	0.960315	-5.332151	-3.356571
1	-0.483084	-6.572889	-2.340922
1	2.295590	-3.846780	-4.184112
1	1.353945	-6.145204	-3.960133
6	2.048435	-4.397982	0.359618
6	3.104954	-5.077052	-0.204537
1	1.216662	-4.938321	0.796860
6	4.151140	-4.315801	-0.742579
6	4.091449	-2.937937	-0.713093
1	4.881671	-2.330933	-1.133905
7	3.049481	-2.269409	-0.176189
8	1.225796	0.002237	0.691699
7	-0.049558	-0.690603	2.440287
6	-0.489452	0.672011	2.704773
1	-1.532281	0.653705	3.038536
1	0.111316	1.144054	3.489687
1	-0.421245	1.265940	1.798052
6	-0.495347	-1.688601	3.413833
1	-1.487325	-2.078706	3.170739
1	0.204136	-2.521135	3.466623
1	-0.523610	-1.213217	4.397697
1	3.123049	-6.161139	-0.226851
35	5.703864	-5.192353	-1.559274
5	-2.598675	-4.710236	1.831470
9	-1.190953	-4.765363	1.814764
9	-3.084750	-4.914887	0.512560
9	-3.121205	-5.687093	2.676038
9	-3.013124	-3.425216	2.265568

[**8-9**]‡ **P1-C2** *endo re-re* [BF_4^-] conf2

Number of imaginary frequencies= 1
The smallest frequencies are=-241.6833 10.6177 12.7392cm(-1)
Electronic energy= -7647.2463107
Zero-point correction= 1.771399
(Hartree/Particle)
Thermal correction to Energy= 1.896249
Thermal correction to Enthalpy= 1.897193
Thermal correction to Gibbs Free Energy= 1.601928
Sum of electronic and zero-point Energies= -7645.474912
Sum of electronic and thermal Energies= -7645.350061
Sum of electronic and thermal Enthalpies= -7645.349117
Sum of electronic and thermal Free Energies= -7645.644383

.....

Cartesian Coordinates

.....

26	7.650844	-2.088963	-1.462913
15	3.218711	0.490143	-2.333527
15	4.463365	0.277974	1.204344
6	6.055729	-0.753252	-1.683725
6	6.093966	-1.302894	-0.349086
6	5.956910	-2.718367	-0.457064
1	5.957001	-3.415986	0.368530
6	5.869206	-3.056226	-1.838062
1	5.801530	-4.056046	-2.244325
6	5.935239	-1.851417	-2.593780
1	5.908063	-1.769663	-3.670510
6	9.480592	-1.375065	-0.791198
1	9.602128	-0.534979	-0.120094
6	9.307986	-2.739404	-0.403222
1	9.270985	-3.113338	0.611213
6	9.145457	-3.518659	-1.589165
1	8.958392	-4.583731	-1.628445
6	9.218908	-2.637189	-2.710723
1	9.100546	-2.916601	-3.749370
6	9.428220	-1.314440	-2.218745
1	9.500543	-0.420810	-2.823444
6	6.045060	0.700685	-2.012560
6	7.228408	1.446136	-1.907996
1	8.131746	0.932757	-1.603805
6	7.262000	2.815015	-2.172573
1	8.189719	3.366359	-2.060239
6	6.095239	3.467800	-2.562847
1	6.103393	4.533264	-2.770496
6	4.903039	2.749940	-2.665093
1	4.000572	3.275372	-2.956324
6	4.849231	1.376605	-2.379404
6	6.181207	-0.480358	0.907133
1	6.821617	0.371180	0.677400
6	6.792066	-1.213823	2.105011
1	6.837045	-0.563500	2.983167
1	6.227696	-2.108847	2.377998
1	7.809768	-1.525596	1.851652
6	1.993735	1.781707	-2.809368
6	1.599946	2.686231	-1.807815
1	2.041820	2.617838	-0.818926
6	0.660636	3.679978	-2.075149
1	0.378222	4.375725	-1.296194
6	0.078901	3.771338	-3.342580
1	-0.667440	4.534915	-3.541645
6	0.457608	2.873267	-4.341719
1	0.009187	2.935126	-5.329218
6	1.413492	1.887168	-4.081156
1	1.691298	1.197966	-4.870138
6	3.285936	-0.646438	-3.770567
6	3.830946	-0.273200	-5.008766
1	4.229923	0.727471	-5.148844
6	3.873070	-1.192221	-6.058588
1	4.294929	-0.899443	-7.015902
6	3.377036	-2.488294	-5.877952
1	3.413265	-3.201146	-6.696973
6	2.845885	-2.867320	-4.642772
1	2.473416	-3.877042	-4.494579
6	2.806094	-1.950601	-3.590386
1	2.450724	-2.247978	-2.608893
6	4.739568	2.102859	1.332044
6	3.599363	2.909534	1.454320
1	2.636212	2.452551	1.629197
6	3.678372	4.296397	1.330379
6	4.900840	4.920163	1.096506
1	4.960842	5.995845	0.973882
6	6.044038	4.125967	1.007355
6	5.972486	2.738164	1.124559
1	6.887843	2.172024	1.028048
6	3.923910	-0.265360	2.872936
6	3.630400	-1.632820	2.995959
1	3.794825	-2.299802	2.157225
6	3.100680	-2.136684	4.180038
6	2.797353	-1.285188	5.242542
1	2.353206	-1.673943	6.152615
6	3.064807	0.076788	5.108401
6	3.640793	0.588635	3.943919
1	3.845812	1.650189	3.876208
29	2.780936	-0.431093	-0.304979
6	2.663441	0.994163	6.230607
6	2.756743	-3.596830	4.285252
6	2.417017	5.108307	1.438225
6	7.359240	4.806551	0.737814
9	7.326584	5.501144	-0.426370
9	8.389191	3.936697	0.653715
9	7.664951	5.699755	1.707273
9	1.365788	4.452411	0.870530
9	2.070266	5.350974	2.721395
9	2.518009	6.301162	0.818941
9	3.086128	2.262876	6.039852
9	1.315511	1.037133	6.366423
9	3.156988	0.578087	7.420426

9	3.066856	-4.097864	5.501666
9	3.406706	-4.341337	3.360884
9	1.430425	-3.815384	4.103138
6	0.774903	0.777926	1.498841
6	0.610467	-1.550773	1.606100
6	0.096367	0.931038	2.694255
1	1.090050	1.636948	0.921669
6	-0.173084	-1.425560	2.786364
6	-0.402090	-0.192429	3.360718
6	0.798984	-2.873136	1.077178
6	1.946229	-3.299470	0.319437
8	2.686150	-2.506467	-0.347962
7	1.069637	-0.428049	0.974897
1	0.265026	-3.627758	1.632395
77	-3.139421	-1.008353	-1.571519
15	-4.803194	0.209968	-0.615932
8	-4.538488	1.371318	0.551592
8	-5.634037	1.136720	-1.728848
7	-5.845730	-0.783736	0.240841
6	-3.927846	2.567446	0.219400
6	-2.621385	2.769235	0.715064
1	-2.176142	1.992048	1.324269
6	-1.958294	3.933723	0.421268
1	-0.965066	4.112971	0.816164
6	-2.550549	4.900177	-0.436209
6	-1.832688	6.062105	-0.830948
1	-0.835553	6.215799	-0.425649
6	-2.380744	6.965116	-1.714580
1	-1.820897	7.845246	-2.017157
6	-3.676975	6.739089	-2.237329
1	-4.098095	7.441162	-2.951304
6	-4.410705	5.638004	-1.850143
1	-5.401558	5.480734	-2.260748
6	-3.882664	4.690491	-0.929597
6	-4.617094	3.524107	-0.509183
6	-6.063559	3.327227	-0.808822
6	-7.051296	4.311255	-0.439756
6	-6.736506	5.465525	0.332048
1	-5.720218	5.614435	0.675833
6	-7.705758	6.386011	0.667570
1	-7.437786	7.252537	1.265459
6	-9.046544	6.210072	0.250564
1	-9.798286	6.947316	0.516928
6	-9.393423	5.092884	-0.474521
1	-10.422960	4.930586	-0.783188
6	-8.421587	4.115600	-0.822365
6	-8.792145	2.934519	-1.519485
1	-9.828432	2.798063	-1.815678
6	-7.861565	1.960351	-1.781795
1	-8.127862	1.033416	-2.278229
6	-6.514838	2.154969	-1.400880
6	-5.497796	-2.230675	0.112606
1	-4.899905	-2.524531	0.980150
6	-6.716055	-3.136443	0.025147
6	-6.724529	-4.355012	0.712933
1	-5.877053	-4.616858	1.338373
6	-7.812606	-5.225419	0.598269
1	-7.809204	-6.164755	1.145222
6	-8.903684	-4.885677	-0.203308
1	-9.756062	-5.555162	-0.281812
6	-8.893564	-3.674578	-0.904879
1	-9.740800	-3.398668	-1.527178
6	-7.803343	-2.813336	-0.798549
1	-7.805237	-1.862268	-1.322375
6	-4.662728	-2.451480	-1.165016
1	-5.346209	-2.466625	-2.022263
1	-4.209662	-3.444710	-1.104153
6	-6.526716	-0.290082	1.489538
1	-6.599172	0.790377	1.358683
6	-7.962290	-0.787300	1.617113
6	-8.975913	-0.107244	0.930268
1	-8.720009	0.763585	0.335067
6	-10.301194	-0.539537	0.991448
1	-11.071535	0.000060	0.446445
6	-10.634486	-1.660822	1.755452
1	-11.663717	-2.006155	1.802506
6	-9.635349	-2.330794	2.465921
1	-9.883717	-3.202445	3.064989
6	-8.311603	-1.891823	2.403371
1	-7.546753	-2.433667	2.948157
6	-5.671519	-0.542963	2.737319
1	-4.719554	-0.016541	2.643456
1	-5.452365	-1.598926	2.901174
1	-6.191849	-0.161170	3.621750
6	-2.222953	-0.904289	0.400346
1	-1.434843	-0.160239	0.386198
1	-2.898443	-0.805030	1.242927
6	-1.958296	-2.246951	-0.013004
1	-2.622058	-2.996578	0.392595
6	-0.788198	-2.732895	-0.653256
1	-0.098749	-2.020233	-1.084721
6	-3.911223	-0.854928	-3.644817
1	-4.972275	-1.094438	-3.621786
6	-3.017200	-1.956939	-3.581981
1	-3.459524	-2.951572	-3.528976
6	-1.601616	-1.944554	-4.133149
1	-1.622914	-2.069758	-5.227663
1	-1.092066	-2.825303	-3.735543
6	-0.787282	-0.686028	-3.767638
1	-0.872037	0.068164	-4.555391
1	0.273679	-0.948710	-3.724803
6	-1.176719	-0.045628	-2.437719
1	-0.435660	-0.109487	-1.645221
6	-2.119245	0.968247	-2.313668
1	-2.031959	1.614320	-1.446709
6	-2.951413	1.530984	-3.448844
1	-3.746450	2.135195	-3.007859
1	-2.326240	2.214654	-4.039644
6	-3.581731	0.457250	-4.361693
1	-2.921721	0.245724	-5.210095
1	-4.504177	0.861610	-4.790441
6	-0.718245	-4.097353	-1.192507
6	-1.582633	-5.130295	-0.773160
6	0.244140	-4.393627	-2.175449
6	-1.491241	-6.400299	-1.339550
1	-2.305023	-4.954953	0.014734
6	0.334930	-5.664902	-2.739257
1	0.919566	-3.611451	-2.499128
6	-0.536080	-6.675815	-2.324812
1	-2.164159	-7.183461	-1.001637
1	1.083845	-5.865025	-3.500645
1	-0.469959	-7.668869	-2.760224
7	2.239631	-4.635378	0.278517
6	3.223434	-5.141568	-0.667898
1	4.124590	-5.492489	-0.147995
1	2.795158	-5.982071	-1.224878
1	3.502642	-4.352353	-1.360828
6	1.560948	-5.650614	1.080376
1	0.641481	-6.001076	0.600062
1	2.237981	-6.500691	1.198763
1	1.322714	-5.279091	2.075691
1	-0.961395	-0.102624	4.285249
1	-0.578400	-2.321548	3.236949
35	-0.099403	2.711242	3.475145
5	-3.014819	-4.021964	2.876344
9	-3.533053	-4.641260	4.013174
9	-3.241149	-2.632442	2.931389
9	-1.628753	-4.273327	2.772477
9	-3.656644	-4.541286	1.716505

[8-9]‡ P1-C2 *exo re-si* [BF_4^-] conf2

Number of imaginary frequencies= 1
The smallest frequencies are= -69.8184 6.9783 7.7797 cm(-1)
Electronic energy= -7647.2255649
Zero-point correction= 1.769579
(Hartree/Particle)
Thermal correction to Energy= 1.894763
Thermal correction to Enthalpy= 1.895708
Thermal correction to Gibbs Free Energy= 1.596992

Sum of electronic and zero-point Energies= -7645.455986
Sum of electronic and thermal Energies= -7645.330801
Sum of electronic and thermal Enthalpies= -7645.329857
Sum of electronic and thermal Free Energies= -7645.628572

.....

Cartesian Coordinates

.....

77	4.083621	-0.739790	-1.577558
15	5.823060	-0.164991	-0.250993
8	6.186270	-0.945256	1.168125
8	7.281177	-0.307216	-1.051900
7	5.608832	1.383067	0.349440
6	6.933018	-2.115040	1.197935
6	6.252456	-3.280829	1.613597
1	5.205548	-3.197911	1.886557
6	6.923573	-4.476811	1.664576
1	6.413851	-5.379266	1.989925
6	8.284992	-4.556499	1.265099
6	8.968137	-5.802716	1.243795
1	8.431956	-6.691822	1.565296
6	10.272868	-5.887522	0.813795
1	10.784290	-6.845458	0.797245
6	10.944045	-4.721672	0.374780
1	11.964776	-4.793898	0.010338
6	10.315132	-3.495617	0.397283
1	10.844577	-2.618506	0.045694
6	8.975332	-3.364210	0.859599
6	8.286153	-2.098316	0.896273
6	8.977768	-0.817915	0.574031
6	10.167658	-0.388367	1.262097
6	10.661956	-1.046254	2.423136
1	10.124612	-1.901366	2.816275
6	11.799356	-0.602199	3.061763
1	12.150179	-1.115673	3.952405
6	12.510967	0.520552	2.574757
1	13.408142	0.855890	3.086753
6	12.053342	1.190919	1.463165
1	12.579277	2.064731	1.087208
6	10.875434	0.768490	0.788414
6	10.374426	1.487322	-0.330359
1	10.925407	2.349413	-0.694693
6	9.183824	1.128806	-0.911973
1	8.762088	1.684999	-1.741497
6	8.483432	0.002772	-0.428449
6	4.575919	2.151051	-0.392201
1	3.688227	2.231295	0.245408
6	5.022226	3.552865	-0.777936
6	4.089700	4.594334	-0.777964
1	3.069497	4.411192	-0.457032
6	4.459945	5.879481	-1.184124
1	3.712644	6.665996	-1.178216
6	5.771829	6.134190	-1.588277
1	6.066504	7.135459	-1.891179
6	6.706391	5.092572	-1.600793
1	7.731921	5.283079	-1.906498
6	6.329828	3.809014	-1.209565
1	7.060047	3.008409	-1.188952
6	4.186847	1.404782	-1.685657
1	4.927983	1.652759	-2.453941
1	3.235465	1.805524	-2.040487
6	5.932421	1.759015	1.768843
1	6.629571	0.995672	2.110043
6	6.675546	3.083804	1.878168
6	8.072286	3.073862	1.783100
1	8.587708	2.126926	1.662417
6	8.804304	4.260847	1.829227
1	9.887590	4.229625	1.747502
6	8.142239	5.481307	1.982937
1	8.705405	6.410137	2.011626
6	6.750568	5.500129	2.109299
1	6.226823	6.443880	2.232122
6	6.024487	4.308948	2.067903
1	4.943940	4.344937	2.151505
6	4.692663	1.669375	2.668156
1	4.287423	0.654273	2.644111
1	3.900924	2.363633	2.375023
1	4.971409	1.903815	3.700107
6	2.946390	-0.977471	0.249431
1	3.070044	-1.971793	0.677221
1	3.080637	-0.185045	0.983665
6	1.890147	-0.793575	-0.715814
1	1.417638	-1.663301	-1.152016
6	1.283802	0.452921	-0.926434
1	1.709917	1.299601	-0.401163
6	5.274959	-0.818315	-3.477298
1	5.883942	0.081856	-3.507790
6	3.908110	-0.656075	-3.802539
1	3.584144	0.346446	-4.081052
6	2.974739	-1.752012	-4.290789
1	3.094142	-1.891198	-5.376449
1	1.950540	-1.394577	-4.138972
6	3.146464	-3.103775	-3.565021
1	3.898050	-3.716310	-4.071703
1	2.206810	-3.662083	-3.631087
6	3.522518	-2.970844	-2.091629
1	2.743383	-3.241717	-1.383592
6	4.821353	-2.973459	-1.600126
1	4.951365	-3.254695	-0.559452
6	6.085768	-3.028678	-2.431846
1	6.915893	-2.729430	-1.788052
1	6.276484	-4.070777	-2.727838
6	6.061745	-2.115158	-3.675188
1	5.654043	-2.653435	-4.536070
1	7.092602	-1.858685	-3.937745
6	0.366993	0.789413	-1.994075
6	-0.269065	-0.183581	-2.798324
6	0.140560	2.154561	-2.271341
6	-1.089308	0.203167	-3.852998
1	-0.127539	-1.238230	-2.592458
6	-0.663781	2.534478	-3.341956
1	0.592992	2.917102	-1.646605
6	-1.280181	1.562089	-4.133342
1	-1.589662	-0.549571	-4.455352
1	-0.812782	3.589666	-3.535399
1	-1.919895	1.857245	-4.958770
26	-6.821179	3.666494	2.113766
15	-4.834843	1.033138	-1.947097
15	-4.891703	-0.654912	1.409581
6	-6.288957	2.381061	0.549232
6	-5.721870	1.941110	1.801901
6	-4.878416	2.983318	2.289111
1	-4.318098	2.962726	3.213314
6	-4.940693	4.073746	1.373876
1	-4.441418	5.026562	1.484878
6	-5.811875	3.708425	0.308517
1	-6.076488	4.326240	-0.536641
6	-8.565262	3.285985	3.178220
1	-8.987320	2.303546	3.343463
6	-7.607966	3.938968	4.013979
1	-7.170883	3.535292	4.917362
6	-7.294785	5.201379	3.424376
1	-6.574255	5.916344	3.799257
6	-8.058939	5.330507	2.224863
1	-8.021317	6.161473	1.532802
6	-8.844197	4.148971	2.072641
1	-9.508884	3.934591	1.246803
6	-7.142774	1.535651	-0.335041
6	-8.469695	1.275372	0.040142
1	-8.840427	1.731158	0.949200
6	-9.301014	0.443602	-0.709100
1	-10.313194	0.242020	-0.373582
6	-8.813693	-0.136575	-1.877464
1	-9.444779	-0.787586	-2.474650
6	-7.497722	0.106640	-2.272362
1	-7.133819	-0.360320	-3.180322
6	-6.638705	0.917157	-1.512480
6	-5.947168	0.579256	2.398289
1	-6.974846	0.304081	2.159026
6	-5.787986	0.515449	3.920059
1	-5.972506	-0.495854	4.293500

1	-4.790901	0.818651	4.247751
1	-6.510596	1.193977	4.382869
6	-4.691932	0.090070	-3.524158
6	-4.650491	-1.312068	-3.429894
1	-4.768861	-1.787721	-2.461516
6	-4.471673	-2.100278	-4.565809
1	-4.455505	-3.181174	-4.470853
6	-4.310287	-1.494074	-5.815925
1	-4.156107	-2.103681	-6.701751
6	-4.350417	-0.102275	-5.920471
1	-4.227527	0.375508	-6.888483
6	-4.548229	0.687013	-4.783693
1	-4.572034	1.766237	-4.883499
6	-4.593954	2.791967	-2.401377
6	-5.536902	3.504680	-3.160616
1	-6.426459	3.004920	-3.534240
6	-5.343071	4.862418	-3.416718
1	-6.074441	5.411588	-4.003482
6	-4.213347	5.516448	-2.909813
1	-4.070457	6.576337	-3.102647
6	-3.273453	4.813523	-2.152679
1	-2.403593	5.317769	-1.744440
6	-3.464190	3.452454	-1.899457
1	-2.758387	2.909909	-1.279868
6	-6.063697	-1.969663	0.855504
6	-5.556405	-2.930158	-0.031584
1	-4.495331	-2.959655	-0.243833
6	-6.404237	-3.834160	-0.671608
6	-7.778083	-3.803877	-0.445449
1	-8.440329	-4.486065	-0.966531
6	-8.284283	-2.861964	0.449757
6	-7.443572	-1.961580	1.102245
1	-7.889097	-1.245323	1.778313
6	-3.767216	-1.470233	2.612824
6	-2.791137	-0.642398	3.195873
1	-2.790590	0.420137	2.984871
6	-1.797311	-1.185623	4.001224
6	-1.723433	-2.564858	4.212461
1	-0.928512	-2.990294	4.814574
6	-2.678174	-3.384797	3.618904
6	-3.704034	-2.848118	2.833824
1	-4.433655	-3.516175	2.390185
29	-3.519767	0.188829	-0.311025
6	-2.548059	-4.878401	3.718586
6	-0.718658	-0.314389	4.580950
6	-5.812822	-4.841156	-1.618911
6	-9.773360	-2.808611	0.659414
9	-10.427607	-2.585433	-0.507366
9	-10.143538	-1.831443	1.515796
9	-10.252281	-3.975703	1.149410
9	-4.793186	-4.303517	-2.337804
9	-5.302903	-5.909974	-0.965291
9	-6.720107	-5.309336	-2.500989
9	-3.751374	-5.492998	3.765070
9	-1.897138	-5.383849	2.638471
9	-1.851056	-5.262991	4.809924
9	-0.602397	-0.479552	5.918228
9	-0.930425	0.999720	4.351825
9	0.501168	-0.616900	4.056378
6	-2.090011	-2.405742	-0.790908
6	-0.870439	-0.999718	0.636079
6	-1.366388	-3.518465	-0.400883
1	-2.854568	-2.478277	-1.555337
6	-0.155755	-2.144760	1.110412
6	-0.398590	-3.402147	0.604987
1	0.581338	-2.006446	1.892347
6	-0.414877	0.276728	1.061724
6	-1.133333	1.519535	1.005121
8	-2.317495	1.624809	0.557265
7	-1.890319	-1.180536	-0.266018
1	0.425072	0.232961	1.738013
7	-0.527143	2.653696	1.480464
6	-1.326836	3.854216	1.697106
1	-1.584465	3.958383	2.762077
1	-0.770026	4.731152	1.370597
1	-2.243661	3.783855	1.118801
6	0.802413	2.672295	2.074243
1	1.485487	2.017945	1.532780
1	1.195090	3.687317	2.001259
1	0.786404	2.365666	3.128398
1	0.139485	-4.267955	0.974354
35	-1.696787	-5.256988	-1.238116
5	0.448269	5.783154	-1.024556
9	-0.752750	6.247650	-0.452656
9	0.205207	5.329489	-2.330672
9	1.396815	6.818200	-1.039645
9	0.942500	4.704663	-0.240401

---

8 P1-C1 *endo re-re*

Number of imaginary frequencies= 0
The smallest frequencies are= 0.2961 8.2522 13.4052 cm(-1)
Electronic energy= -7222.6420682
Zero-point correction= 1.756572
(Hartree/Particle)
Thermal correction to Energy= 1.876002
Thermal correction to Enthalpy= 1.876946
Thermal correction to Gibbs Free Energy= 1.588710
Sum of electronic and zero-point Energies= -7220.885497
Sum of electronic and thermal Energies= -7220.766066
Sum of electronic and thermal Enthalpies= -7220.765122
Sum of electronic and thermal Free Energies= -7221.053358

Cartesian Coordinates

26	4.429627	4.784835	1.752745
15	2.590342	1.576280	-1.898661
15	4.602001	0.105116	0.881224
6	4.058127	3.409803	0.222031
6	4.282766	2.740668	1.481915
6	3.286950	3.193210	2.400907
1	3.195513	2.889401	3.434645
6	2.468162	4.154404	1.736278
1	1.653248	4.708212	2.181614
6	2.941715	4.290370	0.398397
1	2.547383	4.959991	-0.350934
6	6.387461	5.334302	2.177258
1	7.247219	4.688763	2.055202
6	5.576842	5.438264	3.349077
1	5.712598	4.883587	4.267963
6	4.529659	6.371776	3.080763
1	3.729220	6.640227	3.757511
6	4.692548	6.845414	1.743174
1	4.039921	7.538988	1.229463
6	5.840014	6.206554	1.185665
1	6.207374	6.338448	0.177204
6	4.823263	3.114347	-1.023670
6	6.156047	3.537682	-1.133844
1	6.575015	4.124271	-0.325947
6	6.945607	3.203946	-2.234373
1	7.982186	3.523598	-2.275117
6	6.403011	2.436025	-3.262102
1	7.009707	2.152374	-4.115973
6	5.079231	2.003982	-3.176312
1	4.676325	1.390599	-3.974602
6	4.277522	2.321180	-2.068713
6	5.311762	1.665006	1.702135
1	6.195031	1.932920	1.119886
6	5.741425	1.497135	3.162162
1	6.513279	0.728719	3.258736
1	4.907801	1.219161	3.812326
1	6.147100	2.445601	3.527622
6	2.340015	0.630535	-3.464856
6	2.436833	-0.769312	-3.408219
1	2.660529	-1.257820	-2.466904
6	2.194144	-1.540609	-4.548341
1	2.267172	-2.621722	-4.489606
6	1.847709	-0.925228	-5.752259
1	1.646810	-1.526148	-6.634663
6	1.755070	0.468482	-5.817815

1	1.486710	0.954185	-6.751767
6	2.001364	1.242389	-4.683525
1	1.915005	2.321455	-4.749913
6	1.451740	3.007862	-2.119362
6	1.794065	4.143464	-2.871530
1	2.781371	4.224107	-3.316477
6	0.873703	5.179698	-3.041511
1	1.149789	6.054488	-3.623480
6	-0.399517	5.090832	-2.469208
1	-1.118340	5.893632	-2.606695
6	-0.744949	3.966230	-1.716842
1	-1.730603	3.890378	-1.270114
6	0.180796	2.936787	-1.534190
1	-0.083454	2.075123	-0.933647
6	5.826783	-0.422556	-0.391120
6	5.403211	-1.453128	-1.243773
1	4.416789	-1.883115	-1.100669
6	6.239508	-1.916899	-2.259664
6	7.483766	-1.329653	-2.481802
1	8.120430	-1.671085	-3.290261
6	7.888441	-0.284003	-1.652132
6	7.085546	0.151819	-0.598308
1	7.449592	0.951695	0.031707
6	4.697055	-1.254314	2.120914
6	3.773803	-1.217656	3.178397
1	3.095685	-0.378490	3.280709
6	3.683608	-2.281769	4.070779
6	4.468017	-3.424380	3.904225
1	4.357853	-4.272329	4.570855
6	5.360287	-3.473325	2.836858
6	5.496579	-2.391145	1.964523
1	6.200587	-2.465906	1.144869
29	2.452209	0.246879	-0.065844
6	6.172487	-4.716672	2.602352
6	2.630989	-2.289917	5.142475
6	5.805147	-3.101894	-3.076560
6	9.201214	0.389314	-1.943189
9	9.207959	0.942043	-3.182368
9	9.482251	1.378983	-1.067327
9	10.233937	-0.484998	-1.910256
9	6.012574	-4.265374	-2.409796
9	6.467402	-3.193534	-4.248534
9	4.480576	-3.062842	-3.365653
9	7.344363	-4.706807	3.278699
9	6.479691	-4.874928	1.292021
9	5.504624	-5.829089	2.991730
9	3.119784	-2.734223	6.323004
9	2.095721	-1.069833	5.357335
9	1.603704	-3.122126	4.819280
6	1.993048	-2.687579	0.573036
6	1.100542	-2.340917	1.624053
6	0.616464	-1.068276	1.986428
1	0.768402	-3.133790	2.277425
77	-3.333619	-1.316452	-1.274286
15	-5.227325	-0.514560	-0.312508
8	-5.225833	0.663190	0.834052
8	-6.232070	0.160544	-1.444266
7	-5.957234	-1.738883	0.553017
6	-5.021092	2.000576	0.512166
6	-3.825929	2.579375	0.989476
1	-3.155789	1.972373	1.587789
6	-3.545741	3.888170	0.685641
1	-2.637660	4.353008	1.056388
6	-4.417352	4.634606	-0.153373
6	-4.077449	5.949465	-0.572369
1	-3.148258	6.383476	-0.212453
6	-4.897367	6.652682	-1.425963
1	-4.625047	7.653999	-1.746232
6	-6.095551	6.063601	-1.895934
1	-6.730569	6.613885	-2.584150
6	-6.463354	4.797517	-1.493698
1	-7.381136	4.359264	-1.868142
6	-5.646451	4.044810	-0.605180
6	-5.986740	2.709129	-0.185267
6	-7.310654	2.085286	-0.471625
6	-8.544852	2.700529	-0.050916
6	-8.585219	3.889425	0.730889
1	-7.657998	4.358730	1.036114
6	-9.784554	4.444979	1.120836
1	-9.785773	5.349470	1.722300
6	-11.013129	3.846660	0.753520
1	-11.950118	4.300168	1.062949
6	-11.012575	2.681687	0.020836
1	-11.947028	2.198010	-0.251081
6	-9.793382	2.073935	-0.385032
6	-9.795059	0.842834	-1.094512
1	-10.744811	0.382049	-1.350654
6	-8.613674	0.226434	-1.423243
1	-8.587494	-0.729370	-1.935361
6	-7.391499	0.845964	-1.087397
6	-5.409692	-3.082683	0.231014
1	-4.744694	-3.376236	1.050279
6	-6.512360	-4.120836	0.118370
6	-6.324561	-5.399726	0.655035
1	-5.405171	-5.625922	1.190646
6	-7.307189	-6.382701	0.508651
1	-7.150252	-7.370918	0.932009
6	-8.491919	-6.091455	-0.170841
1	-9.259851	-6.852095	-0.279506
6	-8.688494	-4.813377	-0.704564
1	-9.610697	-4.579184	-1.229502
6	-7.704651	-3.835034	-0.562151
1	-7.860006	-2.837758	-0.964412
6	-4.594450	-3.034818	-1.066989
1	-5.281691	-3.057237	-1.920097
1	-3.974083	-3.931492	-1.133713
6	-6.646965	-1.651896	1.890013
1	-7.135499	-2.626578	1.974217
6	-5.635029	-1.570035	3.032359
6	-5.095710	-2.759874	3.547485
1	-5.457505	-3.714693	3.174684
6	-4.116641	-2.737775	4.544420
1	-3.711930	-3.671741	4.924497
6	-3.676121	-1.518468	5.062438
1	-2.918603	-1.495802	5.840981
6	-4.234238	-0.328191	4.586935
1	-3.916845	0.625232	5.000405
6	-5.202801	-0.353575	3.582148
1	-5.619193	0.580518	3.227047
6	-7.766453	-0.614834	1.942828
1	-8.487968	-0.802393	1.144930
1	-7.411106	0.410208	1.847424
1	-8.283323	-0.707916	2.902708
6	-2.493795	-1.105737	0.742453
1	-1.777093	-0.290168	0.719088
1	-3.181962	-1.054177	1.580741
6	-2.084231	-2.411513	0.327130
1	-2.619365	-3.264868	0.731016
6	-1.105427	-2.626561	-0.641960
1	-0.415460	-1.824249	-0.866106
6	-4.192531	-1.063301	-3.348139
1	-5.190917	-1.488166	-3.299794
6	-3.125366	-1.977854	-3.431889
1	-3.374308	-3.038106	-3.452819
6	-1.750226	-1.649389	-3.978054
1	-1.784206	-1.675919	-5.077318
1	-1.071437	-2.449458	-3.674826
6	-1.178861	-0.296954	-3.506350
1	-1.458063	0.501613	-4.199005
1	-0.091927	-0.353955	-3.532561
6	-1.597745	0.109086	-2.101846
1	-0.824440	0.057900	-1.341784
6	-2.694215	0.905384	-1.830151
1	-2.698577	1.439127	-0.885792
6	-3.656336	1.427722	-2.875417
1	-4.520518	1.847428	-2.360596
1	-3.172060	2.261230	-3.403926
6	-4.140074	0.365819	-3.889722
1	-3.508166	0.376883	-4.782925
1	-5.145129	0.639903	-4.221343

6	-0.744417	-3.921633	-1.215282
6	-1.436623	-5.118371	-0.938046
6	0.356709	-3.971732	-2.093139
6	-1.045030	-6.316060	-1.531772
1	-2.275668	-5.115575	-0.250218
6	0.742182	-5.170306	-2.689918
1	0.919854	-3.063066	-2.278748
6	0.040578	-6.347078	-2.414687
1	-1.587484	-7.229914	-1.306371
1	1.597280	-5.188416	-3.359576
1	0.340071	-7.283153	-2.876989
7	2.530483	-3.959082	0.559863
6	3.359387	-4.414467	-0.545016
1	3.047121	-5.417699	-0.855373
1	3.250049	-3.746832	-1.393190
1	4.416971	-4.458463	-0.256013
6	2.305323	-4.947985	1.604665
1	2.185093	-4.478492	2.580336
1	1.422877	-5.569857	1.395675
1	3.179861	-5.601560	1.667039
8	2.327257	-1.895669	-0.379293
6	-0.260746	-0.981230	3.123365
6	-0.757647	0.219206	3.566413
1	-0.516820	-1.893825	3.650942
6	-0.393807	1.379457	2.860009
6	0.450683	1.282155	1.775175
1	0.764551	2.163777	1.230189
7	0.949545	0.105567	1.337133
1	-1.416846	0.264302	4.425186
35	-1.016740	3.142838	3.459647

[8-9]‡ P1-C1 *endo re-re*

Number of imaginary frequencies= 1
The smallest frequencies are=-247.7024 5.0957 10.4338 cm(-1)
Electronic energy= -7222.6348462
Zero-point correction= 1.755700
(Hartree/Particle)
Thermal correction to Energy= 1.874115
Thermal correction to Enthalpy= 1.875059
Thermal correction to Gibbs Free Energy= 1.593083
Sum of electronic and zero-point Energies= -7220.879146
Sum of electronic and thermal Energies= -7220.760731
Sum of electronic and thermal Enthalpies= -7220.759787
Sum of electronic and thermal Free Energies= -7221.041763

.....

Cartesian Coordinates

.....

26	4.295437	4.787355	1.873202
15	2.562805	1.624327	-1.886450
15	4.540775	0.128166	0.933392
6	3.967400	3.424797	0.318842
6	4.154449	2.746058	1.580220
6	3.132327	3.194430	2.473067
1	3.009849	2.884580	3.501734
6	2.334999	4.162811	1.791665
1	1.508954	4.716069	2.216440
6	2.848848	4.307323	0.469963
1	2.478862	4.983288	-0.285896
6	6.237760	5.325940	2.375800
1	7.098839	4.677139	2.283312
6	5.382516	5.426388	3.515834
1	5.479243	4.865002	4.435574
6	4.350403	6.365820	3.212671
1	3.525224	6.633413	3.859406
6	4.567478	6.847204	1.885567
1	3.938634	7.547022	1.351141
6	5.733355	6.207169	1.369596
1	6.141457	6.344865	0.377657
6	4.764269	3.153492	-0.912977
6	6.097323	3.584280	-0.982639
1	6.500778	4.139337	-0.145298
6	6.906087	3.300278	-2.082949
1	7.941613	3.625013	-2.092786
6	6.383592	2.576754	-3.152403
1	7.004122	2.336950	-4.009854
6	5.061542	2.133443	-3.105789
1	4.672316	1.556624	-3.937792
6	4.241815	2.397477	-1.997422
6	5.179769	1.672470	1.830733
1	6.093160	1.961786	1.308082
6	5.519495	1.464681	3.309230
1	6.298243	0.706930	3.429948
1	4.650642	1.149189	3.893039
1	5.881822	2.407557	3.730235
6	2.354461	0.721721	-3.482111
6	2.616243	-0.658015	-3.490617
1	2.930053	-1.152734	-2.579016
6	2.435227	-1.405154	-4.656733
1	2.642167	-2.470234	-4.648829
6	1.979184	-0.786494	-5.822554
1	1.824055	-1.370575	-6.725138
6	1.719168	0.586530	-5.822771
1	1.363613	1.074301	-6.725932
6	1.908661	1.338316	-4.662386
1	1.692248	2.400819	-4.679778
6	1.403676	3.038178	-2.070656
6	1.740556	4.197606	-2.788378
1	2.733256	4.302541	-3.215998
6	0.806428	5.222696	-2.947956
1	1.077442	6.116537	-3.502721
6	-0.475220	5.095145	-2.402608
1	-1.208071	5.886350	-2.533051
6	-0.814284	3.945084	-1.687034
1	-1.807464	3.839152	-1.267659
6	0.124988	2.927386	-1.509523
1	-0.137097	2.044720	-0.936918
6	5.833954	-0.351351	-0.288109
6	5.486642	-1.402292	-1.149405
1	4.518843	-1.879066	-1.036746
6	6.371623	-1.829989	-2.138243
6	7.598250	-1.194274	-2.319206
1	8.275893	-1.511055	-3.103890
6	7.930661	-0.131925	-1.478082
6	7.072228	0.277409	-0.457198
1	7.378658	1.096619	0.178492
6	4.568586	-1.271452	2.131450
6	3.559513	-1.295134	3.107628
1	2.867673	-0.465451	3.195798
6	3.410474	-2.401824	3.940594
6	4.233691	-3.519354	3.798021
1	4.087756	-4.396385	4.418651
6	5.223171	-3.501141	2.818428
6	5.409585	-2.382662	2.005045
1	6.188526	-2.406511	1.253458
29	2.440281	0.234724	-0.102190
6	6.091969	-4.714890	2.637310
6	2.273122	-2.466927	4.920975
6	5.997085	-3.025715	-2.969085
6	9.225234	0.592960	-1.725516
9	9.228151	1.197511	-2.940401
9	9.467207	1.552928	-0.806092
9	10.282676	-0.251335	-1.717126
9	6.178690	-4.181980	-2.282707
9	6.720677	-3.117967	-4.102424
9	4.686754	-3.002237	-3.326825
9	7.068699	-4.789599	3.569641
9	6.695617	-4.731925	1.427184
9	5.369560	-5.858128	2.739829
9	2.644887	-3.031518	6.090498
9	1.757515	-1.251404	5.200191
9	1.250767	-3.226987	4.437728
6	1.975894	-2.751384	0.404035
6	0.812390	-2.465302	1.213731
6	0.453886	-1.190357	1.765515
1	0.409642	-3.292585	1.779814
77	-3.400058	-1.296214	-1.447055
15	-5.267032	-0.538264	-0.377953
8	-5.260515	0.604632	0.820413
8	-6.330094	0.174129	-1.442135

7	-5.966540	-1.799001	0.479356
6	-4.982080	1.930143	0.525274
6	-3.757894	2.439098	1.010716
1	-3.119051	1.781975	1.589817
6	-3.415964	3.740371	0.740351
1	-2.486805	4.152909	1.120380
6	-4.248649	4.546652	-0.083622
6	-3.843320	5.851210	-0.476787
1	-2.895142	6.232401	-0.106594
6	-4.622758	6.608483	-1.322358
1	-4.300125	7.600830	-1.623550
6	-5.844831	6.086323	-1.809761
1	-6.447826	6.678270	-2.492188
6	-6.275796	4.832860	-1.431574
1	-7.211195	4.445828	-1.818952
6	-5.501727	4.025512	-0.552583
6	-5.909897	2.701986	-0.155887
6	-7.269139	2.156938	-0.436261
6	-8.460106	2.845577	-0.001972
6	-8.420903	4.023158	0.796991
1	-7.464244	4.422286	1.110883
6	-9.579451	4.655925	1.192965
1	-9.518930	5.549286	1.807975
6	-10.845783	4.150826	0.814544
1	-11.749891	4.664936	1.127243
6	-10.923652	2.997935	0.066874
1	-11.888643	2.583726	-0.213333
6	-9.748662	2.311610	-0.344190
6	-9.832602	1.090689	-1.066300
1	-10.811106	0.699068	-1.329435
6	-8.695431	0.398867	-1.398607
1	-8.734292	-0.551473	-1.920471
6	-7.430840	0.928255	-1.060056
6	-5.328337	-3.110858	0.180972
1	-4.591423	-3.316290	0.967031
6	-6.342526	-4.240820	0.175098
6	-6.026818	-5.466230	0.773385
1	-5.072363	-5.581304	1.282332
6	-6.925397	-6.535560	0.723005
1	-6.667750	-7.480499	1.193528
6	-8.155374	-6.385415	0.079134
1	-8.858562	-7.212779	0.045011
6	-8.480070	-5.162129	-0.517078
1	-9.437494	-5.037574	-1.015792
6	-7.578937	-4.098569	-0.471435
1	-7.831501	-3.144311	-0.925590
6	-4.594830	-3.051752	-1.163554
1	-5.333876	-3.113068	-1.971371
1	-3.953525	-3.933830	-1.249482
6	-6.667729	-1.732629	1.807972
1	-7.141378	-2.714903	1.886702
6	-5.678308	-1.640575	2.970885
6	-5.126431	-2.826175	3.482675
1	-5.452995	-3.781295	3.079979
6	-4.182184	-2.800242	4.512444
1	-3.769148	-3.731660	4.890196
6	-3.790282	-1.580866	5.068470
1	-3.064029	-1.554831	5.876307
6	-4.357260	-0.394938	4.591550
1	-4.076297	0.558110	5.032312
6	-5.290662	-0.424603	3.553663
1	-5.716327	0.505727	3.199489
6	-7.806830	-0.715833	1.852804
1	-8.514428	-0.911722	1.044022
1	-7.468556	0.315852	1.765797
1	-8.334977	-0.822796	2.805277
6	-2.525378	-1.128243	0.544821
1	-1.882608	-0.253504	0.590611
1	-3.221230	-1.183407	1.377318
6	-1.992560	-2.367340	0.062609
1	-2.496886	-3.272067	0.385508
6	-0.734650	-2.534722	-0.568683
1	-0.209022	-1.652832	-0.907242
6	-4.223052	-1.143972	-3.493042
1	-5.215202	-1.589672	-3.481890
6	-3.126479	-2.048729	-3.521760
1	-3.365222	-3.111893	-3.550807
6	-1.761944	-1.710569	-4.097577
1	-1.805699	-1.728966	-5.197714
1	-1.073388	-2.507899	-3.807469
6	-1.196652	-0.358774	-3.615835
1	-1.429525	0.434488	-4.332820
1	-0.107346	-0.422356	-3.582652
6	-1.691489	0.068035	-2.237650
1	-0.934668	0.084646	-1.459797
6	-2.806514	0.873821	-2.022098
1	-2.816425	1.461214	-1.109695
6	-3.753039	1.359069	-3.101273
1	-4.645283	1.750086	-2.607389
1	-3.289387	2.204787	-3.630586
6	-4.170800	0.260249	-4.102568
1	-3.492722	0.252237	-4.962362
1	-5.160724	0.506430	-4.498882
6	-0.336645	-3.784997	-1.225085
6	-0.871124	-5.040118	-0.873180
6	0.626971	-3.732315	-2.250610
6	-0.457207	-6.196872	-1.530475
1	-1.601547	-5.116434	-0.074047
6	1.036553	-4.889497	-2.909893
1	1.058532	-2.774681	-2.515986
6	0.497635	-6.127752	-2.551846
1	-0.877255	-7.156874	-1.244075
1	1.782672	-4.824824	-3.697000
1	0.817501	-7.032100	-3.061287
7	2.527335	-3.998332	0.475409
6	3.530308	-4.417710	-0.497322
1	3.343462	-5.458859	-0.776613
1	3.460363	-3.806065	-1.391307
1	4.542655	-4.343739	-0.084232
6	2.172731	-5.004927	1.472704
1	1.857177	-4.544831	2.407745
1	1.379541	-5.669547	1.108073
1	3.059622	-5.605100	1.688340
8	2.451419	-1.919421	-0.431553
6	-0.453527	-1.173928	2.861533
6	-0.885357	0.012338	3.418690
1	-0.794742	-2.114293	3.277071
6	-0.417740	1.201507	2.853854
6	0.455954	1.160391	1.781903
1	0.835530	2.067905	1.329475
7	0.890375	0.000915	1.248314
1	-1.574634	0.013224	4.253959
35	-0.962326	2.928041	3.596268

---

9 P1-C1 *endo re-re*

Number of imaginary frequencies= 0
The smallest frequencies are= 11.0939 11.9004 15.4503 cm(-1)
Electronic energy= -7222.6615389
Zero-point correction= 1.759971
(Hartree/Particle)
Thermal correction to Energy= 1.877378
Thermal correction to Enthalpy= 1.878322
Thermal correction to Gibbs Free Energy= 1.600701
Sum of electronic and zero-point Energies= -7220.901568
Sum of electronic and thermal Energies= -7220.784161
Sum of electronic and thermal Enthalpies= -7220.783217
Sum of electronic and thermal Free Energies= -7221.060837

.....

Cartesian Coordinates

.....

26	3.898852	4.895652	1.574662
15	2.505678	1.493604	-2.125655
15	4.288697	0.175760	0.959066
6	3.705985	3.444438	0.076183
6	3.795150	2.839976	1.385025
6	2.704916	3.329922	2.168481
1	2.504626	3.081424	3.200907
6	1.956141	4.247582	1.370366
1	1.097177	4.818407	1.696106

6	2.575495	4.324161	0.088722
1	2.264191	4.953707	-0.730918
6	5.792080	5.494294	2.188071
1	6.669873	4.861403	2.187112
6	4.856658	5.629564	3.259116
1	4.895020	5.110323	4.207423
6	3.833127	6.532902	2.840018
1	2.959487	6.812483	3.413998
6	4.136058	6.958018	1.510580
1	3.534624	7.619056	0.900597
6	5.346139	6.318416	1.108535
1	5.822201	6.417649	0.142497
6	4.601876	3.115393	-1.070793
6	5.931854	3.561327	-1.059641
1	6.261421	4.171234	-0.227766
6	6.829249	3.225715	-2.073325
1	7.859437	3.562799	-2.019111
6	6.400546	2.437933	-3.139203
1	7.088314	2.163539	-3.932731
6	5.082946	1.980105	-3.172868
1	4.764083	1.355996	-4.000352
6	4.176842	2.291200	-2.147363
6	4.811713	1.805365	1.784469
1	5.752783	2.076861	1.304325
6	5.057391	1.721512	3.293739
1	5.830874	0.984693	3.525912
1	4.156839	1.451760	3.851920
1	5.390093	2.700158	3.652133
6	2.428632	0.521864	-3.688723
6	2.852147	-0.816242	-3.642761
1	3.198788	-1.241976	-2.708631
6	2.802474	-1.614770	-4.786679
1	3.139747	-2.644643	-4.734638
6	2.307189	-1.092385	-5.983579
1	2.251864	-1.718018	-6.869740
6	1.879338	0.236563	-6.036056
1	1.490742	0.648092	-6.963134
6	1.945102	1.043281	-4.898745
1	1.603394	2.070385	-4.957956
6	1.336508	2.875912	-2.409276
6	1.672124	3.982612	-3.206747
1	2.662318	4.055669	-3.646738
6	0.740997	4.999371	-3.423022
1	1.009247	5.854494	-4.036807
6	-0.534241	4.914402	-2.854057
1	-1.263253	5.701658	-3.022807
6	-0.871397	3.815359	-2.061827
1	-1.858525	3.744447	-1.623095
6	0.064321	2.806106	-1.828621
1	-0.194066	1.965707	-1.193434
6	5.697310	-0.323147	-0.121857
6	5.459598	-1.417378	-0.964535
1	4.499379	-1.918269	-0.922542
6	6.443022	-1.861064	-1.847170
6	7.664916	-1.198737	-1.942312
1	8.420315	-1.526745	-2.647662
6	7.891725	-0.096161	-1.117536
6	6.932187	0.330273	-0.199030
1	7.159065	1.180042	0.430233
6	4.284222	-1.120836	2.267199
6	3.261048	-1.083798	3.229720
1	2.543213	-0.270423	3.240426
6	3.156952	-2.100436	4.179169
6	4.022675	-3.194066	4.157214
1	3.913604	-3.997554	4.877271
6	5.017017	-3.242328	3.183799
6	5.166913	-2.207576	2.261673
1	5.958559	-2.272909	1.526397
29	2.304474	0.180445	-0.293679
6	5.923673	-4.441784	3.133663
6	2.045863	-2.101369	5.191645
6	6.179031	-3.107291	-2.645813
6	9.187503	0.652943	-1.270096
9	9.300671	1.193357	-2.508789
9	9.309511	1.665366	-0.383888
9	10.257425	-0.158557	-1.106329
9	6.381976	-4.222665	-1.900409
9	6.969383	-3.204166	-3.732114
9	4.890161	-3.170284	-3.072659
9	6.812859	-4.453036	4.150498
9	6.628989	-4.501331	1.981996
9	5.211436	-5.593426	3.225971
9	2.466653	-2.530160	6.399824
9	1.495784	-0.879552	5.361999
9	1.042401	-2.941324	4.815327
6	1.904720	-2.855651	0.275697
6	0.471302	-2.584441	0.720069
6	0.293470	-1.321795	1.528937
1	0.094693	-3.410216	1.320553
77	-3.398990	-1.374753	-1.577203
15	-5.202687	-0.547572	-0.412545
8	-5.095100	0.556870	0.829907
8	-6.311413	0.250549	-1.379204
7	-5.911439	-1.805403	0.452277
6	-4.739953	1.865575	0.562120
6	-3.463728	2.280947	1.005437
1	-2.848336	1.564393	1.537783
6	-3.048163	3.565601	0.759888
1	-2.076417	3.905325	1.105124
6	-3.865358	4.454340	0.007362
6	-3.398937	5.747892	-0.354242
1	-2.414650	6.057170	-0.012221
6	-4.163181	6.581445	-1.139814
1	-3.793667	7.564225	-1.417728
6	-5.430961	6.149392	-1.598070
1	-6.022370	6.800009	-2.235776
6	-5.920968	4.910030	-1.247307
1	-6.891611	4.593281	-1.610658
6	-5.165169	4.026385	-0.427398
6	-5.641663	2.718697	-0.054722
6	-7.046725	2.275014	-0.283614
6	-8.163596	3.037382	0.221348
6	-8.003136	4.187366	1.045704
1	-7.007585	4.504579	1.330384
6	-9.092460	4.897434	1.502718
1	-8.937739	5.767693	2.134236
6	-10.408124	4.501622	1.164997
1	-11.256769	5.076019	1.524781
6	-10.603783	3.376563	0.396724
1	-11.608453	3.044916	0.147213
6	-9.502507	2.612313	-0.076179
6	-9.709209	1.420851	-0.821847
1	-10.724875	1.111694	-1.052178
6	-8.642771	0.655417	-1.219175
1	-8.776182	-0.275106	-1.760695
6	-7.325580	1.075824	-0.926222
6	-5.318610	-3.134465	0.126799
1	-4.566352	-3.366158	0.891324
6	-6.371224	-4.229289	0.147882
6	-6.094524	-5.461548	0.751570
1	-5.137585	-5.608883	1.247618
6	-7.032498	-6.497591	0.720948
1	-6.803539	-7.448006	1.195536
6	-8.264214	-6.307308	0.091318
1	-8.997881	-7.108355	0.071659
6	-8.550879	-5.076750	-0.509846
1	-9.508885	-4.920830	-0.998773
6	-7.610995	-4.046813	-0.482562
1	-7.833035	-3.087152	-0.941240
6	-4.613402	-3.106013	-1.235594
1	-5.374847	-3.161841	-2.023754
1	-4.007562	-4.013187	-1.318606
6	-6.566210	-1.734907	1.802624
1	-7.062251	-2.705112	1.892971
6	-5.542587	-1.674544	2.940006
6	-4.995473	-2.874662	3.422018
1	-5.344589	-3.819636	3.014814
6	-4.027176	-2.876948	4.430088
1	-3.620992	-3.819991	4.786061
6	-3.603492	-1.671633	4.993211

1	-2.859688	-1.668477	5.785575
6	-4.163725	-0.470937	4.545815
1	-3.858830	0.471928	4.992630
6	-5.123025	-0.473293	3.531756
1	-5.544447	0.467780	3.202258
6	-7.678474	-0.691504	1.889878
1	-8.415431	-0.865558	1.102408
1	-7.317948	0.332170	1.797111
1	-8.181026	-0.789747	2.857130
6	-2.471556	-1.319363	0.398784
1	-1.910796	-0.397725	0.518767
1	-3.162842	-1.498940	1.218950
6	-1.885194	-2.434946	-0.268969
1	-2.313888	-3.400077	-0.007558
6	-0.406873	-2.543637	-0.608745
1	-0.059801	-1.663990	-1.149735
6	-4.239387	-1.252429	-3.582268
1	-5.235836	-1.690898	-3.589431
6	-3.139826	-2.174187	-3.601283
1	-3.388244	-3.235393	-3.633973
6	-1.800242	-1.847576	-4.243293
1	-1.900148	-1.824234	-5.340277
1	-1.117488	-2.669422	-4.018108
6	-1.181161	-0.525231	-3.740922
1	-1.355032	0.281458	-4.461532
1	-0.094966	-0.635728	-3.677543
6	-1.693123	-0.076752	-2.373063
1	-0.937085	-0.042359	-1.594558
6	-2.793634	0.761883	-2.177287
1	-2.780716	1.381328	-1.286244
6	-3.726129	1.247210	-3.270477
1	-4.613154	1.663799	-2.786101
1	-3.246153	2.074596	-3.815761
6	-4.161265	0.130836	-4.242923
1	-3.478862	0.087712	-5.099268
1	-5.143239	0.385375	-4.655301
6	-0.079098	-3.776945	-1.436247
6	-0.472375	-5.060694	-1.028142
6	0.711293	-3.657467	-2.586481
6	-0.096577	-6.189997	-1.759944
1	-1.067057	-5.186364	-0.127378
6	1.089017	-4.782598	-3.321554
1	1.041928	-2.673896	-2.898799
6	0.685905	-6.055189	-2.910345
1	-0.412619	-7.175550	-1.428910
1	1.696950	-4.660853	-4.213959
1	0.978240	-6.933756	-3.478527
7	2.500528	-4.005813	0.640755
6	3.651396	-4.502257	-0.117173
1	3.517727	-5.576271	-0.275645
1	3.692381	-4.011682	-1.086091
1	4.590024	-4.340509	0.419302
6	2.021547	-4.887636	1.707248
1	1.540267	-4.321303	2.503987
1	1.331336	-5.643725	1.316432
1	2.887703	-5.390006	2.141916
8	2.451300	-2.061772	-0.525274
6	-0.396134	-1.382809	2.743770
6	-0.696357	-0.219227	3.441644
1	-0.713102	-2.340313	3.137041
6	-0.309761	0.986666	2.869258
6	0.376112	1.001933	1.662213
1	0.692290	1.928165	1.199440
7	0.693420	-0.136518	1.015736
1	-1.230304	-0.260857	4.381885
35	-0.713595	2.671625	3.762128

---

8 P1-C1 *endo si-re*

Number of imaginary frequencies= 0
The smallest frequencies are= 6.7103 10.7191 12.5515 cm(-1)
Electronic energy= -7222.6313862
Zero-point correction= 1.754774
(Hartree/Particle)
Thermal correction to Energy= 1.874755
Thermal correction to Enthalpy= 1.875699
Thermal correction to Gibbs Free Energy= 1.587896
Sum of electronic and zero-point Energies= -7220.876612
Sum of electronic and thermal Energies= -7220.756632
Sum of electronic and thermal Enthalpies= -7220.755688
Sum of electronic and thermal Free Energies= -7221.043491

.....

Cartesian Coordinates

.....

26	3.664540	4.915752	2.324858
15	2.301603	1.884705	-1.677665
15	4.847618	0.531832	0.895544
6	3.428097	3.790679	0.568043
6	4.081870	3.022424	1.595888
6	3.195018	2.946413	2.715012
1	3.399770	2.437762	3.647361
6	2.013720	3.680525	2.398279
1	1.173539	3.848301	3.058804
6	2.159878	4.208570	1.081812
1	1.445466	4.826642	0.557252
6	5.390318	6.052408	2.566718
1	6.349728	5.812212	2.128320
6	4.910786	5.599213	3.833425
1	5.439383	4.948964	4.517517
6	3.589786	6.111536	4.013532
1	2.942158	5.914584	4.857785
6	3.252460	6.880402	2.858136
1	2.306952	7.374220	2.675869
6	4.364599	6.845272	1.964886
1	4.408193	7.311676	0.990014
6	3.985413	4.006117	-0.795795
6	5.023659	4.930415	-0.982547
1	5.371874	5.487664	-0.122557
6	5.613217	5.131353	-2.230776
1	6.422968	5.847235	-2.338262
6	5.154874	4.409390	-3.329920
1	5.598649	4.552289	-4.310460
6	4.127302	3.479696	-3.166203
1	3.795783	2.917532	-4.030651
6	3.544962	3.245332	-1.910031
6	5.375220	2.283247	1.401850
1	5.864259	2.688986	0.511549
6	6.350335	2.371261	2.578213
1	7.247545	1.772090	2.397046
1	5.894725	2.029300	3.511184
1	6.655361	3.412838	2.714922
6	2.203467	1.130534	-3.356081
6	3.297277	0.348027	-3.764475
1	4.177224	0.288068	-3.133206
6	3.285071	-0.319558	-4.986880
1	4.144817	-0.913260	-5.283302
6	2.167608	-0.223663	-5.822599
1	2.148892	-0.750610	-6.771988
6	1.080730	0.561460	-5.433932
1	0.214780	0.651195	-6.083695
6	1.097587	1.238521	-4.209835
1	0.248125	1.849850	-3.927337
6	0.718655	2.797272	-1.462523
6	0.375262	3.893661	-2.270458
1	1.035060	4.202114	-3.076509
6	-0.806247	4.598530	-2.035503
1	-1.067925	5.441515	-2.668708
6	-1.641022	4.230628	-0.974747
1	-2.555562	4.784773	-0.784909
6	-1.293223	3.152783	-0.157946
1	-1.926990	2.883348	0.681504
6	-0.124231	2.426153	-0.403892
1	0.157092	1.595413	0.239850
6	6.160757	-0.043198	-0.254063
6	6.761141	-1.308826	-0.192164
1	6.555445	-1.982364	0.630726
6	7.619142	-1.731518	-1.208797
6	7.872389	-0.928289	-2.319476
1	8.528815	-1.268984	-3.110545
6	7.245785	0.314681	-2.399468

6	6.401401	0.758317	-1.381675
1	5.907470	1.719413	-1.489860
6	5.018653	-0.432753	2.451119
6	3.824046	-0.650368	3.150695
1	2.891447	-0.290985	2.730415
6	3.838115	-1.311438	4.380124
6	5.032820	-1.778134	4.924911
1	5.041372	-2.300157	5.874271
6	6.221846	-1.555918	4.229222
6	6.223839	-0.880159	3.007840
1	7.166122	-0.708384	2.500789
29	2.778057	0.308790	-0.123307
6	7.536708	-1.984624	4.820174
6	2.533140	-1.566892	5.082463
6	8.325242	-3.052707	-1.064398
6	7.408498	1.181108	-3.618254
9	6.274653	1.192214	-4.368515
9	7.660244	2.469165	-3.289297
9	8.408725	0.764755	-4.421629
9	7.572548	-3.959306	-0.403415
9	9.477231	-2.918073	-0.359941
9	8.660198	-3.587904	-2.258501
9	8.172205	-0.949133	5.422037
9	8.379675	-2.455898	3.872558
9	7.389723	-2.951333	5.751251
9	2.697905	-1.788422	6.405051
9	1.683220	-0.520562	4.950946
9	1.891764	-2.652147	4.581568
6	3.717082	-2.199699	-1.422304
6	2.266743	-2.689207	0.364976
6	4.055059	-3.523701	-1.597412
1	4.141850	-1.433780	-2.055417
6	2.631776	-4.070579	0.225988
6	3.511252	-4.494081	-0.742528
1	2.182039	-4.796429	0.896772
6	1.300919	-2.349744	1.344383
6	0.784759	-1.072936	1.671260
8	1.253062	0.044140	1.243250
7	2.858204	-1.774707	-0.476334
1	0.943827	-3.192133	1.919768
7	-0.293757	-0.985039	2.534911
6	-0.644058	0.283469	3.151514
1	-0.622359	0.191916	4.244120
1	-1.654239	0.599007	2.860340
1	0.068291	1.046418	2.843759
6	-1.016273	-2.135229	3.045918
1	-0.590099	-2.507096	3.987782
1	-1.017986	-2.950923	2.322186
1	-2.053266	-1.848256	3.231155
77	-3.752460	-0.928732	-1.451154
15	-5.568317	-0.654832	-0.122233
8	-5.731716	0.592528	0.941835
8	-6.926857	-0.450872	-1.046731
7	-5.679788	-1.946209	0.923955
6	-6.079094	1.876305	0.526745
6	-5.087889	2.867382	0.687864
1	-4.140805	2.581623	1.132009
6	-5.346841	4.153791	0.284855
1	-4.601682	4.932741	0.417204
6	-6.582679	4.476536	-0.338784
6	-6.826075	5.781049	-0.847378
1	-6.054912	6.537066	-0.724863
6	-8.002950	6.078022	-1.496531
1	-8.176155	7.076086	-1.887882
6	-8.984907	5.073404	-1.668016
1	-9.901727	5.304026	-2.202776
6	-8.788405	3.803777	-1.169419
1	-9.548683	3.046233	-1.317589
6	-7.593422	3.465421	-0.475537
6	-7.351341	2.144541	0.048377
6	-8.406894	1.093197	0.060834
6	-9.680334	1.300592	0.702366
6	-9.970510	2.458885	1.476432
1	-9.209141	3.219356	1.601462
6	-11.197327	2.619835	2.083137
1	-11.390402	3.509556	2.675509
6	-12.205999	1.636350	1.948323
1	-13.169816	1.780543	2.427542
6	-11.953325	0.493192	1.224820
1	-12.710481	-0.280633	1.129219
6	-10.693423	0.288080	0.599397
6	-10.414014	-0.916840	-0.100733
1	-11.192078	-1.669867	-0.186801
6	-9.167061	-1.142740	-0.628427
1	-8.915217	-2.069759	-1.132232
6	-8.174915	-0.146216	-0.511464
6	-4.738522	-3.051055	0.586947
1	-3.876222	-2.972082	1.260974
6	-5.368371	-4.419596	0.781810
6	-4.646732	-5.435110	1.418531
1	-3.659501	-5.218212	1.819758
6	-5.188082	-6.717544	1.546711
1	-4.617786	-7.497316	2.043692
6	-6.462396	-6.991841	1.046206
1	-6.887641	-7.985867	1.150775
6	-7.192411	-5.978904	0.415068
1	-8.187311	-6.184951	0.030081
6	-6.647353	-4.702444	0.280632
1	-7.217708	-3.910452	-0.197595
6	-4.273235	-2.910014	-0.866731
1	-5.077190	-3.256898	-1.525495
1	-3.415942	-3.564283	-1.038747
6	-6.245449	-2.023774	2.311838
1	-6.536004	-3.073029	2.404208
6	-5.199301	-1.771074	3.396031
6	-4.730148	-2.854228	4.152685
1	-5.066943	-3.858410	3.908813
6	-3.853357	-2.658591	5.223467
1	-3.508043	-3.511452	5.801195
6	-3.427313	-1.370232	5.550493
1	-2.748147	-1.212812	6.383439
6	-3.871571	-0.284645	4.789882
1	-3.541240	0.720885	5.034889
6	-4.748873	-0.482022	3.721490
1	-5.100088	0.369712	3.151930
6	-7.526802	-1.222171	2.549566
1	-8.291583	-1.490990	1.819569
1	-7.374226	-0.144176	2.521288
1	-7.902556	-1.482962	3.543408
6	-2.587962	-0.315513	0.281443
1	-2.213057	0.684827	0.093668
1	-3.033954	-0.436279	1.264608
6	-1.838612	-1.435361	-0.208268
1	-1.963779	-2.380301	0.305461
6	-1.054309	-1.400529	-1.353484
1	-0.769945	-0.433889	-1.750436
6	-5.087949	-1.187663	-3.283040
1	-5.859481	-1.883561	-2.967586
6	-3.832697	-1.739550	-3.576889
1	-3.724840	-2.818683	-3.479497
6	-2.766276	-1.084494	-4.433055
1	-2.994582	-1.271927	-5.492751
1	-1.819954	-1.591755	-4.230155
6	-2.585718	0.432214	-4.203801
1	-3.258172	0.997209	-4.855299
1	-1.573146	0.703137	-4.505793
6	-2.794553	0.894742	-2.768890
1	-1.906989	1.181492	-2.212768
6	-4.001973	1.337800	-2.272086
1	-3.971677	1.948454	-1.374298
6	-5.298016	1.389930	-3.053668
1	-6.108918	1.570225	-2.349049
1	-5.266403	2.263832	-3.719837
6	-5.616504	0.118110	-3.874450
1	-5.231825	0.217675	-4.893678
1	-6.702811	0.033394	-3.963986
6	-0.403031	-2.548862	-1.975238
6	-0.623965	-3.881078	-1.566788
6	0.491117	-2.314106	-3.039071
6	0.016455	-4.933820	-2.213585

1	-1.282158	-4.095148	-0.731658
6	1.134667	-3.370603	-3.680759
1	0.690370	-1.294219	-3.350691
6	0.894626	-4.684940	-3.275194
1	-0.161389	-5.953795	-1.884894
1	1.829062	-3.162879	-4.488766
1	1.396789	-5.510050	-3.771684
1	3.762749	-5.544306	-0.846572
35	5.257096	-4.025836	-3.061398

[8-9]‡-P1-C1 *endo si-re*

Number of imaginary frequencies= 1
The smallest frequencies are= -207.6434 9.1752 12.4396 cm(-1)
Electronic energy= -7222.6226241
Zero-point correction= 1.754801
(Hartree/Particle)
Thermal correction to Energy= 1.873691
Thermal correction to Enthalpy= 1.874635
Thermal correction to Gibbs Free Energy= 1.591070
Sum of electronic and zero-point Energies= -7220.867823
Sum of electronic and thermal Energies= -7220.748933
Sum of electronic and thermal Enthalpies= -7220.747989
Sum of electronic and thermal Free Energies= -7221.031554

.....

Cartesian Coordinates

.....

26	3.537559	4.933678	2.365887
15	2.430775	1.875807	-1.665330
15	4.905493	0.554700	1.039527
6	3.429227	3.780081	0.619380
6	4.030930	3.035572	1.696227
6	3.078478	2.960040	2.760166
1	3.236207	2.472982	3.713164
6	1.906457	3.668378	2.361093
1	1.023868	3.829111	2.965776
6	2.124278	4.180751	1.048957
1	1.433778	4.779267	0.472552
6	5.226402	6.096288	2.712956
1	6.222867	5.856508	2.366250
6	4.645625	5.680501	3.950010
1	5.121395	5.062442	4.699766
6	3.309717	6.183300	4.000569
1	2.594658	6.009075	4.793896
6	3.064627	6.909198	2.795041
1	2.133867	7.385865	2.517082
6	4.248422	6.856829	2.000515
1	4.368959	7.289547	1.016704
6	4.054965	3.999464	-0.713703
6	5.099945	4.924240	-0.851466
1	5.417968	5.471254	0.026979
6	5.728715	5.142413	-2.077845
1	6.542167	5.858646	-2.149143
6	5.304417	4.439891	-3.203170
1	5.778730	4.600162	-4.166453
6	4.276812	3.503235	-3.086551
1	3.975055	2.948696	-3.967044
6	3.657427	3.251235	-1.852439
6	5.345107	2.315403	1.597922
1	5.895256	2.730304	0.747999
6	6.227529	2.414701	2.844478
1	7.176422	1.890035	2.701335
1	5.735577	1.999638	3.728511
1	6.446755	3.467535	3.042745
6	2.391338	1.092887	-3.332333
6	3.507054	0.326948	-3.714362
1	4.378408	0.285580	-3.070463
6	3.523078	-0.356459	-4.928375
1	4.398868	-0.934860	-5.208336
6	2.411772	-0.299652	-5.775985
1	2.415471	-0.840972	-6.717503
6	1.298533	0.457033	-5.406221
1	0.432020	0.507170	-6.059319
6	1.288060	1.155219	-4.194790
1	0.416130	1.741368	-3.926972
6	0.821357	2.743792	-1.509722
6	0.499895	3.859966	-2.297940
1	1.203277	4.220662	-3.043107
6	-0.720276	4.513852	-2.121386
1	-0.966645	5.373972	-2.737444
6	-1.620643	4.066426	-1.148682
1	-2.570886	4.573649	-1.015495
6	-1.297192	2.964945	-0.353680
1	-1.992309	2.616367	0.403092
6	-0.083017	2.299438	-0.534314
1	0.182698	1.454867	0.094702
6	6.293799	0.064811	-0.065657
6	6.960642	-1.165479	0.020071
1	6.765570	-1.846434	0.839220
6	7.864569	-1.546509	-0.972241
6	8.116221	-0.726633	-2.071256
1	8.809893	-1.035511	-2.843436
6	7.438380	0.487649	-2.166800
6	6.533986	0.883633	-1.180464
1	5.999009	1.821470	-1.298940
6	5.057403	-0.507350	2.534476
6	3.860544	-1.028522	3.037527
1	2.924592	-0.778098	2.550358
6	3.868006	-1.864717	4.156400
6	5.061056	-2.191017	4.793940
1	5.067263	-2.851295	5.652848
6	6.254839	-1.660486	4.299044
6	6.260726	-0.824539	3.183111
1	7.205553	-0.440327	2.816814
29	2.903091	0.325791	-0.082593
6	7.552954	-1.950421	5.003010
6	2.559615	-2.451160	4.607937
6	8.610223	-2.846017	-0.825761
6	7.612303	1.370148	-3.373227
9	6.488334	1.382427	-4.136914
9	7.853824	2.654152	-3.023934
9	8.625305	0.968745	-4.167670
9	7.881874	-3.773729	-0.165950
9	9.758568	-2.681039	-0.124801
9	8.955130	-3.371586	-2.022036
9	7.861216	-0.978438	5.895487
9	8.587481	-2.024083	4.135013
9	7.511463	-3.114038	5.686928
9	2.666246	-3.146959	5.757204
9	1.620683	-1.492507	4.801179
9	2.056466	-3.297205	3.671727
6	3.928713	-2.124015	-1.402345
6	2.015091	-2.667492	-0.167948
6	4.113810	-3.435447	-1.798819
1	4.608779	-1.345105	-1.717953
6	2.191444	-4.030893	-0.536374
6	3.229056	-4.423284	-1.359430
1	1.485060	-4.768909	-0.172994
6	0.853930	-2.324108	0.603451
6	0.674063	-1.140536	1.400386
8	1.299026	-0.049094	1.194626
7	2.905959	-1.737101	-0.620815
1	0.261572	-3.184943	0.877316
7	-0.251755	-1.153567	2.407642
6	-0.606222	0.087336	3.083678
1	-0.164225	0.121637	4.087243
1	-1.693910	0.147711	3.184867
1	-0.242410	0.939027	2.513169
6	-0.863160	-2.350847	2.972582
1	-0.252655	-3.232761	2.791335
1	-1.872361	-2.515991	2.580924
1	-0.937626	-2.223208	4.055264
77	-3.863156	-1.086179	-1.381528
15	-5.660694	-0.580324	-0.078168
8	-5.764089	0.699321	0.970763
8	-6.994161	-0.288662	-1.032086
7	-5.940295	-1.833221	0.996289
6	-6.023332	1.989752	0.524749
6	-4.982236	2.927151	0.699716
1	-4.070876	2.596501	1.185279

6	-5.155612	4.221412	0.276660
1	-4.372862	4.959210	0.427031
6	-6.351918	4.606615	-0.387009
6	-6.506081	5.915526	-0.918754
1	-5.694320	6.626445	-0.787958
6	-7.648784	6.272747	-1.598019
1	-7.753676	7.273583	-2.006419
6	-8.685425	5.325937	-1.777275
1	-9.576029	5.602894	-2.334010
6	-8.575038	4.054329	-1.257603
1	-9.375763	3.340798	-1.411988
6	-7.416561	3.654500	-0.534672
6	-7.266996	2.330411	0.013692
6	-8.389006	1.349658	0.034046
6	-9.651965	1.646237	0.660397
6	-9.883795	2.841636	1.397450
1	-9.083810	3.564312	1.503616
6	-11.102911	3.086672	1.991477
1	-11.250782	4.003801	2.554477
6	-12.161850	2.154315	1.881543
1	-13.119209	2.364828	2.349166
6	-11.966485	0.976865	1.196084
1	-12.763594	0.241918	1.119630
6	-10.716413	0.684867	0.585522
6	-10.498919	-0.555040	-0.074825
1	-11.315085	-1.269218	-0.137580
6	-9.265665	-0.860971	-0.594493
1	-9.061650	-1.814821	-1.069605
6	-8.221940	0.085857	-0.507502
6	-5.148494	-3.050361	0.667266
1	-4.274257	-3.076900	1.332119
6	-5.952390	-4.320737	0.883090
6	-5.363304	-5.428237	1.503569
1	-4.345521	-5.351860	1.879360
6	-6.073078	-6.623823	1.649178
1	-5.603174	-7.475081	2.134108
6	-7.385453	-6.719331	1.182243
1	-7.941236	-7.645164	1.300535
6	-7.983683	-5.614065	0.567314
1	-9.006904	-5.679937	0.207361
6	-7.271194	-4.424888	0.416038
1	-7.737621	-3.560843	-0.049895
6	-4.668892	-2.983773	-0.788970
1	-5.514834	-3.228570	-1.441948
1	-3.919481	-3.764315	-0.945969
6	-6.466387	-1.803597	2.400550
1	-6.834796	-2.821696	2.550373
6	-5.354566	-1.598058	3.427242
6	-4.813040	-2.718634	4.074407
1	-5.182605	-3.708342	3.818319
6	-3.822834	-2.578556	5.050816
1	-3.419601	-3.459926	5.541945
6	-3.360748	-1.308146	5.398238
1	-2.595761	-1.192598	6.160886
6	-3.890203	-0.183843	4.757231
1	-3.540262	0.809085	5.026517
6	-4.875696	-0.326617	3.778253
1	-5.280152	0.553372	3.293144
6	-7.677613	-0.898516	2.632618
1	-8.480922	-1.151682	1.938827
1	-7.453995	0.161838	2.531777
1	-8.039494	-1.074507	3.650323
6	-2.631299	-0.764792	0.388900
1	-2.128352	0.199897	0.350129
1	-3.124181	-0.949664	1.340076
6	-1.997034	-1.875979	-0.260801
1	-2.272389	-2.873770	0.060821
6	-0.841397	-1.762637	-1.071611
1	-0.438422	-0.765154	-1.216620
6	-5.101135	-1.217233	-3.236439
1	-5.980052	-1.803700	-2.984296
6	-3.900060	-1.932990	-3.457096
1	-3.942798	-3.018770	-3.376505
6	-2.756579	-1.417307	-4.312387
1	-3.025622	-1.507390	-5.376257
1	-1.898401	-2.075686	-4.160284
6	-2.338351	0.037730	-4.001485
1	-2.829440	0.731607	-4.692108
1	-1.266187	0.133308	-4.185037
6	-2.613605	0.498739	-2.572049
1	-1.736100	0.712050	-1.972295
6	-3.790272	1.115759	-2.160972
1	-3.725881	1.760556	-1.289438
6	-5.003718	1.352505	-3.039129
1	-5.838780	1.631439	-2.392722
1	-4.808522	2.219146	-3.688235
6	-5.411623	0.130254	-3.891019
1	-4.924819	0.172242	-4.870717
1	-6.487289	0.183527	-4.083905
6	-0.393054	-2.748970	-2.047445
6	-0.905429	-4.060459	-2.105855
6	0.580355	-2.365351	-2.990852
6	-0.466008	-4.948210	-3.084969
1	-1.657338	-4.383180	-1.392787
6	1.017984	-3.255759	-3.969447
1	0.986841	-1.359952	-2.955231
6	0.494723	-4.550225	-4.022320
1	-0.874943	-5.954068	-3.120554
1	1.764446	-2.933662	-4.688414
1	0.831715	-5.245333	-4.785899
1	3.345944	-5.460889	-1.652616
35	5.605669	-3.870390	-2.983613

---

9 P1-C1 *endo si-re*

Number of imaginary frequencies= 0
The smallest frequencies are= 7.3520 12.6874 17.7843 cm(-1)
Electronic energy= -7222.6534935
Zero-point correction= 1.758428
(Hartree/Particle)
Thermal correction to Energy= 1.876614
Thermal correction to Enthalpy= 1.877558
Thermal correction to Gibbs Free Energy= 1.596829
Sum of electronic and zero-point Energies= -7220.895065
Sum of electronic and thermal Energies= -7220.776880
Sum of electronic and thermal Enthalpies= -7220.775935
Sum of electronic and thermal Free Energies= -7221.056665

Cartesian Coordinates

26	3.256921	4.238150	3.458309
15	2.093331	2.283848	-1.218822
15	4.758477	0.407260	0.999729
6	3.109452	3.569550	1.475231
6	3.783381	2.597172	2.297717
6	2.887626	2.210082	3.342722
1	3.109085	1.503464	4.131503
6	1.674997	2.944680	3.184545
1	0.816771	2.904446	3.842099
6	1.814435	3.788870	2.044388
1	1.076660	4.484231	1.670853
6	4.903573	5.374287	4.028178
1	5.888972	5.295373	3.589028
6	4.416070	4.614778	5.135373
1	4.963193	3.852928	5.674277
6	3.061786	5.001072	5.372578
1	2.402666	4.580953	6.120906
6	2.711392	5.997782	4.411340
1	1.741650	6.465515	4.303389
6	3.849201	6.230043	3.582594
1	3.889298	6.908543	2.741451
6	3.667416	4.160287	0.225683
6	4.657531	5.150194	0.303030
1	4.983501	5.472798	1.283455
6	5.224244	5.713082	-0.841397
1	5.994320	6.473051	-0.745449
6	4.795596	5.296460	-2.099054
1	5.224132	5.724827	-2.999647
6	3.822609	4.301467	-2.201892
1	3.516998	3.969163	-3.186749

6	3.263037	3.710249	-1.059008
6	5.120424	1.996016	1.977274
1	5.605115	2.635922	1.233151
6	6.057962	1.858720	3.178987
1	7.043648	1.494495	2.877499
1	5.655039	1.186528	3.941472
1	6.187879	2.843758	3.634533
6	2.014290	1.982817	-3.029288
6	3.082671	1.265690	-3.597401
1	3.912196	0.951445	-2.972439
6	3.097414	0.971644	-4.958967
1	3.934240	0.425132	-5.384271
6	2.032312	1.376392	-5.770619
1	2.034407	1.139143	-6.830407
6	0.965250	2.083343	-5.213850
1	0.132868	2.394598	-5.837976
6	0.954402	2.390374	-3.849571
1	0.114750	2.935892	-3.432911
6	0.487746	3.019227	-0.728007
6	0.111785	4.313032	-1.123026
1	0.731841	4.873375	-1.816808
6	-1.040279	4.897297	-0.594805
1	-1.323620	5.901728	-0.895859
6	-1.814140	4.200844	0.339969
1	-2.690004	4.670794	0.775487
6	-1.451544	2.907641	0.722072
1	-2.042621	2.364368	1.453750
6	-0.306107	2.316346	0.187568
1	0.008214	1.333924	0.521061
6	6.147063	0.335922	-0.216317
6	7.055272	-0.726202	-0.330067
1	7.034965	-1.553645	0.367306
6	7.990288	-0.741984	-1.364472
6	8.035874	0.281507	-2.311324
1	8.757508	0.254711	-3.119152
6	7.122393	1.327894	-2.209193
6	6.184985	1.360166	-1.174920
1	5.470901	2.177478	-1.132471
6	5.044799	-1.026725	2.120036
6	3.969875	-1.903469	2.303155
1	3.025134	-1.695930	1.819432
6	4.111812	-3.050481	3.088243
6	5.319242	-3.334233	3.719492
1	5.433415	-4.228136	4.320876
6	6.390054	-2.454853	3.547799
6	6.263388	-1.315278	2.755045
1	7.124757	-0.673899	2.618096
29	2.732381	0.396551	-0.139466
6	7.690862	-2.709674	4.261892
6	2.930897	-3.969351	3.241419
6	9.003616	-1.852202	-1.454813
6	7.110715	2.441226	-3.222804
9	5.897878	2.550016	-3.821698
9	7.366193	3.639360	-2.648149
9	8.022210	2.259695	-4.199455
9	8.666398	-2.920713	-0.702192
9	10.223813	-1.440348	-1.036569
9	9.158084	-2.283174	-2.729365
9	7.731152	-2.071461	5.455902
9	8.749037	-2.267195	3.546294
9	7.884800	-4.022112	4.509771
9	3.267959	-5.163880	3.764045
9	1.978592	-3.436432	4.046645
9	2.333437	-4.205308	2.044170
6	3.910965	-1.837961	-1.725700
6	1.948717	-2.604274	-0.751934
6	4.285657	-3.127152	-2.075528
1	4.533819	-0.987988	-1.971444
6	2.298084	-3.927036	-1.051880
6	3.482502	-4.206538	-1.723777
1	1.632706	-4.735864	-0.771892
6	0.573425	-2.334681	-0.171872
6	0.624331	-1.519190	1.111551
8	1.177802	-0.391440	1.108697
7	2.767822	-1.580875	-1.066750
1	0.135688	-3.312888	0.014798
7	0.085890	-1.983067	2.251400
6	0.140514	-1.088219	3.412924
1	-0.124934	-1.650263	4.305338
1	-0.561268	-0.256993	3.293325
1	1.146228	-0.679981	3.521454
6	-0.676060	-3.229624	2.370068
1	-0.171850	-4.045480	1.853426
1	-1.690464	-3.112159	1.978651
1	-0.736527	-3.496500	3.423844
77	-3.685349	-0.895944	-1.529037
15	-5.520861	-0.537279	-0.164444
8	-5.720302	0.691081	0.949121
8	-6.924264	-0.315653	-1.058694
7	-5.704047	-1.876460	0.838124
6	-6.166479	1.948579	0.555692
6	-5.227548	3.000369	0.625464
1	-4.228390	2.774149	0.974706
6	-5.592050	4.268243	0.248349
1	-4.877555	5.084445	0.298004
6	-6.898083	4.526993	-0.245559
6	-7.266827	5.822141	-0.700645
1	-6.533759	6.622056	-0.635185
6	-8.517197	6.057963	-1.225293
1	-8.788264	7.050328	-1.573615
6	-9.447674	4.996185	-1.326671
1	-10.424443	5.177392	-1.766082
6	-9.126052	3.732632	-0.880644
1	-9.849441	2.932132	-0.977325
6	-7.852515	3.456691	-0.307350
6	-7.484748	2.148632	0.172240
6	-8.459381	1.024539	0.206576
6	-9.703786	1.098191	0.924453
6	-10.039492	2.192707	1.769977
1	-9.332595	3.005191	1.890435
6	-11.239454	2.227439	2.446429
1	-11.468630	3.071347	3.090907
6	-12.174466	1.172776	2.314398
1	-13.119515	1.217374	2.847715
6	-11.873710	0.087698	1.522588
1	-12.574403	-0.737702	1.426383
6	-10.638138	0.012374	0.823766
6	-10.305462	-1.127428	0.042177
1	-11.026188	-1.935646	-0.045415
6	-9.079670	-1.220530	-0.569718
1	-8.795562	-2.089639	-1.152436
6	-8.158128	-0.156471	-0.452286
6	-4.877380	-3.032223	0.383229
1	-3.967190	-3.061436	0.998242
6	-5.596365	-4.357888	0.569246
6	-4.920855	-5.448204	1.130497
1	-3.899486	-5.320104	1.481635
6	-5.548305	-6.691703	1.251187
1	-5.010925	-7.527823	1.690527
6	-6.866124	-6.855189	0.819394
1	-7.358790	-7.818308	0.918808
6	-7.550924	-5.768913	0.264170
1	-8.578890	-5.886371	-0.068373
6	-6.919175	-4.532097	0.138011
1	-7.453121	-3.684224	-0.278439
6	-4.475049	-2.847314	-1.087529
1	-5.351144	-3.045045	-1.719713
1	-3.735207	-3.612973	-1.337559
6	-6.152112	-1.988814	2.259341
1	-6.519869	-3.015513	2.335321
6	-4.982205	-1.878899	3.234862
6	-4.559456	-3.019458	3.929755
1	-5.051270	-3.970029	3.739369
6	-3.523125	-2.948725	4.865746
1	-3.215641	-3.843303	5.400654
6	-2.891091	-1.729677	5.114720
1	-2.093840	-1.666942	5.849852
6	-3.293898	-0.587535	4.414478
1	-2.805975	0.364961	4.603310
6	-4.329257	-0.660920	3.481534

1	-4.639802	0.230104	2.948021
6	-7.334754	-1.107461	2.669266
1	-8.181077	-1.266250	1.999668
1	-7.095017	-0.045862	2.690593
1	-7.642025	-1.407162	3.676254
6	-2.396365	-0.829956	0.233335
1	-1.917575	0.137564	0.359600
1	-2.881604	-1.183864	1.139669
6	-1.812510	-1.767812	-0.674656
1	-2.037000	-2.812693	-0.466288
6	-0.393376	-1.621371	-1.212434
1	-0.096232	-0.569734	-1.248034
6	-4.940557	-0.807422	-3.325209
1	-5.827553	-1.413592	-3.156048
6	-3.741240	-1.504860	-3.656024
1	-3.804381	-2.589987	-3.735513
6	-2.655671	-0.885144	-4.518266
1	-3.017489	-0.788303	-5.554366
1	-1.815443	-1.577112	-4.552395
6	-2.163881	0.484868	-4.004541
1	-2.631733	1.297702	-4.571933
1	-1.091199	0.564707	-4.191517
6	-2.406107	0.730807	-2.514710
1	-1.510118	0.839448	-1.910484
6	-3.560976	1.338721	-2.010823
1	-3.462444	1.883256	-1.075771
6	-4.768654	1.722552	-2.850457
1	-5.587031	1.961013	-2.166287
1	-4.550260	2.647999	-3.405486
6	-5.237371	0.613049	-3.820680
1	-4.781343	0.755968	-4.806911
1	-6.316771	0.715244	-3.970412
6	-0.171794	-2.236008	-2.581127
6	-0.720311	-3.479617	-2.925085
6	0.650821	-1.586964	-3.510918
6	-0.456391	-4.055906	-4.169169
1	-1.365785	-4.000388	-2.224828
6	0.916553	-2.158701	-4.757148
1	1.083214	-0.624791	-3.258493
6	0.363780	-3.397641	-5.090792
1	-0.895256	-5.017448	-4.421290
1	1.548407	-1.628907	-5.464074
1	0.565098	-3.844685	-6.060216
1	3.756147	-5.226077	-1.971635
35	5.951410	-3.395942	-3.048608

---

8 P1-C1 *exo si-si*

Number of imaginary frequencies= 0
The smallest frequencies are= 12.5000 14.0616 15.2317 cm(-1)
Electronic energy= -7222.6326144
Zero-point correction= 1.756627
(Hartree/Particle)
Thermal correction to Energy= 1.875892
Thermal correction to Enthalpy= 1.876836
Thermal correction to Gibbs Free Energy= 1.593717
Sum of electronic and zero-point Energies= -7220.875988
Sum of electronic and thermal Energies= -7220.756723
Sum of electronic and thermal Enthalpies= -7220.755779
Sum of electronic and thermal Free Energies= -7221.038898

.....

Cartesian Coordinates

.....

26	3.647586	5.476001	1.344250
15	1.261867	1.776080	-1.425452
15	4.554397	0.877020	0.440065
6	2.936411	4.040812	-0.007006
6	3.915793	3.470882	0.882603
6	3.430884	3.618329	2.219074
1	3.946389	3.297904	3.114446
6	2.173494	4.289281	2.165269
1	1.574055	4.584372	3.016111
6	1.870938	4.556784	0.797710
1	0.997735	5.072822	0.425436
6	5.279053	6.640996	0.788594
1	6.057013	6.321308	0.108280
6	5.269557	6.442862	2.202927
1	6.036778	5.945216	2.780683
6	4.048172	6.977150	2.714957
1	3.726304	6.949793	3.747731
6	3.301872	7.504567	1.617470
1	2.316525	7.948300	1.672521
6	4.061845	7.297685	0.427645
1	3.752654	7.563071	-0.574344
6	3.045063	3.994614	-1.491778
6	3.931706	4.859447	-2.149214
1	4.482983	5.574095	-1.552978
6	4.123053	4.807217	-3.530280
1	4.824992	5.486415	-4.005442
6	3.412961	3.878737	-4.286501
1	3.551914	3.817369	-5.361344
6	2.527771	3.005055	-3.653655
1	1.997813	2.279322	-4.257347
6	2.339781	3.034191	-2.262606
6	5.115598	2.692307	0.425270
1	5.266869	2.901143	-0.638379
6	6.412420	3.013122	1.170805
1	7.251821	2.432628	0.777225
1	6.330110	2.815959	2.243221
1	6.643062	4.074339	1.040363
6	0.669682	0.777792	-2.861585
6	1.480237	-0.301093	-3.248935
1	2.371630	-0.525959	-2.674285
6	1.170978	-1.059491	-4.378777
1	1.821416	-1.877857	-4.673458
6	0.028307	-0.760893	-5.126171
1	-0.220974	-1.352376	-6.002255
6	-0.793586	0.302229	-4.741398
1	-1.683241	0.538448	-5.317870
6	-0.472815	1.071526	-3.620421
1	-1.101734	1.911804	-3.355180
6	-0.182623	2.793637	-0.908188
6	-0.653021	3.864107	-1.687564
1	-0.176153	4.099093	-2.634460
6	-1.718494	4.645530	-1.239060
1	-2.078390	5.468593	-1.849627
6	-2.323193	4.366633	-0.008890
1	-3.154275	4.974488	0.337230
6	-1.851781	3.311895	0.775498
1	-2.308661	3.102242	1.737867
6	-0.779355	2.531412	0.334684
1	-0.368037	1.749545	0.966363
6	5.508389	0.116236	-0.942907
6	6.348541	-1.001049	-0.829889
1	6.562244	-1.442955	0.134638
6	6.909987	-1.577099	-1.969634
6	6.629157	-1.080636	-3.242885
1	7.057496	-1.542534	-4.124237
6	5.771499	0.010841	-3.357843
6	5.218579	0.609393	-2.224741
1	4.539173	1.447572	-2.348171
6	5.238470	0.165879	1.993355
6	4.299245	-0.175505	2.976195
1	3.244622	-0.022332	2.781556
6	4.717563	-0.696533	4.201462
6	6.070904	-0.903429	4.464192
1	6.393517	-1.315328	5.412587
6	7.004693	-0.561553	3.487270
6	6.600574	-0.022045	2.264890
1	7.354721	0.246625	1.534152
29	2.265836	0.483744	0.155578
6	8.474385	-0.791064	3.709951
6	3.683360	-1.087610	5.221211
6	7.883518	-2.717386	-1.833746
6	5.390718	0.556677	-4.706772
9	4.047828	0.492159	-4.901366
9	5.734316	1.859659	-4.833942
9	5.971932	-0.114224	-5.722184
9	7.721660	-3.639634	-2.811148
9	7.771724	-3.353908	-0.649078

9	9.164003	-2.279787	-1.926973
9	8.949713	-1.760071	2.890219
9	8.755462	-1.163051	4.975781
9	9.197035	0.323201	3.444089
9	4.190944	-1.130048	6.472755
9	2.643628	-0.218332	5.237849
9	3.161052	-2.312526	4.969276
6	3.054481	-2.293972	-0.577314
6	1.890357	-2.312607	1.466400
6	3.436620	-3.612470	-0.449214
1	3.364723	-1.712909	-1.436701
6	2.265910	-3.688554	1.618045
6	3.034749	-4.339229	0.681229
1	1.936784	-4.220641	2.505485
6	1.101949	-1.724924	2.490903
6	0.775514	-0.361951	2.666078
8	1.203012	0.595960	1.931030
7	2.307657	-1.643993	0.338535
1	0.840303	-2.409315	3.284688
7	-0.060181	0.007867	3.721310
6	0.016631	1.382433	4.206788
1	0.808574	1.499770	4.961756
1	-0.937216	1.662243	4.662268
1	0.228879	2.055396	3.378719
6	-0.481847	-0.965722	4.718075
1	-0.923356	-1.842361	4.238478
1	-1.246341	-0.511408	5.352752
1	0.347400	-1.296312	5.359400
77	-3.122743	-2.219695	-0.659717
15	-4.579835	-0.667152	0.132497
8	-4.409199	0.945899	-0.163624
8	-6.116859	-0.917317	-0.433261
7	-4.518265	-0.655107	1.797901
6	-4.786179	1.510886	-1.376929
6	-3.735662	1.998201	-2.179845
1	-2.726795	1.937629	-1.792276
6	-4.019760	2.545521	-3.405325
1	-3.222104	2.939613	-4.028676
6	-5.357091	2.579305	-3.884774
6	-5.653607	3.060010	-5.189019
1	-4.835547	3.425607	-5.804295
6	-6.942895	3.049324	-5.670739
1	-7.157809	3.412330	-6.671431
6	-7.990599	2.546818	-4.862994
1	-9.003294	2.515498	-5.254243
6	-7.739786	2.090551	-3.586981
1	-8.555524	1.700829	-2.990318
6	-6.423856	2.107029	-3.045747
6	-6.123881	1.624653	-1.719986
6	-7.190046	1.216407	-0.763125
6	-8.265441	2.101426	-0.392347
6	-8.293452	3.473709	-0.768515
1	-7.479231	3.879853	-1.356782
6	-9.328495	4.296652	-0.380578
1	-9.320267	5.342961	-0.671995
6	-10.397553	3.795625	0.400000
1	-11.208766	4.455139	0.693796
6	-10.395830	2.476943	0.795057
1	-11.200336	2.081601	1.409526
6	-9.335212	1.604962	0.426541
6	-9.297212	0.264478	0.893955
1	-10.112888	-0.103657	1.509046
6	-8.216882	-0.536556	0.624006
1	-8.142556	-1.546401	1.011566
6	-7.168674	-0.041218	-0.179208
6	-3.825442	-1.829133	2.384951
1	-2.875587	-1.483442	2.802190
6	-4.627977	-2.485685	3.495034
6	-4.006550	-2.851905	4.692943
1	-2.953214	-2.630889	4.840060
6	-4.735714	-3.479263	5.708085
1	-4.243060	-3.749640	6.637972
6	-6.094014	-3.748050	5.529868
1	-6.664121	-4.227536	6.320478
6	-6.718139	-3.394901	4.328231
1	-7.776339	-3.595459	4.185269
6	-5.988800	-2.771283	3.318342
1	-6.478947	-2.470549	2.397260
6	-3.523042	-2.897884	1.310358
1	-4.387614	-3.562980	1.230568
1	-2.695117	-3.505450	1.681346
6	-4.649906	0.608023	2.611493
1	-4.754342	1.399465	1.873607
6	-5.894017	0.697453	3.491989
6	-6.977439	1.458505	3.035615
1	-6.929101	1.917611	2.052910
6	-8.119574	1.636251	3.819329
1	-8.944895	2.229440	3.436009
6	-8.194840	1.049921	5.083412
1	-9.081843	1.181881	5.697103
6	-7.115748	0.297901	5.557384
1	-7.159818	-0.160548	6.541466
6	-5.973019	0.133310	4.774107
1	-5.148104	-0.449209	5.165816
6	-3.361255	0.901420	3.387078
1	-2.490416	0.859372	2.728535
1	-3.197698	0.207140	4.213734
1	-3.430358	1.906857	3.811935
6	-1.582023	-0.850621	0.114874
1	-1.586311	0.157056	-0.285238
1	-1.574240	-0.896873	1.199461
6	-0.843294	-1.822430	-0.623220
1	-0.436948	-1.521823	-1.582666
6	-0.785133	-3.164254	-0.244897
1	-0.997962	-3.408868	0.789445
6	-4.908649	-3.420802	-1.388926
1	-5.570197	-3.488475	-0.530145
6	-3.792889	-4.274889	-1.379420
1	-3.680619	-4.924942	-0.512310
6	-3.069573	-4.781222	-2.610473
1	-3.637280	-5.631734	-3.015610
1	-2.106062	-5.183820	-2.297305
6	-2.840764	-3.739355	-3.727718
1	-3.694119	-3.725529	-4.411492
1	-1.974251	-4.054525	-4.317065
6	-2.586163	-2.329852	-3.237612
1	-1.555360	-1.999517	-3.237596
6	-3.549857	-1.377522	-3.064611
1	-3.227652	-0.344819	-2.971759
6	-5.029194	-1.608227	-3.278136
1	-5.569212	-0.757970	-2.864418
1	-5.230048	-1.603737	-4.358847
6	-5.593748	-2.911252	-2.659105
1	-5.573832	-3.717894	-3.398889
1	-6.646451	-2.738240	-2.423088
6	-0.155034	-4.238022	-1.013849
6	0.424175	-4.042547	-2.282306
6	-0.137690	-5.532669	-0.461715
6	0.982738	-5.111072	-2.977921
1	0.445686	-3.054057	-2.725684
6	0.421499	-6.601661	-1.159717
1	-0.569174	-5.692527	0.523089
6	0.980118	-6.395363	-2.424211
1	1.432995	-4.941369	-3.951556
1	0.422764	-7.594001	-0.717992
1	1.417393	-7.225969	-2.970434
1	3.311472	-5.380007	0.810723
35	4.540285	-4.439700	-1.834570

[8-9]‡ P1-C1 *exo si-si*

Number of imaginary frequencies= 1
The smallest frequencies are= -121.0528 8.8395 11.1131 cm(-1)
Electronic energy= -7222.6230214
Zero-point correction= 1.755800
(Hartree/Particle)
Thermal correction to Energy= 1.874307
Thermal correction to Enthalpy= 1.875251
Thermal correction to Gibbs Free Energy= 1.593526
Sum of electronic and zero-point Energies= -7220.867221

Sum of electronic and thermal Energies= -7220.748715
Sum of electronic and thermal Enthalpies= -7220.747770
Sum of electronic and thermal Free Energies= -7221.029495

.....

Cartesian Coordinates

.....

26	3.531492	3.834999	4.070237
15	1.204385	2.333391	-0.336032
15	4.538932	0.592510	0.723575
6	2.848457	3.413977	2.131598
6	3.845501	2.462046	2.549815
6	3.360637	1.807680	3.725074
1	3.886234	1.044435	4.283171
6	2.086765	2.361897	4.048883
1	1.481630	2.105100	4.908151
6	1.774455	3.356377	3.075980
1	0.887552	3.972726	3.055945
6	5.133669	5.140507	4.294799
1	5.914251	5.287591	3.560340
6	5.138258	4.164092	5.336999
1	5.916651	3.436139	5.521696
6	3.909631	4.280577	6.055909
1	3.595414	3.655739	6.881622
6	3.144672	5.327983	5.457496
1	2.150207	5.637195	5.751199
6	3.900933	5.860505	4.370650
1	3.578813	6.646511	3.701138
6	2.954776	4.218717	0.881744
6	3.817665	5.322976	0.839076
1	4.346532	5.593019	1.743552
6	4.013950	6.059095	-0.330145
1	4.696396	6.904149	-0.328977
6	3.335414	5.698588	-1.491018
1	3.481139	6.252966	-2.412784
6	2.472715	4.601703	-1.474009
1	1.965313	4.326066	-2.390167
6	2.278062	3.844194	-0.308653
6	5.059794	2.107437	1.742246
1	5.203585	2.885813	0.986926
6	6.351803	1.963344	2.548366
1	7.196778	1.701110	1.904877
1	6.264777	1.202089	3.328317
1	6.575832	2.917783	3.033552
6	0.605187	2.303140	-2.081003
6	1.386018	1.590088	-3.005213
1	2.272631	1.071333	-2.659142
6	1.051976	1.569285	-4.359449
1	1.674595	1.021487	-5.061168
6	-0.082191	2.252954	-4.806667
1	-0.350730	2.233502	-5.858777
6	-0.870128	2.959603	-3.894762
1	-1.756657	3.487855	-4.233791
6	-0.526870	2.990579	-2.541603
1	-1.138063	3.558697	-1.851959
6	-0.239457	2.893392	0.661662
6	-0.685026	4.225929	0.631041
1	-0.195802	4.949665	-0.013768
6	-1.742281	4.633665	1.445297
1	-2.082555	5.664539	1.411533
6	-2.361547	3.716926	2.300653
1	-3.184635	4.034926	2.934112
6	-1.916770	2.393943	2.342300
1	-2.386671	1.685112	3.016202
6	-0.856838	1.981739	1.530517
1	-0.475579	0.968476	1.592968
6	5.513666	0.768644	-0.832464
6	6.404137	-0.181231	-1.353578
1	6.629864	-1.090978	-0.813107
6	7.003666	0.024557	-2.596237
6	6.703723	1.149207	-3.365214
1	7.159471	1.290869	-4.337787
6	5.791006	2.074261	-2.864916
6	5.206379	1.896059	-1.610378
1	4.491357	2.631601	-1.254308
6	5.237355	-0.846606	1.634163
6	4.308727	-1.642738	2.317280
1	3.257596	-1.386138	2.277964
6	4.731340	-2.749286	3.054128
6	6.081189	-3.092212	3.114813
1	6.407036	-3.958480	3.678356
6	7.007874	-2.289976	2.449923
6	6.598048	-1.168927	1.725869
1	7.348350	-0.552485	1.245676
29	2.244787	0.393514	0.262345
6	8.470759	-2.642510	2.455539
6	3.704757	-3.612675	3.733489
6	8.034122	-0.946624	-3.107855
6	5.386769	3.278450	-3.670971
9	4.044630	3.300098	-3.878062
9	5.696535	4.432646	-3.035494
9	5.977311	3.315014	-4.882614
9	7.911559	-1.155065	-4.439618
9	7.960667	-2.147468	-2.496628
9	9.290684	-0.478206	-2.906294
9	8.844594	-3.202721	1.279392
9	8.786995	-3.518004	3.432138
9	9.246728	-1.546404	2.623675
9	4.211668	-4.267394	4.799269
9	2.647114	-2.885702	4.170163
9	3.204795	-4.556725	2.895740
6	3.205686	-1.527663	-1.867108
6	2.205759	-2.725324	-0.123677
6	3.792158	-2.665837	-2.388565
1	3.364641	-0.565015	-2.335352
6	2.847115	-3.906713	-0.599066
6	3.637822	-3.889236	-1.729161
1	2.688845	-4.838406	-0.066331
6	1.275955	-2.865293	0.951660
6	0.804221	-1.831906	1.820954
8	1.124408	-0.606321	1.713349
7	2.436952	-1.534497	-0.761305
1	1.175508	-3.880124	1.304127
7	-0.050102	-2.165798	2.857597
6	-0.148977	-1.226058	3.974838
1	0.729309	-1.294560	4.631928
1	-1.040713	-1.459052	4.559198
1	-0.222208	-0.205120	3.606026
6	-0.354158	-3.556379	3.181326
1	-0.651562	-4.109343	2.288345
1	-1.191659	-3.577505	3.881993
1	0.497986	-4.071292	3.643495
77	-3.072523	-1.482067	-1.762259
15	-4.593017	-0.536388	-0.363487
8	-4.502152	0.999769	0.242329
8	-6.085709	-0.476398	-1.100183
7	-4.654660	-1.387404	1.081199
6	-4.845274	2.106467	-0.525428
6	-3.785910	2.969572	-0.873613
1	-2.794503	2.733561	-0.508281
6	-4.039569	4.075601	-1.644550
1	-3.236204	4.757703	-1.908940
6	-5.351045	4.329203	-2.129627
6	-5.610642	5.423522	-2.998638
1	-4.785727	6.079637	-3.264306
6	-6.871656	5.641488	-3.505446
1	-7.057620	6.477431	-4.173366
6	-7.926892	4.761656	-3.166128
1	-8.915711	4.920313	-3.586694
6	-7.712510	3.701110	-2.312342
1	-8.532002	3.034112	-2.072887
6	-6.427784	3.456833	-1.751125
6	-6.167418	2.353462	-0.860006
6	-7.255938	1.482953	-0.334198
6	-8.391157	2.018356	0.373801
6	-8.476676	3.382885	0.769780
1	-7.659562	4.055471	0.537305
6	-9.571448	3.856670	1.459746
1	-9.606527	4.900177	1.759344
6	-10.646507	2.997111	1.789393
1	-11.505319	3.386489	2.328146

6	-10.589955	1.667174	1.438501
1	-11.399041	0.990254	1.700093
6	-9.467514	1.141786	0.741739
6	-9.378166	-0.243845	0.441834
1	-10.199994	-0.897634	0.718558
6	-8.247662	-0.758718	-0.140257
1	-8.136842	-1.818987	-0.338912
6	-7.192065	0.106991	-0.496913
6	-4.014210	-2.721951	0.966406
1	-3.021473	-2.664961	1.427028
6	-4.800652	-3.818560	1.659715
6	-4.146928	-4.726092	2.499890
1	-3.081727	-4.611201	2.685892
6	-4.854585	-5.764551	3.113160
1	-4.336556	-6.457548	3.770637
6	-6.225486	-5.903995	2.887547
1	-6.779531	-6.704869	3.368982
6	-6.883107	-5.004124	2.041237
1	-7.951489	-5.101013	1.868851
6	-6.174653	-3.971254	1.431252
1	-6.689752	-3.251649	0.802408
6	-3.835335	-3.078667	-0.516376
1	-4.805388	-3.389817	-0.920576
1	-3.184986	-3.952822	-0.588457
6	-4.764888	-0.740720	2.433597
1	-4.836852	0.325708	2.229592
6	-6.031192	-1.100313	3.208690
6	-7.163389	-0.290813	3.050790
1	-7.124545	0.549550	2.364963
6	-8.339950	-0.547086	3.757392
1	-9.203007	0.096005	3.611079
6	-8.399285	-1.621806	4.646368
1	-9.312147	-1.826509	5.199242
6	-7.272696	-2.429608	4.824113
1	-7.306109	-3.269182	5.513109
6	-6.098908	-2.166854	4.116501
1	-5.241756	-2.813580	4.262570
6	-3.482950	-0.948661	3.247645
1	-2.610891	-0.627871	2.673601
1	-3.330173	-1.989597	3.541560
1	-3.537127	-0.351248	4.162354
6	-1.536525	-0.659593	-0.465404
1	-1.264995	0.357011	-0.735547
1	-1.737925	-0.779387	0.596011
6	-0.825932	-1.726175	-1.120392
1	-0.199617	-1.507489	-1.975864
6	-0.769596	-3.011739	-0.564728
1	-1.314767	-3.158435	0.358684
6	-4.587814	-2.077999	-3.304566
1	-5.414749	-2.541833	-2.773581
6	-3.430371	-2.870847	-3.480559
1	-3.464148	-3.887291	-3.089254
6	-2.387237	-2.664396	-4.566415
1	-2.744592	-3.098951	-5.512725
1	-1.502962	-3.241964	-4.281952
6	-1.977873	-1.191168	-4.782645
1	-2.605200	-0.728456	-5.550859
1	-0.954460	-1.159146	-5.170183
6	-2.035127	-0.337858	-3.519244
1	-1.076260	-0.002497	-3.137606
6	-3.140361	0.406229	-3.124232
1	-2.945417	1.258788	-2.483072
6	-4.473617	0.441221	-3.841827
1	-5.198079	0.919992	-3.180503
1	-4.382228	1.088835	-4.726344
6	-5.003883	-0.950466	-4.250491
1	-4.679375	-1.198846	-5.265901
1	-6.096777	-0.911165	-4.282039
6	-0.363186	-4.228522	-1.248620
6	0.274984	-4.226665	-2.504901
6	-0.632705	-5.468420	-0.633835
6	0.608046	-5.424998	-3.132050
1	0.512988	-3.286786	-2.990956
6	-0.292959	-6.665230	-1.259127
1	-1.115247	-5.481073	0.340406
6	0.325687	-6.647292	-2.514108
1	1.096809	-5.405318	-4.101853
1	-0.511619	-7.611107	-0.772140
1	0.589276	-7.579420	-3.005276
1	4.104807	-4.796132	-2.097680
35	4.823869	-2.546664	-4.044691

---

9 P1-C1 *exo si-si*

Number of imaginary frequencies= 0
The smallest frequencies are= 8.7113 13.9586 16.0075 cm(-1)
Electronic energy= -7222.6529593
Zero-point correction= 1.759678
(Hartree/Particle)
Thermal correction to Energy= 1.877518
Thermal correction to Enthalpy= 1.878462
Thermal correction to Gibbs Free Energy= 1.600172
Sum of electronic and zero-point Energies= -7220.893282
Sum of electronic and thermal Energies= -7220.775441
Sum of electronic and thermal Enthalpies= -7220.774497
Sum of electronic and thermal Free Energies= -7221.052787

.....

Cartesian Coordinates

.....

26	3.611430	3.253681	4.433987
15	1.188826	2.471207	-0.065753
15	4.504369	0.442604	0.665531
6	2.902062	3.139132	2.468253
6	3.844826	2.083074	2.738077
6	3.328948	1.301665	3.819378
1	3.814498	0.442414	4.262317
6	2.089015	1.875094	4.230893
1	1.475564	1.537013	5.055329
6	1.828863	3.009498	3.406969
1	0.979090	3.672562	3.480910
6	5.283996	4.428628	4.817483
1	6.073975	4.621311	4.103995
6	5.228095	3.331965	5.730614
1	5.967700	2.548575	5.828997
6	4.004308	3.427693	6.460317
1	3.650507	2.724689	7.202991
6	3.303049	4.582722	5.997942
1	2.326135	4.909218	6.329416
6	4.093525	5.201721	4.984090
1	3.820197	6.082594	4.419214
6	3.033531	4.104152	1.342432
6	3.946390	5.164341	1.427487
1	4.517134	5.278813	2.340155
6	4.133344	6.055606	0.369610
1	4.852846	6.863714	0.464781
6	3.397623	5.899243	-0.802266
1	3.533861	6.581123	-1.635643
6	2.491091	4.844078	-0.913971
1	1.942027	4.722230	-1.839591
6	2.306987	3.932448	0.136282
6	5.047322	1.792160	1.888296
1	5.224946	2.660026	1.245287
6	6.329173	1.493347	2.667489
1	7.167914	1.295592	1.993767
1	6.211799	0.635570	3.335023
1	6.581180	2.363571	3.279296
6	0.626107	2.620122	-1.810236
6	1.431328	2.003800	-2.782718
1	2.313145	1.452124	-2.471160
6	1.123007	2.117846	-4.137648
1	1.760296	1.644942	-4.879275
6	-0.007919	2.836992	-4.535260
1	-0.258309	2.918166	-5.588869
6	-0.819932	3.444046	-3.574532
1	-1.705823	3.994324	-3.877864
6	-0.503583	3.342904	-2.218127
1	-1.137993	3.826935	-1.485381
6	-0.247263	2.939769	0.981672
6	-0.675845	4.273584	1.088775
1	-0.181497	5.053571	0.517758

6	-1.723966	4.607611	1.947332
1	-2.052880	5.640115	2.019927
6	-2.346786	3.616389	2.712133
1	-3.161427	3.878176	3.381028
6	-1.917878	2.290678	2.617521
1	-2.392686	1.522075	3.218437
6	-0.870582	1.952622	1.757874
1	-0.509928	0.932538	1.704739
6	5.481700	0.842180	-0.845900
6	6.460994	0.036413	-1.442592
1	6.737813	-0.918409	-1.017361
6	7.088467	0.451313	-2.616939
6	6.736920	1.648615	-3.239933
1	7.222203	1.956251	-4.158894
6	5.737906	2.432085	-2.667532
6	5.117733	2.040567	-1.480166
1	4.337823	2.666564	-1.056295
6	5.158692	-1.122290	1.378799
6	4.204157	-1.949806	1.982323
1	3.163670	-1.653356	1.975384
6	4.584541	-3.132879	2.617605
6	5.918785	-3.531625	2.640175
1	6.214141	-4.454226	3.125387
6	6.872958	-2.703380	2.048006
6	6.507385	-1.501617	1.440673
1	7.285701	-0.864616	1.040506
29	2.215412	0.468549	0.287701
6	8.322485	-3.109171	2.017690
6	3.515495	-3.983371	3.244858
6	8.180286	-0.377646	-3.240373
6	5.308527	3.722160	-3.314355
9	3.960313	3.780461	-3.448979
9	5.671073	4.796997	-2.575570
9	5.841004	3.883100	-4.542773
9	7.923418	-0.638401	-4.545591
9	8.354089	-1.561710	-2.618104
9	9.366954	0.272705	-3.205831
9	8.659703	-3.634165	0.814752
9	8.615355	-4.035760	2.953016
9	9.139351	-2.050261	2.220340
9	4.011707	-4.891904	4.103946
9	2.613645	-3.228160	3.920635
9	2.801590	-4.669718	2.310289
6	3.176540	-1.457683	-1.989493
6	2.001531	-2.716098	-0.437508
6	3.918320	-2.566090	-2.381129
1	3.338235	-0.488375	-2.445470
6	2.778476	-3.844600	-0.738246
6	3.754797	-3.780676	-1.725693
1	2.597718	-4.779231	-0.221322
6	0.783463	-2.908867	0.436956
6	0.624631	-1.933467	1.596302
8	1.114398	-0.781988	1.584785
7	2.240722	-1.526781	-1.028086
1	0.889876	-3.902855	0.870711
7	-0.084697	-2.340619	2.674480
6	-0.137752	-1.444440	3.834895
1	0.770466	-1.545234	4.439642
1	-1.005069	-1.704763	4.441987
1	-0.224942	-0.410613	3.507287
6	-0.477951	-3.733445	2.917065
1	-0.911177	-4.193022	2.029218
1	-1.237472	-3.743863	3.699720
1	0.377117	-4.329366	3.251563
77	-2.956652	-1.233969	-1.857037
15	-4.569201	-0.418380	-0.443435
8	-4.564976	1.046118	0.354383
8	-6.046114	-0.297710	-1.232367
7	-4.689256	-1.423133	0.905061
6	-4.890501	2.217564	-0.311048
6	-3.836008	3.131445	-0.524289
1	-2.851621	2.872399	-0.155039
6	-4.082307	4.313516	-1.175610
1	-3.282448	5.032870	-1.328075
6	-5.380133	4.601714	-1.678526
6	-5.631539	5.786012	-2.423110
1	-4.812346	6.483828	-2.576761
6	-6.877045	6.039482	-2.951737
1	-7.056780	6.945358	-3.523371
6	-7.923307	5.105137	-2.763543
1	-8.898052	5.293140	-3.204624
6	-7.717218	3.955286	-2.032260
1	-8.528503	3.247930	-1.908380
6	-6.450672	3.671531	-1.448450
6	-6.202631	2.480557	-0.675178
6	-7.294140	1.536056	-0.303702
6	-8.470698	1.961643	0.410573
6	-8.603913	3.266631	0.963445
1	-7.794082	3.977019	0.845542
6	-9.734934	3.633074	1.660365
1	-9.806034	4.632090	2.081036
6	-10.801577	2.720137	1.840296
1	-11.688570	3.024587	2.388101
6	-10.702594	1.445157	1.330516
1	-11.507245	0.728156	1.471800
6	-9.543184	1.029086	0.620327
6	-9.414988	-0.304469	0.146903
1	-10.236084	-0.999327	0.297291
6	-8.249623	-0.724382	-0.442483
1	-8.110575	-1.748360	-0.771737
6	-7.190521	0.190960	-0.630762
6	-4.022173	-2.732471	0.690557
1	-3.068387	-2.717931	1.229318
6	-4.841880	-3.895092	1.219417
6	-4.237691	-4.883290	2.003503
1	-3.187062	-4.786549	2.266239
6	-4.974551	-5.978397	2.465363
1	-4.493132	-6.734746	3.079682
6	-6.328692	-6.092920	2.145839
1	-6.906933	-6.937412	2.510208
6	-6.938566	-5.110683	1.356749
1	-7.994481	-5.187996	1.112273
6	-6.199533	-4.023639	0.895763
1	-6.679711	-3.243069	0.313944
6	-3.715968	-2.943160	-0.805013
1	-4.639627	-3.266453	-1.301591
1	-3.022411	-3.779568	-0.893412
6	-4.865724	-0.930946	2.310321
1	-5.014117	0.142813	2.214960
6	-6.117058	-1.463541	3.007173
6	-7.328085	-0.788497	2.809164
1	-7.348047	0.084767	2.166274
6	-8.505197	-1.219607	3.422644
1	-9.429968	-0.677103	3.246992
6	-8.486266	-2.336526	4.260669
1	-9.399595	-2.678695	4.739783
6	-7.280306	-3.005778	4.485507
1	-7.251582	-3.873994	5.138287
6	-6.106576	-2.567514	3.870218
1	-5.186079	-3.109872	4.051503
6	-3.587271	-1.125156	3.136774
1	-2.735113	-0.670802	2.626590
1	-3.351603	-2.176341	3.319196
1	-3.707872	-0.639887	4.109893
6	-1.474725	-0.611107	-0.381625
1	-1.166408	0.414161	-0.564951
1	-1.752732	-0.797081	0.652524
6	-0.875748	-1.668190	-1.126757
1	-0.161423	-1.383596	-1.891366
6	-0.550402	-2.979583	-0.444266
1	-1.337433	-3.184359	0.282016
6	-4.304487	-1.718729	-3.502643
1	-5.154305	-2.283254	-3.123387
6	-3.086052	-2.454492	-3.673831
1	-3.116835	-3.515818	-3.425003
6	-2.029706	-2.112128	-4.713972
1	-2.358807	-2.431274	-5.715883
1	-1.141086	-2.703408	-4.480058
6	-1.646814	-0.617045	-4.732907
1	-2.231714	-0.080943	-5.487539

1	-0.599781	-0.512267	-5.037077
6	-1.823973	0.075970	-3.384631
1	-0.902793	0.386051	-2.899594
6	-2.974331	0.767755	-3.010937
1	-2.850355	1.566965	-2.287527
6	-4.252084	0.836260	-3.827282
1	-5.038462	1.226630	-3.177012
1	-4.124998	1.567331	-4.640914
6	-4.700465	-0.530815	-4.390097
1	-4.295669	-0.677717	-5.397625
1	-5.789374	-0.521738	-4.503072
6	-0.459264	-4.183402	-1.365934
6	0.144509	-4.110814	-2.628693
6	-0.941973	-5.425416	-0.928796
6	0.241977	-5.242110	-3.441534
1	0.547480	-3.166917	-2.980316
6	-0.848304	-6.559915	-1.737883
1	-1.407572	-5.500446	0.051396
6	-0.256824	-6.470555	-3.000568
1	0.709093	-5.162251	-4.419420
1	-1.238912	-7.509801	-1.383433
1	-0.183793	-7.349957	-3.634090
1	4.341210	-4.654359	-1.987765
35	5.176508	-2.404791	-3.857930

---

8 P1-C1 *exo re-si*

Number of imaginary frequencies= 0
The smallest frequencies are=12.7618 14.8959 15.3289 cm(-1)
Electronic energy= -7222.6420137
Zero-point correction= 1.756579
(Hartree/Particle)
Thermal correction to Energy= 1.875873
Thermal correction to Enthalpy= 1.876817
Thermal correction to Gibbs Free Energy= 1.594748
Sum of electronic and zero-point Energies= -7220.885435
Sum of electronic and thermal Energies= -7220.766141
Sum of electronic and thermal Enthalpies= -7220.765197
Sum of electronic and thermal Free Energies= -7221.047266

.....

Cartesian Coordinates

.....

26	3.853418	5.372567	0.852098
15	1.398131	1.457485	-1.626879
15	4.427099	0.662786	0.401833
6	3.190009	3.755324	-0.306676
6	3.935204	3.303941	0.844421
6	3.260966	3.778266	2.011538
1	3.575576	3.618977	3.033482
6	2.126389	4.539519	1.596367
1	1.436775	5.056365	2.248873
6	2.082918	4.526674	0.172000
1	1.354200	5.027948	-0.447785
6	5.729581	6.188412	0.497437
1	6.580485	5.633929	0.123935
6	5.369196	6.346420	1.870954
1	5.891225	5.923004	2.718640
6	4.166259	7.114461	1.926389
1	3.616617	7.370232	2.822706
6	3.783192	7.432602	0.587724
1	2.897127	7.978980	0.292366
6	4.749021	6.863178	-0.294533
1	4.721821	6.908780	-1.374787
6	3.510462	3.392927	-1.716261
6	4.629087	3.973867	-2.333541
1	5.207494	4.693393	-1.768087
6	5.012620	3.640316	-3.631791
1	5.897410	4.091391	-4.069518
6	4.260659	2.714423	-4.350144
1	4.544190	2.438307	-5.360543
6	3.148010	2.119117	-3.756059
1	2.586364	1.390166	-4.327535
6	2.762323	2.426237	-2.440490
6	5.128056	2.387356	0.784462
1	5.718107	2.667833	-0.090156
6	6.036320	2.457321	2.015318
1	6.901959	1.799247	1.900235
1	5.513907	2.167374	2.931192
1	6.393680	3.484151	2.141629
6	0.840703	0.351400	-2.999411
6	1.501340	-0.880596	-3.146143
1	2.245757	-1.180621	-2.416081
6	1.201262	-1.720004	-4.221689
1	1.740922	-2.652475	-4.340681
6	0.210351	-1.361049	-5.139578
1	-0.031000	-2.021800	-5.967114
6	-0.469645	-0.151063	-4.986029
1	-1.245556	0.134306	-5.690461
6	-0.144807	0.707171	-3.933013
1	-0.652460	1.660737	-3.855027
6	0.022882	2.669535	-1.458995
6	-0.187005	3.706747	-2.382759
1	0.485854	3.825213	-3.227141
6	-1.248385	4.596747	-2.211716
1	-1.404804	5.393664	-2.933114
6	-2.106492	4.465654	-1.114394
1	-2.931858	5.159550	-0.984405
6	-1.898656	3.443184	-0.186681
1	-2.557817	3.335150	0.668514
6	-0.837706	2.551815	-0.358291
1	-0.670478	1.766943	0.369936
6	5.275565	0.063074	-1.119878
6	4.864734	-1.196160	-1.584729
1	4.127287	-1.751279	-1.012593
6	5.370473	-1.709237	-2.779557
6	6.264745	-0.969656	-3.551135
1	6.642848	-1.361526	-4.488329
6	6.654150	0.291681	-3.098370
6	6.181085	0.802875	-1.889777
1	6.508956	1.785320	-1.579040
6	5.042131	-0.469601	1.715587
6	4.376432	-0.396033	2.949400
1	3.592255	0.336713	3.096065
6	4.683864	-1.288056	3.972074
6	5.633473	-2.293084	3.779851
1	5.855313	-3.003964	4.567749
6	6.281874	-2.374466	2.550309
6	6.005249	-1.464726	1.526011
1	6.532868	-1.556642	0.583949
29	2.091232	0.344708	0.218255
6	7.220296	-3.516182	2.282441
6	3.918456	-1.252089	5.265274
6	4.959146	-3.093351	-3.200873
6	7.580395	1.100576	-3.964369
9	7.016924	1.381936	-5.165976
9	7.923372	2.280105	-3.402003
9	8.727807	0.432347	-4.229634
9	3.617167	-3.287047	-3.070835
9	5.548048	-4.044408	-2.435898
9	5.272652	-3.361405	-4.484349
9	6.555336	-4.586017	1.765466
9	7.836283	-3.949313	3.403089
9	8.179139	-3.190821	1.388241
9	4.732738	-1.406272	6.334820
9	3.241674	-0.096370	5.433163
9	3.006453	-2.258219	5.332959
6	2.262119	-2.480738	1.274115
6	1.472450	-2.147900	2.411011
6	0.991437	-0.884209	2.807089
1	1.305139	-2.930083	3.138836
77	-2.852630	-2.440422	-0.622471
15	-4.235835	-0.727928	-0.090766
8	-4.028270	0.806435	-0.654326
8	-5.782404	-1.032241	-0.596138
7	-4.159612	-0.435619	1.550100
6	-4.427344	1.195876	-1.927992
6	-3.386715	1.544212	-2.812804
1	-2.372184	1.516687	-2.437627
6	-3.686565	1.912638	-4.099078
1	-2.895135	2.194436	-4.787616

6	-5.033472	1.900631	-4.553329
6	-5.350035	2.191878	-5.907766
1	-4.539138	2.452898	-6.582772
6	-6.648451	2.129880	-6.360525
1	-6.878310	2.348417	-7.399193
6	-7.685406	1.761882	-5.470823
1	-8.705646	1.686914	-5.835825
6	-7.414733	1.491163	-4.146720
1	-8.222298	1.201708	-3.485213
6	-6.088823	1.568461	-3.636440
6	-5.770097	1.281693	-2.258770
6	-6.825829	1.043586	-1.234860
6	-7.881282	1.994028	-0.989151
6	-7.891154	3.296108	-1.563538
1	-7.075015	3.598252	-2.209174
6	-8.910262	4.183995	-1.295142
1	-8.887993	5.176003	-1.736965
6	-9.980867	3.821092	-0.443433
1	-10.779721	4.529886	-0.246537
6	-9.995232	2.576351	0.144141
1	-10.800495	2.289278	0.815229
6	-8.950328	1.642793	-0.096523
6	-8.927178	0.387549	0.567809
1	-9.741715	0.129810	1.238015
6	-7.861075	-0.461975	0.413503
1	-7.792524	-1.400828	0.952106
6	-6.816836	-0.110958	-0.467165
6	-3.460205	-1.504167	2.309144
1	-2.470585	-1.130850	2.585170
6	-4.183524	-1.887802	3.586081
6	-3.469374	-1.998191	4.783904
1	-2.405440	-1.772827	4.793522
6	-4.119210	-2.371579	5.964207
1	-3.556981	-2.443866	6.891202
6	-5.489582	-2.640025	5.952441
1	-5.998659	-2.921088	6.870059
6	-6.205950	-2.541706	4.754366
1	-7.273763	-2.741920	4.741443
6	-5.555832	-2.170450	3.579203
1	-6.115828	-2.063047	2.654202
6	-3.277078	-2.761592	1.438243
1	-4.200457	-3.349817	1.476331
1	-2.496223	-3.370099	1.900611
6	-4.226424	0.954130	2.135235
1	-4.369559	1.608477	1.278493
6	-5.416647	1.215133	3.054861
6	-6.561679	1.806594	2.507291
1	-6.587222	2.029129	1.445508
6	-7.667835	2.116350	3.300907
1	-8.542639	2.571375	2.845047
6	-7.640920	1.843703	4.669479
1	-8.498199	2.081967	5.293286
6	-6.497488	1.270388	5.233401
1	-6.461861	1.056878	6.298154
6	-5.393987	0.966762	4.435047
1	-4.521695	0.518805	4.895131
6	-2.888300	1.343957	2.764809
1	-2.069898	1.189371	2.057781
1	-2.659961	0.779520	3.670276
1	-2.912685	2.401942	3.036608
6	-1.235960	-1.065855	-0.073046
1	-1.161585	-0.146373	-0.643158
1	-1.224566	-0.912449	1.000628
6	-0.526996	-2.183122	-0.611266
1	-0.091912	-2.063222	-1.593851
6	-0.483070	-3.434999	-0.009506
1	-0.739848	-3.509540	1.039724
6	-4.677283	-3.714920	-1.155793
1	-5.335302	-3.611987	-0.298172
6	-3.586949	-4.581296	-0.998290
1	-3.485799	-5.074125	-0.032064
6	-2.829582	-5.264784	-2.115575
1	-3.386438	-6.164150	-2.416970
1	-1.879960	-5.615892	-1.708945
6	-2.550005	-4.391730	-3.358467
1	-3.377178	-4.469950	-4.070037
1	-1.666156	-4.791471	-3.864574
6	-2.300391	-2.923612	-3.064779
1	-1.272567	-2.589655	-3.128792
6	-3.269750	-1.955585	-3.062633
1	-2.945103	-0.922839	-3.145601
6	-4.743177	-2.210009	-3.288798
1	-5.288147	-1.304536	-3.025790
1	-4.904608	-2.366893	-4.364730
6	-5.336221	-3.402405	-2.498853
1	-5.306857	-4.309474	-3.110866
1	-6.392254	-3.190444	-2.313575
6	0.170420	-4.609388	-0.583210
6	0.712739	-4.625952	-1.884119
6	0.277007	-5.773590	0.201308
6	1.338337	-5.766944	-2.377554
1	0.656494	-3.741333	-2.506901
6	0.900746	-6.917297	-0.295853
1	-0.129982	-5.771666	1.209256
6	1.432135	-6.919080	-1.588766
1	1.763975	-5.755585	-3.376825
1	0.974410	-7.805140	0.325474
1	1.921008	-7.807751	-1.977057
8	2.364090	-1.765481	0.216017
6	0.321254	-0.784866	4.077767
6	-0.037493	0.427210	4.613966
1	0.145801	-1.695506	4.641624
6	0.240996	1.582816	3.862831
6	0.811648	1.462614	2.615206
1	0.996970	2.333881	2.001437
7	1.175266	0.276513	2.080541
6	3.590441	-4.184142	0.093044
1	3.136705	-3.731161	-0.782077
1	4.668896	-3.984591	0.085951
1	3.441877	-5.266872	0.033920
6	3.112161	-4.493898	2.488948
1	3.140010	-3.879831	3.389661
1	2.307195	-5.236951	2.589288
1	4.064171	-5.027556	2.423737
7	2.956788	-3.672178	1.297902
1	-0.516614	0.487740	5.585458
35	-0.232046	3.356751	4.555772

[8-9]‡-P1-C1 *exo re-si*

Number of imaginary frequencies=1
The smallest frequencies are=-148.6503 13.3766 16.1508cm(-1)
Electronic energy= -7222.6391298
Zero-point correction= 1.757111
(Hartree/Particle)
Thermal correction to Energy= 1.874980
Thermal correction to Enthalpy= 1.875924
Thermal correction to Gibbs Free Energy= 1.598871
Sum of electronic and zero-point Energies= -7220.882019
Sum of electronic and thermal Energies= -7220.764150
Sum of electronic and thermal Enthalpies= -7220.763206
Sum of electronic and thermal Free Energies= -7221.040258

.....

Cartesian Coordinates

.....

26	-3.653878	-4.360896	3.266551
15	-1.383041	-2.053272	-0.847871
15	-4.440942	-0.457998	0.640360
6	-3.076080	-3.463516	1.464307
6	-3.810085	-2.538874	2.296364
6	-3.093800	-2.394709	3.524706
1	-3.392565	-1.779748	4.362341
6	-1.942279	-3.237272	3.474161
1	-1.222251	-3.375455	4.268774
6	-1.932733	-3.896132	2.210525
1	-1.202484	-4.616912	1.874178
6	-5.489955	-5.330180	3.366871
1	-6.365886	-5.057233	2.793015
6	-5.132837	-4.809885	4.648507
1	-5.684469	-4.067078	5.209529

6	-3.895822	-5.406903	5.038699
1	-3.344346	-5.192082	5.944569
6	-3.487569	-6.296659	3.998840
1	-2.573913	-6.875998	3.979624
6	-4.471753	-6.250432	2.966942
1	-4.433242	-6.792561	2.031889
6	-3.440056	-3.817858	0.062447
6	-4.561156	-4.629448	-0.165449
1	-5.108841	-4.991610	0.694856
6	-4.985213	-4.958175	-1.452369
1	-5.872661	-5.566750	-1.593171
6	-4.274075	-4.480977	-2.550553
1	-4.592571	-4.720773	-3.559921
6	-3.159602	-3.666068	-2.350471
1	-2.628614	-3.288814	-3.216688
6	-2.733161	-3.309407	-1.060950
6	-5.038292	-1.781562	1.865779
1	-5.661370	-2.462054	1.282888
6	-5.878306	-1.243277	3.027763
1	-6.779410	-0.743895	2.661544
1	-5.323838	-0.527809	3.640975
1	-6.179398	-2.075281	3.671907
6	-0.864089	-1.690596	-2.582618
6	-1.483406	-0.606509	-3.229072
1	-2.176634	0.022329	-2.681572
6	-1.200716	-0.328170	-4.568233
1	-1.697918	0.499879	-5.061661
6	-0.275729	-1.107235	-5.268024
1	-0.049570	-0.882841	-6.306451
6	0.363588	-2.169856	-4.625129
1	1.091876	-2.773494	-5.159163
6	0.064780	-2.467144	-3.294009
1	0.553828	-3.310859	-2.820458
6	0.016253	-3.013115	-0.145669
6	0.245190	-4.360945	-0.468981
1	-0.419639	-4.876051	-1.156135
6	1.314236	-5.048680	0.106484
1	1.487035	-6.089744	-0.150811
6	2.158394	-4.401156	1.014813
1	2.988992	-4.938639	1.462875
6	1.932651	-3.063520	1.344879
1	2.584725	-2.558209	2.048636
6	0.865870	-2.372660	0.766780
1	0.684208	-1.336242	1.026700
6	-5.348557	-0.750464	-0.935305
6	-4.990358	0.084664	-2.003972
1	-4.245637	0.858108	-1.843578
6	-5.573194	-0.086379	-3.259797
6	-6.489833	-1.110656	-3.489010
1	-6.927204	-1.252196	-4.470849
6	-6.825690	-1.954819	-2.430503
6	-6.278061	-1.771907	-1.160882
1	-6.572408	-2.448106	-0.370422
6	-5.098907	1.163491	1.212507
6	-4.422534	1.765941	2.285526
1	-3.619074	1.236811	2.783612
6	-4.747878	3.057251	2.689119
6	-5.730776	3.788890	2.019127
1	-5.962413	4.805840	2.314677
6	-6.396954	3.192313	0.952083
6	-6.098298	1.886120	0.554477
1	-6.636999	1.453258	-0.279932
29	-2.137676	-0.227144	0.246064
6	-7.370805	3.998126	0.139045
6	-3.961186	3.727293	3.780690
6	-5.231261	0.890555	-4.349281
6	-7.765291	-3.098870	-2.698291
9	-7.223158	-3.994689	-3.561241
9	-8.088002	-3.779071	-1.575784
9	-8.920887	-2.677514	-3.262059
9	-3.897042	1.146304	-4.397955
9	-5.835301	2.088491	-4.148205
9	-5.599281	0.458639	-5.571338
9	-6.743598	4.614021	-0.902446
9	-7.964825	4.970172	0.861773
9	-8.344061	3.232398	-0.399772
9	-4.755117	4.437565	4.612130
9	-3.266868	2.846538	4.531968
9	-3.057379	4.607781	3.269836
6	-2.379747	2.744898	-0.332892
6	-1.531176	3.067129	0.783648
6	-1.065097	2.191917	1.808382
1	-1.459548	4.110600	1.050365
77	2.905887	1.854924	-1.750349
15	4.264555	0.521611	-0.508946
8	4.048181	-1.105551	-0.291991
8	5.810405	0.537698	-1.122666
7	4.241061	1.015910	1.096226
6	4.414845	-2.026443	-1.266261
6	3.357614	-2.719450	-1.892951
1	2.346609	-2.516875	-1.564736
6	3.634409	-3.628371	-2.881731
1	2.829111	-4.175107	-3.364110
6	4.973609	-3.844230	-3.306002
6	5.267075	-4.721531	-4.384825
1	4.444104	-5.246734	-4.862730
6	6.559349	-4.892488	-4.827193
1	6.771657	-5.561106	-5.656291
6	7.613471	-4.179048	-4.208816
1	8.628995	-4.294095	-4.576658
6	7.364946	-3.333745	-3.148935
1	8.184772	-2.788799	-2.696557
6	6.045754	-3.150595	-2.647771
6	5.750937	-2.269599	-1.544695
6	6.824494	-1.611695	-0.747447
6	7.869804	-2.362657	-0.099884
6	7.864238	-3.784322	-0.029844
1	7.044294	-4.334534	-0.476135
6	8.874092	-4.469350	0.610393
1	8.840398	-5.554046	0.657945
6	9.950377	-3.775156	1.212927
1	10.741899	-4.329089	1.708978
6	9.979899	-2.399287	1.179899
1	10.790014	-1.851290	1.653845
6	8.945409	-1.660735	0.542864
6	8.939305	-0.240547	0.571908
1	9.758102	0.280591	1.059078
6	7.885768	0.461921	0.044011
1	7.832199	1.543864	0.098982
6	6.834093	-0.233933	-0.588971
6	3.595397	2.346732	1.256224
1	2.561065	2.193140	1.583428
6	4.280111	3.221683	2.288118
6	3.517534	3.849185	3.279648
1	2.445766	3.666620	3.322773
6	4.124902	4.686046	4.220595
1	3.523580	5.160346	4.991516
6	5.503509	4.903876	4.173436
1	5.979871	5.547828	4.907323
6	6.269526	4.286485	3.178318
1	7.343596	4.446322	3.142207
6	5.661219	3.452650	2.242021
1	6.259158	2.946896	1.489340
6	3.568952	3.064996	-0.098918
1	4.583155	3.415181	-0.324231
1	2.955759	3.963572	-0.007125
6	4.242362	0.055995	2.254266
1	4.338412	-0.927545	1.799578
6	5.435897	0.187799	3.198267
6	6.562237	-0.609627	2.958712
1	6.570579	-1.270787	2.098034
6	7.670778	-0.571786	3.806424
1	8.530897	-1.199586	3.591180
6	7.665235	0.266332	4.922802
1	8.524413	0.300652	5.587276
6	6.540875	1.054335	5.184670
1	6.522958	1.708948	6.051783
6	5.435228	1.010666	4.333921
1	4.579508	1.638130	4.553622
6	2.899790	0.071323	2.987751

1	2.077811	-0.105543	2.290446
1	2.706006	1.012686	3.503998
1	2.888842	-0.721838	3.738899
6	1.251863	0.866989	-0.741813
1	0.992129	-0.092264	-1.180617
1	1.365308	0.820317	0.337944
6	0.601067	2.023844	-1.296258
1	0.035989	1.906934	-2.211097
6	0.505463	3.248135	-0.615137
1	1.006435	3.315970	0.340987
6	4.578084	2.719314	-2.955389
1	5.358820	3.012501	-2.258156
6	3.458668	3.581200	-3.043075
1	3.473956	4.475664	-2.421006
6	2.527592	3.684904	-4.239885
1	2.981907	4.325833	-5.011241
1	1.624153	4.203800	-3.905923
6	2.126689	2.326047	-4.854733
1	2.828885	2.042634	-5.644504
1	1.151424	2.431961	-5.341585
6	2.031909	1.187735	-3.844595
1	1.032523	0.824520	-3.636464
6	3.067846	0.319797	-3.538073
1	2.790673	-0.646160	-3.130294
6	4.474811	0.403844	-4.091351
1	5.111281	-0.241447	-3.483607
1	4.481598	-0.017097	-5.107601
6	5.066193	1.830497	-4.101034
1	4.849468	2.325622	-5.052705
1	6.155815	1.753923	-4.039343
6	0.134119	4.526725	-1.213548
6	-0.533802	4.632475	-2.449558
6	0.453550	5.710821	-0.519358
6	-0.865451	5.881353	-2.969850
1	-0.805080	3.738493	-2.999813
6	0.128926	6.959357	-1.045353
1	0.960016	5.640217	0.440193
6	-0.535097	7.049079	-2.272891
1	-1.384295	5.945725	-3.921968
1	0.389101	7.860946	-0.498341
1	-0.794424	8.020392	-2.683780
8	-2.412381	1.597784	-0.884579
6	-0.414134	2.778216	2.936893
6	-0.020418	2.016017	4.015671
1	-0.270068	3.853312	2.956414
6	-0.262051	0.637234	3.959010
6	-0.830976	0.086812	2.827584
1	-0.994355	-0.979419	2.743840
7	-1.221094	0.830633	1.771799
6	-3.774168	3.568413	-2.175580
1	-3.305298	2.749982	-2.715187
1	-4.843042	3.358191	-2.062092
1	-3.666976	4.484989	-2.764343
6	-3.344549	5.055493	-0.261721
1	-3.300235	4.985033	0.824248
1	-2.615766	5.797709	-0.609586
1	-4.347859	5.398417	-0.527145
7	-3.126062	3.753475	-0.883963
1	0.450890	2.473348	4.878783
35	0.212087	-0.518832	5.463187

---

9 P1-C1 *exo re-si*

Number of imaginary frequencies= 0
The smallest frequencies are= 9.8610 14.1888 19.4395 cm(-1)
Electronic energy= -7222.6660768
Zero-point correction= 1.759859
(Hartree/Particle)
Thermal correction to Energy= 1.877368
Thermal correction to Enthalpy= 1.878312
Thermal correction to Gibbs Free Energy= 1.601625
Sum of electronic and zero-point Energies= -7220.906218
Sum of electronic and thermal Energies= -7220.788709
Sum of electronic and thermal Enthalpies= -7220.787765
Sum of electronic and thermal Free Energies= -7221.064452

.....
Cartesian Coordinates
.....

26	-3.675495	-4.160212	3.478700
15	-1.401574	-2.160062	-0.795818
15	-4.409120	-0.373140	0.660570
6	-3.098860	-3.375124	1.624613
6	-3.801072	-2.389738	2.412879
6	-3.068807	-2.198163	3.625788
1	-3.347462	-1.535902	4.433687
6	-1.936951	-3.069884	3.608267
1	-1.213015	-3.186044	4.402755
6	-1.958013	-3.795642	2.381548
1	-1.250110	-4.552480	2.078221
6	-5.531870	-5.078427	3.660635
1	-6.414108	-4.812172	3.093704
6	-5.136781	-4.509744	4.909975
1	-5.659561	-3.729863	5.447580
6	-3.905871	-5.117440	5.302366
1	-3.330536	-4.875164	6.186215
6	-3.540274	-6.063427	4.296974
1	-2.640180	-6.663864	4.285550
6	-4.544380	-6.040688	3.283973
1	-4.537450	-6.624578	2.373589
6	-3.494838	-3.801140	0.251823
6	-4.653237	-4.575596	0.086659
1	-5.206836	-4.858988	0.972569
6	-5.105669	-4.967400	-1.172494
1	-6.021074	-5.542629	-1.265923
6	-4.383904	-4.598620	-2.305112
1	-4.720479	-4.894157	-3.293673
6	-3.233902	-3.821346	-2.168100
1	-2.695274	-3.527739	-3.061411
6	-2.782835	-3.394304	-0.908352
6	-5.014165	-1.629056	1.951943
1	-5.648357	-2.323719	1.398571
6	-5.846312	-1.027641	3.087530
1	-6.737582	-0.527429	2.699271
1	-5.281260	-0.299102	3.675055
1	-6.162938	-1.828945	3.761982
6	-0.905238	-1.921505	-2.552419
6	-1.600277	-0.945676	-3.288118
1	-2.329053	-0.315123	-2.791173
6	-1.355319	-0.781874	-4.652162
1	-1.913014	-0.039452	-5.212442
6	-0.387718	-1.564175	-5.288281
1	-0.187877	-1.428400	-6.347135
6	0.333184	-2.509772	-4.555639
1	1.099236	-3.108031	-5.040432
6	0.071110	-2.695894	-3.196621
1	0.627194	-3.447283	-2.647982
6	-0.014234	-3.072251	-0.014608
6	0.217210	-4.437722	-0.248784
1	-0.424373	-4.990161	-0.929031
6	1.257206	-5.094807	0.410365
1	1.432842	-6.150029	0.222494
6	2.069339	-4.398512	1.311844
1	2.877317	-4.912994	1.823504
6	1.844187	-3.041122	1.549476
1	2.475517	-2.494916	2.242173
6	0.806440	-2.381787	0.888729
1	0.625842	-1.329780	1.074691
6	-5.359605	-0.709067	-0.880348
6	-5.002021	0.062668	-1.994089
1	-4.229018	0.815843	-1.892631
6	-5.614229	-0.148434	-3.228930
6	-6.559920	-1.158276	-3.392280
1	-7.019749	-1.335202	-4.358141
6	-6.895281	-1.943244	-2.288186
6	-6.319279	-1.715229	-1.038332
1	-6.614731	-2.344668	-0.210704
6	-4.999368	1.285744	1.195453
6	-4.273489	1.903433	2.226576
1	-3.471918	1.367717	2.721527
6	-4.561147	3.212068	2.605684

6	-5.556817	3.941455	1.953816
1	-5.763802	4.967381	2.236418
6	-6.273012	3.328209	0.928542
6	-6.009961	2.008353	0.553953
1	-6.585512	1.561565	-0.247790
29	-2.123634	-0.264415	0.197414
6	-7.268018	4.137118	0.142614
6	-3.713676	3.892739	3.643373
6	-5.261455	0.771596	-4.364214
6	-7.859712	-3.081740	-2.485684
9	-7.337634	-4.036605	-3.295068
9	-8.190096	-3.687678	-1.323713
9	-9.008162	-2.670773	-3.069936
9	-3.920671	0.993561	-4.433863
9	-5.832309	1.991917	-4.205368
9	-5.652613	0.297641	-5.561464
9	-6.649539	4.826338	-0.856382
9	-7.901376	5.050382	0.906908
9	-8.207032	3.366432	-0.444248
9	-4.426061	4.745858	4.405790
9	-3.103783	3.012835	4.466421
9	-2.724713	4.628894	3.059635
6	-2.243518	2.732333	-0.578339
6	-1.082697	3.093847	0.329604
6	-0.855027	2.244747	1.562946
1	-1.229686	4.100892	0.712219
77	2.787953	1.610609	-1.888202
15	4.235345	0.413204	-0.569212
8	4.107453	-1.199728	-0.158144
8	5.785760	0.404804	-1.206764
7	4.246448	1.073998	0.985300
6	4.489652	-2.195882	-1.044835
6	3.453296	-2.985527	-1.590507
1	2.437112	-2.785822	-1.276732
6	3.754485	-3.979538	-2.486245
1	2.965412	-4.599752	-2.902433
6	5.097039	-4.193701	-2.900601
6	5.412680	-5.165758	-3.888147
1	4.604650	-5.762621	-4.303436
6	6.707275	-5.339999	-4.322459
1	6.936404	-6.081793	-5.081977
6	7.740770	-4.534052	-3.788684
1	8.757573	-4.653104	-4.151830
6	7.470518	-3.593839	-2.817807
1	8.275148	-2.979666	-2.431866
6	6.148814	-3.402287	-2.325444
6	5.830971	-2.424062	-1.315027
6	6.886449	-1.645187	-0.607792
6	7.966316	-2.279570	0.104031
6	8.017660	-3.683997	0.330115
1	7.215970	-4.310070	-0.043784
6	9.058409	-4.255327	1.029818
1	9.067615	-5.328599	1.197491
6	10.111269	-3.458125	1.539381
1	10.927553	-3.923327	2.084173
6	10.087137	-2.094257	1.353126
1	10.879844	-1.466538	1.752002
6	9.020392	-1.470595	0.649875
6	8.961089	-0.057404	0.515034
1	9.765436	0.545813	0.925853
6	7.877082	0.540811	-0.075952
1	7.786117	1.619277	-0.148124
6	6.841430	-0.258278	-0.608144
6	3.583102	2.404948	1.025739
1	2.566918	2.270162	1.415972
6	4.298574	3.393576	1.925729
6	3.569936	4.151681	2.848909
1	2.499260	3.984797	2.947956
6	4.207224	5.102735	3.651753
1	3.630907	5.678734	4.371019
6	5.583908	5.304651	3.534451
1	6.083809	6.037845	4.161205
6	6.317416	4.554756	2.607679
1	7.390309	4.701425	2.517934
6	5.678528	3.608421	1.809454
1	6.250296	3.002480	1.112822
6	3.469725	2.988874	-0.396630
1	4.457212	3.364459	-0.695186
1	2.821539	3.865478	-0.351720
6	4.281850	0.241589	2.233521
1	4.433119	-0.777839	1.884437
6	5.458599	0.532243	3.164204
6	6.643599	-0.191746	2.982937
1	6.701734	-0.919548	2.180333
6	7.747098	0.003777	3.815454
1	8.653992	-0.570071	3.645843
6	7.677618	0.928742	4.858814
1	8.533176	1.087189	5.509763
6	6.494521	1.643914	5.064532
1	6.426689	2.365874	5.873819
6	5.394829	1.442233	4.229046
1	4.494484	2.020723	4.400095
6	2.933444	0.256226	2.962486
1	2.127843	-0.026276	2.280231
1	2.688697	1.230940	3.388429
1	2.957326	-0.464583	3.784216
6	1.152724	0.808443	-0.683952
1	0.845571	-0.165191	-1.053855
1	1.331693	0.824107	0.386286
6	0.638318	1.977304	-1.316450
1	0.004465	1.812600	-2.180116
6	0.265896	3.217508	-0.534558
1	1.018713	3.395046	0.233933
6	4.293133	2.408654	-3.259966
1	5.108899	2.848280	-2.688739
6	3.101098	3.195515	-3.367824
1	3.113099	4.172998	-2.884519
6	2.145071	3.119680	-4.548447
1	2.576792	3.629477	-5.424584
1	1.250225	3.683153	-4.275618
6	1.734945	1.678630	-4.924894
1	2.363169	1.300023	-5.738049
1	0.711456	1.683270	-5.315344
6	1.793646	0.694852	-3.759246
1	0.835589	0.312388	-3.424130
6	2.903289	-0.089038	-3.456734
1	2.713107	-1.025236	-2.943027
6	4.251048	-0.005509	-4.149634
1	4.971191	-0.546597	-3.531135
1	4.199671	-0.538224	-5.111652
6	4.756330	1.439140	-4.354434
1	4.442374	1.817013	-5.333966
1	5.850944	1.425965	-4.376459
6	0.169077	4.475032	-1.380824
6	-0.509604	4.496754	-2.608372
6	0.696567	5.678232	-0.891463
6	-0.657325	5.687367	-3.322633
1	-0.932808	3.583751	-3.014223
6	0.561198	6.870100	-1.607433
1	1.219179	5.680590	0.062386
6	-0.120923	6.878870	-2.826293
1	-1.189259	5.682374	-4.270062
1	0.985604	7.788685	-1.211815
1	-0.233878	7.803954	-3.384347
8	-2.341542	1.579577	-1.060805
6	-0.287117	2.898921	2.669441
6	-0.006372	2.207103	3.838919
1	-0.083471	3.962168	2.613800
6	-0.305315	0.848799	3.859508
6	-0.848582	0.238421	2.740941
1	-1.077454	-0.818942	2.734009
7	-1.122022	0.924265	1.610348
6	-3.938220	3.499643	-2.138326
1	-3.498994	2.744605	-2.785972
1	-4.942369	3.186710	-1.843691
1	-4.014693	4.438771	-2.691179
6	-3.161376	5.056926	-0.381635
1	-2.929855	5.038404	0.681154
1	-2.493218	5.755182	-0.896826
1	-4.190256	5.406068	-0.483662

7	-3.081420	3.716803	-0.970433
1	0.424379	2.711207	4.696547
35	0.051938	-0.216441	5.449740

[8-9]‡-P1-C1 *endo re-re* conf2

Number of imaginary frequencies= 1
The smallest frequencies are= -255.2870 9.8902 13.3757 cm(-1)
Electronic energy= -7222.6284099
Zero-point correction= 1.754400
(Hartree/Particle)
Thermal correction to Energy= 1.873024
Thermal correction to Enthalpy= 1.873969
Thermal correction to Gibbs Free Energy= 1.592776
Sum of electronic and zero-point Energies= -7220.874010
Sum of electronic and thermal Energies= -7220.755386
Sum of electronic and thermal Enthalpies= -7220.754441
Sum of electronic and thermal Free Energies= -7221.035634

.....

Cartesian Coordinates

.....

26	4.734876	4.665648	1.790828
15	2.778976	1.496143	-1.852997
15	4.720415	-0.025016	0.973603
6	4.311286	3.285680	0.276447
6	4.471768	2.629714	1.554062
6	3.486268	3.159440	2.443433
1	3.357523	2.884734	3.481337
6	2.739763	4.155098	1.744204
1	1.952984	4.767889	2.161824
6	3.247655	4.235424	0.414901
1	2.908977	4.911343	-0.355475
6	6.712328	5.103573	2.249086
1	7.534788	4.406082	2.160754
6	5.884480	5.281748	3.399768
1	5.965066	4.739122	4.332252
6	4.903276	6.271747	3.089069
1	4.107226	6.604164	3.742301
6	5.124386	6.706628	1.746834
1	4.527708	7.428255	1.204558
6	6.242283	5.987554	1.228673
1	6.639690	6.077519	0.227101
6	5.073361	2.936457	-0.957505
6	6.425866	3.293670	-1.059945
1	6.869296	3.852986	-0.245951
6	7.201259	2.932575	-2.161579
1	8.252026	3.201832	-2.196677
6	6.624981	2.202506	-3.198459
1	7.218922	1.901502	-4.055510
6	5.281961	1.832979	-3.119432
1	4.849837	1.249479	-3.924896
6	4.493837	2.177866	-2.010336
6	5.440212	1.509746	1.827295
1	6.364481	1.738298	1.294295
6	5.781844	1.324266	3.308722
1	6.520698	0.529810	3.443456
1	4.904319	1.071833	3.910538
1	6.198353	2.257802	3.699520
6	2.495753	0.578051	-3.427557
6	2.670048	-0.815338	-3.410763
1	2.964223	-1.310811	-2.493196
6	2.423256	-1.573056	-4.557882
1	2.562388	-2.648807	-4.530720
6	1.987530	-0.950144	-5.729121
1	1.780427	-1.541180	-6.616637
6	1.814441	0.436439	-5.754474
1	1.474782	0.927147	-6.662151
6	2.070009	1.198042	-4.613388
1	1.917692	2.271150	-4.648788
6	1.681455	2.957763	-2.032188
6	2.044408	4.089534	-2.780267
1	3.025720	4.142965	-3.242472
6	1.152634	5.154235	-2.922007
1	1.443336	6.027021	-3.499819
6	-0.112128	5.094536	-2.327153
1	-0.811319	5.918001	-2.441125
6	-0.477433	3.971542	-1.582082
1	-1.457338	3.918817	-1.122687
6	0.420052	2.913593	-1.424861
1	0.139551	2.050393	-0.831819
6	5.971003	-0.589798	-0.256482
6	5.553791	-1.626147	-1.104339
1	4.561945	-2.045645	-0.974622
6	6.401443	-2.111379	-2.099470
6	7.659829	-1.547551	-2.299872
1	8.308401	-1.906805	-3.091011
6	8.062994	-0.500968	-1.470279
6	7.242515	-0.036803	-0.441901
1	7.604516	0.766071	0.185457
6	4.702065	-1.400400	2.197776
6	3.709644	-1.360011	3.190328
1	3.061362	-0.495234	3.278179
6	3.521745	-2.447015	4.041263
6	4.285451	-3.606439	3.900939
1	4.105483	-4.466153	4.536604
6	5.258688	-3.650347	2.906114
6	5.486404	-2.552863	2.074913
1	6.251931	-2.624110	1.312639
29	2.608439	0.155047	-0.035119
6	6.064355	-4.907344	2.727315
6	2.402325	-2.444623	5.043561
6	5.953960	-3.292336	-2.914854
6	9.394121	0.146051	-1.738017
9	9.430555	0.703246	-2.974403
9	9.682281	1.126412	-0.853913
9	10.407182	-0.749805	-1.692741
9	6.097249	-4.451938	-2.224925
9	6.648349	-3.424210	-4.062660
9	4.639346	-3.210586	-3.245790
9	7.051545	-5.017031	3.644752
9	6.646343	-4.968888	1.507978
9	5.289495	-6.013049	2.856370
9	2.771513	-3.007454	6.214737
9	1.947293	-1.203105	5.312761
9	1.338807	-3.166055	4.590925
6	2.009404	-2.805056	0.520106
6	0.863432	-2.457954	1.334344
6	0.586916	-1.161900	1.886880
1	0.430912	-3.259962	1.915220
77	-3.322384	-1.086574	-1.263464
15	-5.180379	-0.221177	-0.276298
8	-5.130235	0.890185	0.963847
8	-6.128182	0.604624	-1.364921
7	-6.046986	-1.433860	0.500085
6	-4.741202	2.196185	0.704787
6	-3.487864	2.600235	1.216052
1	-2.907060	1.885957	1.789243
6	-3.039587	3.874474	0.972015
1	-2.085309	4.205274	1.368787
6	-3.795160	4.760783	0.156473
6	-3.284483	6.038911	-0.199631
1	-2.316676	6.337410	0.194550
6	-3.988888	6.871899	-1.039730
1	-3.587029	7.843374	-1.312195
6	-5.237117	6.453771	-1.560084
1	-5.780550	7.103705	-2.239794
6	-5.768606	5.228910	-1.218230
1	-6.721960	4.923497	-1.632906
6	-5.075786	4.346913	-0.342845
6	-5.589839	3.050355	0.018595
6	-6.971883	2.613923	-0.328568
6	-8.127960	3.381716	0.061258
6	-8.043676	4.517441	0.914972
1	-7.079099	4.819624	1.304820
6	-9.170086	5.229009	1.267304
1	-9.077932	6.086915	1.927181
6	-10.445787	4.849572	0.786234
1	-11.323605	5.423823	1.067622
6	-10.568429	3.743489	-0.023494
1	-11.543205	3.427105	-0.385488

6	-9.428917	2.978401	-0.393426
6	-9.561130	1.808581	-1.188721
1	-10.546331	1.519230	-1.543383
6	-8.465132	1.033292	-1.475770
1	-8.546792	0.116087	-2.048937
6	-7.189765	1.428639	-1.015716
6	-5.442938	-2.781203	0.300783
1	-4.790720	-2.998431	1.155926
6	-6.472364	-3.893572	0.199576
6	-6.274070	-5.090790	0.893887
1	-5.410773	-5.192679	1.548194
6	-7.182515	-6.146043	0.768515
1	-7.019263	-7.068470	1.319337
6	-8.303154	-6.008365	-0.051822
1	-9.018595	-6.821068	-0.140955
6	-8.503235	-4.815446	-0.756362
1	-9.377475	-4.698558	-1.390684
6	-7.589015	-3.771233	-0.638620
1	-7.754702	-2.836197	-1.164787
6	-4.592917	-2.785321	-0.981220
1	-5.270255	-2.851645	-1.840252
1	-3.984551	-3.694256	-0.987588
6	-6.809579	-1.156680	1.767566
1	-7.022820	-0.087728	1.739561
6	-8.168874	-1.849830	1.808171
6	-9.226728	-1.293036	1.078526
1	-9.059276	-0.381243	0.515453
6	-10.485268	-1.893670	1.061738
1	-11.289853	-1.444396	0.485453
6	-10.709360	-3.065143	1.789839
1	-11.686381	-3.540249	1.777687
6	-9.668577	-3.616460	2.540364
1	-9.831680	-4.525534	3.112485
6	-8.411284	-3.008653	2.554762
1	-7.614804	-3.461522	3.133835
6	-5.942115	-1.411747	3.006053
1	-5.035254	-0.804049	2.954251
1	-5.648206	-2.459737	3.107965
1	-6.494011	-1.131852	3.908470
6	-2.423526	-0.942308	0.712994
1	-1.732806	-0.103841	0.747850
1	-3.113382	-0.949671	1.551921
6	-1.958862	-2.216281	0.247681
1	-2.509278	-3.086050	0.590555
6	-0.717999	-2.463590	-0.395898
1	-0.157444	-1.617306	-0.768159
6	-4.132566	-0.907129	-3.324558
1	-5.147622	-1.297974	-3.310912
6	-3.087863	-1.867625	-3.343275
1	-3.379627	-2.917487	-3.360667
6	-1.703626	-1.603257	-3.908452
1	-1.739189	-1.625115	-5.008761
1	-1.060923	-2.434164	-3.608493
6	-1.071831	-0.279898	-3.428919
1	-1.254022	0.519770	-4.153522
1	0.011288	-0.402818	-3.385258
6	-1.553349	0.184129	-2.057720
1	-0.801674	0.170190	-1.274931
6	-2.623135	1.052701	-1.861170
1	-2.611944	1.650899	-0.955842
6	-3.525804	1.575691	-2.959091
1	-4.395086	2.033533	-2.483674
1	-3.000766	2.377920	-3.498656
6	-4.001828	0.486802	-3.946223
1	-3.322140	0.429538	-4.802825
1	-4.975615	0.781597	-4.348778
6	-0.402729	-3.745395	-1.039181
6	-1.009892	-4.961363	-0.668111
6	0.556393	-3.765279	-2.070143
6	-0.668875	-6.150014	-1.310659
1	-1.742089	-4.983548	0.132718
6	0.894530	-4.954242	-2.713181
1	1.042081	-2.838933	-2.352651
6	0.284747	-6.153041	-2.335231
1	-1.145863	-7.078559	-1.010034
1	1.639552	-4.945298	-3.503928
1	0.547972	-7.082085	-2.832511
7	2.504851	-4.074127	0.599916
6	3.479588	-4.544778	-0.378463
1	3.255080	-5.584320	-0.634380
1	3.417061	-3.947691	-1.282892
1	4.499727	-4.496321	0.018635
6	2.123175	-5.051184	1.616552
1	1.837413	-4.564482	2.547970
1	1.300225	-5.689286	1.271348
1	2.988540	-5.682263	1.831596
8	2.516492	-2.003332	-0.325648
6	-0.286717	-1.091165	3.007704
6	-0.634782	0.118956	3.573551
1	-0.658035	-2.011796	3.441051
6	-0.116292	1.278133	2.989209
6	0.717805	1.183299	1.889420
1	1.130387	2.066699	1.418588
7	1.071509	0.000310	1.348849
1	-1.286227	0.162370	4.439816
35	-0.517184	3.037021	3.743722

[8-9]$^{+}$-P1-C1 *endo si-re* conf2

Number of imaginary frequencies= 1
The smallest frequencies are= -216.8088 6.9238 9.5093 cm(-1)
Electronic energy= -7222.6176097
Zero-point correction= 1.754258
(Hartree/Particle)
Thermal correction to Energy= 1.873240
Thermal correction to Enthalpy= 1.874184
Thermal correction to Gibbs Free Energy= 1.589712
Sum of electronic and zero-point Energies= -7220.863352
Sum of electronic and thermal Energies= -7220.744370
Sum of electronic and thermal Enthalpies= -7220.743425
Sum of electronic and thermal Free Energies= -7221.027898

.....

Cartesian Coordinates

.....

26	3.751073	4.706004	2.839634
15	2.590871	1.976120	-1.414747
15	5.010192	0.394924	1.200239
6	3.620888	3.680124	1.019391
6	4.188951	2.841943	2.044171
6	3.226776	2.723733	3.094967
1	3.363400	2.170661	4.014529
6	2.081347	3.496316	2.740173
1	1.199599	3.642823	3.349587
6	2.325683	4.092038	1.468420
1	1.657964	4.750164	0.931297
6	5.469358	5.801223	3.255929
1	6.458124	5.562305	2.887453
6	4.884835	5.317391	4.465972
1	5.348323	4.638281	5.168862
6	3.561812	5.846961	4.558718
1	2.847305	5.638679	5.344324
6	3.328870	6.658415	3.406776
1	2.408191	7.173955	3.166807
6	4.506572	6.630737	2.602318
1	4.632577	7.126218	1.649375
6	4.264866	3.978616	-0.289369
6	5.340876	4.875934	-0.351368
1	5.674287	5.339422	0.568029
6	5.981356	5.170980	-1.555234
1	6.818555	5.862848	-1.567468
6	5.537393	4.576642	-2.734017
1	6.019379	4.798521	-3.681114
6	4.481361	3.666050	-2.693064
1	4.166721	3.193099	-3.615471
6	3.849524	3.335221	-1.483675
6	5.483723	2.092680	1.907476
1	6.059566	2.559394	1.102636
6	6.343566	2.073070	3.173575
1	7.289992	1.551775	3.006294
1	5.829853	1.592549	4.010651

1	6.568743	3.103056	3.463729
6	2.563170	1.346159	-3.143306
6	3.655102	0.556909	-3.546052
1	4.483885	0.401820	-2.864129
6	3.699821	-0.001787	-4.821352
1	4.556534	-0.599669	-5.117885
6	2.640442	0.205346	-5.710905
1	2.665818	-0.238256	-6.701857
6	1.551742	0.986605	-5.320387
1	0.726921	1.153883	-6.007058
6	1.513758	1.561270	-4.046016
1	0.662554	2.170128	-3.763065
6	0.997666	2.855443	-1.170792
6	0.676543	4.036867	-1.856945
1	1.360528	4.438020	-2.599331
6	-0.514336	4.708722	-1.574507
1	-0.760172	5.620585	-2.111221
6	-1.381860	4.217113	-0.592860
1	-2.304505	4.744656	-0.372579
6	-1.059992	3.047090	0.098072
1	-1.721861	2.665496	0.869728
6	0.120628	2.361939	-0.193696
1	0.388540	1.466474	0.358343
6	6.402601	-0.039012	0.075946
6	7.045743	-1.285096	0.079880
1	6.828537	-2.020060	0.845048
6	7.958317	-1.610717	-0.924096
6	8.236329	-0.721384	-1.960948
1	8.933056	-0.987920	-2.745966
6	7.580258	0.508168	-1.978452
6	6.673676	0.852189	-0.974755
1	6.160254	1.807386	-1.035321
6	5.124265	-0.793778	2.599171
6	3.916950	-1.351470	3.034081
1	2.988864	-1.053041	2.559096
6	3.904218	-2.286428	4.071335
6	5.086535	-2.675735	4.694698
1	5.076258	-3.409265	5.492204
6	6.290004	-2.109823	4.268205
6	6.316214	-1.175389	3.233135
1	7.267203	-0.765949	2.912543
29	3.025412	0.278329	0.036066
6	7.577864	-2.467329	4.960123
6	2.590167	-2.913776	4.444332
6	8.684891	-2.927683	-0.857230
6	7.775141	1.465982	-3.122472
9	6.654398	1.546948	-3.886887
9	8.036089	2.719821	-2.688038
9	8.784788	1.100960	-3.938537
9	7.938747	-3.886637	-0.265652
9	9.829363	-2.824230	-0.138282
9	9.033840	-3.378549	-2.082505
9	7.901575	-1.552956	5.906290
9	8.615080	-2.512499	4.092971
9	7.510148	-3.666286	5.576818
9	2.651102	-3.607767	5.597933
9	1.612107	-1.985991	4.578342
9	2.168245	-3.776665	3.481457
6	4.049175	-2.089442	-1.454655
6	2.090797	-2.680569	-0.317761
6	4.210990	-3.368778	-1.953269
1	4.759072	-1.308506	-1.690380
6	2.243621	-4.014033	-0.790050
6	3.292751	-4.365737	-1.616481
1	1.510822	-4.760360	-0.504530
6	0.912549	-2.370385	0.442902
6	0.730679	-1.257918	1.337533
8	1.395580	-0.173633	1.268476
7	3.014696	-1.739160	-0.670109
1	0.293217	-3.236036	0.628905
7	-0.246219	-1.348552	2.291811
6	-0.582328	-0.187670	3.105816
1	-0.175924	-0.288549	4.119572
1	-1.671280	-0.091788	3.174989
1	-0.169301	0.712060	2.654622
6	-0.877956	-2.609003	2.678339
1	-0.137793	-3.404908	2.780525
1	-1.648122	-2.922084	1.965969
1	-1.351463	-2.470585	3.652094
77	-3.683484	-0.732043	-1.549594
15	-5.455104	-0.250026	-0.211656
8	-5.522295	0.981458	0.900597
8	-6.806198	0.093143	-1.122734
7	-5.748516	-1.550620	0.814325
6	-5.890401	2.277136	0.555093
6	-4.889503	3.263828	0.692393
1	-3.915934	2.961726	1.059824
6	-5.168888	4.568230	0.371546
1	-4.413062	5.338897	0.491685
6	-6.442317	4.924797	-0.146738
6	-6.714966	6.256182	-0.562612
1	-5.933738	7.003414	-0.449661
6	-7.932524	6.590886	-1.110021
1	-8.129145	7.609851	-1.430121
6	-8.925369	5.595737	-1.272480
1	-9.875664	5.854203	-1.730744
6	-8.698383	4.299537	-0.863007
1	-9.469227	3.552797	-1.008746
6	-7.461413	3.921029	-0.268829
6	-7.189991	2.574029	0.170486
6	-8.247205	1.523930	0.160216
6	-9.508998	1.687730	0.835259
6	-9.769974	2.768234	1.723478
1	-8.992299	3.499194	1.911522
6	-10.987264	2.888929	2.357869
1	-11.158021	3.717933	3.038665
6	-12.015004	1.940567	2.138066
1	-12.970730	2.052357	2.641541
6	-11.792672	0.873757	1.297338
1	-12.566347	0.128754	1.130908
6	-10.543787	0.710956	0.637674
6	-10.295388	-0.416112	-0.191665
1	-11.088795	-1.140667	-0.349835
6	-9.055240	-0.612969	-0.746329
1	-8.830704	-1.483941	-1.351481
6	-8.039255	0.343496	-0.535315
6	-5.042474	-2.781200	0.366018
1	-4.141882	-2.906006	0.979552
6	-5.877488	-4.042494	0.495429
6	-5.294910	-5.211065	0.996125
1	-4.262507	-5.189699	1.339239
6	-6.032816	-6.395169	1.082126
1	-5.569582	-7.292970	1.482468
6	-7.366035	-6.418310	0.669057
1	-7.946882	-7.333004	0.747388
6	-7.951588	-5.254763	0.157206
1	-8.991152	-5.262546	-0.158627
6	-7.209347	-4.079828	0.062391
1	-7.670501	-3.169804	-0.305597
6	-4.609324	-2.613560	-1.103893
1	-5.488934	-2.746347	-1.746792
1	-3.919997	-3.424826	-1.354332
6	-6.097375	-1.380472	2.266505
1	-6.470220	-0.360721	2.345387
6	-7.246331	-2.276329	2.714887
6	-8.556772	-1.839316	2.487061
1	-8.716470	-0.875939	2.016677
6	-9.651055	-2.623532	2.852142
1	-10.658809	-2.264337	2.661697
6	-9.446426	-3.860082	3.469249
1	-10.294104	-4.477511	3.753561
6	-8.143422	-4.292671	3.729662
1	-7.974250	-5.249824	4.215089
6	-7.052692	-3.502657	3.362005
1	-6.048995	-3.861246	3.560845
6	-4.856259	-1.474872	3.163211
1	-4.138042	-0.696877	2.890865
1	-4.355756	-2.444252	3.096129
1	-5.145266	-1.322213	4.207351
6	-2.439592	-0.677393	0.229737

1	-1.883257	0.254737	0.309045
1	-2.943382	-0.948691	1.150702
6	-1.851459	-1.739485	-0.537035
1	-2.183832	-2.752085	-0.341302
6	-0.649194	-1.604807	-1.272609
1	-0.195869	-0.618138	-1.299752
6	-4.905820	-0.606117	-3.420242
1	-5.816126	-1.170797	-3.236525
6	-3.740432	-1.358389	-3.696690
1	-3.848597	-2.442498	-3.730655
6	-2.537736	-0.833601	-4.460667
1	-2.751186	-0.841030	-5.540803
1	-1.715888	-1.536803	-4.305291
6	-2.075934	0.574642	-4.028159
1	-2.548069	1.341604	-4.650632
1	-1.002617	0.653104	-4.210188
6	-2.332979	0.904639	-2.560966
1	-1.452844	0.991458	-1.933541
6	-3.481543	1.528448	-2.089574
1	-3.393951	2.064024	-1.149479
6	-4.676555	1.918176	-2.938584
1	-5.501547	2.162955	-2.265194
1	-4.438677	2.841915	-3.486811
6	-5.140999	0.819957	-3.921892
1	-4.648580	0.944766	-4.891519
1	-6.211525	0.950670	-4.106405
6	-0.201837	-2.515282	-2.319449
6	-0.762290	-3.794389	-2.512783
6	0.822913	-2.092018	-3.188639
6	-0.319222	-4.611873	-3.548943
1	-1.553829	-4.145157	-1.858163
6	1.264399	-2.912869	-4.224721
1	1.267904	-1.112295	-3.049182
6	0.694214	-4.174608	-4.410456
1	-0.765121	-5.592651	-3.688127
1	2.051799	-2.562726	-4.884133
1	1.035124	-4.814461	-5.219298
1	3.392658	-5.378833	-1.989913
35	5.715334	-3.747842	-3.140755

[8-9]‡-P1-C1 *exo si-si* conf2

Number of imaginary frequencies= 1
The smallest frequencies are= -153.7535 8.5286 10.6626 cm(-1)
Electronic energy= -7222.6206504
Zero-point correction= 1.754800
(Hartree/Particle)
Thermal correction to Energy= 1.873746
Thermal correction to Enthalpy= 1.874690
Thermal correction to Gibbs Free Energy= 1.591401
Sum of electronic and zero-point Energies= -7220.865850
Sum of electronic and thermal Energies= -7220.746904
Sum of electronic and thermal Enthalpies= -7220.745960
Sum of electronic and thermal Free Energies= -7221.029250

.....

Cartesian Coordinates

.....

26	3.848815	4.474038	3.163571
15	1.178196	2.281163	-0.762619
15	4.500735	0.586678	0.479637
6	3.024899	3.723646	1.383359
6	3.993749	2.811162	1.934884
6	3.547074	2.432492	3.239977
1	4.065125	1.762936	3.913485
6	2.327904	3.122425	3.509484
1	1.763928	3.081824	4.431821
6	2.013816	3.927019	2.375719
1	1.163357	4.585570	2.281329
6	5.547678	5.667846	3.062478
1	6.305508	5.590952	2.294592
6	5.522980	4.940855	4.291703
1	6.255351	4.213774	4.615529
6	4.335308	5.306043	4.996047
1	4.009366	4.900646	5.944925
6	3.625250	6.257669	4.202055
1	2.669105	6.702386	4.444690
6	4.374341	6.482383	3.008691
1	4.082891	7.128999	2.192228
6	3.093660	4.259107	-0.006428
6	4.022763	5.264815	-0.310069
1	4.632675	5.654343	0.494407
6	4.183964	5.753562	-1.606999
1	4.919114	6.527997	-1.805896
6	3.399995	5.239397	-2.635937
1	3.512157	5.602520	-3.652811
6	2.472360	4.233875	-2.360348
1	1.882781	3.835751	-3.176872
6	2.311541	3.720787	-1.063363
6	5.144042	2.234635	1.164052
1	5.296655	2.843947	0.267845
6	6.465569	2.166542	1.932385
1	7.256091	1.716614	1.324572
1	6.372459	1.589336	2.855956
1	6.774958	3.180889	2.199178
6	0.393806	2.041237	-2.411425
6	1.067586	1.203547	-3.315764
1	1.980172	0.709364	-3.000198
6	0.596199	1.033860	-4.617521
1	1.136267	0.393218	-5.308890
6	-0.568838	1.689520	-5.027015
1	-0.942708	1.555005	-6.037694
6	-1.257600	2.507392	-4.128354
1	-2.172798	3.006321	-4.434356
6	-0.779130	2.685885	-2.828666
1	-1.326732	3.322496	-2.144992
6	-0.125625	3.020655	0.301035
6	-0.593189	2.270094	1.388423
1	-0.219855	1.263219	1.539828
6	-1.487399	2.836209	2.298789
1	-1.831309	2.247395	3.141354
6	-1.927402	4.150313	2.127637
1	-2.621316	4.591014	2.837972
6	-1.472402	4.901078	1.038012
1	-1.812584	5.923383	0.900178
6	-0.571297	4.342086	0.130308
1	-0.190964	4.944910	-0.689166
6	5.435537	0.398634	-1.092956
6	6.286910	-0.660847	-1.430276
1	6.507661	-1.449004	-0.722168
6	6.846374	-0.729863	-2.707556
6	6.547295	0.223174	-3.680227
1	6.969846	0.148552	-4.674646
6	5.669387	1.255628	-3.355214
6	5.123109	1.350992	-2.075786
1	4.428766	2.157069	-1.853612
6	5.123842	-0.668699	1.669124
6	4.155195	-1.205260	2.527467
1	3.124080	-0.891268	2.423723
6	4.512586	-2.123313	3.515007
6	5.836875	-2.533597	3.658500
1	6.114379	-3.252783	4.419869
6	6.803057	-1.994975	2.808349
6	6.459847	-1.060188	1.829654
1	7.241192	-0.641463	1.206850
29	2.216633	0.413509	0.037266
6	8.252356	-2.363175	2.977041
6	3.437891	-2.713807	4.385625
6	7.829741	-1.824940	-3.022557
6	5.253989	2.275056	-4.380508
9	3.903318	2.292336	-4.532239
9	5.614490	3.528138	-4.017635
9	5.788076	2.037435	-5.595171
9	7.806155	-2.171272	-4.328782
9	7.596066	-2.941334	-2.297754
9	9.099940	-1.439115	-2.745267
9	8.874275	-2.494767	1.782384
9	8.411508	-3.523133	3.648435
9	8.929436	-1.410381	3.663059
9	3.919686	-3.145366	5.570564
9	2.453997	-1.821131	4.646779

9	2.842248	-3.782257	3.793898
6	3.022076	-1.777692	-1.904706
6	2.167523	-2.715210	0.063567
6	3.602389	-2.973499	-2.286588
1	3.122605	-0.893822	-2.522858
6	2.824287	-3.936930	-0.260382
6	3.536480	-4.078617	-1.434278
1	2.729286	-4.779147	0.416711
6	1.270084	-2.718815	1.177994
6	0.781542	-1.577089	1.893775
8	1.078883	-0.377610	1.590708
7	2.330323	-1.630305	-0.759229
1	1.212009	-3.671856	1.683712
7	-0.061431	-1.764290	2.958049
6	-0.414954	-0.627611	3.802938
1	0.248955	0.209716	3.597411
1	-0.315969	-0.909920	4.855133
1	-1.449552	-0.315441	3.628521
6	-0.448599	-3.070399	3.475583
1	-0.628499	-3.786038	2.672937
1	-1.379684	-2.958743	4.036294
1	0.317685	-3.481829	4.144105
77	-3.324811	-1.621256	-1.294941
15	-4.944766	-0.732630	0.043854
8	-4.932245	0.801502	0.679756
8	-6.379665	-0.682495	-0.807385
7	-5.080214	-1.627383	1.451612
6	-5.100838	1.896575	-0.167456
6	-3.964235	2.704101	-0.389256
1	-3.040795	2.450732	0.116040
6	-4.056707	3.784010	-1.231606
1	-3.197319	4.427611	-1.389014
6	-5.263702	4.053917	-1.929924
6	-5.336925	5.103715	-2.885262
1	-4.455271	5.718571	-3.046830
6	-6.490004	5.327817	-3.602766
1	-6.533677	6.128024	-4.335789
6	-7.618439	4.499258	-3.394996
1	-8.518939	4.660584	-3.980560
6	-7.585904	3.485363	-2.461972
1	-8.457290	2.856171	-2.326920
6	-6.419077	3.237573	-1.685893
6	-6.344408	2.175751	-0.713059
6	-7.542586	1.375698	-0.335797
6	-8.743531	1.995997	0.164634
6	-8.814779	3.380647	0.485518
1	-7.935058	4.000756	0.360325
6	-9.977994	3.940962	0.967788
1	-10.002459	4.998912	1.213003
6	-11.138276	3.152282	1.152900
1	-12.049693	3.609327	1.526916
6	-11.100024	1.805214	0.872124
1	-11.977294	1.182364	1.026578
6	-9.911774	1.192526	0.389816
6	-9.856604	-0.206691	0.146074
1	-10.751065	-0.804453	0.297176
6	-8.680610	-0.800107	-0.237672
1	-8.601088	-1.871379	-0.389816
6	-7.528643	-0.006530	-0.436996
6	-4.212014	-2.840196	1.444922
1	-3.276873	-2.596094	1.966660
6	-4.851920	-4.024925	2.148608
6	-4.095539	-4.801663	3.033718
1	-3.071960	-4.511962	3.258111
6	-4.644722	-5.940405	3.630441
1	-4.045129	-6.533053	4.315980
6	-5.962397	-6.309191	3.352890
1	-6.393802	-7.189344	3.821095
6	-6.726421	-5.535923	2.471974
1	-7.753905	-5.814785	2.254706
6	-6.173321	-4.405679	1.870770
1	-6.767864	-3.798736	1.192831
6	-3.910916	-3.232060	-0.005204
1	-4.821703	-3.673642	-0.427915
1	-3.159548	-4.022976	-0.015008
6	-5.650712	-1.249653	2.781851
1	-5.949852	-2.208256	3.210562
6	-4.639131	-0.661463	3.766330
6	-4.098088	-1.498204	4.754998
1	-4.330772	-2.559683	4.735497
6	-3.302029	-0.982936	5.781079
1	-2.902687	-1.649006	6.541054
6	-3.038774	0.386632	5.837928
1	-2.436971	0.796838	6.643903
6	-3.554812	1.226927	4.847461
1	-3.362003	2.295375	4.890236
6	-4.337319	0.707763	3.812668
1	-4.736629	1.375023	3.057162
6	-6.934130	-0.420856	2.715089
1	-7.699123	-0.947687	2.142923
1	-6.788751	0.565660	2.276511
1	-7.306909	-0.286089	3.734718
6	-1.821838	-0.703978	-0.028123
1	-1.635621	0.332736	-0.295925
1	-1.996199	-0.841426	1.037346
6	-1.037369	-1.703501	-0.709668
1	-0.457764	-1.410292	-1.575978
6	-0.824305	-2.989951	-0.189307
1	-1.320596	-3.219461	0.745023
6	-4.850463	-2.360752	-2.784668
1	-5.639243	-2.831294	-2.204316
6	-3.665032	-3.103617	-2.959079
1	-3.634376	-4.099957	-2.518856
6	-2.672642	-2.900151	-4.089186
1	-3.057071	-3.370951	-5.007206
1	-1.763747	-3.446973	-3.826480
6	-2.312991	-1.424482	-4.364393
1	-2.961366	-1.011535	-5.144122
1	-1.295404	-1.374193	-4.763490
6	-2.385797	-0.517547	-3.139691
1	-1.437332	-0.119822	-2.796214
6	-3.514431	0.199931	-2.769956
1	-3.352193	1.095514	-2.180559
6	-4.853958	0.129482	-3.472526
1	-5.589780	0.629686	-2.843537
1	-4.791951	0.712250	-4.403690
6	-5.339124	-1.305301	-3.775909
1	-5.035379	-1.603521	-4.784789
1	-6.433030	-1.309260	-3.773348
6	-0.353554	-4.139609	-0.950390
6	0.199482	-4.025599	-2.240705
6	-0.458892	-5.422511	-0.377161
6	0.612432	-5.157345	-2.938996
1	0.318525	-3.047913	-2.693548
6	-0.043634	-6.554039	-1.076074
1	-0.871623	-5.522964	0.623680
6	0.490027	-6.425734	-2.362749
1	1.039111	-5.048856	-3.931915
1	-0.137091	-7.535417	-0.620051
1	0.813350	-7.306753	-2.909456
1	4.006063	-5.021744	-1.691069
35	4.469991	-3.113521	-4.032577

[8-9]‡-P1-C1 *exo re-si* conf2

Number of imaginary frequencies= 1
The smallest frequencies are= -68.1274 8.5848 10.3975 cm(-1)
Electronic energy= -7222.6318937
Zero-point correction= 1.754511
(Hartree/Particle)
Thermal correction to Energy= 1.873363
Thermal correction to Enthalpy= 1.874307
Thermal correction to Gibbs Free Energy= 1.591971
Sum of electronic and zero-point Energies= -7220.877383
Sum of electronic and thermal Energies= -7220.758531
Sum of electronic and thermal Enthalpies= -7220.757587
Sum of electronic and thermal Free Energies= -7221.039922
.....
Cartesian Coordinates
.....

26	-4.419019	-3.967333	3.287124
15	-1.346014	-2.104544	-0.575909
15	-4.499218	-0.254349	0.279185
6	-3.472833	-3.243720	1.557582
6	-4.283754	-2.221881	2.175786
6	-3.795137	-2.019663	3.502849
1	-4.199582	-1.326490	4.227077
6	-2.707132	-2.919390	3.721082
1	-2.151162	-3.029675	4.641190
6	-2.510351	-3.672533	2.526879
1	-1.777430	-4.451684	2.378654
6	-6.312913	-4.812756	3.146998
1	-7.061679	-4.532352	2.418185
6	-6.128541	-4.214357	4.430922
1	-6.705630	-3.395818	4.840310
6	-5.018219	-4.854710	5.060825
1	-4.604080	-4.602251	6.028136
6	-4.514705	-5.847408	4.165922
1	-3.654778	-6.481326	4.337700
6	-5.315066	-5.823538	2.985235
1	-5.167359	-6.441128	2.109948
6	-3.623389	-3.699133	0.145764
6	-4.750014	-4.462670	-0.198738
1	-5.452038	-4.714922	0.585089
6	-4.992253	-4.879197	-1.506422
1	-5.890124	-5.442331	-1.740402
6	-4.080803	-4.550589	-2.506040
1	-4.248893	-4.864325	-3.531326
6	-2.957327	-3.786753	-2.191120
1	-2.272741	-3.528657	-2.989309
6	-2.715592	-3.330397	-0.883694
6	-5.369513	-1.455677	1.467852
1	-5.893126	-2.161993	0.821921
6	-6.396314	-0.809528	2.402182
1	-7.185363	-0.310977	1.832622
1	-5.943561	-0.067984	3.066129
1	-6.854659	-1.583870	3.025517
6	-0.561462	-2.000298	-2.239893
6	-1.113198	-1.078237	-3.146851
1	-1.866038	-0.376987	-2.803802
6	-0.705158	-1.072256	-4.482153
1	-1.157877	-0.375920	-5.178980
6	0.287923	-1.955375	-4.915213
1	0.610966	-1.944253	-5.952049
6	0.876365	-2.839017	-4.007863
1	1.665133	-3.511959	-4.332072
6	0.447095	-2.869696	-2.679676
1	0.894072	-3.579098	-1.993939
6	-0.138125	-3.018900	0.464645
6	0.078352	-4.399085	0.319232
1	-0.466173	-4.956842	-0.437166
6	0.973026	-5.064250	1.158987
1	1.135321	-6.131409	1.037954
6	1.653813	-4.358997	2.155993
1	2.346475	-4.877555	2.812334
6	1.443788	-2.986458	2.307779
1	1.975375	-2.441474	3.080280
6	0.552995	-2.316777	1.464653
1	0.384238	-1.251261	1.585525
6	-5.172449	-0.606922	-1.399077
6	-4.577212	0.111951	-2.446650
1	-3.810155	0.844818	-2.214148
6	-4.949568	-0.126093	-3.769547
6	-5.881960	-1.113268	-4.081603
1	-6.151149	-1.315848	-5.112210
6	-6.454038	-1.844349	-3.039996
6	-6.125393	-1.584330	-1.709396
1	-6.610075	-2.166077	-0.937086
6	-5.136019	1.433286	0.649828
6	-4.622996	2.058195	1.798825
1	-3.949539	1.520531	2.455264
6	-4.948650	3.380359	2.085860
6	-5.767406	4.117787	1.228534
1	-6.002511	5.153488	1.444404
6	-6.269275	3.500060	0.086775
6	-5.967834	2.166278	-0.202386
1	-6.376960	1.716498	-1.099485
29	-2.135055	-0.147363	0.195397
6	-7.067234	4.301941	-0.902546
6	-4.324854	4.072565	3.265141
6	-4.356943	0.732374	-4.851119
6	-7.406627	-2.954998	-3.388286
9	-6.787083	-3.934670	-4.093736
9	-7.948208	-3.537344	-2.296085
9	-8.427199	-2.515944	-4.160639
9	-3.028356	0.951834	-4.651792
9	-4.934414	1.958616	-4.886929
9	-4.490440	0.190576	-6.077527
9	-6.263617	4.822733	-1.870960
9	-7.703479	5.343783	-0.326836
9	-7.995412	3.553572	-1.537193
9	-5.193308	4.906461	3.879203
9	-3.868994	3.202903	4.191957
9	-3.265298	4.835839	2.883677
6	-2.121941	2.779624	-0.546885
6	-1.425030	3.138578	0.653961
6	-1.201499	2.316579	1.788670
1	-1.290944	4.193292	0.844397
77	3.275815	1.440888	-1.593585
15	4.791230	0.444221	-0.228489
8	4.587747	-1.062133	0.433013
8	6.218546	0.217334	-1.054675
7	5.022177	1.361952	1.146026
6	4.774132	-2.217917	-0.324011
6	3.619417	-2.990134	-0.578479
1	2.674363	-2.659467	-0.165997
6	3.720518	-4.134015	-1.329998
1	2.843995	-4.747808	-1.513300
6	4.963472	-4.513539	-1.902963
6	5.059300	-5.639866	-2.764348
1	4.162748	-6.224778	-2.953269
6	6.253713	-5.973633	-3.361466
1	6.314798	-6.831617	-4.024496
6	7.403636	-5.184067	-3.121810
1	8.339429	-5.434487	-3.613204
6	7.348349	-4.096921	-2.276572
1	8.238381	-3.500996	-2.113844
6	6.135942	-3.732620	-1.626287
6	6.040884	-2.595131	-0.745791
6	7.245967	-1.828201	-0.322734
6	8.361178	-2.455512	0.338521
6	8.346275	-3.819576	0.744355
1	7.461484	-4.417838	0.563008
6	9.432044	-4.386420	1.375701
1	9.391786	-5.428140	1.680793
6	10.595758	-3.624584	1.637553
1	11.446303	-4.087339	2.129359
6	10.635976	-2.295405	1.282863
1	11.514334	-1.691891	1.496401
6	9.527647	-1.675258	0.644221
6	9.549369	-0.289751	0.327834
1	10.440000	0.289344	0.554526
6	8.447817	0.316165	-0.223399
1	8.422728	1.379295	-0.437871
6	7.304599	-0.458159	-0.518013
6	4.307425	2.672615	1.078441
1	3.346378	2.558156	1.595149
6	5.079592	3.791423	1.756244
6	4.426966	4.642341	2.655099
1	3.386786	4.452223	2.908669
6	5.103939	5.718363	3.235838
1	4.584527	6.370533	3.932633
6	6.447514	5.946296	2.931055
1	6.977847	6.777291	3.387472
6	7.109600	5.095079	2.039702
1	8.156865	5.263094	1.803507
6	6.428789	4.028386	1.453490
1	6.945528	3.360736	0.768654
6	4.054663	3.039395	-0.383466
1	5.005105	3.359598	-0.825642

1	3.394848	3.907272	-0.422804
6	5.495369	0.999139	2.517477
1	6.155411	1.821469	2.806663
6	4.334637	0.989186	3.501868
6	4.402932	1.776620	4.655722
1	5.267771	2.415376	4.814835
6	3.369017	1.754245	5.594863
1	3.434960	2.368992	6.488372
6	2.250126	0.950215	5.377913
1	1.443003	0.932405	6.102070
6	2.169679	0.168440	4.220550
1	1.293545	-0.446877	4.044645
6	3.207278	0.184449	3.288530
1	3.149142	-0.428148	2.394230
6	6.327502	-0.278554	2.663330
1	7.211387	-0.257486	2.027502
1	5.755599	-1.182002	2.456253
1	6.667118	-0.321393	3.702757
6	1.673532	0.729137	-0.303819
1	1.382752	-0.298403	-0.512495
1	1.852961	0.910124	0.754894
6	0.981058	1.757141	-1.047737
1	0.378097	1.482459	-1.902983
6	0.960355	3.083604	-0.622297
1	1.425172	3.294493	0.336343
6	4.851659	1.956497	-3.139731
1	5.683236	2.389801	-2.591274
6	3.729723	2.784673	-3.336541
1	3.791002	3.800197	-2.946548
6	2.686832	2.606290	-4.424901
1	3.064031	3.026680	-5.369707
1	1.821692	3.213371	-4.145778
6	2.228070	1.148270	-4.638002
1	2.844639	0.658098	-5.398034
1	1.207869	1.151000	-5.033810
6	2.240201	0.300960	-3.371344
1	1.269506	0.009478	-2.992471
6	3.308694	-0.479707	-2.961863
1	3.078743	-1.316907	-2.312718
6	4.641917	-0.564868	-3.671184
1	5.340494	-1.087258	-3.017698
1	4.519351	-1.194298	-4.564833
6	5.239791	0.804209	-4.064726
1	4.953092	1.064195	-5.088765
1	6.330081	0.718273	-4.066006
6	0.598451	4.252504	-1.406709
6	-0.043682	4.172334	-2.659135
6	0.931817	5.526788	-0.902730
6	-0.332129	5.326825	-3.381068
1	-0.331269	3.205526	-3.056622
6	0.649063	6.680492	-1.630343
1	1.419764	5.600600	0.065986
6	0.014666	6.584513	-2.872999
1	-0.831728	5.247554	-4.342062
1	0.919398	7.652801	-1.229024
1	-0.210919	7.482085	-3.441384
8	-2.144660	1.599995	-1.036464
6	-0.775259	2.944424	3.003491
6	-0.766464	2.262086	4.197768
1	-0.526297	4.000297	2.984421
6	-1.142839	0.910296	4.176874
6	-1.417018	0.295481	2.973816
1	-1.639363	-0.761325	2.921081
7	-1.441065	0.963647	1.801198
6	-3.296622	3.510944	-2.573860
1	-2.772745	2.674595	-3.027898
1	-4.368428	3.286752	-2.541379
1	-3.150289	4.395460	-3.200523
6	-2.975560	5.122925	-0.733714
1	-3.086949	5.119344	0.350539
1	-2.154759	5.795955	-1.011726
1	-3.904103	5.510999	-1.159274
7	-2.762648	3.773027	-1.244347
1	-0.491289	2.758444	5.121748
35	-1.287029	-0.113802	5.841464

[8-9]‡-P1-C1 *exo re-re*

Number of imaginary frequencies= 1
The smallest frequencies are= -133.5483 7.6070 11.1405 cm(-1)
Electronic energy= -7222.6211169
Zero-point correction= 1.755465
(Hartree/Particle)
Thermal correction to Energy= 1.873854
Thermal correction to Enthalpy= 1.874798
Thermal correction to Gibbs Free Energy= 1.594441
Sum of electronic and zero-point Energies= -7220.865652
Sum of electronic and thermal Energies= -7220.747263
Sum of electronic and thermal Enthalpies= -7220.746319
Sum of electronic and thermal Free Energies= -7221.026676

.....

Cartesian Coordinates

.....

26	-6.482416	-3.878930	-0.007576
15	-2.916175	-0.738247	-2.191854
15	-4.759485	0.496377	0.795435
6	-5.321963	-2.396768	-0.923561
6	-5.550312	-2.093977	0.470742
6	-5.006110	-3.166321	1.242840
1	-5.031975	-3.245754	2.320934
6	-4.473531	-4.140179	0.345418
1	-4.030761	-5.085183	0.626178
6	-4.665301	-3.667293	-0.985578
1	-4.390911	-4.186874	-1.891589
6	-8.550613	-3.678671	0.024839
1	-9.076179	-2.733453	0.056237
6	-8.106928	-4.428215	1.157186
1	-8.231435	-4.148192	2.194575
6	-7.428893	-5.590771	0.679300
1	-6.946594	-6.341825	1.291055
6	-7.453403	-5.560737	-0.748065
1	-6.995090	-6.285578	-1.407943
6	-8.147269	-4.381773	-1.152707
1	-8.304860	-4.061187	-2.173614
6	-5.668203	-1.482511	-2.048492
6	-7.019190	-1.284259	-2.372795
1	-7.762390	-1.845479	-1.821759
6	-7.418374	-0.377731	-3.353540
1	-8.473831	-0.228226	-3.558685
6	-6.453139	0.351119	-4.043109
1	-6.743278	1.075214	-4.797252
6	-5.104476	0.174234	-3.736294
1	-4.374224	0.774134	-4.264720
6	-4.685329	-0.727867	-2.743656
6	-6.134971	-0.802847	0.980625
1	-6.917605	-0.499456	0.283533
6	-6.751771	-0.896226	2.378746
1	-7.191375	0.059484	2.676966
1	-6.020108	-1.180619	3.139562
1	-7.540087	-1.655429	2.373275
6	-2.067769	0.429893	-3.335130
6	-1.484373	1.581723	-2.789536
1	-1.549925	1.770105	-1.723409
6	-0.811346	2.485746	-3.615579
1	-0.371351	3.376845	-3.181385
6	-0.712921	2.246963	-4.986548
1	-0.188148	2.948946	-5.628349
6	-1.291709	1.098263	-5.536913
1	-1.214083	0.905369	-6.602954
6	-1.963971	0.193909	-4.716720
1	-2.405147	-0.697481	-5.151663
6	-2.204264	-2.351802	-2.700924
6	-2.684981	-3.114077	-3.775371
1	-3.561561	-2.785143	-4.326486
6	-2.046877	-4.305645	-4.126147
1	-2.422995	-4.893318	-4.958855
6	-0.926335	-4.741866	-3.411140
1	-0.430413	-5.666873	-3.690463
6	-0.443829	-3.985887	-2.340223
1	0.429381	-4.315456	-1.784683

6	-1.082010	-2.796455	-1.986442
1	-0.710018	-2.203849	-1.154854
6	-5.414510	1.803492	-0.326065
6	-4.478064	2.760110	-0.746757
1	-3.452437	2.690508	-0.396602
6	-4.859992	3.792268	-1.603633
6	-6.159635	3.860994	-2.102126
1	-6.449102	4.648934	-2.788434
6	-7.078602	2.887291	-1.709584
6	-6.724222	1.880878	-0.811130
1	-7.476683	1.160946	-0.519449
6	-4.587329	1.387149	2.397305
6	-3.975138	0.694983	3.454832
1	-3.712027	-0.350457	3.341801
6	-3.662935	1.357411	4.639063
6	-3.903412	2.724951	4.781823
1	-3.613741	3.243429	5.688908
6	-4.482960	3.415650	3.721802
6	-4.847423	2.753709	2.547915
1	-5.298152	3.323263	1.744789
29	-2.688846	-0.210840	-0.013798
6	-4.710557	4.897810	3.836383
6	-2.933143	0.647590	5.742822
6	-3.861336	4.869373	-1.923763
6	-8.461763	2.934050	-2.298968
9	-8.429511	2.800620	-3.648484
9	-9.263375	1.955651	-1.824054
9	-9.073563	4.114751	-2.046775
9	-3.745572	5.752002	-0.898123
9	-4.196978	5.578324	-3.020816
9	-2.619433	4.365996	-2.131648
9	-5.892055	5.193457	4.423963
9	-4.712163	5.500301	2.623372
9	-3.744950	5.494060	4.576800
9	-3.419070	0.974454	6.960315
9	-2.990691	-0.695008	5.626862
9	-1.613629	0.989235	5.754619
6	-1.234663	1.932605	1.578732
6	-0.635479	0.931538	2.422285
6	-0.966117	-0.457254	2.483049
1	-0.139762	1.288537	3.313363
77	3.761997	-1.555545	0.856584
15	5.080954	-0.424723	-0.715148
8	5.671383	1.130849	-0.550922
8	6.519338	-1.222602	-1.007892
7	4.212961	-0.276706	-2.127869
6	6.474235	1.361362	0.557708
6	5.893150	2.069472	1.631671
1	4.881736	2.438896	1.512816
6	6.616203	2.264975	2.781940
1	6.188310	2.817402	3.613994
6	7.917722	1.706844	2.916770
6	8.635163	1.810575	4.139446
1	8.180542	2.358517	4.960760
6	9.868133	1.217043	4.289646
1	10.404291	1.296703	5.230750
6	10.430494	0.484298	3.217346
1	11.390537	-0.007041	3.346978
6	9.770557	0.382756	2.011626
1	10.212806	-0.190358	1.205486
6	8.505776	1.003075	1.811446
6	7.780044	0.901824	0.569341
6	8.380721	0.308789	-0.656938
6	9.627210	0.812274	-1.186139
6	10.250075	1.990620	-0.686117
1	9.774040	2.547288	0.112042
6	11.439122	2.448756	-1.212340
1	11.885780	3.356410	-0.816379
6	12.078761	1.755549	-2.266487
1	13.018992	2.123972	-2.666221
6	11.493385	0.625461	-2.791628
1	11.960164	0.092102	-3.615795
6	10.259644	0.137652	-2.282694
6	9.627674	-0.998049	-2.857666
1	10.119874	-1.522530	-3.671815
6	8.395389	-1.403570	-2.417317
1	7.874291	-2.240334	-2.869775
6	7.759768	-0.723288	-1.350572
6	2.805641	-0.767261	-2.051934
1	2.153738	0.103271	-1.902250
6	2.409539	-1.456149	-3.350155
6	3.212413	-2.483160	-3.873095
1	4.147938	-2.728422	-3.376837
6	2.826590	-3.174448	-5.019367
1	3.459791	-3.964768	-5.413674
6	1.625188	-2.851122	-5.660328
1	1.317971	-3.392565	-6.550657
6	0.827698	-1.826017	-5.152769
1	-0.103060	-1.566864	-5.644521
6	1.220328	-1.127062	-4.006089
1	0.595977	-0.326730	-3.620211
6	2.592778	-1.772277	-0.890626
1	2.800851	-2.773690	-1.280076
1	1.526289	-1.754817	-0.645178
6	4.532764	0.576439	-3.314442
1	3.947648	0.126445	-4.118891
6	4.062137	2.030170	-3.219862
6	4.848934	3.044050	-2.650865
1	5.791925	2.796414	-2.181284
6	4.440418	4.377015	-2.692966
1	5.066382	5.144508	-2.245826
6	3.244448	4.727671	-3.324242
1	2.934436	5.767946	-3.372876
6	2.452461	3.730419	-3.893417
1	1.529199	3.994746	-4.397826
6	2.854111	2.392798	-3.833363
1	2.234666	1.626093	-4.291702
6	5.993751	0.468482	-3.748610
1	6.265096	-0.576848	-3.910171
1	6.686166	0.900874	-3.025682
1	6.121937	1.006930	-4.692148
6	1.966763	-1.618227	2.027832
1	1.116971	-1.987203	1.458393
1	2.059044	-2.108050	2.989196
6	2.231984	-0.197793	1.980461
1	2.786973	0.256566	2.797156
6	1.518395	0.667042	1.124782
1	0.907098	0.208242	0.353957
6	4.887213	-3.391637	0.356666
1	4.857725	-3.523267	-0.723234
6	3.693857	-3.740667	1.051229
1	2.865841	-4.106415	0.444987
6	3.643318	-4.250369	2.479486
1	3.955913	-5.304727	2.493914
1	2.597420	-4.241842	2.799659
6	4.498319	-3.444366	3.486280
1	5.490513	-3.897410	3.574619
1	4.041591	-3.520194	4.478068
6	4.671392	-1.970638	3.146252
1	4.091539	-1.263005	3.733385
6	5.730056	-1.481728	2.424144
1	5.944485	-0.421192	2.488922
6	6.803313	-2.354162	1.809509
1	7.440567	-1.723632	1.192954
1	7.442790	-2.731695	2.620222
6	6.285881	-3.545881	0.962966
1	6.293566	-4.461638	1.565338
1	6.994162	-3.710578	0.147100
6	1.766786	2.091573	0.954545
6	2.398130	2.877847	1.940063
6	1.322584	2.718836	-0.225988
6	2.591094	4.241657	1.740197
1	2.717094	2.422151	2.872455
6	1.513766	4.084291	-0.420515
1	0.823263	2.127934	-0.986483
6	2.151604	4.850241	0.557903
1	3.079543	4.834816	2.508004
1	1.172494	4.549009	-1.338621
1	2.304873	5.914231	0.403246
7	-1.229282	3.234165	2.002344

6	-1.623486	4.306705	1.096786
1	-0.933636	5.148147	1.217972
1	-1.575642	3.965366	0.067045
1	-2.639694	4.656186	1.313740
6	-0.901595	3.670702	3.356350
1	-1.069120	2.876920	4.082416
1	0.137118	4.014803	3.426575
1	-1.561933	4.500514	3.623727
8	-1.721907	1.674917	0.431896
6	-0.599409	-1.178342	3.655655
6	-0.782843	-2.543024	3.748118
1	-0.183767	-0.634436	4.495089
6	-1.325597	-3.199102	2.640356
6	-1.719129	-2.469576	1.531761
1	-2.174580	-2.950999	0.676075
7	-1.567336	-1.133600	1.452623
1	-0.499961	-3.083261	4.645202
35	-1.550509	-5.143510	2.650606

[8-9]‡-P1-C1 *exo si-re*

Number of imaginary frequencies= 1
The smallest frequencies are= -161.1268 7.3169 11.9812 cm(-1)
Electronic energy= -7222.6073152
Zero-point correction= 1.755306
(Hartree/Particle)
Thermal correction to Energy= 1.874079
Thermal correction to Enthalpy= 1.875023
Thermal correction to Gibbs Free Energy= 1.591574
Sum of electronic and zero-point Energies= -7220.852010
Sum of electronic and thermal Energies= -7220.733236
Sum of electronic and thermal Enthalpies= -7220.732292
Sum of electronic and thermal Free Energies= -7221.015741

.....

Cartesian Coordinates

.....

26	-5.598755	4.384651	-1.540507
15	-2.492914	1.716035	1.652616
15	-5.125201	-0.215715	-0.407475
6	-4.622327	3.311225	-0.027686
6	-5.282422	2.423259	-0.949316
6	-4.728400	2.650792	-2.247237
1	-5.017325	2.137587	-3.154649
6	-3.751328	3.682801	-2.139058
1	-3.184383	4.107802	-2.956178
6	-3.689611	4.096783	-0.776287
1	-3.058339	4.874657	-0.371441
6	-7.560140	4.998947	-1.219100
1	-8.269627	4.488539	-0.581488
6	-7.339899	4.739644	-2.606361
1	-7.845813	3.991904	-3.202055
6	-6.299136	5.607899	-3.057096
1	-5.877683	5.630316	-4.053550
6	-5.874600	6.402111	-1.948646
1	-5.076199	7.132457	-1.957344
6	-6.653995	6.027289	-0.813804
1	-6.551643	6.431173	0.184282
6	-4.860042	3.284818	1.441345
6	-6.016166	3.875169	1.970508
1	-6.681872	4.392976	1.292234
6	-6.325542	3.795384	3.328996
1	-7.232877	4.258870	3.705517
6	-5.469675	3.112963	4.189156
1	-5.698740	3.028261	5.246841
6	-4.312746	2.517233	3.684372
1	-3.670656	1.975066	4.366597
6	-3.993257	2.583417	2.319164
6	-6.223341	1.327984	-0.534443
1	-6.534428	1.518855	0.497296
6	-7.476712	1.197092	-1.402119
1	-8.122948	0.388055	-1.050316
1	-7.231415	1.010516	-2.451067
1	-8.040023	2.132957	-1.349599
6	-1.790514	0.938753	3.167069
6	-2.119513	-0.403945	3.401761
1	-2.715409	-0.935311	2.670762
6	-1.707911	-1.048246	4.568861
1	-1.981860	-2.085588	4.739011
6	-0.949551	-0.353282	5.514129
1	-0.631985	-0.848134	6.427274
6	-0.603561	0.982118	5.284992
1	-0.010783	1.525461	6.015235
6	-1.028947	1.627806	4.122918
1	-0.785211	2.672163	3.970628
6	-1.389605	3.130967	1.246678
6	-1.418234	4.332513	1.973485
1	-2.071942	4.433044	2.834576
6	-0.629630	5.413213	1.577627
1	-0.651880	6.335549	2.150709
6	0.180251	5.311968	0.442436
1	0.784652	6.158179	0.128715
6	0.205249	4.123004	-0.289257
1	0.820875	4.046269	-1.180619
6	-0.569510	3.032583	0.113020
1	-0.581862	2.123712	-0.480363
6	-5.846071	-1.214234	0.963237
6	-6.143668	-2.582171	0.865970
1	-6.079521	-3.099862	-0.082355
6	-6.503507	-3.307010	2.001482
6	-6.557081	-2.700728	3.257062
1	-6.822660	-3.273594	4.137402
6	-6.245532	-1.346733	3.357347
6	-5.894341	-0.606594	2.226969
1	-5.630251	0.440300	2.340893
6	-5.473658	-1.162048	-1.944875
6	-4.458787	-1.176065	-2.907824
1	-3.522885	-0.667052	-2.704768
6	-4.654715	-1.827138	-4.128130
6	-5.852153	-2.480445	-4.405926
1	-5.997721	-2.992332	-5.349441
6	-6.863660	-2.466665	-3.444070
6	-6.685453	-1.810174	-2.227200
1	-7.492078	-1.814739	-1.503003
29	-2.865738	0.213754	-0.029705
6	-8.192985	-3.109639	-3.734358
6	-3.521156	-1.844493	-5.113139
6	-6.893675	-4.755610	1.875839
6	-6.227123	-0.657873	4.695389
9	-4.972652	-0.253034	5.021348
9	-7.002443	0.451231	4.697140
9	-6.658996	-1.454315	5.694233
9	-6.423890	-5.318234	0.742513
9	-8.241125	-4.900985	1.860053
9	-6.437982	-5.490807	2.916582
9	-8.103823	-4.057643	-4.691145
9	-9.100656	-2.198901	-4.161797
9	-8.717071	-3.690841	-2.631126
9	-3.890169	-2.291744	-6.329474
9	-2.988482	-0.608947	-5.277799
9	-2.509455	-2.646042	-4.684630
6	-2.612480	-2.672250	0.680759
6	-1.171429	-2.208352	-1.100237
6	-2.265785	-4.010643	0.688561
1	-3.346895	-2.289656	1.376973
6	-0.814488	-3.585609	-1.140258
6	-1.344427	-4.492198	-0.244040
1	-0.105545	-3.921725	-1.888349
6	-0.517611	-1.322556	-2.019516
6	-1.018712	-0.044204	-2.456858
8	-1.806562	0.683294	-1.773958
7	-2.073177	-1.780007	-0.167187
1	0.133090	-1.841475	-2.708310
7	-0.594380	0.431400	-3.668816
6	-0.981593	1.776780	-4.074596
1	-1.891124	1.762667	-4.689792
1	-0.171875	2.225954	-4.657278
1	-1.172745	2.386289	-3.193001
6	0.010251	-0.421842	-4.693466
1	-0.537398	-1.358512	-4.802962
1	1.058440	-0.645493	-4.477130

1	-0.035197	0.103731	-5.648750
77	4.187467	1.110133	-1.639351
15	5.477586	0.507957	0.222037
8	5.893322	-1.035754	0.715838
8	7.009286	1.167445	0.103306
7	4.733317	1.073657	1.599624
6	6.600441	-1.811729	-0.192657
6	5.894120	-2.858993	-0.824031
1	4.874144	-3.044057	-0.511991
6	6.513449	-3.607199	-1.793714
1	5.986732	-4.423062	-2.280868
6	7.839662	-3.296664	-2.202655
6	8.454774	-3.987972	-3.281604
1	7.899083	-4.784211	-3.770271
6	9.717226	-3.647903	-3.712342
1	10.174593	-4.177225	-4.543098
6	10.414860	-2.591840	-3.079142
1	11.399853	-2.306946	-3.437646
6	9.855841	-1.917148	-2.015311
1	10.402290	-1.105904	-1.549273
6	8.561568	-2.253984	-1.529327
6	7.939136	-1.551847	-0.433937
6	8.683154	-0.569922	0.402443
6	9.912739	-0.942966	1.062962
6	10.389803	-2.283768	1.094612
1	9.808600	-3.066923	0.623267
6	11.569474	-2.608430	1.729984
1	11.903355	-3.642060	1.744070
6	12.344289	-1.613212	2.370307
1	13.275180	-1.882133	2.860902
6	11.900933	-0.309897	2.383120
1	12.471793	0.464451	2.889094
6	10.681492	0.054016	1.751106
6	10.198173	1.389354	1.807926
1	10.792718	2.147017	2.310576
6	8.980597	1.709650	1.267607
1	8.571561	2.712258	1.334345
6	8.213554	0.721889	0.603634
6	3.405276	1.704292	1.358483
1	2.632766	0.949358	1.556702
6	3.185329	2.881846	2.295251
6	1.980777	3.012567	2.988818
1	1.224611	2.241774	2.883977
6	1.747084	4.120342	3.808980
1	0.804786	4.210400	4.341070
6	2.721724	5.109294	3.945869
1	2.543049	5.968752	4.585841
6	3.933196	4.985056	3.256134
1	4.699818	5.748141	3.361302
6	4.161295	3.881618	2.435697
1	5.106924	3.777037	1.910081
6	3.259604	2.212916	-0.094752
1	3.672910	3.227401	-0.133099
1	2.190001	2.308228	-0.284489
6	5.034071	0.719065	3.020970
1	4.632221	1.561584	3.587161
6	4.301951	-0.517422	3.545506
6	3.117334	-0.340850	4.275210
1	2.700041	0.657311	4.380223
6	2.483974	-1.422580	4.890887
1	1.572243	-1.259965	5.455533
6	3.023570	-2.704091	4.781447
1	2.535194	-3.546883	5.263110
6	4.191527	-2.896851	4.039641
1	4.617056	-3.892076	3.942649
6	4.825776	-1.814038	3.429815
1	5.740304	-1.978433	2.874109
6	6.530137	0.689728	3.331943
1	6.992824	1.639466	3.056802
1	7.058621	-0.115948	2.821700
1	6.660926	0.544569	4.408270
6	2.275665	0.999910	-2.639258
1	1.557445	1.722412	-2.255078
1	2.332329	1.013069	-3.721853
6	2.336745	-0.275761	-1.967732
1	2.723845	-1.137138	-2.504938
6	1.520523	-0.538294	-0.834545
1	0.999191	0.317135	-0.412411
6	5.613144	2.760421	-1.997267
1	5.723353	3.311415	-1.066417
6	4.413007	3.004027	-2.722555
1	3.720820	3.727584	-2.293330
6	4.279876	2.873397	-4.228133
1	4.751112	3.742045	-4.710967
1	3.215714	2.930883	-4.474910
6	4.873341	1.569417	-4.811993
1	5.903782	1.744235	-5.136300
1	4.315556	1.298252	-5.713850
6	4.862499	0.377786	-3.861388
1	4.141346	-0.406368	-4.077199
6	5.922810	0.054719	-3.045436
1	5.991890	-0.961275	-2.671723
6	7.178985	0.894900	-2.936512
1	7.798786	0.485432	-2.141586
1	7.754656	0.767710	-3.864681
6	6.939288	2.403586	-2.674633
1	7.003211	2.961497	-3.616132
1	7.753896	2.771209	-2.045326
6	1.592469	-1.692926	0.043106
6	2.268196	-2.879098	-0.304841
6	0.908174	-1.645000	1.275703
6	2.285613	-3.965841	0.565830
1	2.773886	-2.948570	-1.262209
6	0.909802	-2.739464	2.133835
1	0.367605	-0.743522	1.549993
6	1.606014	-3.900805	1.786354
1	2.821325	-4.869348	0.288838
1	0.379869	-2.680091	3.078246
1	1.619561	-4.749968	2.462931
1	-1.053654	-5.536667	-0.268432
35	-3.068785	-5.191748	2.020894

[8-9]^{s}-P1-C1 *endo si-si*

Number of imaginary frequencies= 1
The smallest frequencies are= -150.1039 8.2393 10.3348 cm(-1)
Electronic energy= -7222.6218129
Zero-point correction= 1.754670
(Hartree/Particle)
Thermal correction to Energy= 1.873731
Thermal correction to Enthalpy= 1.874675
Thermal correction to Gibbs Free Energy= 1.590704
Sum of electronic and zero-point Energies= -7220.867143
Sum of electronic and thermal Energies= -7220.748082
Sum of electronic and thermal Enthalpies= -7220.747138
Sum of electronic and thermal Free Energies= -7221.031109

.....

Cartesian Coordinates

.....

26	-7.001877	-3.547878	-0.911926
15	-2.597776	-1.191541	-2.403530
15	-4.668373	0.354317	0.508115
6	-5.432445	-2.383361	-1.681650
6	-5.877104	-1.880038	-0.408055
6	-5.700299	-2.919611	0.558840
1	-5.947674	-2.852849	1.609846
6	-5.171293	-4.063825	-0.110533
1	-4.968395	-5.026358	0.339846
6	-5.016720	-3.738768	-1.490258
1	-4.656505	-4.398710	-2.266346
6	-8.957429	-3.056239	-1.430306
1	-9.297133	-2.059188	-1.676927
6	-8.916943	-3.627384	-0.121918
1	-9.211696	-3.135055	0.795035
6	-8.371960	-4.942899	-0.231965
1	-8.180463	-5.622240	0.588279
6	-8.073385	-5.183921	-1.607776
1	-7.617244	-6.077396	-2.013352
6	-8.436084	-4.019385	-2.348276
1	-8.306122	-3.881913	-3.413065

6	-5.375322	-1.563749	-2.923210
6	-6.559403	-1.284632	-3.620584
1	-7.480616	-1.714005	-3.249823
6	-6.571841	-0.471599	-4.754022
1	-7.508546	-0.268547	-5.265110
6	-5.377461	0.071689	-5.220135
1	-5.363375	0.703183	-6.103336
6	-4.187325	-0.189648	-4.539879
1	-3.271320	0.249425	-4.915018
6	-4.164061	-0.983531	-3.381402
6	-6.252858	-0.448407	-0.155022
1	-6.413210	0.034967	-1.122685
6	-7.506615	-0.252026	0.700172
1	-7.706751	0.808934	0.877748
1	-7.423051	-0.751533	1.669030
1	-8.364482	-0.680176	0.174231
6	-1.380998	-0.214840	-3.384318
6	-1.488529	1.186276	-3.321175
1	-2.291770	1.639041	-2.748370
6	-0.609712	2.002506	-4.029741
1	-0.711770	3.081370	-3.974379
6	0.403803	1.430891	-4.804933
1	1.105332	2.067130	-5.335613
6	0.518348	0.042170	-4.873917
1	1.304325	-0.409685	-5.472366
6	-0.367215	-0.779635	-4.169450
1	-0.259634	-1.856670	-4.232894
6	-2.144091	-2.950891	-2.677511
6	-1.704256	-3.705078	-1.579553
1	-1.635214	-3.238743	-0.602087
6	-1.397149	-5.058744	-1.737902
1	-1.070409	-5.640048	-0.879932
6	-1.520955	-5.665288	-2.989934
1	-1.282926	-6.718176	-3.112345
6	-1.962827	-4.917309	-4.086931
1	-2.067368	-5.387520	-5.060585
6	-2.279534	-3.566968	-3.931826
1	-2.641090	-2.996741	-4.782688
6	-4.746756	2.100570	-0.055424
6	-4.456715	3.195344	0.768045
1	-4.284469	3.061327	1.829215
6	-4.361904	4.479335	0.227860
6	-4.519084	4.698844	-1.138974
1	-4.433699	5.695422	-1.554508
6	-4.770636	3.602117	-1.964521
6	-4.885680	2.317170	-1.436208
1	-5.059058	1.485955	-2.113725
6	-4.935075	0.366944	2.325913
6	-4.297743	-0.653070	3.041849
1	-3.656527	-1.349544	2.516596
6	-4.498239	-0.781103	4.417551
6	-5.319474	0.110773	5.103617
1	-5.464645	0.017061	6.173352
6	-5.956604	1.125987	4.388128
6	-5.781002	1.250894	3.010118
1	-6.306691	2.036534	2.480657
29	-2.671216	-0.522967	-0.226427
6	-6.906219	2.058356	5.090742
6	-3.758050	-1.858407	5.160005
6	-4.130359	5.632400	1.167131
6	-4.828272	3.767861	-3.458341
9	-3.657817	3.384003	-4.035672
9	-5.796502	3.005918	-4.015600
9	-5.049031	5.045266	-3.828446
9	-3.649086	6.723996	0.536158
9	-3.257203	5.307248	2.149800
9	-5.279454	6.004967	1.782181
9	-6.902983	3.289665	4.531387
9	-6.602948	2.204304	6.398593
9	-8.181814	1.605236	5.029660
9	-4.320475	-2.141232	6.353484
9	-3.707153	-3.011171	4.451471
9	-2.472754	-1.496969	5.407532
6	-1.266739	2.088448	0.199442
6	-0.937964	0.689809	2.052098
6	-0.803961	3.198179	0.885120
1	-1.586757	2.164885	-0.831388
6	-0.538362	1.829018	2.810988
6	-0.459305	3.083516	2.234354
1	-0.264167	1.697624	3.851534
6	-0.770436	-0.600790	2.648316
6	-1.279368	-1.854022	2.150290
8	-1.895739	-1.968311	1.045465
7	-1.346183	0.867784	0.754920
1	-0.493010	-0.561639	3.690653
7	-1.122850	-3.002491	2.882601
6	-1.686826	-4.247034	2.372637
1	-2.551844	-4.041884	1.744378
1	-1.992920	-4.869390	3.217852
1	-0.949189	-4.807371	1.780849
6	-0.329133	-3.152921	4.092195
1	0.070220	-2.205009	4.437313
1	0.513305	-3.832939	3.909085
1	-0.945477	-3.575212	4.892087
77	3.025390	-1.225949	-0.871594
15	4.935058	0.113242	-0.557546
8	5.743252	0.487099	0.854109
8	6.210483	-0.534728	-1.428717
7	4.586144	1.665662	-1.082294
6	6.372502	-0.548638	1.535972
6	5.763048	-0.982818	2.731954
1	4.880296	-0.460797	3.074790
6	6.304056	-2.035488	3.426449
1	5.847806	-2.372765	4.352988
6	7.445318	-2.718533	2.923752
6	7.960192	-3.869271	3.580225
1	7.478512	-4.201209	4.496316
6	9.032822	-4.559640	3.062460
1	9.413608	-5.441718	3.568964
6	9.630678	-4.126490	1.855066
1	10.459989	-4.687525	1.433927
6	9.168585	-3.002729	1.204644
1	9.633638	-2.691747	0.276763
6	8.076823	-2.250689	1.721645
6	7.558808	-1.080809	1.056844
6	8.240408	-0.470368	-0.117376
6	9.619278	-0.051611	-0.053417
6	10.365453	-0.051221	1.158708
1	9.885308	-0.364296	2.077967
6	11.682191	0.355355	1.186189
1	12.224908	0.352462	2.127203
6	12.331842	0.782968	0.004185
1	13.371845	1.093877	0.039350
6	11.634286	0.818923	-1.182079
1	12.112832	1.164090	-2.095006
6	10.270906	0.422020	-1.241247
6	9.535499	0.506722	-2.454433
1	10.039473	0.847717	-3.354436
6	8.199699	0.198134	-2.480787
1	7.606970	0.295382	-3.384312
6	7.556066	-0.252378	-1.304950
6	3.189292	1.823585	-1.569880
1	2.570531	2.183448	-0.737798
6	3.082955	2.834396	-2.700678
6	2.051120	3.777648	-2.692660
1	1.372021	3.818000	-1.846652
6	1.877524	4.656943	-3.764839
1	1.069006	5.382934	-3.741576
6	2.741101	4.601655	-4.860560
1	2.612713	5.286468	-5.693974
6	3.780139	3.663296	-4.875024
1	4.460149	3.619034	-5.721478
6	3.947650	2.785245	-3.804275
1	4.757492	2.060406	-3.811372
6	2.634258	0.483321	-2.072003
1	3.054368	0.296089	-3.066398
1	1.558240	0.610641	-2.210588
6	5.295981	2.939737	-0.740282
1	4.930984	3.640007	-1.494559
6	4.887969	3.540403	0.605556

6	3.738100	4.342776	0.668358
1	3.143755	4.493482	-0.227765
6	3.372668	4.990010	1.851486
1	2.483232	5.613743	1.873244
6	4.171498	4.863960	2.989631
1	3.905892	5.383989	3.906027
6	5.316564	4.062997	2.941247
1	5.940499	3.953672	3.824130
6	5.665341	3.399744	1.764002
1	6.554920	2.781127	1.746488
6	6.806996	2.867898	-0.946874
1	7.029169	2.555016	-1.968775
1	7.303562	2.181230	-0.261942
1	7.231963	3.864266	-0.792913
6	0.893744	-1.240541	-0.543256
1	0.334473	-0.767065	-1.341586
1	0.468024	-2.193405	-0.245975
6	1.416447	-0.395205	0.503704
1	1.396331	0.681451	0.378241
6	1.574380	-0.905827	1.814708
1	1.441416	-1.975227	1.931849
6	4.070067	-2.185618	-2.573614
1	4.487615	-1.398139	-3.195694
6	2.668702	-2.391584	-2.697299
1	2.147235	-1.754911	-3.408280
6	1.946129	-3.695890	-2.434987
1	2.053025	-4.361246	-3.305043
1	0.880762	-3.469716	-2.351267
6	2.408797	-4.422138	-1.155477
1	3.230126	-5.107725	-1.384801
1	1.586484	-5.044458	-0.787432
6	2.843953	-3.484664	-0.035018
1	2.151680	-3.402362	0.795083
6	4.149196	-3.091448	0.191754
1	4.405777	-2.729518	1.183846
6	5.319722	-3.469169	-0.694401
1	6.173790	-2.859397	-0.401634
1	5.598135	-4.512178	-0.483771
6	5.067744	-3.287901	-2.210051
1	4.723405	-4.229387	-2.651197
1	6.023354	-3.056447	-2.688353
6	2.199150	-0.253758	2.951750
6	2.484181	1.125176	2.992446
6	2.518094	-1.041770	4.081195
6	3.028640	1.693854	4.144043
1	2.284209	1.751008	2.131060
6	3.071439	-0.472351	5.221632
1	2.334312	-2.110874	4.045772
6	3.318846	0.905344	5.259445
1	3.230467	2.757317	4.164571
1	3.312699	-1.096014	6.077522
1	3.744578	1.359141	6.149675
1	-0.125574	3.940289	2.809546
35	-0.659857	4.909164	-0.050190

[8-9]‡-P1-C1 *endo re-si*

Number of imaginary frequencies= 1
The smallest frequencies are= -212.0251 8.7678 14.5321 cm(-1)
Electronic energy= -7222.6286595
Zero-point correction= 1.756482
(Hartree/Particle)
Thermal correction to Energy= 1.874688
Thermal correction to Enthalpy= 1.875632
Thermal correction to Gibbs Free Energy= 1.596626
Sum of electronic and zero-point Energies= -7220.872177
Sum of electronic and thermal Energies= -7220.753971
Sum of electronic and thermal Enthalpies= -7220.753027
Sum of electronic and thermal Free Energies= -7221.032033

.....

Cartesian Coordinates

.....

77	3.617031	1.685173	-1.313260
15	5.234705	0.304245	-0.330767
8	5.060197	-0.987404	0.709001
8	6.088017	-0.464985	-1.550010
7	6.251110	1.261166	0.592513
6	4.452208	-2.155591	0.264830
6	3.178730	-2.440023	0.801847
1	2.771582	-1.752139	1.530148
6	2.510297	-3.576281	0.421677
1	1.542024	-3.813657	0.852552
6	3.066956	-4.435911	-0.563268
6	2.354312	-5.573853	-1.029917
1	1.394125	-5.804400	-0.575717
6	2.860763	-6.360904	-2.039928
1	2.304581	-7.223641	-2.394769
6	4.106744	-6.033633	-2.626881
1	4.490968	-6.636366	-3.444744
6	4.839731	-4.959512	-2.169212
1	5.792435	-4.725714	-2.629592
6	4.361028	-4.139203	-1.109617
6	5.110549	-3.014428	-0.601918
6	6.530260	-2.774031	-0.980317
6	7.534204	-3.799848	-0.820415
6	7.276465	-5.032125	-0.155718
1	6.294902	-5.215391	0.263864
6	8.258486	-5.989766	-0.018433
1	8.033662	-6.916401	0.502159
6	9.556077	-5.776018	-0.539726
1	10.317468	-6.542999	-0.431845
6	9.850229	-4.585105	-1.164347
1	10.848423	-4.393944	-1.549776
6	8.865845	-3.569811	-1.304628
6	9.188534	-2.317643	-1.894116
1	10.193061	-2.156064	-2.274909
6	8.256344	-1.313895	-1.944155
1	8.490535	-0.334075	-2.347093
6	6.948280	-1.537908	-1.454469
6	5.867962	2.702601	0.594392
1	5.232144	2.886296	1.470279
6	7.081866	3.613322	0.692818
6	7.066818	4.710164	1.561662
1	6.203899	4.869230	2.204232
6	8.148041	5.595251	1.612120
1	8.121619	6.441669	2.292981
6	9.261975	5.385882	0.797128
1	10.106478	6.067903	0.839651
6	9.286809	4.289695	-0.072264
1	10.152262	4.118260	-0.706651
6	8.203372	3.413878	-0.127094
1	8.224426	2.556507	-0.794883
6	5.089628	3.069255	-0.684988
1	5.815095	3.191310	-1.498584
1	4.637417	4.053591	-0.517788
6	7.177636	0.838054	1.691401
1	7.854773	1.688357	1.790707
6	6.514167	0.684171	3.061145
6	6.490380	1.790650	3.923662
1	6.885469	2.741696	3.576178
6	6.006763	1.678091	5.229597
1	6.009964	2.546023	5.883754
6	5.542914	0.447364	5.696897
1	5.176456	0.350489	6.715224
6	5.546166	-0.658554	4.842620
1	5.180137	-1.618810	5.195634
6	6.025847	-0.541676	3.537589
1	6.032016	-1.413154	2.894487
6	8.068968	-0.346826	1.322488
1	8.623367	-0.130729	0.407322
1	7.516788	-1.275162	1.179877
1	8.790704	-0.504828	2.129639
6	4.644301	1.414179	-3.257535
1	5.700390	1.627803	-3.112943
6	3.787857	2.547038	-3.326181
1	4.265895	3.522347	-3.237950
6	2.465991	2.596001	-4.068468
1	2.655019	2.742674	-5.142598
1	1.926585	3.486305	-3.729987
6	1.575212	1.353696	-3.859259

1	1.795802	0.598769	-4.618416
1	0.531043	1.635058	-4.015185
6	1.699830	0.713289	-2.483250
1	0.864901	0.882942	-1.810564
6	2.548278	-0.333631	-2.198881
1	2.328202	-0.940035	-1.323732
6	3.521125	-0.932356	-3.195976
1	4.185788	-1.606512	-2.657640
1	2.951881	-1.557904	-3.895403
6	4.371182	0.093951	-3.982750
1	3.897869	0.318172	-4.945057
1	5.332591	-0.371519	-4.216033
6	-2.244775	-0.069496	3.242668
6	-1.153237	1.807847	2.357390
6	-1.994735	0.334465	4.539300
1	-2.775325	-0.988103	3.033932
6	-0.881926	2.247482	3.682681
6	-1.296297	1.521248	4.778572
1	-0.348713	3.179613	3.825615
6	-0.646871	2.599179	1.272709
6	-1.114118	2.538599	-0.099406
8	-1.408978	1.447744	-0.683074
7	-1.835708	0.639019	2.171117
1	-0.242074	3.547107	1.597720
7	-1.160482	3.699815	-0.819422
6	-1.310144	3.663555	-2.269311
1	-2.313544	3.978669	-2.571981
1	-0.586219	4.348500	-2.725587
1	-1.123889	2.657531	-2.634180
6	-1.020050	5.035656	-0.247361
1	-1.377699	5.064673	0.780589
1	0.021153	5.381874	-0.280167
1	-1.634508	5.724611	-0.832478
6	2.160936	3.238104	-0.941991
1	1.230727	3.097509	-1.477018
1	2.568720	4.240896	-1.059206
6	2.323147	2.616935	0.347598
1	2.966607	3.120054	1.062806
6	1.476249	1.590445	0.858822
1	0.911595	0.997217	0.152200
6	1.682524	0.967117	2.163286
6	2.367595	1.598057	3.219490
6	1.097285	-0.289931	2.404664
6	2.467347	0.983657	4.464301
1	2.809498	2.578500	3.076368
6	1.206809	-0.908777	3.647151
1	0.551681	-0.769494	1.599278
6	1.895058	-0.273285	4.683058
1	2.999152	1.483875	5.265313
1	0.750967	-1.880674	3.807800
1	1.982488	-0.749831	5.655097
1	-1.084385	1.862322	5.785877
35	-2.599275	-0.779716	6.029734
26	-6.539922	-2.911334	2.398187
15	-2.221957	-2.221189	-0.490513
15	-4.611280	0.673053	-0.111081
6	-5.036001	-2.534740	0.984262
6	-5.531721	-1.306012	1.557194
6	-5.311250	-1.364139	2.968217
1	-5.584913	-0.600804	3.682873
6	-4.705053	-2.620121	3.277232
1	-4.448898	-2.974155	4.265978
6	-4.536955	-3.339374	2.058488
1	-4.124989	-4.332520	1.954006
6	-8.525171	-2.978125	1.781222
1	-8.934801	-2.418656	0.950718
6	-8.440209	-2.527693	3.134110
1	-8.764220	-1.564539	3.505445
6	-7.811598	-3.554195	3.902450
1	-7.569139	-3.501305	4.955712
6	-7.507993	-4.639395	3.025106
1	-6.997996	-5.554274	3.296786
6	-7.950247	-4.285131	1.716056
1	-7.837364	-4.889692	0.826509
6	-5.010912	-2.864216	-0.469195
6	-6.214934	-3.168737	-1.122582
1	-7.128242	-3.152396	-0.542607
6	-6.259521	-3.477936	-2.480946
1	-7.211249	-3.682556	-2.960508
6	-5.075998	-3.508984	-3.213948
1	-5.088363	-3.753213	-4.271424
6	-3.868462	-3.197644	-2.589023
1	-2.961811	-3.211514	-3.181326
6	-3.811923	-2.847667	-1.229644
6	-6.084234	-0.147198	0.769380
1	-6.703670	-0.558748	-0.028646
6	-6.944441	0.813140	1.595553
1	-7.370151	1.598332	0.965115
1	-6.375300	1.294945	2.394847
1	-7.763511	0.253315	2.057377
6	-1.068379	-2.287438	-1.926668
6	-1.188787	-1.276047	-2.895517
1	-1.862260	-0.444070	-2.724878
6	-0.465199	-1.349721	-4.085156
1	-0.592257	-0.581028	-4.838062
6	0.425242	-2.405067	-4.300818
1	0.988693	-2.459736	-5.227813
6	0.603092	-3.375620	-3.313633
1	1.317393	-4.181465	-3.453833
6	-0.148557	-3.324111	-2.137667
1	-0.018462	-4.102378	-1.396460
6	-1.673868	-3.586771	0.607505
6	-1.852819	-4.936226	0.262301
1	-2.329221	-5.197022	-0.678316
6	-1.428062	-5.945091	1.128386
1	-1.569850	-6.986639	0.854590
6	-0.827883	-5.615696	2.348820
1	-0.502074	-6.402129	3.023324
6	-0.655375	-4.275292	2.701692
1	-0.198608	-4.017289	3.652650
6	-1.077587	-3.265023	1.834210
1	-0.965899	-2.225091	2.117222
6	-4.970649	0.608936	-1.917294
6	-3.975824	1.140893	-2.750355
1	-3.083388	1.568427	-2.304349
6	-4.120814	1.106069	-4.137874
6	-5.228500	0.498604	-4.724301
1	-5.329145	0.454812	-5.802618
6	-6.201043	-0.059499	-3.894004
6	-6.090501	0.009766	-2.505643
1	-6.876543	-0.425801	-1.905235
6	-4.676696	2.478191	0.260570
6	-4.247204	2.877306	1.537241
1	-3.985688	2.133894	2.280228
6	-4.122192	4.228609	1.848706
6	-4.392156	5.211555	0.895149
1	-4.267569	6.261979	1.132108
6	-4.816115	4.815319	-0.369809
6	-4.972593	3.463824	-0.686872
1	-5.309166	3.197044	-1.681079
29	-2.465066	-0.139101	0.349486
6	-5.001200	5.844480	-1.449287
6	-3.579665	4.651342	3.185120
6	-3.073419	1.770510	-4.985791
6	-7.361062	-0.774419	-4.532514
9	-6.952409	-1.883110	-5.198030
9	-8.285453	-1.172413	-3.630637
9	-7.991782	0.005992	-5.440214
9	-1.816483	1.413972	-4.600903
9	-3.127571	3.120383	-4.876202
9	-3.189308	1.468000	-6.292270
9	-3.844810	6.027950	-2.146837
9	-5.351741	7.049987	-0.956347
9	-5.938337	5.479501	-2.350185
9	-4.201122	5.753969	3.657123
9	-3.695264	3.684946	4.119524
9	-2.256775	4.964472	3.100598

11-P1-C2 *endo si-re*

Number of imaginary frequencies= 0
The smallest frequencies are= 12.2273 13.9943 16.3898 cm(-1)
Electronic energy= -7222.6449288
Zero-point correction= 1.757633
(Hartree/Particle)
Thermal correction to Energy= 1.876644
Thermal correction to Enthalpy= 1.877588
Thermal correction to Gibbs Free Energy= 1.595936
Sum of electronic and zero-point Energies= -7220.887296
Sum of electronic and thermal Energies= -7220.768285
Sum of electronic and thermal Enthalpies= -7220.767341
Sum of electronic and thermal Free Energies= -7221.048993
.....
Cartesian Coordinates
.....

26	7.925814	-0.325224	-1.134485
15	2.922148	0.805089	-2.273970
15	4.030165	0.950354	1.306089
6	5.998236	0.434263	-1.456759
6	6.181396	0.039836	-0.081598
6	6.494505	-1.354101	-0.064761
1	6.703414	-1.945704	0.816129
6	6.539492	-1.817961	-1.413029
1	6.786649	-2.821197	-1.729566
6	6.231513	-0.720903	-2.270311
1	6.204419	-0.743662	-3.349671
6	9.449517	0.946475	-0.519666
1	9.302701	1.824772	0.094856
6	9.684464	-0.379525	-0.042923
1	9.742400	-0.681957	0.994222
6	9.781060	-1.245800	-1.174419
1	9.919926	-2.318443	-1.143464
6	9.604910	-0.456108	-2.351115
1	9.590076	-0.823746	-3.368586
6	9.402240	0.897433	-1.947626
1	9.214803	1.731169	-2.610324
6	5.581058	1.798939	-1.884723
6	6.496532	2.857024	-1.769087
1	7.487919	2.632083	-1.398927
6	6.158489	4.167144	-2.104324
1	6.886855	4.963352	-1.985809
6	4.880405	4.441331	-2.584728
1	4.596885	5.453520	-2.853684
6	3.949029	3.409321	-2.693197
1	2.954232	3.648722	-3.047782
6	4.264640	2.088381	-2.330954
6	5.919411	0.938114	1.094939
1	6.184337	1.955500	0.801017
6	6.718367	0.584953	2.352443
1	6.495671	1.277847	3.168714
1	6.509126	-0.427933	2.706243
1	7.787432	0.646327	2.125911
6	1.448430	1.769654	-2.817881
6	0.689774	2.406650	-1.824343
1	0.916632	2.224623	-0.779689
6	-0.357839	3.259972	-2.173672
1	-0.930258	3.753986	-1.398155
6	-0.681650	3.457819	-3.517713
1	-1.502779	4.116767	-3.785825
6	0.044160	2.795651	-4.512405
1	-0.210690	2.936256	-5.559079
6	1.109999	1.962801	-4.166295
1	1.680649	1.473063	-4.948597
6	3.246914	-0.299572	-3.705513
6	4.024431	0.075192	-4.811141
1	4.489441	1.056046	-4.841388
6	4.214063	-0.816806	-5.869087
1	4.822328	-0.521990	-6.719524
6	3.623844	-2.084206	-5.836469
1	3.776506	-2.776069	-6.659737
6	2.839779	-2.460217	-4.742703
1	2.379132	-3.443346	-4.710467
6	2.657067	-1.571959	-3.682046
1	2.064445	-1.864330	-2.820951
6	3.500772	2.713180	1.328068
6	2.121969	2.921969	1.479330
1	1.469818	2.065264	1.618908
6	1.585456	4.207387	1.398662
6	2.400871	5.305844	1.134333
1	1.980961	6.301780	1.051005
6	3.769925	5.092640	0.962481
6	4.323109	3.816256	1.067320
1	5.388602	3.701662	0.919449
6	3.713243	0.379189	3.025056
6	3.852063	-1.000539	3.246024
1	4.161940	-1.648693	2.434777
6	3.565036	-1.545552	4.493093
6	3.087450	-0.741836	5.530667
1	2.830596	-1.174408	6.490813
6	2.924830	0.620937	5.301693
6	3.249737	1.187842	4.065021
1	3.119609	2.254864	3.923956
29	2.700866	-0.193534	-0.250734
6	2.287902	1.491938	6.345678
6	3.628336	-3.032096	4.701745
6	0.108236	4.377453	1.616582
6	4.637740	6.275913	0.629617
9	4.287974	6.826188	-0.559149
9	5.947621	5.955068	0.550604
9	4.518696	7.257098	1.554576
9	-0.609107	3.450289	0.917727
9	-0.237014	4.213746	2.914325
9	-0.344545	5.587847	1.228843
9	2.855183	2.717586	6.403121
9	0.968579	1.693079	6.071378
9	2.351297	0.953628	7.580985
9	4.179514	-3.350635	5.895001
9	4.339859	-3.660831	3.743098
9	2.384706	-3.585362	4.696763
6	0.708598	-0.836216	1.902132
6	1.145430	-2.184002	1.953592
6	2.019429	-2.861564	1.076952
1	0.782115	-2.794423	2.766981
77	-3.211574	-1.482140	-1.122462
15	-5.072355	-0.469072	-0.309144
8	-5.041297	0.887456	0.620831
8	-6.067192	0.015503	-1.543218
7	-5.835475	-1.520125	0.736256
6	-4.903476	2.165492	0.082417
6	-3.720457	2.860830	0.416048
1	-3.005546	2.390050	1.081903
6	-3.504110	4.111937	-0.106891
1	-2.610258	4.667407	0.154640
6	-4.429819	4.680661	-1.021813
6	-4.159948	5.923329	-1.656847
1	-3.240188	6.444947	-1.405280
6	-5.034120	6.448223	-2.581740
1	-4.815395	7.394207	-3.068253
6	-6.217086	5.744013	-2.910712
1	-6.894207	6.149833	-3.656696
6	-6.517188	4.546090	-2.299105
1	-7.422795	4.017107	-2.571679
6	-5.644538	3.980085	-1.328379
6	-5.915939	2.718918	-0.686572
6	-7.217351	2.012640	-0.854442
6	-8.471583	2.637452	-0.518945
6	-8.551240	3.915745	0.101137
1	-7.639412	4.448055	0.343129
6	-9.769058	4.481302	0.411080
1	-9.801597	5.455367	0.890550
6	-10.976781	3.804320	0.118374
1	-11.928772	4.266696	0.361934
6	-10.937582	2.556030	-0.459983
1	-11.856219	2.015696	-0.672888
6	-9.698168	1.936224	-0.777212
6	-9.655857	0.626591	-1.327494
1	-10.588673	0.109889	-1.534727
6	-8.453258	0.008042	-1.564177
1	-8.393949	-1.002366	-1.953490
6	-7.253863	0.701769	-1.298145

6	-5.336342	-2.916192	0.620096
1	-4.666604	-3.102881	1.466805
6	-6.467569	-3.927946	0.683626
6	-6.284294	-5.130019	1.377392
1	-5.350172	-5.305772	1.906690
6	-7.289861	-6.100122	1.395407
1	-7.135114	-7.028251	1.938636
6	-8.493789	-5.872026	0.725328
1	-9.279300	-6.622170	0.743970
6	-8.685896	-4.670458	0.035597
1	-9.622637	-4.484669	-0.482959
6	-7.678144	-3.706268	0.011943
1	-7.829178	-2.767961	-0.513660
6	-4.544356	-3.093554	-0.683091
1	-5.249358	-3.204875	-1.514899
1	-3.972165	-4.021951	-0.627821
6	-6.526263	-1.209345	2.036833
1	-7.041500	-2.145703	2.266541
6	-5.523556	-0.976156	3.165555
6	-5.028534	-2.082952	3.873462
1	-5.397760	-3.077251	3.636084
6	-4.088861	-1.925666	4.895517
1	-3.720538	-2.797213	5.429609
6	-3.641106	-0.649228	5.240888
1	-2.915134	-0.520817	6.038165
6	-4.143465	0.463192	4.559930
1	-3.813305	1.461817	4.832560
6	-5.073870	0.301304	3.531425
1	-5.450135	1.177166	3.017821
6	-7.619972	-0.149005	1.926030
1	-8.332792	-0.426279	1.146904
1	-7.237701	0.845788	1.701689
1	-8.154188	-0.098597	2.879699
6	-2.362657	-1.104933	0.863865
1	-1.614309	-0.331488	0.736158
1	-3.045478	-0.943347	1.694039
6	-2.010206	-2.460870	0.580295
1	-2.572059	-3.246636	1.072994
6	-1.065027	-2.808574	-0.384659
1	-0.338560	-2.059441	-0.672341
6	-4.067174	-1.434412	-3.227217
1	-5.082178	-1.805557	-3.125945
6	-3.040762	-2.391668	-3.199937
1	-3.332660	-3.435448	-3.092064
6	-1.649344	-2.185603	-3.765441
1	-1.681757	-2.344268	-4.853669
1	-1.009794	-2.973774	-3.363024
6	-1.014042	-0.810886	-3.461598
1	-1.258610	-0.093658	-4.249446
1	0.072165	-0.914731	-3.487306
6	-1.402849	-0.203269	-2.120457
1	-0.632285	-0.174569	-1.354500
6	-2.474868	0.647652	-1.948413
1	-2.458766	1.284001	-1.069642
6	-3.438540	1.069741	-3.037405
1	-4.291752	1.555954	-2.564765
1	-2.945924	1.832806	-3.653656
6	-3.950668	-0.082373	-3.929422
1	-3.305348	-0.200219	-4.805016
1	-4.938933	0.189764	-4.309865
6	-0.760032	-4.170959	-0.822647
6	-1.506417	-5.303644	-0.437704
6	0.349161	-4.362239	-1.669755
6	-1.156086	-6.572150	-0.893974
1	-2.354830	-5.198931	0.230317
6	0.698207	-5.631245	-2.126058
1	0.951638	-3.503591	-1.945698
6	-0.056581	-6.742560	-1.742888
1	-1.741279	-7.433624	-0.584811
1	1.566098	-5.754269	-2.766924
1	0.212762	-7.734347	-2.094270
6	2.256449	-4.260521	1.302117
6	3.092895	-4.991072	0.494639
1	1.754882	-4.743240	2.134381
6	3.725217	-4.321054	-0.566510
6	3.511412	-2.973262	-0.747986
1	4.004475	-2.431397	-1.543307
7	2.689339	-2.247853	0.040284
8	0.877319	-0.044638	0.901305
7	0.025860	-0.333891	2.997855
6	-0.640796	0.957006	2.946396
1	-1.696931	0.851147	3.222895
1	-0.177926	1.666894	3.642681
1	-0.580844	1.359081	1.940471
6	-0.207341	-1.091612	4.219022
1	-1.108677	-1.716421	4.153651
1	0.644840	-1.724226	4.463700
1	-0.340337	-0.386551	5.043792
1	3.250486	-6.050471	0.666791
35	4.892871	-5.296552	-1.807416

[**8-9**]‡**-P1-C2** *endo si-re*

Number of imaginary frequencies= 1
The smallest frequencies are= -255.8377 9.9949 11.5913 cm(-1)
Electronic energy= -7222.6359279
Zero-point correction= 1.754830
(Hartree/Particle)
Thermal correction to Energy= 1.873567
Thermal correction to Enthalpy= 1.874511
Thermal correction to Gibbs Free Energy= 1.591721
Sum of electronic and zero-point Energies= -7220.881098
Sum of electronic and thermal Energies= -7220.762361
Sum of electronic and thermal Enthalpies= -7220.761417
Sum of electronic and thermal Free Energies= -7221.044206

.....

Cartesian Coordinates

.....

26	8.013585	0.343897	-1.088066
15	2.922532	1.119765	-2.182064
15	3.990229	0.789981	1.429510
6	6.009727	0.919138	-1.309794
6	6.234266	0.288003	-0.031298
6	6.714893	-1.035525	-0.275536
1	6.991852	-1.757614	0.480056
6	6.821167	-1.218896	-1.687297
1	7.193866	-2.102310	-2.185261
6	6.384704	-0.020045	-2.323710
1	6.365875	0.166428	-3.387146
6	9.369801	1.645924	-0.202897
1	9.121733	2.363341	0.567879
6	9.768064	0.290874	0.011963
1	9.868212	-0.198103	0.971781
6	9.968867	-0.318377	-1.263998
1	10.240037	-1.351161	-1.439402
6	9.694377	0.659312	-2.268013
1	9.724054	0.498671	-3.337631
6	9.326245	1.872438	-1.613604
1	9.033500	2.790205	-2.104997
6	5.448299	2.287370	-1.493808
6	6.228200	3.396000	-1.127490
1	7.220695	3.213810	-0.736441
6	5.757374	4.702772	-1.243501
1	6.378555	5.534264	-0.925750
6	4.484610	4.926807	-1.762333
1	4.101643	5.936520	-1.869047
6	3.685297	3.841621	-2.119483
1	2.690234	4.036899	-2.499706
6	4.129307	2.516357	-1.968797
6	5.879962	0.906477	1.293815
1	6.095716	1.973722	1.226218
6	6.650607	0.334890	2.486675
1	6.373280	0.846161	3.412751
1	6.465570	-0.733535	2.626049
1	7.723876	0.471584	2.321711
6	1.372942	2.004486	-2.636755
6	0.596619	2.521408	-1.588057
1	0.871447	2.306826	-0.562153
6	-0.516855	3.315024	-1.857986
1	-1.097015	3.719966	-1.039079

6	-0.894043	3.567458	-3.179151
1	-1.768850	4.177171	-3.386267
6	-0.150596	3.022693	-4.228866
1	-0.444707	3.205400	-5.258558
6	0.984828	2.253225	-3.961556
1	1.567529	1.858243	-4.786949
6	3.388234	0.262077	-3.734089
6	4.120953	0.871566	-4.763020
1	4.466335	1.895325	-4.651753
6	4.416914	0.159295	-5.927190
1	4.989510	0.634668	-6.718488
6	3.977008	-1.159910	-6.076442
1	4.211704	-1.711110	-6.982506
6	3.236075	-1.768112	-5.059595
1	2.890969	-2.792220	-5.170375
6	2.946676	-1.059899	-3.892315
1	2.386229	-1.532306	-3.091901
6	3.365067	2.493353	1.742100
6	1.969775	2.608751	1.822245
1	1.363782	1.711991	1.747155
6	1.366465	3.859593	1.950376
6	2.134041	5.022455	1.965849
1	1.664559	5.996572	2.043932
6	3.521414	4.906831	1.862576
6	4.139376	3.659304	1.767062
1	5.217730	3.623620	1.691951
6	3.620326	-0.110043	2.992437
6	3.817723	-1.500192	2.965952
1	4.221766	-1.973060	2.078184
6	3.469084	-2.282548	4.063264
6	2.887458	-1.707057	5.193904
1	2.597672	-2.320527	6.039191
6	2.675268	-0.331111	5.211879
6	3.047389	0.469972	4.128846
1	2.871896	1.538234	4.177447
29	2.774266	-0.168179	-0.329656
6	1.945819	0.286375	6.372373
6	3.605167	-3.777839	4.000112
6	-0.129155	3.921549	2.091867
6	4.340426	6.168202	1.808339
9	4.074819	6.881200	0.686067
9	5.669524	5.925061	1.817700
9	4.070787	6.984207	2.853582
9	-0.749568	3.062411	1.232615
9	-0.537272	3.564982	3.331985
9	-0.626428	5.150700	1.840889
9	2.296359	1.574532	6.571417
9	0.598981	0.279052	6.162938
9	2.158141	-0.380955	7.525952
9	4.008173	-4.298975	5.179179
9	4.481473	-4.176891	3.054785
9	2.412686	-4.368264	3.707710
6	0.684270	-1.248018	1.603274
6	0.979343	-2.614031	1.228778
6	2.125789	-3.069664	0.497687
1	0.548422	-3.383922	1.852395
77	-3.285994	-1.400841	-1.340864
15	-5.130050	-0.468749	-0.389346
8	-5.129980	0.850851	0.608671
8	-6.198061	0.045254	-1.559467
7	-5.836775	-1.580625	0.647523
6	-4.988865	2.141733	0.117587
6	-3.809202	2.825907	0.484014
1	-3.095744	2.325615	1.128465
6	-3.598915	4.102882	0.026441
1	-2.713554	4.653171	0.328165
6	-4.521105	4.706591	-0.870386
6	-4.255578	5.977447	-1.448944
1	-3.340923	6.493310	-1.168274
6	-5.126170	6.536262	-2.357599
1	-4.909479	7.503637	-2.801145
6	-6.302575	5.840109	-2.725166
1	-6.976644	6.273494	-3.458403
6	-6.599625	4.615603	-2.166711
1	-7.500876	4.093093	-2.465823
6	-5.729997	4.013015	-1.215613
6	-6.002414	2.727491	-0.626094
6	-7.311827	2.035310	-0.793625
6	-8.554317	2.660744	-0.415695
6	-8.613518	3.927716	0.230415
1	-7.693760	4.451075	0.461742
6	-9.820338	4.493587	0.580772
1	-9.835357	5.458598	1.079266
6	-11.038694	3.828579	0.305626
1	-11.982209	4.290564	0.580991
6	-11.019193	2.590539	-0.295379
1	-11.945164	2.057694	-0.495514
6	-9.791362	1.971174	-0.655083
6	-9.770946	0.669846	-1.225856
1	-10.712231	0.161365	-1.414815
6	-8.578302	0.050053	-1.503615
1	-8.533575	-0.955622	-1.907759
6	-7.365993	0.731728	-1.260776
6	-5.257581	-2.943055	0.493732
1	-4.516197	-3.087677	1.290022
6	-6.315481	-4.022913	0.632083
6	-6.025570	-5.193709	1.342471
1	-5.058859	-5.295613	1.830990
6	-6.964063	-6.225820	1.428305
1	-6.725267	-7.128468	1.984138
6	-8.208923	-6.091871	0.809744
1	-8.942888	-6.889639	0.880865
6	-8.508546	-4.921993	0.103573
1	-9.477716	-4.808921	-0.374839
6	-7.567748	-3.896147	0.013387
1	-7.802952	-2.981983	-0.524445
6	-4.544156	-3.068651	-0.859606
1	-5.297704	-3.190653	-1.647305
1	-3.944224	-3.983004	-0.850979
6	-6.497243	-1.329322	1.973705
1	-6.976835	-2.286640	2.194633
6	-5.476687	-1.096454	3.088429
6	-4.933107	-2.208517	3.751555
1	-5.273828	-3.205540	3.484266
6	-3.981754	-2.053968	4.763393
1	-3.576546	-2.930020	5.262337
6	-3.568680	-0.775393	5.143393
1	-2.831533	-0.647594	5.931251
6	-4.119314	0.341204	4.507372
1	-3.815321	1.341034	4.805624
6	-5.062545	0.182258	3.490057
1	-5.477042	1.060834	3.011866
6	-7.628632	-0.303576	1.924271
1	-8.357645	-0.587921	1.162658
1	-7.287443	0.707665	1.708018
1	-8.132257	-0.292434	2.895927
6	-2.348044	-1.109401	0.602813
1	-1.665523	-0.267453	0.545778
1	-3.012226	-1.072223	1.463453
6	-1.876670	-2.401500	0.201076
1	-2.397768	-3.262137	0.607984
6	-0.652580	-2.660400	-0.467897
1	-0.109245	-1.817138	-0.872079
6	-4.157221	-1.403955	-3.385837
1	-5.163595	-1.804488	-3.299028
6	-3.092997	-2.339778	-3.364876
1	-3.354414	-3.394594	-3.286062
6	-1.731807	-2.083852	-3.989331
1	-1.804121	-2.178119	-5.084213
1	-1.066468	-2.883897	-3.659208
6	-1.103537	-0.720021	-3.622120
1	-1.306962	0.020496	-4.402154
1	-0.014181	-0.826433	-3.595175
6	-1.559941	-0.148565	-2.280616
1	-0.786661	-0.057986	-1.523445
6	-2.654492	0.696163	-2.123149
1	-2.636668	1.358649	-1.263653
6	-3.612026	1.106893	-3.223777
1	-4.486996	1.559363	-2.753048
1	-3.137817	1.890867	-3.830470

6	-4.071021	-0.063061	-4.118574
1	-3.399358	-0.169034	-4.976699
1	-5.056618	0.175249	-4.530032
6	-0.336898	-3.958646	-1.072350
6	-0.921475	-5.168588	-0.650994
6	0.608250	-4.004979	-2.114296
6	-0.581260	-6.373009	-1.264333
1	-1.638155	-5.172316	0.164094
6	0.944076	-5.207961	-2.732054
1	1.079183	-3.082027	-2.434736
6	0.348895	-6.398983	-2.309381
1	-1.042200	-7.296397	-0.925188
1	1.672913	-5.216163	-3.537420
1	0.609116	-7.339972	-2.785251
6	2.451669	-4.452802	0.569606
6	3.474498	-4.987257	-0.184695
1	1.880098	-5.091581	1.231937
6	4.184930	-4.119330	-1.019837
6	3.867688	-2.774891	-1.048114
1	4.408674	-2.080890	-1.677058
7	2.868225	-2.251627	-0.308050
8	0.967651	-0.249167	0.867839
7	-0.021726	-1.033130	2.752665
6	-0.543942	0.295018	3.057710
1	-1.541339	0.198552	3.492484
1	0.098617	0.816994	3.774276
1	-0.616692	0.884610	2.149455
6	-0.302200	-2.062226	3.751766
1	-1.249953	-2.575782	3.550132
1	0.503026	-2.793752	3.802617
1	-0.372604	-1.582198	4.729720
1	3.710164	-6.044566	-0.133593
35	5.605909	-4.807716	-2.176937

---

9 P1-C2 *endo si-re*

Number of imaginary frequencies= 0
The smallest frequencies are= 7.7509 11.5710 14.5476 cm(-1)
Electronic energy= -7222.663312
Zero-point correction= 1.758579
(Hartree/Particle)
Thermal correction to Energy= 1.876584
Thermal correction to Enthalpy= 1.877528
Thermal correction to Gibbs Free Energy= 1.596755
Sum of electronic and zero-point Energies= -7220.904733
Sum of electronic and thermal Energies= -7220.786728
Sum of electronic and thermal Enthalpies= -7220.785783
Sum of electronic and thermal Free Energies= -7221.066556

.....

Cartesian Coordinates

.....

26	8.026783	0.590559	-1.013377
15	2.955995	1.270479	-2.189525
15	3.932007	0.691861	1.445553
6	6.013767	1.125994	-1.251033
6	6.219869	0.384003	-0.029235
6	6.754721	-0.894584	-0.379394
1	7.033625	-1.675725	0.313851
6	6.906369	-0.942665	-1.799463
1	7.327217	-1.762200	-2.364849
6	6.453570	0.298757	-2.334101
1	6.461868	0.583925	-3.375410
6	9.310548	1.844252	0.035117
1	9.012997	2.484498	0.855115
6	9.738808	0.485776	0.146496
1	9.809943	-0.084890	1.062871
6	10.004068	-0.002674	-1.169118
1	10.308914	-1.009204	-1.423700
6	9.739399	1.053094	-2.093777
1	9.812348	0.988666	-3.171384
6	9.312893	2.193734	-1.350822
1	9.012512	3.144036	-1.770335
6	5.401252	2.483517	-1.327653
6	6.127555	3.585925	-0.851519
1	7.123301	3.412595	-0.463869
6	5.598355	4.875665	-0.853217
1	6.176457	5.700403	-0.448905
6	4.321826	5.090593	-1.366231
1	3.894618	6.088153	-1.382083
6	3.576425	4.009928	-1.837897
1	2.578114	4.195239	-2.215498
6	4.080134	2.698946	-1.804320
6	5.820773	0.863283	1.339394
1	6.010643	1.937025	1.376020
6	6.590118	0.202254	2.486324
1	6.283261	0.611169	3.452800
1	6.438946	-0.880148	2.515657
1	7.660173	0.388548	2.353682
6	1.376747	2.097030	-2.641610
6	0.551808	2.519301	-1.585992
1	0.818118	2.274000	-0.564547
6	-0.598399	3.261635	-1.843443
1	-1.216751	3.593775	-1.019688
6	-0.965340	3.553172	-3.159744
1	-1.870736	4.120229	-3.356245
6	-0.174289	3.098601	-4.216891
1	-0.460661	3.309302	-5.243310
6	0.999260	2.383338	-3.961471
1	1.616356	2.058533	-4.792320
6	3.581388	0.565554	-3.761511
6	4.189636	1.351908	-4.752406
1	4.305579	2.421523	-4.603164
6	4.661759	0.757291	-5.923611
1	5.135616	1.369259	-6.685740
6	4.529044	-0.622327	-6.115125
1	4.902949	-1.081799	-7.025507
6	3.918834	-1.408363	-5.134618
1	3.815775	-2.480358	-5.277869
6	3.449721	-0.815463	-3.961123
1	2.994734	-1.425337	-3.188497
6	3.275164	2.361345	1.864862
6	1.878412	2.472238	1.881083
1	1.275313	1.591813	1.692170
6	1.265097	3.705880	2.093926
6	2.025540	4.862235	2.252417
1	1.548907	5.827083	2.387491
6	3.416872	4.753522	2.213215
6	4.043215	3.518364	2.043142
1	5.124336	3.487428	2.029303
6	3.570882	-0.328697	2.934317
6	3.811507	-1.708378	2.824895
1	4.257008	-2.113599	1.923353
6	3.468305	-2.567308	3.866968
6	2.840251	-2.081313	5.014394
1	2.548311	-2.755474	5.811749
6	2.585235	-0.715917	5.112492
6	2.964383	0.162759	4.095629
1	2.763555	1.221144	4.209568
29	2.796704	-0.131348	-0.425302
6	1.797222	-0.214070	6.291477
6	3.666350	-4.051137	3.725434
6	-0.235694	3.747218	2.173731
6	4.233642	6.013100	2.319443
9	3.964836	6.861213	1.296610
9	5.562986	5.771851	2.297648
9	3.964431	6.688614	3.460084
9	-0.805638	2.915393	1.255609
9	-0.689640	3.334397	3.380452
9	-0.736200	4.980210	1.953793
9	1.893978	1.121479	6.446514
9	0.471562	-0.497526	6.143061
9	2.184753	-0.793980	7.446675
9	4.052835	-4.623803	4.883885
9	4.585873	-4.362074	2.786884
9	2.506038	-4.666252	3.361363
6	0.533026	-1.292173	1.326855
6	0.591575	-2.608455	0.563982
6	1.980789	-3.075217	0.191306
1	0.132993	-3.406397	1.145408
77	-3.367146	-1.333923	-1.544716

15	-5.186469	-0.494315	-0.409813
8	-5.176703	0.778126	0.664626
8	-6.377571	0.045093	-1.456675
7	-5.775954	-1.681042	0.625228
6	-5.062931	2.082761	0.211408
6	-3.860894	2.756314	0.520786
1	-3.109199	2.232931	1.099126
6	-3.676663	4.047496	0.093191
1	-2.772605	4.587213	0.356333
6	-4.654197	4.681003	-0.721088
6	-4.425750	5.970406	-1.273923
1	-3.492170	6.476134	-1.040740
6	-5.355592	6.560806	-2.100220
1	-5.167151	7.542648	-2.524609
6	-6.556706	5.878400	-2.409053
1	-7.278432	6.336812	-3.078977
6	-6.817268	4.635243	-1.874111
1	-7.737880	4.123019	-2.128719
6	-5.885973	3.999822	-1.006113
6	-6.121071	2.694774	-0.444191
6	-7.437794	2.004833	-0.550263
6	-8.654167	2.613615	-0.073412
6	-8.673293	3.855271	0.622550
1	-7.740040	4.369785	0.817070
6	-9.855602	4.404975	1.069378
1	-9.838895	5.349998	1.604873
6	-11.089121	3.748782	0.845132
1	-12.013394	4.197021	1.197727
6	-11.107222	2.535107	0.195973
1	-12.044022	2.008387	0.033510
6	-9.904758	1.933504	-0.264672
6	-9.920014	0.655501	-0.886415
1	-10.871697	0.154027	-1.038994
6	-8.746949	0.047747	-1.256795
1	-8.728470	-0.941934	-1.701069
6	-7.518355	0.717098	-1.058861
6	-5.140423	-3.008302	0.392159
1	-4.343102	-3.140288	1.135648
6	-6.136868	-4.141556	0.565494
6	-5.761754	-5.307764	1.243282
1	-4.769378	-5.371495	1.684425
6	-6.647701	-6.382840	1.359039
1	-6.342250	-7.280336	1.890166
6	-7.925749	-6.298688	0.802766
1	-8.619229	-7.129556	0.897165
6	-8.310657	-5.134758	0.128454
1	-9.305697	-5.060174	-0.302132
6	-7.422512	-4.066060	0.009206
1	-7.724030	-3.156811	-0.503330
6	-4.509170	-3.070501	-1.007194
1	-5.309820	-3.213551	-1.744912
1	-3.880845	-3.964857	-1.050757
6	-6.390670	-1.520067	1.984215
1	-6.843296	-2.497558	2.171547
6	-5.339569	-1.326685	3.079139
6	-4.794139	-2.462247	3.699491
1	-5.143593	-3.447397	3.402201
6	-3.832103	-2.346147	4.706695
1	-3.428229	-3.240261	5.173883
6	-3.405848	-1.082901	5.122090
1	-2.659624	-0.984409	5.906006
6	-3.950467	0.056572	4.521707
1	-3.632130	1.044593	4.843745
6	-4.906531	-0.063915	3.511123
1	-5.318390	0.830881	3.061969
6	-7.546549	-0.521347	2.041737
1	-8.300308	-0.779821	1.295173
1	-7.239634	0.509742	1.873918
1	-8.010976	-0.582549	3.030968
6	-2.294861	-1.133949	0.345743
1	-1.712080	-0.215915	0.360087
1	-2.919145	-1.260168	1.227899
6	-1.765091	-2.291574	-0.304009
1	-2.159300	-3.238143	0.060101
6	-0.314477	-2.429146	-0.737097
1	0.042535	-1.515347	-1.212412
6	-4.341713	-1.346779	-3.499421
1	-5.321924	-1.810827	-3.410445
6	-3.219122	-2.232980	-3.552237
1	-3.432549	-3.301435	-3.516398
6	-1.940549	-1.891682	-4.301656
1	-2.125261	-1.913559	-5.387659
1	-1.216138	-2.682520	-4.101064
6	-1.330290	-0.530668	-3.897673
1	-1.583324	0.239839	-4.634401
1	-0.237591	-0.605343	-3.912955
6	-1.754746	-0.036030	-2.514379
1	-0.947758	0.076811	-1.797459
6	-2.871141	0.773553	-2.284151
1	-2.822150	1.434301	-1.424912
6	-3.885106	1.180852	-3.337021
1	-4.748020	1.606677	-2.818276
1	-3.460275	1.986026	-3.955284
6	-4.358203	0.007091	-4.221523
1	-3.743750	-0.054382	-5.127228
1	-5.377262	0.213138	-4.564581
6	-0.063704	-3.591550	-1.679931
6	-0.588373	-4.871235	-1.447928
6	0.793418	-3.414164	-2.774152
6	-0.264637	-5.938964	-2.288675
1	-1.248328	-5.045252	-0.603209
6	1.126928	-4.478487	-3.613414
1	1.194110	-2.425026	-2.968668
6	0.598441	-5.748932	-3.371390
1	-0.683878	-6.922442	-2.094363
1	1.791394	-4.313133	-4.457360
1	0.852668	-6.581573	-4.021076
6	2.308499	-4.422650	0.384809
6	3.503539	-4.935647	-0.103129
1	1.615464	-5.073331	0.902814
6	4.339454	-4.059878	-0.786218
6	3.988426	-2.725945	-0.930126
1	4.630323	-2.026161	-1.447140
7	2.831751	-2.238530	-0.440453
8	0.874461	-0.234053	0.746241
7	0.002869	-1.260369	2.562712
6	-0.428693	0.030735	3.108251
1	-1.286035	-0.137237	3.758713
1	0.363097	0.515173	3.682198
1	-0.729548	0.687140	2.294315
6	-0.299185	-2.447255	3.368489
1	-1.309990	-2.818225	3.168241
1	0.429108	-3.239030	3.196465
1	-0.229412	-2.165444	4.419611
1	3.760348	-5.979488	0.036953
35	6.006791	-4.696809	-1.572518

---

8 P1-C2 *endo re-re*

Number of imaginary frequencies= 0
The smallest frequencies are= 12.2051 15.9735 17.6675 cm(-1)
Electronic energy= -7222.6397511
Zero-point correction= 1.756337
(Hartree/Particle)
Thermal correction to Energy= 1.875620
Thermal correction to Enthalpy= 1.876564
Thermal correction to Gibbs Free Energy= 1.594294
Sum of electronic and zero-point Energies= -7220.883414
Sum of electronic and thermal Energies= -7220.764131
Sum of electronic and thermal Enthalpies= -7220.763187
Sum of electronic and thermal Free Energies= -7221.045457

.....

Cartesian Coordinates

.....

26	7.441012	-1.991164	-1.488528
15	2.808648	0.278055	-2.408758
15	4.217532	0.443973	1.081482
6	5.747600	-0.784360	-1.768330
6	5.890754	-1.174439	-0.386168
6	5.845281	-2.599618	-0.327343

1	5.935154	-3.197316	0.569395
6	5.713553	-3.097234	-1.657291
1	5.693384	-4.138947	-1.947086
6	5.658625	-1.983541	-2.544030
1	5.574007	-2.027901	-3.619718
6	9.258882	-1.100962	-1.014756
1	9.367275	-0.179530	-0.457816
6	9.188315	-2.414188	-0.457135
1	9.227255	-2.662026	0.595137
6	9.012458	-3.340617	-1.529870
1	8.888847	-4.411034	-1.430536
6	8.974074	-2.600948	-2.750994
1	8.819039	-3.011814	-3.739957
6	9.127706	-1.218486	-2.433748
1	9.113821	-0.403109	-3.144180
6	5.642337	0.627068	-2.239032
6	6.792283	1.431057	-2.248418
1	7.728157	0.982587	-1.941370
6	6.753190	2.774155	-2.620160
1	7.658263	3.372242	-2.590190
6	5.542518	3.339974	-3.011497
1	5.490854	4.384646	-3.301680
6	4.383670	2.562884	-3.007115
1	3.449265	3.024998	-3.303276
6	4.401819	1.216472	-2.607759
6	5.977131	-0.201861	0.756348
1	6.512831	0.668156	0.377911
6	6.743615	-0.717472	1.977623
1	6.776953	0.035556	2.769903
1	6.305764	-1.626336	2.397200
1	7.769436	-0.952002	1.677817
6	1.535708	1.461717	-3.027719
6	1.110655	2.460364	-2.134466
1	1.535135	2.503206	-1.137262
6	0.169587	3.413049	-2.522955
1	-0.125808	4.190594	-1.829107
6	-0.387325	3.363445	-3.803669
1	-1.134154	4.094882	-4.098555
6	0.013823	2.363975	-4.692755
1	-0.417703	2.315082	-5.688606
6	0.974469	1.422227	-4.312297
1	1.275610	0.658486	-5.019963
6	2.909805	-1.026610	-3.698306
6	3.425793	-0.773818	-4.979266
1	3.772387	0.222245	-5.240059
6	3.511201	-1.804985	-5.916315
1	3.911529	-1.603335	-6.905861
6	3.087846	-3.095757	-5.580352
1	3.158965	-3.896633	-6.311061
6	2.585393	-3.353828	-4.302749
1	2.271406	-4.358293	-4.031464
6	2.500354	-2.325496	-3.361474
1	2.166465	-2.530693	-2.348847
6	4.360593	2.286304	0.974393
6	3.161074	3.013615	0.988590
1	2.228038	2.506158	1.189316
6	3.146251	4.382170	0.719880
6	4.327378	5.062468	0.431774
1	4.314256	6.119908	0.191480
6	5.524302	4.348152	0.438180
6	5.549431	2.981391	0.714194
1	6.505190	2.476370	0.698020
6	3.845361	0.094028	2.847545
6	3.759848	-1.261476	3.206327
1	3.974078	-2.032556	2.476597
6	3.358574	-1.625839	4.486913
6	2.990919	-0.657570	5.423030
1	2.651737	-0.945306	6.412193
6	3.054270	0.685022	5.058925
6	3.487566	1.066467	3.786159
1	3.528178	2.120434	3.537416
29	2.479149	-0.419308	-0.265898
6	2.539847	1.725197	6.013853
6	3.217934	-3.074792	4.859036
6	1.840917	5.129600	0.732945
6	6.790316	5.085385	0.094369
9	6.704945	5.666181	-1.127869
9	7.874772	4.280210	0.077651
9	7.040627	6.081134	0.975574
9	0.801699	4.320225	0.390573
9	1.551574	5.636269	1.951810
9	1.837226	6.162238	-0.136395
9	3.062050	2.947930	5.772963
9	1.190526	1.851492	5.920550
9	2.809072	1.412388	7.301352
9	3.846065	-3.357515	6.023138
9	3.719759	-3.904193	3.916721
9	1.915394	-3.422111	5.036767
6	0.378127	0.889630	1.451379
6	0.743636	-1.355641	2.071081
6	-0.174600	1.201046	2.677177
1	0.449915	1.633310	0.665363
6	0.130624	-1.062016	3.337357
6	-0.298220	0.199964	3.656895
6	1.192299	-2.677426	1.861085
6	1.887491	-3.192162	0.740012
8	2.282920	-2.486138	-0.252795
7	0.863996	-0.335852	1.147344
1	1.029060	-3.339242	2.698511
77	-3.268545	-1.641923	-1.104670
15	-4.969048	-0.353688	-0.357085
8	-4.758287	1.005189	0.538919
8	-5.865984	0.245678	-1.613990
7	-5.895745	-1.248926	0.703625
6	-4.348034	2.205928	-0.031564
6	-3.067403	2.659432	0.343418
1	-2.503986	2.073846	1.059445
6	-2.573766	3.815788	-0.205470
1	-1.594225	4.182342	0.081944
6	-3.321612	4.514618	-1.191541
6	-2.769888	5.639704	-1.861899
1	-1.776242	5.975370	-1.576902
6	-3.469466	6.281406	-2.859483
1	-3.034775	7.134688	-3.371689
6	-4.757132	5.820385	-3.224627
1	-5.298065	6.316828	-4.025033
6	-5.330340	4.746122	-2.578532
1	-6.314749	4.402798	-2.875454
6	-4.640692	4.063416	-1.538414
6	-5.195289	2.914162	-0.868624
6	-6.606564	2.470519	-1.053685
6	-7.719195	3.349509	-0.793480
6	-7.557077	4.661602	-0.265887
1	-6.562920	5.024525	-0.035652
6	-8.645288	5.472785	-0.027624
1	-8.493085	6.467507	0.381287
6	-9.958319	5.022019	-0.301760
1	-10.805286	5.675483	-0.114743
6	-10.155602	3.749176	-0.786312
1	-11.159087	3.379858	-0.980865
6	-9.056509	2.880958	-1.028851
6	-9.266879	1.548312	-1.474685
1	-10.281880	1.206308	-1.655709
6	-8.205779	0.694462	-1.644043
1	-8.342303	-0.337231	-1.949976
6	-6.895083	1.163506	-1.414545
6	-5.594514	-2.703771	0.640130
1	-4.961242	-2.953551	1.498192
6	-6.859229	-3.539599	0.721629
6	-6.886814	-4.689997	1.518317
1	-6.012149	-4.952415	2.109284
6	-8.026690	-5.497718	1.559305
1	-8.036405	-6.387582	2.182589
6	-9.153611	-5.155073	0.809238
1	-10.043090	-5.777617	0.845084
6	-9.135009	-4.002612	0.016204
1	-10.011292	-3.728408	-0.564954
6	-7.994649	-3.201015	-0.028230
1	-7.979940	-2.298960	-0.633597
6	-4.821957	-3.032438	-0.643201

1	-5.521696	-3.061716	-1.486394
1	-4.388260	-4.031349	-0.555524
6	-6.520081	-0.798842	1.999463
1	-7.181215	-1.632967	2.250046
6	-5.475830	-0.719264	3.112413
6	-5.174296	-1.882581	3.838499
1	-5.740503	-2.790532	3.646369
6	-4.169908	-1.888175	4.809965
1	-3.952873	-2.801398	5.357407
6	-3.457886	-0.718842	5.082469
1	-2.674901	-0.717511	5.835530
6	-3.771976	0.455034	4.391758
1	-3.232400	1.373359	4.605257
6	-4.773887	0.456211	3.420088
1	-4.999602	1.375973	2.896051
6	-7.421447	0.427047	1.865827
1	-8.181033	0.253080	1.100453
1	-6.881155	1.337254	1.609597
1	-7.929343	0.590781	2.821204
6	-2.408034	-1.329227	0.879479
1	-1.583040	-0.638538	0.752365
1	-3.071837	-1.075092	1.701160
6	-2.201170	-2.724121	0.633458
1	-2.858614	-3.427441	1.133954
6	-1.284628	-3.206409	-0.299696
1	-0.482138	-2.550413	-0.612371
6	-4.084531	-1.537359	-3.229709
1	-5.140955	-1.765904	-3.127117
6	-3.200261	-2.624503	-3.170928
1	-3.631084	-3.614686	-3.028326
6	-1.789899	-2.634442	-3.723970
1	-1.835898	-2.838455	-4.804358
1	-1.266480	-3.482715	-3.278384
6	-0.970276	-1.347578	-3.481726
1	-1.128403	-0.638723	-4.298055
1	0.089822	-1.604209	-3.510739
6	-1.251398	-0.634449	-2.169729
1	-0.492925	-0.710157	-1.394526
6	-2.192278	0.358693	-2.029986
1	-2.099754	1.010049	-1.167905
6	-3.098834	0.863176	-3.132949
1	-3.861552	1.495966	-2.680662
1	-2.507429	1.514523	-3.787813
6	-3.788379	-0.235566	-3.972121
1	-3.187224	-0.471563	-4.855834
1	-4.735503	0.163796	-4.344615
6	-1.132407	-4.605678	-0.698578
6	-1.994584	-5.637450	-0.274323
6	-0.060202	-4.940803	-1.549972
6	-1.795650	-6.949182	-0.699332
1	-2.816691	-5.419695	0.399163
6	0.129918	-6.251844	-1.982759
1	0.631562	-4.162254	-1.855233
6	-0.737385	-7.262433	-1.559358
1	-2.468243	-7.731117	-0.358410
1	0.958573	-6.486411	-2.644666
1	-0.589310	-8.285698	-1.891886
7	2.158470	-4.545926	0.695966
6	3.106355	-5.079581	-0.266505
1	4.002412	-5.468575	0.238243
1	2.654204	-5.899617	-0.836185
1	3.401083	-4.289129	-0.951607
6	1.629918	-5.481947	1.675559
1	0.563686	-5.305847	1.845333
1	1.738968	-6.496459	1.284950
1	2.154402	-5.424434	2.638341
1	-0.715158	0.418342	4.631925
1	0.050027	-1.858649	4.069159
35	-0.691013	3.039733	3.113844

[8-9]‡-P1-C2 *endo re-re*

Number of imaginary frequencies= 1
The smallest frequencies are=-265.7227 12.6739 15.6523cm(-1)
Electronic energy= -7222.6279167
Zero-point correction= 1.756220
(Hartree/Particle)
Thermal correction to Energy= 1.874726
Thermal correction to Enthalpy= 1.875671
Thermal correction to Gibbs Free Energy= 1.594484
Sum of electronic and zero-point Energies= -7220.871696
Sum of electronic and thermal Energies= -7220.753190
Sum of electronic and thermal Enthalpies= -7220.752246
Sum of electronic and thermal Free Energies= -7221.033432

Cartesian Coordinates

26	7.446044	-1.994494	-1.432371
15	2.804950	0.143088	-2.396528
15	4.203109	0.516716	1.047348
6	5.747914	-0.813568	-1.748292
6	5.882726	-1.165584	-0.355363
6	5.849050	-2.589418	-0.263148
1	5.934535	-3.164080	0.648204
6	5.727533	-3.122546	-1.578879
1	5.718781	-4.171674	-1.841401
6	5.668578	-2.032931	-2.493508
1	5.587293	-2.102442	-3.568512
6	9.252220	-1.048363	-1.025935
1	9.352218	-0.090783	-0.532183
6	9.205148	-2.322816	-0.382560
1	9.254811	-2.499891	0.683494
6	9.038339	-3.320495	-1.390670
1	8.931335	-4.383728	-1.220351
6	8.983960	-2.663530	-2.657679
1	8.829995	-3.140891	-3.616514
6	9.117520	-1.260977	-2.433216
1	9.087675	-0.494236	-3.195470
6	5.621999	0.571472	-2.281292
6	6.757307	1.389503	-2.371197
1	7.707429	0.983335	-2.048889
6	6.685108	2.696897	-2.850800
1	7.578574	3.311338	-2.885909
6	5.457933	3.210072	-3.263944
1	5.384107	4.225799	-3.639454
6	4.312361	2.418467	-3.174661
1	3.363445	2.836736	-3.489659
6	4.366319	1.108805	-2.672054
6	5.956553	-0.177670	0.777243
1	6.548166	0.669756	0.429730
6	6.629559	-0.724864	2.040262
1	6.686009	0.040193	2.819342
1	6.100690	-1.587148	2.453888
1	7.645943	-1.043673	1.790931
6	1.487041	1.296524	-2.960167
6	1.109569	2.308575	-2.060583
1	1.610314	2.385381	-1.099675
6	0.119866	3.227778	-2.401179
1	-0.144987	4.012078	-1.705292
6	-0.527714	3.135162	-3.636364
1	-1.312095	3.842316	-3.889593
6	-0.164586	2.128526	-4.532462
1	-0.663203	2.048413	-5.494149
6	0.841744	1.216534	-4.201431
1	1.109436	0.440922	-4.909535
6	2.861782	-1.184534	-3.657816
6	3.298512	-0.966106	-4.973336
1	3.620201	0.024148	-5.283107
6	3.331096	-2.024897	-5.882485
1	3.668357	-1.852378	-6.900543
6	2.933351	-3.305989	-5.483693
1	2.960535	-4.127218	-6.194326
6	2.513045	-3.530270	-4.170420
1	2.216585	-4.526117	-3.853125
6	2.484168	-2.473774	-3.258524
1	2.213633	-2.642363	-2.221235
6	4.348849	2.351175	0.875952
6	3.169297	3.098664	1.005255
1	2.260813	2.621492	1.342477
6	3.139340	4.457900	0.694463

6	4.289658	5.115354	0.266391
1	4.263460	6.168201	0.008473
6	5.472183	4.383030	0.164358
6	5.507908	3.020472	0.458456
1	6.444536	2.497795	0.330791
6	3.807646	0.223484	2.816342
6	3.513278	-1.109823	3.144628
1	3.555803	-1.874530	2.376686
6	3.157207	-1.454231	4.444657
6	3.028718	-0.473998	5.430895
1	2.733988	-0.740213	6.439490
6	3.293767	0.852703	5.096000
6	3.698219	1.205245	3.804507
1	3.917066	2.243870	3.582765
29	2.513651	-0.501220	-0.231243
6	3.077099	1.938411	6.115120
6	2.836308	-2.887883	4.766774
6	1.838007	5.200874	0.824593
6	6.711796	5.100955	-0.298180
9	6.537839	5.653900	-1.522893
9	7.787634	4.287733	-0.375703
9	7.034223	6.114539	0.538308
9	0.791232	4.416825	0.440551
9	1.587458	5.576626	2.098416
9	1.798984	6.311577	0.063049
9	3.921634	2.978261	5.933632
9	1.819216	2.440377	6.037026
9	3.243272	1.494344	7.379928
9	3.197567	-3.217582	6.024826
9	3.458011	-3.745259	3.924082
9	1.505448	-3.146589	4.666306
6	0.469370	0.806528	1.480102
6	0.454674	-1.490388	1.908432
6	-0.205455	1.083661	2.656755
1	0.723520	1.595311	0.784173
6	-0.309157	-1.247762	3.081496
6	-0.617118	0.036005	3.482922
6	0.709586	-2.861920	1.552949
6	1.877914	-3.314470	0.833054
8	2.536509	-2.573405	0.038962
7	0.829135	-0.440287	1.117159
1	0.285698	-3.561034	2.259382
77	-3.381035	-1.624164	-1.235990
15	-5.087347	-0.367642	-0.417419
8	-4.888227	0.976658	0.526153
8	-6.016392	0.279243	-1.636951
7	-5.991633	-1.292386	0.653223
6	-4.361369	2.143310	-0.002330
6	-3.080734	2.516895	0.459481
1	-2.594630	1.883158	1.191648
6	-2.500661	3.665615	-0.016327
1	-1.530579	3.983523	0.348483
6	-3.146844	4.429288	-1.026428
6	-2.510477	5.562165	-1.603278
1	-1.537536	5.859761	-1.220101
6	-3.104275	6.258441	-2.632397
1	-2.605528	7.116426	-3.073468
6	-4.366266	5.846293	-3.124430
1	-4.821335	6.382280	-3.952317
6	-5.024960	4.773437	-2.562765
1	-5.992008	4.473086	-2.949769
6	-4.449081	4.039267	-1.489201
6	-5.109265	2.912505	-0.879280
6	-6.542923	2.583650	-1.124844
6	-7.580814	3.565625	-0.914700
6	-7.323066	4.855998	-0.370709
1	-6.313460	5.121787	-0.083367
6	-8.338065	5.769947	-0.185972
1	-8.110598	6.744085	0.237540
6	-9.671945	5.450874	-0.532807
1	-10.460182	6.184109	-0.389451
6	-9.964632	4.202130	-1.031860
1	-10.987432	3.931237	-1.280672
6	-8.943865	3.230847	-1.218816
6	-9.259327	1.923192	-1.676044
1	-10.291336	1.681268	-1.913784
6	-8.279549	0.969539	-1.783217
1	-8.499451	-0.045557	-2.096510
6	-6.939771	1.302639	-1.484173
6	-5.555086	-2.715488	0.684967
1	-4.859778	-2.837853	1.524549
6	-6.723534	-3.661216	0.896774
6	-6.581554	-4.763091	1.748565
1	-5.648647	-4.900494	2.291035
6	-7.622962	-5.681904	1.904918
1	-7.498775	-6.531378	2.570961
6	-8.823712	-5.501488	1.215110
1	-9.637540	-6.210096	1.340398
6	-8.974876	-4.400622	0.365284
1	-9.908307	-4.252340	-0.171063
6	-7.931444	-3.488723	0.205452
1	-8.049292	-2.628004	-0.447050
6	-4.816873	-3.076028	-0.609576
1	-5.554688	-3.209580	-1.410053
1	-4.320248	-4.041046	-0.470628
6	-6.687144	-0.820372	1.900070
1	-7.304621	-1.677850	2.180686
6	-5.708752	-0.599119	3.056181
6	-5.322093	-1.701802	3.835227
1	-5.765438	-2.674077	3.637555
6	-4.396331	-1.566532	4.873279
1	-4.114139	-2.435558	5.461670
6	-3.854562	-0.313291	5.165571
1	-3.142771	-0.199885	5.978863
6	-4.254530	0.799018	4.418977
1	-3.853841	1.782272	4.649988
6	-5.173338	0.657220	3.377678
1	-5.470451	1.532803	2.814330
6	-7.659685	0.331102	1.650978
1	-8.373334	0.052732	0.871982
1	-7.166296	1.253049	1.345094
1	-8.215429	0.531048	2.572242
6	-2.452207	-1.181895	0.686477
1	-1.713838	-0.400637	0.548203
1	-3.134608	-0.982242	1.508629
6	-2.100657	-2.552783	0.469627
1	-2.717120	-3.278232	0.988707
6	-0.903254	-3.061023	-0.105510
1	-0.268341	-2.382314	-0.659922
6	-4.172185	-1.837046	-3.290237
1	-5.211824	-2.147287	-3.213561
6	-3.198676	-2.852511	-3.075322
1	-3.570877	-3.856545	-2.870240
6	-1.790596	-2.825968	-3.645304
1	-1.806681	-3.136735	-4.701947
1	-1.207177	-3.581885	-3.113141
6	-1.083331	-1.462430	-3.511302
1	-1.253695	-0.852629	-4.402620
1	-0.003855	-1.625622	-3.467458
6	-1.497153	-0.658300	-2.283643
1	-0.743315	-0.554863	-1.507221
6	-2.505240	0.295932	-2.290322
1	-2.446241	1.075217	-1.537933
6	-3.394406	0.616464	-3.474781
1	-4.227392	1.220703	-3.110241
1	-2.829981	1.248368	-4.173938
6	-3.950369	-0.626693	-4.202224
1	-3.285690	-0.914928	-5.023533
1	-4.905749	-0.360551	-4.665147
6	-0.774866	-4.484594	-0.457120
6	-1.629415	-5.480426	0.059293
6	0.234923	-4.882465	-1.352812
6	-1.476539	-6.814711	-0.310915
1	-2.414923	-5.216339	0.758855
6	0.388035	-6.216974	-1.724388
1	0.902373	-4.132516	-1.758563
6	-0.466544	-7.191393	-1.203141
1	-2.146912	-7.564718	0.099175
1	1.175488	-6.495093	-2.419006
1	-0.350017	-8.232701	-1.488848

7	2.268113	-4.615425	0.977785
6	3.309758	-5.166752	0.120480
1	4.215880	-5.384135	0.699985
1	2.955687	-6.097873	-0.334786
1	3.553604	-4.450484	-0.659128
6	1.655765	-5.548460	1.920821
1	0.693704	-5.923014	1.554922
1	2.330276	-6.397675	2.047013
1	1.519495	-5.088848	2.900639
1	-1.172250	0.218686	4.394973
1	-0.621810	-2.088751	3.688999
35	-0.523342	2.932769	3.188581

---

9 P1-C2 *endo re-re*

Number of imaginary frequencies= 0
The smallest frequencies are= 13.1436 14.8842 15.7376 cm(-1)
Electronic energy= -7222.6543802
Zero-point correction= 1.760436
(Hartree/Particle)
Thermal correction to Energy= 1.878042
Thermal correction to Enthalpy= 1.878986
Thermal correction to Gibbs Free Energy= 1.601965
Sum of electronic and zero-point Energies= -7220.893945
Sum of electronic and thermal Energies= -7220.776338
Sum of electronic and thermal Enthalpies= -7220.775394
Sum of electronic and thermal Free Energies= -7221.052416

.....

Cartesian Coordinates

.....

26	7.402476	-2.049259	-1.281595
15	2.782095	0.037806	-2.463580
15	4.090251	0.550071	1.024472
6	5.707118	-0.889985	-1.684451
6	5.803571	-1.193073	-0.276911
6	5.780459	-2.612806	-0.135914
1	5.851971	-3.154758	0.795570
6	5.694461	-3.192871	-1.435079
1	5.699453	-4.250682	-1.661105
6	5.658118	-2.135346	-2.388473
1	5.609495	-2.244295	-3.462116
6	9.199477	-1.089190	-0.858616
1	9.290583	-0.118420	-0.389649
6	9.137822	-2.345250	-0.181313
1	9.163606	-2.492796	0.890018
6	8.994720	-3.370647	-1.164683
1	8.883953	-4.428835	-0.967550
6	8.969840	-2.749370	-2.450376
1	8.837927	-3.253492	-3.398675
6	9.098029	-1.341120	-2.262108
1	9.087682	-0.596422	-3.046353
6	5.592954	0.477797	-2.264234
6	6.729462	1.295228	-2.343729
1	7.669591	0.899994	-1.981282
6	6.671051	2.587612	-2.863680
1	7.565610	3.200637	-2.892126
6	5.455942	3.087833	-3.325244
1	5.392759	4.092360	-3.731557
6	4.308521	2.297761	-3.246481
1	3.368935	2.705810	-3.600433
6	4.349289	1.002470	-2.706652
6	5.845636	-0.168323	0.822113
1	6.450317	0.663451	0.461199
6	6.483669	-0.671410	2.120807
1	6.520277	0.119596	2.874546
1	5.945135	-1.519888	2.550131
1	7.505572	-0.997581	1.906890
6	1.475696	1.164077	-3.101259
6	1.066322	2.207001	-2.251600
1	1.541927	2.330613	-1.283360
6	0.075748	3.100742	-2.651672
1	-0.219979	3.905643	-1.992367
6	-0.536892	2.954408	-3.899318
1	-1.321958	3.641951	-4.199985
6	-0.139760	1.919452	-4.747312
1	-0.612883	1.796987	-5.717299
6	0.864967	1.030368	-4.355073
1	1.155315	0.229635	-5.024944
6	2.909180	-1.333997	-3.666918
6	3.368986	-1.152464	-4.980234
1	3.641733	-0.161151	-5.330606
6	3.493714	-2.250587	-5.832610
1	3.848027	-2.107506	-6.849362
6	3.170839	-3.533908	-5.376962
1	3.274186	-4.386253	-6.042335
6	2.727814	-3.719903	-4.065442
1	2.493245	-4.715770	-3.700927
6	2.601924	-2.622411	-3.212055
1	2.306586	-2.758726	-2.176656
6	4.265837	2.376289	0.779549
6	3.096474	3.147979	0.834707
1	2.166526	2.699572	1.149306
6	3.102926	4.496092	0.476576
6	4.281071	5.119545	0.076437
1	4.283922	6.162261	-0.220890
6	5.453965	4.365630	0.050996
6	5.453623	3.014075	0.392784
1	6.387158	2.475367	0.325827
6	3.666950	0.335805	2.798319
6	3.384504	-0.982872	3.184448
1	3.439728	-1.781114	2.451975
6	3.041296	-1.274916	4.501813
6	2.916702	-0.256830	5.446640
1	2.636476	-0.482523	6.468735
6	3.173306	1.057345	5.054257
6	3.559607	1.359179	3.745993
1	3.772448	2.388366	3.479739
29	2.436171	-0.509549	-0.288472
6	2.973567	2.176165	6.041485
6	2.744914	-2.702735	4.867250
6	1.811040	5.265302	0.519431
6	6.722335	5.047839	-0.388979
9	6.600981	5.559096	-1.637973
9	7.786105	4.215387	-0.399040
9	7.030188	6.085019	0.423081
9	0.769278	4.484852	0.113203
9	1.506828	5.691084	1.765829
9	1.828490	6.347288	-0.281450
9	3.767333	3.235931	5.773328
9	1.695215	2.628735	6.019122
9	3.226860	1.786147	7.309622
9	2.846363	-2.929400	6.190635
9	3.583400	-3.561985	4.236958
9	1.485554	-3.063974	4.501548
6	0.428575	0.869373	1.359105
6	0.245546	-1.396386	1.804903
6	-0.101693	1.194917	2.600379
1	0.676056	1.629471	0.630899
6	-0.312724	-1.123194	3.059516
6	-0.467534	0.189116	3.488323
6	0.275827	-2.822096	1.305970
6	1.697643	-3.295141	1.023801
8	2.438091	-2.610251	0.275810
7	0.652224	-0.402605	0.986205
1	-0.186394	-3.433268	2.076677
77	-3.414678	-1.677748	-1.298318
15	-5.099732	-0.382800	-0.428104
8	-4.869179	0.955115	0.532503
8	-6.079792	0.301702	-1.598950
7	-5.979805	-1.306550	0.669735
6	-4.326972	2.109617	0.001348
6	-3.027912	2.453625	0.435643
1	-2.543223	1.805620	1.156547
6	-2.432470	3.591335	-0.047187
1	-1.449986	3.887787	0.299910
6	-3.082786	4.375321	-1.039052
6	-2.433823	5.496644	-1.625124
1	-1.445323	5.770120	-1.263969
6	-3.035989	6.211564	-2.636606
1	-2.528164	7.059999	-3.085835

6	-4.319136	5.832044	-3.099542
1	-4.781272	6.382691	-3.913840
6	-4.989377	4.772358	-2.526627
1	-5.972209	4.495763	-2.891084
6	-4.404753	4.018552	-1.471518
6	-5.076822	2.904800	-0.851156
6	-6.525775	2.615043	-1.053111
6	-7.529491	3.623318	-0.803067
6	-7.219439	4.904932	-0.265377
1	-6.194177	5.142627	-0.010935
6	-8.202345	5.846021	-0.045623
1	-7.933923	6.812778	0.370916
6	-9.555349	5.564597	-0.348257
1	-10.317970	6.319089	-0.178797
6	-9.898197	4.325054	-0.838393
1	-10.935655	4.082473	-1.053775
6	-8.910891	3.326806	-1.060158
6	-9.276284	2.029809	-1.510133
1	-10.321952	1.815902	-1.712997
6	-8.326341	1.051857	-1.656300
1	-8.585471	0.045282	-1.967192
6	-6.966665	1.345160	-1.404338
6	-5.566579	-2.738335	0.678704
1	-4.858937	-2.882060	1.505071
6	-6.752825	-3.658712	0.906913
6	-6.631965	-4.759761	1.763073
1	-5.698022	-4.918767	2.297711
6	-7.693833	-5.652883	1.932156
1	-7.584154	-6.502232	2.601061
6	-8.895517	-5.447518	1.251168
1	-9.724708	-6.136437	1.385593
6	-9.026502	-4.347038	0.397333
1	-9.959930	-4.179135	-0.133432
6	-7.962994	-3.460975	0.225843
1	-8.065236	-2.600944	-0.429994
6	-4.850156	-3.115345	-0.624922
1	-5.603252	-3.251115	-1.411501
1	-4.373220	-4.088762	-0.474741
6	-6.625741	-0.841589	1.944126
1	-7.254833	-1.688559	2.231767
6	-5.604082	-0.666122	3.071406
6	-5.237227	-1.789343	3.830380
1	-5.729072	-2.740186	3.643840
6	-4.265927	-1.702688	4.831694
1	-4.001742	-2.587242	5.405302
6	-3.653588	-0.478166	5.105303
1	-2.904522	-0.403112	5.888964
6	-4.033812	0.655912	4.381479
1	-3.581044	1.619274	4.600544
6	-5.001285	0.563116	3.379432
1	-5.281771	1.454661	2.833751
6	-7.580087	0.336158	1.751024
1	-8.321405	0.091822	0.986334
1	-7.076738	1.255213	1.453591
1	-8.107121	0.523629	2.691852
6	-2.495281	-1.291362	0.645493
1	-1.836340	-0.433906	0.571339
1	-3.209000	-1.202810	1.461515
6	-2.053590	-2.592634	0.262365
1	-2.608189	-3.402328	0.732123
6	-0.605472	-2.998649	-0.004083
1	-0.144610	-2.359873	-0.757618
6	-4.228243	-1.901645	-3.303251
1	-5.270238	-2.211738	-3.245603
6	-3.249585	-2.929276	-3.088569
1	-3.626534	-3.935303	-2.901045
6	-1.880033	-2.912646	-3.746405
1	-1.972255	-3.128853	-4.823194
1	-1.304239	-3.735648	-3.320033
6	-1.111777	-1.589713	-3.540967
1	-1.208290	-0.950939	-4.424083
1	-0.042406	-1.802374	-3.449433
6	-1.546043	-0.786242	-2.314938
1	-0.788369	-0.666845	-1.544875
6	-2.537727	0.195904	-2.340407
1	-2.451403	0.993139	-1.609127
6	-3.414545	0.526611	-3.533893
1	-4.242232	1.141087	-3.171264
1	-2.843470	1.150323	-4.235873
6	-3.985440	-0.716340	-4.246963
1	-3.318494	-1.027901	-5.059179
1	-4.931672	-0.443369	-4.725948
6	-0.510983	-4.447141	-0.464321
6	-1.094804	-5.488468	0.273886
6	0.206615	-4.780630	-1.618514
6	-0.970488	-6.817313	-0.136476
1	-1.644748	-5.265759	1.183619
6	0.337173	-6.107615	-2.034480
1	0.655038	-3.988866	-2.203214
6	-0.251848	-7.133491	-1.293227
1	-1.433845	-7.606498	0.449316
1	0.892001	-6.334800	-2.940830
1	-0.155782	-8.167350	-1.612437
7	2.139698	-4.462670	1.529097
6	3.458729	-4.955788	1.129231
1	4.190133	-4.755781	1.920281
1	3.397055	-6.036307	0.972636
1	3.774974	-4.469134	0.210592
6	1.457960	-5.336966	2.483222
1	1.166041	-6.269151	1.991052
1	2.149398	-5.561496	3.299576
1	0.576797	-4.872223	2.912343
1	-0.885669	0.413638	4.461920
1	-0.631329	-1.939671	3.695732
35	-0.291327	3.064430	3.097950

---

8 P1-C2 *exo si-si*

Number of imaginary frequencies= 0
The smallest frequencies are= 9.2056 11.6531 13.9144 cm(-1)

Electronic energy= -7222.6394745
Zero-point correction= 1.756770
(Hartree/Particle)
Thermal correction to Energy= 1.875959
Thermal correction to Enthalpy= 1.876903
Thermal correction to Gibbs Free Energy= 1.593668
Sum of electronic and zero-point Energies= -7220.882704
Sum of electronic and thermal Energies= -7220.763515
Sum of electronic and thermal Enthalpies= -7220.762571
Sum of electronic and thermal Free Energies= -7221.045806

.....

Cartesian Coordinates

.....

26	8.187524	0.983036	-0.259123
15	3.230664	1.495266	-1.840112
15	3.898022	0.473492	1.718423
6	6.170438	1.424102	-0.600683
6	6.327879	0.525223	0.519112
6	6.972486	-0.657414	0.042980
1	7.242147	-1.515317	0.643488
6	7.246294	-0.489628	-1.347408
1	7.762968	-1.195636	-1.982733
6	6.754608	0.788428	-1.743901
1	6.831828	1.219145	-2.730681
6	9.267155	2.177105	1.051200
1	8.843625	2.681547	1.909685
6	9.798432	0.850942	1.036719
1	9.844794	0.174387	1.879719
6	10.215285	0.556450	-0.297216
1	10.627345	-0.383066	-0.641353
6	9.940989	1.699424	-1.108363
1	10.109605	1.778375	-2.174266
6	9.355953	2.700455	-0.276372
1	9.007195	3.670261	-0.604401
6	5.452702	2.730609	-0.535000
6	6.036142	3.795724	0.168797
1	7.011567	3.640969	0.612533
6	5.391386	5.022926	0.319797
1	5.860954	5.815573	0.893730

6	4.138181	5.214054	-0.256964
1	3.620219	6.161292	-0.147510
6	3.535067	4.169697	-0.957800
1	2.553271	4.330767	-1.388181
6	4.158720	2.918810	-1.093597
6	5.764109	0.767876	1.893405
1	5.878225	1.830228	2.115760
6	6.445758	-0.033421	3.005552
1	6.010496	0.203241	3.980486
1	6.355051	-1.112028	2.851391
1	7.511645	0.214383	3.030269
6	1.614340	2.243166	-2.326951
6	0.616172	2.318586	-1.342086
1	0.802275	1.901322	-0.359183
6	-0.617508	2.906304	-1.626148
1	-1.372025	2.968751	-0.851643
6	-0.884214	3.395642	-2.907713
1	-1.849264	3.842540	-3.129469
6	0.092261	3.297377	-3.902299
1	-0.108816	3.668438	-4.903325
6	1.337929	2.733860	-3.612439
1	2.091133	2.680916	-4.391144
6	4.062528	1.216245	-3.454551
6	4.757982	2.231379	-4.131656
1	4.824384	3.226118	-3.701152
6	5.380605	1.962454	-5.351505
1	5.920788	2.751915	-5.866509
6	5.310708	0.680639	-5.908074
1	5.801844	0.471831	-6.854342
6	4.607250	-0.328071	-5.246412
1	4.541988	-1.323620	-5.675329
6	3.986240	-0.061419	-4.024292
1	3.436924	-0.845024	-3.515967
6	3.054070	1.991046	2.331746
6	1.656357	1.977460	2.215156
1	1.175605	1.079298	1.840104
6	0.905335	3.106554	2.537732
6	1.527991	4.284461	2.946753
1	0.945172	5.170527	3.172596
6	2.920424	4.303207	3.041713
6	3.681818	3.168431	2.756112
1	4.757724	3.232358	2.845471
6	3.432538	-0.823292	2.939488
6	3.749749	-2.139484	2.569900
1	4.294519	-2.325282	1.651436
6	3.303986	-3.212537	3.334164
6	2.502136	-3.002718	4.457327
1	2.112619	-3.843649	5.021395
6	2.167951	-1.696566	4.810177
6	2.648310	-0.608075	4.076897
1	2.365771	0.395546	4.371042
29	3.007436	-0.199281	-0.355098
6	1.246371	-1.480091	5.979942
6	3.598086	-4.624889	2.911536
6	-0.592102	3.015159	2.464429
6	3.588810	5.597526	3.418474
9	3.359479	6.560673	2.490531
9	4.928735	5.475982	3.539801
9	3.119766	6.081075	4.592584
9	-0.991947	2.274105	1.388533
9	-1.115464	2.398781	3.551450
9	-1.191089	4.216566	2.355615
9	0.734468	-0.226742	6.006067
9	0.190846	-2.334699	5.941830
9	1.862127	-1.682732	7.166582
9	4.252485	-5.310404	3.878730
9	4.350059	-4.687267	1.793119
9	2.455802	-5.318014	2.663095
6	0.835102	-1.845575	0.965364
6	1.297741	-3.030179	0.332265
6	2.405011	-3.193620	-0.529573
1	0.792663	-3.954536	0.577158
77	-3.526199	-1.155425	-1.720107
15	-5.160722	-0.635875	-0.235522
8	-5.120270	0.728081	0.701079
8	-6.617188	-0.439884	-0.992042
7	-5.212627	-1.800641	0.953090
6	-5.217915	1.982055	0.105056
6	-4.064864	2.795385	0.152080
1	-3.202428	2.446563	0.704507
6	-4.070574	4.012263	-0.483454
1	-3.195249	4.654411	-0.443596
6	-5.207234	4.426724	-1.229993
6	-5.186118	5.625279	-1.993435
1	-4.284796	6.232584	-1.978575
6	-6.274710	6.001917	-2.747314
1	-6.245763	6.915566	-3.333599
6	-7.432465	5.188040	-2.768197
1	-8.281289	5.476754	-3.381265
6	-7.493251	4.030743	-2.022213
1	-8.385002	3.415937	-2.055829
6	-6.393079	3.616589	-1.221549
6	-6.415399	2.398040	-0.451673
6	-7.662718	1.610065	-0.239352
6	-8.841494	2.223015	0.326648
6	-8.850482	3.555671	0.826463
1	-7.939905	4.141190	0.800486
6	-9.993793	4.109451	1.361257
1	-9.968525	5.126279	1.742405
6	-11.196015	3.366774	1.426386
1	-12.090784	3.819303	1.843488
6	-11.218241	2.066072	0.976894
1	-12.127330	1.473673	1.039142
6	-10.052321	1.459710	0.435815
6	-10.062959	0.099607	0.024904
1	-10.986825	-0.467098	0.096477
6	-8.913787	-0.500104	-0.422530
1	-8.884729	-1.547163	-0.704512
6	-7.723159	0.253609	-0.519646
6	-4.284708	-2.940146	0.735651
1	-3.415554	-2.791459	1.387272
6	-4.921252	-4.270525	1.104383
6	-4.181305	-5.224628	1.811517
1	-3.172767	-4.982692	2.137720
6	-4.730523	-6.476490	2.102781
1	-4.145316	-7.208126	2.652983
6	-6.031213	-6.781344	1.696579
1	-6.462564	-7.750923	1.928567
6	-6.779123	-5.829771	0.994744
1	-7.793988	-6.058986	0.681500
6	-6.226106	-4.584572	0.697094
1	-6.808117	-3.839228	0.161146
6	-3.819522	-3.006625	-0.729418
1	-4.578219	-3.545475	-1.306070
1	-2.909909	-3.611275	-0.760536
6	-5.729374	-1.685564	2.359470
1	-5.989988	-2.715528	2.614605
6	-4.652812	-1.260095	3.360097
6	-3.996105	-2.248774	4.109561
1	-4.241143	-3.294181	3.939027
6	-3.043337	-1.909491	5.074629
1	-2.539644	-2.689821	5.637695
6	-2.732429	-0.569069	5.308511
1	-1.972565	-0.305321	6.037802
6	-3.379729	0.425224	4.569419
1	-3.136488	1.470180	4.734388
6	-4.330025	0.083564	3.604732
1	-4.825946	0.867099	3.045322
6	-7.027001	-0.888720	2.485315
1	-7.797416	-1.314816	1.839317
1	-6.913227	0.166785	2.239299
1	-7.374767	-0.959132	3.520013
6	-2.211515	-0.518671	-0.104994
1	-2.331834	0.484742	0.285238
1	-2.219207	-1.285205	0.659866
6	-1.297337	-0.665490	-1.192112
1	-0.921441	0.237032	-1.656016
6	-0.993179	-1.894913	-1.764829
1	-1.203755	-2.794421	-1.200770
6	-5.092367	-1.766676	-3.244718

1	-5.748021	-2.452554	-2.714561
6	-3.853136	-2.286340	-3.658542
1	-3.647367	-3.327121	-3.410216
6	-3.018844	-1.766096	-4.810785
1	-3.416921	-2.184123	-5.747255
1	-2.010689	-2.168867	-4.702645
6	-2.934094	-0.228051	-4.935886
1	-3.759614	0.142143	-5.550670
1	-2.011880	0.020272	-5.469942
6	-2.935098	0.525925	-3.619558
1	-1.979723	0.897896	-3.271532
6	-4.063017	1.010890	-3.016515
1	-3.942782	1.757776	-2.237647
6	-5.465874	0.812156	-3.545931
1	-6.167325	1.145510	-2.784446
1	-5.605872	1.485981	-4.403165
6	-5.823249	-0.634765	-3.969788
1	-5.650785	-0.760516	-5.043751
1	-6.896173	-0.773023	-3.813191
6	-0.157173	-2.085983	-2.948921
6	0.304544	-1.020537	-3.748053
6	0.184025	-3.399414	-3.324652
6	1.052370	-1.268297	-4.895392
1	0.084418	0.004612	-3.476472
6	0.947487	-3.644481	-4.465036
1	-0.150929	-4.228531	-2.707612
6	1.376692	-2.579597	-5.261337
1	1.399757	-0.434353	-5.497020
1	1.205495	-4.665104	-4.732108
1	1.963849	-2.767544	-6.155497
6	2.662693	-4.505380	-1.055688
6	3.749324	-4.766244	-1.854381
1	1.977239	-5.307953	-0.800919
6	4.616592	-3.699573	-2.143664
6	4.352862	-2.447398	-1.633939
1	5.006781	-1.610367	-1.841518
7	3.280719	-2.181018	-0.858342
8	1.156924	-0.655997	0.616995
7	-0.054168	-1.975664	2.016966
6	-0.646387	-0.803839	2.641031
1	-1.702141	-0.985759	2.846383
1	-0.158329	-0.551562	3.588753
1	-0.569818	0.042659	1.970911
6	-0.420324	-3.259783	2.597628
1	-1.225745	-3.755240	2.035723
1	0.435614	-3.934364	2.642986
1	-0.769577	-3.096746	3.618652
1	3.929763	-5.762706	-2.244254
35	6.194759	-3.975165	-3.280317

[8-9]‡-P1-C2 *exo si-si*

Number of imaginary frequencies= 1
The smallest frequencies are= -129.6214 8.7202 13.0915 cm(-1)
Electronic energy= -7222.6324643
Zero-point correction= 1.754828
(Hartree/Particle)
Thermal correction to Energy= 1.873410
Thermal correction to Enthalpy= 1.874354
Thermal correction to Gibbs Free Energy= 1.592590
Sum of electronic and zero-point Energies= -7220.877637
Sum of electronic and thermal Energies= -7220.759054
Sum of electronic and thermal Enthalpies= -7220.758110
Sum of electronic and thermal Free Energies= -7221.039875

.....

Cartesian Coordinates

.....

26	8.003890	0.535566	-0.858794
15	2.937988	1.172384	-2.105429
15	3.903793	0.834210	1.536138
6	5.990347	1.055563	-1.115708
6	6.207648	0.424180	0.164300
6	6.729963	-0.884036	-0.076119
1	7.012639	-1.601361	0.681993
6	6.868040	-1.058283	-1.486177
1	7.273277	-1.929953	-1.980245
6	6.410565	0.131149	-2.126277
1	6.407013	0.320672	-3.189396
6	9.301507	1.883611	0.045256
1	9.014316	2.596080	0.807040
6	9.738124	0.543182	0.275880
1	9.835801	0.063437	1.240657
6	9.982438	-0.066493	-0.992189
1	10.289443	-1.091121	-1.155838
6	9.695783	0.896155	-2.007336
1	9.749415	0.730002	-3.075186
6	9.276435	2.100579	-1.367427
1	8.961294	3.005025	-1.869508
6	5.392609	2.409612	-1.299378
6	6.133043	3.535728	-0.904898
1	7.122845	3.377599	-0.497121
6	5.628771	4.830260	-1.016791
1	6.222067	5.674824	-0.680954
6	4.358914	5.025010	-1.553914
1	3.949256	6.024757	-1.653976
6	3.597294	3.922174	-1.938852
1	2.604470	4.094589	-2.335989
6	4.077699	2.608912	-1.800000
6	5.792712	1.016022	1.484079
1	5.982368	2.089455	1.442124
6	6.534867	0.445288	2.695471
1	6.206978	0.929446	3.619615
1	6.378539	-0.630937	2.806653
1	7.609044	0.618500	2.575339
6	1.365084	2.011567	-2.575314
6	0.536934	2.457240	-1.531021
1	0.782039	2.203854	-0.506001
6	-0.586182	3.237088	-1.805196
1	-1.204690	3.590108	-0.990616
6	-0.923816	3.543122	-3.125953
1	-1.808134	4.138311	-3.335526
6	-0.132947	3.064127	-4.172045
1	-0.397336	3.284584	-5.202323
6	1.012603	2.310695	-3.900001
1	1.635356	1.973547	-4.722064
6	3.531091	0.436053	-3.679490
6	4.233159	1.176010	-4.643879
1	4.443656	2.227942	-4.475262
6	4.676108	0.558584	-5.814982
1	5.222360	1.136239	-6.555264
6	4.422340	-0.799447	-6.033291
1	4.776719	-1.279233	-6.941087
6	3.715673	-1.538401	-5.081356
1	3.523036	-2.594971	-5.242819
6	3.270681	-0.921861	-3.910648
1	2.735752	-1.497083	-3.163707
6	3.203815	2.503927	1.868286
6	1.803611	2.563888	1.922557
1	1.236118	1.643447	1.834558
6	1.148962	3.790224	2.034938
6	1.868441	4.982606	2.066686
1	1.359302	5.937613	2.131572
6	3.261061	4.922266	1.993397
6	3.929960	3.700669	1.907468
1	5.009462	3.709763	1.846349
6	3.500589	-0.138279	3.045923
6	3.727933	-1.520681	2.955165
1	4.171269	-1.936818	2.057899
6	3.351204	-2.367602	3.993031
6	2.712721	-1.863475	5.127957
1	2.398448	-2.526595	5.925894
6	2.471183	-0.494005	5.208861
6	2.870839	0.370616	4.185713
1	2.670480	1.431386	4.280891
29	2.787150	-0.157308	-0.283877
6	1.683282	0.045914	6.370248
6	3.524710	-3.854620	3.853161
6	-0.350981	3.792703	2.129852
6	4.026792	6.217386	1.965405
9	3.731786	6.942228	0.857819

9	5.364877	6.031830	1.973323
9	3.720977	7.000060	3.026524
9	-0.904734	2.912419	1.246604
9	-0.787025	3.414231	3.353145
9	-0.890289	5.001200	1.864338
9	1.964132	1.341726	6.622703
9	0.343271	-0.019432	6.128443
9	1.901361	-0.651043	7.505477
9	3.955865	-4.422762	5.000824
9	4.400600	-4.182316	2.880021
9	2.347092	-4.464357	3.543223
6	0.664618	-1.343779	1.568125
6	0.978067	-2.683055	1.144436
6	2.105648	-3.099675	0.371665
1	0.534831	-3.488568	1.711424
77	-3.317360	-1.168261	-1.663083
15	-5.086051	-0.635548	-0.337471
8	-5.147114	0.646869	0.712297
8	-6.419382	-0.301638	-1.273955
7	-5.382708	-1.872892	0.752307
6	-5.093938	1.941340	0.214706
6	-3.922669	2.675242	0.499373
1	-3.159375	2.211649	1.111422
6	-3.785653	3.947113	0.002123
1	-2.908543	4.538430	0.245215
6	-4.776293	4.488919	-0.861866
6	-4.587239	5.747248	-1.495212
1	-3.677494	6.302471	-1.281546
6	-5.523394	6.245101	-2.373624
1	-5.363959	7.202950	-2.860077
6	-6.692360	5.498157	-2.654394
1	-7.418263	5.882659	-3.365069
6	-6.917166	4.285452	-2.039016
1	-7.814683	3.723395	-2.270132
6	-5.978206	3.745382	-1.117032
6	-6.173879	2.470569	-0.473410
6	-7.473496	1.741497	-0.517906
6	-8.698688	2.375843	-0.089723
6	-8.729461	3.667587	0.507785
1	-7.801889	4.202851	0.668885
6	-9.917447	4.244819	0.902321
1	-9.907776	5.229156	1.361672
6	-11.146448	3.567788	0.722654
1	-12.075404	4.038674	1.030497
6	-11.153327	2.305334	0.174465
1	-12.085789	1.760982	0.049612
6	-9.944378	1.675075	-0.226614
6	-9.950186	0.349627	-0.738300
1	-10.897883	-0.169175	-0.851536
6	-8.772557	-0.278082	-1.052212
1	-8.745614	-1.302187	-1.409395
6	-7.547319	0.412849	-0.911950
6	-4.478865	-3.038698	0.557847
1	-3.622325	-2.931166	1.237613
6	-5.160225	-4.360359	0.866996
6	-4.476101	-5.342630	1.592576
1	-3.485519	-5.122596	1.984952
6	-5.055329	-6.594453	1.818986
1	-4.512542	-7.347034	2.384430
6	-6.332526	-6.872698	1.327951
1	-6.788051	-7.842213	1.508564
6	-7.025434	-5.894084	0.607110
1	-8.021626	-6.102745	0.226598
6	-6.441547	-4.648920	0.374838
1	-6.979722	-3.884697	-0.180005
6	-3.981610	-3.056184	-0.891386
1	-4.810426	-3.394618	-1.525733
1	-3.196513	-3.808029	-0.987752
6	-6.060015	-1.787521	2.086950
1	-6.349542	-2.821694	2.288701
6	-5.113751	-1.387694	3.220964
6	-4.455679	-2.398772	3.938012
1	-4.621061	-3.437361	3.663530
6	-3.611561	-2.093375	5.008966
1	-3.114559	-2.894232	5.549218
6	-3.412058	-0.764114	5.385051
1	-2.747936	-0.520000	6.209711
6	-4.068313	0.252366	4.684259
1	-3.926018	1.290361	4.972860
6	-4.911577	-0.055917	3.614710
1	-5.416562	0.745463	3.090342
6	-7.366059	-0.993532	2.066696
1	-8.037607	-1.391153	1.302667
1	-7.225259	0.070737	1.879485
1	-7.854068	-1.102902	3.039908
6	-2.037822	-0.563759	-0.021653
1	-1.867713	0.509758	-0.005942
1	-2.339479	-0.958567	0.946512
6	-1.126730	-1.359133	-0.802591
1	-0.457311	-0.854996	-1.487689
6	-0.890079	-2.720818	-0.540821
1	-1.492548	-3.178405	0.236813
6	-4.591862	-1.533292	-3.475866
1	-5.426017	-2.154432	-3.158489
6	-3.355285	-2.194074	-3.655959
1	-3.341394	-3.269576	-3.479775
6	-2.221618	-1.710671	-4.542860
1	-2.429265	-1.974615	-5.591614
1	-1.325087	-2.270086	-4.259044
6	-1.930652	-0.200554	-4.426890
1	-2.514331	0.358217	-5.165222
1	-0.879790	-0.018640	-4.672220
6	-2.200958	0.382911	-3.042860
1	-1.321846	0.684430	-2.485682
6	-3.398028	0.973716	-2.666098
1	-3.358076	1.692024	-1.853416
6	-4.635510	1.051792	-3.535880
1	-5.470005	1.367339	-2.908603
1	-4.490378	1.848229	-4.281138
6	-5.002847	-0.273467	-4.240052
1	-4.558562	-0.307561	-5.240192
1	-6.086551	-0.297610	-4.388563
6	-0.253048	-3.644818	-1.466985
6	0.551408	-3.206530	-2.538361
6	-0.447676	-5.029189	-1.298871
6	1.130086	-4.121177	-3.412224
1	0.726742	-2.146634	-2.678783
6	0.124863	-5.944817	-2.182095
1	-1.056937	-5.381590	-0.470229
6	0.916524	-5.494688	-3.241414
1	1.746639	-3.763945	-4.231734
1	-0.043494	-7.008489	-2.040384
1	1.366453	-6.205604	-3.928249
6	2.375532	-4.497008	0.298040
6	3.405259	-4.991793	-0.472884
1	1.751333	-5.179032	0.863015
6	4.191349	-4.068646	-1.170036
6	3.927347	-2.717494	-1.060514
1	4.529179	-1.983958	-1.579772
7	2.910818	-2.233947	-0.318995
8	1.010437	-0.304093	0.925976
7	-0.123647	-1.187449	2.678108
6	-0.677401	0.121984	3.001388
1	-1.694729	0.002151	3.380026
1	-0.083392	0.630983	3.768268
1	-0.710999	0.735585	2.107635
6	-0.433338	-2.264960	3.611711
1	-1.335075	-2.818157	3.319425
1	0.401576	-2.959606	3.701103
1	-0.610287	-1.829356	4.596274
1	3.594101	-6.058022	-0.533278
35	5.659027	-4.674031	-2.315731

---

9 P1-C2 *exo si-si*

Number of imaginary frequencies= 0
The smallest frequencies are= 10.8036 13.3986 14.8641 cm(-1)
Electronic energy= -7222.6577931
Zero-point correction= 1.759193
(Hartree/Particle)

Thermal correction to Energy= 1.876944
Thermal correction to Enthalpy= 1.877888
Thermal correction to Gibbs Free Energy= 1.599335
Sum of electronic and zero-point Energies= -7220.898600
Sum of electronic and thermal Energies= -7220.780849
Sum of electronic and thermal Enthalpies= -7220.779905
Sum of electronic and thermal Free Energies= -7221.058458

.....

Cartesian Coordinates

.....

26	7.794310	0.355230	-1.273588
15	2.686650	1.430911	-2.049952
15	3.913434	0.665944	1.481952
6	5.807687	1.024179	-1.343812
6	6.062440	0.262434	-0.144223
6	6.475678	-1.048218	-0.539039
1	6.759077	-1.850497	0.128390
6	6.514000	-1.093369	-1.965338
1	6.835183	-1.931326	-2.565724
6	6.099261	0.176942	-2.460366
1	6.046449	0.468095	-3.498710
6	9.248805	1.508027	-0.335763
1	9.070231	2.158686	0.510162
6	9.592349	0.122812	-0.271004
1	9.711936	-0.461048	0.631904
6	9.706876	-0.366576	-1.607785
1	9.921557	-1.387652	-1.894365
6	9.432980	0.715116	-2.498907
1	9.406405	0.658924	-3.579124
6	9.151979	1.872957	-1.714320
1	8.880132	2.845926	-2.100186
6	5.296914	2.422490	-1.378634
6	6.136314	3.461352	-0.946727
1	7.132636	3.203174	-0.612019
6	5.720478	4.791440	-0.934303
1	6.387307	5.565793	-0.568944
6	4.444164	5.111642	-1.389983
1	4.103202	6.141691	-1.399464
6	3.586932	4.095382	-1.810062
1	2.590536	4.365014	-2.137048
6	3.975462	2.744012	-1.786518
6	5.795345	0.755631	1.251958
1	6.040899	1.819169	1.280535
6	6.610021	0.044176	2.335852
1	6.401188	0.464402	3.323410
1	6.397747	-1.027647	2.374684
1	7.675846	0.168175	2.121673
6	1.171500	2.427487	-2.345152
6	0.444653	2.844187	-1.220045
1	0.739232	2.501661	-0.235121
6	-0.646085	3.699332	-1.363411
1	-1.184734	4.027443	-0.485634
6	-1.051188	4.113800	-2.634627
1	-1.913950	4.765045	-2.742799
6	-0.352468	3.675734	-3.761911
1	-0.668076	3.984672	-4.754264
6	0.762769	2.846323	-3.619525
1	1.310439	2.531763	-4.501697
6	2.992917	0.657142	-3.682532
6	3.750402	1.260676	-4.695933
1	4.225058	2.221882	-4.521008
6	3.902033	0.622162	-5.929026
1	4.494914	1.091323	-6.708939
6	3.290892	-0.613809	-6.161504
1	3.411707	-1.107350	-7.121459
6	2.522902	-1.213307	-5.159224
1	2.041071	-2.170478	-5.336983
6	2.377629	-0.581596	-3.923284
1	1.791882	-1.049811	-3.137543
6	3.333530	2.345148	1.975958
6	1.945731	2.483810	2.126129
1	1.311923	1.611257	2.018820
6	1.375497	3.734767	2.355377
6	2.168493	4.878885	2.413895
1	1.723920	5.856670	2.564122
6	3.548684	4.741092	2.253987
6	4.134541	3.490609	2.050447
1	5.207787	3.436212	1.927366
6	3.595424	-0.383520	2.960947
6	3.747534	-1.770033	2.794226
1	4.121657	-2.167974	1.857340
6	3.397674	-2.644475	3.821552
6	2.859229	-2.163886	5.015868
1	2.564372	-2.848718	5.803322
6	2.698800	-0.789664	5.174460
6	3.078002	0.100132	4.167487
1	2.946397	1.163522	4.325955
29	2.575400	-0.013384	-0.320871
6	2.018857	-0.284107	6.417204
6	3.492116	-4.131863	3.625756
6	-0.115316	3.813331	2.542335
6	4.392610	5.987060	2.271657
9	4.048581	6.832084	1.269546
9	5.710945	5.724202	2.136701
9	4.234535	6.675875	3.425729
9	-0.772294	2.976810	1.688830
9	-0.489603	3.442489	3.788535
9	-0.601829	5.052789	2.323775
9	2.185321	1.041968	6.594986
9	0.677144	-0.508610	6.359959
9	2.464380	-0.907756	7.528696
9	3.938117	-4.761347	4.731978
9	4.305585	-4.469967	2.604306
9	2.266959	-4.667802	3.348964
6	0.537416	-1.307282	1.677552
6	0.583063	-2.637404	0.949269
6	1.862488	-2.990332	0.220002
1	0.432895	-3.445949	1.660331
77	-3.071862	-1.029253	-1.637402
15	-4.941596	-0.548568	-0.384647
8	-5.074949	0.658906	0.762327
8	-6.236870	-0.136064	-1.358032
7	-5.323497	-1.860067	0.596315
6	-4.975997	1.981871	0.369363
6	-3.835294	2.689221	0.809596
1	-3.119132	2.176441	1.440498
6	-3.671335	4.002167	0.446149
1	-2.829207	4.572743	0.824309
6	-4.582098	4.615082	-0.456846
6	-4.341788	5.918716	-0.970190
1	-3.459173	6.454636	-0.630262
6	-5.193617	6.483274	-1.893571
1	-4.994626	7.475240	-2.288404
6	-6.327044	5.761600	-2.338848
1	-6.985335	6.200380	-3.083115
6	-6.601897	4.505868	-1.841371
1	-7.471413	3.964420	-2.196320
6	-5.748799	3.894033	-0.881406
6	-5.997827	2.575096	-0.356999
6	-7.301457	1.874890	-0.536821
6	-8.541648	2.506202	-0.147211
6	-8.591950	3.760983	0.523893
1	-7.669099	4.266865	0.778562
6	-9.793650	4.339340	0.872922
1	-9.797595	5.294648	1.390130
6	-11.019192	3.699553	0.574060
1	-11.958698	4.171115	0.847065
6	-11.009858	2.470596	-0.045778
1	-11.940704	1.952520	-0.261889
6	-9.787607	1.839836	-0.403347
6	-9.781279	0.546579	-0.992001
1	-10.727615	0.052564	-1.194315
6	-8.595989	-0.083359	-1.269408
1	-8.563052	-1.085298	-1.684484
6	-7.368899	0.573213	-1.015814
6	-4.390759	-3.004214	0.407327
1	-3.600654	-2.928453	1.167347
6	-5.080014	-4.347443	0.576869
6	-4.438857	-5.379831	1.272348
1	-3.481943	-5.185779	1.751650

6	-5.016590	-6.649589	1.359470
1	-4.505288	-7.440182	1.902106
6	-6.252070	-6.898261	0.758067
1	-6.706992	-7.882155	0.829556
6	-6.903592	-5.870600	0.067702
1	-7.867255	-6.055390	-0.399487
6	-6.319878	-4.607233	-0.025627
1	-6.826046	-3.806608	-0.558591
6	-3.753031	-2.948111	-0.988443
1	-4.506165	-3.294052	-1.708219
1	-2.947630	-3.679519	-1.021218
6	-6.071530	-1.860603	1.893970
1	-6.391988	-2.899638	2.005104
6	-5.176676	-1.567856	3.101800
6	-4.588350	-2.644880	3.783533
1	-4.776370	-3.657638	3.437799
6	-3.785001	-2.438358	4.908127
1	-3.344789	-3.289405	5.420675
6	-3.557888	-1.142586	5.376009
1	-2.936766	-0.975376	6.251801
6	-4.144828	-0.061292	4.711656
1	-3.985496	0.950807	5.074165
6	-4.946760	-0.271779	3.587840
1	-5.399001	0.577974	3.093086
6	-7.359059	-1.036950	1.868338
1	-7.993496	-1.355485	1.038281
1	-7.186138	0.034603	1.774688
1	-7.905059	-1.211535	2.800510
6	-1.881241	-0.484106	0.106923
1	-1.656728	0.579711	0.088293
1	-2.275259	-0.817695	1.066302
6	-1.075900	-1.393570	-0.645687
1	-0.282224	-0.966599	-1.252997
6	-0.715221	-2.728031	-0.024141
1	-1.522653	-3.004822	0.659633
6	-4.133344	-1.350628	-3.519073
1	-4.971067	-2.026159	-3.358068
6	-2.839230	-1.963278	-3.607421
1	-2.804781	-3.049652	-3.518731
6	-1.698979	-1.392024	-4.436893
1	-1.874909	-1.575012	-5.508989
1	-0.793354	-1.946757	-4.178664
6	-1.451975	0.108980	-4.186626
1	-1.973289	0.716501	-4.933660
1	-0.387735	0.327864	-4.316780
6	-1.869428	0.571937	-2.793265
1	-1.051578	0.854148	-2.139234
6	-3.113996	1.125433	-2.500489
1	-3.164722	1.815720	-1.664089
6	-4.257091	1.228350	-3.492559
1	-5.159174	1.488119	-2.935292
1	-4.061384	2.065828	-4.179760
6	-4.511507	-0.074677	-4.284865
1	-3.971074	-0.051421	-5.237978
1	-5.573973	-0.122402	-4.544698
6	-0.506825	-3.876585	-0.992527
6	0.082969	-3.678898	-2.247025
6	-0.845213	-5.182368	-0.611797
6	0.331317	-4.755978	-3.099191
1	0.355545	-2.677413	-2.555687
6	-0.602609	-6.264151	-1.460938
1	-1.313231	-5.350287	0.355370
6	-0.008707	-6.054607	-2.708396
1	0.790392	-4.581714	-4.068655
1	-0.880081	-7.267595	-1.150091
1	0.182941	-6.893390	-3.371463
6	2.272542	-4.330386	0.278423
6	3.287719	-4.797853	-0.543847
1	1.768904	-5.016515	0.945904
6	3.880069	-3.882566	-1.404965
6	3.500522	-2.548508	-1.374859
1	3.977694	-1.809583	-2.004813
7	2.510570	-2.108378	-0.570692
8	0.949977	-0.259417	1.134215
7	-0.089282	-1.249722	2.871657
6	-0.483803	0.064735	3.389301
1	-1.368132	-0.060543	4.014482
1	0.310614	0.521998	3.984288
1	-0.731842	0.722861	2.558995
6	-0.439675	-2.419286	3.683621
1	-1.392675	-2.858598	3.371786
1	0.347460	-3.172493	3.648130
1	-0.531920	-2.095451	4.720193
1	3.584216	-5.840394	-0.523911
35	5.226376	-4.483798	-2.681852

---

8 P1-C2 *exo re-si*

Number of imaginary frequencies= 0
The smallest frequencies are= 5.1892 6.4945 13.2689 cm(-1)
Electronic energy= -7222.617113
Zero-point correction= 1.754125
(Hartree/Particle)
Thermal correction to Energy= 1.874073
Thermal correction to Enthalpy= 1.875017
Thermal correction to Gibbs Free Energy= 1.587486
Sum of electronic and zero-point Energies= -7220.862988
Sum of electronic and thermal Energies= -7220.743040
Sum of electronic and thermal Enthalpies= -7220.742096
Sum of electronic and thermal Free Energies= -7221.029627

.....

Cartesian Coordinates

.....

77	4.362977	-0.125342	-1.638825
15	6.061223	0.435774	-0.265409
8	6.503065	-0.481815	1.032417
8	7.494338	0.505473	-1.100923
7	5.712911	1.883777	0.489262
6	7.299690	-1.616994	0.894089
6	6.682831	-2.849902	1.197718
1	5.650958	-2.843865	1.532949
6	7.395706	-4.014967	1.060236
1	6.936163	-4.970675	1.295321
6	8.731783	-3.988812	0.577217
6	9.450131	-5.193555	0.347276
1	8.962316	-6.138197	0.572789
6	10.728083	-5.167977	-0.163123
1	11.266305	-6.094361	-0.340775
6	11.337841	-3.928504	-0.471311
1	12.338065	-3.912237	-0.894367
6	10.674774	-2.741643	-0.245498
1	11.155959	-1.803847	-0.496471
6	9.360033	-2.727952	0.298370
6	8.633641	-1.506170	0.534619
6	9.266651	-0.166735	0.378691
6	10.446277	0.212895	1.111772
6	11.021667	-0.609838	2.120395
1	10.558773	-1.559504	2.360227
6	12.147384	-0.210208	2.807176
1	12.562366	-0.853754	3.577510
6	12.764706	1.031642	2.524458
1	13.655960	1.328722	3.069211
6	12.221946	1.863927	1.572143
1	12.674046	2.828789	1.358248
6	11.051218	1.490358	0.857270
6	10.458639	2.372745	-0.086286
1	10.931597	3.330678	-0.282264
6	9.287383	2.034616	-0.718083
1	8.798980	2.703334	-1.418368
6	8.695975	0.780736	-0.454544
6	4.566114	2.593487	-0.138411
1	3.684034	2.434995	0.494120
6	4.805924	4.089060	-0.258226
6	3.757939	4.982323	-0.008464
1	2.797835	4.598189	0.324138
6	3.939280	6.357067	-0.182033
1	3.117459	7.039139	0.018028
6	5.175707	6.852740	-0.601758
1	5.320920	7.921575	-0.730226
6	6.228463	5.965859	-0.850199

1	7.194664	6.344664	-1.172244
6	6.043214	4.593354	-0.683787
1	6.862969	3.903325	-0.862600
6	4.299457	2.011651	-1.528492
1	5.057944	2.404330	-2.216120
1	3.338380	2.375164	-1.894519
6	6.053022	2.393975	1.859304
1	6.143068	3.474270	1.716979
6	4.893219	2.170680	2.824906
6	4.179380	3.271664	3.313805
1	4.455829	4.272043	2.990456
6	3.113428	3.097253	4.201692
1	2.571272	3.963175	4.571354
6	2.739411	1.813320	4.600405
1	1.904274	1.671410	5.278361
6	3.443933	0.707230	4.114058
1	3.151309	-0.293995	4.416025
6	4.515393	0.883971	3.237544
1	5.059892	0.021884	2.867780
6	7.392298	1.943411	2.446567
1	8.214945	2.167742	1.766301
1	7.416073	0.884683	2.699645
1	7.554209	2.514187	3.366152
6	3.267822	-0.591032	0.172735
1	3.532804	-1.544663	0.627579
1	3.280632	0.225838	0.892716
6	2.168545	-0.619805	-0.768411
1	1.822249	-1.574831	-1.142396
6	1.555755	0.534202	-1.222423
1	1.843008	1.469041	-0.755753
6	5.591913	0.112824	-3.544468
1	6.114286	1.059137	-3.437406
6	4.226245	0.189460	-3.869587
1	3.809398	1.185646	-4.013969
6	3.379385	-0.917205	-4.472310
1	3.469676	-0.892180	-5.568590
1	2.332930	-0.684285	-4.248165
6	3.693102	-2.336964	-3.953521
1	4.509020	-2.782607	-4.529079
1	2.817519	-2.970112	-4.127106
6	4.040246	-2.398158	-2.471847
1	3.281111	-2.822225	-1.821610
6	5.316932	-2.324415	-1.952663
1	5.460110	-2.706972	-0.947349
6	6.589967	-2.134722	-2.748215
1	7.380691	-1.852684	-2.050916
1	6.883784	-3.104567	-3.174630
6	6.500319	-1.072026	-3.864714
1	6.166856	-1.529002	-4.800737
1	7.506919	-0.688580	-4.054482
6	0.590941	0.647250	-2.299690
6	-0.031752	-0.466345	-2.902280
6	0.294460	1.934968	-2.791052
6	-0.911066	-0.292173	-3.967091
1	0.160814	-1.464921	-2.526018
6	-0.562135	2.102916	-3.875105
1	0.749534	2.799520	-2.315045
6	-1.169450	0.990451	-4.463591
1	-1.405203	-1.152524	-4.408909
1	-0.776039	3.098881	-4.248649
1	-1.855092	1.120540	-5.294083
26	-6.675169	4.080018	1.291181
15	-4.800380	0.777871	-2.260978
15	-4.733392	-0.294642	1.350875
6	-6.192573	2.519307	-0.018802
6	-5.594742	2.312947	1.279263
6	-4.731185	3.418759	1.541834
1	-4.149269	3.564368	2.441513
6	-4.811855	4.321374	0.442473
1	-4.304519	5.273095	0.362978
6	-5.715085	3.775109	-0.513358
1	-6.004259	4.229251	-1.449345
6	-8.369070	3.923278	2.484995
1	-8.772225	2.994077	2.865762
6	-7.383706	4.736086	3.124987
1	-6.903593	4.528129	4.071786
6	-7.109626	5.850326	2.274250
1	-6.381266	6.628537	2.460953
6	-7.925440	5.727487	1.108353
1	-7.924701	6.395822	0.257458
6	-8.704105	4.538986	1.238762
1	-9.399640	4.157929	0.503570
6	-7.071762	1.540345	-0.721047
6	-8.392937	1.361324	-0.286271
1	-8.741904	1.961379	0.544546
6	-9.245362	0.432456	-0.882716
1	-10.254072	0.301381	-0.505023
6	-8.785070	-0.335187	-1.949917
1	-9.434622	-1.064419	-2.423891
6	-7.472056	-0.180463	-2.396591
1	-7.124688	-0.794416	-3.219794
6	-6.595173	0.731686	-1.789453
6	-5.794994	1.084930	2.122593
1	-6.825369	0.763361	1.972016
6	-5.592035	1.308571	3.623905
1	-5.783868	0.391265	4.187321
1	-4.579700	1.643192	3.863835
1	-6.289577	2.079376	3.966066
6	-4.646104	-0.438061	-3.640241
6	-4.639187	-1.804046	-3.307682
1	-4.802745	-2.107674	-2.279409
6	-4.442269	-2.777886	-4.286082
1	-4.454480	-3.826545	-4.008295
6	-4.227443	-2.398981	-5.614946
1	-4.062598	-3.154766	-6.377577
6	-4.230725	-1.045431	-5.956400
1	-4.068421	-0.742576	-6.987181
6	-4.445410	-0.070074	-4.978320
1	-4.443869	0.975438	-5.264603
6	-4.613038	2.412810	-3.074879
6	-5.598384	2.934508	-3.928783
1	-6.492075	2.356052	-4.145477
6	-5.441577	4.203963	-4.486234
1	-6.207300	4.603907	-5.145008
6	-4.301921	4.961540	-4.191848
1	-4.184638	5.952756	-4.621269
6	-3.321175	4.444766	-3.342372
1	-2.440034	5.034706	-3.104575
6	-3.473911	3.173766	-2.782361
1	-2.735811	2.782634	-2.089993
6	-5.919553	-1.657642	0.958211
6	-5.400415	-2.760275	0.264239
1	-4.337008	-2.820786	0.064454
6	-6.237894	-3.784092	-0.181014
6	-7.611513	-3.726144	0.039508
1	-8.264801	-4.508405	-0.329589
6	-8.129609	-2.633584	0.733921
6	-7.298792	-1.616645	1.201958
1	-7.752242	-0.793138	1.735215
6	-3.711151	-0.999943	2.712850
6	-2.663964	-0.196506	3.196074
1	-2.522488	0.804216	2.807394
6	-1.775320	-0.694701	4.143846
6	-1.879440	-2.009335	4.604662
1	-1.170028	-2.401227	5.324539
6	-2.910045	-2.807074	4.118167
6	-3.829160	-2.308875	3.189127
1	-4.625695	-2.956780	2.842036
29	-3.433097	0.309399	-0.508783
6	-3.002339	-4.251207	4.524943
6	-0.609077	0.134458	4.600637
6	-5.631305	-4.963752	-0.889885
6	-9.618924	-2.565222	0.938718
9	-10.280415	-2.579544	-0.244856
9	-10.003931	-1.449257	1.595946
9	-10.075331	-3.625946	1.644516
9	-4.640221	-4.577931	-1.733731
9	-5.077868	-5.839789	-0.020354
9	-6.537291	-5.645284	-1.621471
9	-4.285202	-4.657263	4.661604

9	-2.437388	-5.060767	3.593823
9	-2.371561	-4.497138	5.693713
9	-0.396627	0.030510	5.932273
9	-0.760201	1.448112	4.320773
9	0.545807	-0.267882	4.003376
6	-1.939592	-2.300606	-0.689398
6	-0.794978	-0.696871	0.598237
6	-1.166184	-3.333445	-0.195288
1	-2.705065	-2.482723	-1.435584
6	-0.020998	-1.759753	1.173280
6	-0.200835	-3.067674	0.788259
1	0.716787	-1.515670	1.928457
6	-0.451814	0.630198	0.947978
6	-1.054894	1.836470	0.496223
8	-2.131598	1.896274	-0.180866
7	-1.794430	-1.021180	-0.291341
1	0.365821	0.703550	1.648568
7	-0.424101	3.036902	0.788981
6	-1.119482	4.293715	0.546543
1	-1.508250	4.725455	1.480897
1	-0.433411	5.021147	0.097241
1	-1.953733	4.121076	-0.129065
6	0.723941	3.107093	1.684724
1	1.546178	2.477942	1.333454
1	1.083509	4.136999	1.717346
1	0.475685	2.804505	2.708642
1	0.390692	-3.864681	1.226544
35	-1.415692	-5.163356	-0.852197

[8-9]‡-P1-C2 *exo re-si*

Number of imaginary frequencies= 1
The smallest frequencies are= -132.9634 4.4564 9.8735 cm(-1)
Electronic energy= -7222.6148776
Zero-point correction= 1.754242
(Hartree/Particle)
Thermal correction to Energy= 1.873142
Thermal correction to Enthalpy= 1.874086
Thermal correction to Gibbs Free Energy= 1.589201
Sum of electronic and zero-point Energies= -7220.860636
Sum of electronic and thermal Energies= -7220.741736
Sum of electronic and thermal Enthalpies= -7220.740791
Sum of electronic and thermal Free Energies= -7221.025677

.....

Cartesian Coordinates

.....

77	4.332396	-0.374629	-1.603431
15	6.025750	0.348253	-0.273900
8	6.544391	-0.442426	1.085853
8	7.452148	0.436447	-1.130948
7	5.630408	1.837402	0.383436
6	7.404842	-1.534014	1.018542
6	6.870200	-2.775879	1.425842
1	5.847254	-2.805383	1.786433
6	7.648829	-3.904255	1.357368
1	7.252601	-4.865284	1.672470
6	8.971623	-3.836502	0.842834
6	9.756983	-5.010419	0.684014
1	9.331298	-5.963224	0.987590
6	11.021358	-4.947369	0.143451
1	11.610485	-5.851316	0.019907
6	11.549151	-3.700160	-0.267815
1	12.537704	-3.656312	-0.715803
6	10.820523	-2.540978	-0.110980
1	11.237540	-1.596890	-0.440850
6	9.518059	-2.564841	0.461554
6	8.725103	-1.373626	0.626852
6	9.276406	-0.014953	0.364525
6	10.442101	0.484438	1.046144
6	11.083222	-0.229751	2.097135
1	10.682692	-1.186344	2.410760
6	12.194677	0.282497	2.730439
1	12.661434	-0.279839	3.534059
6	12.730814	1.535990	2.350071
1	13.611743	1.923086	2.853633
6	12.122640	2.265270	1.353828
1	12.511373	3.237822	1.063215
6	10.965422	1.773674	0.690608
6	10.309336	2.547756	-0.304550
1	10.723091	3.513625	-0.580065
6	9.153135	2.095002	-0.890820
1	8.621576	2.677890	-1.634862
6	8.638216	0.832171	-0.525981
6	4.473202	2.462424	-0.310995
1	3.588658	2.322733	0.322535
6	4.655760	3.953650	-0.538056
6	3.539685	4.797784	-0.479353
1	2.570385	4.383320	-0.215657
6	3.661243	6.160184	-0.762446
1	2.785919	6.802278	-0.711671
6	4.905957	6.696658	-1.101082
1	5.004377	7.757290	-1.314332
6	6.025382	5.860726	-1.159122
1	6.997962	6.271211	-1.416976
6	5.899904	4.498332	-0.883901
1	6.769918	3.849430	-0.915470
6	4.239226	1.769942	-1.660766
1	4.999801	2.125685	-2.367627
1	3.276996	2.095506	-2.060404
6	5.919074	2.430463	1.727104
1	5.917368	3.507670	1.539505
6	4.792885	2.161493	2.722883
6	4.082311	3.239366	3.266005
1	4.326163	4.251238	2.951341
6	3.065153	3.030753	4.202556
1	2.526899	3.880977	4.612188
6	2.729035	1.733808	4.593410
1	1.924223	1.563003	5.301609
6	3.428765	0.650610	4.053264
1	3.167690	-0.361708	4.347880
6	4.457565	0.862301	3.134232
1	5.002695	0.016739	2.731616
6	7.295553	2.120943	2.324049
1	8.091833	2.359130	1.616779
1	7.398614	1.084453	2.641683
1	7.423705	2.759140	3.203909
6	3.162798	-0.687350	0.185106
1	3.357187	-1.657387	0.642379
1	3.208281	0.128467	0.902990
6	2.130595	-0.625976	-0.821616
1	1.746505	-1.549882	-1.234773
6	1.417210	0.550553	-1.111116
1	1.761653	1.465697	-0.647745
6	5.572529	-0.319746	-3.491331
1	6.097222	0.632047	-3.487794
6	4.208452	-0.280733	-3.848576
1	3.795032	0.692537	-4.111720
6	3.389898	-1.453872	-4.362016
1	3.553540	-1.579979	-5.443430
1	2.333374	-1.191502	-4.241446
6	3.661411	-2.787008	-3.631675
1	4.476042	-3.329679	-4.120183
1	2.776195	-3.424857	-3.722590
6	3.988902	-2.628396	-2.148659
1	3.224379	-2.977866	-1.459155
6	5.274710	-2.522152	-1.634638
1	5.412421	-2.808339	-0.596587
6	6.548563	-2.471991	-2.453460
1	7.353730	-2.136574	-1.797015
1	6.809180	-3.492988	-2.768310
6	6.477416	-1.538100	-3.680881
1	6.145473	-2.093894	-4.563300
1	7.488193	-1.185584	-3.906788
6	0.539571	0.718805	-2.256941
6	-0.049480	-0.371389	-2.931896
6	0.295966	2.021280	-2.738852
6	-0.848977	-0.161993	-4.052044
1	0.105626	-1.381169	-2.569131
6	-0.477659	2.224115	-3.878663
1	0.730346	2.868524	-2.215372

6	-1.057791	1.134590	-4.534571
1	-1.317705	-1.007151	-4.547229
1	-0.646583	3.230840	-4.245962
1	-1.680333	1.294533	-5.409291
26	-6.436005	4.125323	1.552940
15	-4.788566	0.969086	-2.212482
15	-4.760229	-0.355784	1.288420
6	-6.075154	2.650657	0.112248
6	-5.529620	2.272533	1.391793
6	-4.571111	3.263789	1.765445
1	-3.999476	3.273139	2.683413
6	-4.539956	4.261994	0.748898
1	-3.941690	5.162490	0.761645
6	-5.466567	3.889206	-0.266531
1	-5.687643	4.442688	-1.167726
6	-8.181348	4.016208	2.675849
1	-8.692739	3.096320	2.927461
6	-7.139714	4.631182	3.436033
1	-6.720922	4.257803	4.361001
6	-6.716157	5.803004	2.737856
1	-5.917868	6.468589	3.039113
6	-7.495468	5.913357	1.546196
1	-7.392553	6.676581	0.786131
6	-8.401884	4.812218	1.508783
1	-9.108815	4.603894	0.717369
6	-7.027495	1.835287	-0.691129
6	-8.384210	1.798518	-0.339825
1	-8.702660	2.368055	0.523534
6	-9.310617	1.053962	-1.070027
1	-10.352428	1.036270	-0.765903
6	-8.887562	0.332725	-2.184542
1	-9.596209	-0.245877	-2.767539
6	-7.538210	0.336223	-2.537883
1	-7.220348	-0.243913	-3.396951
6	-6.591903	1.060790	-1.797027
6	-5.844068	0.986073	2.101867
1	-6.873190	0.717856	1.857606
6	-5.727521	1.064050	3.627042
1	-5.982542	0.107772	4.092229
1	-4.719424	1.336996	3.950217
1	-6.419089	1.826962	3.996330
6	-4.704496	-0.335888	-3.504852
6	-4.883674	-1.664064	-3.076371
1	-5.128530	-1.863508	-2.036563
6	-4.755131	-2.725475	-3.969750
1	-4.903708	-3.741618	-3.617714
6	-4.427299	-2.473744	-5.306761
1	-4.315892	-3.298527	-6.004750
6	-4.246011	-1.158931	-5.740526
1	-3.995069	-0.957947	-6.778363
6	-4.389006	-0.092028	-4.847090
1	-4.246410	0.924323	-5.198044
6	-4.491816	2.565707	-3.066405
6	-5.420651	3.114857	-3.965143
1	-6.327042	2.569409	-4.212343
6	-5.192234	4.370907	-4.527888
1	-5.914128	4.791573	-5.222222
6	-4.039945	5.090236	-4.190505
1	-3.868907	6.072503	-4.622252
6	-3.115352	4.547354	-3.295679
1	-2.222806	5.106177	-3.027665
6	-3.337872	3.287812	-2.733611
1	-2.636787	2.871186	-2.018067
6	-5.903843	-1.728206	0.819084
6	-5.338711	-2.961397	0.453130
1	-4.267887	-3.117777	0.530870
6	-6.147964	-4.007963	0.006237
6	-7.526621	-3.849476	-0.104770
1	-8.150582	-4.668864	-0.441707
6	-8.087558	-2.621686	0.240923
6	-7.292062	-1.568266	0.690627
1	-7.773930	-0.629674	0.929115
6	-3.763388	-1.056926	2.671284
6	-2.636050	-0.308996	3.043079
1	-2.403537	0.610962	2.518671
6	-1.805824	-0.747083	4.072732
6	-2.057869	-1.953420	4.727743
1	-1.401971	-2.301615	5.517020
6	-3.174070	-2.698012	4.353289
6	-4.032897	-2.252456	3.344285
1	-4.904947	-2.846301	3.094511
29	-3.441533	0.389311	-0.476643
6	-3.442929	-4.032697	4.993580
6	-0.574691	0.041776	4.421619
6	-5.512433	-5.310821	-0.396109
6	-9.577955	-2.456271	0.103152
9	-9.952281	-2.346941	-1.194606
9	-10.039019	-1.361644	0.745449
9	-10.240207	-3.525602	0.602787
9	-4.999368	-5.245999	-1.652295
9	-4.495981	-5.642538	0.428165
9	-6.393231	-6.333670	-0.387911
9	-4.765457	-4.237515	5.188454
9	-3.003813	-5.050064	4.212155
9	-2.830776	-4.161256	6.190030
9	-0.262790	-0.043040	5.733331
9	-0.714445	1.354588	4.125262
9	0.516127	-0.402251	3.741355
6	-2.053133	-2.250536	-0.860792
6	-0.757264	-0.782787	0.428466
6	-1.289511	-3.339707	-0.476762
1	-2.871062	-2.357170	-1.563455
6	-0.029133	-1.900264	0.934877
6	-0.280150	-3.177586	0.478766
1	0.744695	-1.730795	1.673075
6	-0.264835	0.521343	0.738458
6	-0.910461	1.778108	0.469995
8	-2.037492	1.883813	-0.097140
7	-1.817135	-1.004201	-0.410820
1	0.547750	0.523283	1.448591
7	-0.243864	2.942370	0.797394
6	-0.945503	4.214628	0.661265
1	-1.405205	4.522147	1.611591
1	-0.234546	4.989540	0.357643
1	-1.728742	4.126063	-0.087247
6	0.892408	2.961566	1.716044
1	1.661660	2.245609	1.426488
1	1.345688	3.953535	1.694960
1	0.590790	2.744341	2.744820
1	0.295838	-4.022463	0.841445
35	-1.597199	-5.089668	-1.291352

---

9 P1-C2 *exo re-si*

Number of imaginary frequencies= 0
The smallest frequencies are= 5.5973 13.7396 15.8178 cm(-1)
Electronic energy= -7222.6463069
Zero-point correction= 1.758931
(Hartree/Particle)
Thermal correction to Energy= 1.876913
Thermal correction to Enthalpy= 1.877857
Thermal correction to Gibbs Free Energy= 1.598010
Sum of electronic and zero-point Energies= -7220.887376
Sum of electronic and thermal Energies= -7220.769394
Sum of electronic and thermal Enthalpies= -7220.768450
Sum of electronic and thermal Free Energies= -7221.048297

.....

Cartesian Coordinates

.....

77	4.127270	-0.436316	-1.492146
15	5.934451	0.283089	-0.262997
8	6.574711	-0.494770	1.067507
8	7.320159	0.414034	-1.198779
7	5.574352	1.772875	0.431295
6	7.433909	-1.575326	0.919210
6	6.942321	-2.834121	1.331236
1	5.941592	-2.886251	1.747045
6	7.730402	-3.949975	1.198352
1	7.365047	-4.922065	1.517159
6	9.021202	-3.854366	0.611540

6	9.812943	-5.013479	0.388753
1	9.419131	-5.977404	0.700527
6	11.044326	-4.922737	-0.219980
1	11.638143	-5.815670	-0.391932
6	11.530325	-3.661008	-0.638590
1	12.491495	-3.594648	-1.140271
6	10.794592	-2.515884	-0.422407
1	11.178949	-1.560460	-0.759360
6	9.525702	-2.568385	0.220134
6	8.726387	-1.392660	0.450786
6	9.237911	-0.021228	0.175780
6	10.430828	0.492646	0.795482
6	11.144210	-0.221023	1.799457
1	10.780694	-1.189435	2.122071
6	12.279164	0.305650	2.376985
1	12.800541	-0.256683	3.146432
6	12.768721	1.574141	1.983656
1	13.668297	1.973662	2.442760
6	12.091997	2.302249	1.031610
1	12.445576	3.285740	0.732930
6	10.909433	1.795539	0.426845
6	10.183632	2.566889	-0.521005
1	10.562968	3.543553	-0.808662
6	9.004139	2.098077	-1.044978
1	8.418678	2.678950	-1.749452
6	8.530013	0.822508	-0.665227
6	4.364374	2.389874	-0.173420
1	3.540523	2.258735	0.538805
6	4.524228	3.879921	-0.432242
6	3.390842	4.703659	-0.400203
1	2.427615	4.274745	-0.136375
6	3.482721	6.059990	-0.718777
1	2.592785	6.683216	-0.688530
6	4.716337	6.614757	-1.070003
1	4.792271	7.671006	-1.312219
6	5.851933	5.800439	-1.105652
1	6.816013	6.222936	-1.376062
6	5.755238	4.443002	-0.793340
1	6.637671	3.811062	-0.813335
6	4.001566	1.697581	-1.499738
1	4.682775	2.077177	-2.272664
1	3.005425	2.025193	-1.796085
6	5.936460	2.356788	1.759240
1	5.903962	3.436681	1.588769
6	4.883569	2.057814	2.826696
6	4.205713	3.117148	3.443862
1	4.421494	4.138278	3.138433
6	3.257403	2.879856	4.444341
1	2.744954	3.716938	4.910564
6	2.956682	1.571910	4.827710
1	2.200200	1.378604	5.582568
6	3.625516	0.507171	4.215932
1	3.395907	-0.514618	4.505804
6	4.585923	0.747376	3.231986
1	5.106571	-0.084100	2.772203
6	7.353391	2.068937	2.267331
1	8.099336	2.323493	1.512552
1	7.494075	1.032516	2.569635
1	7.527517	2.704920	3.141169
6	3.035720	-0.751934	0.373660
1	3.233828	-1.745074	0.777508
1	3.150436	0.035823	1.114756
6	2.059634	-0.579915	-0.658265
1	1.586015	-1.475516	-1.048861
6	1.115682	0.611617	-0.610984
1	1.683353	1.487640	-0.298314
6	5.092262	-0.333014	-3.455431
1	5.575985	0.635361	-3.570272
6	3.671842	-0.353768	-3.632944
1	3.193032	0.594216	-3.879068
6	2.896016	-1.562936	-4.133051
1	3.030045	-1.680622	-5.220031
1	1.835135	-1.354768	-3.976032
6	3.264661	-2.876821	-3.411146
1	4.033642	-3.418186	-3.971259
1	2.389861	-3.535833	-3.390193
6	3.750989	-2.674061	-1.977229
1	3.076165	-3.029895	-1.200998
6	5.092360	-2.545081	-1.623880
1	5.369688	-2.835291	-0.615762
6	6.248906	-2.474264	-2.606978
1	7.127756	-2.130352	-2.055388
1	6.483086	-3.487901	-2.966152
6	5.998166	-1.521995	-3.797988
1	5.570060	-2.074013	-4.641882
1	6.963043	-1.141664	-4.148371
6	0.473520	0.947838	-1.943332
6	-0.078293	-0.033017	-2.781212
6	0.453998	2.280116	-2.382297
6	-0.630601	0.306676	-4.017168
1	-0.070722	-1.071695	-2.475189
6	-0.074925	2.621883	-3.629322
1	0.869913	3.056465	-1.745161
6	-0.623741	1.635267	-4.449895
1	-1.063361	-0.466999	-4.644452
1	-0.069596	3.658557	-3.952051
1	-1.047746	1.897697	-5.414590
26	-6.479467	4.008003	1.490923
15	-4.505868	1.026240	-2.300025
15	-4.693422	-0.434886	1.233552
6	-5.956740	2.577324	0.053624
6	-5.433177	2.226975	1.353427
6	-4.566660	3.277885	1.776019
1	-4.033707	3.314108	2.715723
6	-4.569892	4.289783	0.771986
1	-4.044496	5.233909	0.818946
6	-5.428084	3.864449	-0.282939
1	-5.654396	4.419327	-1.180995
6	-8.243476	3.772956	2.562936
1	-8.686112	2.820163	2.821259
6	-7.283573	4.490393	3.340425
1	-6.867401	4.174203	4.287640
6	-6.936612	5.678208	2.627051
1	-6.206597	6.414356	2.936766
6	-7.683150	5.696677	1.409358
1	-7.617774	6.447943	0.633399
6	-8.490766	4.521267	1.369942
1	-9.146416	4.232916	0.559656
6	-6.820414	1.686884	-0.776314
6	-8.151847	1.465428	-0.392664
1	-8.526705	1.984647	0.480240
6	-8.984384	0.588320	-1.087565
1	-9.998422	0.414213	-0.742399
6	-8.498829	-0.070195	-2.214695
1	-9.135054	-0.751364	-2.771861
6	-7.178797	0.134414	-2.619455
1	-6.813822	-0.394654	-3.492500
6	-6.317538	0.982412	-1.905063
6	-5.727021	0.933897	2.057221
1	-6.752282	0.673668	1.796132
6	-5.633668	1.004609	3.583665
1	-5.867988	0.039029	4.040720
1	-4.641439	1.307515	3.927271
1	-6.352520	1.744787	3.947575
6	-4.301775	-0.043154	-3.782010
6	-4.361177	-1.435234	-3.593129
1	-4.609824	-1.837426	-2.616262
6	-4.130267	-2.309152	-4.654186
1	-4.195115	-3.379973	-4.490266
6	-3.816967	-1.801769	-5.919431
1	-3.624326	-2.479902	-6.745689
6	-3.755942	-0.421134	-6.116571
1	-3.515623	-0.020569	-7.097320
6	-4.001622	0.456300	-5.056553
1	-3.945702	1.525371	-5.227916
6	-4.197481	2.730743	-2.888443
6	-5.106651	3.409330	-3.715721
1	-6.007738	2.909010	-4.058986
6	-4.863860	4.733983	-4.079885
1	-5.570607	5.257791	-4.717114

6	-3.714994	5.387886	-3.619006
1	-3.532578	6.422177	-3.896800
6	-2.805738	4.712262	-2.802329
1	-1.913805	5.217672	-2.443211
6	-3.045423	3.386071	-2.436815
1	-2.355554	2.863327	-1.783268
6	-5.922905	-1.745715	0.800674
6	-5.504574	-2.753089	-0.079235
1	-4.461943	-2.829506	-0.349385
6	-6.421732	-3.634292	-0.651186
6	-7.779966	-3.533945	-0.356974
1	-8.500168	-4.188096	-0.835825
6	-8.196597	-2.554019	0.542706
6	-7.283730	-1.678801	1.129344
1	-7.660451	-0.932666	1.814587
6	-3.628199	-1.132511	2.553879
6	-2.631693	-0.275622	3.050927
1	-2.570540	0.744311	2.687959
6	-1.712604	-0.735583	3.988904
6	-1.737855	-2.063356	4.420940
1	-1.008288	-2.427182	5.136065
6	-2.712050	-2.916598	3.906649
6	-3.659585	-2.461036	2.985418
1	-4.408302	-3.147646	2.607000
29	-3.313077	0.294062	-0.521884
6	-2.682798	-4.374232	4.278214
6	-0.602297	0.165939	4.449476
6	-5.941920	-4.684111	-1.617350
6	-9.670195	-2.418568	0.820611
9	-10.373351	-2.307708	-0.332520
9	-9.958306	-1.331147	1.569562
9	-10.161556	-3.496922	1.471629
9	-4.826401	-4.279026	-2.278621
9	-5.625618	-5.842307	-0.994293
9	-6.873730	-4.977395	-2.547406
9	-3.896081	-4.954450	4.165147
9	-1.840983	-5.067537	3.466487
9	-2.250158	-4.567533	5.542221
9	-0.350523	0.046695	5.768877
9	-0.864308	1.469208	4.197893
9	0.565631	-0.126134	3.810558
6	-2.044939	-2.386417	-0.619059
6	-0.630919	-0.924952	0.495732
6	-1.569212	-3.467384	0.110314
1	-2.779057	-2.510643	-1.405775
6	-0.121426	-1.983534	1.264260
6	-0.608300	-3.273619	1.097847
1	0.649573	-1.786691	1.998700
6	0.074648	0.408491	0.585993
6	-0.801818	1.645420	0.729583
8	-1.991487	1.673994	0.347037
7	-1.622564	-1.129010	-0.394378
1	0.699074	0.339157	1.474463
7	-0.238071	2.770066	1.230218
6	-1.049706	3.986198	1.296969
1	-1.538673	4.075362	2.274688
1	-0.397782	4.851470	1.151776
1	-1.813830	3.964819	0.523943
6	1.001628	2.833075	2.006230
1	1.660997	1.996189	1.800219
1	1.536839	3.750433	1.755831
1	0.774994	2.842308	3.074783
1	-0.249304	-4.090866	1.711180
35	-2.295810	-5.242507	-0.222670

[8-9]‡-P1-C2 *endo si-re* conf2

Number of imaginary frequencies= 1
The smallest frequencies are= -267.9727 7.6782 11.0818 cm(-1)
Electronic energy= -7222.6289103
Zero-point correction= 1.754635
(Hartree/Particle)
Thermal correction to Energy= 1.873395
Thermal correction to Enthalpy= 1.874339
Thermal correction to Gibbs Free Energy= 1.590919
Sum of electronic and zero-point Energies= -7220.874275
Sum of electronic and thermal Energies= -7220.755515
Sum of electronic and thermal Enthalpies= -7220.754571
Sum of electronic and thermal Free Energies= -7221.037991

.....

Cartesian Coordinates

.....

26	8.164627	0.057258	-1.065056
15	3.103215	1.071739	-2.100875
15	4.188583	0.684021	1.495427
6	6.189305	0.736413	-1.267302
6	6.395438	0.096480	0.009527
6	6.803895	-1.250638	-0.237111
1	7.046643	-1.986448	0.517012
6	6.886909	-1.440226	-1.649618
1	7.207327	-2.342424	-2.150055
6	6.506085	-0.221142	-2.283619
1	6.484707	-0.035891	-3.347268
6	9.603795	1.270912	-0.185159
1	9.409258	1.994807	0.595273
6	9.926972	-0.107268	0.009603
1	10.010702	-0.613254	0.962148
6	10.076161	-0.711579	-1.275898
1	10.286432	-1.755699	-1.466962
6	9.844918	0.291956	-2.265243
1	9.852705	0.142690	-3.336881
6	9.556076	1.516207	-1.592551
1	9.310740	2.455236	-2.069711
6	5.687471	2.127783	-1.444822
6	6.520940	3.200170	-1.089263
1	7.509097	2.971867	-0.711177
6	6.106729	4.526498	-1.198552
1	6.767927	5.329763	-0.889183
6	4.838039	4.806492	-1.700072
1	4.498189	5.832040	-1.801561
6	3.986762	3.757676	-2.046174
1	2.996266	3.996837	-2.412938
6	4.373487	2.413945	-1.900997
6	6.080420	0.732436	1.335960
1	6.333268	1.791008	1.260490
6	6.845595	0.140099	2.522346
1	6.595096	0.662999	3.449630
1	6.628981	-0.921518	2.667768
1	7.920604	0.242918	2.344627
6	1.588256	2.028907	-2.520716
6	0.854192	2.565279	-1.451744
1	1.135358	2.319372	-0.434517
6	-0.224853	3.414332	-1.691563
1	-0.772275	3.834021	-0.857674
6	-0.609956	3.704561	-3.002644
1	-1.458429	4.357514	-3.186282
6	0.089245	3.140346	-4.072380
1	-0.212843	3.351726	-5.094226
6	1.190974	2.314111	-3.835221
1	1.740995	1.903498	-4.675341
6	3.509487	0.207207	-3.665494
6	4.242699	0.799502	-4.704237
1	4.621911	1.811291	-4.593517
6	4.494589	0.085449	-5.877629
1	5.067255	0.547452	-6.676739
6	4.010711	-1.218413	-6.025923
1	4.211234	-1.771012	-6.939299
6	3.270233	-1.809574	-4.998783
1	2.891297	-2.821777	-5.108627
6	3.024733	-1.099685	-3.822499
1	2.463757	-1.559055	-3.014833
6	3.628067	2.407084	1.823032
6	2.240256	2.573630	1.936669
1	1.598047	1.701166	1.877043
6	1.686858	3.846352	2.075416
6	2.496697	4.980207	2.070209
1	2.064452	5.970660	2.157203
6	3.876055	4.813822	1.934770
6	4.444576	3.544227	1.826131
1	5.518449	3.466908	1.725256

6	3.813247	-0.208535	3.060639
6	3.953177	-1.605412	3.026630
1	4.319934	-2.091735	2.130204
6	3.596890	-2.375974	4.129803
6	3.066368	-1.780576	5.275698
1	2.771185	-2.384507	6.125832
6	2.916692	-0.396811	5.303276
6	3.295856	0.390940	4.212801
1	3.170008	1.465730	4.269138
29	2.914389	-0.222419	-0.250930
6	2.249939	0.256051	6.481960
6	3.672285	-3.875360	4.060073
6	0.197558	3.963067	2.247629
6	4.738377	6.045317	1.864166
9	4.463300	6.776960	0.756422
9	6.057682	5.755554	1.830887
9	4.530439	6.861124	2.923739
9	-0.470335	3.133043	1.394911
9	-0.198654	3.612299	3.492956
9	-0.259078	5.210987	2.013743
9	2.716304	1.503103	6.706278
9	0.908081	0.375665	6.278115
9	2.405996	-0.451977	7.619593
9	4.076246	-4.416492	5.229632
9	4.514138	-4.305467	3.097178
9	2.452208	-4.416622	3.787833
6	0.794431	-1.230090	1.704803
6	1.032434	-2.604850	1.318073
6	2.160810	-3.099280	0.581783
1	0.578073	-3.361320	1.941823
77	-3.150248	-1.209094	-1.279168
15	-4.969673	-0.206197	-0.363083
8	-4.906103	1.091553	0.671777
8	-5.977806	0.396016	-1.542326
7	-5.781249	-1.285238	0.636034
6	-4.737106	2.390790	0.215375
6	-3.534557	3.030063	0.588299
1	-2.825818	2.487869	1.203111
6	-3.295559	4.317217	0.177371
1	-2.390918	4.830795	0.487255
6	-4.215290	4.980298	-0.678977
6	-3.925776	6.268675	-1.204750
1	-2.995146	6.748843	-0.913348
6	-4.793704	6.888768	-2.075136
1	-4.559551	7.869942	-2.477539
6	-5.990066	6.236662	-2.457820
1	-6.662314	6.717237	-3.162781
6	-6.309535	4.995453	-1.950757
1	-7.225643	4.508827	-2.263904
6	-5.445243	4.330559	-1.036623
6	-5.742922	3.027629	-0.496323
6	-7.065426	2.369024	-0.700156
6	-8.303484	3.008170	-0.332868
6	-8.351307	4.234255	0.388649
1	-7.425616	4.710223	0.689592
6	-9.554354	4.816360	0.724215
1	-9.562232	5.747676	1.283257
6	-10.779386	4.210049	0.356587
1	-11.719380	4.683912	0.623714
6	-10.772150	3.013970	-0.324112
1	-11.704305	2.526230	-0.597187
6	-9.549171	2.379077	-0.674232
6	-9.542772	1.120606	-1.334249
1	-10.489076	0.657902	-1.599548
6	-8.358714	0.473582	-1.587626
1	-8.328875	-0.509454	-2.045150
6	-7.139114	1.094955	-1.242775
6	-5.288977	-2.680555	0.489171
1	-4.625244	-2.904366	1.333081
6	-6.406358	-3.709268	0.471281
6	-6.247922	-4.922587	1.148004
1	-5.344924	-5.096874	1.729607
6	-7.245138	-5.900790	1.098804
1	-7.112177	-6.835860	1.636321
6	-8.414162	-5.670503	0.371596
1	-9.197211	-6.423017	0.342538
6	-8.574169	-4.462231	-0.316409
1	-9.485282	-4.271920	-0.877004
6	-7.573663	-3.493785	-0.273904
1	-7.708082	-2.543396	-0.781634
6	-4.481752	-2.823384	-0.818203
1	-5.189316	-2.934270	-1.648145
1	-3.915436	-3.757515	-0.765689
6	-6.412671	-0.852692	1.931326
1	-6.571832	0.218423	1.817575
6	-7.794520	-1.452908	2.161222
6	-8.903473	-0.808050	1.600233
1	-8.755903	0.106445	1.037050
6	-10.190381	-1.325304	1.751519
1	-11.034508	-0.809937	1.300956
6	-10.388724	-2.496572	2.486437
1	-11.387626	-2.907417	2.604529
6	-9.293547	-3.130036	3.079569
1	-9.437447	-4.037735	3.658924
6	-8.008772	-2.606538	2.925138
1	-7.170992	-3.119755	3.383866
6	-5.452989	-1.041281	3.112248
1	-4.539112	-0.465571	2.943836
1	-5.178459	-2.087017	3.273580
1	-5.923841	-0.676867	4.030315
6	-2.211349	-0.949093	0.664911
1	-1.486568	-0.142814	0.610226
1	-2.877946	-0.874836	1.519657
6	-1.803542	-2.266255	0.277710
1	-2.370507	-3.095565	0.687714
6	-0.583919	-2.588666	-0.374943
1	-0.002701	-1.773371	-0.784455
6	-4.003435	-1.173992	-3.334234
1	-5.026108	-1.534114	-3.259055
6	-2.980269	-2.154369	-3.305783
1	-3.288377	-3.196737	-3.231164
6	-1.603539	-1.956038	-3.915390
1	-1.666414	-2.055688	-5.010388
1	-0.973590	-2.778802	-3.572018
6	-0.928652	-0.614885	-3.549963
1	-1.105923	0.131550	-4.330499
1	0.155780	-0.759474	-3.523157
6	-1.364575	-0.027204	-2.208830
1	-0.591475	0.027085	-1.448133
6	-2.424440	0.861223	-2.055503
1	-2.387926	1.519427	-1.193202
6	-3.353834	1.313672	-3.163631
1	-4.210623	1.806001	-2.699853
1	-2.839314	2.074057	-3.767211
6	-3.858263	0.164662	-4.061951
1	-3.188775	0.032729	-4.918127
1	-4.831859	0.444521	-4.475569
6	-0.332417	-3.902849	-0.976818
6	-0.980416	-5.079744	-0.554989
6	0.609486	-3.999896	-2.018315
6	-0.707569	-6.300270	-1.170134
1	-1.695585	-5.045282	0.260748
6	0.878579	-5.218901	-2.637400
1	1.132495	-3.104430	-2.336763
6	0.218407	-6.375738	-2.216531
1	-1.218099	-7.197441	-0.831647
1	1.606273	-5.266146	-3.442538
1	0.425975	-7.328863	-2.694156
6	2.439914	-4.491991	0.654309
6	3.434671	-5.063463	-0.110404
1	1.853719	-5.109753	1.323792
6	4.162758	-4.222890	-0.957634
6	3.892060	-2.868232	-0.985269
1	4.447336	-2.195952	-1.625001
7	2.921474	-2.308020	-0.233194
8	1.106842	-0.239353	0.971772
7	0.110066	-0.996949	2.865573
6	-0.376830	0.341672	3.180703
1	-1.377473	0.267450	3.618817
1	0.277053	0.842017	3.902282

1	-0.435635	0.940033	2.277296
6	-0.169849	-2.010177	3.880411
1	-1.149658	-2.480153	3.723726
1	0.599318	-2.780768	3.897645
1	-0.170951	-1.524820	4.859250
1	3.634474	-6.128068	-0.059188
35	5.540006	-4.964556	-2.134005

[8-9]‡-P1-C2 *endo re-re* conf2

Number of imaginary frequencies= 1
The smallest frequencies are=-266.9227 14.6030 16.4956cm(-1)
Electronic energy= -7222.6225041
Zero-point correction= 1.755305
(Hartree/Particle)
Thermal correction to Energy= 1.873789
Thermal correction to Enthalpy= 1.874733
Thermal correction to Gibbs Free Energy= 1.596155
Sum of electronic and zero-point Energies= -7220.867200
Sum of electronic and thermal Energies= -7220.748715
Sum of electronic and thermal Enthalpies= -7220.747771
Sum of electronic and thermal Free Energies= -7221.026349

.....

Cartesian Coordinates

.....

26	7.587737	-2.030120	-1.503578
15	2.982145	0.290134	-2.301438
15	4.408503	0.363313	1.158495
6	5.910194	-0.797811	-1.737637
6	6.045487	-1.241406	-0.371125
6	5.984273	-2.666595	-0.366827
1	6.061588	-3.298816	0.506460
6	5.847183	-3.111998	-1.714095
1	5.816015	-4.141703	-2.043405
6	5.805672	-1.965233	-2.558266
1	5.719254	-1.966488	-3.634902
6	9.411110	-1.164151	-1.007964
1	9.524467	-0.257497	-0.428184
6	9.332159	-2.490786	-0.483910
1	9.370071	-2.765494	0.561692
6	9.150577	-3.388404	-1.579896
1	9.020587	-4.460268	-1.508050
6	9.116668	-2.617626	-2.781714
1	8.958973	-3.002187	-3.780748
6	9.278997	-1.244724	-2.429334
1	9.270492	-0.411021	-3.118186
6	5.813259	0.628040	-2.160974
6	6.966849	1.425874	-2.171613
1	7.906619	0.967310	-1.892626
6	6.926067	2.776475	-2.516030
1	7.833657	3.370536	-2.489856
6	5.711640	3.356397	-2.874325
1	5.660840	4.406631	-3.143498
6	4.548595	2.585868	-2.864101
1	3.610231	3.056927	-3.132745
6	4.570425	1.231128	-2.495048
6	6.147653	-0.315184	0.808645
1	6.710589	0.554532	0.470750
6	6.880430	-0.900879	2.019068
1	6.922259	-0.181175	2.841372
1	6.407743	-1.812402	2.392121
1	7.903848	-1.152778	1.725778
6	1.696044	1.506233	-2.806632
6	1.308245	2.452313	-1.842264
1	1.780838	2.450113	-0.865178
6	0.340765	3.411024	-2.134609
1	0.063706	4.138879	-1.384071
6	-0.272839	3.426692	-3.389954
1	-1.040171	4.163886	-3.607896
6	0.102141	2.488160	-4.352854
1	-0.369765	2.492138	-5.331237
6	1.084434	1.535572	-4.067389
1	1.358886	0.813545	-4.827830
6	3.024373	-0.958034	-3.641947
6	3.483239	-0.670641	-4.936489
1	3.835003	0.327737	-5.180319
6	3.500509	-1.672787	-5.908177
1	3.855396	-1.447454	-6.909791
6	3.064349	-2.964904	-5.593817
1	3.079468	-3.741132	-6.353684
6	2.621482	-3.258475	-4.301722
1	2.294495	-4.263382	-4.049774
6	2.609322	-2.259187	-3.327461
1	2.323342	-2.483730	-2.305137
6	4.586523	2.202559	1.171447
6	3.406763	2.947169	1.308168
1	2.486690	2.444570	1.568588
6	3.392252	4.323874	1.083888
6	4.559426	4.998675	0.735291
1	4.544650	6.063574	0.531420
6	5.743208	4.268481	0.633010
6	5.765116	2.891021	0.849402
1	6.707336	2.373713	0.735995
6	3.984023	-0.127869	2.874739
6	3.800150	-1.506259	3.073924
1	3.981371	-2.198174	2.259017
6	3.351382	-1.985637	4.299730
6	3.023056	-1.105273	5.331860
1	2.644004	-1.478063	6.277408
6	3.175939	0.263913	5.120270
6	3.668938	0.757962	3.909861
1	3.786002	1.827315	3.780416
29	2.671094	-0.489416	-0.185857
6	2.712818	1.206199	6.197233
6	3.121335	-3.457736	4.496390
6	2.092172	5.070769	1.207198
6	6.996213	5.003425	0.237303
9	6.842756	5.633724	-0.952664
9	8.065468	4.186331	0.121469
9	7.316338	5.959702	1.139242
9	1.048641	4.307505	0.774004
9	1.814905	5.412257	2.484499
9	2.076139	6.203968	0.477696
9	3.100815	2.479518	5.975162
9	1.357473	1.211062	6.283723
9	3.174111	0.845838	7.416237
9	3.629667	-3.895178	5.668971
9	3.670476	-4.201419	3.510756
9	1.793668	-3.755215	4.519455
6	0.655877	0.743710	1.630039
6	0.638721	-1.572463	1.927870
6	0.065667	0.958541	2.864419
1	0.869166	1.568309	0.961855
6	-0.020897	-1.391874	3.172509
6	-0.281009	-0.129956	3.668636
6	0.830053	-2.923155	1.463339
6	1.981571	-3.354441	0.703627
8	2.674443	-2.568196	-0.014418
7	0.983157	-0.482844	1.177981
1	0.396854	-3.657551	2.127216
77	-3.249702	-1.353953	-1.191222
15	-4.980383	-0.111354	-0.400278
8	-4.786750	1.132620	0.694008
8	-5.791872	0.691865	-1.604590
7	-6.025333	-1.086679	0.486867
6	-4.165387	2.307615	0.299515
6	-2.885259	2.561738	0.839178
1	-2.460850	1.840555	1.528158
6	-2.218962	3.709108	0.488588
1	-1.248093	3.929903	0.915264
6	-2.775601	4.600843	-0.467735
6	-2.052354	5.743244	-0.908393
1	-1.083531	5.947966	-0.459549
6	-2.558960	6.563232	-1.891720
1	-1.995281	7.428200	-2.228564
6	-3.815955	6.269698	-2.473442
1	-4.201616	6.903069	-3.267098
6	-4.557010	5.190135	-2.042460
1	-5.517664	4.981791	-2.498886
6	-4.074030	4.330988	-1.016403

6	-4.821494	3.193713	-0.539746
6	-6.247008	2.965437	-0.908242
6	-7.249032	3.982496	-0.696563
6	-6.982310	5.187734	0.012310
1	-5.996154	5.353524	0.428541
6	-7.962015	6.139720	0.195545
1	-7.731517	7.045817	0.748646
6	-9.265030	5.946545	-0.321017
1	-10.024430	6.709253	-0.175741
6	-9.566726	4.782288	-0.990153
1	-10.568243	4.607887	-1.374807
6	-8.584255	3.773004	-1.180717
6	-8.909765	2.551198	-1.827940
1	-9.914821	2.408384	-2.214461
6	-7.976183	1.551583	-1.935139
1	-8.207728	0.599236	-2.400263
6	-6.669172	1.753820	-1.437371
6	-5.503862	-2.482518	0.608196
1	-4.826803	-2.526032	1.471196
6	-6.594349	-3.515506	0.822127
6	-6.500817	-4.410780	1.892276
1	-5.669207	-4.324837	2.588272
6	-7.469792	-5.400752	2.082399
1	-7.386643	-6.085136	2.922383
6	-8.546678	-5.499720	1.200720
1	-9.308449	-6.259650	1.350951
6	-8.643363	-4.611633	0.122885
1	-9.484150	-4.677443	-0.561974
6	-7.670748	-3.633504	-0.068620
1	-7.762044	-2.929414	-0.889730
6	-4.701377	-2.822897	-0.653531
1	-5.400111	-2.951205	-1.488719
1	-4.204870	-3.785707	-0.504651
6	-6.838547	-0.514542	1.613808
1	-6.918846	0.551492	1.391314
6	-8.271917	-1.044484	1.628640
6	-9.136787	-0.659239	0.596078
1	-8.769013	0.004679	-0.177798
6	-10.453131	-1.114706	0.548968
1	-11.103648	-0.803250	-0.264173
6	-10.934077	-1.964616	1.549127
1	-11.957839	-2.326918	1.516299
6	-10.088629	-2.337583	2.595309
1	-10.450863	-2.995556	3.380435
6	-8.770401	-1.875485	2.638058
1	-8.131015	-2.190353	3.454715
6	-6.105061	-0.643980	2.952757
1	-5.121362	-0.174050	2.880776
1	-5.971500	-1.686373	3.253771
1	-6.671785	-0.137031	3.739421
6	-2.318315	-1.070200	0.755855
1	-1.559398	-0.299935	0.679539
1	-3.003253	-0.913907	1.585731
6	-1.998348	-2.432440	0.445753
1	-2.635957	-3.175261	0.912855
6	-0.817255	-2.930609	-0.174793
1	-0.168654	-2.225006	-0.676007
6	-4.022496	-1.428697	-3.273842
1	-5.069154	-1.720004	-3.222733
6	-3.074783	-2.474430	-3.115846
1	-3.468441	-3.480273	-2.970482
6	-1.662516	-2.437511	-3.672419
1	-1.680858	-2.665149	-4.749895
1	-1.101479	-3.246424	-3.199723
6	-0.923776	-1.105375	-3.433387
1	-1.067264	-0.431602	-4.282261
1	0.150876	-1.297224	-3.390687
6	-1.332603	-0.373143	-2.159149
1	-0.588904	-0.340278	-1.367119
6	-2.317779	0.603716	-2.123063
1	-2.263352	1.332004	-1.320746
6	-3.167382	1.014023	-3.309561
1	-3.978624	1.641595	-2.937885
1	-2.558247	1.645894	-3.969469
6	-3.763633	-0.168918	-4.105441
1	-3.109604	-0.426838	-4.945559
1	-4.711027	0.153960	-4.547676
6	-0.732928	-4.322475	-0.646696
6	-1.632388	-5.328497	-0.237527
6	0.281065	-4.677026	-1.556531
6	-1.516381	-6.630094	-0.720953
1	-2.426262	-5.100209	0.464569
6	0.398245	-5.978573	-2.040027
1	0.980711	-3.918388	-1.884172
6	-0.499392	-6.963978	-1.622039
1	-2.221314	-7.388102	-0.391630
1	1.190821	-6.222555	-2.741667
1	-0.411355	-7.980124	-1.995193
7	2.319757	-4.676802	0.726304
6	3.368129	-5.177616	-0.152904
1	4.255889	-5.464131	0.425316
1	3.004638	-6.058515	-0.692500
1	3.645772	-4.403945	-0.863112
6	1.663159	-5.672476	1.570751
1	0.686093	-5.961851	1.171121
1	2.297112	-6.560357	1.606387
1	1.545581	-5.312153	2.593206
1	-0.731780	0.007933	4.644936
1	-0.271878	-2.266163	3.762167
35	-0.201993	2.776895	3.513522

[8-9]‡-P1-C2 *exo si-si* conf2

Number of imaginary frequencies= 1
The smallest frequencies are= -137.3513 7.2662 8.6309 cm(-1)
Electronic energy= -7222.6278115
Zero-point correction= 1.754809
(Hartree/Particle)
Thermal correction to Energy= 1.873359
Thermal correction to Enthalpy= 1.874303
Thermal correction to Gibbs Free Energy= 1.591806
Sum of electronic and zero-point Energies= -7220.873003
Sum of electronic and thermal Energies= -7220.754453
Sum of electronic and thermal Enthalpies= -7220.753509
Sum of electronic and thermal Free Energies= -7221.036005

.....

Cartesian Coordinates

.....

26	8.123816	0.204442	-0.683955
15	3.132810	1.198662	-1.972731
15	4.000928	0.629832	1.659858
6	6.156735	0.873616	-0.966352
6	6.291601	0.146301	0.273613
6	6.735765	-1.174944	-0.041473
1	6.940851	-1.960815	0.672408
6	6.909649	-1.263471	-1.455759
1	7.271915	-2.125593	-1.997291
6	6.552780	-0.006101	-2.024642
1	6.595303	0.253525	-3.071855
6	9.466962	1.393982	0.361338
1	9.192959	2.071497	1.159293
6	9.802185	0.013380	0.513001
1	9.819586	-0.539353	1.442767
6	10.059706	-0.523777	-0.785284
1	10.303390	-1.553912	-1.009533
6	9.883634	0.523902	-1.739685
1	9.973178	0.428006	-2.813733
6	9.519567	1.708256	-1.032429
1	9.289825	2.665246	-1.480752
6	5.636403	2.266411	-1.076911
6	6.429857	3.327957	-0.614881
1	7.410048	3.096796	-0.218372
6	5.987407	4.649693	-0.645587
1	6.618355	5.442517	-0.256671
6	4.728644	4.937369	-1.166654
1	4.365751	5.959468	-1.200870
6	3.917556	3.898767	-1.623591
1	2.935155	4.142773	-2.009012
6	4.336169	2.558577	-1.570047
6	5.896694	0.683226	1.622907

1	6.155978	1.743103	1.643536
6	6.590079	-0.005930	2.801370
1	6.291556	0.445426	3.751619
1	6.357761	-1.073461	2.848293
1	7.674059	0.098261	2.691776
6	1.621021	2.143083	-2.443718
6	0.769851	2.550895	-1.402421
1	0.958775	2.208899	-0.391093
6	-0.304121	3.402474	-1.661729
1	-0.942332	3.724083	-0.849313
6	-0.567222	3.823139	-2.967586
1	-1.412709	4.475377	-3.167053
6	0.246194	3.385331	-4.014498
1	0.038502	3.695760	-5.034483
6	1.341372	2.556771	-3.754943
1	1.981961	2.249277	-4.574726
6	3.732023	0.499314	-3.560843
6	4.464915	1.253884	-4.490384
1	4.701303	2.293063	-4.281400
6	4.905683	0.666850	-5.677663
1	5.474969	1.255919	-6.391067
6	4.620403	-0.675906	-5.946365
1	4.972158	-1.131973	-6.867301
6	3.886058	-1.430036	-5.027974
1	3.668577	-2.475109	-5.228772
6	3.443306	-0.843657	-3.840690
1	2.886366	-1.431735	-3.120347
6	3.415880	2.330178	2.055388
6	2.023206	2.495491	2.067662
1	1.387575	1.629686	1.911685
6	1.460151	3.760108	2.235633
6	2.265560	4.889999	2.361761
1	1.826439	5.875919	2.466776
6	3.651380	4.724869	2.334540
6	4.228110	3.461492	2.199776
1	5.306873	3.386915	2.186304
6	3.510529	-0.363082	3.129093
6	3.637443	-1.755559	3.002582
1	4.068762	-2.180401	2.103742
6	3.176955	-2.599786	4.008644
6	2.557702	-2.081335	5.147177
1	2.181739	-2.741959	5.920170
6	2.419954	-0.700448	5.265042
6	2.900642	0.159323	4.273764
1	2.780079	1.228842	4.399057
29	2.839669	-0.191748	-0.212912
6	1.651498	-0.137346	6.427632
6	3.240867	-4.091124	3.829625
6	-0.037633	3.866968	2.295731
6	4.515686	5.952941	2.424772
9	4.284020	6.798037	1.390016
9	5.835279	5.662441	2.413470
9	4.267249	6.655281	3.554832
9	-0.627740	3.065491	1.360624
9	-0.527579	3.462704	3.490621
9	-0.486137	5.118578	2.075401
9	2.008727	1.132572	6.713329
9	0.315331	-0.115704	6.164066
9	1.809306	-0.870987	7.549838
9	3.569313	-4.723409	4.977460
9	4.135009	-4.459054	2.888356
9	2.035589	-4.596987	3.446103
6	0.597146	-1.310859	1.558994
6	0.840214	-2.647740	1.083441
6	1.978550	-3.108201	0.349186
1	0.324523	-3.444471	1.600192
77	-3.154510	-0.810413	-1.893736
15	-4.874625	-0.232858	-0.533667
8	-4.808645	1.011541	0.566522
8	-6.215701	0.219663	-1.404793
7	-5.231873	-1.484887	0.534976
6	-4.834384	2.332076	0.143947
6	-3.650123	3.074387	0.337131
1	-2.810203	2.588381	0.815615
6	-3.598397	4.385009	-0.066113
1	-2.704424	4.976359	0.111510
6	-4.705298	4.972065	-0.738197
6	-4.629997	6.292293	-1.258589
1	-3.710568	6.853565	-1.113002
6	-5.688789	6.845021	-1.943290
1	-5.617823	7.852751	-2.341933
6	-6.869770	6.090427	-2.140183
1	-7.695009	6.520200	-2.700609
6	-6.982623	4.814012	-1.632311
1	-7.892140	4.248524	-1.798618
6	-5.916363	4.216566	-0.904321
6	-5.999614	2.882091	-0.365447
6	-7.272408	2.106585	-0.332079
6	-8.464171	2.635660	0.284542
6	-8.474041	3.855788	1.017436
1	-7.552102	4.411654	1.137341
6	-9.631994	4.333009	1.592500
1	-9.608174	5.262765	2.153694
6	-10.848791	3.621437	1.467576
1	-11.754661	4.013637	1.920344
6	-10.872265	2.425062	0.787752
1	-11.793853	1.855363	0.701672
6	-9.692385	1.896292	0.197031
6	-9.706340	0.635447	-0.457560
1	-10.642182	0.088971	-0.533008
6	-8.545759	0.096264	-0.953946
1	-8.522835	-0.882238	-1.421599
6	-7.339458	0.824287	-0.857885
6	-4.400367	-2.691751	0.281392
1	-3.515882	-2.649081	0.929544
6	-5.113073	-4.002842	0.558404
6	-4.455682	-5.008262	1.274582
1	-3.465111	-4.815265	1.681826
6	-5.065919	-6.247769	1.488149
1	-4.545851	-7.017068	2.052634
6	-6.345979	-6.489785	0.987844
1	-6.829544	-7.446836	1.162316
6	-7.006713	-5.490350	0.263942
1	-8.006956	-5.669006	-0.120718
6	-6.390460	-4.260799	0.042986
1	-6.911501	-3.476974	-0.498102
6	-3.937165	-2.681535	-1.180723
1	-4.794666	-2.948261	-1.809519
1	-3.197460	-3.471797	-1.318506
6	-5.700346	-1.204214	1.936245
1	-6.162596	-0.218115	1.886488
6	-6.802940	-2.156882	2.388866
6	-8.101863	-1.950034	1.906875
1	-8.291759	-1.115806	1.240055
6	-9.146449	-2.802569	2.262131
1	-10.144962	-2.624941	1.871402
6	-8.907720	-3.877998	3.122068
1	-9.716166	-4.548819	3.399247
6	-7.622496	-4.078556	3.629706
1	-7.425944	-4.908962	4.302166
6	-6.580453	-3.220075	3.271500
1	-5.588310	-3.404061	3.668035
6	-4.517737	-1.101550	2.906447
1	-3.825470	-0.331141	2.559695
1	-3.968153	-2.041920	3.001299
1	-4.875232	-0.824122	3.902667
6	-1.893456	-0.285120	-0.200779
1	-1.666373	0.777359	-0.166937
1	-2.242174	-0.672986	0.754081
6	-1.006502	-1.118792	-0.963638
1	-0.284026	-0.647084	-1.616820
6	-0.870825	-2.499055	-0.722476
1	-1.539057	-2.932239	0.011057
6	-4.420274	-1.061213	-3.710464
1	-5.288135	-1.650420	-3.425474
6	-3.212391	-1.779691	-3.897265
1	-3.256700	-2.859764	-3.758216
6	-2.048120	-1.327633	-4.762364
1	-2.251572	-1.561522	-5.819029
1	-1.179007	-1.928879	-4.477630

6	-1.696782	0.166303	-4.609404
1	-2.253419	0.767157	-5.335253
1	-0.637998	0.312095	-4.845477
6	-1.949544	0.721380	-3.210431
1	-1.060652	0.960597	-2.638791
6	-3.119953	1.354705	-2.815977
1	-3.048752	2.046134	-1.982022
6	-4.351512	1.521064	-3.682056
1	-5.174005	1.839460	-3.038707
1	-4.174833	2.341378	-4.393740
6	-4.766645	0.239797	-4.439011
1	-4.311872	0.221647	-5.434557
1	-5.848390	0.267208	-4.601119
6	-0.262590	-3.443811	-1.647603
6	0.595368	-3.035893	-2.688415
6	-0.544718	-4.816480	-1.510407
6	1.149540	-3.969463	-3.558087
1	0.825271	-1.984745	-2.814551
6	0.000759	-5.750143	-2.391592
1	-1.199533	-5.144507	-0.706889
6	0.852754	-5.330741	-3.416286
1	1.810703	-3.635362	-4.352194
1	-0.234497	-6.804089	-2.274940
1	1.282619	-6.056217	-4.100798
6	2.182287	-4.515468	0.264062
6	3.216321	-5.049725	-0.473927
1	1.507133	-5.174107	0.797206
6	4.072210	-4.156973	-1.126233
6	3.866898	-2.796386	-1.009951
1	4.521441	-2.087579	-1.498400
7	2.845987	-2.273465	-0.300631
8	1.038171	-0.269573	0.983245
7	-0.230440	-1.149008	2.642719
6	-0.668969	0.189251	3.023564
1	-1.672590	0.128868	3.453596
1	-0.002984	0.636568	3.769730
1	-0.704499	0.830184	2.147772
6	-0.617923	-2.233345	3.541005
1	-1.546279	-2.725152	3.219717
1	0.170331	-2.982217	3.620689
1	-0.777032	-1.818596	4.538575
1	3.356666	-6.122895	-0.542105
35	5.555314	-4.822259	-2.217582

[8-9]‡-P1-C2 *exo re-si* conf2

Number of imaginary frequencies= 1
The smallest frequencies are= -133.9785 4.3747 7.6585 cm(-1)
Electronic energy= -7222.6089123
Zero-point correction= 1.754200
(Hartree/Particle)
Thermal correction to Energy= 1.873225
Thermal correction to Enthalpy= 1.874170
Thermal correction to Gibbs Free Energy= 1.588051
Sum of electronic and zero-point Energies= -7220.854713
Sum of electronic and thermal Energies= -7220.735687
Sum of electronic and thermal Enthalpies= -7220.734743
Sum of electronic and thermal Free Energies= -7221.020862

.....

Cartesian Coordinates

.....

77	-4.163394	-0.905691	1.466574
15	-5.888732	-0.077176	0.255889
8	-6.427972	-0.741237	-1.163095
8	-7.297192	-0.051063	1.141311
7	-5.526030	1.472669	-0.289678
6	-7.373590	-1.759853	-1.201906
6	-6.930404	-3.001340	-1.708319
1	-5.902321	-3.086230	-2.044108
6	-7.803080	-4.058401	-1.773576
1	-7.477209	-5.015994	-2.169464
6	-9.135200	-3.923533	-1.298271
6	-10.023451	-5.033099	-1.288988
1	-9.668713	-5.983292	-1.679548
6	-11.298091	-4.914661	-0.783544
1	-11.967334	-5.769982	-0.776304
6	-11.731230	-3.675381	-0.255291
1	-12.728349	-3.589994	0.167011
6	-10.900216	-2.575970	-0.264725
1	-11.249247	-1.640940	0.156110
6	-9.584273	-2.653321	-0.801413
6	-8.686878	-1.524912	-0.823998
6	-9.131060	-0.165153	-0.405705
6	-10.259841	0.499136	-1.003412
6	-10.915591	0.001273	-2.163882
1	-10.555157	-0.910042	-2.626731
6	-11.987146	0.669155	-2.715540
1	-12.464602	0.274149	-3.607647
6	-12.468408	1.868040	-2.136575
1	-13.316937	2.380022	-2.580770
6	-11.849689	2.386489	-1.021775
1	-12.197906	3.314493	-0.575657
6	-10.732372	1.731089	-0.435400
6	-10.060291	2.289718	0.685321
1	-10.435007	3.211361	1.120941
6	-8.922668	1.701285	1.180411
1	-8.369978	2.130370	2.008630
6	-8.456944	0.499467	0.606157
6	-4.345464	2.037661	0.409395
1	-3.475895	1.937405	-0.248412
6	-4.479223	3.501004	0.794688
6	-3.349177	4.325700	0.743645
1	-2.408198	3.923255	0.376287
6	-3.421402	5.659652	1.152933
1	-2.537528	6.289938	1.099395
6	-4.629058	6.182399	1.619946
1	-4.692686	7.222365	1.927488
6	-5.758075	5.358610	1.686749
1	-6.703280	5.759160	2.042741
6	-5.680374	4.026139	1.285875
1	-6.561794	3.395180	1.308350
6	-4.090902	1.230695	1.694764
1	-4.846156	1.521440	2.435655
1	-3.129220	1.533692	2.111887
6	-5.851346	1.915907	-1.689169
1	-6.709416	1.311991	-1.980335
6	-6.320023	3.363303	-1.753660
6	-7.675308	3.635094	-1.531301
1	-8.355308	2.811640	-1.343467
6	-8.157419	4.943962	-1.539939
1	-9.212871	5.130450	-1.360139
6	-7.283810	6.006417	-1.785454
1	-7.651586	7.028748	-1.788952
6	-5.934698	5.744749	-2.038152
1	-5.248907	6.563868	-2.235720
6	-5.459112	4.432178	-2.030150
1	-4.406439	4.249913	-2.217050
6	-4.716799	1.588847	-2.667699
1	-4.525778	0.512819	-2.668453
1	-3.784830	2.105667	-2.426314
1	-5.006847	1.887374	-3.679864
6	-3.037761	-1.080624	-0.376645
1	-3.250356	-2.010803	-0.903345
1	-3.087164	-0.209065	-1.026858
6	-1.984389	-1.105518	0.609651
1	-1.588149	-2.058477	0.936665
6	-1.304706	0.055352	1.014936
1	-1.665432	0.999067	0.627751
6	-5.355750	-1.009332	3.368924
1	-5.874425	-0.059149	3.466968
6	-3.980141	-1.004088	3.690594
1	-3.560276	-0.059059	4.035427
6	-3.157283	-2.218362	4.088608
1	-3.287247	-2.422849	5.162474
1	-2.103019	-1.955203	3.952852
6	-3.466178	-3.489944	3.270072
1	-4.279888	-4.054185	3.734456
1	-2.590283	-4.146401	3.293166
6	-3.819448	-3.212938	1.811765
1	-3.066339	-3.501265	1.083016

6	-5.110879	-3.051851	1.328960
1	-5.266572	-3.239446	0.270670
6	-6.370373	-3.061186	2.171244
1	-7.185337	-2.666713	1.560383
1	-6.633552	-4.103002	2.405119
6	-6.266219	-2.234389	3.472491
1	-5.920150	-2.865608	4.296711
1	-7.269243	-1.896164	3.748739
6	-0.423209	0.153847	2.164323
6	0.190956	-0.969778	2.757292
6	-0.198213	1.423973	2.733367
6	0.990330	-0.824057	3.887410
1	0.051263	-1.953761	2.324037
6	0.578047	1.562088	3.881018
1	-0.649202	2.297584	2.271117
6	1.177606	0.439613	4.458778
1	1.474135	-1.692758	4.324302
1	0.733247	2.544433	4.314785
1	1.798768	0.546885	5.341817
26	6.182655	4.443637	-1.331342
15	4.813475	0.900663	2.229912
15	4.756076	-0.116499	-1.412197
6	5.924551	2.827050	-0.026656
6	5.288438	2.580247	-1.300279
6	4.306299	3.595846	-1.500767
1	3.667186	3.693252	-2.367563
6	4.348928	4.486628	-0.389097
1	3.752940	5.380879	-0.267624
6	5.347345	4.020444	0.513389
1	5.632775	4.486764	1.444599
6	7.804480	4.453376	-2.625421
1	8.258833	3.566263	-3.046045
6	6.716421	5.187950	-3.189295
1	6.197197	4.951456	-4.108485
6	6.401779	6.262154	-2.302183
1	5.601844	6.979220	-2.431923
6	7.296340	6.194415	-1.191038
1	7.293580	6.849928	-0.330173
6	8.164057	5.080245	-1.391604
1	8.937161	4.753802	-0.709786
6	6.926451	1.926641	0.615918
6	8.235968	1.882156	0.115661
1	8.486421	2.528081	-0.716152
6	9.199158	1.022607	0.643357
1	10.194829	0.993768	0.213130
6	8.865845	0.192000	1.710186
1	9.602504	-0.484701	2.132527
6	7.568772	0.215485	2.225078
1	7.323067	-0.445760	3.048463
6	6.581271	1.053817	1.684943
6	5.592384	1.404758	-2.187844
1	6.659145	1.207138	-2.082992
6	5.312956	1.642793	-3.674790
1	5.558061	0.758184	-4.268888
1	4.270127	1.901548	-3.870563
1	5.932302	2.475941	-4.019818
6	4.832566	-0.341420	3.590852
6	4.982076	-1.692853	3.234217
1	5.154299	-1.956329	2.196432
6	4.925585	-2.697515	4.199229
1	5.059960	-3.732836	3.904035
6	4.693236	-2.366047	5.537861
1	4.636775	-3.147090	6.290717
6	4.536101	-1.027543	5.901859
1	4.356510	-0.762363	6.940056
6	4.611110	-0.018733	4.937015
1	4.484713	1.014691	5.238777
6	4.476299	2.496678	3.068280
6	5.423281	3.105152	3.907920
1	6.374780	2.616378	4.098643
6	5.151979	4.346145	4.484839
1	5.888353	4.814377	5.131856
6	3.935081	4.987469	4.225671
1	3.728014	5.956514	4.671261
6	2.991291	4.383776	3.391554
1	2.049578	4.884174	3.182256
6	3.259576	3.141808	2.810831
1	2.547905	2.684885	2.131796
6	6.128990	-1.322825	-1.131467
6	5.826478	-2.456672	-0.364250
1	4.807677	-2.632814	-0.044362
6	6.824244	-3.357184	0.008806
6	8.151655	-3.135562	-0.350068
1	8.932326	-3.815841	-0.027884
6	8.455763	-2.010062	-1.114552
6	7.459706	-1.123004	-1.520511
1	7.750484	-0.272111	-2.120345
6	3.720982	-0.910581	-2.712345
6	2.643019	-0.169266	-3.225360
1	2.493700	0.860122	-2.922970
6	1.740703	-0.755385	-4.108772
6	1.852598	-2.101908	-4.460003
1	1.134019	-2.562042	-5.128793
6	2.903508	-2.843656	-3.928025
6	3.840846	-2.256425	-3.074861
1	4.652923	-2.864304	-2.694553
29	3.478791	0.287427	0.508578
6	2.971086	-4.322740	-4.187502
6	0.566128	0.029074	-4.620566
6	6.457123	-4.587657	0.791600
6	9.898203	-1.746514	-1.454179
9	10.659046	-1.675956	-0.334110
9	10.070351	-0.586200	-2.124887
9	10.424146	-2.733441	-2.215285
9	5.388490	-4.367756	1.598683
9	6.122872	-5.616422	-0.020799
9	7.471253	-5.012830	1.574262
9	4.232457	-4.799503	-4.107389
9	2.235026	-5.010097	-3.275891
9	2.485976	-4.650737	-5.404812
9	0.321670	-0.218033	-5.924952
9	0.740385	1.364091	-4.485193
9	-0.578905	-0.284780	-3.952431
6	2.356620	-2.512084	0.583757
6	0.967546	-1.038396	-0.593572
6	1.741845	-3.619834	0.027717
1	3.149185	-2.620661	1.314884
6	0.345298	-2.159338	-1.221581
6	0.728888	-3.449304	-0.923198
1	-0.431922	-1.980638	-1.955736
6	0.396240	0.245862	-0.838233
6	0.914031	1.530791	-0.468855
8	1.983153	1.704604	0.187551
7	2.009585	-1.249411	0.268601
1	-0.399330	0.226632	-1.565823
7	0.169645	2.648404	-0.800301
6	0.727213	3.975139	-0.561924
1	1.136639	4.408406	-1.485448
1	-0.057007	4.642527	-0.188565
1	1.526033	3.907564	0.172572
6	-0.942249	2.592833	-1.745971
1	-1.674453	1.837856	-1.454604
1	-1.448073	3.559864	-1.745668
1	-0.607981	2.377763	-2.767387
1	0.262844	-4.297558	-1.411398
35	2.293185	-5.420096	0.559052

[8-9]‡-P1-C2 *exo si-re*

Number of imaginary frequencies= 1
The smallest frequencies are= -203.7211 9.5009 13.8096 cm(-1)
Electronic energy= -7222.6216665
Zero-point correction= 1.756224
(Hartree/Particle)
Thermal correction to Energy= 1.874396
Thermal correction to Enthalpy= 1.875340
Thermal correction to Gibbs Free Energy= 1.596320
Sum of electronic and zero-point Energies= -7220.865442
Sum of electronic and thermal Energies= -7220.747271
Sum of electronic and thermal Enthalpies= -7220.746327

Sum of electronic and thermal Free Energies= -7221.025346

.....

Cartesian Coordinates

.....

26	-7.113289	3.462019	0.401115
15	-3.294569	1.186117	-2.368655
15	-4.516794	-0.539422	0.748118
6	-5.817688	2.297932	-0.761513
6	-5.808180	1.873496	0.618379
6	-5.381577	2.981080	1.413904
1	-5.284851	2.987554	2.490781
6	-5.161228	4.093375	0.548122
1	-4.872171	5.087794	0.855571
6	-5.429424	3.675797	-0.787767
1	-5.378129	4.297133	-1.668693
6	-9.084764	2.853777	0.650119
1	-9.414112	1.823231	0.660160
6	-8.651419	3.607975	1.783474
1	-8.587958	3.248362	2.801656
6	-8.271432	4.907923	1.329888
1	-7.865470	5.701372	1.943523
6	-8.470419	4.958391	-0.083261
1	-8.243046	5.796859	-0.728357
6	-8.974061	3.691426	-0.503194
1	-9.197917	3.406551	-1.522331
6	-6.110564	1.387222	-1.904513
6	-7.427513	0.946648	-2.107691
1	-8.200494	1.336960	-1.458400
6	-7.749940	0.013892	-3.092670
1	-8.774463	-0.327728	-3.203290
6	-6.744000	-0.489231	-3.913760
1	-6.972202	-1.225689	-4.676832
6	-5.427741	-0.066814	-3.731137
1	-4.657237	-0.486660	-4.366205
6	-5.083580	0.857629	-2.730227
6	-6.096490	0.471731	1.076359
1	-6.850968	0.060322	0.403965
6	-6.635096	0.383578	2.507149
1	-6.867460	-0.649612	2.779011
1	-5.926605	0.773530	3.242984
1	-7.550783	0.977648	2.576217
6	-2.418552	0.304218	-3.727151
6	-1.743448	-0.887547	-3.429769
1	-1.705953	-1.243341	-2.405420
6	-1.109325	-1.605933	-4.448414
1	-0.590894	-2.527835	-4.216817
6	-1.132006	-1.134373	-5.761376
1	-0.629218	-1.691085	-6.546956
6	-1.793698	0.060161	-6.062395
1	-1.808742	0.435361	-7.081618
6	-2.433770	0.775907	-5.051802
1	-2.945571	1.700765	-5.296840
6	-2.989122	2.943440	-2.805489
6	-3.785939	3.679768	-3.694126
1	-4.669593	3.227844	-4.135315
6	-3.455226	5.002268	-3.997251
1	-4.078955	5.569888	-4.682046
6	-2.327035	5.595741	-3.421515
1	-2.076180	6.626148	-3.656634
6	-1.524902	4.862287	-2.542943
1	-0.647663	5.315706	-2.090311
6	-1.856820	3.541800	-2.235774
1	-1.240073	2.969924	-1.549749
6	-5.003566	-1.921488	-0.371936
6	-3.937194	-2.650708	-0.918195
1	-2.919078	-2.381869	-0.656002
6	-4.180086	-3.695129	-1.810800
6	-5.479480	-3.998223	-2.214304
1	-5.664855	-4.789424	-2.932442
6	-6.535770	-3.252371	-1.690442
6	-6.310400	-2.239668	-0.757743
1	-7.160662	-1.700557	-0.362031
6	-4.169643	-1.407179	2.334201
6	-3.563514	-0.656441	3.353409
1	-3.337724	0.391607	3.196682
6	-3.238070	-1.253953	4.569188
6	-3.490187	-2.608509	4.791772
1	-3.215875	-3.075336	5.730600
6	-4.083278	-3.353153	3.775736
6	-4.425520	-2.763903	2.555737
1	-4.889454	-3.370733	1.786272
29	-2.716793	0.572549	-0.263089
6	-4.260257	-4.837292	3.933247
6	-2.479705	-0.469666	5.601981
6	-3.024910	-4.527612	-2.294605
6	-7.926812	-3.541827	-2.185924
9	-8.023494	-3.342798	-3.523800
9	-8.859789	-2.760006	-1.600201
9	-8.280936	-4.828893	-1.964607
9	-1.906255	-3.780060	-2.483691
9	-2.691042	-5.485215	-1.394201
9	-3.286343	-5.152917	-3.459353
9	-5.404719	-5.276438	3.365112
9	-3.245533	-5.510980	3.326349
9	-4.269467	-5.222023	5.225608
9	-2.760937	-0.869522	6.858901
9	-2.725622	0.855341	5.526289
9	-1.132828	-0.624942	5.440021
6	-0.812623	-1.269109	1.160874
6	-0.435409	-0.241353	2.111134
6	-0.962047	1.091585	2.183471
1	-0.031320	-0.584251	3.050978
77	4.378743	-1.572575	1.493309
15	5.232450	-0.710391	-0.519941
8	5.342302	0.893987	-0.974416
8	6.834860	-1.147767	-0.713109
7	4.339376	-1.320950	-1.796537
6	6.061571	1.712187	-0.111926
6	5.317806	2.584518	0.710684
1	4.244132	2.625339	0.579902
6	5.969081	3.352834	1.642861
1	5.410999	4.036097	2.277086
6	7.375454	3.232554	1.818750
6	8.048313	3.941380	2.850901
1	7.467053	4.604925	3.486095
6	9.400078	3.780228	3.055956
1	9.902338	4.321049	3.852714
6	10.134431	2.891486	2.235012
1	11.195450	2.744787	2.415749
6	9.516389	2.205698	1.211636
1	10.093180	1.523425	0.598562
6	8.125594	2.363445	0.955982
6	7.444363	1.644891	-0.092288
6	8.174203	0.843096	-1.113260
6	9.214791	1.440977	-1.917437
6	9.487826	2.837943	-1.901392
1	8.887440	3.490076	-1.279006
6	10.490875	3.379482	-2.676659
1	10.670391	4.450529	-2.648902
6	11.282590	2.558041	-3.512950
1	12.074505	2.997306	-4.112493
6	11.029890	1.206105	-3.574600
1	11.613862	0.562834	-4.227750
6	9.992489	0.620051	-2.800446
6	9.697142	-0.766410	-2.902150
1	10.301234	-1.389694	-3.555517
6	8.641669	-1.303157	-2.212983
1	8.371872	-2.349693	-2.305734
6	7.863997	-0.489855	-1.353472
6	3.116661	-2.051609	-1.376582
1	2.276208	-1.345268	-1.391141
6	2.773681	-3.202315	-2.310587
6	1.431191	-3.493484	-2.576642
1	0.660748	-2.831298	-2.193545
6	1.078250	-4.621405	-3.323497
1	0.030254	-4.837684	-3.505340
6	2.071521	-5.461685	-3.830331
1	1.801287	-6.334883	-4.417412
6	3.416974	-5.171943	-3.579186
1	4.195546	-5.818955	-3.974305

6	3.764622	-4.055914	-2.817712
1	4.809358	-3.832784	-2.617215
6	3.268688	-2.650546	0.039740
1	3.759063	-3.624376	-0.072248
1	2.254870	-2.855998	0.398827
6	4.341048	-0.829296	-3.212161
1	3.904145	-1.659749	-3.771130
6	3.423224	0.368951	-3.461994
6	2.076054	0.137056	-3.776471
1	1.699812	-0.881700	-3.804451
6	1.214766	1.193597	-4.085104
1	0.180068	0.990756	-4.331606
6	1.695879	2.503231	-4.101586
1	1.030565	3.324863	-4.353155
6	3.035082	2.748511	-3.785162
1	3.418123	3.765449	-3.789566
6	3.888657	1.692452	-3.465091
1	4.923735	1.902656	-3.224022
6	5.748703	-0.644493	-3.773679
1	6.325100	-1.564197	-3.653928
1	6.296816	0.170011	-3.300012
1	5.676308	-0.420114	-4.841900
6	2.635942	-1.759777	2.746889
1	1.922428	-2.455555	2.320947
1	2.819967	-1.930831	3.804452
6	2.585304	-0.390834	2.308729
1	2.939609	0.358796	3.009370
6	1.774222	0.093493	1.241015
1	1.498392	-0.598996	0.458667
6	6.011918	-3.076039	1.406075
1	6.009092	-3.525103	0.415696
6	4.997875	-3.527201	2.294042
1	4.314779	-4.283682	1.910175
6	5.118877	-3.552583	3.806536
1	5.741587	-4.408391	4.106439
1	4.122576	-3.743953	4.215572
6	5.683906	-2.253073	4.420374
1	6.770047	-2.331577	4.528350
1	5.287744	-2.135898	5.433947
6	5.361231	-0.992639	3.627341
1	4.612913	-0.333946	4.059224
6	6.207153	-0.456749	2.679846
1	6.089274	0.591149	2.421603
6	7.504785	-1.108685	2.250672
1	7.896417	-0.554954	1.400025
1	8.238006	-0.982863	3.060304
6	7.392772	-2.608083	1.876114
1	7.693427	-3.231091	2.726326
1	8.111407	-2.811731	1.078144
6	1.725695	1.510969	0.894056
6	1.986961	2.518942	1.848668
6	1.379341	1.905147	-0.412630
6	1.916860	3.865666	1.505725
1	2.232782	2.250752	2.869247
6	1.326139	3.255177	-0.755756
1	1.172089	1.150050	-1.164593
6	1.588046	4.239926	0.199873
1	2.113704	4.623926	2.258054
1	1.081445	3.536980	-1.771690
1	1.539606	5.290783	-0.070777
6	-0.687987	1.849057	3.355103
6	-1.065283	3.174054	3.455694
1	-0.180637	1.369331	4.183568
6	-1.717920	3.745246	2.361923
6	-2.015759	2.969979	1.254802
1	-2.555692	3.379774	0.411247
7	-1.666570	1.673435	1.165754
8	-1.192714	-1.005700	-0.022379
7	-0.657308	-2.586558	1.523968
6	-0.795394	-3.640980	0.526456
1	-0.010802	-4.389855	0.681815
1	-1.766228	-4.143754	0.611745
1	-0.700356	-3.229317	-0.472527
6	-0.590105	-3.098866	2.889800
1	0.358894	-3.617109	3.068685
1	-0.705580	-2.310326	3.627461
1	-1.397452	-3.823023	3.037536
1	-0.845161	3.749108	4.348772
35	-2.211992	5.638486	2.380165

[8-9]‡-P1-C2 *exo re-re*

Number of imaginary frequencies= 1
The smallest frequencies are=-159.3210 10.5794 11.5867cm(-1)
Electronic energy= -7222.6196948
Zero-point correction= 1.754881
(Hartree/Particle)
Thermal correction to Energy= 1.873735
Thermal correction to Enthalpy= 1.874679
Thermal correction to Gibbs Free Energy= 1.591336
Sum of electronic and zero-point Energies= -7220.864813
Sum of electronic and thermal Energies= -7220.745960
Sum of electronic and thermal Enthalpies= -7220.745015
Sum of electronic and thermal Free Energies= -7221.028359

Cartesian Coordinates

26	-5.900050	4.224129	1.355207
15	-2.101593	1.905616	-1.425708
15	-4.755698	-0.305295	0.316320
6	-4.648665	3.154903	0.058699
6	-5.257507	2.284577	1.038382
6	-4.855019	2.735537	2.332422
1	-5.154540	2.298033	3.274762
6	-4.033203	3.887775	2.169275
1	-3.607818	4.483107	2.965784
6	-3.911088	4.151245	0.774693
1	-3.372055	4.972890	0.328210
6	-7.911616	4.428106	0.880804
1	-8.490539	3.695835	0.333540
6	-7.729743	4.464456	2.297389
1	-8.140344	3.761202	3.009676
6	-6.870307	5.563551	2.603734
1	-6.515327	5.837735	3.588566
6	-6.520632	6.206493	1.377162
1	-5.855107	7.052840	1.269658
6	-7.163919	5.506557	0.313319
1	-7.070713	5.734444	-0.739796
6	-4.755888	2.965790	-1.417509
6	-5.993861	3.180335	-2.042831
1	-6.819458	3.520893	-1.431422
6	-6.184583	2.953111	-3.406067
1	-7.161475	3.120512	-3.850630
6	-5.117617	2.511939	-4.184529
1	-5.244789	2.322637	-5.245498
6	-3.877429	2.286461	-3.586194
1	-3.065556	1.914683	-4.199637
6	-3.676279	2.490547	-2.211075
6	-6.035742	1.045992	0.698723
1	-6.498996	1.196498	-0.281282
6	-7.133395	0.667676	1.695293
1	-7.653692	-0.240961	1.378160
1	-6.740795	0.498574	2.700952
1	-7.863771	1.480852	1.752022
6	-1.094374	1.337320	-2.857293
6	-1.101431	-0.038351	-3.133559
1	-1.651796	-0.707651	-2.481032
6	-0.420615	-0.545732	-4.240182
1	-0.446686	-1.611163	-4.449517
6	0.301621	0.318376	-5.068102
1	0.842616	-0.074730	-5.924147
6	0.332699	1.687462	-4.788430
1	0.905707	2.362108	-5.417030
6	-0.369528	2.197123	-3.694875
1	-0.340555	3.261539	-3.496851
6	-1.267410	3.419329	-0.810670
6	-1.375552	4.664334	-1.449094
1	-1.951335	4.758880	-2.364990
6	-0.771882	5.793058	-0.890848
1	-0.864475	6.755040	-1.386730

6	-0.053415	5.685842	0.305135
1	0.413558	6.565965	0.738030
6	0.060128	4.447175	0.942918
1	0.616400	4.362196	1.870905
6	-0.547225	3.318236	0.389373
1	-0.514598	2.367170	0.910832
6	-5.534548	-1.181061	-1.097637
6	-4.931838	-1.000425	-2.350711
1	-4.018654	-0.421489	-2.427892
6	-5.496598	-1.562324	-3.493232
6	-6.663374	-2.324491	-3.407493
1	-7.093928	-2.774692	-4.294228
6	-7.261320	-2.504628	-2.162228
6	-6.713243	-1.930185	-1.011758
1	-7.198811	-2.086352	-0.053647
6	-4.783241	-1.488293	1.716564
6	-4.491002	-0.971675	2.990214
1	-4.347275	0.093616	3.124520
6	-4.339359	-1.827818	4.076643
6	-4.431134	-3.212816	3.918022
1	-4.301093	-3.876888	4.765266
6	-4.684671	-3.724376	2.648221
6	-4.866455	-2.875496	1.552890
1	-5.060408	-3.310811	0.580202
29	-2.523547	0.315019	0.095579
6	-4.693140	-5.214008	2.437726
6	-4.097915	-1.275914	5.453458
6	-4.881125	-1.313871	-4.843372
6	-8.527211	-3.306715	-2.022602
9	-9.569373	-2.521809	-1.657506
9	-8.405658	-4.254621	-1.063867
9	-8.874682	-3.929105	-3.167220
9	-3.598616	-0.894777	-4.751326
9	-4.889024	-2.428554	-5.608971
9	-5.559197	-0.364048	-5.532330
9	-5.455070	-5.574071	1.381576
9	-3.444247	-5.689210	2.198593
9	-5.158082	-5.875764	3.520472
9	-5.186622	-1.416809	6.245949
9	-3.789556	0.041081	5.436795
9	-3.082679	-1.920831	6.078901
6	-2.115199	-2.561640	-0.489835
6	-1.138647	-2.016016	1.567477
6	-1.818389	-3.903714	-0.339991
1	-2.645632	-2.206488	-1.365869
6	-0.797420	-3.387495	1.741085
6	-1.135128	-4.339184	0.798234
6	-0.728252	-1.087575	2.577777
6	-1.322495	0.195566	2.854698
8	-1.970872	0.877256	2.001210
7	-1.777547	-1.634273	0.420767
1	-0.193173	-1.554510	3.391758
77	3.228805	-1.095254	-0.952156
15	4.973146	0.384320	-0.473046
8	5.809958	0.533671	0.969356
8	6.274228	0.106374	-1.491721
7	4.426655	1.938578	-0.671215
6	6.450976	-0.617149	1.416169
6	5.844842	-1.305049	2.488761
1	4.961931	-0.870562	2.939933
6	6.382999	-2.488625	2.928066
1	5.933043	-3.022527	3.760768
6	7.510913	-3.052217	2.270616
6	8.014508	-4.327871	2.643900
1	7.539037	-4.850137	3.470094
6	9.067085	-4.899660	1.965856
1	9.439131	-5.878202	2.254979
6	9.654719	-4.215205	0.875354
1	10.466823	-4.679898	0.323636
6	9.204100	-2.967335	0.502134
1	9.660960	-2.463585	-0.341153
6	8.133781	-2.334284	1.193904
6	7.626568	-1.037617	0.816302
6	8.306385	-0.185009	-0.196937
6	9.697540	0.175478	-0.055810
6	10.447709	-0.110106	1.119642
1	9.962917	-0.603303	1.953394
6	11.775873	0.244399	1.223775
1	12.320203	0.020186	2.136807
6	12.434768	0.902169	0.158775
1	13.483657	1.168312	0.251282
6	11.734339	1.216567	-0.984069
1	12.218999	1.740282	-1.804022
6	10.360034	0.880383	-1.115418
6	9.622941	1.249820	-2.273242
1	10.132550	1.764054	-3.083229
6	8.279196	0.992854	-2.351620
1	7.687034	1.300340	-3.207226
6	7.621676	0.312777	-1.297848
6	3.022071	2.087417	-1.140195
1	2.461619	2.546021	-0.316825
6	2.972244	3.034044	-2.331809
6	2.098103	4.122858	-2.338109
1	1.480398	4.311978	-1.468422
6	2.008422	4.961590	-3.453639
1	1.318583	5.801084	-3.439129
6	2.802633	4.720373	-4.575623
1	2.738648	5.371090	-5.443247
6	3.693596	3.639401	-4.571385
1	4.323062	3.450709	-5.436997
6	3.778160	2.805021	-3.457900
1	4.478987	1.974335	-3.451428
6	2.333903	0.745458	-1.525633
1	2.251802	0.716852	-2.614126
1	1.308723	0.792978	-1.151153
6	5.075495	3.228530	-0.288437
1	4.712773	3.937671	-1.036857
6	4.603443	3.759795	1.062845
6	5.151712	3.317304	2.276095
1	5.882561	2.517416	2.274848
6	4.770606	3.904409	3.482342
1	5.210378	3.554810	4.412041
6	3.825905	4.935608	3.500493
1	3.536948	5.395452	4.441614
6	3.256726	5.367856	2.302047
1	2.520759	6.167323	2.302049
6	3.647240	4.783908	1.093372
1	3.216071	5.137597	0.160873
6	6.598026	3.233875	-0.420983
1	6.888807	2.997365	-1.445692
1	7.093273	2.535234	0.254002
1	6.961318	4.239503	-0.189788
6	1.257567	-1.798598	-0.445155
1	0.481249	-1.141927	-0.827731
1	1.058884	-2.842039	-0.662770
6	1.798312	-1.484601	0.856338
1	2.269234	-2.278936	1.429088
6	1.417541	-0.322011	1.562033
1	0.874777	0.431942	0.999991
6	4.073396	-1.347319	-2.978981
1	4.203057	-0.358698	-3.413956
6	2.737913	-1.837477	-2.960144
1	1.977899	-1.183202	-3.377346
6	2.347521	-3.301314	-3.014804
1	2.467806	-3.667848	-4.044827
1	1.278146	-3.369238	-2.793755
6	3.131174	-4.213177	-2.042963
1	3.996074	-4.645364	-2.555942
1	2.495945	-5.057353	-1.756552
6	3.616812	-3.522859	-0.775545
1	3.088179	-3.766853	0.142089
6	4.858962	-2.944884	-0.661278
1	5.254798	-2.778648	0.334869
6	5.852479	-2.860026	-1.800205
1	6.703482	-2.271034	-1.464391
1	6.238164	-3.871681	-1.991630
6	5.296293	-2.259313	-3.116709
1	5.039478	-3.065900	-3.813760
1	6.097526	-1.687501	-3.591675
6	1.966632	0.124978	2.835560

6	2.629175	-0.742799	3.729046
6	1.793415	1.470771	3.211096
6	3.117794	-0.271214	4.943568
1	2.749981	-1.791187	3.475327
6	2.274189	1.937982	4.432226
1	1.283437	2.148503	2.533045
6	2.942387	1.071734	5.301026
1	3.629572	-0.950855	5.618893
1	2.136208	2.979533	4.699660
1	3.319820	1.436323	6.251865
7	-1.138921	0.750963	4.092877
6	-1.525852	2.136578	4.323209
1	-2.488137	2.194715	4.847900
1	-0.763761	2.622725	4.941368
1	-1.614191	2.659892	3.373627
6	-0.684936	0.031324	5.277596
1	0.384467	0.177893	5.454727
1	-1.236784	0.406879	6.143380
1	-0.899561	-1.032987	5.199698
1	-0.889474	-5.384268	0.947858
1	-0.281075	-3.688718	2.646717
35	-2.392121	-5.164067	-1.720141

[8-9]‡-P1-C2 *endo si-si*

Number of imaginary frequencies= 1
The smallest frequencies are=-180.7054 11.6134 14.5069cm(-1)
Electronic energy= -7222.6307633
Zero-point correction= 1.755896
(Hartree/Particle)
Thermal correction to Energy= 1.874226
Thermal correction to Enthalpy= 1.875170
Thermal correction to Gibbs Free Energy= 1.595804
Sum of electronic and zero-point Energies= -7220.874868
Sum of electronic and thermal Energies= -7220.756538
Sum of electronic and thermal Enthalpies= -7220.755593
Sum of electronic and thermal Free Energies= -7221.034960

.....

Cartesian Coordinates

.....

26	6.791719	-3.245451	1.102479
15	2.484432	-1.598787	-1.497132
15	4.666575	0.928280	0.262182
6	5.290347	-2.398989	-0.098147
6	5.750121	-1.469810	0.906060
6	5.506037	-2.055669	2.187051
1	5.750597	-1.610958	3.142034
6	4.940489	-3.350403	1.985900
1	4.681185	-4.056998	2.760891
6	4.803044	-3.560542	0.581945
1	4.423843	-4.452474	0.105142
6	8.789636	-3.000150	0.583499
1	9.188678	-2.137679	0.066236
6	8.655818	-3.139565	1.998880
1	8.930624	-2.400486	2.739457
6	8.054385	-4.407723	2.263170
1	7.788564	-4.793818	3.238424
6	7.815832	-5.052520	1.011629
1	7.340908	-6.014667	0.871700
6	8.270729	-4.184695	-0.025335
1	8.201858	-4.380436	-1.086654
6	5.306564	-2.143071	-1.565560
6	6.544419	-2.098118	-2.226996
1	7.438873	-2.261026	-1.640461
6	6.645586	-1.847063	-3.593949
1	7.621455	-1.798540	-4.066545
6	5.485671	-1.654299	-4.340015
1	5.539380	-1.465037	-5.407036
6	4.246271	-1.673024	-3.701859
1	3.359168	-1.492471	-4.296000
6	4.128289	-1.887664	-2.316912
6	6.235190	-0.074812	0.616566
1	6.780854	-0.098025	-0.328430
6	7.154321	0.514226	1.689997
1	7.486221	1.518779	1.412539
1	6.660960	0.581544	2.663212
1	8.035592	-0.124992	1.802005
6	1.429974	-1.094231	-2.919876
6	1.370369	0.270482	-3.241121
1	1.883332	0.990985	-2.614229
6	0.651174	0.703490	-4.356391
1	0.620879	1.760643	-4.596460
6	-0.033862	-0.222205	-5.148910
1	-0.603236	0.115705	-6.010213
6	0.009037	-1.580771	-4.827543
1	-0.534920	-2.305455	-5.426030
6	0.746396	-2.016428	-3.725098
1	0.780101	-3.074418	-3.495705
6	1.814738	-3.244191	-1.037764
6	2.241983	-4.447969	-1.616287
1	3.013208	-4.439423	-2.381067
6	1.684882	-5.660978	-1.202963
1	2.021814	-6.589674	-1.654597
6	0.702389	-5.681473	-0.207867
1	0.278269	-6.627165	0.117194
6	0.266459	-4.483825	0.366195
1	-0.499281	-4.490663	1.134341
6	0.813774	-3.270826	-0.053422
1	0.473581	-2.340779	0.393744
6	4.903041	1.770350	-1.356921
6	3.846741	2.596220	-1.767914
1	3.006957	2.750554	-1.099172
6	3.840169	3.162210	-3.042051
6	4.868314	2.899632	-3.944059
1	4.854002	3.323671	-4.941613
6	5.910369	2.061796	-3.540512
6	5.940246	1.505707	-2.261131
1	6.761835	0.852221	-1.999268
6	4.603176	2.287840	1.499487
6	4.164374	1.920283	2.781384
1	3.950982	0.880705	3.002756
6	3.957215	2.887213	3.760541
6	4.147068	4.240679	3.476659
1	3.961543	4.996858	4.230953
6	4.571292	4.604430	2.200834
6	4.815606	3.640662	1.218338
1	5.150248	3.956936	0.237084
29	2.591822	-0.137994	0.227299
6	4.669204	6.063252	1.852757
6	3.423968	2.493220	5.109691
6	2.684477	4.050562	-3.411273
6	6.989147	1.742766	-4.539614
9	6.497643	1.045347	-5.593267
9	7.991433	1.008432	-4.009205
9	7.541089	2.868402	-5.050435
9	1.487844	3.447137	-3.146618
9	2.683451	5.200272	-2.695051
9	2.676580	4.383957	-4.715144
9	5.538138	6.295750	0.846770
9	3.462906	6.547974	1.446161
9	5.049723	6.815854	2.906934
9	4.020125	3.179425	6.108833
9	3.585233	1.177944	5.363854
9	2.090441	2.752640	5.210600
6	1.161085	2.353613	1.308430
6	0.671555	1.613459	2.445856
6	1.134287	0.333988	2.904920
1	0.217091	2.197515	3.233295
77	-3.042671	1.137995	-1.161454
15	-4.798710	-0.358150	-0.763792
8	-5.554637	-0.753470	0.671734
8	-6.144025	0.146826	-1.629879
7	-4.321434	-1.886650	-1.243961
6	-6.225826	0.255868	1.349674
6	-5.609648	0.753813	2.517443
1	-4.686131	0.294541	2.845531
6	-6.191270	1.791570	3.201494
1	-5.731217	2.177589	4.106967
6	-7.381381	2.397729	2.713091
6	-7.941379	3.536255	3.354017

1	-7.454829	3.918250	4.247917
6	-9.063521	4.153235	2.848575
1	-9.478945	5.026646	3.342721
6	-9.667775	3.655955	1.669477
1	-10.537177	4.159783	1.256912
6	-9.161679	2.541799	1.035492
1	-9.633491	2.181992	0.129014
6	-8.017189	1.864079	1.541036
6	-7.452778	0.707137	0.891092
6	-8.129629	0.027017	-0.247591
6	-9.483869	-0.458946	-0.132071
6	-10.194548	-0.464090	1.101306
1	-9.705582	-0.103446	1.998175
6	-11.487770	-0.935082	1.178922
1	-12.002300	-0.933615	2.135647
6	-12.148746	-1.427139	0.028921
1	-13.170150	-1.788732	0.103344
6	-11.484157	-1.460575	-1.176226
1	-11.969971	-1.854564	-2.065233
6	-10.145261	-0.997190	-1.286402
6	-9.441585	-1.079204	-2.518501
1	-9.952888	-1.469182	-3.394155
6	-8.124199	-0.707722	-2.591689
1	-7.552454	-0.801917	-3.508933
6	-7.467840	-0.193529	-1.448512
6	-2.914144	-1.942319	-1.737372
1	-2.269233	-2.230337	-0.896288
6	-2.751985	-2.984528	-2.834817
6	-1.752970	-3.958191	-2.742303
1	-1.121887	-3.991081	-1.860895
6	-1.552801	-4.879588	-3.774454
1	-0.768542	-5.626028	-3.681684
6	-2.358632	-4.839282	-4.913435
1	-2.209075	-5.555633	-5.716387
6	-3.369634	-3.875250	-5.010190
1	-4.007355	-3.843404	-5.889505
6	-3.563055	-2.955822	-3.979650
1	-4.354517	-2.214431	-4.052262
6	-2.463519	-0.569638	-2.277113
1	-2.865893	-0.456094	-3.289813
1	-1.375981	-0.603608	-2.377659
6	-4.945904	-3.201616	-0.897742
1	-4.531382	-3.881998	-1.643900
6	-4.529869	-3.779568	0.457858
6	-3.435847	-4.655839	0.510134
1	-2.868274	-4.852669	-0.394716
6	-3.091403	-5.311297	1.696238
1	-2.254242	-6.003935	1.706978
6	-3.839137	-5.097816	2.855587
1	-3.582536	-5.614115	3.776595
6	-4.920974	-4.213330	2.820685
1	-5.506693	-4.035055	3.718366
6	-5.263779	-3.563501	1.634483
1	-6.115668	-2.895139	1.624109
6	-6.458075	-3.228182	-1.115233
1	-6.694749	-2.932485	-2.139225
1	-7.001305	-2.574518	-0.433113
1	-6.818577	-4.249573	-0.960772
6	-0.936590	1.508277	-0.892753
1	-0.341104	1.140620	-1.717205
1	-0.712302	2.534698	-0.635712
6	-1.224348	0.592974	0.177770
1	-0.990769	-0.456613	0.025535
6	-1.463234	1.032592	1.505218
1	-1.673083	2.085005	1.644547
6	-4.154368	1.947704	-2.889895
1	-4.476851	1.112694	-3.506458
6	-2.780991	2.306932	-2.999207
1	-2.174891	1.720204	-3.688609
6	-2.226844	3.699355	-2.760619
1	-2.427095	4.326736	-3.642172
1	-1.138307	3.619308	-2.687114
6	-2.777008	4.393339	-1.493597
1	-3.661375	4.986429	-1.744357
1	-2.029416	5.104482	-1.127153
6	-3.131962	3.445106	-0.354829
1	-2.442697	3.442267	0.482677
6	-4.386912	2.917093	-0.144287
1	-4.623619	2.541180	0.846833
6	-5.568743	3.146664	-1.066430
1	-6.361889	2.461072	-0.773424
1	-5.956410	4.160911	-0.891924
6	-5.268024	2.950143	-2.571931
1	-5.015382	3.910134	-3.035861
1	-6.185847	2.608090	-3.058018
6	-1.895354	0.168460	2.600578
6	-1.855033	-1.235791	2.520608
6	-2.341589	0.758977	3.799326
6	-2.261744	-2.017833	3.598926
1	-1.508269	-1.721050	1.614747
6	-2.753915	-0.024185	4.875434
1	-2.366800	1.843141	3.875323
6	-2.718673	-1.418509	4.776632
1	-2.232880	-3.097714	3.514127
1	-3.104505	0.451108	5.787031
1	-3.042044	-2.034496	5.610689
6	0.838382	-0.028262	4.247816
6	1.112930	-1.292974	4.726293
1	0.381073	0.704976	4.899684
6	1.718610	-2.195356	3.849709
6	2.052836	-1.796686	2.568860
1	2.547990	-2.469809	1.883034
7	1.772918	-0.564697	2.096823
8	1.674104	1.808810	0.287759
7	0.972430	3.714271	1.291416
6	1.217231	4.464024	0.064152
1	0.498030	5.286852	-0.001248
1	2.226064	4.890761	0.043804
1	1.088119	3.817320	-0.798996
6	0.697465	4.520821	2.477999
1	-0.376133	4.710259	2.610176
1	1.090541	4.047591	3.377469
1	1.205795	5.482425	2.368033
1	0.861907	-1.570456	5.744138
35	2.073399	-4.034667	4.414989

[**8-9**]‡**-P1-C2** *endo re-si*

Number of imaginary frequencies= 1
The smallest frequencies are= -73.8742 13.1378 15.6372 cm(-1)
Electronic energy= -7222.6203364
Zero-point correction= 1.756912
(Hartree/Particle)
Thermal correction to Energy= 1.875122
Thermal correction to Enthalpy= 1.876066
Thermal correction to Gibbs Free Energy= 1.597000
Sum of electronic and zero-point Energies= -7220.863425
Sum of electronic and thermal Energies= -7220.745215
Sum of electronic and thermal Enthalpies= -7220.744271
Sum of electronic and thermal Free Energies= -7221.023337

.....

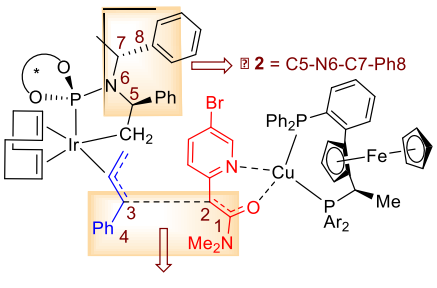
Cartesian Coordinates

.....

77	-3.917185	-0.752632	-1.985459
15	-5.573902	-0.442159	-0.362628
8	-5.396538	0.083956	1.208338
8	-6.674955	0.691943	-0.904556
7	-6.329944	-1.906327	-0.076414
6	-4.845095	1.344519	1.396746
6	-3.526753	1.386139	1.894599
1	-3.053740	0.453513	2.170332
6	-2.885181	2.592239	2.012691
1	-1.871963	2.635206	2.396408
6	-3.526447	3.789391	1.591125
6	-2.833571	5.029538	1.592579
1	-1.807855	5.049280	1.948992
6	-3.434458	6.177246	1.126905
1	-2.888768	7.116194	1.118634
6	-4.761758	6.126764	0.638743
1	-5.226501	7.028217	0.249667

6	-5.470489	4.944192	0.646582
1	-6.483194	4.922999	0.261367
6	-4.886495	3.741199	1.132036
6	-5.586442	2.480370	1.116625
6	-7.039618	2.373537	0.806850
6	-8.015458	3.128319	1.558095
6	-7.672778	3.900080	2.704143
1	-6.645382	3.917837	3.046402
6	-8.627675	4.611754	3.398500
1	-8.336841	5.185399	4.274001
6	-9.981649	4.596498	2.989217
1	-10.722089	5.167792	3.541419
6	-10.354974	3.839566	1.901713
1	-11.394307	3.798032	1.586172
6	-9.397601	3.082099	1.174280
6	-9.792541	2.258346	0.085699
1	-10.837433	2.238708	-0.210781
6	-8.873515	1.472322	-0.559007
1	-9.156372	0.806289	-1.367263
6	-7.512572	1.511635	-0.174436
6	-5.716970	-3.040971	-0.820484
1	-4.950583	-3.499250	-0.181582
6	-6.737888	-4.109460	-1.177807
6	-6.422056	-5.462777	-1.012980
1	-5.466123	-5.737754	-0.573070
6	-7.321668	-6.458143	-1.405956
1	-7.061987	-7.504460	-1.270420
6	-8.553477	-6.107709	-1.961549
1	-9.257218	-6.879158	-2.260928
6	-8.878816	-4.756938	-2.126862
1	-9.837499	-4.476980	-2.555056
6	-7.976007	-3.766314	-1.742295
1	-8.229676	-2.716328	-1.862808
6	-5.060987	-2.540475	-2.119933
1	-5.857260	-2.377467	-2.856271
1	-4.440248	-3.356888	-2.503414
6	-7.170835	-2.269447	1.109174
1	-7.698707	-3.167553	0.781997
6	-6.362555	-2.686742	2.339380
6	-5.948258	-4.022521	2.453958
1	-6.184969	-4.723417	1.658274
6	-5.270317	-4.473509	3.589724
1	-4.967383	-5.514753	3.660155
6	-5.007006	-3.592383	4.640196
1	-4.493382	-3.940641	5.532123
6	-5.409612	-2.257981	4.535897
1	-5.206993	-1.564119	5.347207
6	-6.080078	-1.810180	3.397071
1	-6.390391	-0.773944	3.338630
6	-8.257194	-1.236652	1.403631
1	-8.858197	-1.061950	0.508621
1	-7.862770	-0.279205	1.743858
1	-8.913496	-1.626249	2.187528
6	-5.232656	0.209663	-3.485237
1	-6.213188	-0.255211	-3.421791
6	-4.230921	-0.549036	-4.152777
1	-4.535177	-1.518745	-4.544672
6	-3.029390	0.035762	-4.871978
1	-3.337878	0.402237	-5.862326
1	-2.322134	-0.780064	-5.052805
6	-2.318622	1.158413	-4.088918
1	-2.746727	2.130620	-4.351120
1	-1.267886	1.196622	-4.391817
6	-2.375687	0.986268	-2.576508
1	-1.443305	0.689820	-2.107918
6	-3.332608	1.577630	-1.773928
1	-3.092709	1.730007	-0.726409
6	-4.485256	2.401397	-2.311895
1	-5.169333	2.607509	-1.490760
1	-4.090346	3.376765	-2.632696
6	-5.268281	1.739841	-3.470021
1	-4.900126	2.104760	-4.435238
1	-6.312371	2.056692	-3.401657
6	1.152120	-1.312638	-1.688559
6	0.848882	-2.322046	-0.706223
6	1.404153	-2.424841	0.601752
1	0.407932	-3.240558	-1.064053
6	-2.233271	-1.987347	-2.511728
1	-1.400107	-1.436930	-2.932244
1	-2.508864	-2.860426	-3.099419
6	-2.290680	-2.113243	-1.074955
1	-2.768470	-2.989603	-0.648156
6	-1.468272	-1.331014	-0.228810
1	-0.970134	-0.475180	-0.662271
6	-1.418993	-1.387063	1.217019
6	-2.074598	-2.378058	1.976783
6	-0.644065	-0.419696	1.895182
6	-1.960169	-2.392044	3.363540
1	-2.678290	-3.133987	1.485230
6	-0.539731	-0.432402	3.281573
1	-0.116428	0.334692	1.319716
6	-1.196470	-1.420694	4.020297
1	-2.472616	-3.158155	3.933517
1	0.058252	0.317188	3.784744
1	-1.113419	-1.434541	5.103323
6	1.156392	-3.621889	1.337543
6	1.708457	-3.824599	2.583178
1	0.544160	-4.394746	0.886475
6	2.519248	-2.809691	3.104814
6	2.712511	-1.647458	2.384145
1	3.328743	-0.850678	2.777052
7	2.160749	-1.437168	1.175152
8	1.395968	-0.100014	-1.385670
7	1.103936	-1.649580	-3.018313
6	1.160846	-0.615596	-4.043610
1	0.247079	-0.636940	-4.652481
1	2.016038	-0.788024	-4.706252
1	1.262204	0.360002	-3.573702
6	0.935777	-3.006861	-3.525748
1	-0.114618	-3.232048	-3.747738
1	1.316139	-3.743383	-2.820486
1	1.509077	-3.107846	-4.450300
1	1.525432	-4.741745	3.132437
35	3.399699	-3.022492	4.838745
26	5.074278	3.714224	-3.249707
15	2.341285	2.486228	1.047457
15	4.776693	-0.191232	-0.489234
6	4.279343	3.215126	-1.370158
6	4.813978	2.053119	-2.038669
6	4.104197	1.901946	-3.273389
1	4.274675	1.140494	-4.021327
6	3.157378	2.963232	-3.379760
1	2.499633	3.145071	-4.219227
6	3.271890	3.777272	-2.216249
1	2.708055	4.674423	-2.005830
6	7.072125	4.274698	-3.378685
1	7.852366	3.936134	-2.710265
6	6.658850	3.623887	-4.581235
1	7.063740	2.701300	-4.975357
6	5.584225	4.378050	-5.143382
1	5.029963	4.124600	-6.037606
6	5.332038	5.493657	-4.288065
1	4.555401	6.235186	-4.421940
6	6.251437	5.431026	-3.198893
1	6.292848	6.119724	-2.366149
6	4.693689	3.698040	-0.022046
6	5.936807	4.330271	0.127547
1	6.560505	4.443199	-0.749167
6	6.377391	4.809970	1.361214
1	7.348553	5.290109	1.439636
6	5.558120	4.679676	2.478877
1	5.872862	5.062078	3.445274
6	4.326000	4.035481	2.359099
1	3.713356	3.924028	3.244963
6	3.886720	3.513239	1.132199
6	5.798510	1.112171	-1.397601
1	6.232374	1.642156	-0.542331
6	6.962047	0.633452	-2.271989
1	7.573775	-0.103405	-1.741731
1	6.633846	0.189502	-3.212571

1	7.594570	1.491173	-2.519237
6	1.763176	2.463799	2.799330
6	2.485427	1.682687	3.717925
1	3.363013	1.139397	3.390566
6	2.107064	1.619275	5.057617
1	2.696339	1.026860	5.750359
6	0.975973	2.315430	5.496458
1	0.669601	2.258039	6.536779
6	0.242754	3.084159	4.590239
1	-0.638203	3.627017	4.920857
6	0.640576	3.169010	3.252440
1	0.074839	3.788510	2.566465
6	1.144650	3.571514	0.176976
6	1.127983	4.960243	0.389131
1	1.814251	5.409100	1.101303
6	0.243874	5.768691	-0.324879
1	0.234067	6.841448	-0.154205
6	-0.625550	5.197299	-1.259902
1	-1.313554	5.826578	-1.816898
6	-0.611114	3.818015	-1.474891
1	-1.280102	3.376441	-2.204843
6	0.268202	3.001797	-0.757744
1	0.305611	1.932216	-0.948105
6	5.861286	-0.637407	0.930688
6	5.729328	0.177259	2.064860
1	5.055526	1.027493	2.038603
6	6.437723	-0.108744	3.229800
6	7.296897	-1.206309	3.286503
1	7.837168	-1.438120	4.196804
6	7.448135	-1.999989	2.150401
6	6.740973	-1.724040	0.976928
1	6.873413	-2.367916	0.114713
6	4.669619	-1.724526	-1.492276
6	4.344389	-2.930929	-0.847881
1	4.279443	-2.975995	0.232124
6	4.074510	-4.076616	-1.591904
6	4.120774	-4.058198	-2.986950
1	3.900489	-4.951707	-3.559879
6	4.416456	-2.857163	-3.624866
6	4.677785	-1.700243	-2.890956
1	4.867510	-0.784199	-3.427371
29	2.651684	0.413008	0.220353
6	4.476063	-2.800238	-5.125847
6	3.596995	-5.325520	-0.905090
6	6.166719	0.703341	4.466096
6	8.316279	-3.227942	2.206914
9	9.283921	-3.127155	3.142575
9	8.919124	-3.473609	1.021771
9	7.586538	-4.330017	2.509172
9	5.076715	0.225747	5.126815
9	7.194973	0.678059	5.337258
9	5.901531	1.997203	4.177706
9	4.198191	-1.556990	-5.595301
9	5.699213	-3.129225	-5.598776
9	3.592071	-3.649881	-5.699807
9	2.245177	-5.449703	-1.013160
9	3.887742	-5.339858	0.412170
9	4.126840	-6.440713	-1.454028



C1-P1 *re-re*_1

Number of imaginary frequencies= 1

The smallest frequencies are= -208.3273 7.6812 12.1104 cm(-1)
Electronic energy= -7222.6357129
Zero-point correction= 1.756033
(Hartree/Particle)
Thermal correction to Energy= 1.874272
Thermal correction to Enthalpy= 1.875216
Thermal correction to Gibbs Free Energy= 1.594952
Sum of electronic and zero-point Energies= -7220.879680
Sum of electronic and thermal Energies= -7220.761441
Sum of electronic and thermal Enthalpies= -7220.760497
Sum of electronic and thermal Free Energies= -7221.040761

.....

Cartesian Coordinates

.....

26	-3.649716	-3.884826	3.789579
15	-1.482765	-2.060473	-0.606649
15	-4.596284	-0.382582	0.700313
6	-3.112134	-3.223545	1.876075
6	-3.859689	-2.214117	2.590619
6	-3.132328	-1.889180	3.776957
1	-3.437348	-1.177099	4.531464
6	-1.961947	-2.706301	3.822712
1	-1.231703	-2.724702	4.619890
6	-1.951245	-3.528639	2.658434
1	-1.207938	-4.272036	2.413123
6	-5.483411	-4.813437	4.086595
1	-6.382623	-4.591045	3.527574
6	-5.058256	-4.161469	5.284436
1	-5.573746	-3.353758	5.786635
6	-3.807116	-4.728154	5.675508
1	-3.208154	-4.421987	6.523122
6	-3.459293	-5.732043	4.721147
1	-2.553133	-6.323420	4.720771
6	-4.494627	-5.786372	3.741221
1	-4.506715	-6.429105	2.871632
6	-3.487137	-3.751378	0.531344
6	-4.599695	-4.598156	0.411167
1	-5.125622	-4.881431	1.313965
6	-5.050761	-5.054906	-0.826891
1	-5.933937	-5.683152	-0.884366
6	-4.375036	-4.677926	-1.984722
1	-4.717250	-5.016956	-2.957451
6	-3.264530	-3.838481	-1.892812
1	-2.757172	-3.542564	-2.803861
6	-2.812807	-3.353056	-0.655229
6	-5.122014	-1.570116	2.084573
1	-5.704578	-2.348662	1.589603
6	-5.988507	-0.939632	3.177768
1	-6.911916	-0.531037	2.758062
1	-5.470746	-0.130063	3.700070
1	-6.248948	-1.703773	3.916410
6	-0.961158	-1.899025	-2.367365
6	-1.568255	-0.891421	-3.135663
1	-2.273830	-0.210875	-2.672079
6	-1.250959	-0.749187	-4.488110
1	-1.734225	0.025954	-5.073911
6	-0.308457	-1.592940	-5.080574
1	-0.052871	-1.472457	-6.129446
6	0.308749	-2.589376	-4.319491
1	1.048841	-3.243476	-4.771453
6	-0.022155	-2.748020	-2.973068
1	0.451827	-3.533515	-2.396960
6	-0.069806	-2.901280	0.216256
6	0.171732	-4.277998	0.072593
1	-0.482513	-4.883233	-0.547922
6	1.235238	-4.878864	0.747353
1	1.416308	-5.943185	0.628054
6	2.062597	-4.115718	1.577885
1	2.887707	-4.586882	2.103843
6	1.827556	-2.747714	1.727479
1	2.466874	-2.149698	2.368136
6	0.766715	-2.144034	1.048874
1	0.578766	-1.084999	1.174393
6	-5.537348	-0.879096	-0.801354
6	-5.177935	-0.222388	-1.987088

1	-4.420313	0.554059	-1.953974
6	-5.774319	-0.574027	-3.197618
6	-6.702892	-1.611080	-3.261587
1	-7.141875	-1.904676	-4.208664
6	-7.043764	-2.275524	-2.082898
6	-6.488838	-1.903575	-0.858536
1	-6.793552	-2.437080	0.031534
6	-5.276353	1.277269	1.108922
6	-4.571776	2.008548	2.078421
1	-3.730979	1.556074	2.589661
6	-4.915684	3.327360	2.356145
6	-5.950197	3.956596	1.660289
1	-6.198181	4.992913	1.858779
6	-6.643454	3.232474	0.694077
6	-6.322368	1.899050	0.421581
1	-6.882393	1.365220	-0.337699
29	-2.316360	-0.137261	0.241172
6	-7.675411	3.918225	-0.156376
6	-4.091183	4.131173	3.322459
6	-5.421418	0.217830	-4.425393
6	-7.987452	-3.443507	-2.168686
9	-7.467307	-4.439418	-2.929289
9	-8.266363	-3.975950	-0.958330
9	-9.164610	-3.099930	-2.740184
9	-4.089643	0.480331	-4.489269
9	-6.042960	1.423970	-4.434930
9	-5.761250	-0.413537	-5.566359
9	-7.120605	4.382847	-1.311315
9	-8.232090	4.980135	0.461069
9	-8.672693	3.083733	-0.521016
9	-4.853926	4.946647	4.082379
9	-3.367893	3.351529	4.155072
9	-3.205775	4.931987	2.668783
6	-2.675215	2.730787	-0.735925
6	-1.737037	3.213478	0.249897
6	-1.231080	2.503283	1.384655
1	-1.667853	4.285573	0.360771
77	2.926648	1.743362	-1.610752
15	4.401385	0.391576	-0.503008
8	4.192610	-1.208945	-0.132411
8	5.835260	0.310493	-1.354219
7	4.651121	1.007078	1.040555
6	4.414873	-2.210427	-1.075077
6	3.278069	-2.921201	-1.514091
1	2.315095	-2.668185	-1.091628
6	3.418599	-3.912610	-2.451511
1	2.552977	-4.475887	-2.787270
6	4.689634	-4.199003	-3.016088
6	4.831283	-5.167645	-4.046551
1	3.946473	-5.708320	-4.372813
6	6.054735	-5.405707	-4.630276
1	6.151548	-6.143655	-5.421292
6	7.188269	-4.670748	-4.208376
1	8.147776	-4.839667	-4.688735
6	7.087693	-3.737724	-3.198966
1	7.966512	-3.179268	-2.900238
6	5.844546	-3.482251	-2.554211
6	5.701046	-2.510362	-1.498335
6	6.878004	-1.809743	-0.915507
6	7.996553	-2.520328	-0.351515
6	7.982376	-3.926995	-0.135171
1	7.097945	-4.494774	-0.399504
6	9.065223	-4.571462	0.422412
1	9.025188	-5.644319	0.587691
6	10.226077	-3.849603	0.790211
1	11.073625	-4.372366	1.223594
6	10.268683	-2.485401	0.610261
1	11.146396	-1.914966	0.902762
6	9.162510	-1.786847	0.053835
6	9.179979	-0.372208	-0.073651
1	10.070734	0.173584	0.223220
6	8.070097	0.301405	-0.517769
1	8.048371	1.383006	-0.587409
6	6.922773	-0.424175	-0.903688
6	4.218312	2.428225	1.136931
1	3.239927	2.455688	1.629039
6	5.167578	3.287810	1.949581
6	4.667321	4.109723	2.965206
1	3.602308	4.094472	3.188624
6	5.524378	4.932758	3.702142
1	5.123959	5.560053	4.493945
6	6.893146	4.939795	3.426319
1	7.563071	5.571277	4.003104
6	7.398311	4.126765	2.405412
1	8.463483	4.121561	2.191008
6	6.540329	3.310545	1.671766
1	6.934202	2.655311	0.902334
6	4.057027	3.005749	-0.280041
1	5.049881	3.193230	-0.707041
1	3.563162	3.978043	-0.201398
6	4.713377	0.172690	2.287413
1	4.660512	-0.857871	1.939430
6	6.034956	0.291195	3.046524
6	7.103204	-0.530220	2.665106
1	6.973851	-1.218528	1.836596
6	8.328396	-0.479325	3.332087
1	9.138933	-1.128081	3.012700
6	8.503077	0.398177	4.404094
1	9.455023	0.443764	4.926160
6	7.440205	1.211259	4.806175
1	7.562432	1.897305	5.639863
6	6.216129	1.151949	4.138107
1	5.410868	1.800470	4.462475
6	3.488327	0.400901	3.180660
1	2.563925	0.226610	2.625494
1	3.443898	1.409191	3.597734
1	3.518097	-0.300227	4.018737
6	1.405672	1.187666	-0.177037
1	0.696157	0.472618	-0.591579
1	1.766019	0.898060	0.804943
6	1.159219	2.586241	-0.406895
1	1.585692	3.299293	0.289329
6	0.130179	3.060528	-1.253751
1	-0.411077	2.313733	-1.821374
6	4.407298	2.161353	-3.248681
1	5.354987	2.369794	-2.761105
6	3.447780	3.195949	-3.241972
1	3.734034	4.137894	-2.774567
6	2.315131	3.319958	-4.247936
1	2.708127	3.707765	-5.200463
1	1.622697	4.075345	-3.870576
6	1.535426	2.008026	-4.498139
1	1.938397	1.483543	-5.370893
1	0.499332	2.258052	-4.749114
6	1.519613	1.046121	-3.312257
1	0.549847	0.871725	-2.863041
6	2.464825	0.043896	-3.103966
1	2.139520	-0.812964	-2.522927
6	3.682117	-0.201598	-3.974063
1	4.342032	-0.890030	-3.443156
1	3.365617	-0.720196	-4.891027
6	4.469707	1.078445	-4.326640
1	4.109717	1.496447	-5.272258
1	5.517751	0.810495	-4.491120
6	0.012186	4.429541	-1.747950
6	0.717887	5.510814	-1.184201
6	-0.843939	4.679135	-2.838789
6	0.561432	6.797992	-1.691694
1	1.389893	5.341415	-0.348890
6	-0.997596	5.968025	-3.345872
1	-1.384861	3.850750	-3.286144
6	-0.298113	7.033750	-2.771400
1	1.111510	7.622212	-1.246523
1	-1.660075	6.141337	-4.189109
1	-0.416191	8.039463	-3.164018
8	-2.706355	1.521089	-1.130457
6	-0.505546	3.244922	2.360275
6	0.003430	2.639266	3.492163
1	-0.378535	4.312662	2.217493
6	-0.216923	1.266509	3.645712

6	-0.895930	0.566451	2.665950
1	-1.066549	-0.498312	2.757059
7	-1.378022	1.155286	1.554492
6	-4.213165	3.261992	-2.560918
1	-3.690467	2.459764	-3.077638
1	-5.232315	2.932475	-2.332747
1	-4.274070	4.130279	-3.223748
6	-3.750787	4.989251	-0.857768
1	-3.581521	5.053029	0.215722
1	-3.127736	5.733708	-1.368103
1	-4.802120	5.223880	-1.040952
7	-3.487412	3.640072	-1.353026
1	0.540399	3.214325	4.239019
35	0.402353	0.321820	5.239910

C1-P1 *re-re_2*

Number of imaginary frequencies= 1
The smallest frequencies are= -204.7451 6.0926 12.6994 cm(-1)
Electronic energy= -7222.6357296
Zero-point correction= 1.756081
(Hartree/Particle)
Thermal correction to Energy= 1.874315
Thermal correction to Enthalpy= 1.875259
Thermal correction to Gibbs Free Energy= 1.595318
Sum of electronic and zero-point Energies= -7220.879649
Sum of electronic and thermal Energies= -7220.761415
Sum of electronic and thermal Enthalpies= -7220.760470
Sum of electronic and thermal Free Energies= -7221.040412

.....

Cartesian Coordinates

.....

26	-3.590371	-3.885361	3.799579
15	-1.457814	-2.062168	-0.611400
15	-4.570627	-0.396323	0.705988
6	-3.066686	-3.227495	1.880959
6	-3.810546	-2.217526	2.598450
6	-3.075182	-1.888830	3.778864
1	-3.375648	-1.175409	4.533926
6	-1.903685	-2.704660	3.818314
1	-1.168941	-2.722338	4.611395
6	-1.900223	-3.529770	2.655968
1	-1.157862	-4.272866	2.406808
6	-5.420004	-4.818231	4.109312
1	-6.322729	-4.600426	3.554122
6	-4.990545	-4.160879	5.302668
1	-5.505826	-3.353052	5.804888
6	-3.735809	-4.722661	5.689290
1	-3.133341	-4.411813	6.532710
6	-3.390099	-5.728941	4.736716
1	-2.482380	-6.317918	4.733891
6	-4.430265	-5.789606	3.762306
1	-4.444977	-6.435651	2.895240
6	-3.449443	-3.758148	0.539536
6	-4.557405	-4.611891	0.428364
1	-5.074981	-4.897454	1.335234
6	-5.014197	-5.072935	-0.806006
1	-5.893314	-5.707424	-0.856441
6	-4.350186	-4.691561	-1.969181
1	-4.697983	-5.033183	-2.939011
6	-3.244734	-3.844409	-1.886301
1	-2.746368	-3.544967	-2.801222
6	-2.786417	-3.356490	-0.652272
6	-5.078983	-1.578623	2.100900
1	-5.664463	-2.361024	1.615569
6	-5.936610	-0.944784	3.199130
1	-6.866715	-0.543950	2.786847
1	-5.417818	-0.128842	3.710329
1	-6.185162	-1.704962	3.945875
6	-0.945050	-1.898348	-2.375136
6	-1.549628	-0.883712	-3.136070
1	-2.248950	-0.201337	-2.666093
6	-1.236642	-0.735743	-4.488971
1	-1.717573	0.045530	-5.068557
6	-0.301070	-1.581057	-5.089826
1	-0.048811	-1.456218	-6.138995
6	0.313057	-2.585256	-4.336505
1	1.047612	-3.241124	-4.794851
6	-0.013475	-2.749411	-2.989689
1	0.458283	-3.541521	-2.420831
6	-0.042068	-2.909125	0.200232
6	0.195456	-4.285280	0.044266
1	-0.464902	-4.884460	-0.575553
6	1.262979	-4.893773	0.705434
1	1.440857	-5.957468	0.576171
6	2.098322	-4.138709	1.535178
1	2.926970	-4.615188	2.050686
6	1.866574	-2.771735	1.697922
1	2.512767	-2.181304	2.338296
6	0.801702	-2.160009	1.032766
1	0.616493	-1.101443	1.168451
6	-5.516896	-0.911005	-0.786813
6	-5.166459	-0.263716	-1.980404
1	-4.410359	0.514535	-1.958709
6	-5.770928	-0.625822	-3.183875
6	-6.698371	-1.664597	-3.232843
1	-7.142961	-1.967096	-4.174450
6	-7.029992	-2.319966	-2.046585
6	-6.467614	-1.936996	-0.829043
1	-6.765359	-2.463973	0.067311
6	-5.266634	1.259013	1.105166
6	-4.567164	2.007039	2.065722
1	-3.719124	1.568676	2.577604
6	-4.927156	3.323757	2.333394
6	-5.972653	3.933610	1.636531
1	-6.233073	4.968259	1.827509
6	-6.660714	3.192763	0.679592
6	-6.323387	1.861463	0.417077
1	-6.879807	1.314050	-0.335172
29	-2.292198	-0.138168	0.238162
6	-7.706188	3.855264	-0.172820
6	-4.110427	4.148770	3.288318
6	-5.428108	0.155653	-4.421128
6	-7.971326	-3.490731	-2.117847
9	-7.456418	-4.487642	-2.880798
9	-8.235651	-4.019933	-0.902831
9	-9.155444	-3.152560	-2.678077
9	-4.098095	0.423361	-4.494709
9	-6.055638	1.358727	-4.439756
9	-5.771268	-0.488566	-5.554043
9	-7.166590	4.301648	-1.342086
9	-8.265090	4.924244	0.429998
9	-8.700488	3.006245	-0.511386
9	-4.881993	4.959076	4.044934
9	-3.370709	3.388453	4.124252
9	-3.241677	4.957834	2.622366
6	-2.688127	2.718667	-0.768294
6	-1.757673	3.221047	0.214034
6	-1.243961	2.528303	1.355541
1	-1.701428	4.294975	0.314217
77	2.928883	1.759844	-1.618323
15	4.386573	0.398025	-0.502155
8	4.177905	-1.206392	-0.150434
8	5.832590	0.329479	-1.334011
7	4.610688	0.997478	1.051336
6	4.413931	-2.197939	-1.099995
6	3.284111	-2.906786	-1.559309
1	2.316296	-2.661429	-1.143937
6	3.436926	-3.886161	-2.507233
1	2.575831	-4.446331	-2.859389
6	4.714822	-4.162569	-3.061322
6	4.870110	-5.117543	-4.102518
1	3.990156	-5.655848	-4.445463
6	6.100486	-5.345355	-4.675699
1	6.207709	-6.072714	-5.475125
6	7.227588	-4.613538	-4.231695
1	8.192741	-4.774137	-4.703523
6	7.113734	-3.693935	-3.211423
1	7.987968	-3.137527	-2.895867
6	5.862920	-3.449233	-2.577455

6	5.705512	-2.490213	-1.511761
6	6.874049	-1.793828	-0.907220
6	7.987185	-2.508521	-0.337719
6	7.973933	-3.917740	-0.138907
1	7.094434	-4.484259	-0.421679
6	9.051355	-4.566447	0.424248
1	9.012086	-5.641386	0.575548
6	10.205556	-3.846366	0.815699
1	11.048913	-4.372372	1.253299
6	10.247013	-2.479983	0.652912
1	11.119740	-1.911188	0.962985
6	9.146353	-1.777307	0.090830
6	9.162847	-0.361353	-0.021356
1	10.049051	0.182793	0.291726
6	8.057236	0.314896	-0.471972
1	8.034393	1.397097	-0.530602
6	6.915806	-0.408410	-0.879066
6	4.182783	2.419454	1.154110
1	3.198099	2.447756	1.632956
6	5.124303	3.266135	1.989278
6	4.614175	4.073716	3.011460
1	3.546576	4.057877	3.222106
6	5.464614	4.882515	3.771424
1	5.056457	5.498670	4.568011
6	6.836670	4.889185	3.512647
1	7.501402	5.509382	4.107407
6	7.351851	4.090484	2.485452
1	8.419547	4.085131	2.283970
6	6.500400	3.288726	1.728560
1	6.901578	2.644412	0.953757
6	4.042418	3.009137	-0.260022
1	5.041126	3.198803	-0.671491
1	3.549210	3.981744	-0.179981
6	4.649637	0.152336	2.291672
1	4.602619	-0.875261	1.934153
6	5.958150	0.265340	3.073941
6	7.040968	-0.535516	2.689814
1	6.931360	-1.207331	1.845167
6	8.256127	-0.485064	3.374740
1	9.078411	-1.117663	3.052886
6	8.405978	0.371095	4.467654
1	9.350303	0.416509	5.003387
6	7.328123	1.162577	4.872703
1	7.430779	1.831440	5.722824
6	6.113837	1.103344	4.186773
1	5.295841	1.733938	4.514650
6	3.409391	0.375300	3.165057
1	2.494192	0.203109	2.594009
1	3.357622	1.381659	3.585709
1	3.425339	-0.329432	4.000514
6	1.390843	1.202958	-0.205753
1	0.685259	0.486752	-0.625529
1	1.742071	0.913271	0.779368
6	1.141885	2.601925	-0.435863
1	1.561773	3.315281	0.264047
6	0.117702	3.072742	-1.289047
1	-0.419428	2.323717	-1.857759
6	4.432292	2.185631	-3.236463
1	5.374796	2.387575	-2.736266
6	3.475431	3.221937	-3.231982
1	3.757958	4.158619	-2.752021
6	2.353246	3.358000	-4.247915
1	2.755972	3.755507	-5.192323
1	1.657565	4.109994	-3.869291
6	1.574649	2.049773	-4.520263
1	1.987915	1.532915	-5.392715
1	0.542411	2.304508	-4.782125
6	1.541521	1.076334	-3.343909
1	0.566267	0.900749	-2.907323
6	2.482287	0.071048	-3.132038
1	2.149190	-0.789501	-2.560882
6	3.710361	-0.169604	-3.988403
1	4.362737	-0.862952	-3.454708
1	3.404484	-0.681370	-4.912825
6	4.504167	1.111351	-4.322218
1	4.155241	1.537559	-5.268266
1	5.553356	0.842425	-4.477532
6	-0.005521	4.440944	-1.782865
6	0.697624	5.524311	-1.219791
6	-0.864109	4.687830	-2.872473
6	0.536171	6.811061	-1.726656
1	1.371749	5.356359	-0.385910
6	-1.022713	5.976372	-3.378837
1	-1.404110	3.857934	-3.318236
6	-0.325769	7.044175	-2.805062
1	1.084257	7.636998	-1.282222
1	-1.687163	6.147913	-4.220880
1	-0.447695	8.049590	-3.197265
8	-2.705879	1.504890	-1.150809
6	-0.540781	3.293406	2.329366
6	-0.038839	2.710715	3.475678
1	-0.430432	4.361371	2.175638
6	-0.236935	1.336133	3.642602
6	-0.882226	0.610166	2.658556
1	-1.028618	-0.457980	2.756382
7	-1.363645	1.178446	1.535282
6	-4.232927	3.216585	-2.597137
1	-3.704605	2.412290	-3.104620
1	-5.249908	2.882693	-2.365381
1	-4.299861	4.076766	-3.270053
6	-3.793029	4.962196	-0.908083
1	-3.623821	5.036799	0.164729
1	-3.181421	5.711930	-1.424545
1	-4.847869	5.180288	-1.092164
7	-3.510497	3.613347	-1.393591
1	0.475828	3.304177	4.223819
35	0.360882	0.433238	5.268625

C1-P1 *re-re*_3

Number of imaginary frequencies= 1
The smallest frequencies are= -255.2870 9.8902 13.3757 cm(-1)
Electronic energy= -7222.6284099
Zero-point correction= 1.754400
(Hartree/Particle)
Thermal correction to Energy= 1.873024
Thermal correction to Enthalpy= 1.873969
Thermal correction to Gibbs Free Energy= 1.592776
Sum of electronic and zero-point Energies= -7220.874010
Sum of electronic and thermal Energies= -7220.755386
Sum of electronic and thermal Enthalpies= -7220.754441
Sum of electronic and thermal Free Energies= -7221.035634

.....

Cartesian Coordinates

.....

26	4.734876	4.665648	1.790828
15	2.778976	1.496143	-1.852997
15	4.720415	-0.025016	0.973603
6	4.311286	3.285680	0.276447
6	4.471768	2.629714	1.554062
6	3.486268	3.159440	2.443433
1	3.357523	2.884734	3.481337
6	2.739763	4.155098	1.744204
1	1.952984	4.767889	2.161824
6	3.247655	4.235424	0.414901
1	2.908977	4.911343	-0.355475
6	6.712328	5.103573	2.249086
1	7.534788	4.406082	2.160754
6	5.884480	5.281748	3.399768
1	5.965066	4.739122	4.332252
6	4.903276	6.271747	3.089069
1	4.107226	6.604164	3.742301
6	5.124386	6.706628	1.746834
1	4.527708	7.428255	1.204558
6	6.242283	5.987554	1.228673
1	6.639690	6.077519	0.227101
6	5.073361	2.936457	-0.957505
6	6.425866	3.293670	-1.059945
1	6.869296	3.852986	-0.245951
6	7.201259	2.932575	-2.161579

1	8.252026	3.201832	-2.196677
6	6.624981	2.202506	-3.198459
1	7.218922	1.901502	-4.055510
6	5.281961	1.832979	-3.119432
1	4.849837	1.249479	-3.924896
6	4.493837	2.177866	-2.010336
6	5.440212	1.509746	1.827295
1	6.364481	1.738298	1.294295
6	5.781844	1.324266	3.308722
1	6.520698	0.529810	3.443456
1	4.904319	1.071833	3.910538
1	6.198353	2.257802	3.699520
6	2.495753	0.578051	-3.427557
6	2.670048	-0.815338	-3.410763
1	2.964223	-1.310811	-2.493196
6	2.423256	-1.573056	-4.557882
1	2.562388	-2.648807	-4.530720
6	1.987530	-0.950144	-5.729121
1	1.780427	-1.541180	-6.616637
6	1.814441	0.436439	-5.754474
1	1.474782	0.927147	-6.662151
6	2.070009	1.198042	-4.613388
1	1.917692	2.271150	-4.648788
6	1.681455	2.957763	-2.032188
6	2.044408	4.089534	-2.780267
1	3.025720	4.142965	-3.242472
6	1.152634	5.154235	-2.922007
1	1.443336	6.027021	-3.499819
6	-0.112128	5.094536	-2.327153
1	-0.811319	5.918001	-2.441125
6	-0.477433	3.971542	-1.582082
1	-1.457338	3.918817	-1.122687
6	0.420052	2.913593	-1.424861
1	0.139551	2.050393	-0.831819
6	5.971003	-0.589798	-0.256482
6	5.553791	-1.626147	-1.104339
1	4.561945	-2.045645	-0.974622
6	6.401443	-2.111379	-2.099470
6	7.659829	-1.547551	-2.299872
1	8.308401	-1.906805	-3.091011
6	8.062994	-0.500968	-1.470279
6	7.242515	-0.036803	-0.441901
1	7.604516	0.766071	0.185457
6	4.702065	-1.400400	2.197776
6	3.709644	-1.360011	3.190328
1	3.061362	-0.495234	3.278179
6	3.521745	-2.447015	4.041263
6	4.285451	-3.606439	3.900939
1	4.105483	-4.466153	4.536604
6	5.258688	-3.650347	2.906114
6	5.486404	-2.552863	2.074913
1	6.251931	-2.624110	1.312639
29	2.608439	0.155047	-0.035119
6	6.064355	-4.907344	2.727315
6	2.402325	-2.444623	5.043561
6	5.953960	-3.292336	-2.914854
6	9.394121	0.146051	-1.738017
9	9.430555	0.703246	-2.974403
9	9.682281	1.126412	-0.853913
9	10.407182	-0.749805	-1.692741
9	6.097249	-4.451938	-2.224925
9	6.648349	-3.424210	-4.062660
9	4.639346	-3.210586	-3.245790
9	7.051545	-5.017031	3.644752
9	6.646343	-4.968888	1.507978
9	5.289495	-6.013049	2.856370
9	2.771513	-3.007454	6.214737
9	1.947293	-1.203105	5.312761
9	1.338807	-3.166055	4.590925
6	2.009404	-2.805056	0.520106
6	0.863432	-2.457954	1.334344
6	0.586916	-1.161900	1.886880
1	0.430912	-3.259962	1.915220
77	-3.322384	-1.086574	-1.263464
15	-5.180379	-0.221177	-0.276298
8	-5.130235	0.890185	0.963847
8	-6.128182	0.604624	-1.364921
7	-6.046986	-1.433860	0.500085
6	-4.741202	2.196185	0.704787
6	-3.487864	2.600235	1.216052
1	-2.907060	1.885957	1.789243
6	-3.039587	3.874474	0.972015
1	-2.085309	4.205274	1.368787
6	-3.795160	4.760783	0.156473
6	-3.284483	6.038911	-0.199631
1	-2.316676	6.337410	0.194550
6	-3.988888	6.871899	-1.039730
1	-3.587029	7.843374	-1.312195
6	-5.237117	6.453771	-1.560084
1	-5.780550	7.103705	-2.239794
6	-5.768606	5.228910	-1.218230
1	-6.721960	4.923497	-1.632906
6	-5.075786	4.346913	-0.342845
6	-5.589839	3.050355	0.018595
6	-6.971883	2.613923	-0.328568
6	-8.127960	3.381716	0.061258
6	-8.043676	4.517441	0.914972
1	-7.079099	4.819624	1.304820
6	-9.170086	5.229009	1.267304
1	-9.077932	6.086915	1.927181
6	-10.445787	4.849572	0.786234
1	-11.323605	5.423823	1.067622
6	-10.568429	3.743489	-0.023494
1	-11.543205	3.427105	-0.385488
6	-9.428917	2.978401	-0.393426
6	-9.561130	1.808581	-1.188721
1	-10.546331	1.519230	-1.543383
6	-8.465132	1.033292	-1.475770
1	-8.546792	0.116087	-2.048937
6	-7.189765	1.428639	-1.015716
6	-5.442938	-2.781203	0.300783
1	-4.790720	-2.998431	1.155926
6	-6.472364	-3.893572	0.199576
6	-6.274070	-5.090790	0.893887
1	-5.410773	-5.192679	1.548194
6	-7.182515	-6.146043	0.768515
1	-7.019263	-7.068470	1.319337
6	-8.303154	-6.008365	-0.051822
1	-9.018595	-6.821068	-0.140955
6	-8.503235	-4.815446	-0.756362
1	-9.377475	-4.698558	-1.390684
6	-7.589015	-3.771233	-0.638620
1	-7.754702	-2.836197	-1.164787
6	-4.592917	-2.785321	-0.981220
1	-5.270255	-2.851645	-1.840252
1	-3.984551	-3.694256	-0.987588
6	-6.809579	-1.156680	1.767566
1	-7.022820	-0.087728	1.739561
6	-8.168874	-1.849830	1.808171
6	-9.226728	-1.293036	1.078526
1	-9.059276	-0.381243	0.515453
6	-10.485268	-1.893670	1.061738
1	-11.289853	-1.444396	0.485453
6	-10.709360	-3.065143	1.789839
1	-11.686381	-3.540249	1.777687
6	-9.668577	-3.616460	2.540364
1	-9.831680	-4.525534	3.112485
6	-8.411284	-3.008653	2.554762
1	-7.614804	-3.461522	3.133835
6	-5.942115	-1.411747	3.006053
1	-5.035254	-0.804049	2.954251
1	-5.648206	-2.459737	3.107965
1	-6.494011	-1.131852	3.908470
6	-2.423526	-0.942308	0.712994
1	-1.732806	-0.103841	0.747850
1	-3.113382	-0.949671	1.551921
6	-1.958862	-2.216281	0.247681
1	-2.509278	-3.086050	0.590555
6	-0.717999	-2.463590	-0.395898
1	-0.157444	-1.617306	-0.768159

6	-4.132566	-0.907129	-3.324558
1	-5.147622	-1.297974	-3.310912
6	-3.087863	-1.867625	-3.343275
1	-3.379627	-2.917487	-3.360667
6	-1.703626	-1.603257	-3.908452
1	-1.739189	-1.625115	-5.008761
1	-1.060923	-2.434164	-3.608493
6	-1.071831	-0.279898	-3.428919
1	-1.254022	0.519770	-4.153522
1	0.011288	-0.402818	-3.385258
6	-1.553349	0.184129	-2.057720
1	-0.801674	0.170190	-1.274931
6	-2.623135	1.052701	-1.861170
1	-2.611944	1.650899	-0.955842
6	-3.525804	1.575691	-2.959091
1	-4.395086	2.033533	-2.483674
1	-3.000766	2.377920	-3.498656
6	-4.001828	0.486802	-3.946223
1	-3.322140	0.429538	-4.802825
1	-4.975615	0.781597	-4.348778
6	-0.402729	-3.745395	-1.039181
6	-1.009892	-4.961363	-0.668111
6	0.556393	-3.765279	-2.070143
6	-0.668875	-6.150014	-1.310659
1	-1.742089	-4.983548	0.132718
6	0.894530	-4.954242	-2.713181
1	1.042081	-2.838933	-2.352651
6	0.284747	-6.153041	-2.335231
1	-1.145863	-7.078559	-1.010034
1	1.639552	-4.945298	-3.503928
1	0.547972	-7.082085	-2.832511
7	2.504851	-4.074127	0.599916
6	3.479588	-4.544778	-0.378463
1	3.255080	-5.584320	-0.634380
1	3.417061	-3.947691	-1.282892
1	4.499727	-4.496321	0.018635
6	2.123175	-5.051184	1.616552
1	1.837413	-4.564482	2.547970
1	1.300225	-5.689286	1.271348
1	2.988540	-5.682263	1.831596
8	2.516492	-2.003332	-0.325648
6	-0.286717	-1.091165	3.007704
6	-0.634782	0.118956	3.573551
1	-0.658035	-2.011796	3.441051
6	-0.116292	1.278133	2.989209
6	0.717805	1.183299	1.889420
1	1.130387	2.066699	1.418588
7	1.071509	0.000310	1.348849
1	-1.286227	0.162370	4.439816
35	-0.517184	3.037021	3.743722

C1-P1 *re-re*_4

Number of imaginary frequencies= 1
The smallest frequencies are=-280.6810 10.2421 14.1723cm(-1)
Electronic energy= -7222.6274683
Zero-point correction= 1.756318
(Hartree/Particle)
Thermal correction to Energy= 1.874582
Thermal correction to Enthalpy= 1.875527
Thermal correction to Gibbs Free Energy= 1.595160
Sum of electronic and zero-point Energies= -7220.871151
Sum of electronic and thermal Energies= -7220.752886
Sum of electronic and thermal Enthalpies= -7220.751942
Sum of electronic and thermal Free Energies= -7221.032308

.....

Cartesian Coordinates

.....

26	-8.485868	-1.159941	-0.400074
15	-3.890269	0.488585	-2.289694
15	-4.442076	0.587633	1.414697
6	-6.733614	-0.183022	-1.004959
6	-6.624601	-0.668396	0.351238
6	-6.791957	-2.087148	0.323926
1	-6.779286	-2.741573	1.184732
6	-7.035535	-2.482206	-1.026076
1	-7.242945	-3.487407	-1.365825
6	-7.005950	-1.313406	-1.841140
1	-7.177059	-1.278757	-2.906398
6	-9.981751	-0.053489	0.524802
1	-9.808666	0.826261	1.130704
6	-10.001644	-1.402926	0.992684
1	-9.841816	-1.724812	2.013169
6	-10.223555	-2.256837	-0.130393
1	-10.255773	-3.338294	-0.109908
6	-10.341809	-1.435783	-1.292822
1	-10.480035	-1.785103	-2.307577
6	-10.194122	-0.075533	-0.888755
1	-10.208502	0.783223	-1.546153
6	-6.506517	1.236807	-1.406448
6	-7.480631	2.198945	-1.101209
1	-8.393601	1.865712	-0.625080
6	-7.292838	3.553469	-1.375505
1	-8.057215	4.273646	-1.101416
6	-6.109703	3.973204	-1.978033
1	-5.940391	5.024875	-2.185652
6	-5.124804	3.036252	-2.291931
1	-4.203483	3.380059	-2.748135
6	-5.294442	1.671667	-2.009556
6	-6.293866	0.192129	1.539855
1	-6.802610	1.146649	1.397041
6	-6.740406	-0.391702	2.882974
1	-6.513849	0.294128	3.703854
1	-6.256012	-1.347271	3.100626
1	-7.820941	-0.561331	2.858641
6	-2.601243	1.528963	-3.098480
6	-1.603780	2.075398	-2.274544
1	-1.574582	1.820933	-1.221160
6	-0.637141	2.928863	-2.810133
1	0.121433	3.355642	-2.162329
6	-0.645400	3.229869	-4.174273
1	0.106627	3.895331	-4.587061
6	-1.617595	2.667304	-5.005241
1	-1.621572	2.889142	-6.068654
6	-2.593920	1.824523	-4.471006
1	-3.346946	1.402022	-5.127392
6	-4.530306	-0.596210	-3.625788
6	-5.407786	-0.127443	-4.617302
1	-5.714646	0.914269	-4.624738
6	-5.914946	-1.004456	-5.577029
1	-6.595384	-0.635054	-6.338999
6	-5.556523	-2.356694	-5.551675
1	-5.960464	-3.039524	-6.293725
6	-4.681974	-2.827355	-4.569614
1	-4.400027	-3.876159	-4.544278
6	-4.172186	-1.949737	-3.610757
1	-3.497574	-2.314531	-2.845819
6	-4.305581	2.423793	1.368901
6	-3.018207	2.925851	1.130661
1	-2.189064	2.233085	1.024062
6	-2.805738	4.300195	1.026101
6	-3.867316	5.197726	1.111270
1	-3.701775	6.264009	1.004180
6	-5.150378	4.693241	1.324674
6	-5.371630	3.324333	1.475845
1	-6.381371	2.981902	1.655338
6	-3.681160	0.149628	3.031546
6	-3.492546	-1.217419	3.294594
1	-3.860358	-1.962659	2.598880
6	-2.797691	-1.625190	4.429405
6	-2.248681	-0.689371	5.307944
1	-1.673590	-1.012458	6.168004
6	-2.415274	0.664499	5.032753
6	-3.141040	1.087453	3.916883
1	-3.247503	2.149422	3.731423
29	-3.198164	-0.384344	-0.315704
6	-1.793151	1.692998	5.936056
6	-2.500570	-3.080134	4.657377
6	-1.394927	4.792301	0.880946
6	-6.300196	5.662774	1.351848

9	-6.435060	6.302801	0.163526
9	-7.481618	5.061469	1.613391
9	-6.120784	6.625820	2.285452
9	-0.744520	4.768175	2.074186
9	-1.318880	6.054699	0.415060
9	-0.676223	4.008708	0.038383
9	-2.631900	2.090688	6.919120
9	-1.436372	2.806629	5.251096
9	-0.675263	1.221141	6.537798
9	-2.649472	-3.431120	5.953198
9	-3.285075	-3.892700	3.919711
9	-1.209734	-3.371070	4.328897
6	-0.651968	-0.379857	1.403282
6	-0.566397	-1.827466	1.357112
6	-1.602997	-2.725388	0.915396
1	0.062825	-2.278519	2.110382
77	4.030787	-1.613993	-0.760359
15	5.634521	-0.000450	-0.570165
8	6.196891	0.633728	0.857002
8	7.070454	-0.539596	-1.232905
7	5.108842	1.403426	-1.312713
6	7.093439	-0.077609	1.646333
6	6.600133	-0.559689	2.878549
1	5.570784	-0.340843	3.142804
6	7.425333	-1.284566	3.702083
1	7.062791	-1.654779	4.656927
6	8.755128	-1.588338	3.302670
6	9.593241	-2.405814	4.108734
1	9.203360	-2.773366	5.054382
6	10.864022	-2.738743	3.697760
1	11.493832	-3.368788	4.318957
6	11.345498	-2.269879	2.452219
1	12.339476	-2.553892	2.118671
6	10.564927	-1.460860	1.655137
1	10.948451	-1.118661	0.701338
6	9.254560	-1.077958	2.056711
6	8.410493	-0.239289	1.244408
6	8.903203	0.410967	-0.002760
6	10.043335	1.290325	-0.011202
6	10.704100	1.702958	1.179944
1	10.339973	1.351672	2.137942
6	11.788157	2.552477	1.134954
1	12.269819	2.857549	2.059589
6	12.277179	3.036296	-0.101934
1	13.137039	3.699448	-0.122035
6	11.649466	2.675758	-1.272620
1	12.001993	3.054308	-2.228448
6	10.518989	1.814197	-1.261068
6	9.841001	1.481086	-2.465175
1	10.218543	1.866905	-3.407793
6	8.705777	0.709546	-2.435174
1	8.151152	0.467434	-3.335497
6	8.235378	0.211236	-1.200349
6	3.905085	1.191467	-2.158409
1	3.038267	1.598105	-1.621094
6	4.015880	1.901410	-3.499012
6	2.860327	2.403561	-4.107780
1	1.911239	2.335310	-3.585159
6	2.916974	2.974482	-5.381358
1	2.009258	3.350898	-5.844614
6	4.136616	3.061003	-6.056983
1	4.184288	3.510740	-7.044736
6	5.296517	2.565612	-5.453016
1	6.249995	2.631778	-5.970300
6	5.235575	1.984895	-4.185588
1	6.136322	1.605898	-3.711876
6	3.676025	-0.306964	-2.419646
1	4.327386	-0.612328	-3.246664
1	2.646980	-0.445174	-2.761686
6	5.372234	2.840985	-0.978696
1	5.200807	3.357895	-1.926436
6	4.338762	3.390371	0.000851
6	3.274050	4.159199	-0.490836
1	3.197352	4.337418	-1.561037
6	2.320323	4.704840	0.372968
1	1.501075	5.294872	-0.025074
6	2.422142	4.488733	1.748149
1	1.679115	4.905628	2.419606
6	3.477202	3.720803	2.249738
1	3.564098	3.551493	3.319881
6	4.425734	3.172472	1.384374
1	5.239632	2.580225	1.784984
6	6.811456	3.179401	-0.584913
1	7.509970	2.834727	-1.349127
1	7.107949	2.757394	0.373588
1	6.893300	4.268678	-0.516546
6	2.926676	-0.615817	0.846786
1	2.993476	-1.215428	1.752253
1	3.164330	0.432742	1.010726
6	1.917899	-0.892317	-0.124069
1	1.643844	-0.052239	-0.751865
6	1.061163	-2.034169	-0.219269
1	1.348697	-2.928086	0.315880
6	5.264864	-2.857789	-2.116680
1	5.684853	-2.200070	-2.872810
6	3.906860	-3.239476	-2.287151
1	3.389236	-2.863216	-3.168949
6	3.327445	-4.532241	-1.740553
1	3.670242	-5.379199	-2.355137
1	2.245395	-4.485023	-1.868699
6	3.655098	-4.793340	-0.253916
1	4.524851	-5.452348	-0.164650
1	2.821413	-5.335157	0.205465
6	3.912031	-3.529543	0.565482
1	3.172403	-3.319730	1.334513
6	5.171799	-2.962004	0.750669
1	5.319139	-2.371437	1.649633
6	6.449352	-3.447982	0.094156
1	7.209239	-2.676304	0.234683
1	6.808935	-4.342907	0.623375
6	6.302384	-3.738831	-1.415053
1	6.048299	-4.791774	-1.577419
1	7.272928	-3.583834	-1.895816
6	0.284153	-2.272376	-1.446400
6	-0.064988	-1.240757	-2.340847
6	-0.101093	-3.587302	-1.769861
6	-0.712386	-1.527749	-3.540311
1	0.155492	-0.208213	-2.101151
6	-0.753469	-3.874476	-2.968477
1	0.127084	-4.389910	-1.076206
6	-1.042913	-2.846668	-3.868857
1	-0.971582	-0.715908	-4.212699
1	-1.024493	-4.900294	-3.201793
1	-1.546262	-3.064038	-4.805628
7	0.072989	0.273749	2.360595
6	0.277422	1.714731	2.266188
1	1.296480	1.949106	2.583656
1	0.149137	2.047440	1.239595
1	-0.417366	2.262472	2.913052
6	0.647502	-0.340194	3.554104
1	0.149707	-1.274884	3.804807
1	1.722352	-0.520895	3.435897
1	0.505169	0.339463	4.399052
8	-1.280881	0.303097	0.540744
6	-1.472848	-4.097325	1.263375
6	-2.393275	-5.036639	0.842807
1	-0.640566	-4.403161	1.887403
6	-3.462671	-4.586276	0.064591
6	-3.569419	-3.244665	-0.250116
1	-4.399563	-2.873953	-0.836929
7	-2.664988	-2.330089	0.153660
1	-2.288557	-6.081230	1.115485
35	-4.814999	-5.836447	-0.594539

C1-P1 *re-re_5*

Number of imaginary frequencies= 1
The smallest frequencies are= -180.7742 8.6804 12.4610 cm(-1)
Electronic energy= -7222.6357815

Zero-point correction= 1.756784
(Hartree/Particle)
Thermal correction to Energy= 1.874600
Thermal correction to Enthalpy= 1.875544
Thermal correction to Gibbs Free Energy= 1.596819
Sum of electronic and zero-point Energies= -7220.878997
Sum of electronic and thermal Energies= -7220.761181
Sum of electronic and thermal Enthalpies= -7220.760237
Sum of electronic and thermal Free Energies= -7221.038962

Cartesian Coordinates

26	-8.542937	-0.875966	0.241093
15	-4.045284	-0.270153	-2.340607
15	-4.260155	0.966463	1.202010
6	-6.786609	-0.271264	-0.722541
6	-6.602300	-0.346793	0.708562
6	-6.860546	-1.692856	1.112893
1	-6.823933	-2.067641	2.126402
6	-7.234877	-2.442534	-0.042280
1	-7.534578	-3.481146	-0.055788
6	-7.192531	-1.570530	-1.168540
1	-7.444417	-1.834749	-2.184071
6	-9.884203	0.562252	0.912364
1	-9.606972	1.551338	1.252997
6	-9.967906	-0.611388	1.722440
1	-9.758911	-0.669171	2.782318
6	-10.332222	-1.704997	0.879109
1	-10.442475	-2.736295	1.187738
6	-10.473766	-1.208110	-0.452337
1	-10.711621	-1.795436	-1.329512
6	-10.198493	0.191532	-0.432070
1	-10.196059	0.846369	-1.292761
6	-6.499909	0.945189	-1.538176
6	-7.352371	2.054686	-1.436167
1	-8.228177	1.967602	-0.806029
6	-7.085986	3.253023	-2.098037
1	-7.751235	4.101549	-1.973245
6	-5.948307	3.359138	-2.894654
1	-5.718911	4.289191	-3.405274
6	-5.085226	2.269362	-3.014265
1	-4.194451	2.370443	-3.624278
6	-5.331899	1.062694	-2.340455
6	-6.115377	0.787352	1.568631
1	-6.576327	1.702462	1.193693
6	-6.476914	0.647632	3.050139
1	-6.141965	1.518815	3.619668
1	-6.033678	-0.241817	3.505643
1	-7.563985	0.565649	3.145380
6	-2.747429	0.328732	-3.505344
6	-1.589659	0.898895	-2.955619
1	-1.486186	0.973205	-1.879557
6	-0.550380	1.328917	-3.784248
1	0.338764	1.773913	-3.348720
6	-0.653392	1.184201	-5.169048
1	0.159382	1.511058	-5.811667
6	-1.805287	0.618425	-5.725210
1	-1.891683	0.504227	-6.802165
6	-2.848567	0.195963	-4.900069
1	-3.732809	-0.247924	-5.345159
6	-4.826410	-1.659380	-3.252476
6	-5.801861	-1.465223	-4.243472
1	-6.127042	-0.460688	-4.498341
6	-6.378946	-2.562924	-4.884016
1	-7.136836	-2.405290	-5.646231
6	-5.987460	-3.861780	-4.541791
1	-6.444156	-4.714449	-5.036152
6	-5.009122	-4.059782	-3.564455
1	-4.697514	-5.065619	-3.296933
6	-4.431492	-2.962555	-2.922612
1	-3.670555	-3.115378	-2.165873
6	-4.008114	2.692548	0.608198
6	-2.738174	2.972834	0.085864
1	-1.984989	2.191432	0.074560
6	-2.446911	4.240637	-0.420958
6	-3.421363	5.233819	-0.467379
1	-3.201749	6.206656	-0.892801
6	-4.693895	4.941651	0.025141
6	-4.984784	3.695340	0.578635
1	-5.981624	3.523005	0.960584
6	-3.393905	0.958693	2.823045
6	-3.281954	-0.285408	3.463392
1	-3.747596	-1.161373	3.025868
6	-2.542949	-0.408131	4.635708
6	-1.867377	0.690071	5.173052
1	-1.256456	0.581106	6.061824
6	-1.949178	1.914282	4.515125
6	-2.722038	2.059998	3.360353
1	-2.763820	3.026541	2.872533
29	-3.276374	-0.598660	-0.228136
6	-1.176907	3.098222	5.030216
6	-2.338360	-1.760797	5.257092
6	-1.054883	4.496529	-0.923070
6	-5.767213	5.986278	-0.110492
9	-6.023758	6.257452	-1.415158
9	-6.935966	5.607420	0.450933
9	-5.404974	7.158287	0.459818
9	-0.154970	4.589434	0.090619
9	-0.952146	5.629662	-1.647532
9	-0.633446	3.475847	-1.710901
9	-1.904259	3.867624	5.869829
9	-0.767111	3.902649	4.017296
9	-0.064362	2.718209	5.704711
9	-2.396570	-1.713763	6.605597
9	-3.246724	-2.666318	4.837645
9	-1.111300	-2.263264	4.943587
6	-0.643923	-0.379156	1.242117
6	-0.672872	-1.757543	1.668027
6	-1.753703	-2.680203	1.479873
1	-0.020939	-2.028614	2.485115
77	3.930696	-1.592419	-0.893671
15	5.550459	-0.054628	-0.430077
8	6.285326	0.141105	1.045770
8	6.888207	-0.313047	-1.390973
7	4.930343	1.481678	-0.655625
6	7.323852	-0.688567	1.459446
6	7.044822	-1.537535	2.552955
1	6.063599	-1.482553	3.012723
6	8.009272	-2.402945	3.005284
1	7.808912	-3.056697	3.849358
6	9.271121	-2.477756	2.356254
6	10.248945	-3.425306	2.763881
1	10.019121	-4.078256	3.601868
6	11.453841	-3.525777	2.106137
1	12.192114	-4.256677	2.422609
6	11.724435	-2.682300	1.002394
1	12.665757	-2.780078	0.469317
6	10.804134	-1.742115	0.592100
1	11.026750	-1.112127	-0.260716
6	9.556809	-1.594097	1.261343
6	8.570442	-0.625631	0.853818
6	8.850418	0.389554	-0.200456
6	9.942863	1.321710	-0.102127
6	10.764450	1.423919	1.055509
1	10.564966	0.783629	1.906451
6	11.799106	2.332035	1.115673
1	12.407334	2.393692	2.013559
6	12.073948	3.188904	0.023117
1	12.897713	3.894195	0.082452
6	11.284435	3.135153	-1.102981
1	11.470800	3.800548	-1.941991
6	10.199362	2.220918	-1.192285
6	9.352118	2.202050	-2.333567
1	9.561562	2.879058	-3.156852
6	8.263533	1.366497	-2.380221
1	7.577750	1.360553	-3.221128
6	8.016528	0.489537	-1.301804
6	3.613611	1.459558	-1.358215
1	2.828996	1.581005	-0.600363
6	3.480891	2.605654	-2.343912

6	2.358758	3.436176	-2.281071
1	1.638119	3.287469	-1.486567
6	2.167354	4.456239	-3.217168
1	1.282458	5.083054	-3.151863
6	3.118201	4.665244	-4.218023
1	2.980467	5.459796	-4.946047
6	4.256782	3.852141	-4.274567
1	5.004654	4.019289	-5.045104
6	4.436569	2.826869	-3.345656
1	5.326177	2.203290	-3.381690
6	3.412577	0.115812	-2.072814
1	4.009476	0.109509	-2.993340
1	2.366217	0.042921	-2.381544
6	5.222324	2.783125	0.026392
1	5.006195	3.530357	-0.741772
6	4.264734	3.063587	1.184901
6	3.357399	4.127935	1.087307
1	3.308654	4.702099	0.166125
6	2.514824	4.456211	2.153540
1	1.806932	5.273482	2.048205
6	2.566066	3.718888	3.337859
1	1.898091	3.955234	4.160152
6	3.460426	2.648918	3.442210
1	3.503386	2.065982	4.358253
6	4.300792	2.321578	2.375458
1	4.994919	1.493723	2.469399
6	6.678278	3.024747	0.434700
1	7.346954	2.910689	-0.418962
1	7.011552	2.370623	1.238901
1	6.754281	4.058641	0.785543
6	2.938583	-0.939173	0.913684
1	3.116285	-1.627343	1.741336
1	3.111430	0.099200	1.183702
6	1.845119	-1.220466	0.024937
1	1.434888	-0.391137	-0.540010
6	1.051096	-2.395389	0.071081
1	1.349402	-3.164556	0.774441
6	5.054064	-2.427093	-2.641065
1	5.394560	-1.575074	-3.222426
6	3.691848	-2.784084	-2.769676
1	3.086130	-2.199300	-3.461669
6	3.135039	-4.169446	-2.485647
1	3.359767	-4.839103	-3.330162
1	2.047250	-4.083894	-2.443760
6	3.636866	-4.804918	-1.168952
1	4.516057	-5.428581	-1.358795
1	2.863037	-5.480371	-0.789780
6	3.979255	-3.802453	-0.069259
1	3.326400	-3.807393	0.798280
6	5.239951	-3.249612	0.119616
1	5.472060	-2.887397	1.116456
6	6.449586	-3.499030	-0.760525
1	7.203936	-2.751125	-0.509699
1	6.881731	-4.477826	-0.505423
6	6.156216	-3.421875	-2.274221
1	5.887917	-4.410578	-2.660176
1	7.075279	-3.132041	-2.792327
6	0.201301	-2.853434	-1.020858
6	-0.087608	-2.046454	-2.138176
6	-0.284655	-4.176640	-1.004751
6	-0.801100	-2.557881	-3.217377
1	0.257459	-1.021841	-2.167254
6	-1.006964	-4.685646	-2.082808
1	-0.072733	-4.808613	-0.147515
6	-1.255002	-3.881893	-3.199319
1	-1.007793	-1.921521	-4.071688
1	-1.363563	-5.711448	-2.058282
1	-1.810424	-4.277109	-4.044123
7	0.169155	0.492020	1.913129
6	0.487452	1.786917	1.326189
1	1.560385	1.966009	1.411832
1	0.206353	1.796545	0.276283
1	-0.035046	2.597141	1.844554
6	0.795179	0.234947	3.204861
1	0.254472	-0.524569	3.764103
1	1.839726	-0.074411	3.096391
1	0.777293	1.155071	3.793182
8	-1.253336	0.038444	0.208263
6	-1.674381	-3.935691	2.146557
6	-2.663535	-4.887860	2.007221
1	-0.819675	-4.137392	2.783597
6	-3.752965	-4.572464	1.189034
6	-3.811166	-3.341383	0.563837
1	-4.653031	-3.068896	-0.059436
7	-2.842553	-2.413495	0.694775
1	-2.595169	-5.841680	2.519306
35	-5.201254	-5.860062	0.914978

C1-P1 *si-re*_1

Number of imaginary frequencies= 1
The smallest frequencies are= -209.3974 6.2346 12.4896 cm(-1)
Electronic energy= -7222.6227613
Zero-point correction= 1.755738
(Hartree/Particle)
Thermal correction to Energy= 1.874328
Thermal correction to Enthalpy= 1.875272
Thermal correction to Gibbs Free Energy= 1.592693
Sum of electronic and zero-point Energies= -7220.867023
Sum of electronic and thermal Energies= -7220.748433
Sum of electronic and thermal Enthalpies= -7220.747489
Sum of electronic and thermal Free Energies= -7221.030068

Cartesian Coordinates

26	3.572952	4.879751	2.501907
15	2.418129	1.927009	-1.598467
15	4.924159	0.536289	1.045293
6	3.445587	3.768283	0.729847
6	4.054105	2.996938	1.783670
6	3.110520	2.898802	2.853375
1	3.275385	2.390576	3.793998
6	1.937416	3.619918	2.481491
1	1.060388	3.768378	3.097246
6	2.145605	4.162631	1.180128
1	1.451774	4.776030	0.623643
6	5.269727	6.026613	2.861980
1	6.262474	5.790685	2.502144
6	4.696892	5.586050	4.094140
1	5.175506	4.948440	4.825530
6	3.363717	6.093255	4.166478
1	2.654370	5.905167	4.961777
6	3.112633	6.847192	2.979564
1	2.182021	7.334474	2.720013
6	4.289656	6.807100	2.174429
1	4.404676	7.261566	1.199888
6	4.059044	4.019560	-0.603018
6	5.110630	4.938984	-0.725743
1	5.445815	5.454597	0.165162
6	5.724185	5.191531	-1.953134
1	6.543335	5.902305	-2.012683
6	5.276805	4.530560	-3.094518
1	5.738356	4.718428	-4.058980
6	4.244288	3.597735	-2.992832
1	3.927271	3.072808	-3.885969
6	3.640977	3.309816	-1.758606
6	5.366543	2.277138	1.659822
1	5.917807	2.719475	0.824558
6	6.246311	2.331862	2.911026
1	7.193943	1.809206	2.754124
1	5.750575	1.888277	3.778871
1	6.467296	3.376836	3.145718
6	2.369558	1.197541	-3.287919
6	3.478061	0.428191	-3.683506
1	4.338910	0.351849	-3.028763
6	3.499079	-0.211653	-4.920690
1	4.369666	-0.792629	-5.211132
6	2.398558	-0.108088	-5.778077
1	2.405282	-0.615977	-6.737998
6	1.292273	0.651920	-5.394490

1	0.434607	0.738265	-6.055365
6	1.277971	1.308257	-4.159682
1	0.412164	1.899247	-3.882431
6	0.805375	2.778847	-1.388601
6	0.454534	3.913388	-2.136827
1	1.133030	4.297866	-2.892995
6	-0.761467	4.557750	-1.903205
1	-1.029769	5.433150	-2.487763
6	-1.627352	4.084186	-0.911502
1	-2.571521	4.588601	-0.731488
6	-1.275906	2.962428	-0.157669
1	-1.939538	2.595623	0.619344
6	-0.067242	2.305514	-0.397687
1	0.221891	1.446807	0.200695
6	6.302347	0.083958	-0.089659
6	6.973271	-1.146744	-0.047335
1	6.787933	-1.852863	0.752444
6	7.870788	-1.494951	-1.057264
6	8.108461	-0.643251	-2.134968
1	8.796303	-0.926994	-2.921864
6	7.424003	0.569468	-2.190180
6	6.528688	0.934800	-1.183641
1	5.990910	1.874590	-1.272099
6	5.091444	-0.574631	2.502196
6	3.898581	-1.101886	3.008657
1	2.956523	-0.825242	2.548126
6	3.918209	-1.978544	4.095818
6	5.120044	-2.341445	4.696586
1	5.136134	-3.034345	5.529258
6	6.309715	-1.804809	4.198581
6	6.303166	-0.925601	3.116342
1	7.244282	-0.535400	2.746323
29	2.917459	0.333519	-0.067233
6	7.619610	-2.139922	4.859317
6	2.612289	-2.569372	4.549458
6	8.627671	-2.792355	-0.955207
6	7.579848	1.484385	-3.374779
9	6.443221	1.519470	-4.118413
9	7.830663	2.757781	-2.994438
9	8.577926	1.102979	-4.197636
9	7.923550	-3.737762	-0.294633
9	9.794008	-2.632646	-0.283303
9	8.944335	-3.292032	-2.170568
9	7.973446	-1.198373	5.767257
9	8.628379	-2.212012	3.961181
9	7.571792	-3.320200	5.513414
9	2.729858	-3.293780	5.679977
9	1.681109	-1.610992	4.777625
9	2.092325	-3.390298	3.599886
6	3.935070	-2.087640	-1.451342
6	2.028659	-2.656797	-0.217100
6	4.117984	-3.390747	-1.875394
1	4.613519	-1.302627	-1.755690
6	2.202224	-4.012011	-0.615471
6	3.235552	-4.387396	-1.451653
1	1.497935	-4.757520	-0.263523
6	0.871990	-2.329912	0.568414
6	0.703758	-1.169883	1.400876
8	1.338591	-0.078509	1.226974
7	2.916537	-1.716903	-0.656347
1	0.276156	-3.195034	0.820516
7	-0.218480	-1.205434	2.410666
6	-0.561927	0.017185	3.124358
1	-0.141610	0.004317	4.137638
1	-1.649964	0.098671	3.204479
1	-0.167028	0.880529	2.593673
6	-0.841092	-2.414260	2.937350
1	-0.232257	-3.293802	2.738444
1	-1.847280	-2.564235	2.532012
1	-0.925952	-2.314369	4.022175
77	-3.841043	-1.026078	-1.389123
15	-5.659637	-0.552855	-0.100806
8	-5.795202	0.731242	0.939830
8	-6.997396	-0.294416	-1.061569
7	-5.924545	-1.815150	0.967997
6	-6.125221	2.006614	0.491059
6	-5.122654	2.992264	0.621112
1	-4.175524	2.709017	1.065324
6	-5.369715	4.274286	0.197964
1	-4.614398	5.046249	0.311887
6	-6.607010	4.603832	-0.417544
6	-6.840869	5.903858	-0.941919
1	-6.058449	6.651455	-0.840242
6	-8.023019	6.207044	-1.578396
1	-8.189292	7.201538	-1.981868
6	-9.019687	5.212278	-1.720873
1	-9.941758	5.446743	-2.244989
6	-8.831135	3.947331	-1.207538
1	-9.602770	3.197621	-1.335218
6	-7.630125	3.602636	-0.526252
6	-7.397705	2.287473	0.015413
6	-8.465507	1.249374	0.045086
6	-9.731421	1.468081	0.695270
6	-10.010094	2.633850	1.462540
1	-9.244507	3.392620	1.572245
6	-11.230148	2.804226	2.080218
1	-11.414830	3.699976	2.666281
6	-12.242872	1.822254	1.964565
1	-13.201914	1.974052	2.451094
6	-12.000539	0.671697	1.249064
1	-12.761446	-0.100130	1.167408
6	-10.747514	0.456553	0.613189
6	-10.478551	-0.754100	-0.081589
1	-11.259625	-1.505652	-0.153478
6	-9.238676	-0.986209	-0.623808
1	-8.997863	-1.915748	-1.128085
6	-8.240784	0.007576	-0.524975
6	-5.116226	-3.019519	0.628152
1	-4.238541	-3.036202	1.288362
6	-5.893704	-4.306278	0.842454
6	-5.275050	-5.405328	1.449613
1	-4.255989	-5.309343	1.817409
6	-5.957271	-6.617068	1.592573
1	-5.464786	-7.461344	2.067184
6	-7.271491	-6.737817	1.136502
1	-7.805986	-7.676340	1.252892
6	-7.898951	-5.641495	0.535131
1	-8.923673	-5.726821	0.183608
6	-7.213695	-4.436005	0.386459
1	-7.702598	-3.579062	-0.068230
6	-4.646176	-2.934295	-0.830229
1	-5.496500	-3.167771	-1.481997
1	-3.898540	-3.712634	-1.005353
6	-6.444134	-1.803427	2.374562
1	-6.803128	-2.826004	2.516589
6	-5.329446	-1.596523	3.397406
6	-4.786491	-2.714749	4.046712
1	-5.153947	-3.705599	3.792165
6	-3.795876	-2.570777	5.022251
1	-3.391038	-3.450363	5.515254
6	-3.335170	-1.298949	5.365967
1	-2.569684	-1.180523	6.127650
6	-3.865201	-0.176937	4.721166
1	-3.515151	0.816981	4.986660
6	-4.850423	-0.323589	3.742671
1	-5.255041	0.554124	3.253129
6	-7.660391	-0.910026	2.624262
1	-8.465991	-1.159368	1.932091
1	-7.443429	0.152852	2.536777
1	-8.014908	-1.101888	3.641708
6	-2.615237	-0.742190	0.393493
1	-2.109473	0.221315	0.377166
1	-3.110563	-0.945541	1.339555
6	-1.980954	-1.839666	-0.279256
1	-2.256391	-2.844423	0.019436
6	-0.824869	-1.709633	-1.087186
1	-0.419532	-0.709714	-1.205571
6	-5.065657	-1.129784	-3.258112
1	-5.943097	-1.723867	-3.019229
6	-3.859416	-1.833569	-3.482691

1	-3.893845	-2.920790	-3.419875
6	-2.717103	-1.291392	-4.323186
1	-2.988725	-1.350614	-5.388475
1	-1.858142	-1.953019	-4.193314
6	-2.299038	0.155558	-3.972001
1	-2.778001	0.866864	-4.653685
1	-1.224439	0.250748	-4.139361
6	-2.591230	0.588115	-2.536868
1	-1.721152	0.798499	-1.924994
6	-3.775526	1.189506	-2.124735
1	-3.719894	1.818317	-1.241008
6	-4.985510	1.434146	-3.005544
1	-5.828139	1.688104	-2.358558
1	-4.796178	2.318446	-3.632164
6	-5.375320	0.228719	-3.888871
1	-4.875397	0.294755	-4.860610
1	-6.448567	0.280791	-4.095115
6	-0.378734	-2.670246	-2.089277
6	-0.895893	-3.977548	-2.185546
6	0.597722	-2.263610	-3.019823
6	-0.459966	-4.838127	-3.190162
1	-1.648623	-4.317867	-1.481533
6	1.032396	-3.127056	-4.023493
1	1.009304	-1.261856	-2.953623
6	0.502884	-4.416848	-4.115088
1	-0.873082	-5.840787	-3.255370
1	1.781570	-2.787804	-4.731578
1	0.836979	-5.090499	-4.898920
1	3.351171	-5.418830	-1.766153
35	5.603698	-3.802582	-3.076109

C1-P1 *si-re_2*

Number of imaginary frequencies= 1
The smallest frequencies are= -216.8139 6.5130 9.5023 cm(-1)
Electronic energy= -7222.6176109
Zero-point correction= 1.754240
(Hartree/Particle)
Thermal correction to Energy= 1.873228
Thermal correction to Enthalpy= 1.874173
Thermal correction to Gibbs Free Energy= 1.589602
Sum of electronic and zero-point Energies= -7220.863371
Sum of electronic and thermal Energies= -7220.744382
Sum of electronic and thermal Enthalpies= -7220.743438
Sum of electronic and thermal Free Energies= -7221.028008

.....

Cartesian Coordinates

.....

26	3.750607	4.705403	2.840742
15	2.590679	1.976356	-1.414242
15	5.010277	0.394881	1.200302
6	3.620554	3.679845	1.020323
6	4.188778	2.841560	2.044930
6	3.226651	2.722991	3.095725
1	3.363379	2.169748	4.015168
6	2.081083	3.495447	2.741104
1	1.199318	3.641675	3.350562
6	2.325284	4.091448	1.469456
1	1.657445	4.749574	0.932483
6	5.468728	5.800839	3.257170
1	6.457527	5.562139	2.888641
6	4.884311	5.316723	4.467151
1	5.347931	4.637585	5.169928
6	3.561208	5.846068	4.560015
1	2.846762	5.637566	5.345618
6	3.328105	6.657660	3.408205
1	2.407338	7.173091	3.168343
6	4.505791	6.630297	2.603711
1	4.631689	7.125949	1.650842
6	4.264480	3.978728	-0.288373
6	5.340427	4.876139	-0.350146
1	5.673812	5.339397	0.569376
6	5.980872	5.171550	-1.553940
1	6.818023	5.863480	-1.566000
6	5.536939	4.577496	-2.732878
1	6.018896	4.799667	-3.679921
6	4.480979	3.666809	-2.692154
1	4.166363	3.194072	-3.614680
6	3.849183	3.335608	-1.482846
6	5.483642	2.092489	1.908031
1	6.059425	2.559482	1.103312
6	6.343499	2.072651	3.174114
1	7.289940	1.551425	3.006720
1	5.829820	1.591946	4.011104
1	6.568638	3.102590	3.464470
6	2.563007	1.346779	-3.142949
6	3.655126	0.557941	-3.545999
1	4.484058	0.402985	-2.864226
6	3.699833	-0.000518	-4.821403
1	4.556680	-0.598096	-5.118155
6	2.640278	0.206472	-5.710779
1	2.665661	-0.236921	-6.701823
6	1.551396	0.987324	-5.319962
1	0.726444	1.154497	-6.006501
6	1.513388	1.561714	-4.045466
1	0.662007	2.170215	-3.762268
6	0.997360	2.855389	-1.170097
6	0.676025	4.036921	-1.855951
1	1.359978	4.438421	-2.598180
6	-0.515034	4.708414	-1.573413
1	-0.761033	5.620379	-2.109879
6	-1.382550	4.216302	-0.592007
1	-2.305339	4.743577	-0.371687
6	-1.060471	3.046150	0.098612
1	-1.722333	2.664073	0.870031
6	0.120361	2.361403	-0.193223
1	0.388458	1.465855	0.358583
6	6.402732	-0.038677	0.075922
6	7.045867	-1.284766	0.079510
1	6.828656	-2.019939	0.844477
6	7.958435	-1.610131	-0.924557
6	8.236436	-0.720522	-1.961174
1	8.933155	-0.986840	-2.746273
6	7.580386	0.509047	-1.978327
6	6.673814	0.852813	-0.974535
1	6.160414	1.808037	-1.034872
6	5.124426	-0.794139	2.598954
6	3.917159	-1.352025	3.033755
1	2.989047	-1.053618	2.558807
6	3.904508	-2.287124	4.070881
6	5.086857	-2.676387	4.694217
1	5.076638	-3.410010	5.491640
6	6.290276	-2.110304	4.267813
6	6.316408	-1.175733	3.232861
1	7.267359	-0.766147	2.912328
29	3.025509	0.278342	0.036196
6	7.578183	-2.467740	4.959681
6	2.590505	-2.914631	4.443787
6	8.684988	-2.927129	-0.858040
6	7.775248	1.467142	-3.122112
9	6.654586	1.548057	-3.886655
9	8.035907	2.720939	-2.687389
9	8.785067	1.102468	-3.938119
9	7.938797	-3.886247	-0.266784
9	9.829422	-2.823902	-0.138997
9	9.033997	-3.377644	-2.083427
9	7.902000	-1.553217	5.905667
9	8.615321	-2.513065	4.092442
9	7.510502	-3.666596	5.576570
9	2.651475	-3.608716	5.597330
9	1.612359	-1.986944	4.577849
9	2.168680	-3.777474	3.480828
6	4.049268	-2.088867	-1.455307
6	2.091015	-2.680425	-0.318430
6	4.211158	-3.368067	-1.954244
1	4.759060	-1.307810	-1.690927
6	2.243936	-4.013768	-0.791021
6	3.293048	-4.365192	-1.617604
1	1.511216	-4.760223	-0.505634
6	0.912740	-2.370477	0.442310

6	0.730838	-1.258273	1.337277
8	1.395740	-0.173968	1.268586
7	3.014822	-1.738861	-0.670598
1	0.293447	-3.236204	0.628082
7	-0.246102	-1.349196	2.291480
6	-0.582338	-0.188522	3.105735
1	-0.175816	-0.289505	4.119435
1	-1.671302	-0.092870	3.175029
1	-0.169532	0.711372	2.654666
6	-0.877754	-2.609784	2.677697
1	-0.137556	-3.405703	2.779542
1	-1.648012	-2.922653	1.965329
1	-1.351127	-2.471688	3.651564
77	-3.683379	-0.732019	-1.549892
15	-5.454939	-0.249849	-0.211904
8	-5.522152	0.981890	0.900073
8	-6.806182	0.092955	-1.122912
7	-5.748164	-1.550276	0.814362
6	-5.890734	2.277405	0.554432
6	-4.890114	3.264443	0.691266
1	-3.916329	2.962793	1.058463
6	-5.170004	4.568702	0.370282
1	-4.414372	5.339620	0.490047
6	-6.443698	4.924797	-0.147665
6	-6.716896	6.256041	-0.563631
1	-5.935873	7.003537	-0.451012
6	-7.934727	6.590283	-1.110715
1	-8.131776	7.609145	-1.430883
6	-8.927296	5.594790	-1.272751
1	-9.877813	5.852890	-1.730763
6	-8.699769	4.298715	-0.863183
1	-9.470415	3.551712	-1.008607
6	-7.462503	3.920684	-0.269314
6	-7.190516	2.573835	0.170121
6	-8.247399	1.523401	0.160194
6	-9.509104	1.686849	0.835486
6	-9.770218	2.767306	1.723722
1	-8.992723	3.498505	1.911578
6	-10.987412	2.887654	2.358365
1	-11.158276	3.716629	3.039170
6	-12.014912	1.938976	2.138808
1	-12.970564	2.050492	2.642483
6	-11.792438	0.872210	1.298061
1	-12.565927	0.126974	1.131809
6	-10.543643	0.709764	0.638139
6	-10.295080	-0.417249	-0.191226
1	-11.088315	-1.142029	-0.349234
6	-9.054982	-0.613762	-0.746126
1	-8.830325	-1.484666	-1.351330
6	-8.039230	0.342998	-0.535327
6	-5.042076	-2.780884	0.366199
1	-4.141385	-2.905490	0.979630
6	-5.876904	-4.042265	0.495932
6	-5.294013	-5.210717	0.996547
1	-4.261529	-5.189164	1.339407
6	-6.031707	-6.394933	1.082802
1	-5.568229	-7.292636	1.483081
6	-7.365025	-6.418311	0.670064
1	-7.945707	-7.333093	0.748590
6	-7.950890	-5.254886	0.158296
1	-8.990533	-5.262850	-0.157271
6	-7.208863	-4.079835	0.063230
1	-7.670260	-3.169900	-0.304667
6	-4.609157	-2.613472	-1.103806
1	-5.488869	-2.746363	-1.746546
1	-3.919871	-3.424775	-1.354235
6	-6.096822	-1.379842	2.266557
1	-6.469921	-0.360167	2.345233
6	-7.245469	-2.275892	2.715339
6	-8.556062	-1.839252	2.487689
1	-8.716089	-0.875993	2.017179
6	-9.650078	-2.623688	2.853102
1	-10.657959	-2.264780	2.662788
6	-9.445015	-3.860090	3.470359
1	-10.292480	-4.477696	3.754923
6	-8.141851	-4.292306	3.730595
1	-7.972344	-5.249342	4.216136
6	-7.051392	-3.502067	3.362617
1	-6.047562	-3.860363	3.561318
6	-4.855535	-1.473690	3.163088
1	-4.137636	-0.695475	2.890526
1	-4.354707	-2.442907	3.096047
1	-5.144427	-1.320998	4.207255
6	-2.439417	-0.677362	0.229388
1	-1.883119	0.254780	0.308715
1	-2.943192	-0.948719	1.150341
6	-1.851271	-1.739400	-0.537441
1	-2.183576	-2.752028	-0.341733
6	-0.648991	-1.604648	-1.273002
1	-0.195699	-0.617963	-1.300069
6	-4.905902	-0.606344	-3.420442
1	-5.816163	-1.171041	-3.236556
6	-3.740513	-1.358594	-3.696931
1	-3.848630	-2.442711	-3.730760
6	-2.537924	-0.833824	-4.461085
1	-2.751500	-0.841353	-5.541196
1	-1.716024	-1.536972	-4.305749
6	-2.076148	0.574482	-4.028760
1	-2.548434	1.341353	-4.651227
1	-1.002867	0.653017	-4.210995
6	-2.333014	0.904589	-2.561554
1	-1.452816	0.991498	-1.934225
6	-3.481563	1.528403	-2.090116
1	-3.393917	2.064061	-1.150073
6	-4.676652	1.918013	-2.939080
1	-5.501585	2.162886	-2.265652
1	-4.438823	2.841681	-3.487448
6	-5.141196	0.819670	-3.922206
1	-4.648925	0.944396	-4.891919
1	-6.211754	0.950326	-4.106574
6	-0.201671	-2.515000	-2.319968
6	-0.762089	-3.794108	-2.513391
6	0.822982	-2.091602	-3.189204
6	-0.319094	-4.611452	-3.549693
1	-1.553553	-4.144979	-1.858732
6	1.264397	-2.912312	-4.225428
1	1.267942	-1.111874	-3.049695
6	0.694239	-4.174049	-4.411258
1	-0.764971	-5.592231	-3.688947
1	2.051722	-2.562053	-4.884872
1	1.035089	-4.813793	-5.220212
1	3.393029	-5.378199	-1.991261
35	5.715417	-3.746642	-3.141995

C1-P1 *si-re*_3

Number of imaginary frequencies= 1
The smallest frequencies are= -197.1989 8.6085 13.7259 cm(-1)
Electronic energy= -7222.6148556
Zero-point correction= 1.754949
(Hartree/Particle)
Thermal correction to Energy= 1.873794
Thermal correction to Enthalpy= 1.874739
Thermal correction to Gibbs Free Energy= 1.591463
Sum of electronic and zero-point Energies= -7220.859906
Sum of electronic and thermal Energies= -7220.741061
Sum of electronic and thermal Enthalpies= -7220.740117
Sum of electronic and thermal Free Energies= -7221.023393

.....

Cartesian Coordinates

.....

26	3.528601	4.903890	2.540814
15	2.483930	1.882572	-1.541068
15	5.013984	0.585536	1.145216
6	3.448653	3.768440	0.781108
6	4.073219	3.028227	1.848084
6	3.125227	2.912800	2.911998
1	3.298121	2.418099	3.858415
6	1.933266	3.593364	2.524110
1	1.046845	3.719385	3.131448

6	2.134050	4.127768	1.218251
1	1.425762	4.713804	0.650702
6	5.188166	6.103891	2.899930
1	6.190541	5.890923	2.552695
6	4.616213	5.663516	4.132721
1	5.106094	5.051265	4.878127
6	3.268422	6.133268	4.185969
1	2.557588	5.936634	4.977864
6	3.006866	6.863034	2.986272
1	2.064946	7.318847	2.711043
6	4.192414	6.846262	2.192717
1	4.302511	7.289831	1.212583
6	4.064568	4.023735	-0.550071
6	5.092343	4.969741	-0.672666
1	5.404663	5.502762	0.216326
6	5.710212	5.227093	-1.896897
1	6.510352	5.959258	-1.956082
6	5.291411	4.543388	-3.035693
1	5.756624	4.734493	-3.997772
6	4.282557	3.584847	-2.934412
1	3.987348	3.043941	-3.825475
6	3.675642	3.292660	-1.703027
6	5.405997	2.344848	1.741505
1	5.949252	2.788938	0.901867
6	6.278879	2.442914	2.994967
1	7.243003	1.948478	2.846670
1	5.794361	1.995467	3.867185
1	6.466682	3.497241	3.216606
6	2.458898	1.141285	-3.226528
6	3.588554	0.399374	-3.615339
1	4.449462	0.348947	-2.958318
6	3.631534	-0.242093	-4.851130
1	4.517125	-0.802345	-5.136686
6	2.534872	-0.163840	-5.715750
1	2.560175	-0.669795	-6.676353
6	1.409063	0.570555	-5.339793
1	0.556327	0.639571	-6.008860
6	1.368272	1.222832	-4.103199
1	0.484481	1.788692	-3.829084
6	0.854191	2.703911	-1.346888
6	0.490797	3.836069	-2.092431
1	1.165203	4.230735	-2.846981
6	-0.730650	4.468223	-1.853575
1	-1.007527	5.344601	-2.432616
6	-1.589410	3.983436	-0.860994
1	-2.533186	4.483991	-0.670865
6	-1.228796	2.858923	-0.115627
1	-1.886286	2.484749	0.663632
6	-0.013811	2.215874	-0.359709
1	0.289045	1.361490	0.237712
6	6.417499	0.158062	0.032015
6	7.136464	-1.043375	0.106526
1	6.974793	-1.737246	0.922185
6	8.051274	-1.379395	-0.892220
6	8.261526	-0.543294	-1.987607
1	8.963643	-0.817800	-2.765096
6	7.533314	0.642051	-2.071677
6	6.618334	0.993995	-1.078396
1	6.046509	1.910991	-1.189091
6	5.187639	-0.512282	2.611220
6	4.004047	-1.090312	3.083195
1	3.065068	-0.854450	2.595107
6	4.028068	-1.964439	4.171965
6	5.225045	-2.272317	4.811926
1	5.244443	-2.960839	5.648212
6	6.404569	-1.683652	4.350160
6	6.393803	-0.809768	3.263291
1	7.329054	-0.381549	2.921582
29	3.020806	0.320595	0.012771
6	7.705114	-1.949253	5.058983
6	2.736340	-2.612401	4.586006
6	8.854931	-2.645324	-0.758537
6	7.667459	1.541841	-3.270395
9	6.530542	1.539584	-4.014499
9	7.888079	2.826402	-2.909186
9	8.674464	1.171599	-4.087157
9	8.176930	-3.605835	-0.092135
9	10.004381	-2.431117	-0.072563
9	9.207404	-3.152249	-1.960810
9	7.981350	-0.981704	5.966528
9	8.746707	-1.982149	4.196686
9	7.691622	-3.123162	5.725827
9	2.843333	-3.303483	5.737972
9	1.747547	-1.700288	4.749733
9	2.300075	-3.481883	3.636345
6	4.141254	-2.086212	-1.323601
6	2.232969	-2.697387	-0.113160
6	4.370083	-3.388354	-1.727640
1	4.801408	-1.285844	-1.628287
6	2.454334	-4.052126	-0.490192
6	3.511766	-4.406310	-1.304436
1	1.766791	-4.813916	-0.139551
6	1.052305	-2.397424	0.644060
6	0.814467	-1.232284	1.449890
8	1.419684	-0.122472	1.289580
7	3.099657	-1.735882	-0.548592
1	0.471687	-3.276111	0.885870
7	-0.148077	-1.293612	2.422726
6	-0.539432	-0.085927	3.137139
1	-0.095029	-0.064641	4.140077
1	-1.629740	-0.058915	3.239534
1	-0.206532	0.794205	2.591207
6	-0.736250	-2.534792	2.917014
1	-0.011582	-3.348525	2.905114
1	-1.621472	-2.829390	2.341241
1	-1.037454	-2.384613	3.956597
77	-3.637088	-1.138790	-1.433773
15	-5.408193	-0.561772	-0.132310
8	-5.580272	0.833721	0.737650
8	-6.801111	-0.551163	-1.034384
7	-5.530560	-1.667629	1.143465
6	-6.035123	2.010905	0.153211
6	-5.110653	3.076647	0.100524
1	-4.125354	2.926702	0.525776
6	-5.476666	4.266797	-0.475588
1	-4.780665	5.099918	-0.509264
6	-6.760236	4.417151	-1.064455
6	-7.117044	5.613843	-1.743228
1	-6.394037	6.424755	-1.776949
6	-8.341837	5.739591	-2.358122
1	-8.602899	6.655525	-2.880069
6	-9.257256	4.660840	-2.324888
1	-10.212221	4.750595	-2.834623
6	-8.949170	3.494700	-1.658225
1	-9.661425	2.678608	-1.655748
6	-7.702451	3.336794	-0.989287
6	-7.345873	2.129267	-0.285338
6	-8.331375	1.033900	-0.070724
6	-9.604409	1.262615	0.561499
6	-9.935181	2.492780	1.194305
1	-9.202965	3.291015	1.215842
6	-11.158860	2.674713	1.800956
1	-11.381916	3.619802	2.287843
6	-12.123383	1.638910	1.806933
1	-13.085248	1.797632	2.285766
6	-11.830347	0.429163	1.219071
1	-12.552920	-0.382664	1.233189
6	-10.572912	0.204677	0.596189
6	-10.250201	-1.059497	0.035100
1	-10.997394	-1.847941	0.043745
6	-8.999350	-1.294117	-0.478556
1	-8.723817	-2.255726	-0.896691
6	-8.046164	-0.254063	-0.491018
6	-4.819007	-2.933488	0.813426
1	-3.865837	-2.954218	1.351589
6	-5.596904	-4.182054	1.190564
6	-4.929656	-5.272086	1.762428
1	-3.869922	-5.188808	1.994390
6	-5.614378	-6.455354	2.050865
1	-5.083847	-7.290404	2.500295

6	-6.979629	-6.560295	1.773485
1	-7.515451	-7.476671	2.004308
6	-7.652568	-5.476514	1.200904
1	-8.714957	-5.547729	0.983415
6	-6.963759	-4.298693	0.908678
1	-7.484304	-3.452878	0.475298
6	-4.500704	-2.962370	-0.694206
1	-5.416119	-3.194142	-1.252575
1	-3.808730	-3.788062	-0.881448
6	-5.571076	-1.174216	2.568224
1	-4.885278	-0.324837	2.645187
6	-6.948678	-0.682686	2.989429
6	-7.101422	0.618020	3.484186
1	-6.251291	1.295175	3.475411
6	-8.331497	1.054043	3.981449
1	-8.434687	2.069049	4.354858
6	-9.428697	0.190915	3.986408
1	-10.390377	0.530537	4.358664
6	-9.287998	-1.104734	3.483062
1	-10.140821	-1.777737	3.469996
6	-8.057235	-1.538469	2.989089
1	-7.953166	-2.548320	2.606954
6	-5.073312	-2.216905	3.581189
1	-4.038382	-2.516202	3.394643
1	-5.702350	-3.108163	3.602269
1	-5.108390	-1.754768	4.571966
6	-2.384210	-0.807877	0.309809
1	-1.859194	0.143048	0.266673
1	-2.862978	-0.975691	1.270496
6	-1.759292	-1.933287	-0.332390
1	-2.039002	-2.932003	-0.017626
6	-0.587105	-1.820020	-1.113546
1	-0.177751	-0.822036	-1.234873
6	-4.896221	-1.328842	-3.275879
1	-5.783604	-1.883148	-2.985314
6	-3.712817	-2.077072	-3.466274
1	-3.779758	-3.156792	-3.333079
6	-2.550227	-1.627829	-4.333003
1	-2.801285	-1.780764	-5.394043
1	-1.704303	-2.285544	-4.122584
6	-2.110462	-0.162801	-4.109078
1	-2.600324	0.497402	-4.832552
1	-1.039815	-0.094264	-4.310625
6	-2.360990	0.383082	-2.704821
1	-1.475287	0.605052	-2.118206
6	-3.527473	1.026522	-2.309541
1	-3.447724	1.702438	-1.463457
6	-4.749955	1.241128	-3.181703
1	-5.573998	1.549843	-2.534487
1	-4.558335	2.084433	-3.861672
6	-5.181672	-0.004547	-3.985329
1	-4.695125	-0.010937	-4.965800
1	-6.256431	0.062047	-4.180070
6	-0.105997	-2.798443	-2.078549
6	-0.602166	-4.115862	-2.149127
6	0.879680	-2.399414	-3.002869
6	-0.133857	-4.995573	-3.121281
1	-1.365142	-4.446744	-1.451367
6	1.344898	-3.281822	-3.975950
1	1.273873	-1.389495	-2.956547
6	0.838775	-4.582416	-4.040327
1	-0.529235	-6.006324	-3.167454
1	2.099379	-2.948780	-4.681548
1	1.197666	-5.271389	-4.799472
1	3.664168	-5.437707	-1.602858
35	5.880248	-3.771109	-2.907254

C1-P1 *si-si_*1

Number of imaginary frequencies= 1
The smallest frequencies are= -123.2430 6.5976 9.6602 cm(-1)
Electronic energy= -7222.6139549
Zero-point correction= 1.754755
(Hartree/Particle)
Thermal correction to Energy= 1.873208
Thermal correction to Enthalpy= 1.874152
Thermal correction to Gibbs Free Energy= 1.591107
Sum of electronic and zero-point Energies= -7220.859199
Sum of electronic and thermal Energies= -7220.740747
Sum of electronic and thermal Enthalpies= -7220.739803
Sum of electronic and thermal Free Energies= -7221.022848

.....

Cartesian Coordinates

.....

26	5.035540	4.254583	2.966468
15	3.561049	2.295706	-1.620015
15	4.951451	-0.123056	1.058023
6	4.786274	3.443273	1.052508
6	4.926098	2.403798	2.039746
6	3.863602	2.556667	2.983544
1	3.698047	1.934565	3.852886
6	3.085930	3.687663	2.601372
1	2.237095	4.085076	3.139354
6	3.650688	4.234979	1.413943
1	3.304397	5.110035	0.882210
6	6.955507	4.669372	3.651684
1	7.846447	4.133736	3.352093
6	6.099384	4.329154	4.743521
1	6.223790	3.485593	5.409207
6	5.025574	5.270791	4.771618
1	4.190823	5.261747	5.460152
6	5.216943	6.191408	3.696725
1	4.555637	7.005357	3.430404
6	6.409951	5.822127	3.006985
1	6.809845	6.312328	2.129722
6	5.641668	3.583221	-0.154849
6	6.946651	4.081872	-0.031134
1	7.292206	4.370947	0.952957
6	7.793013	4.201483	-1.133400
1	8.801487	4.583466	-1.003407
6	7.335055	3.826959	-2.394035
1	7.978829	3.910666	-3.264049
6	6.046781	3.311399	-2.536465
1	5.720612	2.995985	-3.519532
6	5.191082	3.164061	-1.432438
6	5.902412	1.265634	1.943467
1	6.689924	1.548025	1.238468
6	6.556394	0.875020	3.271241
1	7.262531	0.050067	3.140221
1	5.816887	0.576471	4.019308
1	7.103212	1.737149	3.663580
6	3.644415	1.727885	-3.369028
6	4.236069	0.476326	-3.598783
1	4.598305	-0.104717	-2.755973
6	4.376696	-0.017410	-4.894934
1	4.840491	-0.986365	-5.056209
6	3.917334	0.734662	-5.979834
1	4.018587	0.350436	-6.990736
6	3.329514	1.983976	-5.761235
1	2.974349	2.572925	-6.602171
6	3.194802	2.481864	-4.462659
1	2.737237	3.453448	-4.307392
6	2.311328	3.644733	-1.623630
6	1.019500	3.338959	-1.167521
1	0.817847	2.348136	-0.778363
6	0.022472	4.316253	-1.165737
1	-0.971341	4.071513	-0.801145
6	0.308625	5.609572	-1.611276
1	-0.464912	6.372421	-1.604432
6	1.597083	5.924040	-2.054844
1	1.825360	6.930166	-2.394999
6	2.595897	4.947490	-2.061285
1	3.595821	5.201641	-2.400735
6	6.191891	-0.944994	-0.030792
6	6.356181	-2.337801	-0.111769
1	5.822683	-3.000961	0.556448
6	7.209643	-2.891945	-1.064236
6	7.888125	-2.086438	-1.980407
1	8.543286	-2.525103	-2.724029
6	7.702099	-0.708193	-1.921904

6	6.867243	-0.136824	-0.958832
1	6.733250	0.940434	-0.957584
6	4.553942	-1.348013	2.375641
6	3.221528	-1.386129	2.803457
1	2.500771	-0.711965	2.358390
6	2.821409	-2.283402	3.797150
6	3.738443	-3.157788	4.375241
1	3.425685	-3.862541	5.136499
6	5.069793	-3.111322	3.957944
6	5.482497	-2.210714	2.976170
1	6.524351	-2.196499	2.677850
29	3.130558	0.589568	-0.176657
6	6.091965	-4.000740	4.612839
6	1.370356	-2.337081	4.192284
6	7.458273	-4.376472	-1.104799
6	8.358066	0.196827	-2.930266
9	7.441768	0.751447	-3.763384
9	9.008955	1.222356	-2.333682
9	9.252364	-0.453903	-3.702994
9	7.260205	-4.882364	-2.345572
9	6.666840	-5.061059	-0.254296
9	8.741338	-4.664113	-0.776241
9	7.067758	-4.361860	3.748901
9	5.541081	-5.132761	5.101390
9	6.700882	-3.377719	5.650520
9	1.184025	-2.883061	5.412533
9	0.817977	-1.101425	4.215207
9	0.633974	-3.075433	3.321343
6	2.936145	-2.189322	-1.185528
6	1.108732	-1.780339	0.221149
6	2.688471	-3.549797	-1.205471
1	3.771343	-1.767187	-1.729747
6	0.837690	-3.178241	0.237508
6	1.620029	-4.069870	-0.469736
1	-0.001258	-3.541417	0.821201
6	0.191428	-0.914324	0.902779
6	0.450775	0.437412	1.327051
8	1.470026	1.100761	0.968828
7	2.179468	-1.318970	-0.495263
1	-0.584421	-1.449580	1.428747
7	-0.468249	1.095314	2.116119
6	-0.199867	2.480752	2.482453
1	0.374090	2.974139	1.701803
1	0.365357	2.544156	3.422785
1	-1.154695	2.998174	2.621518
6	-1.442158	0.445319	2.980932
1	-1.688445	-0.551582	2.637987
1	-2.366310	1.029308	2.997148
1	-1.064198	0.372541	4.007812
77	-4.207658	0.693955	-1.558242
15	-5.861341	-0.304227	-0.354238
8	-6.293499	0.131352	1.185835
8	-7.326813	-0.145424	-1.133122
7	-5.497212	-1.919441	-0.089014
6	-7.074101	1.261574	1.407926
6	-6.438235	2.348372	2.046740
1	-5.398192	2.239450	2.336237
6	-7.143095	3.502667	2.282421
1	-6.669335	4.344254	2.779741
6	-8.491924	3.623394	1.851481
6	-9.207757	4.839864	2.019542
1	-8.707420	5.671556	2.508688
6	-10.499398	4.969435	1.562003
1	-11.035365	5.905184	1.690704
6	-11.126113	3.882206	0.907373
1	-12.137030	3.994677	0.526292
6	-10.465827	2.683809	0.743066
1	-10.959663	1.865841	0.232091
6	-9.137439	2.505844	1.221606
6	-8.416795	1.268899	1.061412
6	-9.060602	0.038223	0.520593
6	-10.226836	-0.548762	1.127181
6	-10.781283	-0.070042	2.347485
1	-10.312374	0.766074	2.852401
6	-11.894970	-0.661255	2.903536
1	-12.293973	-0.280571	3.839400
6	-12.520305	-1.762763	2.272109
1	-13.401391	-2.214032	2.718806
6	-11.998221	-2.266677	1.102497
1	-12.457091	-3.123553	0.616083
6	-10.841388	-1.690762	0.510182
6	-10.272682	-2.242196	-0.669925
1	-10.753185	-3.096386	-1.138524
6	-9.112984	-1.725135	-1.192355
1	-8.638361	-2.150063	-2.070284
6	-8.509113	-0.609243	-0.573306
6	-4.362469	-2.378411	-0.927135
1	-3.468882	-2.401763	-0.292395
6	-4.571226	-3.777322	-1.478889
6	-3.493235	-4.669855	-1.521897
1	-2.536281	-4.368950	-1.100706
6	-3.638931	-5.935077	-2.096418
1	-2.793796	-6.617530	-2.123583
6	-4.871780	-6.324011	-2.625270
1	-4.990215	-7.309672	-3.066277
6	-5.955345	-5.440453	-2.578777
1	-6.918314	-5.740081	-2.983466
6	-5.805380	-4.174493	-2.011978
1	-6.646823	-3.488383	-1.966545
6	-4.132932	-1.399923	-2.083708
1	-4.898127	-1.583535	-2.847170
1	-3.170379	-1.618595	-2.548435
6	-5.767722	-2.792761	1.102326
1	-5.686977	-3.802735	0.691128
6	-4.667143	-2.676504	2.157564
6	-3.579407	-3.562967	2.105613
1	-3.545227	-4.314203	1.320967
6	-2.553556	-3.506196	3.053635
1	-1.716385	-4.195401	2.992603
6	-2.612531	-2.572121	4.089613
1	-1.815121	-2.524610	4.825641
6	-3.697102	-1.691803	4.159339
1	-3.751662	-0.962104	4.962692
6	-4.708269	-1.734244	3.196410
1	-5.535739	-1.036848	3.258129
6	-7.182593	-2.699028	1.673551
1	-7.919072	-2.889571	0.891282
1	-7.406083	-1.736359	2.129281
1	-7.291307	-3.472567	2.440098
6	-3.112255	0.735374	0.313012
1	-3.304507	1.659261	0.855627
1	-3.241877	-0.148475	0.934244
6	-2.022546	0.712566	-0.626499
1	-1.551600	1.638780	-0.938844
6	-1.401323	-0.504861	-0.972567
1	-1.854168	-1.393270	-0.553646
6	-5.403607	1.018238	-3.411100
1	-5.938327	0.093811	-3.615758
6	-4.027546	1.034328	-3.754119
1	-3.624370	0.132318	-4.214090
6	-3.205224	2.281227	-4.039908
1	-3.372558	2.616156	-5.075358
1	-2.150087	1.993530	-3.978462
6	-3.465308	3.443644	-3.059015
1	-4.264266	4.090300	-3.434259
1	-2.568380	4.069457	-3.003719
6	-3.817627	2.986304	-1.645366
1	-3.060540	3.186768	-0.890792
6	-5.115394	2.802882	-1.171233
1	-5.261409	2.884149	-0.098444
6	-6.382015	2.930437	-1.994277
1	-7.192856	2.468283	-1.426060
1	-6.638923	3.995043	-2.098033
6	-6.293493	2.262153	-3.382556
1	-5.934746	2.978110	-4.128746
1	-7.301948	1.976292	-3.696770
6	-0.578593	-0.755700	-2.143216
6	0.018410	0.264859	-2.910124
6	-0.419719	-2.092319	-2.565615
6	0.744046	-0.047816	-4.054811

1	-0.086814	1.300788	-2.610139
6	0.323251	-2.403898	-3.701939
1	-0.888884	-2.886624	-1.995184
6	0.908718	-1.380766	-4.450360
1	1.195550	0.745068	-4.638359
1	0.441440	-3.440553	-4.003353
1	1.489391	-1.612846	-5.338043
1	1.406114	-5.133352	-0.455857
35	3.836318	-4.714453	-2.273222

C1-P1 *si-si_2*

Number of imaginary frequencies= 1
The smallest frequencies are= -137.4056 8.9684 11.7779 cm(-1)
Electronic energy= -7222.6224907
Zero-point correction= 1.755417
(Hartree/Particle)
Thermal correction to Energy= 1.873917
Thermal correction to Enthalpy= 1.874862
Thermal correction to Gibbs Free Energy= 1.593551
Sum of electronic and zero-point Energies= -7220.867073
Sum of electronic and thermal Energies= -7220.748573
Sum of electronic and thermal Enthalpies= -7220.747629
Sum of electronic and thermal Free Energies= -7221.028940

.....

Cartesian Coordinates

.....

26	3.553249	5.046322	2.234886
15	2.258195	1.915635	-1.698219
15	4.679298	0.568674	1.023704
6	3.361399	3.846684	0.523002
6	3.934571	3.106577	1.617797
6	2.990953	3.116651	2.692892
1	3.133540	2.653601	3.660178
6	1.854544	3.875379	2.282060
1	0.989414	4.104864	2.889879
6	2.086282	4.333540	0.952099
1	1.424204	4.951502	0.362846
6	5.306005	6.129042	2.522573
1	6.280392	5.829949	2.159826
6	4.731437	5.769021	3.779708
1	5.190080	5.140755	4.531609
6	3.424136	6.340333	3.846259
1	2.717830	6.217210	4.656730
6	3.190429	7.052857	2.630590
1	2.278984	7.569998	2.360966
6	4.353037	6.923893	1.813835
1	4.475812	7.329184	0.818644
6	3.977802	3.999845	-0.823701
6	5.055791	4.879659	-0.999139
1	5.412577	5.428629	-0.137251
6	5.665906	5.054341	-2.241334
1	6.506498	5.734862	-2.340937
6	5.183203	4.358651	-3.347292
1	5.635472	4.491773	-4.325365
6	4.121655	3.466567	-3.193119
1	3.773054	2.920786	-4.061386
6	3.526791	3.247655	-1.940098
6	5.210459	2.319627	1.531356
1	5.775351	2.688006	0.670026
6	6.104315	2.404763	2.770820
1	7.019406	1.819882	2.640895
1	5.593599	2.046556	3.668887
1	6.385601	3.448386	2.935991
6	2.188332	1.061324	-3.328139
6	3.346713	0.419328	-3.801677
1	4.281234	0.517127	-3.260231
6	3.321995	-0.311742	-4.987617
1	4.232029	-0.785271	-5.344190
6	2.131037	-0.433269	-5.710826
1	2.108311	-1.007168	-6.632617
6	0.971302	0.184725	-5.239812
1	0.040000	0.090528	-5.790640
6	0.999831	0.931406	-4.058383
1	0.093600	1.410436	-3.707246
6	0.672798	2.835092	-1.581351
6	-0.187212	2.547478	-0.512112
1	0.077982	1.769010	0.197359
6	-1.370396	3.273573	-0.356273
1	-2.025304	3.055430	0.479325
6	-1.713258	4.269565	-1.272136
1	-2.642460	4.819240	-1.154887
6	-0.860810	4.553753	-2.344981
1	-1.122073	5.330127	-3.058314
6	0.332767	3.846338	-2.494458
1	1.000738	4.081570	-3.318326
6	6.026985	-0.019270	-0.082018
6	6.595904	-1.296854	0.009897
1	6.336027	-1.963750	0.822872
6	7.494065	-1.739799	-0.962041
6	7.826953	-0.939172	-2.052953
1	8.516989	-1.293878	-2.808373
6	7.237040	0.319383	-2.161511
6	6.345595	0.779385	-1.191589
1	5.883906	1.753393	-1.319437
6	4.811329	-0.442751	2.554701
6	3.599867	-0.816131	3.146588
1	2.668025	-0.506162	2.687573
6	3.590075	-1.581059	4.315676
6	4.781761	-1.985866	4.910151
1	4.773355	-2.589974	5.809571
6	5.991313	-1.604932	4.323687
6	6.013944	-0.834894	3.161837
1	6.967941	-0.557220	2.729079
29	2.668430	0.393062	-0.078721
6	7.290267	-1.983612	4.982739
6	2.262842	-2.005319	4.881286
6	8.144891	-3.086178	-0.790344
6	7.494514	1.181479	-3.367588
9	6.423385	1.186772	-4.206377
9	7.718190	2.470495	-3.026349
9	8.554253	0.760494	-4.087010
9	8.566792	-3.604388	-1.963616
9	7.304205	-3.981603	-0.224696
9	9.230560	-3.009028	0.018418
9	8.285222	-2.136964	4.080157
9	7.187482	-3.138530	5.675792
9	7.699460	-1.033792	5.858147
9	2.371509	-2.545424	6.112153
9	1.403110	-0.962079	4.970515
9	1.660401	-2.931941	4.092139
6	3.622368	-2.034940	-1.458929
6	1.942795	-2.627881	0.064235
6	3.900152	-3.356154	-1.755957
1	4.169865	-1.229708	-1.927966
6	2.242767	-3.999025	-0.179083
6	3.207450	-4.372882	-1.093852
1	1.682212	-4.761545	0.350448
6	0.835539	-2.331086	0.924799
6	0.514138	-1.064181	1.523061
8	1.054040	0.036301	1.180009
7	2.668739	-1.669981	-0.585378
1	0.447710	-3.210027	1.417321
7	-0.440976	-1.012455	2.501785
6	-0.745803	0.249082	3.163206
1	0.022868	0.983775	2.933967
1	-0.786431	0.090448	4.244943
1	-1.719925	0.634068	2.834618
6	-1.216908	-2.142510	2.991620
1	-1.211365	-2.976253	2.293773
1	-2.253771	-1.828957	3.124211
1	-0.835455	-2.489741	3.957683
77	-3.707888	-0.850276	-1.543522
15	-5.448924	-0.714589	-0.076332
8	-5.607665	0.426957	1.123414
8	-6.869798	-0.450085	-0.905915
7	-5.512792	-2.100000	0.860186
6	-5.790655	1.759994	0.779499
6	-4.714777	2.632063	1.051315
1	-3.836126	2.222442	1.536429

6	-4.807767	3.954689	0.696516
1	-3.992761	4.640081	0.909499
6	-5.954423	4.432297	0.004880
6	-6.019960	5.771232	-0.467986
1	-5.183158	6.434326	-0.263841
6	-7.109974	6.216688	-1.181111
1	-7.146439	7.239304	-1.544836
6	-8.181912	5.333375	-1.452945
1	-9.030074	5.680807	-2.035753
6	-8.159321	4.035510	-0.989887
1	-8.986007	3.371189	-1.212720
6	-7.057074	3.544319	-0.236513
6	-6.996040	2.188092	0.247676
6	-8.166413	1.267524	0.194369
6	-9.430453	1.628646	0.789898
6	-9.606276	2.808934	1.566171
1	-8.761897	3.465585	1.736120
6	-10.828545	3.123513	2.120183
1	-10.930841	4.027358	2.713973
6	-11.947972	2.279291	1.930952
1	-12.906616	2.543988	2.367317
6	-11.809031	1.115784	1.208791
1	-12.652828	0.444431	1.071993
6	-10.558742	0.754182	0.637913
6	-10.404490	-0.473038	-0.061694
1	-11.266415	-1.122437	-0.185676
6	-9.176444	-0.849646	-0.542530
1	-9.023838	-1.798714	-1.045762
6	-8.065912	0.009809	-0.382109
6	-4.501921	-3.118500	0.457995
1	-3.629021	-3.010065	1.116018
6	-5.023434	-4.538024	0.603354
6	-4.222087	-5.519251	1.197639
1	-3.254336	-5.240838	1.608630
6	-4.659035	-6.845007	1.275352
1	-4.026154	-7.596156	1.739958
6	-5.910337	-7.199472	0.767254
1	-6.255572	-8.227297	0.833297
6	-6.720642	-6.222648	0.178300
1	-7.697960	-6.490987	-0.213504
6	-6.277998	-4.903052	0.093097
1	-6.909418	-4.140114	-0.355085
6	-4.089888	-2.884641	-1.000589
1	-4.911856	-3.235071	-1.635955
1	-3.234954	-3.518607	-1.237735
6	-6.123175	-2.312939	2.210306
1	-6.355628	-3.380393	2.222160
6	-5.147451	-2.084111	3.365651
6	-4.611870	-3.197659	4.029655
1	-4.852347	-4.195276	3.672202
6	-3.791357	-3.044072	5.150712
1	-3.394122	-3.921854	5.653014
6	-3.487745	-1.766524	5.624259
1	-2.852972	-1.641965	6.497006
6	-4.002776	-0.648065	4.962436
1	-3.771648	0.350791	5.322621
6	-4.824772	-0.804546	3.844175
1	-5.228227	0.069976	3.349837
6	-7.461572	-1.604149	2.426798
1	-8.172297	-1.884760	1.647135
1	-7.377345	-0.518128	2.448044
1	-7.867784	-1.931238	3.388568
6	-2.409812	-0.296112	0.108386
1	-2.356429	0.779221	0.246792
1	-2.632504	-0.831062	1.026802
6	-1.469224	-0.900134	-0.799432
1	-0.893359	-0.264651	-1.462908
6	-1.091118	-2.255970	-0.684132
1	-1.618536	-2.825742	0.070706
6	-5.027942	-1.169314	-3.307416
1	-5.735886	-1.951828	-3.043774
6	-3.717441	-1.608239	-3.632754
1	-3.543473	-2.684087	-3.608405
6	-2.729067	-0.857784	-4.510125
1	-2.939581	-1.059692	-5.572099
1	-1.732271	-1.265556	-4.312520
6	-2.712851	0.659854	-4.252819
1	-3.480782	1.155419	-4.852598
1	-1.761236	1.074769	-4.593088
6	-2.911798	1.025805	-2.787287
1	-2.028262	1.355916	-2.249450
6	-4.140183	1.381395	-2.256233
1	-4.137643	1.982577	-1.353050
6	-5.441042	1.376231	-3.034584
1	-6.257101	1.504336	-2.323848
1	-5.459655	2.258655	-3.690997
6	-5.691587	0.093028	-3.863322
1	-5.368527	0.237585	-4.899464
1	-6.770852	-0.080248	-3.904612
6	-0.457270	-3.051854	-1.722450
6	0.291787	-2.484568	-2.773272
6	-0.610582	-4.452514	-1.684501
6	0.852440	-3.294878	-3.756096
1	0.448403	-1.413375	-2.813282
6	-0.062559	-5.259682	-2.680552
1	-1.170748	-4.903515	-0.869257
6	0.672324	-4.682903	-3.719268
1	1.433945	-2.840353	-4.551264
1	-0.201887	-6.336155	-2.641063
1	1.109308	-5.308525	-4.492277
1	3.408223	-5.419594	-1.293729
35	5.243145	-3.767622	-3.113830

C1-P1 *si-si_*3

Number of imaginary frequencies= 1
The smallest frequencies are= -153.6881 8.3775 10.6465 cm(-1)
Electronic energy= -7222.62065
Zero-point correction= 1.754803
(Hartree/Particle)
Thermal correction to Energy= 1.873748
Thermal correction to Enthalpy= 1.874692
Thermal correction to Gibbs Free Energy= 1.591384
Sum of electronic and zero-point Energies= -7220.865847
Sum of electronic and thermal Energies= -7220.746902
Sum of electronic and thermal Enthalpies= -7220.745958
Sum of electronic and thermal Free Energies= -7221.029266

.....

Cartesian Coordinates

.....

26	3.848819	4.474283	3.163302
15	1.178209	2.281145	-0.762769
15	4.500708	0.586735	0.479643
6	3.024928	3.723749	1.383135
6	3.993776	2.811314	1.934741
6	3.547088	2.432744	3.239859
1	4.065136	1.763240	3.913422
6	2.327912	3.122690	3.509300
1	1.763926	3.082151	4.431633
6	2.013831	3.927192	2.375468
1	1.163368	4.585731	2.281021
6	5.547755	5.667987	3.062239
1	6.305671	5.590942	2.294452
6	5.522873	4.941171	4.291565
1	6.255172	4.214109	4.615597
6	4.335137	5.306523	4.995717
1	4.009062	4.901281	5.944615
6	3.625225	6.258076	4.201508
1	2.669078	6.702885	4.443966
6	4.374470	6.482581	3.008201
1	4.083149	7.129097	2.191613
6	3.093700	4.259112	-0.006689
6	4.022822	5.264784	-0.310391
1	4.632757	5.654333	0.494057
6	4.184005	5.753477	-1.607344
1	4.919165	6.527891	-1.806286
6	3.400000	5.239290	-2.636242
1	3.512140	5.602377	-3.653132
6	2.472362	4.233786	-2.360597
1	1.882765	3.835637	-3.177095

6	2.311564	3.720749	-1.063589
6	5.144069	2.234710	1.163966
1	5.296733	2.843966	0.267729
6	6.465568	2.166602	1.932345
1	7.256095	1.716619	1.324578
1	6.372406	1.589436	2.855936
1	6.774983	3.180950	2.199109
6	0.393841	2.041141	-2.411573
6	1.067668	1.203452	-3.315877
1	1.980277	0.709333	-3.000282
6	0.596304	1.033693	-4.617632
1	1.136412	0.393055	-5.308972
6	-0.568762	1.689279	-5.027160
1	-0.942618	1.554707	-6.037836
6	-1.257566	2.507159	-4.128538
1	-2.172781	3.006040	-4.434568
6	-0.779114	2.685727	-2.828853
1	-1.326746	3.322348	-2.145215
6	-0.125620	3.020705	0.300825
6	-0.593197	2.270210	1.388253
1	-0.219851	1.263351	1.539739
6	-1.487436	2.836374	2.298559
1	-1.831361	2.247610	3.141152
6	-1.927450	4.150463	2.127312
1	-2.621388	4.591200	2.837600
6	-1.472429	4.901163	1.037651
1	-1.812616	5.923456	0.899746
6	-0.571297	4.342122	0.130005
1	-0.190951	4.944895	-0.689500
6	5.435463	0.398553	-1.092958
6	6.286664	-0.661066	-1.430276
1	6.507317	-1.449239	-0.722155
6	6.846088	-0.730199	-2.707567
6	6.547120	0.222850	-3.680259
1	6.969642	0.148144	-4.674684
6	5.669381	1.255448	-3.355247
6	5.123158	1.350936	-2.075805
1	4.428959	2.157139	-1.853630
6	5.123819	-0.668581	1.669191
6	4.155203	-1.205005	2.527652
1	3.124104	-0.890941	2.423965
6	4.512604	-2.123019	3.515225
6	5.836872	-2.533404	3.658627
1	6.114385	-3.252565	4.420016
6	6.803026	-1.994915	2.808357
6	6.459806	-1.060160	1.829635
1	7.241128	-0.641538	1.206732
29	2.216608	0.413531	0.037248
6	8.252313	-2.363202	2.976967
6	3.437939	-2.713367	4.385979
6	7.829324	-1.825408	-3.022511
6	5.254087	2.274895	-4.380564
9	3.903434	2.292144	-4.532466
9	5.614509	3.527973	-4.017604
9	5.788331	2.037324	-5.595167
9	7.805924	-2.171607	-4.328772
9	7.595332	-2.941836	-2.297859
9	9.099534	-1.439822	-2.744936
9	8.874177	-2.494772	1.782280
9	8.411429	-3.523197	3.648303
9	8.929473	-1.410475	3.663001
9	3.919794	-3.144814	5.570935
9	2.454102	-1.820618	4.647097
9	2.842209	-3.781858	3.794415
6	3.021907	-1.777740	-1.904670
6	2.167577	-2.715146	0.063756
6	3.602165	-2.973571	-2.286561
1	3.122378	-0.893907	-2.522884
6	2.824318	-3.936880	-0.260199
6	3.536372	-4.078634	-1.434171
1	2.729397	-4.779059	0.416954
6	1.270267	-2.718700	1.178280
6	0.781649	-1.576942	1.893963
8	1.078908	-0.377469	1.590791
7	2.330292	-1.630285	-0.759120
1	1.212286	-3.671699	1.684084
7	-0.061312	-1.764092	2.958255
6	-0.414931	-0.627346	3.803012
1	0.248974	0.209982	3.597473
1	-0.316030	-0.909569	4.855238
1	-1.449523	-0.315214	3.628489
6	-0.448460	-3.070141	3.475949
1	-0.627818	-3.786026	2.673404
1	-1.379810	-2.958540	4.036234
1	0.317624	-3.481235	4.144909
77	-3.324642	-1.621299	-1.294851
15	-4.944643	-0.732540	0.043809
8	-4.932145	0.801641	0.679589
8	-6.379497	-0.682462	-0.807514
7	-5.080180	-1.627181	1.451633
6	-5.100774	1.896646	-0.167704
6	-3.964191	2.704181	-0.389575
1	-3.040737	2.450861	0.115718
6	-4.056706	3.784046	-1.231977
1	-3.197338	4.427660	-1.389436
6	-5.263724	4.053896	-1.930278
6	-5.336995	5.103659	-2.885651
1	-4.455362	5.718532	-3.047263
6	-6.490098	5.327708	-3.603134
1	-6.533811	6.127889	-4.336182
6	-7.618508	4.499129	-3.395307
1	-8.519027	4.660412	-3.980854
6	-7.585925	3.485267	-2.462249
1	-8.457292	2.856058	-2.327152
6	-6.419073	3.237535	-1.686188
6	-6.344359	2.175761	-0.713306
6	-7.542507	1.375686	-0.335997
6	-8.743468	1.995955	0.164429
6	-8.814764	3.380612	0.485271
1	-7.935068	4.000750	0.360040
6	-9.977991	3.940896	0.967546
1	-10.002493	4.998852	1.212731
6	-11.138238	3.152175	1.152705
1	-12.049665	3.609194	1.526728
6	-11.099940	1.805100	0.871968
1	-11.977183	1.182221	1.026458
6	-9.911675	1.192444	0.389654
6	-9.856455	-0.206779	0.145953
1	-10.750890	-0.804571	0.297085
6	-8.680442	-0.800162	-0.237790
1	-8.600879	-1.871435	-0.389903
6	-7.528510	-0.006543	-0.437150
6	-4.212015	-2.840017	1.445056
1	-3.276879	-2.595896	1.966795
6	-4.851954	-4.024690	2.148805
6	-4.095567	-4.801431	3.033908
1	-3.071968	-4.511759	3.258255
6	-4.644765	-5.940140	3.630678
1	-4.045167	-6.532792	4.316210
6	-5.962462	-6.308890	3.353181
1	-6.393880	-7.189018	3.821423
6	-6.726491	-5.535619	2.472273
1	-7.753992	-5.814453	2.255047
6	-6.173375	-4.405407	1.871021
1	-6.767922	-3.798463	1.193087
6	-3.910899	-3.231993	-0.005033
1	-4.821695	-3.673559	-0.427742
1	-3.159564	-4.022940	-0.014769
6	-5.650701	-1.249343	2.781834
1	-5.949910	-2.207906	3.210586
6	-4.639110	-0.661164	3.766310
6	-4.098134	-1.497888	4.755029
1	-4.330872	-2.559357	4.735570
6	-3.302073	-0.982616	5.781105
1	-2.902781	-1.648672	6.541119
6	-3.038756	0.386943	5.837904
1	-2.436956	0.797155	6.643878
6	-3.554729	1.227220	4.847388
1	-3.361872	2.295660	4.890126
6	-4.337230	0.708048	3.812593

1	-4.736483	1.375295	3.057045
6	-6.934065	-0.420467	2.715006
1	-7.699089	-0.947278	2.142862
1	-6.788614	0.566015	2.276376
1	-7.306845	-0.285621	3.734624
6	-1.821642	-0.703976	-0.028111
1	-1.635323	0.332679	-0.296065
1	-1.996050	-0.841237	1.037375
6	-1.037238	-1.703688	-0.709463
1	-0.457572	-1.410696	-1.575806
6	-0.824306	-2.990047	-0.188832
1	-1.320578	-3.219276	0.745581
6	-4.850255	-2.360839	-2.784622
1	-5.639110	-2.831256	-2.204272
6	-3.664863	-3.103798	-2.958871
1	-3.634302	-4.100095	-2.518546
6	-2.672384	-2.900508	-4.088932
1	-3.056806	-3.371339	-5.006939
1	-1.763558	-3.447402	-3.826132
6	-2.312571	-1.424893	-4.364233
1	-2.960821	-1.011953	-5.144070
1	-1.294937	-1.374735	-4.763224
6	-2.385423	-0.517842	-3.139621
1	-1.436961	-0.120114	-2.796131
6	-3.514041	0.199736	-2.770012
1	-3.351771	1.095364	-2.180690
6	-4.853531	0.129334	-3.472657
1	-5.589360	0.629613	-2.843732
1	-4.791438	0.712052	-4.403847
6	-5.338757	-1.305436	-3.775992
1	-5.034925	-1.603745	-4.784820
1	-6.432663	-1.309331	-3.773543
6	-0.353701	-4.139954	-0.949616
6	0.199388	-4.026353	-2.239944
6	-0.459283	-5.422702	-0.376075
6	0.612141	-5.158344	-2.937956
1	0.318636	-3.048795	-2.693010
6	-0.044223	-6.554473	-1.074711
1	-0.872054	-5.522841	0.624781
6	0.489483	-6.426573	-2.361409
1	1.038874	-5.050168	-3.930888
1	-0.137868	-7.535724	-0.618454
1	0.812653	-7.307781	-2.907900
1	4.005926	-5.021776	-1.690962
35	4.469497	-3.113695	-4.032676

C1-P1 *si-si_*4

Number of imaginary frequencies= 2
The smallest frequencies are=-150.0093 -2.3103 11.0100cm(-1)
Electronic energy= -7222.6173492
Zero-point correction= 1.754340
(Hartree/Particle)
Thermal correction to Energy= 1.872225
Thermal correction to Enthalpy= 1.873170
Thermal correction to Gibbs Free Energy= 1.594755
Sum of electronic and zero-point Energies= -7220.863009
Sum of electronic and thermal Energies= -7220.745124
Sum of electronic and thermal Enthalpies= -7220.744180
Sum of electronic and thermal Free Energies= -7221.022594

.....

Cartesian Coordinates

.....

26	-7.190961	-2.567863	2.869730
15	-5.003359	-1.675470	-1.741316
15	-4.423367	0.892806	1.129024
6	-6.554572	-1.928662	0.980697
6	-5.978186	-1.122548	2.026955
6	-5.213391	-1.988421	2.871215
1	-4.658873	-1.686093	3.748886
6	-5.330740	-3.317976	2.371319
1	-4.900280	-4.204496	2.817133
6	-6.159240	-3.284643	1.212650
1	-6.459225	-4.134294	0.616324
6	-8.908072	-1.730530	3.686032
1	-9.253091	-0.724528	3.488603
6	-8.002711	-2.118288	4.721000
1	-7.538141	-1.456622	5.439830
6	-7.781590	-3.525054	4.608781
1	-7.118533	-4.115375	5.227599
6	-8.547825	-4.006290	3.503568
1	-8.568940	-5.024784	3.139005
6	-9.244680	-2.898726	2.934735
1	-9.888733	-2.934862	2.066658
6	-7.345279	-1.390897	-0.160247
6	-8.653426	-0.931305	0.050845
1	-9.063573	-0.995168	1.050450
6	-9.419836	-0.399845	-0.986696
1	-10.426930	-0.044630	-0.788318
6	-8.886949	-0.332766	-2.271884
1	-9.470615	0.073170	-3.092200
6	-7.580744	-0.765367	-2.500662
1	-7.171041	-0.682047	-3.500164
6	-6.787788	-1.272250	-1.459241
6	-6.009272	0.378744	2.048138
1	-6.825645	0.715712	1.402887
6	-6.186120	1.004762	3.433190
1	-6.149363	2.097269	3.381888
1	-5.413577	0.671946	4.131783
1	-7.158495	0.711020	3.839812
6	-4.710028	-1.116748	-3.470629
6	-4.585035	0.266165	-3.688544
1	-4.724606	0.955018	-2.860708
6	-4.307574	0.764084	-4.960400
1	-4.223660	1.836383	-5.113605
6	-4.137853	-0.118117	-6.032855
1	-3.911786	0.265991	-7.023396
6	-4.266959	-1.493256	-5.826415
1	-4.142673	-2.182869	-6.656650
6	-4.557269	-1.992495	-4.553246
1	-4.655374	-3.062756	-4.406639
6	-4.977965	-3.508255	-1.828976
6	-3.828382	-4.173134	-1.380227
1	-2.994790	-3.595887	-0.996666
6	-3.774902	-5.568638	-1.396948
1	-2.882679	-6.076292	-1.041100
6	-4.866560	-6.306979	-1.859695
1	-4.827756	-7.392780	-1.864982
6	-6.013517	-5.647182	-2.314558
1	-6.863597	-6.218532	-2.676761
6	-6.071039	-4.252734	-2.300094
1	-6.968404	-3.746314	-2.643575
6	-4.878985	2.418297	0.204021
6	-4.120192	3.598672	0.182584
1	-3.230508	3.702376	0.787962
6	-4.495382	4.663664	-0.635814
6	-5.589685	4.561724	-1.494808
1	-5.868407	5.388504	-2.137173
6	-6.309226	3.369602	-1.517493
6	-5.970430	2.310714	-0.673224
1	-6.547140	1.392104	-0.724754
6	-3.288957	1.364788	2.500010
6	-2.505807	0.309347	2.988611
1	-2.580418	-0.666226	2.525222
6	-1.651209	0.505133	4.073010
6	-1.520783	1.762201	4.657386
1	-0.839738	1.918296	5.486438
6	-2.286626	2.816989	4.161276
6	-3.191783	2.619145	3.117457
1	-3.814226	3.447061	2.803661
29	-3.541061	-0.713997	-0.308693
6	-2.061160	4.195686	4.716991
6	-0.801278	-0.628452	4.570886
6	-3.770520	5.979714	-0.542237
6	-7.441102	3.176530	-2.490214
9	-7.119580	2.260724	-3.439363
9	-8.557781	2.722315	-1.876644
9	-7.768900	4.315832	-3.133905
9	-3.595023	6.549521	-1.756278
9	-2.557307	5.863304	0.037347

9	-4.476360	6.868545	0.200732
9	-3.079412	5.037084	4.442880
9	-0.936973	4.749586	4.187390
9	-1.888441	4.182758	6.056657
9	-0.598067	-0.565788	5.903724
9	-1.354420	-1.832863	4.297856
9	0.431894	-0.621637	3.994521
6	-1.905586	1.461549	-1.474394
6	-0.673844	0.291914	0.142697
6	-1.071408	2.560481	-1.393614
1	-2.740474	1.441131	-2.163406
6	0.162327	1.435753	0.302414
6	-0.033594	2.573811	-0.454442
1	0.970147	1.405098	1.023846
6	-0.289940	-0.920572	0.801840
6	-1.125150	-2.081408	1.000584
8	-2.329415	-2.144983	0.606960
7	-1.737213	0.363839	-0.716001
1	0.552982	-0.799920	1.464573
7	-0.623626	-3.195367	1.632563
6	-1.529893	-4.303345	1.917086
1	-2.326546	-4.344316	1.178450
1	-1.979316	-4.194726	2.914333
1	-0.963641	-5.239651	1.894810
6	0.634091	-3.276950	2.365061
1	1.261677	-2.410180	2.194336
1	1.189312	-4.167218	2.049036
1	0.439306	-3.355842	3.440833
77	4.399960	-1.802450	-1.255164
15	5.682243	-0.120317	-0.422533
8	6.172492	-0.032309	1.157977
8	7.156116	-0.063494	-1.196816
7	4.856302	1.328506	-0.538438
6	7.233613	-0.799651	1.629103
6	6.909646	-1.814814	2.555826
1	5.873162	-1.930050	2.855383
6	7.902172	-2.624144	3.049992
1	7.668359	-3.404263	3.768782
6	9.243168	-2.473531	2.604205
6	10.265772	-3.355901	3.047084
1	10.004056	-4.137412	3.755612
6	11.555060	-3.235385	2.580455
1	12.327729	-3.918137	2.921443
6	11.870687	-2.226404	1.639533
1	12.883184	-2.148682	1.254004
6	10.906054	-1.344785	1.202060
1	11.165946	-0.585313	0.474446
6	9.567725	-1.424246	1.679234
6	8.534307	-0.521872	1.238514
6	8.829824	0.654143	0.373138
6	9.772156	1.672040	0.759361
6	10.386496	1.702079	2.042721
1	10.138121	0.936711	2.768228
6	11.277444	2.697137	2.381896
1	11.725841	2.701342	3.371259
6	11.608867	3.717317	1.458540
1	12.318185	4.490726	1.737975
6	11.016678	3.732921	0.216176
1	11.245677	4.520814	-0.496588
6	10.080374	2.731494	-0.159761
6	9.430057	2.775910	-1.422777
1	9.683947	3.569300	-2.119980
6	8.470212	1.848730	-1.745176
1	7.937517	1.878434	-2.689401
6	8.159993	0.821204	-0.827779
6	3.687796	1.259719	-1.454555
1	2.781838	1.287908	-0.835589
6	3.641902	2.424559	-2.434519
6	2.406775	2.863458	-2.927360
1	1.492183	2.414247	-2.555089
6	2.340804	3.866328	-3.897372
1	1.371972	4.193371	-4.263263
6	3.512845	4.447571	-4.386861
1	3.462724	5.231801	-5.136954
6	4.750229	4.014426	-3.901843
1	5.668071	4.462178	-4.273479
6	4.813646	3.007709	-2.937241
1	5.774904	2.678460	-2.555904
6	3.711630	-0.046377	-2.269053
1	4.372977	0.109412	-3.129279
1	2.714865	-0.214408	-2.681675
6	4.878944	2.556088	0.316255
1	4.674234	3.368111	-0.386378
6	3.747593	2.580078	1.343445
6	2.854696	3.660474	1.345921
1	2.947128	4.429349	0.582204
6	1.855618	3.766055	2.317858
1	1.170870	4.609399	2.307989
6	1.725932	2.777420	3.294209
1	0.946746	2.861333	4.043835
6	2.600170	1.686061	3.293201
1	2.493159	0.907105	4.042235
6	3.609323	1.592945	2.331045
1	4.302360	0.759693	2.352986
6	6.220326	2.909021	0.968011
1	7.016118	2.963561	0.223984
1	6.508949	2.208430	1.750074
1	6.114795	3.899412	1.421321
6	3.259947	-1.589228	0.567926
1	3.702031	-2.135946	1.400507
1	3.022576	-0.558452	0.822645
6	2.302009	-2.291337	-0.247800
1	2.213209	-3.364976	-0.138883
6	1.288295	-1.622210	-0.958881
1	1.399200	-0.551277	-1.061035
6	5.735013	-2.201645	-3.006380
1	5.973499	-1.239122	-3.451637
6	4.445665	-2.716378	-3.284061
1	3.811397	-2.122207	-3.941613
6	4.051979	-4.184820	-3.228481
1	4.354377	-4.689094	-4.159258
1	2.957768	-4.232250	-3.196916
6	4.622226	-4.946399	-2.012736
1	5.601076	-5.370296	-2.254650
1	3.970437	-5.797209	-1.789255
6	4.750261	-4.096061	-0.752808
1	4.044189	-4.322128	0.042266
6	5.896473	-3.410442	-0.378329
1	6.002897	-3.171697	0.675189
6	7.176286	-3.330286	-1.185738
1	7.786198	-2.527990	-0.765892
1	7.744840	-4.261205	-1.044615
6	6.959617	-3.062558	-2.691378
1	6.881565	-4.007143	-3.238712
1	7.847281	-2.557214	-3.083313
6	0.376964	-2.243454	-1.906272
6	0.117826	-3.631020	-1.923392
6	-0.269719	-1.425224	-2.854602
6	-0.750466	-4.172866	-2.865544
1	0.589536	-4.279554	-1.192484
6	-1.143680	-1.970874	-3.792499
1	-0.077962	-0.357412	-2.848969
6	-1.387192	-3.346090	-3.799502
1	-0.947046	-5.240687	-2.866852
1	-1.642338	-1.326070	-4.509202
1	-2.077185	-3.771271	-4.521533
1	0.612974	3.434284	-0.332364
35	-1.348273	4.067460	-2.605480

C1-P1 *si-si_5*

Number of imaginary frequencies= 1
The smallest frequencies are= -120.6364 8.8364 11.1071 cm(-1)
Electronic energy= -7222.6230217
Zero-point correction= 1.755803
(Hartree/Particle)
Thermal correction to Energy= 1.874309
Thermal correction to Enthalpy= 1.875253
Thermal correction to Gibbs Free Energy= 1.593538
Sum of electronic and zero-point Energies= -7220.867219

Sum of electronic and thermal Energies= -7220.748713
Sum of electronic and thermal Enthalpies= -7220.747769
Sum of electronic and thermal Free Energies= -7221.029484

.....

Cartesian Coordinates

.....

26	3.531371	3.835178	4.070051
15	1.204308	2.333378	-0.336164
15	4.538934	0.592577	0.723550
6	2.848414	3.414022	2.131425
6	3.845496	2.462162	2.549711
6	3.360639	1.807826	3.724989
1	3.886264	1.044631	4.283128
6	2.086730	2.361988	4.048739
1	1.481589	2.105189	4.908003
6	1.774386	3.356401	3.075779
1	0.887450	3.972701	3.055709
6	5.133569	5.140653	4.294612
1	5.914240	5.287600	3.560220
6	5.138004	4.164380	5.336946
1	5.916345	3.436420	5.521832
6	3.909301	4.281011	6.055704
1	3.594963	3.656305	6.881471
6	3.144450	5.328365	5.457064
1	2.149966	5.637662	5.750613
6	3.900851	5.860709	4.370228
1	3.578839	6.646640	3.700576
6	2.954742	4.218710	0.881538
6	3.817707	5.322908	0.838801
1	4.346621	5.592949	1.743249
6	4.014014	6.058967	-0.330453
1	4.696520	6.903972	-0.329336
6	3.335426	5.698460	-1.491296
1	3.481169	6.252789	-2.413088
6	2.472660	4.601629	-1.474222
1	1.965237	4.325971	-2.390362
6	2.277985	3.844179	-0.308831
6	5.059805	2.107545	1.742170
1	5.203604	2.885893	0.986824
6	6.351796	1.963487	2.548325
1	7.196786	1.701215	1.904872
1	6.264748	1.202275	3.328314
1	6.575819	2.917951	3.033467
6	0.605086	2.303090	-2.081136
6	1.385703	1.589728	-3.005285
1	2.272192	1.070785	-2.659182
6	1.051599	1.568828	-4.359507
1	1.674050	1.020779	-5.061177
6	-0.082427	2.252703	-4.806766
1	-0.351027	2.233160	-5.858859
6	-0.870140	2.959686	-3.894925
1	-1.756542	3.488129	-4.233989
6	-0.526802	2.990777	-2.541790
1	-1.137746	3.559240	-1.852209
6	-0.239568	2.893392	0.661486
6	-0.685080	4.225950	0.630909
1	-0.195739	4.949720	-0.013771
6	-1.742431	4.633669	1.445051
1	-2.082651	5.664562	1.411323
6	-2.361876	3.716883	2.300226
1	-3.185064	4.034857	2.933568
6	-1.917163	2.393878	2.341826
1	-2.387255	1.684992	3.015536
6	-0.857110	1.981699	1.530186
1	-0.475903	0.968416	1.592618
6	5.513677	0.768645	-0.832491
6	6.404156	-0.181247	-1.353565
1	6.629864	-1.090981	-0.813067
6	7.003717	0.024516	-2.596212
6	6.703794	1.149150	-3.365221
1	7.159570	1.290796	-4.337784
6	5.791040	2.074198	-2.864979
6	5.206387	1.896026	-1.610450
1	4.491339	2.631562	-1.254421
6	5.237359	-0.846487	1.634223
6	4.308741	-1.642550	2.317432
1	3.257608	-1.385956	2.278107
6	4.731367	-2.749019	3.054395
6	6.081218	-3.091925	3.115108
1	6.407079	-3.958121	3.678754
6	7.007896	-2.289755	2.450125
6	6.598057	-1.168790	1.725950
1	7.348354	-0.552391	1.245698
29	2.244759	0.393549	0.262353
6	8.470777	-2.642307	2.455794
6	3.704808	-3.612338	3.733885
6	8.034164	-0.946685	-3.107813
6	5.386815	3.278364	-3.671072
9	4.044655	3.300106	-3.878014
9	5.696744	4.432582	-3.035711
9	5.977226	3.314799	-4.882782
9	7.911474	-1.155298	-4.439537
9	7.960829	-2.147455	-2.496429
9	9.290727	-0.478180	-2.906448
9	8.844510	-3.203169	1.279926
9	8.787077	-3.517283	3.432841
9	9.246778	-1.546126	2.623280
9	4.211755	-4.266906	4.799745
9	2.647159	-2.885336	4.170482
9	3.204860	-4.556517	2.896275
6	3.205760	-1.527776	-1.866993
6	2.205912	-2.725323	-0.123421
6	3.792239	-2.665970	-2.388385
1	3.364695	-0.565156	-2.335303
6	2.847273	-3.906743	-0.598771
6	3.637931	-3.889333	-1.728891
1	2.689036	-4.838404	-0.065969
6	1.276265	-2.865214	0.952023
6	0.804309	-1.831780	1.821076
8	1.124359	-0.606149	1.713383
7	2.437058	-1.534537	-0.761165
1	1.175793	-3.880022	1.304549
7	-0.050095	-2.165616	2.857691
6	-0.149016	-1.225787	3.974853
1	0.729476	-1.293851	4.631713
1	-1.040500	-1.459071	4.559481
1	-0.222766	-0.204915	3.605958
6	-0.354166	-3.556181	3.181448
1	-0.651518	-4.109159	2.288452
1	-1.191703	-3.577298	3.882071
1	0.497948	-4.071101	3.643672
77	-3.072559	-1.482184	-1.762288
15	-4.593006	-0.536469	-0.363508
8	-4.502112	0.999706	0.242214
8	-6.085708	-0.476523	-1.100167
7	-4.654591	-1.387416	1.081214
6	-4.845296	2.106381	-0.525557
6	-3.785954	2.969463	-0.873859
1	-2.794513	2.733389	-0.508664
6	-4.039676	4.075496	-1.644773
1	-3.236343	4.757605	-1.909244
6	-5.351201	4.329110	-2.129712
6	-5.610876	5.423448	-2.998677
1	-4.785985	6.079570	-3.264400
6	-6.871935	5.641422	-3.505372
1	-7.057959	6.477382	-4.173253
6	-7.927137	4.761574	-3.165991
1	-8.915990	4.920233	-3.586474
6	-7.712678	3.701009	-2.312248
1	-8.532146	3.034000	-2.072745
6	-6.427907	3.456731	-1.751135
6	-6.167468	2.353361	-0.860034
6	-7.255939	1.482832	-0.334160
6	-8.391136	2.018220	0.373889
6	-8.476654	3.382747	0.769876
1	-7.659558	4.055344	0.537368
6	-9.571399	3.856517	1.459895
1	-9.606476	4.900021	1.759501
6	-10.646435	2.996946	1.789584
1	-11.505228	3.386311	2.328377

6	-10.589884	1.667010	1.438685
1	-11.398949	0.990080	1.700311
6	-9.467465	1.141637	0.741875
6	-9.378110	-0.243994	0.441976
1	-10.199917	-0.897793	0.718735
6	-8.247621	-0.758853	-0.140156
1	-8.136796	-1.819121	-0.338815
6	-7.192052	0.106869	-0.496860
6	-4.014179	-2.721980	0.966435
1	-3.021417	-2.664996	1.427004
6	-4.800603	-3.818563	1.659807
6	-4.146850	-4.726077	2.499978
1	-3.081642	-4.611190	2.685933
6	-4.854491	-5.764514	3.113306
1	-4.336439	-6.457497	3.770778
6	-6.225403	-5.903951	2.887754
1	-6.779434	-6.704807	3.369235
6	-6.883053	-5.004095	2.041451
1	-7.951443	-5.100978	1.869114
6	-6.174616	-3.971248	1.431408
1	-6.689736	-3.251652	0.802573
6	-3.835395	-3.078736	-0.516347
1	-4.805475	-3.389860	-0.920502
1	-3.185078	-3.952911	-0.588442
6	-4.764769	-0.740686	2.433601
1	-4.836704	0.325739	2.229565
6	-6.031062	-1.100224	3.208737
6	-7.163233	-0.290681	3.050880
1	-7.124389	0.549671	2.365041
6	-8.339771	-0.546897	3.757542
1	-9.202808	0.096230	3.611267
6	-8.399109	-1.621606	4.646531
1	-9.311952	-1.826264	5.199451
6	-7.272547	-2.429455	4.824227
1	-7.305962	-3.269022	5.513233
6	-6.098780	-2.166755	4.116561
1	-5.241646	-2.813513	4.262598
6	-3.482826	-0.948653	3.247631
1	-2.610765	-0.627822	2.673613
1	-3.330040	-1.989603	3.541492
1	-3.537007	-0.351293	4.162374
6	-1.536550	-0.659667	-0.465503
1	-1.265005	0.356929	-0.735661
1	-1.737896	-0.779453	0.595922
6	-0.825926	-1.726227	-1.120511
1	-0.199629	-1.507520	-1.975991
6	-0.769742	-3.011812	-0.564998
1	-1.314810	-3.158530	0.358473
6	-4.587873	-2.078126	-3.304613
1	-5.414798	-2.541972	-2.773623
6	-3.430433	-2.870966	-3.480598
1	-3.464214	-3.887405	-3.089277
6	-2.387264	-2.664514	-4.566418
1	-2.744589	-3.099100	-5.512724
1	-1.502987	-3.242063	-4.281916
6	-1.977916	-1.191286	-4.782683
1	-2.605250	-0.728599	-5.550905
1	-0.954505	-1.159269	-5.170225
6	-2.035162	-0.337945	-3.519305
1	-1.076297	-0.002593	-3.137662
6	-3.140396	0.406128	-3.124288
1	-2.945455	1.258674	-2.483111
6	-4.473654	0.441110	-3.841876
1	-5.198109	0.919918	-3.180571
1	-4.382249	1.088694	-4.726412
6	-5.003950	-0.950577	-4.250512
1	-4.679487	-1.198965	-5.265935
1	-6.096844	-0.911259	-4.282015
6	-0.363084	-4.228535	-1.248810
6	0.275234	-4.226617	-2.505021
6	-0.632504	-5.468456	-0.634025
6	0.608531	-5.424916	-3.132102
1	0.513179	-3.286715	-2.991061
6	-0.292519	-6.665233	-1.259250
1	-1.115156	-5.481151	0.340161
6	0.326267	-6.647235	-2.514161
1	1.097409	-5.405194	-4.101845
1	-0.511099	-7.611130	-0.772266
1	0.590043	-7.579338	-3.005276
1	4.104913	-4.796248	-2.097368
35	4.823940	-2.546896	-4.044531

C1-P1 *si-si_6*

Number of imaginary frequencies= 1
The smallest frequencies are=-184.1952 10.0009 14.2259cm(-1)
Electronic energy= -7222.619327
Zero-point correction= 1.755410
(Hartree/Particle)
Thermal correction to Energy= 1.874062
Thermal correction to Enthalpy= 1.875006
Thermal correction to Gibbs Free Energy= 1.592536
Sum of electronic and zero-point Energies= -7220.863917
Sum of electronic and thermal Energies= -7220.745265
Sum of electronic and thermal Enthalpies= -7220.744321
Sum of electronic and thermal Free Energies= -7221.026791

.....

Cartesian Coordinates

.....

26	3.594610	4.429288	3.241035
15	2.513187	2.139896	-1.283945
15	4.846396	0.307284	1.178649
6	3.493798	3.601526	1.316702
6	4.041921	2.659524	2.257781
6	3.060378	2.435633	3.272750
1	3.173363	1.782124	4.127290
6	1.923664	3.246980	2.981676
1	1.031538	3.331785	3.587898
6	2.193276	3.972421	1.784195
1	1.539695	4.689650	1.309078
6	5.303740	5.480681	3.788546
1	6.295134	5.292940	3.398571
6	4.719765	4.852495	4.930794
1	5.186484	4.100137	5.551983
6	3.392612	5.357916	5.081176
1	2.678180	5.050904	5.833597
6	3.155296	6.297179	4.031919
1	2.229476	6.826605	3.848752
6	4.335589	6.374004	3.233804
1	4.459842	6.978168	2.345392
6	4.158511	4.028240	0.054734
6	5.216517	4.947848	0.101612
1	5.521760	5.327828	1.068290
6	5.870446	5.371973	-1.055206
1	6.693356	6.077369	-0.984647
6	5.455962	4.890302	-2.294837
1	5.945750	5.217113	-3.206973
6	4.417336	3.961517	-2.363261
1	4.124185	3.583340	-3.335021
6	3.777030	3.495066	-1.203948
6	5.333853	1.921501	2.057546
1	5.921935	2.468283	1.315194
6	6.181066	1.762956	3.322235
1	7.117858	1.240047	3.111471
1	5.652144	1.215986	4.107242
1	6.424002	2.756563	3.709346
6	2.570147	1.571698	-3.033952
6	3.775700	1.041892	-3.527948
1	4.673581	1.079571	-2.920658
6	3.844665	0.500992	-4.809947
1	4.790334	0.113309	-5.177270
6	2.701173	0.458932	-5.614195
1	2.750452	0.032172	-6.611700
6	1.496930	0.972021	-5.129031
1	0.604216	0.943129	-5.747207
6	1.431014	1.530673	-3.849042
1	0.491522	1.933872	-3.488391
6	0.920837	3.040903	-1.116819
6	0.623307	4.174259	-1.890901
1	1.317418	4.505513	-2.658294

6	-0.557677	4.884004	-1.670438
1	-0.785134	5.756798	-2.275740
6	-1.436977	4.482880	-0.658135
1	-2.349941	5.043156	-0.477660
6	-1.139242	3.361212	0.117240
1	-1.810298	3.055631	0.913408
6	0.027948	2.629610	-0.117656
1	0.260064	1.753585	0.480894
6	6.223359	-0.021452	-0.000339
6	6.784053	-1.295257	-0.176124
1	6.499171	-2.120650	0.464434
6	7.709307	-1.525371	-1.194138
6	8.080868	-0.508966	-2.073307
1	8.793601	-0.697019	-2.867133
6	7.503997	0.750027	-1.916403
6	6.585107	0.997862	-0.894841
1	6.141938	1.985802	-0.819720
6	4.990113	-1.006216	2.459291
6	3.791567	-1.553057	2.926144
1	2.850950	-1.203177	2.517493
6	3.804891	-2.541772	3.914326
6	5.005689	-3.002702	4.443271
1	5.013907	-3.777640	5.201364
6	6.204104	-2.453734	3.977569
6	6.203425	-1.462327	2.999632
1	7.146836	-1.057684	2.653533
29	2.829484	0.343387	0.071229
6	7.499803	-2.911938	4.591384
6	2.496209	-3.142355	4.344222
6	8.363635	-2.876460	-1.303737
6	7.809639	1.854332	-2.892236
9	6.783613	2.039673	-3.765420
9	8.000432	3.038057	-2.267470
9	8.910141	1.600599	-3.628728
9	8.696851	-3.176318	-2.578476
9	7.567042	-3.865708	-0.843198
9	9.508727	-2.927786	-0.579227
9	7.708417	-2.329609	5.796663
9	8.565552	-2.612534	3.817869
9	7.509797	-4.247897	4.799101
9	2.601085	-3.864418	5.477226
9	1.554971	-2.190845	4.553353
9	1.998799	-3.972509	3.388491
6	3.714725	-1.885271	-1.657351
6	1.969809	-2.640610	-0.289756
6	3.954651	-3.155510	-2.147341
1	4.299086	-1.038829	-1.991755
6	2.224826	-3.967140	-0.735600
6	3.206197	-4.233977	-1.670485
1	1.618513	-4.778364	-0.347766
6	0.838896	-2.430269	0.573695
6	0.596089	-1.269328	1.393384
8	1.164765	-0.146727	1.217102
7	2.748574	-1.622858	-0.759747
1	0.395914	-3.356306	0.911672
7	-0.326216	-1.369109	2.399054
6	-0.601506	-0.226268	3.259965
1	-1.657703	0.060300	3.193348
1	0.016176	0.614967	2.953443
1	-0.373905	-0.476260	4.302307
6	-1.004241	-2.616887	2.735106
1	-1.640352	-2.964818	1.914883
1	-1.641763	-2.440224	3.601352
1	-0.293740	-3.405679	2.993941
77	-3.489748	-0.393341	-1.687887
15	-5.254890	-0.206432	-0.270345
8	-5.409334	0.954127	0.909670
8	-6.670767	0.039246	-1.114022
7	-5.374173	-1.577328	0.694085
6	-5.905830	2.223541	0.642316
6	-4.993808	3.290766	0.795158
1	-3.984646	3.061962	1.117507
6	-5.400583	4.576332	0.542098
1	-4.710432	5.405983	0.667592
6	-6.721104	4.835861	0.086362
6	-7.129705	6.153544	-0.255080
1	-6.415327	6.963846	-0.134660
6	-8.394261	6.398922	-0.739909
1	-8.695024	7.408933	-1.002366
6	-9.299574	5.325281	-0.912978
1	-10.287967	5.515817	-1.321154
6	-8.939705	4.038243	-0.576131
1	-9.645343	3.230800	-0.728031
6	-7.650120	3.748793	-0.047659
6	-7.239687	2.413586	0.312756
6	-8.192058	1.266970	0.282709
6	-9.437504	1.275505	1.005785
6	-9.765535	2.281846	1.957025
1	-9.053395	3.073659	2.158393
6	-10.964205	2.254431	2.636095
1	-11.186264	3.028918	3.364606
6	-11.906168	1.224423	2.400041
1	-12.848407	1.219235	2.940005
6	-11.616433	0.226083	1.497891
1	-12.322460	-0.580597	1.318308
6	-10.382752	0.215062	0.791163
6	-10.058424	-0.844154	-0.099271
1	-10.784360	-1.634523	-0.266835
6	-8.823973	-0.897693	-0.697471
1	-8.534214	-1.719432	-1.342958
6	-7.897847	0.143736	-0.474769
6	-4.511344	-2.684135	0.207620
1	-3.610782	-2.722619	0.832326
6	-5.185272	-4.043430	0.260412
6	-4.459078	-5.162168	0.681024
1	-3.434088	-5.037008	1.024239
6	-5.044523	-6.431558	0.685245
1	-4.471225	-7.290849	1.022680
6	-6.367499	-6.591105	0.269240
1	-6.829872	-7.574057	0.282778
6	-7.096767	-5.476686	-0.160753
1	-8.129909	-5.591968	-0.476882
6	-6.506922	-4.214759	-0.173003
1	-7.080874	-3.345272	-0.476656
6	-4.083647	-2.408359	-1.247183
1	-4.929180	-2.656565	-1.899996
1	-3.288614	-3.108467	-1.508765
6	-5.743280	-1.507747	2.149520
1	-6.241960	-0.547145	2.263779
6	-6.765424	-2.557577	2.570084
6	-8.124383	-2.263485	2.407684
1	-8.410718	-1.297237	2.009001
6	-9.109248	-3.190071	2.751405
1	-10.157308	-2.939019	2.611865
6	-8.744052	-4.429876	3.281160
1	-9.505214	-5.158125	3.547231
6	-7.391889	-4.722311	3.478930
1	-7.097162	-5.680812	3.896948
6	-6.412006	-3.789808	3.134327
1	-5.368481	-4.042232	3.284963
6	-4.495122	-1.476722	3.037163
1	-3.850887	-0.644705	2.742173
1	-3.914229	-2.398680	2.977361
1	-4.787962	-1.335512	4.082028
6	-2.207084	-0.135959	0.047335
1	-2.098328	0.902087	0.340777
1	-2.468891	-0.786098	0.877306
6	-1.284776	-0.655600	-0.925722
1	-0.649156	0.031635	-1.470647
6	-0.970673	-2.035027	-1.004763
1	-1.568425	-2.691593	-0.384602
6	-4.796352	-0.467904	-3.490031
1	-5.575783	-1.198752	-3.290918
6	-3.524766	-0.991620	-3.835234
1	-3.437889	-2.077099	-3.886804
6	-2.465807	-0.252496	-4.635823
1	-2.686416	-0.330978	-5.711984
1	-1.512277	-0.767384	-4.482362
6	-2.310091	1.229551	-4.240813
1	-3.008626	1.849909	-4.808928

1	-1.312933	1.571852	-4.526133
6	-2.509301	1.496407	-2.752887
1	-1.615159	1.716739	-2.178496
6	-3.716035	1.899704	-2.203719
1	-3.676637	2.424964	-1.254256
6	-5.008482	2.063268	-2.980610
1	-5.821018	2.160469	-2.258218
1	-4.969647	3.010643	-3.538114
6	-5.332134	0.893907	-3.941672
1	-4.957289	1.110295	-4.946908
1	-6.419588	0.819532	-4.033631
6	-0.358463	-2.672062	-2.164599
6	0.458469	-1.969336	-3.072332
6	-0.593112	-4.041501	-2.392411
6	1.008398	-2.615064	-4.175677
1	0.675079	-0.920985	-2.906152
6	-0.056604	-4.682495	-3.509030
1	-1.206917	-4.599333	-1.689634
6	0.747477	-3.971630	-4.403442
1	1.643913	-2.057405	-4.856062
1	-0.258851	-5.736657	-3.675661
1	1.174617	-4.470335	-5.268749
1	3.376695	-5.244071	-2.026056
35	5.326223	-3.409244	-3.513751

C1-P1 *si-si_7*

Number of imaginary frequencies= 1
The smallest frequencies are= -187.6124 6.9636 11.0676 cm(-1)
Electronic energy= -7222.6193586
Zero-point correction= 1.755050
(Hartree/Particle)
Thermal correction to Energy= 1.873850
Thermal correction to Enthalpy= 1.874795
Thermal correction to Gibbs Free Energy= 1.591033
Sum of electronic and zero-point Energies= -7220.864308
Sum of electronic and thermal Energies= -7220.745508
Sum of electronic and thermal Enthalpies= -7220.744564
Sum of electronic and thermal Free Energies= -7221.028326

.....

Cartesian Coordinates

.....

26	3.550937	4.404932	3.282371
15	2.504507	2.147182	-1.267645
15	4.838037	0.309906	1.189014
6	3.464854	3.593595	1.349670
6	4.013463	2.646947	2.285808
6	3.027443	2.408371	3.293169
1	3.139243	1.748394	4.142879
6	1.887972	3.216045	3.003156
1	0.992177	3.290458	3.605360
6	2.160005	3.953453	1.813549
1	1.505012	4.671099	1.341013
6	5.251306	5.458734	3.852579
1	6.246306	5.279006	3.468073
6	4.661636	4.816815	4.984227
1	5.126931	4.060345	5.601485
6	3.331048	5.314710	5.129488
1	2.612291	4.996598	5.873119
6	3.097286	6.263095	4.087642
1	2.170448	6.790138	3.902742
6	4.283247	6.353097	3.299304
1	4.411313	6.966245	2.417623
6	4.132848	4.034169	0.094275
6	5.184612	4.960208	0.153473
1	5.482614	5.334662	1.124585
6	5.840853	5.398156	-0.996866
1	6.658688	6.108430	-0.916819
6	5.435057	4.923971	-2.242240
1	5.926618	5.261594	-3.149464
6	4.402789	3.989111	-2.323001
1	4.116409	3.617271	-3.299200
6	3.760543	3.508736	-1.170455
6	5.310979	1.918160	2.087057
1	5.901995	2.476156	1.355445
6	6.148487	1.749355	3.356982
1	7.089093	1.232293	3.148647
1	5.615201	1.191674	4.131545
1	6.384184	2.739605	3.756909
6	2.574630	1.591986	-3.021124
6	3.786745	1.073701	-3.511025
1	4.680009	1.113460	-2.897174
6	3.867288	0.541155	-4.795800
1	4.817701	0.161999	-5.159753
6	2.728971	0.496467	-5.607184
1	2.787190	0.076352	-6.607030
6	1.518307	0.998316	-5.126238
1	0.629897	0.966850	-5.750477
6	1.440568	1.548400	-3.843141
1	0.495781	1.941696	-3.485174
6	0.906744	3.038677	-1.102917
6	0.604982	4.174843	-1.871176
1	1.299972	4.515544	-2.633605
6	-0.581505	4.875505	-1.650948
1	-0.812219	5.750567	-2.251719
6	-1.462452	4.462331	-0.644846
1	-2.380077	5.015083	-0.464929
6	-1.160373	3.337870	0.124668
1	-1.832746	3.021132	0.915465
6	0.012680	2.615771	-0.109950
1	0.248288	1.737542	0.483880
6	6.221009	0.000835	0.011254
6	6.787422	-1.268911	-0.176052
1	6.503833	-2.102416	0.454537
6	7.717723	-1.484476	-1.192544
6	8.088317	-0.457479	-2.059734
1	8.804862	-0.634261	-2.852734
6	7.505834	0.797441	-1.891714
6	6.582487	1.031080	-0.870743
1	6.135496	2.016582	-0.787057
6	4.987517	-1.015906	2.456272
6	3.790666	-1.575062	2.916770
1	2.848392	-1.224580	2.512320
6	3.808799	-2.575743	3.890993
6	5.012607	-3.038742	4.415424
1	5.025166	-3.823223	5.162662
6	6.206362	-2.479060	3.956553
6	6.200980	-1.473726	2.990356
1	7.143944	-1.062629	2.648310
29	2.823378	0.342269	0.076018
6	7.520880	-2.916985	4.544457
6	2.503684	-3.190118	4.312009
6	8.379525	-2.831050	-1.312436
6	7.810207	1.912950	-2.855063
9	6.788095	2.100307	-3.732352
9	7.989935	3.091681	-2.217786
9	8.916549	1.673195	-3.587542
9	8.717639	-3.117600	-2.588979
9	7.587389	-3.828733	-0.862701
9	9.523123	-2.882380	-0.585589
9	7.444452	-4.139462	5.111489
9	7.943065	-2.059414	5.504772
9	8.496166	-2.961199	3.608410
9	2.609869	-3.915539	5.442844
9	1.552262	-2.248532	4.520089
9	2.018349	-4.021542	3.351054
6	3.725554	-1.868663	-1.667216
6	1.976385	-2.642192	-0.315705
6	3.970547	-3.133400	-2.168909
1	4.309284	-1.017670	-1.991299
6	2.235558	-3.963374	-0.774679
6	3.221907	-4.218390	-1.707495
1	1.628655	-4.779679	-0.398622
6	0.840704	-2.443486	0.544284
6	0.592852	-1.294001	1.378619
8	1.161259	-0.168492	1.221485
7	2.754778	-1.617714	-0.771093
1	0.397771	-3.374437	0.868332
7	-0.336897	-1.409057	2.375798
6	-0.623974	-0.277019	3.247043

1	-0.309666	-0.497412	4.274059
1	-1.698470	-0.064402	3.250257
1	-0.085437	0.598952	2.892500
6	-0.995175	-2.668760	2.706754
1	-1.642432	-3.012266	1.893237
1	-1.617421	-2.511879	3.587864
1	-0.272155	-3.453366	2.941689
77	-3.486366	-0.396203	-1.707225
15	-5.254054	-0.194251	-0.298755
8	-5.400796	0.977635	0.870916
8	-6.672339	0.046508	-1.139904
7	-5.380209	-1.557168	0.677257
6	-5.919742	2.238743	0.608503
6	-5.022602	3.320256	0.750542
1	-4.006109	3.108302	1.061051
6	-5.452829	4.599502	0.504377
1	-4.773937	5.439568	0.621733
6	-6.783433	4.839312	0.067604
6	-7.217562	6.151077	-0.265083
1	-6.514151	6.972205	-0.153489
6	-8.492835	6.377537	-0.730667
1	-8.813225	7.383215	-0.986454
6	-9.383675	5.290145	-0.892598
1	-10.380958	5.465856	-1.285524
6	-8.998727	4.008244	-0.563993
1	-9.694002	3.190265	-0.707195
6	-7.697051	3.738004	-0.055311
6	-7.260612	2.408897	0.296885
6	-8.195777	1.248016	0.276706
6	-9.431307	1.235433	1.016400
6	-9.760084	2.232235	1.977280
1	-9.056324	3.032987	2.172849
6	-10.948494	2.184044	2.673035
1	-11.171256	2.951354	3.408876
6	-11.878968	1.141920	2.444575
1	-12.813380	1.120583	2.997595
6	-11.587893	0.152408	1.533155
1	-12.284794	-0.663405	1.359305
6	-10.364265	0.162679	0.809248
6	-10.037212	-0.887181	-0.091355
1	-10.754596	-1.686318	-0.254246
6	-8.809832	-0.920622	-0.705537
1	-8.517752	-1.734003	-1.360466
6	-7.895313	0.132244	-0.488944
6	-4.514627	-2.668445	0.205559
1	-3.615739	-2.699734	0.832772
6	-5.181433	-4.031035	0.270345
6	-4.437685	-5.143897	0.676478
1	-3.407436	-5.009415	1.000159
6	-5.011011	-6.418408	0.690299
1	-4.423626	-7.272715	1.016030
6	-6.340137	-6.589599	0.299084
1	-6.793434	-7.576641	0.320561
6	-7.087107	-5.481414	-0.115947
1	-8.124987	-5.605584	-0.412605
6	-6.508796	-4.213992	-0.139026
1	-7.095731	-3.349805	-0.432039
6	-4.084779	-2.407245	-1.251955
1	-4.930887	-2.659656	-1.902673
1	-3.291507	-3.112071	-1.506410
6	-5.744090	-1.458844	2.132482
1	-6.286757	-0.519291	2.219246
6	-6.715200	-2.540490	2.588127
6	-8.086865	-2.310437	2.428818
1	-8.418581	-1.368008	2.008905
6	-9.027359	-3.271707	2.799702
1	-10.086426	-3.070407	2.662227
6	-8.603941	-4.482623	3.352474
1	-9.329880	-5.238424	3.639270
6	-7.238889	-4.710821	3.545949
1	-6.899652	-5.646499	3.981523
6	-6.303417	-3.743189	3.175431
1	-5.248592	-3.944890	3.325064
6	-4.493918	-1.340619	3.010155
1	-3.903819	-0.476208	2.695393
1	-3.860467	-2.228298	2.960477
1	-4.785849	-1.198925	4.055310
6	-2.206016	-0.143103	0.029955
1	-2.098138	0.893756	0.326879
1	-2.467879	-0.795501	0.858029
6	-1.281740	-0.658883	-0.943487
1	-0.646643	0.030836	-1.485919
6	-0.965059	-2.037646	-1.027908
1	-1.562817	-2.698114	-0.411732
6	-4.789581	-0.477286	-3.513144
1	-5.569959	-1.206570	-3.311946
6	-3.517664	-1.002572	-3.852946
1	-3.429739	-2.088187	-3.898690
6	-2.456149	-0.265944	-4.652569
1	-2.674305	-0.346455	-5.729067
1	-1.503817	-0.781716	-4.495558
6	-2.298581	1.217150	-4.260940
1	-2.992852	1.837665	-4.834166
1	-1.299118	1.555605	-4.542657
6	-2.503522	1.490013	-2.774873
1	-1.611869	1.713442	-2.197684
6	-3.712416	1.895125	-2.231908
1	-3.676301	2.424540	-1.284585
6	-5.002187	2.055790	-3.013947
1	-5.817515	2.155589	-2.294967
1	-4.961188	3.001240	-3.574550
6	-5.322134	0.883241	-3.972260
1	-4.941706	1.095664	-4.976207
1	-6.409146	0.809531	-4.069779
6	-0.350814	-2.666356	-2.191670
6	0.469140	-1.956543	-3.091034
6	-0.584901	-4.033698	-2.431364
6	1.023015	-2.593163	-4.197725
1	0.685029	-0.909593	-2.915485
6	-0.044456	-4.665630	-3.551363
1	-1.201381	-4.597240	-1.735571
6	0.762822	-3.947801	-4.437303
1	1.660858	-2.029859	-4.871314
1	-0.246283	-5.718375	-3.727238
1	1.192902	-4.439682	-5.305056
1	3.396181	-5.224224	-2.073195
35	5.349575	-3.371245	-3.530345

C1-P1 *si-si_*8

Number of imaginary frequencies= 1
The smallest frequencies are= -153.7535 8.5286 10.6626 cm(-1)
Electronic energy= -7222.6206504
Zero-point correction= 1.754800
(Hartree/Particle)
Thermal correction to Energy= 1.873746
Thermal correction to Enthalpy= 1.874690
Thermal correction to Gibbs Free Energy= 1.591401
Sum of electronic and zero-point Energies= -7220.865850
Sum of electronic and thermal Energies= -7220.746904
Sum of electronic and thermal Enthalpies= -7220.745960
Sum of electronic and thermal Free Energies= -7221.029250

.....

Cartesian Coordinates

.....

26	3.848815	4.474038	3.163571
15	1.178196	2.281163	-0.762619
15	4.500735	0.586678	0.479637
6	3.024899	3.723646	1.383359
6	3.993749	2.811162	1.934884
6	3.547074	2.432492	3.239977
1	4.065125	1.762936	3.913485
6	2.327904	3.122425	3.509484
1	1.763928	3.081824	4.431821
6	2.013816	3.927019	2.375719
1	1.163357	4.585570	2.281329
6	5.547678	5.667846	3.062478
1	6.305508	5.590952	2.294592
6	5.522980	4.940855	4.291703
1	6.255351	4.213774	4.615529

6	4.335308	5.306043	4.996047
1	4.009366	4.900646	5.944925
6	3.625250	6.257669	4.202055
1	2.669105	6.702386	4.444690
6	4.374341	6.482383	3.008691
1	4.082891	7.128999	2.192228
6	3.093660	4.259107	-0.006428
6	4.022763	5.264815	-0.310069
1	4.632675	5.654343	0.494407
6	4.183964	5.753562	-1.606999
1	4.919114	6.527997	-1.805896
6	3.399995	5.239397	-2.635937
1	3.512157	5.602520	-3.652811
6	2.472360	4.233875	-2.360348
1	1.882781	3.835751	-3.176872
6	2.311541	3.720787	-1.063363
6	5.144042	2.234635	1.164052
1	5.296655	2.843947	0.267845
6	6.465569	2.166542	1.932385
1	7.256091	1.716614	1.324572
1	6.372459	1.589336	2.855956
1	6.774958	3.180889	2.199178
6	0.393806	2.041237	-2.411425
6	1.067586	1.203547	-3.315764
1	1.980172	0.709364	-3.000198
6	0.596199	1.033860	-4.617521
1	1.136267	0.393218	-5.308890
6	-0.568838	1.689520	-5.027015
1	-0.942708	1.555005	-6.037694
6	-1.257600	2.507392	-4.128354
1	-2.172798	3.006321	-4.434356
6	-0.779130	2.685885	-2.828666
1	-1.326732	3.322496	-2.144992
6	-0.125625	3.020655	0.301035
6	-0.593189	2.270094	1.388423
1	-0.219855	1.263219	1.539828
6	-1.487399	2.836209	2.298789
1	-1.831309	2.247395	3.141354
6	-1.927402	4.150313	2.127637
1	-2.621316	4.591014	2.837972
6	-1.472402	4.901078	1.038012
1	-1.812584	5.923383	0.900178
6	-0.571297	4.342086	0.130308
1	-0.190964	4.944910	-0.689166
6	5.435537	0.398634	-1.092956
6	6.286910	-0.660847	-1.430276
1	6.507661	-1.449004	-0.722168
6	6.846374	-0.729863	-2.707556
6	6.547295	0.223174	-3.680227
1	6.969846	0.148552	-4.674646
6	5.669387	1.255628	-3.355214
6	5.123109	1.350992	-2.075786
1	4.428766	2.157069	-1.853612
6	5.123842	-0.668699	1.669124
6	4.155195	-1.205260	2.527467
1	3.124080	-0.891268	2.423723
6	4.512586	-2.123313	3.515007
6	5.836875	-2.533597	3.658500
1	6.114379	-3.252783	4.419869
6	6.803057	-1.994975	2.808349
6	6.459847	-1.060188	1.829654
1	7.241192	-0.641463	1.206850
29	2.216633	0.413509	0.037266
6	8.252356	-2.363175	2.977041
6	3.437891	-2.713807	4.385625
6	7.829741	-1.824940	-3.022557
6	5.253989	2.275056	-4.380508
9	3.903318	2.292336	-4.532239
9	5.614490	3.528138	-4.017635
9	5.788076	2.037435	-5.595171
9	7.806155	-2.171272	-4.328782
9	7.596066	-2.941334	-2.297754
9	9.099940	-1.439115	-2.745267
9	8.874275	-2.494767	1.782384
9	8.411508	-3.523133	3.648435
9	8.929436	-1.410381	3.663059
9	3.919686	-3.145366	5.570564
9	2.453997	-1.821131	4.646779
9	2.842248	-3.782257	3.793898
6	3.022076	-1.777692	-1.904706
6	2.167523	-2.715210	0.063567
6	3.602389	-2.973499	-2.286588
1	3.122605	-0.893822	-2.522858
6	2.824287	-3.936930	-0.260382
6	3.536480	-4.078617	-1.434278
1	2.729286	-4.779147	0.416711
6	1.270084	-2.718815	1.177994
6	0.781542	-1.577089	1.893775
8	1.078883	-0.377610	1.590708
7	2.330323	-1.630305	-0.759229
1	1.212009	-3.671856	1.683712
7	-0.061431	-1.764290	2.958049
6	-0.414954	-0.627611	3.802938
1	0.248955	0.209716	3.597411
1	-0.315969	-0.909920	4.855133
1	-1.449552	-0.315441	3.628521
6	-0.448599	-3.070399	3.475583
1	-0.628499	-3.786038	2.672937
1	-1.379684	-2.958743	4.036294
1	0.317685	-3.481829	4.144105
77	-3.324811	-1.621256	-1.294941
15	-4.944766	-0.732630	0.043854
8	-4.932245	0.801502	0.679756
8	-6.379665	-0.682495	-0.807385
7	-5.080214	-1.627383	1.451612
6	-5.100838	1.896575	-0.167456
6	-3.964235	2.704101	-0.389256
1	-3.040795	2.450732	0.116040
6	-4.056707	3.784010	-1.231606
1	-3.197319	4.427611	-1.389014
6	-5.263702	4.053917	-1.929924
6	-5.336925	5.103715	-2.885262
1	-4.455271	5.718571	-3.046830
6	-6.490004	5.327817	-3.602766
1	-6.533677	6.128024	-4.335789
6	-7.618439	4.499258	-3.394996
1	-8.518939	4.660584	-3.980560
6	-7.585904	3.485363	-2.461972
1	-8.457290	2.856171	-2.326920
6	-6.419077	3.237573	-1.685893
6	-6.344408	2.175751	-0.713059
6	-7.542586	1.375698	-0.335797
6	-8.743531	1.995997	0.164634
6	-8.814779	3.380647	0.485518
1	-7.935058	4.000756	0.360325
6	-9.977994	3.940962	0.967788
1	-10.002459	4.998912	1.213003
6	-11.138276	3.152282	1.152900
1	-12.049693	3.609327	1.526916
6	-11.100024	1.805214	0.872124
1	-11.977294	1.182364	1.026578
6	-9.911774	1.192526	0.389816
6	-9.856604	-0.206691	0.146074
1	-10.751065	-0.804453	0.297176
6	-8.680610	-0.800107	-0.237672
1	-8.601088	-1.871379	-0.389816
6	-7.528643	-0.006530	-0.436996
6	-4.212014	-2.840196	1.444922
1	-3.276873	-2.596094	1.966660
6	-4.851920	-4.024925	2.148608
6	-4.095539	-4.801663	3.033718
1	-3.071960	-4.511962	3.258111
6	-4.644722	-5.940405	3.630441
1	-4.045129	-6.533053	4.315980
6	-5.962397	-6.309191	3.352890
1	-6.393802	-7.189344	3.821095
6	-6.726421	-5.535923	2.471974
1	-7.753905	-5.814785	2.254706
6	-6.173321	-4.405679	1.870770
1	-6.767864	-3.798736	1.192831

6	-3.910916	-3.232060	-0.005204
1	-4.821703	-3.673642	-0.427915
1	-3.159548	-4.022976	-0.015008
6	-5.650712	-1.249653	2.781851
1	-5.949852	-2.208256	3.210562
6	-4.639131	-0.661463	3.766330
6	-4.098088	-1.498204	4.754998
1	-4.330772	-2.559683	4.735497
6	-3.302029	-0.982936	5.781079
1	-2.902687	-1.649006	6.541054
6	-3.038774	0.386632	5.837928
1	-2.436971	0.796838	6.643903
6	-3.554812	1.226927	4.847461
1	-3.362003	2.295375	4.890236
6	-4.337319	0.707763	3.812668
1	-4.736629	1.375023	3.057162
6	-6.934130	-0.420856	2.715089
1	-7.699123	-0.947687	2.142923
1	-6.788751	0.565660	2.276511
1	-7.306909	-0.286089	3.734718
6	-1.821838	-0.703978	-0.028123
1	-1.635621	0.332736	-0.295925
1	-1.996199	-0.841426	1.037346
6	-1.037369	-1.703501	-0.709668
1	-0.457764	-1.410292	-1.575978
6	-0.824305	-2.989951	-0.189307
1	-1.320596	-3.219461	0.745023
6	-4.850463	-2.360752	-2.784668
1	-5.639243	-2.831294	-2.204316
6	-3.665032	-3.103617	-2.959079
1	-3.634376	-4.099957	-2.518856
6	-2.672642	-2.900151	-4.089186
1	-3.057071	-3.370951	-5.007206
1	-1.763747	-3.446973	-3.826480
6	-2.312991	-1.424482	-4.364393
1	-2.961366	-1.011535	-5.144122
1	-1.295404	-1.374193	-4.763490
6	-2.385797	-0.517547	-3.139691
1	-1.437332	-0.119822	-2.796214
6	-3.514431	0.199931	-2.769956
1	-3.352193	1.095514	-2.180559
6	-4.853958	0.129482	-3.472526
1	-5.589780	0.629686	-2.843537
1	-4.791951	0.712250	-4.403690
6	-5.339124	-1.305301	-3.775909
1	-5.035379	-1.603521	-4.784789
1	-6.433030	-1.309260	-3.773348
6	-0.353554	-4.139609	-0.950390
6	0.199482	-4.025599	-2.240705
6	-0.458892	-5.422511	-0.377161
6	0.612432	-5.157345	-2.938996
1	0.318525	-3.047913	-2.693548
6	-0.043634	-6.554039	-1.076074
1	-0.871623	-5.522964	0.623680
6	0.490027	-6.425734	-2.362749
1	1.039111	-5.048856	-3.931915
1	-0.137091	-7.535417	-0.620051
1	0.813350	-7.306753	-2.909456
1	4.006063	-5.021744	-1.691069
35	4.469991	-3.113521	-4.032577

C1-P1 *re-si_*1

Number of imaginary frequencies= 1
The smallest frequencies are= -138.3855 7.8376 9.4099 cm(-1)
Electronic energy= -7222.6241764
Zero-point correction= 1.754258
(Hartree/Particle)
Thermal correction to Energy= 1.873058
Thermal correction to Enthalpy= 1.874002
Thermal correction to Gibbs Free Energy= 1.591132
Sum of electronic and zero-point Energies= -7220.869918
Sum of electronic and thermal Energies= -7220.751118
Sum of electronic and thermal Enthalpies= -7220.750174
Sum of electronic and thermal Free Energies= -7221.033045

.....
Cartesian Coordinates
.....

26	-8.571311	-1.286216	0.529375
15	-4.315801	-0.218965	-2.304923
15	-4.433480	0.950588	1.258540
6	-6.949038	-0.504018	-0.534920
6	-6.673923	-0.553744	0.882388
6	-6.762362	-1.917191	1.299706
1	-6.622789	-2.280161	2.308873
6	-7.122195	-2.707738	0.167372
1	-7.308350	-3.772834	0.170028
6	-7.242069	-1.841039	-0.957864
1	-7.526420	-2.136075	-1.956070
6	-10.007696	0.005358	1.287063
1	-9.810015	1.015820	1.620078
6	-9.928029	-1.173829	2.089992
1	-9.653550	-1.214732	3.135652
6	-10.227823	-2.295677	1.258238
1	-10.214620	-3.333738	1.563189
6	-10.493390	-1.810862	-0.058636
1	-10.720876	-2.415971	-0.926386
6	-10.359930	-0.390479	-0.040894
1	-10.472966	0.264724	-0.893966
6	-6.834008	0.737182	-1.356043
6	-7.792121	1.751514	-1.204733
1	-8.624798	1.572524	-0.535987
6	-7.682571	2.974647	-1.866163
1	-8.425364	3.749032	-1.701700
6	-6.603616	3.201132	-2.717246
1	-6.497083	4.151763	-3.229539
6	-5.639840	2.207199	-2.888634
1	-4.797360	2.401533	-3.543115
6	-5.725656	0.979515	-2.213089
6	-6.250309	0.630741	1.704936
1	-6.794337	1.499990	1.331969
6	-6.538231	0.494154	3.202518
1	-6.248179	1.399995	3.741954
1	-6.005706	-0.348281	3.652190
1	-7.610521	0.330563	3.347153
6	-3.165843	0.505432	-3.551167
6	-2.017649	1.157794	-3.076967
1	-1.835731	1.220820	-2.009660
6	-1.085852	1.688731	-3.972232
1	-0.195636	2.180193	-3.595058
6	-1.290176	1.570994	-5.348078
1	-0.559507	1.975249	-6.043069
6	-2.434335	0.927334	-5.828814
1	-2.599328	0.833020	-6.898498
6	-3.368142	0.397951	-4.937188
1	-4.245342	-0.107430	-5.326420
6	-5.032043	-1.668418	-3.181211
6	-6.078064	-1.548066	-4.110489
1	-6.498043	-0.571986	-4.334433
6	-6.604296	-2.684468	-4.726682
1	-7.416332	-2.582834	-5.441160
6	-6.093660	-3.950349	-4.420083
1	-6.510536	-4.833903	-4.895024
6	-5.048750	-4.075255	-3.501532
1	-4.645862	-5.054641	-3.259094
6	-4.521778	-2.938761	-2.884756
1	-3.712971	-3.037668	-2.170794
6	-4.338658	2.696390	0.680530
6	-3.111259	3.066853	0.114264
1	-2.306536	2.339776	0.085369
6	-2.936717	4.340126	-0.427115
6	-3.989202	5.252551	-0.456320
1	-3.862795	6.231614	-0.905134
6	-5.218206	4.871097	0.083992
6	-5.393838	3.615961	0.667563
1	-6.362557	3.367538	1.080326
6	-3.516795	0.965093	2.850436
6	-3.212361	-0.290929	3.398049
1	-3.543194	-1.193406	2.897807
6	-2.460424	-0.385908	4.564827

6	-1.970951	0.760986	5.193493
1	-1.367439	0.682968	6.090369
6	-2.257427	2.005062	4.636779
6	-3.032340	2.115484	3.478492
1	-3.243762	3.097591	3.070514
29	-3.366760	-0.483912	-0.254386
6	-1.640860	3.245715	5.219049
6	-2.059534	-1.736219	5.089426
6	-1.579411	4.710463	-0.955275
6	-6.372638	5.828307	-0.030091
9	-6.698726	6.054814	-1.327754
9	-7.487455	5.374288	0.582909
9	-6.078271	7.035500	0.505327
9	-1.011481	3.671140	-1.623645
9	-0.718781	5.031427	0.042969
9	-1.612313	5.757346	-1.803215
9	-0.484062	3.561761	4.572545
9	-1.330339	3.104873	6.523982
9	-2.449406	4.321420	5.102319
9	-2.060615	-1.775240	6.439393
9	-2.870344	-2.721828	4.648862
9	-0.797314	-2.065017	4.696639
6	-0.657939	0.017735	1.102677
6	-0.530777	-1.370626	1.459918
6	-1.506182	-2.401030	1.297503
1	0.231414	-1.616091	2.182956
77	4.142479	-2.013477	-0.789625
15	5.595667	-0.383365	-0.202853
8	6.314576	-0.299866	1.288353
8	6.936756	-0.353577	-1.190589
7	4.823673	1.105674	-0.209523
6	7.490158	-0.974658	1.592946
6	7.388024	-1.993736	2.565451
1	6.420020	-2.181794	3.017767
6	8.504606	-2.707995	2.920508
1	8.441878	-3.487511	3.674508
6	9.751686	-2.456855	2.287811
6	10.896980	-3.240530	2.594879
1	10.803626	-4.020946	3.345669
6	12.093559	-3.028374	1.948722
1	12.961793	-3.635291	2.188082
6	12.186039	-2.024899	0.955298
1	13.123307	-1.876307	0.426778
6	11.098191	-1.237663	0.645141
1	11.189142	-0.483773	-0.127210
6	9.851915	-1.409090	1.310988
6	8.693648	-0.602736	1.013459
6	8.766941	0.554536	0.076972
6	9.698542	1.637574	0.257862
6	10.473334	1.791851	1.441301
1	10.360056	1.074885	2.246064
6	11.349515	2.845619	1.584355
1	11.922037	2.946993	2.501837
6	11.506002	3.801754	0.552137
1	12.204249	4.623965	0.678052
6	10.762353	3.692069	-0.600822
1	10.859857	4.427233	-1.395395
6	9.838592	2.625662	-0.775369
6	9.034066	2.536630	-1.943341
1	9.160672	3.274572	-2.730159
6	8.073997	1.561499	-2.055246
1	7.423198	1.497201	-2.920020
6	7.929696	0.605869	-1.026789
6	3.514702	1.075011	-0.912115
1	2.714456	1.087725	-0.161269
6	3.315406	2.250221	-1.858847
6	2.059624	2.853471	-1.977501
1	1.237603	2.505373	-1.360915
6	1.858831	3.916694	-2.863673
1	0.883004	4.386886	-2.925031
6	2.914385	4.379033	-3.651217
1	2.764492	5.212379	-4.331879
6	4.168534	3.767897	-3.551246
1	4.999308	4.126223	-4.153009
6	4.363484	2.709575	-2.666444
1	5.344199	2.260536	-2.561914
6	3.403116	-0.226048	-1.731938
1	3.973419	-0.087898	-2.658113
1	2.363837	-0.350710	-2.041600
6	5.090114	2.141102	0.847552
1	6.088838	1.912579	1.215669
6	5.164521	3.559744	0.300666
6	6.403021	4.040412	-0.139968
1	7.274496	3.399485	-0.066663
6	6.528335	5.323347	-0.673747
1	7.499639	5.673506	-1.013020
6	5.407679	6.152422	-0.763096
1	5.496868	7.151171	-1.181554
6	4.171172	5.692791	-0.301259
1	3.294576	6.331647	-0.362788
6	4.053271	4.409357	0.234088
1	3.082419	4.065105	0.574213
6	4.121055	1.986442	2.023844
1	4.219818	0.987632	2.456546
1	3.081247	2.130760	1.725272
1	4.350211	2.724980	2.798070
6	3.170187	-1.741846	1.119350
1	3.672942	-2.257750	1.937276
1	2.955285	-0.700249	1.348658
6	2.161683	-2.482785	0.399174
1	2.092111	-3.553781	0.551045
6	1.123965	-1.863413	-0.321079
1	1.181017	-0.788374	-0.428704
6	5.274973	-2.476102	-2.691216
1	5.485987	-1.519559	-3.161651
6	3.959911	-2.963816	-2.828070
1	3.263042	-2.353602	-3.401625
6	3.525316	-4.410282	-2.678228
1	3.681967	-4.948881	-3.625451
1	2.445475	-4.403738	-2.502915
6	4.212476	-5.168579	-1.522868
1	5.143134	-5.629070	-1.867142
1	3.564965	-5.994628	-1.211244
6	4.506574	-4.304722	-0.299882
1	3.893327	-4.502097	0.575075
6	5.703290	-3.643086	-0.067982
1	5.935679	-3.393047	0.963162
6	6.884786	-3.606105	-1.015348
1	7.557753	-2.812977	-0.683212
1	7.443689	-4.548530	-0.920825
6	6.507049	-3.359619	-2.492346
1	6.348071	-4.311514	-3.007838
1	7.355916	-2.882299	-2.990503
6	0.264461	-2.542879	-1.277869
6	0.080383	-3.940956	-1.285651
6	-0.377497	-1.772292	-2.265828
6	-0.693742	-4.545147	-2.273947
1	0.545143	-4.553007	-0.520539
6	-1.134498	-2.380269	-3.263959
1	-0.273552	-0.693864	-2.243762
6	-1.289162	-3.769757	-3.274957
1	-0.826649	-5.623252	-2.269911
1	-1.614413	-1.769470	-4.021270
1	-1.886591	-4.243180	-4.048009
8	-1.382403	0.429426	0.142007
6	-1.226200	-3.670449	1.884064
6	-2.113186	-4.721602	1.783504
1	-0.300898	-3.796820	2.435980
6	-3.306603	-4.497485	1.088021
6	-3.554223	-3.258903	0.529123
1	-4.475741	-3.059798	-0.002932
7	-2.681831	-2.234458	0.614558
6	0.106080	2.330465	1.364831
1	-0.639699	2.905716	1.926483
1	1.086457	2.776968	1.550698
1	-0.118629	2.404291	0.305463
6	0.767899	0.668019	3.061690
1	0.291395	-0.159777	3.582859
1	1.833852	0.446633	2.944512
1	0.667907	1.554762	3.691986

7	0.119933	0.931946	1.776571
1	-1.892311	-5.682449	2.236076
35	-4.635338	-5.922098	0.891954

C1-P1 *re-si_2*

Number of imaginary frequencies= 1
The smallest frequencies are=-212.3847 11.3265 12.5086cm(-1)
Electronic energy= -7222.6317145
Zero-point correction= 1.755524
(Hartree/Particle)
Thermal correction to Energy= 1.874043
Thermal correction to Enthalpy= 1.874987
Thermal correction to Gibbs Free Energy= 1.595134
Sum of electronic and zero-point Energies= -7220.876191
Sum of electronic and thermal Energies= -7220.757672
Sum of electronic and thermal Enthalpies= -7220.756728
Sum of electronic and thermal Free Energies= -7221.036581

.....

Cartesian Coordinates

.....

26	4.283280	3.820783	3.517524
15	1.367622	2.086474	-0.504156
15	4.554921	0.254983	0.360415
6	3.413989	3.165503	1.724286
6	4.236201	2.135908	2.315575
6	3.709391	1.845850	3.611834
1	4.113380	1.128493	4.312666
6	2.588343	2.701323	3.840437
1	1.999086	2.746820	4.745786
6	2.410637	3.515145	2.683688
1	1.660849	4.281327	2.555308
6	6.145631	4.745422	3.461426
1	6.918194	4.540359	2.731789
6	5.965814	4.065049	4.704266
1	6.569880	3.247666	5.075361
6	4.820218	4.621654	5.350475
1	4.402093	4.296106	6.293933
6	4.291023	5.645609	4.506843
1	3.402993	6.232960	4.699679
6	5.109144	5.722340	3.340419
1	4.951398	6.383588	2.499288
6	3.594343	3.685416	0.337685
6	4.715873	4.481531	0.056668
1	5.381678	4.726830	0.874064
6	4.997378	4.936781	-1.230617
1	5.891488	5.523422	-1.416554
6	4.131936	4.615731	-2.273104
1	4.334601	4.956877	-3.283219
6	3.010074	3.826384	-2.020208
1	2.357922	3.576244	-2.848319
6	2.729363	3.334272	-0.734486
6	5.363663	1.437073	1.606221
1	5.873289	2.185954	0.997958
6	6.390492	0.789113	2.538595
1	7.211479	0.344130	1.969733
1	5.947361	0.003673	3.157055
1	6.802668	1.551837	3.206695
6	0.613818	2.010127	-2.183147
6	1.152179	1.069274	-3.079132
1	1.886440	0.351923	-2.727617
6	0.752290	1.059600	-4.417267
1	1.192989	0.344459	-5.103176
6	-0.211103	1.966765	-4.867312
1	-0.525861	1.955289	-5.906619
6	-0.783624	2.873800	-3.972193
1	-1.550126	3.565621	-4.309571
6	-0.369368	2.900957	-2.638878
1	-0.808483	3.624318	-1.962434
6	0.143573	2.954343	0.556064
6	-0.099880	4.333060	0.442533
1	0.414956	4.915287	-0.316123
6	-0.976874	4.967840	1.323605
1	-1.160057	6.034138	1.227770
6	-1.611640	4.234658	2.331064
1	-2.289278	4.730878	3.019505
6	-1.374464	2.863383	2.450970
1	-1.870638	2.294734	3.230515
6	-0.501865	2.224898	1.566395
1	-0.309732	1.162211	1.665180
6	5.289975	0.648870	-1.282057
6	4.727116	-0.034795	-2.369688
1	3.963152	-0.781663	-2.181047
6	5.109101	0.272063	-3.674691
6	6.028581	1.288196	-3.927926
1	6.303926	1.546422	-4.944339
6	6.574341	1.979209	-2.845496
6	6.228618	1.656848	-1.532493
1	6.685093	2.216755	-0.727556
6	5.167931	-1.434382	0.754298
6	4.531871	-2.078331	1.827282
1	3.784092	-1.552797	2.406895
6	4.823585	-3.404168	2.131380
6	5.746530	-4.121760	1.369336
1	5.962452	-5.159788	1.595160
6	6.380118	-3.481059	0.306628
6	6.102817	-2.146137	-0.003080
1	6.605916	-1.679336	-0.842297
29	2.209171	0.121090	0.194019
6	7.301334	-4.273180	-0.578115
6	4.055173	-4.108980	3.214424
6	4.532555	-0.535199	-4.804150
6	7.511973	3.119903	-3.131351
9	6.891114	4.107458	-3.824536
9	8.009654	3.679259	-2.006828
9	8.563368	2.726791	-3.887137
9	3.216067	-0.823265	-4.600693
9	5.157968	-1.730076	-4.936276
9	4.621595	0.096468	-5.990963
9	6.606667	-4.912165	-1.559183
9	7.969409	-5.227429	0.104728
9	8.215289	-3.494781	-1.195305
9	4.827786	-4.976466	3.902654
9	3.512002	-3.248000	4.102515
9	3.026662	-4.834914	2.696901
6	2.234627	-2.769580	-0.736163
6	1.264677	-3.148446	0.269404
6	1.004508	-2.415215	1.471809
1	1.073769	-4.208544	0.371407
77	-3.304172	-1.406542	-1.558923
15	-4.875441	-0.536030	-0.169564
8	-4.718079	0.942160	0.580147
8	-6.314048	-0.302192	-0.975279
7	-5.082606	-1.534858	1.150487
6	-4.818303	2.111261	-0.169251
6	-3.627470	2.848369	-0.351341
1	-2.717807	2.485189	0.108819
6	-3.649605	3.998815	-1.099441
1	-2.745230	4.585570	-1.225459
6	-4.843480	4.415588	-1.746044
6	-4.852088	5.545067	-2.608776
1	-3.928438	6.103412	-2.738475
6	-5.995774	5.913104	-3.280382
1	-5.990277	6.772960	-3.943846
6	-7.180435	5.156064	-3.116785
1	-8.075222	5.432748	-3.666974
6	-7.210279	4.067616	-2.271742
1	-8.125053	3.496332	-2.168454
6	-6.053113	3.668831	-1.545520
6	-6.045160	2.527613	-0.664078
6	-7.295447	1.797295	-0.313885
6	-8.428714	2.468207	0.271514
6	-8.385613	3.829481	0.685136
1	-7.465572	4.390309	0.571838
6	-9.488286	4.440504	1.241933
1	-9.424912	5.478418	1.556127
6	-10.699328	3.729144	1.415124
1	-11.562354	4.226215	1.848238
6	-10.770649	2.404221	1.048968
1	-11.687457	1.838826	1.194079

6	-9.646785	1.739272	0.487555
6	-9.704852	0.357961	0.157860
1	-10.634920	-0.182401	0.309745
6	-8.591713	-0.292580	-0.311655
1	-8.596180	-1.355103	-0.530914
6	-7.393112	0.428749	-0.511025
6	-4.245485	-2.770860	1.088624
1	-3.343729	-2.589769	1.685313
6	-4.956726	-3.977497	1.677653
6	-4.296195	-4.795737	2.600460
1	-3.297047	-4.524357	2.932739
6	-4.914283	-5.943456	3.104957
1	-4.389134	-6.568955	3.821692
6	-6.207993	-6.277172	2.699064
1	-6.693547	-7.164304	3.095841
6	-6.878639	-5.459958	1.782474
1	-7.887817	-5.710679	1.467013
6	-6.255055	-4.321411	1.272925
1	-6.777893	-3.680253	0.567783
6	-3.838925	-3.079915	-0.358189
1	-4.688087	-3.563722	-0.854875
1	-3.041069	-3.825041	-0.322626
6	-5.652536	-1.266219	2.506394
1	-6.270729	-2.140855	2.727405
6	-4.554955	-1.219180	3.561976
6	-4.652476	-2.047266	4.685710
1	-5.484111	-2.742497	4.763861
6	-3.691360	-1.994630	5.697573
1	-3.782479	-2.641836	6.565597
6	-2.613150	-1.116501	5.586543
1	-1.860390	-1.073448	6.366486
6	-2.500220	-0.296876	4.458685
1	-1.652839	0.373865	4.366700
6	-3.465695	-0.343446	3.452446
1	-3.379704	0.299211	2.581440
6	-6.576292	-0.052500	2.650681
1	-7.422695	-0.107450	1.966412
1	-6.055641	0.893147	2.505778
1	-6.973023	-0.070472	3.670373
6	-1.774056	-0.770874	-0.135122
1	-1.639020	0.306303	-0.085842
1	-1.908542	-1.225735	0.844688
6	-0.989638	-1.463911	-1.118575
1	-0.471288	-0.854845	-1.846909
6	-0.669796	-2.839567	-1.108360
1	-1.158600	-3.465170	-0.373627
6	-4.895384	-2.025464	-3.031028
1	-5.653388	-2.549649	-2.454569
6	-3.716524	-2.745259	-3.319606
1	-3.656400	-3.768588	-2.950802
6	-2.798108	-2.467609	-4.493378
1	-3.238457	-2.888184	-5.410731
1	-1.870939	-3.014785	-4.319908
6	-2.460878	-0.976397	-4.717846
1	-3.153114	-0.536988	-5.443557
1	-1.464639	-0.904784	-5.165262
6	-2.471791	-0.115985	-3.461567
1	-1.508032	0.231966	-3.115148
6	-3.572608	0.577382	-3.012186
1	-3.393845	1.420098	-2.353648
6	-4.954720	0.504467	-3.620531
1	-5.651775	0.978039	-2.929928
1	-4.962079	1.113659	-4.536724
6	-5.447089	-0.925420	-3.939362
1	-5.206727	-1.182140	-4.976879
1	-6.538512	-0.934980	-3.868016
6	-0.148547	-3.532532	-2.290866
6	0.488069	-2.849102	-3.346465
6	-0.297789	-4.928022	-2.391502
6	0.949722	-3.539356	-4.463449
1	0.641640	-1.779198	-3.284035
6	0.156571	-5.617069	-3.515749
1	-0.780852	-5.469053	-1.581540
6	0.783146	-4.925205	-4.556978
1	1.455516	-2.994057	-5.255209
1	0.022714	-6.693215	-3.579203
1	1.141340	-5.461094	-5.431158
8	2.366246	-1.574454	-1.147083
6	0.373152	-3.091323	2.557611
6	0.295016	-2.517105	3.809775
1	0.011510	-4.103251	2.405059
6	0.827751	-1.230745	3.964737
6	1.306928	-0.550417	2.864410
1	1.662714	0.468707	2.945253
7	1.382555	-1.110985	1.639886
6	3.734447	-3.472671	-2.541552
1	3.294559	-2.631130	-3.065213
1	4.784737	-3.258781	-2.317507
1	3.690317	-4.345762	-3.198671
6	3.095450	-5.113346	-0.812001
1	2.981170	-5.133372	0.271037
1	2.359060	-5.786275	-1.268731
1	4.097521	-5.481544	-1.046531
7	2.974411	-3.752659	-1.328486
1	-0.143322	-3.053391	4.643799
35	0.980977	-0.401965	5.730726

C1-P1 *re-si*_3

Number of imaginary frequencies= 1
The smallest frequencies are= -50.1004 11.0874 12.5338 cm(-1)
Electronic energy= -7222.6312683
Zero-point correction= 1.755056
(Hartree/Particle)
Thermal correction to Energy= 1.873591
Thermal correction to Enthalpy= 1.874536
Thermal correction to Gibbs Free Energy= 1.593392
Sum of electronic and zero-point Energies= -7220.876212
Sum of electronic and thermal Energies= -7220.757677
Sum of electronic and thermal Enthalpies= -7220.756733
Sum of electronic and thermal Free Energies= -7221.037876
.....
Cartesian Coordinates
.....

26	4.332351	4.770046	2.089876
15	2.533156	1.718804	-1.760630
15	4.617029	0.151016	0.938765
6	3.961879	3.466281	0.493366
6	4.234704	2.736842	1.709765
6	3.250870	3.114733	2.675203
1	3.192475	2.753293	3.692495
6	2.392574	4.089297	2.083088
1	1.574135	4.596753	2.574150
6	2.827845	4.305085	0.742987
1	2.396790	5.000257	0.038482
6	6.282628	5.384433	2.463682
1	7.166321	4.795065	2.257341
6	5.527297	5.366389	3.675822
1	5.735245	4.758479	4.546170
6	4.426019	6.262815	3.523687
1	3.648165	6.443087	4.253976
6	4.499963	6.835416	2.217479
1	3.790079	7.528346	1.785257
6	5.646426	6.294161	1.562944
1	5.956060	6.509383	0.549207
6	4.706655	3.295584	-0.788248
6	6.018429	3.783570	-0.890428
1	6.440782	4.297187	-0.036358
6	6.781453	3.611990	-2.045155
1	7.802093	3.979462	-2.079938
6	6.229485	2.953919	-3.141562
1	6.809755	2.809047	-4.046932
6	4.929267	2.455001	-3.063383
1	4.519325	1.930911	-3.919271
6	4.159022	2.595814	-1.897858
6	5.289270	1.672610	1.853985
1	6.163367	1.994129	1.285428
6	5.726697	1.412216	3.298241
1	6.519877	0.660546	3.336474
1	4.901122	1.060722	3.923234

1	6.105947	2.341866	3.733607
6	2.319982	0.911784	-3.404858
6	2.873231	-0.367684	-3.579755
1	3.358028	-0.863903	-2.746159
6	2.789558	-1.008370	-4.817236
1	3.247413	-1.982180	-4.947910
6	2.115890	-0.400180	-5.879518
1	2.039165	-0.907128	-6.837094
6	1.540562	0.860806	-5.705519
1	1.013174	1.339080	-6.525956
6	1.650809	1.519719	-4.478752
1	1.213309	2.505816	-4.365475
6	1.265143	3.041943	-1.791166
6	1.461241	4.293076	-2.396218
1	2.419431	4.535793	-2.846253
6	0.427318	5.231605	-2.413007
1	0.585769	6.199051	-2.881062
6	-0.809809	4.926284	-1.834739
1	-1.615380	5.654890	-1.853193
6	-1.009154	3.680815	-1.235208
1	-1.965656	3.434307	-0.790260
6	0.026619	2.746597	-1.208716
1	-0.120180	1.780248	-0.737520
6	5.875585	-0.317319	-0.321252
6	5.537229	-1.408022	-1.136127
1	4.606195	-1.936883	-0.954232
6	6.369028	-1.790800	-2.188417
6	7.530026	-1.076612	-2.476168
1	8.164135	-1.361294	-3.308055
6	7.854023	0.020945	-1.677318
6	7.050005	0.392304	-0.599811
1	7.344941	1.247422	-0.007588
6	4.642449	-1.257250	2.125069
6	3.619114	-1.275196	3.087225
1	2.921654	-0.448283	3.151194
6	3.464603	-2.369410	3.933114
6	4.304292	-3.479752	3.824468
1	4.167216	-4.342008	4.466611
6	5.312427	-3.464867	2.864956
6	5.494658	-2.361077	2.026587
1	6.290606	-2.383905	1.291254
29	2.497905	0.252365	-0.051837
6	6.154676	-4.690536	2.647740
6	2.312053	-2.423640	4.896801
6	5.996614	-3.010920	-2.983703
6	9.080354	0.818716	-2.027922
9	8.964816	1.392962	-3.251222
9	9.325175	1.812290	-1.145383
9	10.186864	0.040457	-2.075234
9	4.683110	-2.999431	-3.339016
9	6.178517	-4.146560	-2.265694
9	6.714719	-3.134476	-4.116947
9	5.632338	-5.473240	1.662280
9	6.238033	-5.462076	3.751533
9	7.413010	-4.383619	2.265163
9	2.668818	-2.967273	6.081643
9	1.788928	-1.205197	5.147958
9	1.298736	-3.194259	4.413073
6	1.983263	-2.685062	0.409219
6	0.882735	-2.394831	1.284453
6	0.478187	-1.129213	1.793844
1	0.452182	-3.230533	1.816490
77	-3.361313	-1.003969	-1.721116
15	-5.130744	-0.723169	-0.316345
8	-5.244770	0.434580	0.865852
8	-6.488733	-0.365632	-1.208248
7	-5.343109	-2.086801	0.632569
6	-5.291511	1.776469	0.511263
6	-4.167975	2.559825	0.856574
1	-3.356349	2.089255	1.400062
6	-4.142730	3.889387	0.513689
1	-3.300378	4.514522	0.794741
6	-5.195075	4.453895	-0.257749
6	-5.120147	5.792011	-0.730569
1	-4.252285	6.388429	-0.460936
6	-6.114228	6.317648	-1.524742
1	-6.042986	7.338172	-1.889194
6	-7.227983	5.519020	-1.878479
1	-7.999341	5.928438	-2.524361
6	-7.342896	4.226057	-1.415260
1	-8.200445	3.627602	-1.699764
6	-6.341878	3.653763	-0.582167
6	-6.423708	2.300522	-0.092571
6	-7.669476	1.490258	-0.203205
6	-8.925585	1.979931	0.314739
6	-9.031535	3.183502	1.067734
1	-8.139023	3.757565	1.284428
6	-10.248126	3.624261	1.542762
1	-10.296214	4.542869	2.120509
6	-11.431590	2.890328	1.293845
1	-12.384325	3.254400	1.666863
6	-11.363644	1.706206	0.595454
1	-12.259411	1.117834	0.414211
6	-10.122781	1.215526	0.106387
6	-10.047778	-0.034170	-0.566005
1	-10.959813	-0.600296	-0.732755
6	-8.836490	-0.534801	-0.968326
1	-8.746027	-1.504046	-1.447286
6	-7.659707	0.218112	-0.756355
6	-4.354894	-3.155201	0.325541
1	-3.502304	-3.043463	1.008838
6	-4.929104	-4.548760	0.512250
6	-4.162272	-5.539332	1.136667
1	-3.186184	-5.281776	1.542016
6	-4.641385	-6.847931	1.245657
1	-4.035115	-7.606593	1.732922
6	-5.900096	-7.175817	0.738029
1	-6.277795	-8.190367	0.827564
6	-6.675518	-6.189589	0.118707
1	-7.658118	-6.437389	-0.273416
6	-6.191595	-4.886761	0.003228
1	-6.795036	-4.116662	-0.470184
6	-3.881275	-2.999703	-1.121352
1	-4.695050	-3.331885	-1.776516
1	-3.045211	-3.677280	-1.300872
6	-6.016058	-2.180043	1.968140
1	-6.179158	-3.253269	2.091725
6	-5.124121	-1.757856	3.136616
6	-4.262227	-2.708093	3.706323
1	-4.230278	-3.712203	3.292046
6	-3.477181	-2.395884	4.819444
1	-2.823756	-3.150167	5.249508
6	-3.558609	-1.126308	5.395901
1	-2.966034	-0.884030	6.273749
6	-4.411640	-0.169852	4.836163
1	-4.483997	0.819730	5.279330
6	-5.181647	-0.480930	3.713972
1	-5.840607	0.271878	3.298319
6	-7.405441	-1.546139	1.987778
1	-8.026724	-1.982477	1.202783
1	-7.387663	-0.465343	1.849357
1	-7.875706	-1.754733	2.953310
6	-2.087303	-0.379894	-0.087680
1	-1.974383	0.700945	-0.046493
1	-2.358569	-0.803448	0.875211
6	-1.139897	-1.120783	-0.887210
1	-0.496290	-0.595049	-1.583062
6	-0.889051	-2.477274	-0.644559
1	-1.471169	-2.939071	0.143973
6	-4.648179	-1.314924	-3.532399
1	-5.428063	-2.018144	-3.249736
6	-3.370536	-1.869480	-3.780063
1	-3.279122	-2.951562	-3.688296
6	-2.284409	-1.239880	-4.636569
1	-2.472823	-1.456965	-5.699378
1	-1.340430	-1.735019	-4.386422
6	-2.125130	0.278053	-4.425178
1	-2.783613	0.829769	-5.102497
1	-1.103383	0.567850	-4.687792
6	-2.393972	0.724747	-2.992458

1	-1.518631	1.033507	-2.433516
6	-3.618838	1.193897	-2.535913
1	-3.611655	1.836238	-1.659857
6	-4.881607	1.255875	-3.369941
1	-5.717371	1.453582	-2.698672
1	-4.814542	2.119733	-4.047386
6	-5.171941	-0.030378	-4.176516
1	-4.758308	0.052473	-5.186457
1	-6.254991	-0.124158	-4.298444
6	-0.199907	-3.401191	-1.525027
6	0.549326	-2.983334	-2.644628
6	-0.314612	-4.783669	-1.268562
6	1.140689	-3.922356	-3.484358
1	0.675229	-1.927913	-2.852559
6	0.279996	-5.720112	-2.110395
1	-0.880949	-5.115916	-0.402319
6	1.008548	-5.291230	-3.224269
1	1.713081	-3.585636	-4.342115
1	0.176308	-6.780590	-1.899961
1	1.474309	-6.017627	-3.883900
8	2.482719	-1.850517	-0.412960
6	-0.506577	-1.103263	2.826754
6	-0.988634	0.084584	3.330220
1	-0.882064	-2.041476	3.220657
6	-0.474355	1.272534	2.798308
6	0.495838	1.224344	1.818972
1	0.921316	2.127744	1.403410
7	0.963958	0.062287	1.319779
6	3.399245	-4.389666	-0.641470
1	3.297531	-3.740871	-1.505859
1	4.439164	-4.379573	-0.297078
1	3.146977	-5.410932	-0.944114
6	2.185672	-4.969850	1.419571
1	1.926408	-4.511162	2.372867
1	1.369649	-5.633678	1.103973
1	3.081542	-5.575504	1.580061
7	2.485010	-3.962329	0.409205
1	-1.748877	0.089835	4.100864
35	-1.136161	3.006497	3.427532

C1-P1 *re-si*_4

Number of imaginary frequencies= 1
The smallest frequencies are= -68.1590 8.5309 10.3557 cm(-1)
Electronic energy= -7222.6318939
Zero-point correction= 1.754512
(Hartree/Particle)
Thermal correction to Energy= 1.873365
Thermal correction to Enthalpy= 1.874310
Thermal correction to Gibbs Free Energy= 1.591948
Sum of electronic and zero-point Energies= -7220.877382
Sum of electronic and thermal Energies= -7220.758529
Sum of electronic and thermal Enthalpies= -7220.757584
Sum of electronic and thermal Free Energies= -7221.039946

.....

Cartesian Coordinates

.....

26	-4.418478	-3.968074	3.286596
15	-1.345928	-2.104418	-0.576348
15	-4.499164	-0.254368	0.279527
6	-3.472622	-3.243938	1.557089
6	-4.283432	-2.222275	2.175738
6	-3.794582	-2.020454	3.502773
1	-4.198909	-1.327494	4.227267
6	-2.706533	-2.920232	3.720557
1	-2.150412	-3.030775	4.640544
6	-2.509971	-3.673038	2.526104
1	-1.777094	-4.452164	2.377555
6	-6.312933	-4.812345	3.147567
1	-7.062282	-4.530791	2.419796
6	-6.126885	-4.215376	4.431922
1	-6.703098	-3.396962	4.842789
6	-5.016244	-4.856984	5.059998
1	-4.600949	-4.605738	6.027130
6	-4.514213	-5.849033	4.163544
1	-3.654470	-6.483625	4.333743
6	-5.315831	-5.823528	2.983750
1	-5.169407	-6.440373	2.107726
6	-3.623390	-3.698928	0.145155
6	-4.750230	-4.462084	-0.199490
1	-5.452338	-4.714246	0.584292
6	-4.992611	-4.878295	-1.507243
1	-5.890645	-5.441130	-1.741311
6	-4.081102	-4.549724	-2.506818
1	-4.249303	-4.863221	-3.532160
6	-2.957453	-3.786193	-2.191782
1	-2.272844	-3.528072	-2.989943
6	-2.715571	-3.330155	-0.884270
6	-5.369288	-1.455787	1.468251
1	-5.893256	-2.161889	0.822379
6	-6.395673	-0.809622	2.403033
1	-7.184853	-0.310884	1.833821
1	-5.942586	-0.068232	3.066925
1	-6.853908	-1.583986	3.026426
6	-0.561417	-1.999952	-2.240337
6	-1.113132	-1.077713	-3.147125
1	-1.865883	-0.376447	-2.803920
6	-0.705169	-1.071562	-4.482449
1	-1.157882	-0.375093	-5.179148
6	0.287824	-1.954689	-4.915695
1	0.610809	-1.943439	-5.952548
6	0.876262	-2.838501	-4.008507
1	1.664969	-3.511446	-4.332858
6	0.447066	-2.869348	-2.680299
1	0.894045	-3.578874	-1.994690
6	-0.138010	-3.018894	0.464067
6	0.078545	-4.399042	0.318423
1	-0.465917	-4.956693	-0.438099
6	0.973185	-5.064314	1.158128
1	1.135538	-6.131445	1.036920
6	1.653857	-4.359207	2.155316
1	2.346488	-4.877851	2.811623
6	1.443762	-2.986704	2.307326
1	1.975260	-2.441834	3.079968
6	0.553008	-2.316914	1.464245
1	0.384196	-1.251426	1.585291
6	-5.172675	-0.606801	-1.398651
6	-4.577395	0.111938	-2.446293
1	-3.810130	0.844620	-2.213885
6	-4.950033	-0.125960	-3.769136
6	-5.882743	-1.112877	-4.081066
1	-6.152125	-1.315374	-5.111639
6	-6.454870	-1.843820	-3.039394
6	-6.125963	-1.583909	-1.708834
1	-6.610714	-2.165492	-0.936439
6	-5.135943	1.433242	0.650329
6	-4.622838	2.058110	1.799310
1	-3.949339	1.520421	2.455684
6	-4.948457	3.380270	2.086406
6	-5.767267	4.117733	1.229161
1	-6.002345	5.153431	1.445079
6	-6.269225	3.500045	0.087421
6	-5.967813	2.166270	-0.201802
1	-6.377003	1.716526	-1.098890
29	-2.134978	-0.147374	0.195299
6	-7.067266	4.301944	-0.901818
6	-4.324565	4.072438	3.265658
6	-4.357409	0.732385	-4.850808
6	-7.407735	-2.954264	-3.387579
9	-6.788464	-3.934047	-4.093123
9	-7.949279	-3.536524	-2.295314
9	-8.428321	-2.515007	-4.159793
9	-3.028848	0.951958	-4.651466
9	-4.934964	1.958581	-4.886833
9	-4.490826	0.190389	-6.077140
9	-6.263753	4.822644	-1.870365
9	-7.703367	5.343846	-0.326060
9	-7.995582	3.553606	-1.536303
9	-5.192957	4.906340	3.879798
9	-3.868659	3.202747	4.192423

9	-3.265021	4.835697	2.884130
6	-2.121897	2.779638	-0.546769
6	-1.424876	3.138515	0.654046
6	-1.201330	2.316438	1.788711
1	-1.290792	4.193216	0.844555
77	3.275870	1.440995	-1.593615
15	4.791238	0.444259	-0.228509
8	4.587728	-1.062123	0.432929
8	6.218589	0.217387	-1.054648
7	5.022151	1.361945	1.146046
6	4.774129	-2.217863	-0.324162
6	3.619408	-2.990020	-0.578785
1	2.674327	-2.659347	-0.166372
6	3.720530	-4.133850	-1.330377
1	2.843995	-4.747592	-1.513797
6	4.963522	-4.513391	-1.903248
6	5.059387	-5.639676	-2.764683
1	4.162832	-6.224545	-2.953717
6	6.253844	-5.973460	-3.361705
1	6.314959	-6.831415	-4.024770
6	7.403774	-5.183950	-3.121902
1	8.339604	-5.434380	-3.613221
6	7.348449	-4.096843	-2.276617
1	8.238488	-3.500960	-2.113778
6	6.135997	-3.732531	-1.626421
6	6.040901	-2.595084	-0.745874
6	7.245968	-1.828179	-0.322727
6	8.361145	-2.455511	0.338564
6	8.346205	-3.819579	0.744382
1	7.461413	-4.417826	0.562989
6	9.431938	-4.386443	1.375773
1	9.391651	-5.428166	1.680855
6	10.595650	-3.624625	1.637683
1	11.446166	-4.087397	2.129524
6	10.635904	-2.295445	1.283004
1	11.514262	-1.691946	1.496585
6	9.527611	-1.675277	0.644319
6	9.549366	-0.289768	0.327942
1	10.439998	0.289313	0.554670
6	8.447841	0.316170	-0.223320
1	8.422774	1.379303	-0.437780
6	7.304619	-0.458133	-0.517977
6	4.307366	2.672593	1.078506
1	3.346309	2.558081	1.595183
6	5.079480	3.791393	1.756381
6	4.426793	4.642268	2.655232
1	3.386608	4.452114	2.908753
6	5.103711	5.718295	3.236027
1	4.584251	6.370433	3.932817
6	6.447292	5.946276	2.931304
1	6.977581	6.777275	3.387763
6	7.109438	5.095101	2.039957
1	8.156708	5.263154	1.803807
6	6.428683	4.028403	1.453688
1	6.945467	3.360788	0.768853
6	4.054641	3.039443	-0.383389
1	5.005089	3.359696	-0.825516
1	3.394799	3.907303	-0.422703
6	5.495310	0.999086	2.517495
1	6.155305	1.821431	2.806743
6	4.334559	0.989023	3.501862
6	4.402773	1.776443	4.655729
1	5.267542	2.415290	4.814852
6	3.368868	1.753926	5.594879
1	3.434747	2.368659	6.488402
6	2.250075	0.949762	5.377926
1	1.442968	0.931834	6.102098
6	2.169700	0.168013	4.220540
1	1.293638	-0.447407	4.044630
6	3.207284	0.184171	3.288506
1	3.149217	-0.428402	2.394185
6	6.327501	-0.278573	2.663302
1	7.211402	-0.257422	2.027501
1	5.755651	-1.182039	2.456155
1	6.667090	-0.321456	3.702736
6	1.673541	0.729213	-0.303939
1	1.382780	-0.298324	-0.512659
1	1.852922	0.910167	0.754789
6	0.981092	1.757239	-1.047847
1	0.378188	1.482581	-1.903141
6	0.960256	3.083677	-0.622302
1	1.425045	3.294549	0.336354
6	4.851818	1.956627	-3.139655
1	5.683373	2.389885	-2.591129
6	3.729921	2.784844	-3.336489
1	3.791211	3.800347	-2.946443
6	2.687071	2.606560	-4.424904
1	3.064307	3.027012	-5.369668
1	1.821928	3.213634	-4.145766
6	2.228300	1.148563	-4.638117
1	2.844914	0.658424	-5.398134
1	1.208124	1.151323	-5.033990
6	2.240341	0.301199	-3.371499
1	1.269620	0.009733	-2.992685
6	3.308778	-0.479534	-2.961998
1	3.078760	-1.316753	-2.312905
6	4.642038	-0.564707	-3.671243
1	5.340559	-1.087151	-3.017741
1	4.519507	-1.194086	-4.564932
6	5.239978	0.804372	-4.064680
1	4.953350	1.064417	-5.088724
1	6.330265	0.718405	-4.065896
6	0.598341	4.252586	-1.406703
6	-0.043795	4.172420	-2.659128
6	0.931688	5.526867	-0.902708
6	-0.332271	5.326916	-3.381041
1	-0.331368	3.205612	-3.056629
6	0.648912	6.680576	-1.630306
1	1.419639	5.600675	0.066007
6	0.014504	6.584603	-2.872957
1	-0.831880	5.247650	-4.342031
1	0.919234	7.652885	-1.228977
1	-0.211102	7.482179	-3.441326
8	-2.144635	1.600043	-1.036421
6	-0.775076	2.944202	3.003565
6	-0.766321	2.261796	4.197806
1	-0.526083	4.000068	2.984560
6	-1.142750	0.910024	4.176833
6	-1.416920	0.295279	2.973736
1	-1.639312	-0.761516	2.920940
7	-1.440919	0.963513	1.801158
6	-3.296820	3.511003	-2.573568
1	-2.772897	2.674756	-3.027742
1	-4.368588	3.286651	-2.540947
1	-3.150705	4.395588	-3.200181
6	-2.975535	5.122945	-0.733406
1	-3.086848	5.119322	0.350856
1	-2.154741	5.795968	-1.011448
1	-3.904103	5.511050	-1.158881
7	-2.762685	3.773063	-1.244112
1	-0.491142	2.758092	5.121818
35	-1.287056	-0.114156	5.841357

C2-P1 *re-re*_1

Number of imaginary frequencies= 1
The smallest frequencies are= -185.2916 8.1656 11.5906 cm(-1)
Electronic energy= -7222.6155244
Zero-point correction= 1.755258
(Hartree/Particle)
Thermal correction to Energy= 1.873470
Thermal correction to Enthalpy= 1.874414
Thermal correction to Gibbs Free Energy= 1.594351
Sum of electronic and zero-point Energies= -7220.860266
Sum of electronic and thermal Energies= -7220.742054
Sum of electronic and thermal Enthalpies= -7220.741110
Sum of electronic and thermal Free Energies= -7221.021174
.....
Cartesian Coordinates
.....

77	4.096977	-1.312390	-0.962602
15	5.786597	0.009988	-0.168643
8	6.602896	-0.240053	1.255370
8	7.067103	0.036151	-1.237686
7	5.194091	1.554806	0.095324
6	7.632324	-1.172197	1.349117
6	7.381214	-2.302846	2.156848
1	6.426754	-2.372411	2.667927
6	8.340104	-3.277570	2.277194
1	8.161463	-4.149713	2.899641
6	9.565810	-3.174743	1.565593
6	10.532895	-4.214981	1.618679
1	10.323820	-5.084810	2.235934
6	11.700726	-4.132328	0.894899
1	12.430795	-4.935254	0.938095
6	11.943268	-3.002064	0.078260
1	12.854551	-2.950304	-0.510578
6	11.032886	-1.969324	0.016550
1	11.233083	-1.117156	-0.621958
6	9.824411	-2.009833	0.767259
6	8.848222	-0.951504	0.719638
6	9.104483	0.326924	-0.000394
6	10.224569	1.174522	0.313741
6	11.099678	0.917373	1.406187
1	10.922342	0.053922	2.036117
6	12.157013	1.756364	1.683330
1	12.805603	1.541432	2.527784
6	12.403177	2.898221	0.883922
1	13.244850	3.546064	1.110627
6	11.563948	3.190668	-0.167116
1	11.728595	4.074761	-0.777585
6	10.453944	2.355802	-0.470411
6	9.553785	2.687954	-1.519312
1	9.742316	3.577387	-2.113871
6	8.442041	1.917168	-1.754506
1	7.718747	2.169461	-2.522416
6	8.221551	0.761063	-0.974996
6	3.830253	1.734717	-0.489317
1	3.099175	1.588680	0.313521
6	3.619611	3.135417	-1.037983
6	2.518106	3.888261	-0.613310
1	1.855631	3.480789	0.144695
6	2.257932	5.147067	-1.161116
1	1.392377	5.713321	-0.827492
6	3.109502	5.672926	-2.134602
1	2.912425	6.651691	-2.562642
6	4.222986	4.935079	-2.552607
1	4.894503	5.343473	-3.302939
6	4.475390	3.675422	-2.008726
1	5.346108	3.108171	-2.326721
6	3.592899	0.678852	-1.575775
1	4.173000	0.943465	-2.468209
1	2.540359	0.701384	-1.866020
6	5.552920	2.592568	1.111612
1	5.322504	3.536551	0.610444
6	4.659745	2.526744	2.349346
6	3.835973	3.616162	2.663155
1	3.805783	4.470999	1.992625
6	3.060366	3.619648	3.826135
1	2.433861	4.477649	4.054866
6	3.091189	2.523030	4.689590
1	2.489991	2.520864	5.594493
6	3.899695	1.425177	4.379588
1	3.929832	0.567555	5.046258
6	4.679630	1.427498	3.221167
1	5.317149	0.579548	2.998607
6	7.031595	2.684511	1.500135
1	7.660053	2.809559	0.617901
1	7.378092	1.822022	2.067335
1	7.151755	3.573072	2.127719
6	3.168442	-1.165385	0.993543
1	3.357465	-2.058096	1.591355
1	3.371362	-0.245059	1.532760
6	2.058542	-1.181336	0.083998
1	1.645086	-0.230890	-0.234408
6	1.234213	-2.319093	-0.152169
1	1.491786	-3.229285	0.380140
6	5.141929	-1.625488	-2.911372
1	5.491959	-0.649903	-3.237613
6	3.767278	-1.904197	-3.094563
1	3.160336	-1.131388	-3.566404
6	3.195173	-3.305499	-3.223389
1	3.429710	-3.707230	-4.221074
1	2.108207	-3.226737	-3.173601
6	3.676132	-4.294789	-2.136100
1	4.522879	-4.882841	-2.505568
1	2.872820	-5.011228	-1.936280
6	4.077970	-3.646996	-0.811761
1	3.453535	-3.889668	0.042081
6	5.366815	-3.211069	-0.515959
1	5.638066	-3.164780	0.534392
6	6.543047	-3.239759	-1.473311
1	7.339030	-2.629231	-1.042459
1	6.933543	-4.266537	-1.530655
6	6.218996	-2.711359	-2.887462
1	5.910215	-3.535349	-3.539203
1	7.135575	-2.304751	-3.325238
6	0.418390	-2.508723	-1.339935
6	0.126068	-1.452205	-2.220805
6	-0.080170	-3.791258	-1.641428
6	-0.654850	-1.664679	-3.350239
1	0.523294	-0.467282	-2.023820
6	-0.866828	-4.002810	-2.771908
1	0.153947	-4.619648	-0.979802
6	-1.165835	-2.937896	-3.626994
1	-0.870329	-0.833001	-4.010983
1	-1.250720	-4.995940	-2.984665
1	-1.791595	-3.094509	-4.500493
26	-2.993647	4.930987	1.168654
15	-3.273113	1.106713	-2.310361
15	-4.619759	0.408625	1.114931
6	-3.469534	3.456386	-0.239197
6	-3.539761	2.929593	1.099016
6	-2.247895	3.077370	1.690460
1	-1.977853	2.780210	2.693922
6	-1.390496	3.710323	0.744723
1	-0.361348	3.995636	0.912948
6	-2.140148	3.947053	-0.442970
1	-1.781799	4.423859	-1.344153
6	-4.524196	6.137605	1.895263
1	-5.559382	5.833468	1.978126
6	-3.516086	5.962661	2.892139
1	-3.652467	5.500704	3.860875
6	-2.285933	6.465934	2.369668
1	-1.327567	6.446827	2.871931
6	-2.533060	6.952898	1.050187
1	-1.795570	7.367205	0.375283
6	-3.914864	6.752456	0.757613
1	-4.403888	6.996724	-0.175610
6	-4.564207	3.407823	-1.245188
6	-5.614194	4.335235	-1.186665
1	-5.609451	5.063426	-0.386279
6	-6.641272	4.336038	-2.129688
1	-7.443679	5.063874	-2.056941
6	-6.629320	3.398735	-3.160313
1	-7.418356	3.388594	-3.904681
6	-5.613647	2.444629	-3.214826
1	-5.634060	1.704371	-4.006320
6	-4.584197	2.419411	-2.260300
6	-4.734979	2.228580	1.682930
1	-5.630272	2.636044	1.208534
6	-4.874199	2.406897	3.198682
1	-5.790341	1.942241	3.571431
1	-4.030583	1.973679	3.744051
1	-4.909601	3.476192	3.425347
6	-3.936426	-0.062156	-3.574345
6	-5.027873	-0.857256	-3.181968
1	-5.465315	-0.718898	-2.198753
6	-5.563804	-1.814192	-4.041439
1	-6.401871	-2.419140	-3.710547

6	-5.009842	-1.995978	-5.312599
1	-5.418510	-2.745978	-5.983669
6	-3.931947	-1.205706	-5.716128
1	-3.500881	-1.335633	-6.704894
6	-3.399593	-0.240012	-4.855669
1	-2.565481	0.366652	-5.190057
6	-1.882655	1.989901	-3.122587
6	-2.070805	2.784401	-4.265734
1	-3.059112	2.878317	-4.706455
6	-0.992561	3.463543	-4.834446
1	-1.146229	4.075996	-5.718455
6	0.279548	3.358841	-4.263039
1	1.119921	3.891517	-4.698989
6	0.468479	2.582901	-3.117502
1	1.450218	2.522955	-2.663815
6	-0.609988	1.907839	-2.540779
1	-0.482724	1.341512	-1.623235
6	-6.234317	0.010037	0.305541
6	-6.545444	-1.352196	0.141933
1	-5.884855	-2.115851	0.537734
6	-7.710431	-1.737983	-0.516785
6	-8.587651	-0.785043	-1.033785
1	-9.501618	-1.089530	-1.531613
6	-8.275987	0.563073	-0.882179
6	-7.106150	0.965683	-0.231614
1	-6.896990	2.024993	-0.152822
6	-4.769647	-0.579563	2.668258
6	-3.599610	-1.058060	3.264931
1	-2.636695	-0.866402	2.804326
6	-3.665416	-1.794255	4.453316
6	-4.888839	-2.072543	5.054832
1	-4.936259	-2.646488	5.972228
6	-6.056144	-1.591823	4.458342
6	-6.002716	-0.848847	3.281846
1	-6.925317	-0.480593	2.848010
29	-2.865545	-0.020154	-0.350295
6	-7.395016	-1.924001	5.059558
6	-2.383049	-2.262228	5.082387
6	-8.022731	-3.195371	-0.720402
6	-9.225641	1.579735	-1.457399
9	-9.100100	1.673417	-2.803655
9	-9.031185	2.814915	-0.949178
9	-10.514335	1.243907	-1.216372
9	-7.683157	-3.603398	-1.971329
9	-7.362303	-3.984591	0.150856
9	-9.343214	-3.449260	-0.581721
9	-7.912440	-3.055529	4.523845
9	-7.316995	-2.120463	6.393568
9	-8.299076	-0.941804	4.843930
9	-2.581936	-2.996403	6.193913
9	-1.595244	-1.212612	5.428823
9	-1.649735	-3.021394	4.227023
6	-3.399329	-2.935892	-0.794552
6	-1.689834	-2.678615	0.783029
6	-3.519511	-4.287692	-0.517039
1	-4.005508	-2.465256	-1.558763
6	-1.832516	-4.046634	1.138490
6	-2.743991	-4.860475	0.492645
1	-1.201745	-4.456471	1.920485
6	-0.615878	-1.939058	1.386994
6	-0.449168	-0.505101	1.352501
8	-0.924560	0.230542	0.433882
7	-2.525249	-2.139641	-0.155026
1	-0.132006	-2.468930	2.193364
7	0.342729	0.078469	2.306892
6	0.814681	1.444844	2.122981
1	0.357141	2.121279	2.853958
1	1.897885	1.479859	2.262295
1	0.555286	1.782334	1.124010
6	0.871178	-0.599494	3.485023
1	1.862902	-1.027937	3.299128
1	0.964445	0.133302	4.291274
1	0.201168	-1.382461	3.829774
1	-2.836729	-5.909468	0.752943
35	-4.726981	-5.392140	-1.583718

C2-P1 *re-re_2*

Number of imaginary frequencies= 1
The smallest frequencies are=-227.2969 11.5199 13.3150cm(-1)
Electronic energy= -7222.6110077
Zero-point correction= 1.754688
(Hartree/Particle)
Thermal correction to Energy= 1.873132
Thermal correction to Enthalpy= 1.874076
Thermal correction to Gibbs Free Energy= 1.593819
Sum of electronic and zero-point Energies= -7220.856320
Sum of electronic and thermal Energies= -7220.737876
Sum of electronic and thermal Enthalpies= -7220.736932
Sum of electronic and thermal Free Energies= -7221.017189

.....

Cartesian Coordinates

.....

26	-3.617782	-3.632523	-4.194816
15	-1.785632	-2.510082	0.520230
15	-4.661583	-0.460481	-0.751923
6	-3.187839	-3.334846	-2.168828
6	-3.930512	-2.225032	-2.709383
6	-3.159054	-1.663254	-3.773247
1	-3.448091	-0.821035	-4.387136
6	-1.966038	-2.430046	-3.913246
1	-1.199791	-2.280681	-4.660782
6	-1.981116	-3.458557	-2.927848
1	-1.225922	-4.217909	-2.781764
6	-5.369217	-4.633010	-4.696005
1	-6.269423	-4.632380	-4.095812
6	-5.035162	-3.679537	-5.705870
1	-5.634958	-2.828524	-5.999691
6	-3.748776	-4.019021	-6.225493
1	-3.203130	-3.468192	-6.980349
6	-3.286875	-5.181607	-5.536438
1	-2.330206	-5.667220	-5.676924
6	-4.288156	-5.562460	-4.593944
1	-4.221507	-6.391277	-3.902360
6	-3.586953	-4.127097	-0.974302
6	-4.584028	-5.107541	-1.081781
1	-5.042000	-5.270188	-2.048821
6	-4.987373	-5.863628	0.018826
1	-5.767888	-6.610066	-0.093948
6	-4.387299	-5.651300	1.258078
1	-4.691625	-6.229570	2.124020
6	-3.411516	-4.663742	1.392469
1	-2.971277	-4.492021	2.368241
6	-3.009537	-3.883375	0.296999
6	-5.199524	-1.685078	-2.112871
1	-5.694807	-2.503615	-1.587260
6	-6.187821	-1.112280	-3.133131
1	-7.083571	-0.722807	-2.641061
1	-5.748526	-0.303482	-3.722782
1	-6.485882	-1.908137	-3.821549
6	-1.635200	-2.410763	2.352531
6	-2.626992	-1.661083	3.009300
1	-3.414313	-1.193165	2.426861
6	-2.615505	-1.516404	4.395777
1	-3.395616	-0.936124	4.879202
6	-1.596522	-2.112060	5.146195
1	-1.573809	-1.992553	6.225457
6	-0.608654	-2.862346	4.503935
1	0.185590	-3.325153	5.082151
6	-0.632219	-3.023095	3.115028
1	0.130283	-3.623433	2.634101
6	-0.224201	-3.235165	-0.117639
6	0.144208	-4.569949	0.111204
1	-0.488473	-5.213987	0.715074
6	1.317349	-5.078747	-0.449781
1	1.600846	-6.110760	-0.264349
6	2.120809	-4.264867	-1.255376
1	3.029497	-4.665685	-1.694967
6	1.748145	-2.940423	-1.500047
1	2.363254	-2.309348	-2.135410

6	0.580637	-2.425093	-0.932976
1	0.267851	-1.408979	-1.151936
6	-5.628147	-0.894174	0.757207
6	-5.709802	0.052980	1.793707
1	-5.290849	1.045465	1.667912
6	-6.341399	-0.268280	2.994543
6	-6.878116	-1.537167	3.204656
1	-7.378317	-1.777099	4.136039
6	-6.769709	-2.485677	2.191310
6	-6.145550	-2.178404	0.981285
1	-6.067259	-2.955311	0.231301
6	-5.352952	1.158287	-1.295740
6	-4.607247	1.834214	-2.273097
1	-3.698286	1.389467	-2.657599
6	-5.019212	3.078917	-2.742011
6	-6.168524	3.687027	-2.234129
1	-6.479296	4.663096	-2.588913
6	-6.913776	3.010820	-1.271125
6	-6.522365	1.750392	-0.810279
1	-7.138232	1.246178	-0.074764
29	-2.382876	-0.482635	-0.324266
6	-8.125799	3.661034	-0.660893
6	-4.178003	3.821585	-3.741682
6	-6.407129	0.739070	4.109870
6	-7.312611	-3.866700	2.445997
9	-6.478592	-4.588831	3.233946
9	-7.495516	-4.568812	1.307641
9	-8.502783	-3.820562	3.087357
9	-5.398366	0.554938	5.001139
9	-6.314975	2.005517	3.656287
9	-7.559396	0.639127	4.808905
9	-9.092713	2.757699	-0.381887
9	-7.817833	4.274483	0.508109
9	-8.665377	4.598810	-1.468276
9	-4.929051	4.500721	-4.633236
9	-3.362242	2.997607	-4.436825
9	-3.376313	4.743281	-3.135696
6	-2.385630	1.653475	1.860233
6	-2.136748	2.534262	-0.293105
6	-2.903496	2.846087	2.336067
1	-2.239195	0.804156	2.516702
6	-2.804724	3.717213	0.125890
6	-3.177752	3.887798	1.445303
1	-2.978215	4.507194	-0.595040
6	-1.470502	2.546662	-1.565060
6	-1.035428	1.384111	-2.303260
8	-1.117977	0.207745	-1.843694
7	-2.034516	1.479016	0.572016
1	-1.639582	3.452702	-2.123755
77	3.523850	2.347193	-0.180770
15	4.757479	0.485705	0.286328
8	5.123518	-0.743399	-0.760790
8	6.277304	0.935270	0.780174
7	3.983686	-0.422548	1.481700
6	6.163174	-0.640903	-1.676444
6	5.788392	-0.616738	-3.037822
1	4.734433	-0.694895	-3.283661
6	6.752312	-0.499471	-4.007248
1	6.478086	-0.489183	-5.058341
6	8.119584	-0.357123	-3.647756
6	9.117855	-0.155020	-4.639150
1	8.814457	-0.139459	-5.682689
6	10.435857	0.030371	-4.288980
1	11.190337	0.187634	-5.054147
6	10.804660	0.033275	-2.922825
1	11.840376	0.207776	-2.645833
6	9.863379	-0.175825	-1.938238
1	10.167530	-0.159100	-0.898892
6	8.495383	-0.399475	-2.262467
6	7.485910	-0.623766	-1.256639
6	7.836451	-0.793655	0.181680
6	8.778464	-1.785910	0.630608
6	9.305956	-2.788101	-0.230056
1	8.985099	-2.821452	-1.264329
6	10.197953	-3.729744	0.235448
1	10.577312	-4.490560	-0.440796
6	10.617049	-3.721937	1.587066
1	11.324635	-4.466820	1.939303
6	10.109847	-2.779982	2.453351
1	10.403442	-2.775801	3.499837
6	9.175533	-1.805813	2.009490
6	8.599584	-0.880896	2.920315
1	8.913142	-0.899149	3.960130
6	7.627761	-0.007029	2.502317
1	7.146316	0.686431	3.183155
6	7.245004	0.007320	1.144645
6	2.942325	0.395742	2.164536
1	1.964165	0.149089	1.736882
6	2.870461	0.165641	3.663146
6	1.621207	0.060499	4.287015
1	0.717380	0.072486	3.682277
6	1.528000	-0.086407	5.673061
1	0.550619	-0.180834	6.137509
6	2.686881	-0.132238	6.451962
1	2.617015	-0.254070	7.529243
6	3.938047	-0.025008	5.836041
1	4.844425	-0.060789	6.434621
6	4.028114	0.127280	4.451398
1	4.998477	0.201982	3.970932
6	3.213002	1.885127	1.892655
1	4.081266	2.205096	2.482206
1	2.361418	2.459596	2.262171
6	3.764048	-1.901818	1.284735
1	3.527847	-2.059576	0.231878
6	4.980391	-2.757276	1.604821
6	5.504056	-3.605592	0.621614
1	5.111130	-3.551498	-0.389772
6	6.517883	-4.516359	0.927675
1	6.914317	-5.165442	0.152156
6	7.026241	-4.585179	2.225900
1	7.820809	-5.285137	2.465616
6	6.522574	-3.729131	3.209210
1	6.923529	-3.766091	4.218551
6	5.506868	-2.823613	2.901473
1	5.109629	-2.172466	3.673452
6	2.560612	-2.438823	2.067498
1	1.639965	-1.913284	1.814804
1	2.709285	-2.396282	3.147078
1	2.429008	-3.484688	1.779633
6	1.978586	1.037701	-0.997120
1	1.975303	1.070297	-2.085480
1	1.958300	0.025842	-0.603590
6	1.237828	2.028025	-0.270808
1	0.896185	1.761429	0.723096
6	0.678371	3.206494	-0.829612
1	0.916121	3.428686	-1.859917
6	5.172938	3.726614	0.414563
1	5.566884	3.354054	1.355572
6	3.957110	4.447270	0.471724
1	3.507956	4.594657	1.453716
6	3.532366	5.470870	-0.567134
1	4.111563	6.396570	-0.427752
1	2.491038	5.730797	-0.369730
6	3.663113	4.989230	-2.031319
1	4.609721	5.332133	-2.461872
1	2.874495	5.459790	-2.627858
6	3.563080	3.475005	-2.218582
1	2.703637	3.127494	-2.785244
6	4.655746	2.609721	-2.185588
1	4.555374	1.672900	-2.726667
6	6.086773	3.015001	-1.884062
1	6.659782	2.104406	-1.697487
1	6.524414	3.480575	-2.779500
6	6.229119	3.954707	-0.667704
1	6.191841	5.000446	-0.989744
1	7.219675	3.807223	-0.226976
6	0.252565	4.361496	-0.033562
6	0.241257	4.354775	1.372565
6	-0.157444	5.533729	-0.697730
6	-0.153419	5.484035	2.087199

1	0.539896	3.465259	1.913868
6	-0.555638	6.661899	0.015854
1	-0.161905	5.550888	-1.784708
6	-0.552456	6.642612	1.414312
1	-0.154552	5.456506	3.173054
1	-0.865081	7.556465	-0.517054
1	-0.858720	7.521654	1.973872
7	-0.456773	1.551306	-3.538852
6	0.130667	0.408446	-4.225269
1	-0.387648	0.221217	-5.174085
1	1.186324	0.610827	-4.449508
1	0.055330	-0.474031	-3.596456
6	-0.268021	2.816815	-4.235410
1	0.779405	3.145322	-4.182116
1	-0.523207	2.682838	-5.291973
1	-0.906129	3.604285	-3.845734
1	-3.636723	4.811942	1.778506
35	-3.161731	3.087895	4.258275

C2-P1 *re-re*_3

Number of imaginary frequencies= 1
The smallest frequencies are=-243.3633 5.1929 11.3286 cm(-1)
Electronic energy= -7222.6143593
Zero-point correction= 1.755753
(Hartree/Particle)
Thermal correction to Energy= 1.873982
Thermal correction to Enthalpy= 1.874926
Thermal correction to Gibbs Free Energy= 1.595009
Sum of electronic and zero-point Energies= -7220.858606
Sum of electronic and thermal Energies= -7220.740377
Sum of electronic and thermal Enthalpies= -7220.739433
Sum of electronic and thermal Free Energies= -7221.019351

.....

Cartesian Coordinates

.....

26	3.098552	4.346842	-2.946487
15	2.723955	1.778242	1.595644
15	4.662810	0.171975	-1.198096
6	3.306451	3.357167	-1.108541
6	3.463878	2.443095	-2.214772
6	2.252988	2.461451	-2.969471
1	2.062134	1.889919	-3.866411
6	1.363192	3.397739	-2.368806
1	0.375680	3.659591	-2.723591
6	2.013460	3.957349	-1.232335
1	1.604568	4.704531	-0.568390
6	4.787638	5.141194	-3.860085
1	5.786850	4.737222	-3.762289
6	3.822969	4.764758	-4.844341
1	3.960524	4.023414	-5.620177
6	2.627981	5.507249	-4.598358
1	1.701955	5.422780	-5.151875
6	2.853511	6.344472	-3.463473
1	2.129974	7.006535	-3.006327
6	4.187102	6.120458	-3.008917
1	4.647275	6.591305	-2.151244
6	4.292657	3.552661	-0.006946
6	5.445922	4.313135	-0.247322
1	5.573347	4.745836	-1.231144
6	6.418071	4.509936	0.732880
1	7.308668	5.086430	0.505792
6	6.244019	3.943881	1.993062
1	6.991600	4.083066	2.767876
6	5.108893	3.175373	2.254982
1	4.995236	2.734632	3.238670
6	4.131175	2.952557	1.272790
6	4.682566	1.596176	-2.459617
1	5.546982	2.199633	-2.180450
6	4.866719	1.168543	-3.918547
1	5.785689	0.590083	-4.046769
1	4.033525	0.562498	-4.283916
1	4.928771	2.063543	-4.544285
6	2.935230	1.277019	3.354536
6	3.958183	0.357405	3.646158
1	4.620305	0.020327	2.855882
6	4.147086	-0.112732	4.944300
1	4.950287	-0.813393	5.147889
6	3.300226	0.316311	5.971205
1	3.437614	-0.055818	6.982309
6	2.275013	1.221826	5.690777
1	1.611610	1.556659	6.483182
6	2.092782	1.704175	4.390818
1	1.289258	2.405020	4.192815
6	1.257298	2.875700	1.574121
6	1.276705	4.136089	2.193073
1	2.137339	4.438712	2.782723
6	0.206569	5.014809	2.024279
1	0.224789	5.989068	2.504304
6	-0.876164	4.647634	1.219210
1	-1.699759	5.336812	1.068344
6	-0.901289	3.392740	0.606487
1	-1.732637	3.120962	-0.033055
6	0.154665	2.499478	0.793959
1	0.163945	1.544056	0.277598
6	6.242684	0.327386	-0.251892
6	6.405520	-0.541350	0.836230
1	5.678619	-1.322724	1.013041
6	7.482372	-0.402261	1.710972
6	8.426650	0.603474	1.520542
1	9.248513	0.730054	2.216386
6	8.278039	1.457683	0.428674
6	7.207504	1.322638	-0.454743
1	7.132597	2.021026	-1.276505
6	4.871468	-1.383548	-2.156494
6	3.768799	-1.794599	-2.922655
1	2.875694	-1.180804	-2.960475
6	3.811956	-2.989566	-3.634851
6	4.923678	-3.830732	-3.554262
1	4.946259	-4.770575	-4.093006
6	6.004674	-3.435024	-2.771346
6	5.994071	-2.214180	-2.089876
1	6.864618	-1.926988	-1.510735
29	2.753746	0.037544	0.146468
6	7.188241	-4.346665	-2.594247
6	2.613713	-3.416221	-4.434464
6	7.613051	-1.356852	2.865633
6	9.287522	2.559200	0.248888
9	9.352550	3.351123	1.347280
9	9.004365	3.358367	-0.802951
9	10.532938	2.066720	0.056962
9	6.396003	-1.690817	3.369814
9	8.209479	-2.513682	2.498303
9	8.337522	-0.838027	3.877862
9	8.355066	-3.662927	-2.606535
9	7.131954	-4.994732	-1.404132
9	7.259561	-5.291470	-3.555416
9	2.953432	-4.157459	-5.508580
9	1.899622	-2.355661	-4.878540
9	1.757426	-4.175338	-3.695669
6	3.496618	-2.626341	1.184771
6	1.812732	-2.842681	-0.417829
6	3.837452	-3.964946	1.080434
1	3.982458	-1.978916	1.904378
6	2.134308	-4.216389	-0.553049
6	3.163573	-4.784331	0.174985
1	1.572200	-4.821336	-1.255099
6	0.640538	-2.349851	-1.107672
6	0.501247	-1.004525	-1.631432
8	1.051091	0.003734	-1.103951
7	2.543447	-2.058763	0.425200
1	0.171513	-3.124017	-1.698212
77	-3.976706	-1.556195	0.982391
15	-5.584482	-0.021394	0.433059
8	-6.115986	0.323675	-1.104779
8	-7.035782	-0.448497	1.144644
7	-5.090929	1.506450	0.900726
6	-6.994253	-0.525274	-1.769483
6	-6.472886	-1.218475	-2.884478
1	-5.439179	-1.043874	-3.164104

6	-7.275670	-2.086682	-3.581334
1	-6.890019	-2.619471	-4.445921
6	-8.612514	-2.325148	-3.162304
6	-9.428069	-3.281482	-3.826063
1	-9.014629	-3.809989	-4.681100
6	-10.706495	-3.545480	-3.389532
1	-11.319433	-4.282340	-3.900263
6	-11.217440	-2.865058	-2.258685
1	-12.217095	-3.093376	-1.900319
6	-10.458519	-1.919868	-1.603038
1	-10.864447	-1.416822	-0.733612
6	-9.141511	-1.603120	-2.039681
6	-8.319817	-0.624005	-1.373791
6	-8.849527	0.232424	-0.275626
6	-9.997895	1.082956	-0.450557
6	-10.626833	1.273899	-1.712860
1	-10.229100	0.769684	-2.585520
6	-11.721433	2.100633	-1.844882
1	-12.177994	2.234842	-2.821395
6	-12.252950	2.781658	-0.723740
1	-13.120834	3.423775	-0.841753
6	-11.655680	2.639310	0.508191
1	-12.040161	3.171338	1.374546
6	-10.515026	1.807958	0.676200
6	-9.866565	1.701877	1.936777
1	-10.274929	2.240223	2.787432
6	-8.719909	0.958664	2.070063
1	-8.183647	0.893037	3.010800
6	-8.210442	0.259542	0.953273
6	-3.901159	1.474834	1.798216
1	-3.030917	1.776889	1.204227
6	-4.035669	2.418411	2.984259
6	-2.887116	3.004654	3.530630
1	-1.925157	2.834814	3.058379
6	-2.969857	3.802552	4.673939
1	-2.068678	4.255333	5.078892
6	-4.205014	4.023980	5.287828
1	-4.271780	4.649418	6.173626
6	-5.355571	3.436355	4.752834
1	-6.321001	3.602665	5.223431
6	-5.270680	2.635814	3.612664
1	-6.166143	2.184265	3.194337
6	-3.664854	0.055280	2.348232
1	-4.336739	-0.093389	3.201688
1	-2.645128	0.010783	2.740255
6	-5.417417	2.857846	0.356311
1	-5.338270	3.517162	1.224321
6	-4.402690	3.373576	-0.662743
6	-3.932527	4.687420	-0.525658
1	-4.244388	5.275857	0.334021
6	-3.069496	5.246853	-1.470307
1	-2.713109	6.264821	-1.340749
6	-2.656400	4.493406	-2.571224
1	-1.985072	4.923379	-3.309436
6	-3.123988	3.184938	-2.721298
1	-2.821907	2.599395	-3.584550
6	-3.992396	2.629315	-1.777518
1	-4.369314	1.623910	-1.919148
6	-6.843202	3.053655	-0.174444
1	-7.583886	2.780054	0.577142
1	-7.033273	2.491965	-1.087741
1	-6.967790	4.117546	-0.398130
6	-2.755634	-0.843256	-0.667956
1	-2.840742	-1.515738	-1.518320
1	-2.885841	0.201107	-0.936061
6	-1.788942	-1.116307	0.353746
1	-1.448779	-0.250349	0.911351
6	-0.985791	-2.296782	0.500758
1	-1.344958	-3.199652	0.030013
6	-5.262764	-2.528004	2.524103
1	-5.685333	-1.735112	3.136015
6	-3.914886	-2.880029	2.786021
1	-3.410984	-2.348868	3.593502
6	-3.315218	-4.240353	2.477239
1	-3.639899	-4.971324	3.233952
1	-2.232935	-4.150061	2.583097
6	-3.638167	-4.770056	1.062978
1	-4.519233	-5.419234	1.090494
1	-2.809900	-5.401555	0.723792
6	-3.868792	-3.678147	0.019773
1	-3.123988	-3.614270	-0.768792
6	-5.119131	-3.145299	-0.282437
1	-5.246545	-2.719350	-1.272921
6	-6.411231	-3.498924	0.428390
1	-7.161128	-2.762613	0.135671
1	-6.766559	-4.473767	0.062926
6	-6.295456	-3.511851	1.968420
1	-6.054838	-4.519904	2.322316
1	-7.273890	-3.266283	2.392041
6	-0.188202	-2.516683	1.714152
6	0.220852	-1.471957	2.565717
6	0.214367	-3.828388	2.035472
6	0.987071	-1.735693	3.699512
1	-0.043973	-0.444624	2.340402
6	0.995558	-4.089935	3.158072
1	-0.087340	-4.645087	1.386040
6	1.384351	-3.041966	3.997229
1	1.287645	-0.917963	4.343911
1	1.301200	-5.108684	3.377847
1	1.993782	-3.238780	4.874548
7	-0.314673	-0.807853	-2.712395
6	-0.725240	0.542841	-3.076130
1	-0.231616	0.869728	-3.999901
1	-1.806783	0.551213	-3.241061
1	-0.471942	1.235857	-2.278557
6	-0.867063	-1.856158	-3.563136
1	-1.888785	-2.125738	-3.266678
1	-0.900588	-1.484476	-4.591396
1	-0.246469	-2.748210	-3.563089
1	3.420218	-5.831527	0.057872
35	5.254624	-4.692806	2.205930

C2-P1 *re-re_*4

Number of imaginary frequencies= 1
The smallest frequencies are=-266.9227 14.6030 16.4956cm(-1)
Electronic energy= -7222.6225041
Zero-point correction= 1.755305
(Hartree/Particle)
Thermal correction to Energy= 1.873789
Thermal correction to Enthalpy= 1.874733
Thermal correction to Gibbs Free Energy= 1.596155
Sum of electronic and zero-point Energies= -7220.867200
Sum of electronic and thermal Energies= -7220.748715
Sum of electronic and thermal Enthalpies= -7220.747771
Sum of electronic and thermal Free Energies= -7221.026349

.....

Cartesian Coordinates

.....

26	7.587737	-2.030120	-1.503578
15	2.982145	0.290134	-2.301438
15	4.408503	0.363313	1.158495
6	5.910194	-0.797811	-1.737637
6	6.045487	-1.241406	-0.371125
6	5.984273	-2.666595	-0.366827
1	6.061588	-3.298816	0.506460
6	5.847183	-3.111998	-1.714095
1	5.816015	-4.141703	-2.043405
6	5.805672	-1.965233	-2.558266
1	5.719254	-1.966488	-3.634902
6	9.411110	-1.164151	-1.007964
1	9.524467	-0.257497	-0.428184
6	9.332159	-2.490786	-0.483910
1	9.370071	-2.765494	0.561692
6	9.150577	-3.388404	-1.579896
1	9.020587	-4.460268	-1.508050
6	9.116668	-2.617626	-2.781714
1	8.958973	-3.002187	-3.780748
6	9.278997	-1.244724	-2.429334
1	9.270492	-0.411021	-3.118186

6	5.813259	0.628040	-2.160974
6	6.966849	1.425874	-2.171613
1	7.906619	0.967310	-1.892626
6	6.926067	2.776475	-2.516030
1	7.833657	3.370536	-2.489856
6	5.711640	3.356397	-2.874325
1	5.660840	4.406631	-3.143498
6	4.548595	2.585868	-2.864101
1	3.610231	3.056927	-3.132745
6	4.570425	1.231128	-2.495048
6	6.147653	-0.315184	0.808645
1	6.710589	0.554532	0.470750
6	6.880430	-0.900879	2.019068
1	6.922259	-0.181175	2.841372
1	6.407743	-1.812402	2.392121
1	7.903848	-1.152778	1.725778
6	1.696044	1.506233	-2.806632
6	1.308245	2.452313	-1.842264
1	1.780838	2.450113	-0.865178
6	0.340765	3.411024	-2.134609
1	0.063706	4.138879	-1.384071
6	-0.272839	3.426692	-3.389954
1	-1.040171	4.163886	-3.607896
6	0.102141	2.488160	-4.352854
1	-0.369765	2.492138	-5.331237
6	1.084434	1.535572	-4.067389
1	1.358886	0.813545	-4.827830
6	3.024373	-0.958034	-3.641947
6	3.483239	-0.670641	-4.936489
1	3.835003	0.327737	-5.180319
6	3.500509	-1.672787	-5.908177
1	3.855396	-1.447454	-6.909791
6	3.064349	-2.964904	-5.593817
1	3.079468	-3.741132	-6.353684
6	2.621482	-3.258475	-4.301722
1	2.294495	-4.263382	-4.049774
6	2.609322	-2.259187	-3.327461
1	2.323342	-2.483730	-2.305137
6	4.586523	2.202559	1.171447
6	3.406763	2.947169	1.308168
1	2.486690	2.444570	1.568588
6	3.392252	4.323874	1.083888
6	4.559426	4.998675	0.735291
1	4.544650	6.063574	0.531420
6	5.743208	4.268481	0.633010
6	5.765116	2.891021	0.849402
1	6.707336	2.373713	0.735995
6	3.984023	-0.127869	2.874739
6	3.800150	-1.506259	3.073924
1	3.981371	-2.198174	2.259017
6	3.351382	-1.985637	4.299730
6	3.023056	-1.105273	5.331860
1	2.644004	-1.478063	6.277408
6	3.175939	0.263913	5.120270
6	3.668938	0.757962	3.909861
1	3.786002	1.827315	3.780416
29	2.671094	-0.489416	-0.185857
6	2.712818	1.206199	6.197233
6	3.121335	-3.457736	4.496390
6	2.092172	5.070769	1.207198
6	6.996213	5.003425	0.237303
9	6.842756	5.633724	-0.952664
9	8.065468	4.186331	0.121469
9	7.316338	5.959702	1.139242
9	1.048641	4.307505	0.774004
9	1.814905	5.412257	2.484499
9	2.076139	6.203968	0.477696
9	3.100815	2.479518	5.975162
9	1.357473	1.211062	6.283723
9	3.174111	0.845838	7.416237
9	3.629667	-3.895178	5.668971
9	3.670476	-4.201419	3.510756
9	1.793668	-3.755215	4.519455
6	0.655877	0.743710	1.630039
6	0.638721	-1.572463	1.927870
6	0.065667	0.958541	2.864419
1	0.869166	1.568309	0.961855
6	-0.020897	-1.391874	3.172509
6	-0.281009	-0.129956	3.668636
6	0.830053	-2.923155	1.463339
6	1.981571	-3.354441	0.703627
8	2.674443	-2.568196	-0.014418
7	0.983157	-0.482844	1.177981
1	0.396854	-3.657551	2.127216
77	-3.249702	-1.353953	-1.191222
15	-4.980383	-0.111354	-0.400278
8	-4.786750	1.132620	0.694008
8	-5.791872	0.691865	-1.604590
7	-6.025333	-1.086679	0.486867
6	-4.165387	2.307615	0.299515
6	-2.885259	2.561738	0.839178
1	-2.460850	1.840555	1.528158
6	-2.218962	3.709108	0.488588
1	-1.248093	3.929903	0.915264
6	-2.775601	4.600843	-0.467735
6	-2.052354	5.743244	-0.908393
1	-1.083531	5.947966	-0.459549
6	-2.558960	6.563232	-1.891720
1	-1.995281	7.428200	-2.228564
6	-3.815955	6.269698	-2.473442
1	-4.201616	6.903069	-3.267098
6	-4.557010	5.190135	-2.042460
1	-5.517664	4.981791	-2.498886
6	-4.074030	4.330988	-1.016403
6	-4.821494	3.193713	-0.539746
6	-6.247008	2.965437	-0.908242
6	-7.249032	3.982496	-0.696563
6	-6.982310	5.187734	0.012310
1	-5.996154	5.353524	0.428541
6	-7.962015	6.139720	0.195545
1	-7.731517	7.045817	0.748646
6	-9.265030	5.946545	-0.321017
1	-10.024430	6.709253	-0.175741
6	-9.566726	4.782288	-0.990153
1	-10.568243	4.607887	-1.374807
6	-8.584255	3.773004	-1.180717
6	-8.909765	2.551198	-1.827940
1	-9.914821	2.408384	-2.214461
6	-7.976183	1.551583	-1.935139
1	-8.207728	0.599236	-2.400263
6	-6.669172	1.753820	-1.437371
6	-5.503862	-2.482518	0.608196
1	-4.826803	-2.526032	1.471196
6	-6.594349	-3.515506	0.822127
6	-6.500817	-4.410780	1.892276
1	-5.669207	-4.324837	2.588272
6	-7.469792	-5.400752	2.082399
1	-7.386643	-6.085136	2.922383
6	-8.546678	-5.499720	1.200720
1	-9.308449	-6.259650	1.350951
6	-8.643363	-4.611633	0.122885
1	-9.484150	-4.677443	-0.561974
6	-7.670748	-3.633504	-0.068620
1	-7.762044	-2.929414	-0.889730
6	-4.701377	-2.822897	-0.653531
1	-5.400111	-2.951205	-1.488719
1	-4.204870	-3.785707	-0.504651
6	-6.838547	-0.514542	1.613808
1	-6.918846	0.551492	1.391314
6	-8.271917	-1.044484	1.628640
6	-9.136787	-0.659239	0.596078
1	-8.769013	0.004679	-0.177798
6	-10.453131	-1.114706	0.548968
1	-11.103648	-0.803250	-0.264173
6	-10.934077	-1.964616	1.549127
1	-11.957839	-2.326918	1.516299
6	-10.088629	-2.337583	2.595309
1	-10.450863	-2.995556	3.380435
6	-8.770401	-1.875485	2.638058
1	-8.131015	-2.190353	3.454715

6	-6.105061	-0.643980	2.952757
1	-5.121362	-0.174050	2.880776
1	-5.971500	-1.686373	3.253771
1	-6.671785	-0.137031	3.739421
6	-2.318315	-1.070200	0.755855
1	-1.559398	-0.299935	0.679539
1	-3.003253	-0.913907	1.585731
6	-1.998348	-2.432440	0.445753
1	-2.635957	-3.175261	0.912855
6	-0.817255	-2.930609	-0.174793
1	-0.168654	-2.225006	-0.676007
6	-4.022496	-1.428697	-3.273842
1	-5.069154	-1.720004	-3.222733
6	-3.074783	-2.474430	-3.115846
1	-3.468441	-3.480273	-2.970482
6	-1.662516	-2.437511	-3.672419
1	-1.680858	-2.665149	-4.749895
1	-1.101479	-3.246424	-3.199723
6	-0.923776	-1.105375	-3.433387
1	-1.067264	-0.431602	-4.282261
1	0.150876	-1.297224	-3.390687
6	-1.332603	-0.373143	-2.159149
1	-0.588904	-0.340278	-1.367119
6	-2.317779	0.603716	-2.123063
1	-2.263352	1.332004	-1.320746
6	-3.167382	1.014023	-3.309561
1	-3.978624	1.641595	-2.937885
1	-2.558247	1.645894	-3.969469
6	-3.763633	-0.168918	-4.105441
1	-3.109604	-0.426838	-4.945559
1	-4.711027	0.153960	-4.547676
6	-0.732928	-4.322475	-0.646696
6	-1.632388	-5.328497	-0.237527
6	0.281065	-4.677026	-1.556531
6	-1.516381	-6.630094	-0.720953
1	-2.426262	-5.100209	0.464569
6	0.398245	-5.978573	-2.040027
1	0.980711	-3.918388	-1.884172
6	-0.499392	-6.963978	-1.622039
1	-2.221314	-7.388102	-0.391630
1	1.190821	-6.222555	-2.741667
1	-0.411355	-7.980124	-1.995193
7	2.319757	-4.676802	0.726304
6	3.368129	-5.177616	-0.152904
1	4.255889	-5.464131	0.425316
1	3.004638	-6.058515	-0.692500
1	3.645772	-4.403945	-0.863112
6	1.663159	-5.672476	1.570751
1	0.686093	-5.961851	1.171121
1	2.297112	-6.560357	1.606387
1	1.545581	-5.312153	2.593206
1	-0.731780	0.007933	4.644936
1	-0.271878	-2.266163	3.762167
35	-0.201993	2.776895	3.513522

C2-P1 *si-re*_1

Number of imaginary frequencies=1
The smallest frequencies are= -266.5782 8.9694 12.2158 cm(-1)
Electronic energy= -7222.6288434
Zero-point correction= 1.755010
(Hartree/Particle)
Thermal correction to Energy= 1.873675
Thermal correction to Enthalpy= 1.874619
Thermal correction to Gibbs Free Energy= 1.591955
Sum of electronic and zero-point Energies= -7220.873833
Sum of electronic and thermal Energies= -7220.755168
Sum of electronic and thermal Enthalpies= -7220.754224
Sum of electronic and thermal Free Energies= -7221.036889

.....

Cartesian Coordinates

.....

26	8.173479	0.126622	-1.046102
15	3.105130	1.081939	-2.104116
15	4.181241	0.712969	1.497141
6	6.191743	0.782250	-1.260198
6	6.398708	0.147056	0.018896
6	6.823828	-1.195723	-0.222994
1	7.071930	-1.927036	0.533746
6	6.916169	-1.387003	-1.634717
1	7.249864	-2.286256	-2.131767
6	6.524832	-0.173516	-2.273013
1	6.507144	0.009607	-3.337064
6	9.591264	1.359005	-0.158807
1	9.381651	2.080819	0.619551
6	9.930463	-0.014732	0.040055
1	10.014025	-0.518305	0.993879
6	10.095671	-0.618956	-1.243534
1	10.319878	-1.660725	-1.431581
6	9.858569	0.380250	-2.235851
1	9.875228	0.229649	-3.307201
6	9.549981	1.601765	-1.566885
1	9.296348	2.536986	-2.047165
6	5.675318	2.167851	-1.441739
6	6.495671	3.249989	-1.085088
1	7.485757	3.033720	-0.704963
6	6.066322	4.571439	-1.195369
1	6.717849	5.382326	-0.885284
6	4.795154	4.836642	-1.698553
1	4.443382	5.858151	-1.800035
6	3.956792	3.778016	-2.046262
1	2.964125	4.005815	-2.414387
6	4.359042	2.438885	-1.900829
6	6.072221	0.783363	1.342356
1	6.311817	1.844760	1.263598
6	6.841574	0.204931	2.532790
1	6.581689	0.727523	3.457658
1	6.638014	-0.858867	2.681092
1	7.915675	0.320898	2.357787
6	1.582349	2.020357	-2.538139
6	0.833090	2.550727	-1.476866
1	1.108614	2.311522	-0.456536
6	-0.254064	3.386100	-1.727871
1	-0.813345	3.801012	-0.899507
6	-0.631651	3.668381	-3.042823
1	-1.486103	4.310838	-3.235468
6	0.083578	3.110371	-4.105236
1	-0.212270	3.315851	-5.130111
6	1.192997	2.297991	-3.856712
1	1.754873	1.892089	-4.691224
6	3.529597	0.216634	-3.663587
6	4.264158	0.812188	-4.699472
1	4.634804	1.827179	-4.589085
6	4.528760	0.097300	-5.869547
1	5.102528	0.561901	-6.666359
6	4.056094	-1.210692	-6.017512
1	4.266487	-1.763964	-6.928261
6	3.313909	-1.805027	-4.993443
1	2.943505	-2.820380	-5.103146
6	3.055640	-1.094244	-3.820432
1	2.493088	-1.556040	-3.015237
6	3.600033	2.430466	1.817849
6	2.209408	2.580771	1.918846
1	1.578904	1.700044	1.855346
6	1.639579	3.847114	2.048749
6	2.436161	4.990382	2.048330
1	1.991663	5.975992	2.128357
6	3.818629	4.839929	1.926249
6	4.403297	3.576947	1.825817
1	5.478949	3.512512	1.734470
6	3.812556	-0.179726	3.063736
6	3.969735	-1.574882	3.033955
1	4.342472	-2.059214	2.138861
6	3.622966	-2.346443	4.139455
6	3.085032	-1.754213	5.283477
1	2.797592	-2.359048	6.135636
6	2.916973	-0.372468	5.306322
6	3.286058	0.416648	4.213403
1	3.145515	1.489863	4.265852
29	2.923102	-0.209205	-0.251598

6	2.240972	0.275285	6.482516
6	3.715418	-3.844998	4.073674
6	0.147429	3.947550	2.206310
6	4.667083	6.081259	1.860284
9	4.390252	6.809289	0.750577
9	5.989773	5.806473	1.834923
9	4.443569	6.894973	2.918274
9	-0.503238	3.100586	1.356959
9	-0.255872	3.605936	3.451877
9	-0.321638	5.187488	1.954720
9	2.692111	1.528378	6.704283
9	0.897943	0.378418	6.276718
9	2.403932	-0.428076	7.622065
9	4.121452	-4.378816	5.245827
9	4.565315	-4.267963	3.114631
9	2.502229	-4.400354	3.798675
6	0.812662	-1.236523	1.705658
6	1.067586	-2.609704	1.324877
6	2.200684	-3.093095	0.588749
1	0.622624	-3.369309	1.951598
77	-3.134078	-1.268589	-1.268067
15	-4.959371	-0.293010	-0.325044
8	-4.920781	1.024690	0.684221
8	-5.992180	0.261247	-1.505768
7	-5.710316	-1.383800	0.706052
6	-4.764172	2.316091	0.199809
6	-3.571888	2.977413	0.567449
1	-2.862557	2.458604	1.201564
6	-3.341709	4.255875	0.125525
1	-2.445102	4.786152	0.430562
6	-4.258447	4.886110	-0.758370
6	-3.974767	6.160767	-1.319543
1	-3.051818	6.658379	-1.033060
6	-4.838385	6.745674	-2.218264
1	-4.608338	7.716065	-2.648252
6	-6.024637	6.071310	-2.593842
1	-6.693005	6.523811	-3.320723
6	-6.338925	4.843540	-2.052018
1	-7.247207	4.339013	-2.359781
6	-5.478579	4.214901	-1.109115
6	-5.770684	2.925427	-0.534683
6	-7.088322	2.254637	-0.725316
6	-8.330292	2.898471	-0.376846
6	-8.385579	4.145329	0.307508
1	-7.462989	4.640091	0.586600
6	-9.591982	4.724153	0.637321
1	-9.604783	5.671259	1.169053
6	-10.813490	4.093808	0.300569
1	-11.756209	4.564609	0.563419
6	-10.798929	2.878735	-0.346126
1	-11.727882	2.373270	-0.597142
6	-9.572087	2.246890	-0.688366
6	-9.558758	0.964294	-1.298944
1	-10.502809	0.482222	-1.535432
6	-8.371860	0.318987	-1.536332
1	-8.335960	-0.680577	-1.955552
6	-7.155538	0.962548	-1.223769
6	-5.228741	-2.777456	0.508417
1	-4.540905	-3.016814	1.326605
6	-6.358851	-3.790670	0.520366
6	-6.239949	-4.969182	1.263888
1	-5.350204	-5.133268	1.868198
6	-7.260142	-5.925468	1.249219
1	-7.159140	-6.833090	1.838129
6	-8.409013	-5.709745	0.485713
1	-9.206908	-6.447045	0.479244
6	-8.529596	-4.536698	-0.267888
1	-9.425153	-4.357949	-0.856626
6	-7.510719	-3.586831	-0.251857
1	-7.617203	-2.660309	-0.808483
6	-4.453598	-2.897375	-0.817897
1	-5.173833	-2.997943	-1.637835
1	-3.880450	-3.828576	-0.789866
6	-6.310065	-1.000710	2.031657
1	-6.197399	0.079875	2.087405
6	-7.810641	-1.260609	2.148750
6	-8.693384	-0.238845	1.776531
1	-8.292940	0.696244	1.397975
6	-10.075679	-0.401347	1.885751
1	-10.735336	0.408308	1.586469
6	-10.599671	-1.596441	2.382140
1	-11.674585	-1.730054	2.469017
6	-9.729678	-2.617365	2.774825
1	-10.124686	-3.551545	3.164590
6	-8.348789	-2.447278	2.665610
1	-7.694955	-3.257511	2.966230
6	-5.505225	-1.583609	3.199836
1	-4.451718	-1.297092	3.116680
1	-5.561408	-2.673272	3.259287
1	-5.897007	-1.179904	4.138071
6	-2.203071	-1.009234	0.680503
1	-1.489875	-0.192447	0.633349
1	-2.875870	-0.949863	1.532407
6	-1.775661	-2.317946	0.285333
1	-2.329427	-3.159498	0.688435
6	-0.551485	-2.617812	-0.369162
1	0.017503	-1.792389	-0.775284
6	-3.987196	-1.235922	-3.320249
1	-5.005765	-1.607438	-3.246520
6	-2.951259	-2.203768	-3.294128
1	-3.246098	-3.250407	-3.224828
6	-1.578505	-1.985461	-3.906596
1	-1.644032	-2.076406	-5.002184
1	-0.938357	-2.804121	-3.572350
6	-0.917243	-0.639824	-3.531694
1	-1.097714	0.108859	-4.309373
1	0.168427	-0.774548	-3.500559
6	-1.364443	-0.062442	-2.189772
1	-0.592999	0.001359	-1.427943
6	-2.435762	0.812254	-2.034454
1	-2.405596	1.469078	-1.170925
6	-3.372899	1.256783	-3.139337
1	-4.238971	1.728791	-2.671708
1	-2.873072	2.031798	-3.736695
6	-3.856397	0.105530	-4.045147
1	-3.180312	-0.014758	-4.897853
1	-4.831253	0.373730	-4.463694
6	-0.278320	-3.925986	-0.974505
6	-0.905256	-5.115139	-0.555109
6	0.664891	-4.004078	-2.016361
6	-0.609577	-6.329599	-1.171741
1	-1.621408	-5.095133	0.260248
6	0.956520	-5.216988	-2.637135
1	1.170936	-3.098660	-2.333693
6	0.318184	-6.386550	-2.217668
1	-1.103622	-7.236460	-0.834639
1	1.684749	-5.249722	-3.442456
1	0.543660	-7.335043	-2.696382
6	2.496027	-4.482333	0.664891
6	3.497859	-5.043931	-0.097873
1	1.917235	-5.105073	1.336152
6	4.217018	-4.196946	-0.946439
6	3.930382	-2.845671	-0.977806
1	4.478808	-2.168269	-1.618111
7	2.952163	-2.295276	-0.228367
8	1.111520	-0.245169	0.967572
7	0.126791	-1.006379	2.866197
6	-0.375934	0.327560	3.176243
1	-1.375529	0.242963	3.614864
1	0.272218	0.838046	3.895856
1	-0.441983	0.922338	2.270895
6	-0.143418	-2.019043	3.884079
1	-1.118971	-2.498385	3.728890
1	0.632763	-2.782448	3.903088
1	-0.148687	-1.530994	4.861539
1	3.710091	-6.105990	-0.043765
35	5.604807	-4.925348	-2.118787

C2-P1 *si-re*_2

Number of imaginary frequencies= 1
The smallest frequencies are= -267.9420 7.6459 11.1107 cm(-1)
Electronic energy= -7222.6289103
Zero-point correction= 1.754635
(Hartree/Particle)
Thermal correction to Energy= 1.873394
Thermal correction to Enthalpy= 1.874339
Thermal correction to Gibbs Free Energy= 1.590922
Sum of electronic and zero-point Energies= -7220.874276
Sum of electronic and thermal Energies= -7220.755516
Sum of electronic and thermal Enthalpies= -7220.754572
Sum of electronic and thermal Free Energies= -7221.037988
.....
Cartesian Coordinates
.....

26	8.164596	0.057089	-1.065021
15	3.103223	1.071702	-2.100878
15	4.188561	0.684018	1.495436
6	6.189305	0.736313	-1.267302
6	6.395395	0.096392	0.009540
6	6.803807	-1.250745	-0.237072
1	7.046516	-1.986556	0.517061
6	6.886832	-1.440358	-1.649576
1	7.207218	-2.342574	-2.149999
6	6.506061	-0.221269	-2.283599
1	6.484705	-0.036040	-3.347252
6	9.603761	1.270656	-0.185019
1	9.409197	1.994515	0.595439
6	9.926895	-0.107543	0.009688
1	10.010555	-0.613585	0.962210
6	10.076116	-0.711796	-1.275836
1	10.286363	-1.755911	-1.466947
6	9.844939	0.291794	-2.265142
1	9.852769	0.142583	-3.336788
6	9.556107	1.516021	-1.592401
1	9.310821	2.455078	-2.069532
6	5.687507	2.127693	-1.444852
6	6.521001	3.200066	-1.089314
1	7.509152	2.971749	-0.711222
6	6.106821	4.526402	-1.198629
1	6.768038	5.329658	-0.889273
6	4.838139	4.806418	-1.700158
1	4.498315	5.831971	-1.801671
6	3.986838	3.757615	-2.046240
1	2.996348	3.996792	-2.413012
6	4.373531	2.413878	-1.901034
6	6.080397	0.732386	1.335960
1	6.333263	1.790951	1.260462
6	6.845569	0.140065	2.522356
1	6.595070	0.662979	3.449632
1	6.628949	-0.921550	2.667793
1	7.920578	0.242877	2.344635
6	1.588280	2.028895	-2.520715
6	0.854220	2.565275	-1.451744
1	1.135384	2.319370	-0.434517
6	-0.224819	3.414335	-1.691568
1	-0.772237	3.834032	-0.857681
6	-0.609920	3.704560	-3.002651
1	-1.458390	4.357516	-3.186291
6	0.089280	3.140339	-4.072384
1	-0.212805	3.351720	-5.094232
6	1.191005	2.314099	-3.835222
1	1.741030	1.903483	-4.675338
6	3.509439	0.207130	-3.665490
6	4.242777	0.799321	-4.704202
1	4.622138	1.811052	-4.593463
6	4.494598	0.085240	-5.877593
1	5.067364	0.547162	-6.676677
6	4.010517	-1.218543	-6.025919
1	4.210982	-1.771163	-6.939296
6	3.269900	-1.809595	-4.998815
1	2.890790	-2.821728	-5.108692
6	3.024478	-1.099682	-3.822531
1	2.463354	-1.558946	-3.014907
6	3.628086	2.407097	1.823019
6	2.240280	2.573681	1.936675
1	1.598043	1.701237	1.877077
6	1.686918	3.846419	2.075413
6	2.496784	4.980255	2.070181
1	2.064565	5.970719	2.157174
6	3.876136	4.813833	1.934720
6	4.444622	3.544223	1.826081
1	5.518492	3.466877	1.725185
6	3.813212	-0.208515	3.060659
6	3.953117	-1.605395	3.026667
1	4.319876	-2.091733	2.130250
6	3.596810	-2.375937	4.129847
6	3.066286	-1.780517	5.275729
1	2.771081	-2.384435	6.125866
6	2.916633	-0.396749	5.303290
6	3.295824	0.390983	4.212810
1	3.170003	1.465777	4.269136
29	2.914361	-0.222418	-0.250912
6	2.249877	0.256142	6.481955
6	3.672185	-3.875325	4.060136
6	0.197625	3.963171	2.247647
6	4.738491	6.045303	1.864087
9	4.463466	6.776909	0.756305
9	6.057789	5.755501	1.830854
9	4.530547	6.861158	2.923621
9	-0.470298	3.133147	1.394953
9	-0.198577	3.612434	3.492986
9	-0.258986	5.211097	2.013746
9	2.716292	1.503175	6.706284
9	0.908031	0.375817	6.278072
9	2.405871	-0.451891	7.619594
9	4.076128	-4.416446	5.229706
9	4.514040	-4.305457	3.097254
9	2.452103	-4.416574	3.787892
6	0.794376	-1.230034	1.704829
6	1.032368	-2.604798	1.318116
6	2.160729	-3.099255	0.581827
1	0.577978	-3.361257	1.941858
77	-3.150279	-1.209019	-1.279288
15	-4.969726	-0.206119	-0.363253
8	-4.906117	1.091578	0.671674
8	-5.977820	0.396197	-1.542473
7	-5.781403	-1.285182	0.635780
6	-4.737058	2.390831	0.215341
6	-3.534484	3.030035	0.588302
1	-2.825761	2.487773	1.203073
6	-3.295448	4.317211	0.177467
1	-2.390793	4.830743	0.487385
6	-4.215164	4.980388	-0.678822
6	-3.925619	6.268806	-1.204478
1	-2.994975	6.748923	-0.913035
6	-4.793537	6.889004	-2.074800
1	-4.559363	7.870210	-2.477109
6	-5.989917	6.236962	-2.457538
1	-6.662158	6.717621	-3.162449
6	-6.309412	4.995713	-1.950592
1	-7.225536	4.509139	-2.263776
6	-5.445134	4.330713	-1.036522
6	-5.742849	3.027750	-0.496322
6	-7.065374	2.369199	-0.700191
6	-8.303408	3.008364	-0.332853
6	-8.351185	4.234407	0.388740
1	-7.425476	4.710324	0.689708
6	-9.554210	4.816532	0.724350
1	-9.562053	5.747814	1.283449
6	-10.779265	4.210286	0.356690
1	-11.719241	4.684165	0.623848
6	-10.772073	3.014246	-0.324078
1	-11.704246	2.526553	-0.597175
6	-9.549117	2.379330	-0.674239
6	-9.542766	1.120897	-1.334328
1	-10.489087	0.658240	-1.599647
6	-8.358730	0.473847	-1.587753
1	-8.328934	-0.509160	-2.045344
6	-7.139107	1.095161	-1.242878

6	-5.288916	-2.680451	0.489108
1	-4.625090	-2.904031	1.333007
6	-6.406104	-3.709375	0.471441
6	-6.247398	-4.922542	1.148375
1	-5.344342	-5.096541	1.729974
6	-7.244412	-5.900959	1.099385
1	-7.111238	-6.835906	1.637062
6	-8.413510	-5.671041	0.372179
1	-9.196407	-6.423720	0.343283
6	-8.573788	-4.462925	-0.316036
1	-9.484958	-4.272903	-0.876635
6	-7.573476	-3.494269	-0.273745
1	-7.708096	-2.544006	-0.781655
6	-4.481756	-2.823316	-0.818293
1	-5.189365	-2.934201	-1.648198
1	-3.915443	-3.757449	-0.765796
6	-6.412893	-0.852560	1.931022
1	-6.572347	0.218491	1.817066
6	-7.794571	-1.453105	2.161082
6	-8.903723	-0.808695	1.599969
1	-8.756435	0.105708	1.036563
6	-10.190481	-1.326272	1.751424
1	-11.034769	-0.811252	1.300764
6	-10.388473	-2.497416	2.486633
1	-11.387256	-2.908512	2.604857
6	-9.293101	-3.130427	3.079885
1	-9.436728	-4.038024	3.659469
6	-8.008477	-2.606604	2.925292
1	-7.170541	-3.119467	3.384134
6	-5.453105	-1.040678	3.111932
1	-4.539489	-0.464576	2.943454
1	-5.178114	-2.086289	3.273283
1	-5.924080	-0.676436	4.030004
6	-2.211414	-0.948938	0.664811
1	-1.486620	-0.142668	0.610105
1	-2.878030	-0.874641	1.519539
6	-1.803609	-2.266116	0.277670
1	-2.370587	-3.095407	0.687690
6	-0.583987	-2.588567	-0.374959
1	-0.002725	-1.773293	-0.784453
6	-4.003453	-1.173954	-3.334358
1	-5.026124	-1.534087	-3.259187
6	-2.980285	-2.154330	-3.305886
1	-3.288398	-3.196696	-3.231257
6	-1.603541	-1.956016	-3.915466
1	-1.666374	-2.055741	-5.010459
1	-0.973587	-2.778745	-3.572015
6	-0.928697	-0.614830	-3.550096
1	-1.106033	0.131585	-4.330637
1	0.155741	-0.759368	-3.523330
6	-1.364605	-0.027155	-2.208957
1	-0.591504	0.027126	-1.448263
6	-2.424463	0.861284	-2.055641
1	-2.387954	1.519497	-1.193345
6	-3.353845	1.313721	-3.163783
1	-4.210627	1.806076	-2.700019
1	-2.839309	2.074082	-3.767379
6	-3.858290	0.164698	-4.062084
1	-3.188817	0.032754	-4.918270
1	-4.831893	0.444553	-4.475688
6	-0.332517	-3.902762	-0.976821
6	-0.980602	-5.079626	-0.555033
6	0.609420	-3.999850	-2.018281
6	-0.707810	-6.300157	-1.170191
1	-1.695800	-5.045136	0.260676
6	0.878459	-5.218860	-2.637381
1	1.132501	-3.104412	-2.336690
6	0.218197	-6.375663	-2.216559
1	-1.218409	-7.197302	-0.831740
1	1.606178	-5.266137	-3.442493
1	0.425720	-7.328792	-2.694197
6	2.439817	-4.491969	0.654367
6	3.434545	-5.063464	-0.110365
1	1.853635	-5.109713	1.323878
6	4.162617	-4.222916	-0.957633
6	3.891941	-2.868253	-0.985277
1	4.447199	-2.195988	-1.625042
7	2.921393	-2.308018	-0.233172
8	1.106818	-0.239302	0.971804
7	0.109987	-0.996879	2.865584
6	-0.376885	0.341754	3.180696
1	-1.377492	0.267545	3.618895
1	0.277053	0.842137	3.902199
1	-0.435768	0.940081	2.277270
6	-0.169926	-2.010091	3.880438
1	-1.149738	-2.480066	3.723768
1	0.599238	-2.780685	3.897675
1	-0.171017	-1.524723	4.859270
1	3.634336	-6.128071	-0.059138
35	5.539805	-4.964628	-2.134047

C2-P1 *si-re*_3

Number of imaginary frequencies= 1
The smallest frequencies are=-151.4891 10.4142 12.5611cm(-1)
Electronic energy= -7222.6271114
Zero-point correction= 1.755475
(Hartree/Particle)
Thermal correction to Energy= 1.873703
Thermal correction to Enthalpy= 1.874647
Thermal correction to Gibbs Free Energy= 1.595076
Sum of electronic and zero-point Energies= -7220.871636
Sum of electronic and thermal Energies= -7220.753408
Sum of electronic and thermal Enthalpies= -7220.752464
Sum of electronic and thermal Free Energies= -7221.032035

.....

Cartesian Coordinates

.....

26	-4.703316	4.864637	1.510872
15	-1.968104	1.590501	-1.525797
15	-4.729643	0.191844	0.600289
6	-3.935303	3.477491	0.144183
6	-4.502374	2.819748	1.298288
6	-3.793209	3.270937	2.453908
1	-3.991948	2.975056	3.474842
6	-2.816633	4.223855	2.033908
1	-2.151718	4.779338	2.680581
6	-2.907912	4.356301	0.617848
1	-2.318943	5.021697	0.006026
6	-6.697907	5.430963	1.378593
1	-7.497552	4.792330	1.027115
6	-6.241528	5.537042	2.727980
1	-6.629706	4.988742	3.575910
6	-5.152271	6.460379	2.754751
1	-4.567214	6.727332	3.625046
6	-4.936020	6.927212	1.422389
1	-4.161066	7.612525	1.105284
6	-5.890831	6.293266	0.572913
1	-5.964697	6.420128	-0.498729
6	-4.336940	3.173893	-1.261579
6	-5.591825	3.600843	-1.722503
1	-6.206097	4.193377	-1.056625
6	-6.069345	3.261593	-2.988096
1	-7.058917	3.581746	-3.298624
6	-5.279701	2.487920	-3.834924
1	-5.641183	2.203732	-4.818011
6	-4.026171	2.054113	-3.403365
1	-3.427372	1.442011	-4.068281
6	-3.541975	2.370220	-2.124247
6	-5.575977	1.768811	1.236742
1	-6.274682	2.062380	0.451861
6	-6.361406	1.600409	2.539857
1	-7.156872	0.858761	2.425783
1	-5.723779	1.283256	3.369438
1	-6.814218	2.558527	2.812495
6	-1.303626	0.720716	-3.007530
6	-1.575619	-0.651670	-3.130450
1	-2.129089	-1.166211	-2.351844
6	-1.120971	-1.361376	-4.244500
1	-1.356819	-2.415664	-4.339946

6	-0.363396	-0.719420	-5.227307
1	0.001689	-1.277548	-6.084841
6	-0.078895	0.642960	-5.104481
1	0.517662	1.150089	-5.857220
6	-0.559281	1.362149	-4.009563
1	-0.339163	2.419514	-3.938761
6	-0.848529	3.033208	-1.303808
6	-0.950400	4.179677	-2.109555
1	-1.682088	4.218041	-2.910598
6	-0.136735	5.287275	-1.866941
1	-0.223194	6.168231	-2.496321
6	0.777947	5.265986	-0.808986
1	1.401651	6.132510	-0.610350
6	0.889670	4.127395	-0.007621
1	1.600082	4.107201	0.812216
6	0.087312	3.011289	-0.260346
1	0.173955	2.127107	0.364180
6	-5.656583	-0.327273	-0.904822
6	-5.073225	-1.370307	-1.639001
1	-4.163158	-1.830312	-1.267536
6	-5.643988	-1.797643	-2.837543
6	-6.779162	-1.171666	-3.349170
1	-7.207877	-1.485016	-4.294573
6	-7.345003	-0.120153	-2.627141
6	-6.808311	0.289937	-1.406219
1	-7.289190	1.101427	-0.877107
6	-5.106239	-1.121589	1.829520
6	-4.323940	-1.113691	2.995191
1	-3.588366	-0.332861	3.147230
6	-4.461197	-2.122588	3.942379
6	-5.362171	-3.171055	3.742249
1	-5.452944	-3.968166	4.471265
6	-6.130306	-3.181469	2.581277
6	-6.014884	-2.163326	1.629217
1	-6.625787	-2.198555	0.734008
29	-2.410679	0.194977	0.199909
6	-7.028666	-4.349347	2.286546
6	-3.550362	-2.155515	5.137089
6	-5.036179	-2.976563	-3.546011
6	-8.520776	0.603681	-3.223502
9	-8.180125	1.230263	-4.378452
9	-9.023315	1.546798	-2.396964
9	-9.529534	-0.243418	-3.532701
9	-3.678800	-2.955679	-3.491640
9	-5.418356	-4.148176	-2.978065
9	-5.383987	-3.035980	-4.847354
9	-8.157753	-3.973222	1.647519
9	-6.407953	-5.249646	1.473970
9	-7.390500	-5.017087	3.401108
9	-4.195490	-2.549668	6.256319
9	-2.988930	-0.953336	5.388893
9	-2.526930	-3.034169	4.953178
6	-2.239519	-2.787264	0.831445
6	-1.262323	-2.573214	1.870209
6	-0.905633	-1.314236	2.446267
1	-1.048546	-3.412630	2.516390
77	3.322308	-1.995212	-0.770188
15	4.789639	-0.281638	-0.528835
8	5.402195	0.186997	0.922334
8	6.205136	-0.550804	-1.381854
7	4.044075	1.128132	-0.993369
6	6.539651	-0.327423	1.514012
6	6.348015	-0.973142	2.756465
1	5.344141	-1.009446	3.166090
6	7.422929	-1.516876	3.412185
1	7.290817	-2.007705	4.372253
6	8.720301	-1.467712	2.833127
6	9.827579	-2.094860	3.465684
1	9.665206	-2.595085	4.416964
6	11.075233	-2.083800	2.883951
1	11.913512	-2.570567	3.373707
6	11.260108	-1.449086	1.632998
1	12.238865	-1.463321	1.162097
6	10.210205	-0.817696	1.001247
1	10.372068	-0.347734	0.038678
6	8.911891	-0.787361	1.583295
6	7.791170	-0.137280	0.949531
6	7.955982	0.683040	-0.282071
6	8.874174	1.791179	-0.342303
6	9.529738	2.303463	0.812669
1	9.331908	1.851779	1.777636
6	10.391547	3.375129	0.723709
1	10.870609	3.755131	1.621500
6	10.653940	3.990153	-0.524059
1	11.341773	4.828827	-0.579512
6	10.022021	3.533366	-1.658432
1	10.197374	4.009688	-2.619564
6	9.110352	2.444071	-1.599026
6	8.404534	2.012714	-2.754882
1	8.600041	2.500282	-3.705783
6	7.448075	1.032974	-2.660622
1	6.852022	0.732276	-3.514389
6	7.210449	0.405772	-1.417843
6	2.879476	0.918995	-1.907172
1	2.000895	1.294922	-1.370313
6	3.050484	1.752888	-3.173317
6	2.306581	2.922709	-3.351593
1	1.590576	3.215663	-2.594262
6	2.474135	3.717648	-4.489066
1	1.881657	4.621232	-4.604201
6	3.400916	3.351730	-5.466034
1	3.536127	3.965571	-6.352141
6	4.161114	2.189129	-5.292892
1	4.891010	1.899668	-6.044122
6	3.988348	1.400314	-4.155961
1	4.592051	0.506997	-4.029292
6	2.660961	-0.578968	-2.231307
1	3.178585	-0.827243	-3.160888
1	1.595055	-0.715565	-2.433425
6	4.243649	2.538587	-0.515868
1	3.291252	3.014606	-0.767358
6	4.371382	2.647097	1.002162
6	3.292981	2.246199	1.803111
1	2.380841	1.896727	1.329948
6	3.386845	2.255634	3.193467
1	2.544702	1.924756	3.791751
6	4.562012	2.692815	3.812519
1	4.640451	2.698674	4.896228
6	5.629591	3.127245	3.025395
1	6.547265	3.473306	3.493406
6	5.533812	3.106095	1.631327
1	6.389046	3.418257	1.042615
6	5.331362	3.288454	-1.283946
1	5.178353	3.183004	-2.358051
1	6.327856	2.920214	-1.044391
1	5.291072	4.353120	-1.030385
6	2.090734	-1.092918	0.762709
1	2.335236	-1.437122	1.768004
1	2.022854	-0.012126	0.696658
6	1.132684	-1.856395	0.004651
1	0.573925	-1.361009	-0.782314
6	0.680288	-3.127364	0.418321
1	1.111090	-3.521200	1.331057
6	4.650842	-2.953625	-2.332594
1	4.879320	-2.165605	-3.044115
6	3.372498	-3.537570	-2.414784
1	2.704489	-3.177251	-3.196870
6	3.040698	-4.928861	-1.905193
1	3.438309	-5.677030	-2.607927
1	1.956113	-5.040085	-1.925442
6	3.550405	-5.241959	-0.477946
1	4.517081	-5.754236	-0.526644
1	2.855442	-5.947044	-0.012260
6	3.693759	-4.032779	0.441727
1	3.024084	-3.995715	1.293137
6	4.846780	-3.275097	0.546219
1	4.983371	-2.710499	1.463660
6	6.107918	-3.496730	-0.264776
1	6.765259	-2.639987	-0.112429
1	6.634776	-4.370406	0.145989

6	5.872547	-3.687241	-1.780398
1	5.778624	-4.752696	-2.014833
1	6.759445	-3.333213	-2.313505
6	0.036088	-4.121239	-0.428581
6	-0.433891	-3.824076	-1.722123
6	-0.067486	-5.445749	0.037215
6	-0.978785	-4.823248	-2.522836
1	-0.353050	-2.814366	-2.099025
6	-0.607143	-6.446923	-0.767051
1	0.290916	-5.685941	1.034720
6	-1.065097	-6.138433	-2.051841
1	-1.344289	-4.580251	-3.515850
1	-0.669489	-7.465448	-0.395071
1	-1.486250	-6.916208	-2.682208
6	-0.137615	-1.320360	3.648484
6	0.139662	-0.155431	4.332324
1	0.194846	-2.271336	4.051320
6	-0.346592	1.043683	3.795090
6	-1.027510	1.029823	2.593772
1	-1.393357	1.946053	2.146449
7	-1.289144	-0.108722	1.918483
8	-2.426846	-1.966177	-0.122052
7	-2.932684	-3.966474	0.827362
6	-3.710756	-4.358514	-0.341577
1	-3.614018	-5.437899	-0.488946
1	-4.772559	-4.120822	-0.213590
1	-3.327739	-3.859740	-1.225789
6	-2.971633	-4.906384	1.943143
1	-2.225632	-5.702251	1.826623
1	-2.812328	-4.399775	2.893601
1	-3.963990	-5.362260	1.974603
1	0.698157	-0.174105	5.261970
35	-0.122089	2.736121	4.751963

C2-P1 *si-re_*4

Number of imaginary frequencies= 1
The smallest frequencies are= -192.1184 6.9342 12.9296 cm(-1)
Electronic energy= -7222.6277096
Zero-point correction= 1.756077
(Hartree/Particle)
Thermal correction to Energy= 1.874298
Thermal correction to Enthalpy= 1.875242
Thermal correction to Gibbs Free Energy= 1.594238
Sum of electronic and zero-point Energies= -7220.871633
Sum of electronic and thermal Energies= -7220.753412
Sum of electronic and thermal Enthalpies= -7220.752467
Sum of electronic and thermal Free Energies= -7221.033471

.....

Cartesian Coordinates

.....

26	-7.069352	-3.098020	-2.145295
15	-5.001012	-0.832388	2.068271
15	-4.596823	0.882428	-1.284847
6	-6.456923	-1.892342	-0.548376
6	-5.801999	-1.508007	-1.777220
6	-5.060745	-2.635115	-2.248521
1	-4.470866	-2.668476	-3.154440
6	-5.275857	-3.720710	-1.348342
1	-4.881926	-4.721641	-1.455647
6	-6.132651	-3.266141	-0.303916
1	-6.499091	-3.859569	0.519964
6	-8.679830	-2.502214	-3.311441
1	-8.945602	-1.473048	-3.513338
6	-7.778414	-3.301065	-4.079737
1	-7.236549	-2.981903	-4.959955
6	-7.680330	-4.581712	-3.454775
1	-7.047559	-5.398624	-3.776066
6	-8.520667	-4.575308	-2.300108
1	-8.636745	-5.385661	-1.592596
6	-9.139235	-3.292538	-2.212048
1	-9.809580	-2.968739	-1.427692
6	-7.247223	-0.967541	0.315217
6	-8.502307	-0.516555	-0.121051
1	-8.878311	-0.882615	-1.068337
6	-9.257730	0.390953	0.621804
1	-10.213136	0.738894	0.242081
6	-8.769316	0.858278	1.839834
1	-9.342550	1.567671	2.427707
6	-7.520900	0.430099	2.291704
1	-7.142699	0.815080	3.232270
6	-6.738910	-0.462805	1.542690
6	-5.808919	-0.117356	-2.349968
1	-6.791978	0.312846	-2.154151
6	-5.554482	-0.054956	-3.858648
1	-5.603143	0.975052	-4.222436
1	-4.577362	-0.462144	-4.131888
1	-6.319367	-0.643684	-4.374751
6	-4.770992	0.137592	3.617053
6	-4.293409	1.452863	3.500282
1	-4.054642	1.851356	2.521055
6	-4.092010	2.234251	4.638819
1	-3.733431	3.252554	4.536585
6	-4.338342	1.701024	5.906968
1	-4.168091	2.304934	6.793866
6	-4.797967	0.387629	6.031880
1	-4.987473	-0.033325	7.015329
6	-5.021996	-0.388938	4.893132
1	-5.385317	-1.405028	5.004427
6	-5.058881	-2.567209	2.665016
6	-6.238066	-3.175452	3.122630
1	-7.171188	-2.620028	3.126900
6	-6.218278	-4.501404	3.559376
1	-7.135737	-4.967795	3.907165
6	-5.022894	-5.227540	3.549119
1	-5.012338	-6.260715	3.884340
6	-3.843010	-4.620856	3.111147
1	-2.910229	-5.177784	3.106883
6	-3.861744	-3.296147	2.670886
1	-2.946352	-2.821638	2.335720
6	-5.539436	2.319685	-0.619003
6	-4.825082	3.165998	0.241664
1	-3.779117	2.957163	0.443540
6	-5.454864	4.251293	0.850998
6	-6.812755	4.491611	0.653517
1	-7.304773	5.322927	1.145167
6	-7.527941	3.632747	-0.181661
6	-6.901167	2.568089	-0.829118
1	-7.496123	1.935167	-1.472754
6	-3.386763	1.676055	-2.430178
6	-2.381799	0.852336	-2.964862
1	-2.386178	-0.211662	-2.760483
6	-1.354547	1.398782	-3.730310
6	-1.281372	2.775604	-3.951135
1	-0.462519	3.201517	-4.519795
6	-2.269215	3.592373	-3.409834
6	-3.323886	3.052469	-2.668958
1	-4.077735	3.720273	-2.269396
29	-3.527326	-0.247511	0.453859
6	-2.145457	5.086018	-3.514967
6	-0.222105	0.536057	-4.213613
6	-4.624223	5.180588	1.690310
6	-9.005270	3.866291	-0.345581
9	-9.666595	3.701638	0.826675
9	-9.569181	3.024910	-1.239791
9	-9.267741	5.128625	-0.757656
9	-3.796330	4.499921	2.526259
9	-3.821985	5.957638	0.919973
9	-5.369505	6.005885	2.450259
9	-3.347817	5.695020	-3.595207
9	-1.525708	5.598283	-2.415040
9	-1.417728	5.469050	-4.584451
9	0.157485	0.845755	-5.472055
9	-0.523607	-0.779281	-4.191144
9	0.886039	0.700128	-3.434040
6	-1.117908	1.561780	0.138246
6	-0.352904	0.469250	-0.405170
6	-0.749334	-0.889744	-0.611611
1	0.517635	0.736270	-0.979135
77	4.234866	0.147758	1.712140

15	6.013290	-0.327371	0.372997
8	6.376971	0.503934	-1.011781
8	7.455046	-0.186710	1.195345
7	5.830132	-1.874114	-0.250532
6	7.080575	1.703685	-0.981929
6	6.368076	2.856656	-1.378174
1	5.335196	2.744138	-1.691153
6	6.993929	4.078265	-1.363314
1	6.460565	4.972471	-1.673110
6	8.338175	4.194395	-0.916850
6	8.973063	5.462885	-0.827053
1	8.413720	6.344314	-1.129701
6	10.261471	5.577161	-0.356331
1	10.735676	6.551721	-0.287226
6	10.965439	4.420003	0.054187
1	11.973379	4.515286	0.447645
6	10.384183	3.173724	-0.034489
1	10.936081	2.300759	0.292929
6	9.062343	3.014088	-0.537093
6	8.424492	1.726732	-0.641503
6	9.156010	0.456464	-0.373697
6	10.349057	0.089947	-1.091182
6	10.851073	0.848353	-2.185896
1	10.319883	1.737073	-2.505070
6	11.992130	0.462285	-2.855060
1	12.349994	1.055074	-3.691989
6	12.698457	-0.701832	-2.468802
1	13.599989	-0.989554	-3.001695
6	12.229023	-1.472829	-1.429750
1	12.749894	-2.380038	-1.134926
6	11.046365	-1.112102	-0.728153
6	10.532837	-1.935017	0.310786
1	11.075543	-2.833701	0.589571
6	9.349894	-1.618160	0.931773
1	8.921517	-2.246927	1.704802
6	8.665040	-0.441138	0.559873
6	4.764021	-2.635355	0.457965
1	3.858414	-2.601396	-0.160529
6	5.134240	-4.093804	0.659266
6	4.157655	-5.083961	0.495832
1	3.159810	-4.799778	0.168241
6	4.455789	-6.426077	0.745410
1	3.687851	-7.183629	0.614211
6	5.740588	-6.792712	1.152682
1	5.976808	-7.836229	1.340868
6	6.723436	-5.810063	1.309800
1	7.727013	-6.089610	1.619145
6	6.421412	-4.469703	1.067595
1	7.186063	-3.706021	1.174822
6	4.459260	-1.980184	1.811990
1	5.261947	-2.230236	2.516439
1	3.539753	-2.415522	2.213500
6	6.134977	-2.403735	-1.624677
1	6.205036	-3.482996	-1.463711
6	4.955981	-2.183756	-2.571886
6	4.038044	-3.225685	-2.768211
1	4.204866	-4.179543	-2.274248
6	2.913502	-3.052599	-3.580452
1	2.218305	-3.875537	-3.723107
6	2.686090	-1.826263	-4.207524
1	1.803400	-1.679451	-4.821385
6	3.603088	-0.785370	-4.032439
1	3.432396	0.170380	-4.519431
6	4.730646	-0.963713	-3.228426
1	5.429632	-0.146393	-3.098556
6	7.485552	-1.987085	-2.207008
1	8.290639	-2.219855	-1.507700
1	7.541442	-0.930357	-2.460932
1	7.651256	-2.566053	-3.121008
6	3.108779	0.235539	-0.138455
1	2.896079	1.265122	-0.425234
1	3.493313	-0.358336	-0.963371
6	2.209462	-0.422813	0.766185
1	2.170819	-1.503884	0.714993
6	1.148557	0.212549	1.452713
1	1.143131	1.293295	1.487751
6	5.427863	0.317908	3.587222
1	6.102813	-0.533840	3.618039
6	4.077513	0.062080	3.934340
1	3.827660	-0.957562	4.227083
6	3.096706	1.102062	4.452685
1	3.263769	1.272483	5.527465
1	2.093049	0.676982	4.358493
6	3.138028	2.447061	3.694917
1	3.841489	3.134322	4.174267
1	2.154517	2.923148	3.767293
6	3.501588	2.320532	2.217473
1	2.702576	2.545924	1.517054
6	4.794855	2.412476	1.711433
1	4.892010	2.707004	0.671043
6	6.059616	2.576360	2.532042
1	6.906072	2.338182	1.883025
1	6.170548	3.632512	2.818863
6	6.116858	1.670605	3.779483
1	5.677163	2.180469	4.642285
1	7.166389	1.494274	4.034102
6	0.302555	-0.449513	2.438301
6	0.278262	-1.851290	2.600887
6	-0.519313	0.335030	3.272805
6	-0.519278	-2.437123	3.579709
1	0.886375	-2.484545	1.964414
6	-1.317970	-0.254261	4.250609
1	-0.530223	1.412678	3.143515
6	-1.318638	-1.642089	4.409384
1	-0.522934	-3.517248	3.694932
1	-1.946984	0.365482	4.880629
1	-1.948080	-2.102808	5.164653
6	0.174942	-1.749645	-1.274599
6	-0.083066	-3.097528	-1.422613
1	1.090244	-1.333744	-1.676699
6	-1.295335	-3.584646	-0.926390
6	-2.195253	-2.718498	-0.333429
1	-3.155578	-3.063070	0.025496
7	-1.937418	-1.406261	-0.173799
8	-2.172492	1.417002	0.829721
7	-0.619339	2.834504	-0.032225
6	-1.185446	3.951268	0.714064
1	-0.374630	4.549962	1.145697
1	-1.781405	4.604034	0.065881
1	-1.813982	3.579481	1.518257
6	0.494261	3.185591	-0.907328
1	1.455709	3.173895	-0.375226
1	0.558720	2.519422	-1.765576
1	0.325689	4.194376	-1.292569
1	0.631291	-3.745487	-1.917915
35	-1.735620	-5.486848	-1.073150

C2-P1 *si-re_5*

Number of imaginary frequencies= 1
The smallest frequencies are= -199.8191 4.9171 11.4236 cm(-1)
Electronic energy= -7222.624432
Zero-point correction= 1.755119
(Hartree/Particle)
Thermal correction to Energy= 1.873743
Thermal correction to Enthalpy= 1.874687
Thermal correction to Gibbs Free Energy= 1.590645
Sum of electronic and zero-point Energies= -7220.869313
Sum of electronic and thermal Energies= -7220.750689
Sum of electronic and thermal Enthalpies= -7220.749745
Sum of electronic and thermal Free Energies= -7221.033787

.....

Cartesian Coordinates

.....

26	8.310019	-1.881266	1.008163
15	4.672251	-0.243612	-2.339006
15	4.497913	0.963224	1.230877
6	6.976428	-0.872883	-0.250214
6	6.506934	-0.881995	1.115899
6	6.341480	-2.244389	1.513670

1	6.015386	-2.583150	2.487609
6	6.735937	-3.078443	0.424854
1	6.769344	-4.159226	0.432550
6	7.131387	-2.237843	-0.656168
1	7.504230	-2.569360	-1.613048
6	9.790536	-0.824787	2.010162
1	9.689775	0.195126	2.357369
6	9.435283	-1.998996	2.742638
1	9.012508	-2.025185	3.738124
6	9.692008	-3.132357	1.912157
1	9.493261	-4.165015	2.167207
6	10.205637	-2.659796	0.666110
1	10.467032	-3.270709	-0.187844
6	10.269186	-1.235780	0.727177
1	10.595106	-0.584326	-0.072310
6	7.146473	0.368053	-1.061202
6	8.205606	1.240642	-0.771091
1	8.905621	0.952797	0.003117
6	8.356907	2.460725	-1.429979
1	9.169915	3.126802	-1.158985
6	7.443216	2.827556	-2.415268
1	7.540359	3.778964	-2.928464
6	6.382048	1.975827	-2.724834
1	5.669072	2.278339	-3.483995
6	6.206384	0.755079	-2.054983
6	6.164698	0.351275	1.905135
1	6.888454	1.120566	1.631822
6	6.218055	0.159133	3.423257
1	5.996461	1.093632	3.945798
1	5.507552	-0.596220	3.770329
1	7.222755	-0.168930	3.706807
6	3.783444	0.636374	-3.696024
6	2.775470	1.544709	-3.333549
1	2.538645	1.698393	-2.287606
6	2.049240	2.224618	-4.313711
1	1.277404	2.928173	-4.017678
6	2.311594	1.995108	-5.666004
1	1.739527	2.515526	-6.428955
6	3.310810	1.090637	-6.035322
1	3.519502	0.907261	-7.085610
6	4.046408	0.417527	-5.058150
1	4.817101	-0.282268	-5.362876
6	5.295562	-1.771570	-3.149551
6	6.447557	-1.775813	-3.952818
1	6.999875	-0.855509	-4.117912
6	6.903728	-2.966244	-4.521058
1	7.798266	-2.961037	-5.137407
6	6.215633	-4.162538	-4.292806
1	6.577109	-5.089073	-4.729635
6	5.064235	-4.162957	-3.501841
1	4.524504	-5.088245	-3.320570
6	4.607821	-2.972709	-2.932273
1	3.716237	-2.976729	-2.317504
6	4.772165	2.695198	0.664352
6	3.712462	3.275060	-0.047950
1	2.800731	2.706722	-0.199131
6	3.833383	4.561771	-0.572749
6	5.019091	5.280575	-0.433251
1	5.121381	6.269935	-0.864973
6	6.078834	4.693093	0.258445
6	5.957153	3.422612	0.821613
1	6.801681	3.011921	1.357934
6	3.390004	1.170975	2.685800
6	2.798743	0.004149	3.195874
1	3.042668	-0.957311	2.760489
6	1.877239	0.076560	4.237018
6	1.502799	1.310533	4.773196
1	0.767603	1.368983	5.567312
6	2.078707	2.467308	4.255672
6	3.023455	2.406260	3.227081
1	3.454015	3.326437	2.847702
29	3.460688	-0.328538	-0.419233
6	1.612668	3.818481	4.718776
6	1.177562	-1.169110	4.704683
6	2.644815	5.174667	-1.259499
6	7.380306	5.443196	0.341188
9	7.909859	5.648577	-0.891229
9	8.312275	4.788164	1.067679
9	7.221212	6.666455	0.897133
9	1.977294	4.267401	-2.017327
9	1.744217	5.653887	-0.363544
9	2.983633	6.199993	-2.066543
9	2.633555	4.695104	4.837789
9	0.742548	4.361986	3.822248
9	0.972438	3.769436	5.904332
9	0.908506	-1.136550	6.026875
9	1.889764	-2.287388	4.454673
9	-0.024120	-1.325707	4.075702
6	0.718926	0.640856	0.529845
6	0.346562	-0.700308	0.902347
6	1.154838	-1.879551	0.884989
1	-0.524764	-0.798276	1.529710
77	-4.128176	-0.698639	-1.564754
15	-6.000312	-0.472545	-0.294581
8	-6.266562	0.768025	0.765847
8	-7.377040	-0.370773	-1.226520
7	-6.096522	-1.772172	0.764262
6	-6.732795	2.006253	0.339237
6	-5.837667	3.091454	0.461932
1	-4.860611	2.908684	0.897173
6	-6.222625	4.337959	0.034465
1	-5.546772	5.183390	0.126479
6	-7.497591	4.533606	-0.562432
6	-7.876350	5.800198	-1.084514
1	-7.174788	6.626045	-0.999634
6	-9.096129	5.976378	-1.697728
1	-9.373070	6.946960	-2.098679
6	-9.987249	4.883469	-1.819012
1	-10.939363	5.019855	-2.323715
6	-9.657110	3.646299	-1.309699
1	-10.348101	2.819126	-1.420500
6	-8.413368	3.431288	-0.652674
6	-8.033739	2.149094	-0.118054
6	-8.977793	0.997446	-0.066967
6	-10.242296	1.073989	0.617707
6	-10.633046	2.206756	1.385616
1	-9.957659	3.049598	1.470764
6	-11.848893	2.242529	2.033206
1	-12.119935	3.116796	2.618174
6	-12.744956	1.150161	1.949966
1	-13.702654	1.195724	2.460053
6	-12.390450	0.028399	1.235507
1	-13.060033	-0.825893	1.178339
6	-11.137319	-0.048038	0.568706
6	-10.749599	-1.225077	-0.127117
1	-11.440323	-2.062237	-0.173778
6	-9.508297	-1.315867	-0.706859
1	-9.179975	-2.211973	-1.221878
6	-8.629494	-0.212990	-0.643631
6	-5.178150	-2.874522	0.369801
1	-4.285576	-2.816541	1.003370
6	-5.808252	-4.238493	0.587280
6	-5.034384	-5.283904	1.105706
1	-4.002125	-5.092239	1.391234
6	-5.575487	-6.563110	1.258937
1	-4.963019	-7.364291	1.663517
6	-6.903833	-6.807234	0.903351
1	-7.329169	-7.799062	1.027923
6	-7.686019	-5.765622	0.393530
1	-8.722636	-5.946844	0.122271
6	-7.141458	-4.490990	0.235501
1	-7.751086	-3.677189	-0.144415
6	-4.734566	-2.701960	-1.089205
1	-5.552451	-3.005507	-1.754226
1	-3.899915	-3.381892	-1.281889
6	-6.457380	-1.766159	2.226243
1	-6.567024	-2.830266	2.454172
6	-5.292718	-1.255014	3.074741
6	-4.289206	-2.157172	3.465366
1	-4.407948	-3.214207	3.240640

6	-3.142651	-1.719151	4.133253
1	-2.367038	-2.427763	4.408147
6	-2.993958	-0.367478	4.450277
1	-2.101592	-0.026545	4.965434
6	-4.008377	0.532962	4.113030
1	-3.913725	1.582666	4.378269
6	-5.145777	0.093884	3.431903
1	-5.913177	0.809737	3.166054
6	-7.812082	-1.131875	2.536872
1	-8.590195	-1.594261	1.925618
1	-7.837632	-0.057089	2.365318
1	-8.047602	-1.314503	3.590128
6	-3.071106	-0.309201	0.281815
1	-2.706711	0.715517	0.308272
1	-3.568910	-0.602456	1.201147
6	-2.247479	-1.290167	-0.369180
1	-2.374081	-2.328505	-0.082541
6	-1.053220	-0.962165	-1.050534
1	-0.876940	0.083551	-1.261640
6	-5.211316	-0.867105	-3.515815
1	-6.021075	-1.577002	-3.366744
6	-3.916753	-1.415690	-3.675500
1	-3.835459	-2.502428	-3.660940
6	-2.751164	-0.723836	-4.363665
1	-2.849244	-0.820799	-5.456007
1	-1.842095	-1.264486	-4.085743
6	-2.575545	0.763651	-3.984013
1	-3.119489	1.403375	-4.686054
1	-1.518401	1.029687	-4.089250
6	-3.017325	1.106976	-2.562461
1	-2.223016	1.396828	-1.880642
6	-4.295324	1.532342	-2.213375
1	-4.379585	2.117348	-1.303089
6	-5.475837	1.664601	-3.155345
1	-6.377281	1.759472	-2.545629
1	-5.380729	2.602938	-3.721525
6	-5.644780	0.470959	-4.117268
1	-5.087440	0.647050	-5.042768
1	-6.697952	0.400205	-4.406050
6	-0.271148	-1.883452	-1.859991
6	-0.448113	-3.281391	-1.821276
6	0.690887	-1.348334	-2.740149
6	0.298170	-4.109825	-2.657156
1	-1.172823	-3.719319	-1.143632
6	1.422071	-2.176852	-3.585720
1	0.860076	-0.277090	-2.750699
6	1.227484	-3.561333	-3.547715
1	0.150158	-5.185359	-2.620302
1	2.151563	-1.743986	-4.262245
1	1.803776	-4.209032	-4.201717
6	0.598451	-3.061893	1.452651
6	1.292389	-4.254547	1.449865
1	-0.385457	-3.010030	1.905703
6	2.569052	-4.258809	0.879030
6	3.090242	-3.094181	0.347852
1	4.084413	-3.069458	-0.079786
7	2.407333	-1.932605	0.337549
8	1.617578	0.897065	-0.330441
7	-0.021658	1.683177	1.036179
6	0.140284	3.023632	0.487223
1	-0.830331	3.531058	0.498103
1	0.841043	3.622807	1.081070
1	0.500852	2.972365	-0.537589
6	-0.835325	1.628643	2.248434
1	-1.903707	1.710724	2.021002
1	-0.665476	0.710327	2.803392
1	-0.559655	2.466369	2.895724
1	0.861060	-5.151431	1.881308
35	3.632769	-5.900379	0.823677

C2-P1 *si-re_6*

Number of imaginary frequencies= 1
The smallest frequencies are=-248.5005 10.0000 13.1047cm(-1)
Electronic energy= -7222.6257487
Zero-point correction= 1.754465
(Hartree/Particle)
Thermal correction to Energy= 1.873243
Thermal correction to Enthalpy= 1.874187
Thermal correction to Gibbs Free Energy= 1.591464
Sum of electronic and zero-point Energies= -7220.871284
Sum of electronic and thermal Energies= -7220.752506
Sum of electronic and thermal Enthalpies= -7220.751562
Sum of electronic and thermal Free Energies= -7221.034284
.....
Cartesian Coordinates
.....

26	8.171352	0.400264	-0.958048
15	3.085816	1.016431	-2.164600
15	4.107150	0.913566	1.472824
6	6.163942	0.929946	-1.249987
6	6.376207	0.381543	0.067724
6	6.877733	-0.947986	-0.086649
1	7.152668	-1.617624	0.716925
6	7.012186	-1.214371	-1.482496
1	7.406374	-2.120317	-1.919606
6	6.569918	-0.063265	-2.198315
1	6.565983	0.056778	-3.271434
6	9.487853	1.772900	-0.122959
1	9.211619	2.531625	0.596958
6	9.900238	0.439638	0.181717
1	9.984676	0.010357	1.171166
6	10.139559	-0.241567	-1.050424
1	10.429511	-1.278614	-1.157079
6	9.875125	0.669894	-2.117425
1	9.932438	0.446702	-3.174669
6	9.474562	1.914018	-1.545475
1	9.182024	2.797107	-2.097082
6	5.580578	2.273591	-1.525755
6	6.336946	3.417716	-1.226608
1	7.327854	3.278995	-0.814767
6	5.844621	4.704996	-1.434722
1	6.448499	5.566850	-1.168819
6	4.573318	4.870997	-1.978747
1	4.174318	5.864279	-2.156035
6	3.796291	3.750287	-2.268522
1	2.801785	3.900612	-2.670334
6	4.262421	2.446620	-2.025279
6	5.993165	1.076572	1.345210
1	6.183098	2.142316	1.207734
6	6.767818	0.606401	2.579257
1	6.464181	1.164472	3.469342
1	6.613545	-0.456716	2.781545
1	7.837920	0.766972	2.415564
6	1.517469	1.839410	-2.670439
6	0.728505	2.402337	-1.654965
1	1.010280	2.262250	-0.617739
6	-0.407259	3.145283	-1.972804
1	-0.999438	3.585229	-1.180855
6	-0.792865	3.300697	-3.306472
1	-1.684878	3.870860	-3.549642
6	-0.035736	2.709891	-4.320717
1	-0.336082	2.816969	-5.359216
6	1.121104	1.991270	-4.007411
1	1.713490	1.559432	-4.807137
6	3.576269	0.089231	-3.668282
6	4.329449	0.650123	-4.709874
1	4.678474	1.675969	-4.637139
6	4.640975	-0.113630	-5.836812
1	5.229790	0.324141	-6.637848
6	4.195391	-1.435455	-5.936981
1	4.441366	-2.026124	-6.814722
6	3.433901	-1.995437	-4.907591
1	3.083520	-3.021099	-4.981052
6	3.130215	-1.236219	-3.776723
1	2.555117	-1.671193	-2.965615
6	3.426446	2.612038	1.682206
6	2.029308	2.686222	1.773477
1	1.452539	1.767133	1.772268
6	1.385068	3.922731	1.811706

6	2.111703	5.108299	1.729414
1	1.608471	6.068431	1.737739
6	3.501144	5.031969	1.618546
6	4.160524	3.802259	1.608403
1	5.238168	3.796635	1.518459
6	3.754814	0.084734	3.077701
6	3.974664	-1.301763	3.111190
1	4.375163	-1.806536	2.239554
6	3.653867	-2.039654	4.246913
6	3.073836	-1.423474	5.356711
1	2.802449	-2.002192	6.232183
6	2.838021	-0.051749	5.314677
6	3.185936	0.706819	4.193346
1	2.993390	1.773627	4.196537
29	2.935672	-0.167548	-0.242190
6	2.096885	0.602942	6.446470
6	3.821607	-3.533398	4.250155
6	-0.110929	3.942683	1.954101
6	4.274385	6.314049	1.465368
9	3.977678	6.933805	0.296380
9	5.611065	6.119761	1.483587
9	3.979329	7.194268	2.449877
9	-0.701200	3.035790	1.122548
9	-0.507282	3.611638	3.204838
9	-0.648911	5.145104	1.663801
9	2.433071	1.901235	6.598045
9	0.752320	0.573420	6.225238
9	2.306594	-0.017628	7.625950
9	4.238274	-3.992021	5.449971
9	4.704078	-3.954907	3.320541
9	2.642169	-4.162869	3.987426
6	0.843076	-1.212898	1.716931
6	1.172598	-2.587651	1.405314
6	2.336716	-3.048117	0.702959
1	0.761949	-3.337349	2.066485
77	-3.139462	-1.581887	-1.194792
15	-4.969431	-0.610966	-0.264716
8	-4.979220	0.775639	0.634258
8	-6.064701	-0.233332	-1.451510
7	-5.629202	-1.640161	0.899673
6	-4.890346	2.031346	0.052830
6	-3.733276	2.775026	0.370819
1	-3.008751	2.341172	1.049676
6	-3.554325	4.020548	-0.175329
1	-2.684410	4.613533	0.088907
6	-4.490012	4.531535	-1.114558
6	-4.256254	5.764617	-1.781629
1	-3.358345	6.324684	-1.533463
6	-5.134509	6.232224	-2.733106
1	-4.941875	7.171311	-3.243566
6	-6.285801	5.476005	-3.057426
1	-6.965224	5.833794	-3.825696
6	-6.552362	4.286887	-2.413284
1	-7.434875	3.719203	-2.683341
6	-5.676694	3.779574	-1.412918
6	-5.919948	2.531166	-0.731398
6	-7.212508	1.800430	-0.864513
6	-8.474074	2.440304	-0.587280
6	-8.564881	3.736231	-0.007832
1	-7.656789	4.269613	0.245464
6	-9.786970	4.312121	0.263952
1	-9.826525	5.297745	0.718902
6	-10.989973	3.629375	-0.034376
1	-11.946266	4.097774	0.179525
6	-10.939950	2.366218	-0.579386
1	-11.854792	1.819659	-0.793331
6	-9.695889	1.736462	-0.853888
6	-9.645882	0.403632	-1.342319
1	-10.575626	-0.117594	-1.552326
6	-8.441371	-0.233712	-1.498600
1	-8.375392	-1.264482	-1.830055
6	-7.244230	0.465443	-1.233612
6	-5.122406	-3.030967	0.742061
1	-4.373200	-3.218922	1.520211
6	-6.227649	-4.067346	0.855829
6	-6.005568	-5.264879	1.544582
1	-5.055854	-5.422032	2.051320
6	-6.995519	-6.249665	1.598900
1	-6.810052	-7.171806	2.143118
6	-8.222865	-6.045431	0.964125
1	-8.996461	-6.806648	1.011853
6	-8.450183	-4.853407	0.268527
1	-9.401883	-4.686392	-0.229004
6	-7.457979	-3.874137	0.211612
1	-7.634761	-2.945289	-0.322202
6	-4.424006	-3.198730	-0.622416
1	-5.186161	-3.335963	-1.398683
1	-3.842523	-4.124675	-0.591178
6	-5.948064	-1.126449	2.282981
1	-5.101361	-0.514843	2.611211
6	-7.191498	-0.249358	2.326483
6	-7.112778	1.048046	2.846741
1	-6.142458	1.454416	3.119409
6	-8.262485	1.823384	3.010654
1	-8.182890	2.831964	3.406490
6	-9.509881	1.307397	2.654092
1	-10.404592	1.912072	2.767012
6	-9.595920	0.017916	2.123833
1	-10.560993	-0.384614	1.829149
6	-8.445403	-0.754754	1.961320
1	-8.519538	-1.758229	1.554576
6	-6.104609	-2.247305	3.323402
1	-5.206331	-2.862148	3.415323
1	-6.955020	-2.894860	3.106043
1	-6.280471	-1.769971	4.291898
6	-2.181762	-1.249102	0.720077
1	-1.517403	-0.394114	0.648731
1	-2.833506	-1.215138	1.590779
6	-1.679832	-2.540552	0.340723
1	-2.180655	-3.406355	0.763046
6	-0.434432	-2.777130	-0.296953
1	0.075481	-1.930303	-0.736024
6	-4.022457	-1.671812	-3.240999
1	-5.029824	-2.063254	-3.127690
6	-2.962806	-2.608451	-3.179946
1	-3.229203	-3.656944	-3.048479
6	-1.597978	-2.389820	-3.808486
1	-1.661746	-2.546523	-4.896701
1	-0.936443	-3.170124	-3.427088
6	-0.968387	-1.008286	-3.516506
1	-1.178041	-0.310212	-4.332977
1	0.121301	-1.113356	-3.492165
6	-1.415064	-0.366395	-2.203245
1	-0.639246	-0.240905	-1.453538
6	-2.511444	0.480157	-2.077790
1	-2.491145	1.181892	-1.249710
6	-3.478618	0.839667	-3.188270
1	-4.353825	1.304456	-2.730944
1	-3.014485	1.602514	-3.828422
6	-3.936163	-0.366317	-4.032658
1	-3.264168	-0.509222	-4.884992
1	-4.921706	-0.146129	-4.454367
6	-0.058808	-4.084712	-0.844712
6	-0.556959	-5.301701	-0.341610
6	0.862803	-4.131509	-1.907224
6	-0.159063	-6.515939	-0.898290
1	-1.245260	-5.300789	0.497762
6	1.256397	-5.344707	-2.468369
1	1.264920	-3.200658	-2.291735
6	0.745003	-6.543726	-1.965918
1	-0.552147	-7.445289	-0.496032
1	1.964674	-5.354620	-3.291843
1	1.051270	-7.492413	-2.396928
6	2.695018	-4.417577	0.842188
6	3.730470	-4.963552	0.113460
1	2.137090	-5.037426	1.533418
6	4.422086	-4.119547	-0.760605
6	4.075532	-2.784985	-0.850776
1	4.604556	-2.108988	-1.508905
7	3.062404	-2.251105	-0.137151

8	1.100745	-0.242518	0.936661
7	0.131004	-0.965683	2.858689
6	-0.460183	0.346315	3.096538
1	-1.473536	0.220276	3.492329
1	0.123488	0.916169	3.826576
1	-0.516880	0.904594	2.167675
6	-0.107884	-1.948062	3.912827
1	-1.046612	-2.494707	3.753149
1	0.713674	-2.658506	3.986010
1	-0.172364	-1.419482	4.866890
1	3.989890	-6.011654	0.213961
35	5.857954	-4.829666	-1.885014

C2-P1 *si-re_7*

Number of imaginary frequencies=1
The smallest frequencies are=-267.9727 7.6782 11.0818 cm(-1)
Electronic energy= -7222.6289103
Zero-point correction= 1.754635
(Hartree/Particle)
Thermal correction to Energy= 1.873395
Thermal correction to Enthalpy= 1.874339
Thermal correction to Gibbs Free Energy= 1.590919
Sum of electronic and zero-point Energies= -7220.874275
Sum of electronic and thermal Energies= -7220.755515
Sum of electronic and thermal Enthalpies= -7220.754571
Sum of electronic and thermal Free Energies= -7221.037991

.....

Cartesian Coordinates

.....

26	8.164627	0.057258	-1.065056
15	3.103215	1.071739	-2.100875
15	4.188583	0.684021	1.495427
6	6.189305	0.736413	-1.267302
6	6.395438	0.096480	0.009527
6	6.803895	-1.250638	-0.237111
1	7.046643	-1.986448	0.517012
6	6.886909	-1.440226	-1.649618
1	7.207327	-2.342424	-2.150055
6	6.506085	-0.221142	-2.283619
1	6.484707	-0.035891	-3.347268
6	9.603795	1.270912	-0.185159
1	9.409258	1.994807	0.595273
6	9.926972	-0.107268	0.009603
1	10.010702	-0.613254	0.962148
6	10.076161	-0.711579	-1.275898
1	10.286432	-1.755699	-1.466962
6	9.844918	0.291956	-2.265243
1	9.852705	0.142690	-3.336881
6	9.556076	1.516207	-1.592551
1	9.310740	2.455236	-2.069711
6	5.687471	2.127783	-1.444822
6	6.520940	3.200170	-1.089263
1	7.509097	2.971867	-0.711177
6	6.106729	4.526498	-1.198552
1	6.767927	5.329763	-0.889183
6	4.838039	4.806492	-1.700072
1	4.498189	5.832040	-1.801561
6	3.986762	3.757676	-2.046174
1	2.996266	3.996837	-2.412938
6	4.373487	2.413945	-1.900997
6	6.080420	0.732436	1.335960
1	6.333268	1.791008	1.260490
6	6.845595	0.140099	2.522346
1	6.595096	0.662999	3.449630
1	6.628981	-0.921518	2.667768
1	7.920604	0.242918	2.344627
6	1.588256	2.028907	-2.520716
6	0.854192	2.565279	-1.451744
1	1.135358	2.319372	-0.434517
6	-0.224853	3.414332	-1.691563
1	-0.772275	3.834021	-0.857674
6	-0.609956	3.704561	-3.002644
1	-1.458429	4.357514	-3.186282
6	0.089245	3.140346	-4.072380
1	-0.212843	3.351726	-5.094226
6	1.190974	2.314111	-3.835221
1	1.740995	1.903498	-4.675341
6	3.509487	0.207207	-3.665494
6	4.242699	0.799502	-4.704237
1	4.621911	1.811291	-4.593517
6	4.494589	0.085449	-5.877629
1	5.067255	0.547452	-6.676739
6	4.010711	-1.218413	-6.025923
1	4.211234	-1.771012	-6.939299
6	3.270233	-1.809574	-4.998783
1	2.891297	-2.821777	-5.108627
6	3.024733	-1.099685	-3.822499
1	2.463757	-1.559055	-3.014833
6	3.628067	2.407084	1.823032
6	2.240256	2.573630	1.936669
1	1.598047	1.701166	1.877043
6	1.686858	3.846352	2.075416
6	2.496697	4.980207	2.070209
1	2.064452	5.970660	2.157203
6	3.876055	4.813822	1.934770
6	4.444576	3.544227	1.826131
1	5.518449	3.466908	1.725256
6	3.813247	-0.208535	3.060639
6	3.953177	-1.605412	3.026630
1	4.319934	-2.091735	2.130204
6	3.596890	-2.375974	4.129803
6	3.066368	-1.780576	5.275698
1	2.771185	-2.384507	6.125832
6	2.916692	-0.396811	5.303276
6	3.295856	0.390940	4.212801
1	3.170008	1.465730	4.269138
29	2.914389	-0.222419	-0.250930
6	2.249939	0.256051	6.481960
6	3.672285	-3.875360	4.060073
6	0.197558	3.963067	2.247629
6	4.738377	6.045317	1.864166
9	4.463300	6.776960	0.756422
9	6.057682	5.755554	1.830887
9	4.530439	6.861124	2.923739
9	-0.470335	3.133043	1.394911
9	-0.198654	3.612299	3.492956
9	-0.259078	5.210987	2.013743
9	2.716304	1.503103	6.706278
9	0.908081	0.375665	6.278115
9	2.405996	-0.451977	7.619593
9	4.076246	-4.416492	5.229632
9	4.514138	-4.305467	3.097178
9	2.452208	-4.416622	3.787833
6	0.794431	-1.230090	1.704803
6	1.032434	-2.604850	1.318073
6	2.160810	-3.099280	0.581783
1	0.578073	-3.361320	1.941823
77	-3.150248	-1.209094	-1.279168
15	-4.969673	-0.206197	-0.363083
8	-4.906103	1.091553	0.671777
8	-5.977806	0.396016	-1.542326
7	-5.781249	-1.285238	0.636034
6	-4.737106	2.390790	0.215375
6	-3.534557	3.030063	0.588299
1	-2.825818	2.487869	1.203111
6	-3.295559	4.317217	0.177371
1	-2.390918	4.830795	0.487255
6	-4.215290	4.980298	-0.678977
6	-3.925776	6.268675	-1.204750
1	-2.995146	6.748843	-0.913348
6	-4.793704	6.888768	-2.075136
1	-4.559551	7.869942	-2.477539
6	-5.990066	6.236662	-2.457820
1	-6.662314	6.717237	-3.162781
6	-6.309535	4.995453	-1.950757
1	-7.225643	4.508827	-2.263904
6	-5.445243	4.330559	-1.036623
6	-5.742922	3.027629	-0.496323
6	-7.065426	2.369024	-0.700156

6	-8.303484	3.008170	-0.332868
6	-8.351307	4.234255	0.388649
1	-7.425616	4.710223	0.689592
6	-9.554354	4.816360	0.724215
1	-9.562232	5.747676	1.283257
6	-10.779386	4.210049	0.356587
1	-11.719380	4.683912	0.623714
6	-10.772150	3.013970	-0.324112
1	-11.704305	2.526230	-0.597187
6	-9.549171	2.379077	-0.674232
6	-9.542772	1.120606	-1.334249
1	-10.489076	0.657902	-1.599548
6	-8.358714	0.473582	-1.587626
1	-8.328875	-0.509454	-2.045150
6	-7.139114	1.094955	-1.242775
6	-5.288977	-2.680555	0.489171
1	-4.625244	-2.904366	1.333081
6	-6.406358	-3.709268	0.471281
6	-6.247922	-4.922587	1.148004
1	-5.344924	-5.096874	1.729607
6	-7.245138	-5.900790	1.098804
1	-7.112177	-6.835860	1.636321
6	-8.414162	-5.670503	0.371596
1	-9.197211	-6.423017	0.342538
6	-8.574169	-4.462231	-0.316409
1	-9.485282	-4.271920	-0.877004
6	-7.573663	-3.493785	-0.273904
1	-7.708082	-2.543396	-0.781634
6	-4.481752	-2.823384	-0.818203
1	-5.189316	-2.934270	-1.648145
1	-3.915436	-3.757515	-0.765689
6	-6.412671	-0.852692	1.931326
1	-6.571832	0.218423	1.817575
6	-7.794520	-1.452908	2.161222
6	-8.903473	-0.808050	1.600233
1	-8.755903	0.106445	1.037050
6	-10.190381	-1.325304	1.751519
1	-11.034508	-0.809937	1.300956
6	-10.388724	-2.496572	2.486437
1	-11.387626	-2.907417	2.604529
6	-9.293547	-3.130036	3.079569
1	-9.437447	-4.037735	3.658924
6	-8.008772	-2.606538	2.925138
1	-7.170992	-3.119755	3.383866
6	-5.452989	-1.041281	3.112248
1	-4.539112	-0.465571	2.943836
1	-5.178459	-2.087017	3.273580
1	-5.923841	-0.676867	4.030315
6	-2.211349	-0.949093	0.664911
1	-1.486568	-0.142814	0.610226
1	-2.877946	-0.874836	1.519657
6	-1.803542	-2.266255	0.277710
1	-2.370507	-3.095565	0.687714
6	-0.583919	-2.588666	-0.374943
1	-0.002701	-1.773371	-0.784455
6	-4.003435	-1.173992	-3.334234
1	-5.026108	-1.534114	-3.259055
6	-2.980269	-2.154369	-3.305783
1	-3.288377	-3.196737	-3.231164
6	-1.603539	-1.956038	-3.915390
1	-1.666414	-2.055688	-5.010388
1	-0.973590	-2.778802	-3.572018
6	-0.928652	-0.614885	-3.549963
1	-1.105923	0.131550	-4.330499
1	0.155780	-0.759474	-3.523157
6	-1.364575	-0.027204	-2.208830
1	-0.591475	0.027085	-1.448133
6	-2.424440	0.861223	-2.055503
1	-2.387926	1.519427	-1.193202
6	-3.353834	1.313672	-3.163631
1	-4.210623	1.806001	-2.699853
1	-2.839314	2.074057	-3.767211
6	-3.858263	0.164662	-4.061951
1	-3.188775	0.032729	-4.918127
1	-4.831859	0.444521	-4.475569
6	-0.332417	-3.902849	-0.976818
6	-0.980416	-5.079744	-0.554989
6	0.609486	-3.999896	-2.018315
6	-0.707569	-6.300270	-1.170134
1	-1.695585	-5.045282	0.260748
6	0.878579	-5.218901	-2.637400
1	1.132495	-3.104430	-2.336763
6	0.218407	-6.375738	-2.216531
1	-1.218099	-7.197441	-0.831647
1	1.606273	-5.266146	-3.442538
1	0.425975	-7.328863	-2.694156
6	2.439914	-4.491991	0.654309
6	3.434671	-5.063463	-0.110404
1	1.853719	-5.109753	1.323792
6	4.162758	-4.222890	-0.957634
6	3.892060	-2.868232	-0.985269
1	4.447336	-2.195952	-1.625001
7	2.921474	-2.308020	-0.233194
8	1.106842	-0.239353	0.971772
7	0.110066	-0.996949	2.865573
6	-0.376830	0.341672	3.180703
1	-1.377473	0.267450	3.618817
1	0.277053	0.842017	3.902282
1	-0.435635	0.940033	2.277296
6	-0.169849	-2.010177	3.880411
1	-1.149658	-2.480153	3.723726
1	0.599318	-2.780768	3.897645
1	-0.170951	-1.524820	4.859250
1	3.634474	-6.128068	-0.059188
35	5.540006	-4.964556	-2.134005

C2-P1 *si-si*_1

Number of imaginary frequencies= 1
The smallest frequencies are=-140.2026 11.8716 12.8133cm(-1)
Electronic energy= -7222.6277013
Zero-point correction= 1.756519
(Hartree/Particle)
Thermal correction to Energy= 1.874655
Thermal correction to Enthalpy= 1.875599
Thermal correction to Gibbs Free Energy= 1.595400
Sum of electronic and zero-point Energies= -7220.871182
Sum of electronic and thermal Energies= -7220.753046
Sum of electronic and thermal Enthalpies= -7220.752102
Sum of electronic and thermal Free Energies= -7221.032301

.....

Cartesian Coordinates

.....

26	8.099631	0.502906	-0.733919
15	3.044641	1.442877	-1.834633
15	4.010285	0.578992	1.700866
6	6.108555	1.130246	-0.930538
6	6.291835	0.319628	0.249556
6	6.764823	-0.962213	-0.169932
1	7.011537	-1.790213	0.480553
6	6.912653	-0.941280	-1.589442
1	7.290771	-1.748986	-2.199538
6	6.507640	0.342893	-2.058169
1	6.521958	0.678906	-3.084115
6	9.429658	1.657482	0.368282
1	9.153607	2.271831	1.215259
6	9.805420	0.280150	0.419181
1	9.852366	-0.333334	1.309118
6	10.052640	-0.160105	-0.917000
1	10.320525	-1.165192	-1.215162
6	9.829910	0.944626	-1.794212
1	9.902758	0.924853	-2.873594
6	9.446226	2.067059	-1.001341
1	9.182504	3.045690	-1.378421
6	5.544381	2.510249	-0.919997
6	6.317704	3.556830	-0.392774
1	7.315816	3.326226	-0.043619
6	5.833449	4.860760	-0.300554
1	6.450843	5.639397	0.136117
6	4.552509	5.148798	-0.764247

1	4.157628	6.157674	-0.703396
6	3.762429	4.125028	-1.286357
1	2.763621	4.367699	-1.627764
6	4.222406	2.798519	-1.352913
6	5.898551	0.744085	1.637553
1	6.096490	1.813915	1.722373
6	6.654260	0.023328	2.756709
1	6.344756	0.390415	3.739304
1	6.490697	-1.057415	2.734885
1	7.727456	0.203276	2.640273
6	1.500462	2.380076	-2.201644
6	0.649035	2.673276	-1.122987
1	0.859722	2.257767	-0.143781
6	-0.452305	3.511066	-1.301605
1	-1.079248	3.760330	-0.455022
6	-0.745713	4.024521	-2.567031
1	-1.614118	4.662066	-2.705770
6	0.068756	3.699667	-3.653640
1	-0.161108	4.084907	-4.642918
6	1.194189	2.892090	-3.471680
1	1.835469	2.674854	-4.319271
6	3.601617	0.887524	-3.493175
6	4.335039	1.704784	-4.367093
1	4.614612	2.709845	-4.065349
6	4.716705	1.223413	-5.620834
1	5.288476	1.859412	-6.290604
6	4.366598	-0.072612	-6.013702
1	4.669999	-0.445244	-6.987842
6	3.628713	-0.887390	-5.151384
1	3.357806	-1.896698	-5.448472
6	3.250341	-0.408201	-3.896190
1	2.697034	-1.044997	-3.215360
6	3.339975	2.203247	2.255286
6	1.940415	2.283870	2.305323
1	1.354707	1.398757	2.079805
6	1.306360	3.491186	2.595133
6	2.047976	4.652707	2.800130
1	1.556512	5.598370	2.999695
6	3.440162	4.576562	2.723709
6	4.088766	3.366469	2.473670
1	5.169720	3.359839	2.425814
6	3.625457	-0.569335	3.084647
6	3.816813	-1.935162	2.821856
1	4.227610	-2.250926	1.870237
6	3.443306	-2.893147	3.759604
6	2.843695	-2.516807	4.962913
1	2.527922	-3.265347	5.680834
6	2.644009	-1.162361	5.217284
6	3.042455	-0.188882	4.296615
1	2.874657	0.856888	4.526245
29	2.833047	-0.122771	-0.215867
6	1.886924	-0.750351	6.448369
6	3.575263	-4.356711	3.442463
6	-0.193852	3.500344	2.700452
6	4.228912	5.847659	2.882676
9	3.901053	6.753351	1.927872
9	5.562192	5.646621	2.799495
9	3.984473	6.442877	4.073422
9	-0.773535	2.787610	1.689030
9	-0.620864	2.922770	3.848647
9	-0.713877	4.741289	2.653013
9	2.215039	0.492226	6.862206
9	0.545945	-0.740602	6.212608
9	2.091325	-1.594547	7.481743
9	4.025904	-5.062662	4.502893
9	4.413535	-4.589334	2.410929
9	2.373279	-4.900894	3.103966
6	0.719404	-1.518585	1.531865
6	1.013475	-2.790757	0.929927
6	2.138110	-3.117931	0.109775
1	0.555089	-3.658185	1.383041
77	-2.997266	-0.810485	-1.913630
15	-4.703352	-0.241234	-0.528701
8	-4.722996	1.083782	0.470185
8	-6.081842	0.037773	-1.416609
7	-4.940296	-1.436800	0.627163
6	-4.966311	2.358140	-0.025738
6	-3.884208	3.262344	0.031762
1	-2.959516	2.929436	0.488475
6	-4.030711	4.528382	-0.476454
1	-3.208331	5.236983	-0.432137
6	-5.250638	4.918170	-1.093411
6	-5.386676	6.193641	-1.705364
1	-4.541472	6.876377	-1.671762
6	-6.554929	6.554187	-2.338012
1	-6.646386	7.529396	-2.807147
6	-7.636579	5.643046	-2.389321
1	-8.548571	5.919984	-2.910321
6	-7.543182	4.404913	-1.791151
1	-8.378492	3.717487	-1.850955
6	-6.359146	4.004474	-1.111009
6	-6.224910	2.711464	-0.488284
6	-7.371947	1.767940	-0.360071
6	-8.603783	2.138534	0.289369
6	-8.766778	3.369195	0.985620
1	-7.936351	4.063257	1.038926
6	-9.955084	3.682163	1.609530
1	-10.049254	4.623594	2.143150
6	-11.050988	2.787421	1.569674
1	-11.982537	3.050236	2.062252
6	-10.924355	1.580824	0.919183
1	-11.750941	0.875413	0.893917
6	-9.707572	1.219161	0.278895
6	-9.557136	-0.053567	-0.333997
1	-10.399322	-0.739292	-0.339124
6	-8.349352	-0.433483	-0.862014
1	-8.193034	-1.417173	-1.291772
6	-7.268911	0.473686	-0.846418
6	-4.225476	-2.692818	0.282646
1	-3.308940	-2.739129	0.882269
6	-5.046994	-3.935731	0.567299
6	-4.474810	-5.014748	1.249197
1	-3.452108	-4.937586	1.612225
6	-5.210978	-6.180671	1.481698
1	-4.757407	-7.008496	2.019987
6	-6.528797	-6.275549	1.030161
1	-7.106032	-7.176772	1.216751
6	-7.103984	-5.202665	0.339779
1	-8.132008	-5.267090	-0.005931
6	-6.367161	-4.043099	0.109040
1	-6.822179	-3.196355	-0.396768
6	-3.826968	-2.670626	-1.200279
1	-4.714354	-2.898095	-1.801972
1	-3.120621	-3.482465	-1.381694
6	-5.270899	-1.153588	2.067018
1	-5.365971	-0.071506	2.124093
6	-6.616280	-1.706228	2.533924
6	-7.745545	-0.883763	2.430201
1	-7.644015	0.106144	1.996275
6	-8.997438	-1.313219	2.874492
1	-9.854803	-0.653081	2.778247
6	-9.138177	-2.580798	3.442314
1	-10.109537	-2.921163	3.790846
6	-8.017330	-3.406551	3.565254
1	-8.113564	-4.395201	4.005770
6	-6.768105	-2.970083	3.121714
1	-5.915958	-3.632252	3.220106
6	-4.108029	-1.537515	2.990308
1	-3.186352	-1.060170	2.649953
1	-3.940640	-2.615826	3.044122
1	-4.324345	-1.185313	4.003263
6	-1.691874	-0.340174	-0.242144
1	-1.432081	0.713696	-0.181073
1	-2.026754	-0.749874	0.707945
6	-0.841222	-1.177512	-1.044647
1	-0.119443	-0.712602	-1.704053
6	-0.745448	-2.565619	-0.841083
1	-1.405564	-2.996916	-0.098812
6	-4.284287	-1.029999	-3.728597
1	-5.152810	-1.615975	-3.440678

6	-3.080763	-1.746956	-3.933459
1	-3.123250	-2.828643	-3.805833
6	-1.924113	-1.279006	-4.801788
1	-2.146930	-1.478674	-5.861466
1	-1.058089	-1.897973	-4.550376
6	-1.550385	0.206798	-4.611495
1	-2.095088	0.833063	-5.325179
1	-0.488282	0.339673	-4.842369
6	-1.799397	0.735686	-3.201388
1	-0.909803	0.979396	-2.630993
6	-2.972237	1.355166	-2.788462
1	-2.893729	2.028829	-1.942244
6	-4.211026	1.544309	-3.639340
1	-5.030922	1.836592	-2.979678
1	-4.044398	2.388631	-4.324783
6	-4.624955	0.285439	-4.431384
1	-4.162994	0.290883	-5.423699
1	-5.705596	0.319004	-4.599710
6	-0.173810	-3.510330	-1.790296
6	0.656284	-3.105603	-2.854314
6	-0.462609	-4.881194	-1.650149
6	1.175376	-4.039285	-3.745786
1	0.891582	-2.055993	-2.979149
6	0.049512	-5.815359	-2.550330
1	-1.093992	-5.207301	-0.827296
6	0.871569	-5.398372	-3.600507
1	1.816542	-3.708803	-4.558063
1	-0.189601	-6.868051	-2.430165
1	1.274479	-6.124665	-4.300326
6	2.420515	-4.498944	-0.100087
6	3.437862	-4.906831	-0.934788
1	1.818277	-5.238609	0.413528
6	4.200641	-3.913274	-1.557248
6	3.925911	-2.581908	-1.315999
1	4.510060	-1.796130	-1.775519
7	2.919406	-2.181340	-0.511429
8	1.094954	-0.406769	1.048022
7	-0.079595	-1.492856	2.649830
6	-0.497100	-0.199708	3.184379
1	-1.380115	-0.338937	3.809818
1	0.284317	0.259603	3.798511
1	-0.748171	0.478686	2.371858
6	-0.380071	-2.677791	3.451076
1	-1.269946	-3.208441	3.087249
1	0.462314	-3.370744	3.462618
1	-0.562544	-2.368022	4.481533
1	3.634933	-5.960489	-1.099110
35	5.647883	-4.397114	-2.783950

C2-P1 *si-si_2*

Number of imaginary frequencies= 1
The smallest frequencies are= -129.6160 8.7205 13.0915 cm(-1)
Electronic energy= -7222.6324644
Zero-point correction= 1.754828
(Hartree/Particle)
Thermal correction to Energy= 1.873410
Thermal correction to Enthalpy= 1.874354
Thermal correction to Gibbs Free Energy= 1.592590
Sum of electronic and zero-point Energies= -7220.877637
Sum of electronic and thermal Energies= -7220.759054
Sum of electronic and thermal Enthalpies= -7220.758110
Sum of electronic and thermal Free Energies= -7221.039874

.....

Cartesian Coordinates

.....

26	8.003884	0.535572	-0.858814
15	2.937978	1.172396	-2.105426
15	3.903795	0.834200	1.536135
6	5.990341	1.055570	-1.115717
6	6.207646	0.424178	0.164285
6	6.729960	-0.884036	-0.076144
1	7.012639	-1.601366	0.681961
6	6.868033	-1.058273	-1.486205
1	7.273268	-1.929939	-1.980279
6	6.410555	0.131163	-2.126295
1	6.407000	0.320694	-3.189412
6	9.301505	1.883611	0.045241
1	9.014316	2.596076	0.807030
6	9.738121	0.543180	0.275857
1	9.835801	0.063431	1.240631
6	9.982431	-0.066488	-0.992217
1	10.289436	-1.091115	-1.155872
6	9.695775	0.896166	-2.007358
1	9.749405	0.730018	-3.075208
6	9.276429	2.100586	-1.367441
1	8.961288	3.005036	-1.869516
6	5.392602	2.409621	-1.299377
6	6.133038	3.535734	-0.904894
1	7.122842	3.377603	-0.497125
6	5.628766	4.830266	-1.016776
1	6.222063	5.674828	-0.680939
6	4.358904	5.025020	-1.553889
1	3.949245	6.024768	-1.653941
6	3.597282	3.922186	-1.938830
1	2.604456	4.094603	-2.335960
6	4.077689	2.608923	-1.799990
6	5.792714	1.016011	1.484070
1	5.982371	2.089444	1.442123
6	6.534874	0.445267	2.695455
1	6.206988	0.929418	3.619604
1	6.378547	-0.630959	2.806629
1	7.609050	0.618480	2.575321
6	1.365072	2.011582	-2.575301
6	0.536925	2.457247	-1.531003
1	0.782031	2.203854	-0.505985
6	-0.586191	3.237098	-1.805170
1	-1.204698	3.590112	-0.990586
6	-0.923828	3.543141	-3.125924
1	-1.808147	4.138332	-3.335491
6	-0.132961	3.064154	-4.172022
1	-0.397353	3.284618	-5.202298
6	1.012589	2.310720	-3.899985
1	1.635340	1.973577	-4.722052
6	3.531077	0.436076	-3.679493
6	4.233139	1.176041	-4.643880
1	4.443634	2.227973	-4.475258
6	4.676087	0.558623	-5.814987
1	5.222334	1.136283	-6.555269
6	4.422323	-0.799408	-6.033303
1	4.776701	-1.279187	-6.941104
6	3.715663	-1.538370	-5.081370
1	3.523029	-2.594940	-5.242838
6	3.270672	-0.921838	-3.910657
1	2.735748	-1.497067	-3.163718
6	3.203819	2.503915	1.868294
6	1.803615	2.563877	1.922569
1	1.236121	1.643437	1.834567
6	1.148967	3.790213	2.034958
6	1.868448	4.982594	2.066710
1	1.359310	5.937601	2.131603
6	3.261068	4.922253	1.993418
6	3.929965	3.700657	1.907480
1	5.009467	3.709750	1.846357
6	3.500598	-0.138297	3.045917
6	3.727943	-1.520698	2.955153
1	4.171277	-1.936831	2.057884
6	3.351217	-2.367624	3.993016
6	2.712737	-1.863502	5.127946
1	2.398466	-2.526625	5.925881
6	2.471198	-0.494033	5.208857
6	2.870850	0.370593	4.185711
1	2.670491	1.431362	4.280895
29	2.787146	-0.157307	-0.283882
6	1.683300	0.045881	6.370248
6	3.524724	-3.854641	3.853140
6	-0.350975	3.792693	2.129877
6	4.026799	6.217373	1.965437
9	3.731767	6.942241	0.857875
9	5.364884	6.031817	1.973319

9	3.721010	7.000022	3.026581
9	-0.904732	2.912411	1.246629
9	-0.787016	3.414220	3.353170
9	-0.890283	5.001191	1.864365
9	1.964150	1.341692	6.622708
9	0.343289	-0.019464	6.128446
9	1.901382	-0.651080	7.505473
9	3.955881	-4.422788	5.000799
9	4.400611	-4.182333	2.879996
9	2.347104	-4.464377	3.543201
6	0.664620	-1.343787	1.568122
6	0.978069	-2.683061	1.144427
6	2.105648	-3.099677	0.371651
1	0.534834	-3.488576	1.711411
77	-3.317360	-1.168254	-1.663083
15	-5.086051	-0.635547	-0.337468
8	-5.147113	0.646866	0.712306
8	-6.419381	-0.301632	-1.273951
7	-5.382708	-1.872896	0.752305
6	-5.093938	1.941339	0.214721
6	-3.922670	2.675241	0.499392
1	-3.159375	2.211645	1.111439
6	-3.785654	3.947114	0.002149
1	-2.908545	4.538430	0.245245
6	-4.776295	4.488924	-0.861837
6	-4.587242	5.747256	-1.495177
1	-3.677497	6.302479	-1.281508
6	-5.523396	6.245112	-2.373587
1	-5.363961	7.202964	-2.860036
6	-6.692362	5.498169	-2.654362
1	-7.418264	5.882674	-3.365035
6	-6.917166	4.285461	-2.038989
1	-7.814683	3.723404	-2.270109
6	-5.978207	3.745387	-1.117008
6	-6.173879	2.470571	-0.473392
6	-7.473496	1.741498	-0.517892
6	-8.698688	2.375843	-0.089706
6	-8.729462	3.667583	0.507809
1	-7.801889	4.202847	0.668911
6	-9.917448	4.244813	0.902347
1	-9.907777	5.229148	1.361703
6	-11.146448	3.567782	0.722677
1	-12.075404	4.038667	1.030522
6	-11.153327	2.305331	0.174481
1	-12.085789	1.760980	0.049625
6	-9.944378	1.675074	-0.226600
6	-9.950185	0.349629	-0.738293
1	-10.897882	-0.169173	-0.851531
6	-8.772557	-0.278079	-1.052207
1	-8.745613	-1.302182	-1.409395
6	-7.547319	0.412852	-0.911943
6	-4.478865	-3.038700	0.557839
1	-3.622324	-2.931172	1.237606
6	-5.160225	-4.360363	0.866982
6	-4.476100	-5.342638	1.592556
1	-3.485518	-5.122606	1.984933
6	-5.055328	-6.594462	1.818960
1	-4.512540	-7.347046	2.384400
6	-6.332525	-6.872705	1.327925
1	-6.788050	-7.842221	1.508533
6	-7.025433	-5.894087	0.607089
1	-8.021626	-6.102746	0.226577
6	-6.441547	-4.648921	0.374824
1	-6.979723	-3.884696	-0.180016
6	-3.981609	-3.056180	-0.891394
1	-4.810425	-3.394612	-1.525742
1	-3.196512	-3.808024	-0.987763
6	-6.060014	-1.787530	2.086948
1	-6.349541	-2.821704	2.288694
6	-5.113749	-1.387708	3.220963
6	-4.455675	-2.398789	3.938005
1	-4.621056	-3.437377	3.663518
6	-3.611556	-2.093396	5.008959
1	-3.114552	-2.894256	5.549206
6	-3.412055	-0.764138	5.385051
1	-2.747932	-0.520027	6.209711
6	-4.068312	0.252346	4.684265
1	-3.926018	1.290340	4.972872
6	-4.911577	-0.055932	3.614715
1	-5.416563	0.745449	3.090352
6	-7.366058	-0.993542	2.066698
1	-8.037607	-1.391159	1.302667
1	-7.225258	0.070728	1.879491
1	-7.854067	-1.102915	3.039909
6	-2.037822	-0.563758	-0.021649
1	-1.867714	0.509759	-0.005933
1	-2.339479	-0.958571	0.946514
6	-1.126730	-1.359128	-0.802592
1	-0.457311	-0.854987	-1.487687
6	-0.890079	-2.720814	-0.540829
1	-1.492548	-3.178405	0.236803
6	-4.591862	-1.533278	-3.475866
1	-5.426016	-2.154420	-3.158492
6	-3.355284	-2.194058	-3.655963
1	-3.341393	-3.269562	-3.479783
6	-2.221617	-1.710651	-4.542862
1	-2.429264	-1.974592	-5.591617
1	-1.325087	-2.270066	-4.259048
6	-1.930652	-0.200535	-4.426885
1	-2.514332	0.358239	-5.165215
1	-0.879791	-0.018619	-4.672216
6	-2.200959	0.382924	-3.042853
1	-1.321846	0.684441	-2.485674
6	-3.398029	0.973727	-2.666088
1	-3.358076	1.692032	-1.853403
6	-4.635510	1.051807	-3.535869
1	-5.470006	1.367351	-2.908592
1	-4.490379	1.848247	-4.281124
6	-5.002847	-0.273450	-4.240047
1	-4.558563	-0.307539	-5.240188
1	-6.086551	-0.297592	-4.388558
6	-0.253049	-3.644810	-1.466998
6	0.551407	-3.206516	-2.538373
6	-0.447678	-5.029182	-1.298891
6	1.130084	-4.121159	-3.412241
1	0.726740	-2.146620	-2.678790
6	0.124860	-5.944805	-2.182121
1	-1.056939	-5.381587	-0.470251
6	0.916521	-5.494671	-3.241438
1	1.746636	-3.763923	-4.231749
1	-0.043497	-7.008477	-2.040415
1	1.366449	-6.205583	-3.928277
6	2.375532	-4.497009	0.298019
6	3.405258	-4.991791	-0.472909
1	1.751336	-5.179037	0.862994
6	4.191345	-4.068640	-1.170060
6	3.927343	-2.717489	-1.060531
1	4.529173	-1.983950	-1.579787
7	2.910815	-2.233945	-0.319008
8	1.010437	-0.304098	0.925978
7	-0.123642	-1.187463	2.678109
6	-0.677395	0.121969	3.001396
1	-1.694722	0.002134	3.380036
1	-0.083385	0.630964	3.768277
1	-0.710996	0.735574	2.107646
6	-0.433329	-2.264978	3.611708
1	-1.335066	-2.818175	3.319422
1	0.401586	-2.959623	3.701094
1	-0.610275	-1.829378	4.596273
1	3.594100	-6.058020	-0.533308
35	5.659020	-4.674019	-2.315761

C2-P1 *si-si_*3

Number of imaginary frequencies= 1
The smallest frequencies are=-144.5181 11.5388 11.9627cm(-1)
Electronic energy= -7222.6282241
Zero-point correction= 1.756203
(Hartree/Particle)
Thermal correction to Energy= 1.874354

Thermal correction to Enthalpy= 1.875298
Thermal correction to Gibbs Free Energy= 1.595172
Sum of electronic and zero-point Energies= -7220.872021
Sum of electronic and thermal Energies= -7220.753870
Sum of electronic and thermal Enthalpies= -7220.752926
Sum of electronic and thermal Free Energies= -7221.033052

.....

Cartesian Coordinates

.....

26	8.092456	0.520782	-0.649762
15	3.054031	1.500962	-1.795088
15	3.972654	0.521829	1.730185
6	6.103351	1.153527	-0.851510
6	6.273186	0.306954	0.305064
6	6.751376	-0.961422	-0.148749
1	6.991041	-1.809095	0.478660
6	6.916825	-0.896084	-1.564898
1	7.302180	-1.684618	-2.195259
6	6.516845	0.402161	-1.998324
1	6.542510	0.769819	-3.013192
6	9.407516	1.637457	0.508017
1	9.122472	2.222290	1.372716
6	9.785035	0.259813	0.515243
1	9.823720	-0.384103	1.383864
6	10.048776	-0.133152	-0.832455
1	10.322523	-1.126684	-1.162385
6	9.834717	1.001345	-1.673139
1	9.921046	1.019619	-2.751557
6	9.440038	2.094843	-0.846014
1	9.179285	3.086140	-1.190849
6	5.539586	2.532587	-0.806571
6	6.303127	3.560121	-0.229996
1	7.291265	3.314140	0.136192
6	5.821107	4.862579	-0.110494
1	6.430155	5.625525	0.363981
6	4.552992	5.169464	-0.597232
1	4.160690	6.178038	-0.517938
6	3.771704	4.164137	-1.165873
1	2.782108	4.420370	-1.523842
6	4.228231	2.837973	-1.258847
6	5.861336	0.688781	1.700006
1	6.057034	1.755641	1.820109
6	6.602726	-0.063039	2.808556
1	6.280341	0.276919	3.796807
1	6.440400	-1.142866	2.755692
1	7.677353	0.120181	2.710981
6	1.514434	2.450703	-2.149022
6	0.660769	2.724590	-1.066949
1	0.866836	2.287623	-0.095991
6	-0.434864	3.572894	-1.230695
1	-1.059769	3.811669	-0.379412
6	-0.721782	4.114685	-2.485895
1	-1.585514	4.760875	-2.613119
6	0.093965	3.808168	-3.576963
1	-0.130747	4.215931	-4.558360
6	1.215147	2.991626	-3.408701
1	1.859325	2.790456	-4.258090
6	3.625865	0.991762	-3.463452
6	4.375644	1.828605	-4.304315
1	4.660248	2.821821	-3.969715
6	4.766973	1.382136	-5.568036
1	5.351637	2.033039	-6.211862
6	4.409491	0.102175	-6.004370
1	4.719893	-0.243129	-6.986357
6	3.654931	-0.731601	-5.175293
1	3.377419	-1.728696	-5.505812
6	3.267812	-0.287707	-3.909912
1	2.701009	-0.939560	-3.255387
6	3.293739	2.124502	2.335622
6	1.893619	2.203115	2.374426
1	1.310151	1.325244	2.116467
6	1.256507	3.402180	2.690686
6	1.995129	4.557564	2.937097
1	1.501105	5.497054	3.158632
6	3.388098	4.483941	2.872382
6	4.039455	3.281855	2.592286
1	5.120539	3.276874	2.550506
6	3.571900	-0.683951	3.059237
6	3.764982	-2.037282	2.738932
1	4.182717	-2.311440	1.777460
6	3.384149	-3.034215	3.632092
6	2.776737	-2.709408	4.846470
1	2.457331	-3.487954	5.530123
6	2.575653	-1.367047	5.157617
6	2.980340	-0.355356	4.281981
1	2.810953	0.679788	4.554167
29	2.817728	-0.106381	-0.220078
6	1.813696	-1.006381	6.401870
6	3.518824	-4.482971	3.254496
6	-0.245089	3.408484	2.772806
6	4.174646	5.750804	3.071949
9	3.870882	6.672916	2.124751
9	5.509374	5.549479	3.017106
9	3.902190	6.326470	4.266125
9	-0.807711	2.732192	1.726861
9	-0.691134	2.791286	3.892362
9	-0.764665	4.650522	2.760208
9	2.147653	0.214002	6.873210
9	0.474146	-0.976646	6.159889
9	2.006680	-1.897424	7.397452
9	3.967663	-5.231883	4.285829
9	4.360361	-4.671288	2.216647
9	2.318372	-5.013766	2.890636
6	0.683793	-1.563762	1.447691
6	0.977509	-2.808047	0.791128
6	2.107544	-3.107001	-0.032029
1	0.507316	-3.692094	1.197816
77	-3.030878	-0.701125	-1.967298
15	-4.737343	-0.154320	-0.582609
8	-4.719668	1.136120	0.461512
8	-6.124743	0.177434	-1.438508
7	-5.011786	-1.380061	0.537298
6	-4.965277	2.428488	0.018642
6	-3.875520	3.323078	0.074713
1	-2.940211	2.967223	0.490051
6	-4.029911	4.607904	-0.381679
1	-3.201947	5.310121	-0.337886
6	-5.267138	5.027792	-0.942049
6	-5.415223	6.327424	-1.497689
1	-4.564169	7.003039	-1.467747
6	-6.602953	6.720864	-2.071686
1	-6.703645	7.714981	-2.497233
6	-7.693195	5.819737	-2.119348
1	-8.621770	6.124093	-2.593643
6	-7.587901	4.557629	-1.575849
1	-8.430815	3.879089	-1.631133
6	-6.382708	4.122282	-0.956975
6	-6.234807	2.805150	-0.391802
6	-7.378465	1.857202	-0.261430
6	-8.584490	2.198623	0.447952
6	-8.726234	3.406510	1.187583
1	-7.896282	4.101571	1.234050
6	-9.894653	3.697711	1.857498
1	-9.973512	4.622836	2.421269
6	-10.990045	2.801773	1.825202
1	-11.906212	3.048068	2.353886
6	-10.881895	1.614896	1.136983
1	-11.707499	0.908252	1.118618
6	-9.686183	1.276224	0.446403
6	-9.557631	0.028588	-0.221622
1	-10.399315	-0.658178	-0.224502
6	-8.370992	-0.325052	-0.815281
1	-8.230934	-1.289315	-1.292321
6	-7.292852	0.585175	-0.806650
6	-4.255427	-2.614532	0.208628
1	-3.348959	-2.642446	0.826575
6	-5.032172	-3.897516	0.445661
6	-4.373604	-5.014787	0.970107
1	-3.329465	-4.931693	1.265045
6	-5.049607	-6.226328	1.138438

1	-4.528171	-7.083584	1.555765
6	-6.396353	-6.328608	0.785056
1	-6.929383	-7.264414	0.927589
6	-7.057810	-5.216939	0.251158
1	-8.108406	-5.286786	-0.017092
6	-6.377700	-4.013894	0.073773
1	-6.896449	-3.142117	-0.312938
6	-3.843885	-2.571929	-1.272690
1	-4.731342	-2.799296	-1.875215
1	-3.136524	-3.380278	-1.462449
6	-5.348256	-1.073852	1.971897
1	-5.838514	-0.101747	1.942575
6	-6.369926	-2.036538	2.563240
6	-7.730848	-1.777420	2.358419
1	-8.024018	-0.893722	1.802490
6	-8.709407	-2.642846	2.847716
1	-9.759380	-2.424795	2.671046
6	-8.336916	-3.781652	3.565935
1	-9.093874	-4.462328	3.945695
6	-6.983329	-4.034819	3.801411
1	-6.683867	-4.915180	4.363190
6	-6.008875	-3.163772	3.310892
1	-4.962577	-3.384350	3.491614
6	-4.079348	-0.915832	2.817678
1	-3.462001	-0.114806	2.407121
1	-3.478894	-1.828809	2.853659
1	-4.347260	-0.654565	3.846118
6	-1.714135	-0.267995	-0.295767
1	-1.455470	0.784305	-0.208249
1	-2.041987	-0.702163	0.645459
6	-0.863570	-1.079696	-1.125668
1	-0.146974	-0.592832	-1.775248
6	-0.771644	-2.474580	-0.973675
1	-1.430206	-2.928961	-0.244894
6	-4.331247	-0.898759	-3.780788
1	-5.195855	-1.490554	-3.492754
6	-3.129054	-1.610209	-4.005568
1	-3.166713	-2.693282	-3.889590
6	-1.979532	-1.125907	-4.874029
1	-2.209562	-1.311736	-5.934641
1	-1.109801	-1.745362	-4.637829
6	-1.608935	0.358676	-4.667519
1	-2.163242	0.992099	-5.367237
1	-0.549825	0.497629	-4.908183
6	-1.844079	0.869909	-3.248812
1	-0.949404	1.104704	-2.682198
6	-3.013080	1.481843	-2.816429
1	-2.928329	2.143864	-1.961339
6	-4.262158	1.676835	-3.650611
1	-5.075811	1.956392	-2.977424
1	-4.107128	2.531265	-4.326150
6	-4.680349	0.428186	-4.457607
1	-4.227750	0.450710	-5.453933
1	-5.762534	0.462211	-4.615167
6	-0.202634	-3.387209	-1.955789
6	0.632649	-2.947758	-3.001522
6	-0.498586	-4.761076	-1.868313
6	1.150681	-3.849843	-3.925728
1	0.871746	-1.895294	-3.088539
6	0.011080	-5.663123	-2.802048
1	-1.133660	-5.116002	-1.060534
6	0.839215	-5.211632	-3.833036
1	1.796478	-3.491663	-4.722529
1	-0.234245	-6.718228	-2.722425
1	1.240802	-5.913408	-4.558163
6	2.381366	-4.479342	-0.302506
6	3.406095	-4.856741	-1.142700
1	1.766734	-5.237240	0.168018
6	4.185420	-3.842184	-1.708106
6	3.918765	-2.521217	-1.407888
1	4.516464	-1.720367	-1.821561
7	2.904398	-2.149799	-0.599398
8	1.067157	-0.432660	1.017895
7	-0.125537	-1.585979	2.558748
6	-0.547696	-0.318080	3.147809
1	-1.438415	-0.485719	3.754213
1	0.227304	0.110937	3.791321
1	-0.788515	0.397777	2.365091
6	-0.434143	-2.803526	3.306135
1	-1.330184	-3.309571	2.921736
1	0.401513	-3.504214	3.283248
1	-0.610164	-2.539292	4.350401
1	3.596697	-5.903337	-1.353284
35	5.644478	-4.279987	-2.938442

C2-P1 *si-si_4*

Number of imaginary frequencies= 1
The smallest frequencies are= -85.0501 8.7684 12.6547 cm(-1)
Electronic energy= -7222.6286078
Zero-point correction= 1.755409
(Hartree/Particle)
Thermal correction to Energy= 1.873899
Thermal correction to Enthalpy= 1.874843
Thermal correction to Gibbs Free Energy= 1.593613
Sum of electronic and zero-point Energies= -7220.873199
Sum of electronic and thermal Energies= -7220.754709
Sum of electronic and thermal Enthalpies= -7220.753764
Sum of electronic and thermal Free Energies= -7221.034995

.....

Cartesian Coordinates

.....

26	-7.835704	2.630500	0.942235
15	-4.584026	0.210632	-2.343153
15	-4.518735	-0.774960	1.278003
6	-6.704372	1.355528	-0.269583
6	-6.230632	1.338663	1.093900
6	-5.831146	2.666715	1.436144
1	-5.446908	2.985409	2.395498
6	-6.083841	3.511506	0.313705
1	-5.927799	4.580754	0.276613
6	-6.621451	2.707917	-0.734318
1	-6.936455	3.058807	-1.705457
6	-9.510846	1.869082	1.909937
1	-9.620620	0.844945	2.241378
6	-8.942605	2.938145	2.668127
1	-8.537790	2.862806	3.668540
6	-8.959195	4.113012	1.856347
1	-8.565551	5.082161	2.133200
6	-9.537730	3.770948	0.596320
1	-9.661281	4.435734	-0.248467
6	-9.878570	2.385852	0.628683
1	-10.310918	1.822942	-0.187302
6	-7.112118	0.132592	-1.020443
6	-8.317473	-0.506259	-0.692479
1	-8.940640	-0.058401	0.070759
6	-8.712537	-1.695404	-1.305105
1	-9.639377	-2.176703	-1.009111
6	-7.900637	-2.266217	-2.282212
1	-8.188914	-3.194535	-2.764493
6	-6.695532	-1.651847	-2.622919
1	-6.067636	-2.114582	-3.375748
6	-6.274171	-0.467618	-1.997700
6	-6.085162	0.091122	1.919550
1	-6.910028	-0.570532	1.650449
6	-6.138570	0.325875	3.431427
1	-6.053005	-0.616297	3.979800
1	-5.341740	0.989343	3.777771
1	-7.095489	0.791494	3.686274
6	-3.919774	-0.926969	-3.630842
6	-3.139596	-2.010707	-3.198147
1	-2.922182	-2.127791	-2.142506
6	-2.609040	-2.911984	-4.122694
1	-2.015284	-3.750941	-3.775903
6	-2.833784	-2.727613	-5.489496
1	-2.411547	-3.422726	-6.209803
6	-3.599871	-1.644104	-5.928010
1	-3.775440	-1.493670	-6.989569
6	-4.145989	-0.750843	-5.004140
1	-4.738902	0.085285	-5.359322

6	-4.929514	1.764748	-3.261880
6	-6.085804	1.938413	-4.039508
1	-6.812040	1.135166	-4.120764
6	-6.317020	3.149924	-4.693146
1	-7.216123	3.277840	-5.289296
6	-5.397272	4.197581	-4.577035
1	-5.583494	5.142061	-5.080461
6	-4.240130	4.026784	-3.813390
1	-3.520901	4.835866	-3.720859
6	-4.008922	2.815633	-3.158332
1	-3.112555	2.683600	-2.564817
6	-5.028409	-2.478078	0.792060
6	-4.028594	-3.261167	0.196156
1	-3.029410	-2.850828	0.086485
6	-4.318463	-4.545392	-0.265191
6	-5.610971	-5.059318	-0.180565
1	-5.839025	-6.049232	-0.559226
6	-6.608041	-4.269216	0.391806
6	-6.323863	-2.998881	0.892401
1	-7.128412	-2.427770	1.334976
6	-3.460087	-1.067567	2.756483
6	-2.805824	0.046916	3.303721
1	-2.942720	1.029534	2.864392
6	-1.964430	-0.101548	4.405434
6	-1.707523	-1.361439	4.947387
1	-1.032169	-1.475378	5.786477
6	-2.325439	-2.470932	4.375507
6	-3.210045	-2.329772	3.304357
1	-3.691365	-3.213022	2.901252
29	-3.315129	0.259136	-0.459285
6	-1.987499	-3.857662	4.845237
6	-1.354371	1.124833	5.022988
6	-3.199369	-5.388240	-0.808822
6	-8.010743	-4.810221	0.428779
9	-8.496268	-5.012669	-0.821399
9	-8.871933	-3.981961	1.059046
9	-8.067533	-6.007045	1.058123
9	-2.345686	-4.662827	-1.577053
9	-2.448210	-5.918106	0.189738
9	-3.640591	-6.415435	-1.561559
9	-3.072651	-4.662666	4.870178
9	-1.091511	-4.451351	4.008193
9	-1.438923	-3.869707	6.076795
9	-0.252072	0.837426	5.754444
9	-2.220756	1.756266	5.848219
9	-0.985811	2.030722	4.083637
6	-0.749904	-0.946408	0.607561
6	-0.253737	0.349790	0.976208
6	-0.876572	1.619441	0.813514
1	0.625481	0.376314	1.604438
77	4.180867	-0.260119	-1.753589
15	5.855185	0.321354	-0.341730
8	6.401547	-0.635434	0.889732
8	7.274701	0.588151	-1.171072
7	5.410008	1.685301	0.527965
6	7.305140	-1.670013	0.664967
6	6.818481	-2.980302	0.864055
1	5.791088	-3.107310	1.189124
6	7.648870	-4.051320	0.645782
1	7.290073	-5.064957	0.799849
6	8.979001	-3.850739	0.187476
6	9.823017	-4.953711	-0.114754
1	9.435182	-5.958142	0.033469
6	11.097414	-4.757847	-0.596391
1	11.732432	-5.607665	-0.828810
6	11.576071	-3.442266	-0.804204
1	12.573654	-3.290702	-1.206286
6	10.788411	-2.351076	-0.507762
1	11.170349	-1.352372	-0.682758
6	9.473594	-2.514023	0.012016
6	8.621747	-1.395926	0.327720
6	9.107388	0.012004	0.273368
6	10.237245	0.465646	1.041969
6	10.897901	-0.358101	1.996110
1	10.541712	-1.367475	2.163336
6	11.972379	0.112078	2.719473
1	12.454200	-0.535201	3.446651
6	12.450323	1.430766	2.530136
1	13.303081	1.784591	3.102035
6	11.821022	2.263547	1.633002
1	12.164963	3.284749	1.490874
6	10.699699	1.815935	0.882506
6	10.017760	2.691419	-0.005563
1	10.384581	3.706113	-0.131103
6	8.891687	2.272389	-0.670009
1	8.335501	2.930277	-1.328788
6	8.437551	0.947037	-0.498627
6	4.218096	2.351965	-0.057398
1	3.342704	2.060445	0.535962
6	4.324054	3.866171	-0.010877
6	3.190470	4.629263	0.295759
1	2.259274	4.126887	0.544232
6	3.245906	6.025179	0.280370
1	2.358185	6.604408	0.520487
6	4.442670	6.673941	-0.032050
1	4.490579	7.759164	-0.037639
6	5.581060	5.918368	-0.331257
1	6.517057	6.416898	-0.568522
6	5.521376	4.524381	-0.323360
1	6.407665	3.936410	-0.541789
6	4.014587	1.873464	-1.498009
1	4.765491	2.358507	-2.133778
1	3.042220	2.213240	-1.858397
6	5.635317	2.001231	1.979757
1	5.433488	3.074820	2.030037
6	4.588008	1.323786	2.861364
6	3.397000	2.009880	3.145626
1	3.264467	3.020101	2.765788
6	2.390063	1.423490	3.917603
1	1.478247	1.972157	4.127092
6	2.566753	0.136105	4.428543
1	1.790403	-0.318671	5.034613
6	3.752924	-0.553928	4.162414
1	3.902537	-1.551636	4.566425
6	4.754472	0.033709	3.386719
1	5.667069	-0.515866	3.191051
6	7.074820	1.829354	2.463000
1	7.758190	2.390306	1.822524
1	7.402362	0.791847	2.489002
1	7.145754	2.234407	3.477307
6	3.147713	-0.927215	0.044990
1	3.425085	-1.943337	0.321863
1	3.216513	-0.232782	0.880892
6	2.040015	-0.770183	-0.861761
1	1.652012	-1.637480	-1.382002
6	1.339323	0.440204	-0.978846
1	1.707965	1.270318	-0.392369
6	5.351743	0.137442	-3.618577
1	5.834681	1.102404	-3.488288
6	3.975385	0.166890	-3.943427
1	3.516534	1.149452	-4.052612
6	3.203874	-0.943846	-4.634687
1	3.350065	-0.878428	-5.723959
1	2.140050	-0.756576	-4.458238
6	3.551921	-2.363810	-4.141348
1	4.381150	-2.777600	-4.722786
1	2.696061	-3.021359	-4.324861
6	3.903320	-2.436154	-2.658524
1	3.168030	-2.921599	-2.022737
6	5.191975	-2.349151	-2.149013
1	5.363149	-2.788284	-1.171390
6	6.448324	-2.101525	-2.959124
1	7.244565	-1.830725	-2.261571
1	6.757962	-3.043044	-3.435724
6	6.307119	-0.988213	-4.018854
1	5.980736	-1.410180	-4.974238
1	7.295220	-0.554895	-4.199996
6	0.450573	0.807886	-2.067877
6	-0.095783	-0.128623	-2.968019
6	0.200584	2.178993	-2.288304

6	-0.823855	0.298061	-4.074460
1	0.048632	-1.189738	-2.802006
6	-0.527884	2.602489	-3.397242
1	0.596508	2.909004	-1.589138
6	-1.034789	1.662781	-4.299358
1	-1.235031	-0.433871	-4.760710
1	-0.701608	3.662762	-3.556685
1	-1.607854	1.988241	-5.162156
6	-0.162756	2.769337	1.271717
6	-0.681080	4.038715	1.135546
1	0.803511	2.627636	1.744382
6	-1.940748	4.163067	0.534469
6	-2.612330	3.035264	0.105739
1	-3.591063	3.104995	-0.350453
7	-2.102514	1.793288	0.228018
8	-1.661839	-1.142855	-0.257991
7	-0.128635	-2.042106	1.160630
6	-0.353827	-3.371423	0.613356
1	0.596039	-3.918030	0.588421
1	-1.058251	-3.949205	1.224527
1	-0.745277	-3.296977	-0.398155
6	0.686261	-1.999942	2.369411
1	1.759265	-1.979638	2.147061
1	0.438646	-1.131307	2.976429
1	0.469558	-2.889505	2.966875
1	-0.132424	4.906190	1.486921
35	-2.758559	5.925349	0.285171

C2-P1 *si-si_5*

Number of imaginary frequencies= 1
The smallest frequencies are= -137.3513 7.2662 8.6309 cm(-1)
Electronic energy= -7222.6278115
Zero-point correction= 1.754809
(Hartree/Particle)
Thermal correction to Energy= 1.873359
Thermal correction to Enthalpy= 1.874303
Thermal correction to Gibbs Free Energy= 1.591806
Sum of electronic and zero-point Energies= -7220.873003
Sum of electronic and thermal Energies= -7220.754453
Sum of electronic and thermal Enthalpies= -7220.753509
Sum of electronic and thermal Free Energies= -7221.036005

.....

Cartesian Coordinates

.....

26	8.123816	0.204442	-0.683955
15	3.132810	1.198662	-1.972731
15	4.000928	0.629832	1.659858
6	6.156735	0.873616	-0.966352
6	6.291601	0.146301	0.273613
6	6.735765	-1.174944	-0.041473
1	6.940851	-1.960815	0.672408
6	6.909649	-1.263471	-1.455759
1	7.271915	-2.125593	-1.997291
6	6.552780	-0.006101	-2.024642
1	6.595303	0.253525	-3.071855
6	9.466962	1.393982	0.361338
1	9.192959	2.071497	1.159293
6	9.802185	0.013380	0.513001
1	9.819586	-0.539353	1.442767
6	10.059706	-0.523777	-0.785284
1	10.303390	-1.553912	-1.009533
6	9.883634	0.523902	-1.739685
1	9.973178	0.428006	-2.813733
6	9.519567	1.708256	-1.032429
1	9.289825	2.665246	-1.480752
6	5.636403	2.266411	-1.076911
6	6.429857	3.327957	-0.614881
1	7.410048	3.096796	-0.218372
6	5.987407	4.649693	-0.645587
1	6.618355	5.442517	-0.256671
6	4.728644	4.937369	-1.166654
1	4.365751	5.959468	-1.200870
6	3.917556	3.898767	-1.623591
1	2.935155	4.142773	-2.009012
6	4.336169	2.558577	-1.570047
6	5.896694	0.683226	1.622907
1	6.155978	1.743103	1.643536
6	6.590079	-0.005930	2.801370
1	6.291556	0.445426	3.751619
1	6.357761	-1.073461	2.848293
1	7.674059	0.098261	2.691776
6	1.621021	2.143083	-2.443718
6	0.769851	2.550895	-1.402421
1	0.958775	2.208899	-0.391093
6	-0.304121	3.402474	-1.661729
1	-0.942332	3.724083	-0.849313
6	-0.567222	3.823139	-2.967586
1	-1.412709	4.475377	-3.167053
6	0.246194	3.385331	-4.014498
1	0.038502	3.695760	-5.034483
6	1.341372	2.556771	-3.754943
1	1.981961	2.249277	-4.574726
6	3.732023	0.499314	-3.560843
6	4.464915	1.253884	-4.490384
1	4.701303	2.293063	-4.281400
6	4.905683	0.666850	-5.677663
1	5.474969	1.255919	-6.391067
6	4.620403	-0.675906	-5.946365
1	4.972158	-1.131973	-6.867301
6	3.886058	-1.430036	-5.027974
1	3.668577	-2.475109	-5.228772
6	3.443306	-0.843657	-3.840690
1	2.886366	-1.431735	-3.120347
6	3.415880	2.330178	2.055388
6	2.023206	2.495491	2.067662
1	1.387575	1.629686	1.911685
6	1.460151	3.760108	2.235633
6	2.265560	4.889999	2.361761
1	1.826439	5.875919	2.466776
6	3.651380	4.724869	2.334540
6	4.228110	3.461492	2.199776
1	5.306873	3.386915	2.186304
6	3.510529	-0.363082	3.129093
6	3.637443	-1.755559	3.002582
1	4.068762	-2.180401	2.103742
6	3.176955	-2.599786	4.008644
6	2.557702	-2.081335	5.147177
1	2.181739	-2.741959	5.920170
6	2.419954	-0.700448	5.265042
6	2.900642	0.159323	4.273764
1	2.780079	1.228842	4.399057
29	2.839669	-0.191748	-0.212912
6	1.651498	-0.137346	6.427632
6	3.240867	-4.091124	3.829625
6	-0.037633	3.866968	2.295731
6	4.515686	5.952941	2.424772
9	4.284020	6.798037	1.390016
9	5.835279	5.662441	2.413470
9	4.267249	6.655281	3.554832
9	-0.627740	3.065491	1.360624
9	-0.527579	3.462704	3.490621
9	-0.486137	5.118578	2.075401
9	2.008727	1.132572	6.713329
9	0.315331	-0.115704	6.164066
9	1.809306	-0.870987	7.549838
9	3.569313	-4.723409	4.977460
9	4.135009	-4.459054	2.888356
9	2.035589	-4.596987	3.446103
6	0.597146	-1.310859	1.558994
6	0.840214	-2.647740	1.083441
6	1.978550	-3.108201	0.349186
1	0.324523	-3.444471	1.600192
77	-3.154510	-0.810413	-1.893736
15	-4.874625	-0.232858	-0.533667
8	-4.808645	1.011541	0.566522
8	-6.215701	0.219663	-1.404793
7	-5.231873	-1.484887	0.534976
6	-4.834384	2.332076	0.143947
6	-3.650123	3.074387	0.337131

1	-2.810203	2.588381	0.815615
6	-3.598397	4.385009	-0.066113
1	-2.704424	4.976359	0.111510
6	-4.705298	4.972065	-0.738197
6	-4.629997	6.292293	-1.258589
1	-3.710568	6.853565	-1.113002
6	-5.688789	6.845021	-1.943290
1	-5.617823	7.852751	-2.341933
6	-6.869770	6.090427	-2.140183
1	-7.695009	6.520200	-2.700609
6	-6.982623	4.814012	-1.632311
1	-7.892140	4.248524	-1.798618
6	-5.916363	4.216566	-0.904321
6	-5.999614	2.882091	-0.365447
6	-7.272408	2.106585	-0.332079
6	-8.464171	2.635660	0.284542
6	-8.474041	3.855788	1.017436
1	-7.552102	4.411654	1.137341
6	-9.631994	4.333009	1.592500
1	-9.608174	5.262765	2.153694
6	-10.848791	3.621437	1.467576
1	-11.754661	4.013637	1.920344
6	-10.872265	2.425062	0.787752
1	-11.793853	1.855363	0.701672
6	-9.692385	1.896292	0.197031
6	-9.706340	0.635447	-0.457560
1	-10.642182	0.088971	-0.533008
6	-8.545759	0.096264	-0.953946
1	-8.522835	-0.882238	-1.421599
6	-7.339458	0.824287	-0.857885
6	-4.400367	-2.691751	0.281392
1	-3.515882	-2.649081	0.929544
6	-5.113073	-4.002842	0.558404
6	-4.455682	-5.008262	1.274582
1	-3.465111	-4.815265	1.681826
6	-5.065919	-6.247769	1.488149
1	-4.545851	-7.017068	2.052634
6	-6.345979	-6.489785	0.987844
1	-6.829544	-7.446836	1.162316
6	-7.006713	-5.490350	0.263942
1	-8.006956	-5.669006	-0.120718
6	-6.390460	-4.260799	0.042986
1	-6.911501	-3.476974	-0.498102
6	-3.937165	-2.681535	-1.180723
1	-4.794666	-2.948261	-1.809519
1	-3.197460	-3.471797	-1.318506
6	-5.700346	-1.204214	1.936245
1	-6.162596	-0.218115	1.886488
6	-6.802940	-2.156882	2.388866
6	-8.101863	-1.950034	1.906875
1	-8.291759	-1.115806	1.240055
6	-9.146449	-2.802569	2.262131
1	-10.144962	-2.624941	1.871402
6	-8.907720	-3.877998	3.122068
1	-9.716166	-4.548819	3.399247
6	-7.622496	-4.078556	3.629706
1	-7.425944	-4.908962	4.302166
6	-6.580453	-3.220075	3.271500
1	-5.588310	-3.404061	3.668035
6	-4.517737	-1.101550	2.906447
1	-3.825470	-0.331141	2.559695
1	-3.968153	-2.041920	3.001299
1	-4.875232	-0.824122	3.902667
6	-1.893456	-0.285120	-0.200779
1	-1.666373	0.777359	-0.166937
1	-2.242174	-0.672986	0.754081
6	-1.006502	-1.118792	-0.963638
1	-0.284026	-0.647084	-1.616820
6	-0.870825	-2.499055	-0.722476
1	-1.539057	-2.932239	0.011057
6	-4.420274	-1.061213	-3.710464
1	-5.288135	-1.650420	-3.425474
6	-3.212391	-1.779691	-3.897265
1	-3.256700	-2.859764	-3.758216
6	-2.048120	-1.327633	-4.762364
1	-2.251572	-1.561522	-5.819029
1	-1.179007	-1.928879	-4.477630
6	-1.696782	0.166303	-4.609404
1	-2.253419	0.767157	-5.335253
1	-0.637998	0.312095	-4.845477
6	-1.949544	0.721380	-3.210431
1	-1.060652	0.960597	-2.638791
6	-3.119953	1.354705	-2.815977
1	-3.048752	2.046134	-1.982022
6	-4.351512	1.521064	-3.682056
1	-5.174005	1.839460	-3.038707
1	-4.174833	2.341378	-4.393740
6	-4.766645	0.239797	-4.439011
1	-4.311872	0.221647	-5.434557
1	-5.848390	0.267208	-4.601119
6	-0.262590	-3.443811	-1.647603
6	0.595368	-3.035893	-2.688415
6	-0.544718	-4.816480	-1.510407
6	1.149540	-3.969463	-3.558087
1	0.825271	-1.984745	-2.814551
6	0.000759	-5.750143	-2.391592
1	-1.199533	-5.144507	-0.706889
6	0.852754	-5.330741	-3.416286
1	1.810703	-3.635362	-4.352194
1	-0.234497	-6.804089	-2.274940
1	1.282619	-6.056217	-4.100798
6	2.182287	-4.515468	0.264062
6	3.216321	-5.049725	-0.473927
1	1.507133	-5.174107	0.797206
6	4.072210	-4.156973	-1.126233
6	3.866898	-2.796386	-1.009951
1	4.521441	-2.087579	-1.498400
7	2.845987	-2.273465	-0.300631
8	1.038171	-0.269573	0.983245
7	-0.230440	-1.149008	2.642719
6	-0.668969	0.189251	3.023564
1	-1.672590	0.128868	3.453596
1	-0.002984	0.636568	3.769730
1	-0.704499	0.830184	2.147772
6	-0.617923	-2.233345	3.541005
1	-1.546279	-2.725152	3.219717
1	0.170331	-2.982217	3.620689
1	-0.777032	-1.818596	4.538575
1	3.356666	-6.122895	-0.542105
35	5.555314	-4.822259	-2.217582

C2-P1 *re-si*_1

Number of imaginary frequencies= 1
The smallest frequencies are= -109.7588 7.2168 10.9356 cm(-1)

Electronic energy= -7222.6051215
Zero-point correction= 1.755752
(Hartree/Particle)
Thermal correction to Energy= 1.874136
Thermal correction to Enthalpy= 1.875080
Thermal correction to Gibbs Free Energy= 1.592739
Sum of electronic and zero-point Energies= -7220.849369
Sum of electronic and thermal Energies= -7220.730985
Sum of electronic and thermal Enthalpies= -7220.730041
Sum of electronic and thermal Free Energies= -7221.012382

.....

Cartesian Coordinates

.....

26	3.691301	4.212964	-3.467863
15	2.121518	2.499022	1.191326
15	4.584788	0.388958	-0.705458
6	3.367073	3.634746	-1.481144
6	3.912833	2.548935	-2.253005
6	2.998932	2.275090	-3.317970
1	3.126766	1.518776	-4.080419
6	1.916060	3.197483	-3.227072
1	1.089270	3.277743	-3.917293
6	2.138889	4.033012	-2.096807
1	1.508595	4.845156	-1.762138

6	5.523459	5.055217	-3.977729
1	6.457493	4.845652	-3.473402
6	4.985357	4.327894	-5.083272
1	5.435306	3.468351	-5.560947
6	3.724280	4.906676	-5.421069
1	3.052773	4.558855	-6.195061
6	3.481959	5.991298	-4.524910
1	2.595526	6.611537	-4.500636
6	4.593326	6.085034	-3.635427
1	4.696748	6.796479	-2.827529
6	3.934622	4.187906	-0.224863
6	5.012557	5.082709	-0.277977
1	5.428106	5.324574	-1.247229
6	5.540902	5.659172	0.876399
1	6.379995	6.344842	0.805344
6	4.983826	5.349750	2.114887
1	5.378584	5.792671	3.023195
6	3.935803	4.433146	2.192037
1	3.537945	4.180111	3.167489
6	3.408121	3.826253	1.039772
6	5.149069	1.773783	-1.887819
1	5.795894	2.425603	-1.296124
6	5.951728	1.275861	-3.095079
1	6.847110	0.732711	-2.781709
1	5.361738	0.611666	-3.733218
1	6.261616	2.136248	-3.694328
6	2.134599	2.183430	3.009259
6	3.125346	1.314950	3.497037
1	3.824939	0.860235	2.804463
6	3.227522	1.042407	4.861009
1	3.999772	0.367043	5.215562
6	2.327886	1.630086	5.755666
1	2.397399	1.414733	6.818019
6	1.333027	2.486006	5.278074
1	0.625494	2.936331	5.968366
6	1.235164	2.765221	3.912294
1	0.454370	3.429495	3.556511
6	0.511647	3.320428	0.880364
6	0.279869	4.686940	1.100816
1	1.092873	5.331074	1.423647
6	-0.997907	5.218698	0.909536
1	-1.171233	6.277697	1.079116
6	-2.053920	4.389258	0.516601
1	-3.050951	4.799916	0.382665
6	-1.824617	3.029501	0.292663
1	-2.641207	2.374385	0.008858
6	-0.543782	2.500986	0.453724
1	-0.354294	1.454846	0.237094
6	5.638734	0.511542	0.804963
6	5.674183	-0.605176	1.659946
1	5.170006	-1.524696	1.383298
6	6.360600	-0.546533	2.870513
6	7.008660	0.622157	3.268724
1	7.549616	0.659144	4.207603
6	6.957240	1.734397	2.433225
6	6.272534	1.691689	1.215827
1	6.241696	2.586963	0.607581
6	5.192815	-1.172180	-1.483561
6	4.347900	-1.802958	-2.405281
1	3.375292	-1.379334	-2.628613
6	4.748322	-2.981300	-3.039762
6	5.982942	-3.561750	-2.757118
1	6.286801	-4.479903	-3.244840
6	6.827750	-2.927539	-1.847058
6	6.447776	-1.739372	-1.222676
1	7.139452	-1.263864	-0.536595
29	2.386573	0.560797	0.015571
6	8.152575	-3.541921	-1.483594
6	3.810726	-3.632903	-4.017928
6	6.362061	-1.727584	3.801660
6	7.627760	3.002174	2.891514
9	6.874711	3.657538	3.808392
9	7.858651	3.860325	1.875368
9	8.817889	2.748310	3.482733
9	5.438341	-1.576593	4.786652
9	6.079781	-2.881285	3.163260
9	7.555868	-1.880857	4.416115
9	9.120596	-2.604528	-1.360031
9	8.085729	-4.187913	-0.294416
9	8.571016	-4.439335	-2.400659
9	4.415290	-4.576583	-4.765138
9	3.273578	-2.723776	-4.867132
9	2.762040	-4.237261	-3.394882
6	2.251231	-1.841940	1.826107
6	1.627823	-2.381280	-0.368792
6	2.402396	-3.176413	2.164731
1	2.420424	-1.055900	2.551930
6	1.899107	-3.751884	-0.088906
6	2.266632	-4.158960	1.178933
1	1.791874	-4.482086	-0.881917
6	1.056887	-2.062135	-1.642974
6	0.801814	-0.741872	-2.160172
8	0.853676	0.303247	-1.445392
7	1.887447	-1.441865	0.595102
1	1.091564	-2.880196	-2.340384
77	-4.323843	-1.620371	-1.577345
15	-5.103615	-0.406037	0.183200
8	-4.905920	1.238930	0.305267
8	-6.770405	-0.501013	0.283098
7	-4.387236	-0.930633	1.598785
6	-5.723178	2.114512	-0.405669
6	-5.105680	2.858354	-1.436915
1	-4.046002	2.720590	-1.618133
6	-5.851021	3.732672	-2.188684
1	-5.382059	4.314197	-2.977363
6	-7.248609	3.862077	-1.970682
6	-8.046415	4.701162	-2.795117
1	-7.558488	5.265873	-3.585345
6	-9.407545	4.786873	-2.609122
1	-10.009383	5.426465	-3.248027
6	-10.027489	4.024781	-1.590023
1	-11.104774	4.075483	-1.460756
6	-9.280002	3.214423	-0.763281
1	-9.773817	2.632106	0.005663
6	-7.867873	3.117272	-0.911485
6	-7.059268	2.276822	-0.066441
6	-7.621916	1.579402	1.122767
6	-8.258264	2.287983	2.203143
6	-8.332118	3.708432	2.256667
1	-7.892940	4.294522	1.458559
6	-8.939638	4.350292	3.313966
1	-8.977250	5.435765	3.332301
6	-9.508213	3.611987	4.379188
1	-9.990196	4.132001	5.201813
6	-9.431570	2.237909	4.374531
1	-9.845601	1.657491	5.194875
6	-8.798718	1.544498	3.307139
6	-8.671096	0.129248	3.331440
1	-9.092136	-0.423634	4.166427
6	-8.002044	-0.528860	2.329538
1	-7.870812	-1.605217	2.337366
6	-7.468471	0.208165	1.250608
6	-3.680292	-2.236831	1.420532
1	-2.610406	-2.023343	1.356031
6	-3.884503	-3.201366	2.575560
6	-2.786686	-3.909614	3.079104
1	-1.793266	-3.701559	2.688426
6	-2.953440	-4.856647	4.091352
1	-2.090721	-5.395806	4.473332
6	-4.223315	-5.096670	4.622675
1	-4.354218	-5.825265	5.417851
6	-5.324327	-4.389939	4.129160
1	-6.314264	-4.567269	4.540860
6	-5.155678	-3.453956	3.107558
1	-6.009644	-2.901456	2.726443
6	-4.125419	-2.909243	0.122030
1	-5.099170	-3.382976	0.290624
1	-3.423198	-3.710637	-0.112270
6	-4.229610	-0.303502	2.952666
1	-4.822820	-0.912083	3.642992

6	-2.772308	-0.395097	3.385904
6	-2.430092	-0.917368	4.635858
1	-3.213616	-1.273234	5.299957
6	-1.089596	-1.014971	5.020118
1	-0.835119	-1.424523	5.993886
6	-0.080185	-0.609216	4.146026
1	0.960834	-0.692884	4.437749
6	-0.417995	-0.078519	2.896710
1	0.355617	0.239373	2.208487
6	-1.755430	0.040087	2.529218
1	-2.021629	0.447812	1.560592
6	-4.699882	1.146471	3.114421
1	-5.750712	1.278021	2.864881
1	-4.103358	1.838368	2.518280
1	-4.570614	1.404851	4.170070
6	-2.495434	-0.453080	-1.468490
1	-2.549700	0.431914	-2.100005
1	-2.132109	-0.229970	-0.467750
6	-2.034879	-1.683075	-2.061915
1	-2.009386	-1.782082	-3.139336
6	-1.354864	-2.660253	-1.305160
1	-1.253216	-2.459411	-0.243331
6	-6.278166	-2.638744	-1.998468
1	-6.673293	-2.965136	-1.039799
6	-5.236865	-3.425935	-2.545475
1	-4.932117	-4.304418	-1.977231
6	-4.860211	-3.493190	-4.015623
1	-5.524552	-4.194218	-4.544276
1	-3.854833	-3.922854	-4.070433
6	-4.859799	-2.124840	-4.727560
1	-5.847116	-1.911578	-5.147352
1	-4.173208	-2.167265	-5.579712
6	-4.439496	-0.964565	-3.828672
1	-3.465400	-0.534075	-4.049200
6	-5.320011	-0.159305	-3.114320
1	-4.974583	0.836761	-2.857607
6	-6.821704	-0.346815	-3.040571
1	-7.191495	0.257841	-2.209611
1	-7.281077	0.061114	-3.953052
6	-7.259746	-1.812237	-2.830797
1	-7.416676	-2.305232	-3.795265
1	-8.230732	-1.816155	-2.326389
6	-1.182784	-4.053682	-1.686757
6	-1.248090	-4.496087	-3.025393
6	-0.964581	-5.008042	-0.672645
6	-1.089893	-5.842454	-3.332429
1	-1.409392	-3.777684	-3.821284
6	-0.815249	-6.360418	-0.984056
1	-0.923791	-4.681112	0.361661
6	-0.871984	-6.781041	-2.313597
1	-1.135561	-6.167887	-4.367792
1	-0.652922	-7.081818	-0.188501
1	-0.750014	-7.831795	-2.559793
7	0.399541	-0.608368	-3.471464
6	-0.134486	0.661280	-3.940609
1	0.506462	1.087747	-4.721574
1	-1.132056	0.502612	-4.370783
1	-0.199564	1.358235	-3.110329
6	0.416470	-1.638430	-4.500239
1	0.835908	-2.575640	-4.151558
1	-0.600119	-1.828518	-4.869069
1	1.019676	-1.296209	-5.349659
1	2.434904	-5.208050	1.398410
35	2.781039	-3.671041	4.016972

C2-P1 *re-si_2*

Number of imaginary frequencies= 1
The smallest frequencies are= -157.4297 6.6090 8.1764 cm(-1)
Electronic energy= -7222.6051024
Zero-point correction= 1.753731
(Hartree/Particle)
Thermal correction to Energy= 1.872606
Thermal correction to Enthalpy= 1.873551
Thermal correction to Gibbs Free Energy= 1.588744
Sum of electronic and zero-point Energies= -7220.851372
Sum of electronic and thermal Energies= -7220.732496
Sum of electronic and thermal Enthalpies= -7220.731552
Sum of electronic and thermal Free Energies= -7221.016359

.....

Cartesian Coordinates

.....

77	4.093730	-0.613844	-1.540111
15	5.812917	0.197980	-0.300611
8	6.418242	-0.503008	1.065429
8	7.175259	0.322794	-1.234544
7	5.393970	1.701232	0.353534
6	7.319171	-1.560745	1.010103
6	6.856398	-2.793739	1.520111
1	5.857108	-2.835907	1.940508
6	7.669345	-3.898143	1.473038
1	7.327003	-4.850158	1.868425
6	8.954853	-3.818982	0.873598
6	9.769843	-4.975449	0.737405
1	9.398249	-5.919200	1.127859
6	10.993986	-4.908175	0.111886
1	11.606679	-5.798790	0.007649
6	11.446714	-3.674653	-0.413460
1	12.400137	-3.628663	-0.931835
6	10.688237	-2.531570	-0.281731
1	11.049549	-1.600361	-0.700724
6	9.428676	-2.556476	0.380941
6	8.608337	-1.379181	0.530213
6	9.107494	-0.026574	0.154684
6	10.328916	0.514281	0.693390
6	11.048605	-0.116794	1.745592
1	10.666372	-1.035627	2.173474
6	12.206203	0.435833	2.248405
1	12.729392	-0.060653	3.060634
6	12.713606	1.649479	1.726236
1	13.629530	2.071619	2.129338
6	12.033124	2.297284	0.720284
1	12.398967	3.240913	0.323724
6	10.828069	1.761961	0.189863
6	10.092074	2.464329	-0.801067
1	10.485036	3.400710	-1.186770
6	8.880865	1.988089	-1.236033
1	8.285950	2.518574	-1.971387
6	8.394882	0.763594	-0.731530
6	4.249621	2.289645	-0.391299
1	3.343431	2.162352	0.208563
6	4.416152	3.768372	-0.693198
6	3.291745	4.603656	-0.683370
1	2.323959	4.195062	-0.402653
6	3.403918	5.953212	-1.025049
1	2.523084	6.589620	-1.006464
6	4.646317	6.485102	-1.380179
1	4.737510	7.536304	-1.638443
6	5.771485	5.655199	-1.399446
1	6.741461	6.059720	-1.676109
6	5.655504	4.305319	-1.062863
1	6.527898	3.661157	-1.071528
6	4.044171	1.531334	-1.715046
1	4.819964	1.843488	-2.425490
1	3.093883	1.849029	-2.149290
6	5.502595	1.939746	1.840895
1	5.107434	1.054230	2.349622
6	6.934641	2.141491	2.317449
6	7.463820	1.306325	3.308649
1	6.883813	0.454078	3.652313
6	8.725116	1.553886	3.854012
1	9.123651	0.890845	4.616885
6	9.475768	2.644861	3.412081
1	10.462605	2.833099	3.823618
6	8.960656	3.476316	2.414639
1	9.544632	4.318676	2.055055
6	7.699866	3.226199	1.871128
1	7.302064	3.882521	1.104250
6	4.658974	3.132383	2.319650
1	3.596542	3.009879	2.102175

1	4.999366	4.075949	1.890377
1	4.769112	3.195217	3.406081
6	2.983054	-0.810706	0.312751
1	3.190403	-1.752556	0.819986
1	3.046733	0.047474	0.981244
6	1.921939	-0.809531	-0.666133
1	1.525237	-1.757212	-1.007654
6	1.224996	0.353182	-1.037947
1	1.582650	1.293141	-0.640676
6	5.257813	-0.678653	-3.458012
1	5.777136	0.272373	-3.542776
6	3.876480	-0.666350	-3.757934
1	3.451692	0.285509	-4.076858
6	3.048497	-1.872126	-4.172316
1	3.169409	-2.057419	-5.250771
1	1.996005	-1.609464	-4.023144
6	3.360559	-3.159002	-3.378902
1	4.163444	-3.721545	-3.863978
1	2.479876	-3.809159	-3.399379
6	3.737920	-2.907552	-1.921854
1	2.997699	-3.211435	-1.185806
6	5.037705	-2.755149	-1.457706
1	5.209311	-2.968606	-0.407037
6	6.285291	-2.749431	-2.317658
1	7.105459	-2.357601	-1.712983
1	6.551324	-3.786814	-2.567474
6	6.161070	-1.904400	-3.603862
1	5.795917	-2.520546	-4.431225
1	7.160180	-1.566146	-3.894551
6	0.334107	0.468425	-2.179486
6	-0.271583	-0.645743	-2.797955
6	0.090159	1.750354	-2.713630
6	-1.084807	-0.479104	-3.915605
1	-0.114676	-1.639582	-2.394804
6	-0.699518	1.910218	-3.848997
1	0.536272	2.616781	-2.233356
6	-1.293388	0.796996	-4.450037
1	-1.563848	-1.341317	-4.370289
1	-0.869881	2.901762	-4.255334
1	-1.926010	0.921133	-5.322766
26	-6.495305	4.278278	1.436723
15	-4.933990	0.895355	-2.199234
15	-4.825224	-0.204469	1.417687
6	-6.147213	2.707414	0.097168
6	-5.520753	2.454518	1.373771
6	-4.587516	3.505767	1.618009
1	-3.967612	3.606308	2.498306
6	-4.650391	4.421923	0.527909
1	-4.091282	5.343371	0.438975
6	-5.613539	3.937598	-0.403100
1	-5.904862	4.415861	-1.326347
6	-8.136677	4.189989	2.701655
1	-8.561377	3.276583	3.096266
6	-7.090609	4.956875	3.300879
1	-6.577953	4.722303	4.224213
6	-6.806447	6.062805	2.442991
1	-6.038353	6.808440	2.601281
6	-7.678079	5.982453	1.314500
1	-7.687324	6.655706	0.467569
6	-8.501394	4.828500	1.475202
1	-9.246643	4.483988	0.771587
6	-7.101757	1.778499	-0.575321
6	-8.409863	1.659177	-0.082968
1	-8.696432	2.274447	0.760591
6	-9.326988	0.764659	-0.634173
1	-10.321909	0.677379	-0.209954
6	-8.948434	-0.025985	-1.716381
1	-9.649029	-0.729087	-2.156030
6	-7.651595	0.071214	-2.222688
1	-7.369032	-0.560123	-3.057612
6	-6.709297	0.945447	-1.659404
6	-5.780526	1.235308	2.213274
1	-6.829085	0.977597	2.063482
6	-5.566033	1.437864	3.716048
1	-5.770003	0.517819	4.270962
1	-4.549031	1.757180	3.955338
1	-6.250502	2.215609	4.067583
6	-4.880057	-0.325755	-3.577612
6	-4.954377	-1.689520	-3.243980
1	-5.121720	-1.980890	-2.212375
6	-4.834729	-2.672278	-4.225764
1	-4.910954	-3.718639	-3.949422
6	-4.614691	-2.305121	-5.557278
1	-4.509364	-3.068701	-6.322688
6	-4.533643	-0.953831	-5.898176
1	-4.365058	-0.661079	-6.930792
6	-4.671628	0.032211	-4.916990
1	-4.604740	1.076336	-5.200599
6	-4.679799	2.521090	-3.010341
6	-5.660196	3.100118	-3.832144
1	-6.587658	2.569496	-4.028839
6	-5.453134	4.365076	-4.383270
1	-6.215194	4.810603	-5.016433
6	-4.267777	5.059816	-4.115586
1	-4.111619	6.047754	-4.539945
6	-3.290493	4.484955	-3.299928
1	-2.372958	5.025915	-3.084329
6	-3.494356	3.218922	-2.745707
1	-2.756629	2.781724	-2.081948
6	-6.096789	-1.511704	1.110320
6	-5.695453	-2.624800	0.358185
1	-4.655971	-2.738382	0.078924
6	-6.621667	-3.583609	-0.053495
6	-7.972845	-3.445744	0.253096
1	-8.696146	-4.173550	-0.097302
6	-8.375194	-2.341692	1.003722
6	-7.452552	-1.395182	1.445975
1	-7.817077	-0.562960	2.030855
6	-3.726973	-0.910685	2.714879
6	-2.706059	-0.078756	3.205476
1	-2.634420	0.950853	2.874751
6	-1.761838	-0.575683	4.099046
6	-1.773921	-1.918560	4.480860
1	-1.021142	-2.308118	5.157187
6	-2.765810	-2.750064	3.967782
6	-3.745952	-2.253675	3.104716
1	-4.510865	-2.927373	2.737040
29	-3.567222	0.335787	-0.476213
6	-2.718954	-4.224014	4.261965
6	-0.650365	0.306127	4.592950
6	-6.143012	-4.779246	-0.829779
6	-9.843307	-2.171475	1.288378
9	-10.562306	-2.115390	0.140102
9	-10.110913	-1.042258	1.980148
9	-10.338929	-3.209194	2.000910
9	-5.124893	-4.451429	-1.666146
9	-5.676374	-5.752875	-0.014951
9	-7.120755	-5.324016	-1.582444
9	-3.936973	-4.801960	4.180491
9	-1.918990	-4.871317	3.375097
9	-2.224142	-4.483768	5.491963
9	-0.408272	0.124818	5.908464
9	-0.914351	1.619945	4.405333
9	0.522839	0.047225	3.950971
6	-2.274010	-2.397065	-0.570818
6	-0.961514	-0.847993	0.596274
6	-1.611249	-3.468539	0.002575
1	-3.054636	-2.549171	-1.307836
6	-0.289537	-1.930409	1.239079
6	-0.613125	-3.240077	0.956564
1	0.475463	-1.707063	1.973579
6	-0.447929	0.464226	0.823338
6	-1.054221	1.717707	0.477995
8	-2.152934	1.825854	-0.141923
7	-1.989453	-1.116084	-0.266487
1	0.352283	0.487984	1.545910
7	-0.374299	2.878975	0.793760
6	-1.032730	4.165220	0.591893
1	-1.458957	4.547171	1.530429
1	-0.304748	4.895969	0.224149

1	-1.835067	4.055288	-0.133251
6	0.764168	2.897858	1.708628
1	1.519071	2.165101	1.419249
1	1.229545	3.884209	1.665430
1	0.466186	2.699840	2.744877
1	-0.113725	-4.060079	1.459612
35	-2.074867	-5.299841	-0.501215

C2-P1 *re-si_3*

Number of imaginary frequencies= 1
The smallest frequencies are= -180.2500 9.1061 9.9596 cm(-1)
Electronic energy= -7222.6127823
Zero-point correction= 1.754790
(Hartree/Particle)
Thermal correction to Energy= 1.873573
Thermal correction to Enthalpy= 1.874518
Thermal correction to Gibbs Free Energy= 1.590856
Sum of electronic and zero-point Energies= -7220.857992
Sum of electronic and thermal Energies= -7220.739209
Sum of electronic and thermal Enthalpies= -7220.738265
Sum of electronic and thermal Free Energies= -7221.021926

.....

Cartesian Coordinates

.....

77	-4.080831	2.333505	0.420612
15	-4.859186	0.258181	-0.081606
8	-5.131437	-0.959346	1.010266
8	-6.369988	0.384241	-0.770509
7	-3.796341	-0.531158	-1.113528
6	-6.294699	-1.032248	1.767119
6	-6.136206	-0.864607	3.160440
1	-5.136027	-0.708465	3.550917
6	-7.235369	-0.910703	3.980269
1	-7.124889	-0.792630	5.054443
6	-8.534850	-1.083455	3.432458
6	-9.687246	-1.052655	4.263811
1	-9.548958	-0.920443	5.333737
6	-10.949507	-1.172133	3.728477
1	-11.823909	-1.142923	4.371971
6	-11.106982	-1.316162	2.329636
1	-12.104576	-1.383033	1.905142
6	-10.009200	-1.365898	1.497830
1	-10.155761	-1.464305	0.429200
6	-8.687125	-1.272138	2.016959
6	-7.516476	-1.318630	1.175019
6	-7.611940	-1.613027	-0.283411
6	-8.253370	-2.798023	-0.793461
6	-8.671545	-3.867430	0.046936
1	-8.501100	-3.799356	1.114948
6	-9.269723	-4.992481	-0.477727
1	-9.569317	-5.799641	0.184565
6	-9.491057	-5.111281	-1.870766
1	-9.969397	-6.001349	-2.268732
6	-9.084616	-4.103632	-2.715894
1	-9.232634	-4.187268	-3.789435
6	-8.447994	-2.937223	-2.210050
6	-7.964179	-1.930544	-3.088409
1	-8.119641	-2.043418	-4.157268
6	-7.258305	-0.860470	-2.598894
1	-6.833396	-0.106206	-3.252170
6	-7.073524	-0.729225	-1.206157
6	-2.787039	0.412890	-1.666950
1	-1.874360	0.338596	-1.064897
6	-2.406537	0.113023	-3.102838
6	-1.053921	-0.014998	-3.433492
1	-0.311057	0.054952	-2.644632
6	-0.661315	-0.255644	-4.752711
1	0.392271	-0.364833	-4.993310
6	-1.626728	-0.369615	-5.755158
1	-1.328306	-0.564952	-6.781371
6	-2.982424	-0.238349	-5.431025
1	-3.737341	-0.337580	-6.206212
6	-3.369754	0.004030	-4.114259
1	-4.422997	0.072432	-3.857627
6	-3.330548	1.841986	-1.541444
1	-4.139650	1.978061	-2.269616
1	-2.546987	2.544290	-1.825034
6	-3.447550	-1.988175	-0.987367
1	-4.167863	-2.386152	-0.274923
6	-3.653739	-2.791328	-2.268841
6	-4.923573	-3.326262	-2.520178
1	-5.720682	-3.151744	-1.806330
6	-5.176650	-4.085192	-3.663272
1	-6.172219	-4.486952	-3.830584
6	-4.148257	-4.332644	-4.575552
1	-4.337632	-4.921478	-5.469102
6	-2.870256	-3.828255	-4.322250
1	-2.057866	-4.021484	-5.016414
6	-2.623555	-3.071529	-3.175503
1	-1.625077	-2.690103	-3.005705
6	-2.063290	-2.170515	-0.360994
1	-2.023347	-1.656719	0.601002
1	-1.250993	-1.790967	-0.984767
1	-1.876263	-3.233251	-0.188893
6	-2.482386	1.403334	1.572744
1	-2.787071	1.130937	2.582843
1	-1.971196	0.594842	1.057735
6	-1.971241	2.736943	1.386347
1	-2.101692	3.460639	2.181483
6	-1.166505	3.122359	0.294736
1	-1.015523	2.388193	-0.485251
6	-5.813978	3.370996	-0.569310
1	-5.950909	2.890216	-1.533780
6	-4.742975	4.285437	-0.469210
1	-4.150687	4.453905	-1.368622
6	-4.628348	5.396697	0.559821
1	-5.218556	6.268046	0.236731
1	-3.583981	5.721662	0.572494
6	-5.041544	4.984025	1.989564
1	-6.109407	5.164443	2.144569
1	-4.519261	5.626214	2.706235
6	-4.730821	3.529289	2.332479
1	-3.936686	3.375845	3.058033
6	-5.626411	2.478186	2.174562
1	-5.470236	1.598746	2.792230
6	-7.016029	2.595435	1.579555
1	-7.377497	1.587029	1.369802
1	-7.691924	3.016031	2.338460
6	-7.080868	3.435179	0.284817
1	-7.298836	4.481258	0.521722
1	-7.921404	3.078204	-0.317530
6	-0.925955	4.511467	-0.090470
6	-0.927089	5.573136	0.837712
6	-0.687025	4.806287	-1.446173
6	-0.690540	6.879020	0.420410
1	-1.097456	5.369812	1.890040
6	-0.469807	6.120429	-1.865197
1	-0.680519	3.998221	-2.171059
6	-0.464497	7.159588	-0.933972
1	-0.682658	7.684064	1.149770
1	-0.293906	6.327081	-2.916970
1	-0.283812	8.181234	-1.255277
26	4.515873	-2.243117	4.828356
15	1.952821	-2.722825	0.278429
15	4.496174	0.107281	0.655196
6	3.810208	-2.491199	2.870783
6	4.236290	-1.131445	3.107834
6	3.446047	-0.602796	4.173687
1	3.535954	0.389250	4.594941
6	2.561762	-1.628135	4.622676
1	1.864935	-1.551177	5.445981
6	2.791244	-2.790004	3.830729
1	2.291768	-3.740295	3.941082
6	6.538778	-2.487782	5.235433
1	7.336844	-2.262385	4.540499
6	5.953209	-1.575586	6.165619
1	6.223080	-0.536007	6.294151
6	4.913125	-2.262395	6.862778
1	4.257764	-1.833545	7.609488

6	4.857104	-3.600157	6.366490
1	4.155555	-4.364694	6.673219
6	5.861407	-3.740289	5.363412
1	6.054541	-4.633112	4.784413
6	4.324233	-3.341347	1.756153
6	5.628021	-3.854648	1.836130
1	6.194336	-3.664247	2.738890
6	6.210716	-4.562357	0.785473
1	7.234518	-4.913219	0.868238
6	5.477479	-4.789534	-0.376503
1	5.918018	-5.329018	-1.209319
6	4.175737	-4.297777	-0.478793
1	3.625258	-4.469163	-1.397037
6	3.585150	-3.561760	0.561570
6	5.290142	-0.425471	2.302596
1	6.012922	-1.187861	2.011129
6	6.050820	0.661378	3.069102
1	6.800840	1.142796	2.436030
1	5.392452	1.439611	3.462151
1	6.561349	0.199677	3.918888
6	1.363901	-3.421179	-1.324618
6	1.743627	-2.734713	-2.487912
1	2.329089	-1.829159	-2.398117
6	1.395524	-3.211920	-3.751917
1	1.719523	-2.675125	-4.636752
6	0.638790	-4.379125	-3.866283
1	0.359990	-4.753986	-4.846471
6	0.229788	-5.056647	-2.714650
1	-0.378222	-5.952506	-2.798429
6	0.592844	-4.587325	-1.451053
1	0.263683	-5.128682	-0.571957
6	0.844839	-3.454671	1.544078
6	0.895989	-4.817119	1.881897
1	1.606020	-5.475759	1.390102
6	0.055329	-5.325610	2.872891
1	0.099394	-6.380465	3.128578
6	-0.834613	-4.477219	3.540969
1	-1.484007	-4.874756	4.315894
6	-0.879803	-3.119807	3.215635
1	-1.560401	-2.454808	3.740518
6	-0.042267	-2.607554	2.222199
1	-0.049828	-1.547693	1.991377
6	5.530746	-0.724263	-0.631135
6	4.938330	-0.879034	-1.890899
1	3.966134	-0.443297	-2.068929
6	5.573174	-1.601716	-2.897442
6	6.810999	-2.199794	-2.663864
1	7.292143	-2.794675	-3.433745
6	7.408028	-2.038834	-1.415377
6	6.788092	-1.296555	-0.409276
1	7.291832	-1.197929	0.543276
6	4.890486	1.893108	0.452287
6	4.312634	2.788295	1.367537
1	3.709457	2.417071	2.187108
6	4.485800	4.160896	1.217619
6	5.201840	4.676473	0.135702
1	5.318059	5.746901	0.008885
6	5.756575	3.789207	-0.783082
6	5.614773	2.407510	-0.627489
1	6.062813	1.745395	-1.359624
29	2.233927	-0.457934	0.284737
6	6.428924	4.324876	-2.016491
6	3.804163	5.108078	2.164549
6	4.896875	-1.843855	-4.218214
6	8.713212	-2.740390	-1.153639
9	8.604333	-4.072928	-1.382179
9	9.136578	-2.589275	0.119955
9	9.697981	-2.289475	-1.963401
9	3.751033	-1.134418	-4.351346
9	5.693445	-1.519953	-5.260148
9	4.570921	-3.150918	-4.366949
9	7.375812	3.484391	-2.487714
9	5.532843	4.504751	-3.022045
9	7.015651	5.521857	-1.799890
9	4.563745	6.187868	2.440443
9	3.485686	4.518479	3.338956
9	2.636315	5.584263	1.643083
6	2.094641	1.194154	-2.371828
6	1.678299	2.468190	-0.453986
6	2.518241	2.303983	-3.082375
1	2.051278	0.220712	-2.847186
6	2.129225	3.627181	-1.150110
6	2.563704	3.553240	-2.456850
1	2.145623	4.576592	-0.630150
6	1.163844	2.661611	0.869799
6	0.850279	1.638239	1.829057
8	0.795710	0.405336	1.526305
7	1.714908	1.250183	-1.079884
1	1.335613	3.656612	1.242373
7	0.538778	1.995398	3.117649
6	0.165247	0.972497	4.085502
1	0.698908	1.146061	5.026653
1	-0.912910	1.010473	4.292016
1	0.421000	-0.011590	3.703730
6	0.489482	3.351881	3.648536
1	0.611299	4.105237	2.876854
1	-0.479187	3.518804	4.134379
1	1.276361	3.498522	4.398016
1	2.927644	4.433331	-2.973347
35	3.072554	2.123120	-4.949532

C2-P1 *re-si*_4

Number of imaginary frequencies= 1
The smallest frequencies are= -133.9785 4.3747 7.6585 cm(-1)
Electronic energy= -7222.6089123
Zero-point correction= 1.754200
(Hartree/Particle)
Thermal correction to Energy= 1.873225
Thermal correction to Enthalpy= 1.874170
Thermal correction to Gibbs Free Energy= 1.588051
Sum of electronic and zero-point Energies= -7220.854713
Sum of electronic and thermal Energies= -7220.735687
Sum of electronic and thermal Enthalpies= -7220.734743
Sum of electronic and thermal Free Energies= -7221.020862

.....

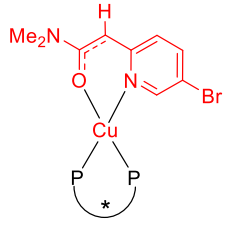
Cartesian Coordinates

.....

77	-4.163394	-0.905691	1.466574
15	-5.888732	-0.077176	0.255889
8	-6.427972	-0.741237	-1.163095
8	-7.297192	-0.051063	1.141311
7	-5.526030	1.472669	-0.289678
6	-7.373590	-1.759853	-1.201906
6	-6.930404	-3.001340	-1.708319
1	-5.902321	-3.086230	-2.044108
6	-7.803080	-4.058401	-1.773576
1	-7.477209	-5.015994	-2.169464
6	-9.135200	-3.923533	-1.298271
6	-10.023451	-5.033099	-1.288988
1	-9.668713	-5.983292	-1.679548
6	-11.298091	-4.914661	-0.783544
1	-11.967334	-5.769982	-0.776304
6	-11.731230	-3.675381	-0.255291
1	-12.728349	-3.589994	0.167011
6	-10.900216	-2.575970	-0.264725
1	-11.249247	-1.640940	0.156110
6	-9.584273	-2.653321	-0.801413
6	-8.686878	-1.524912	-0.823998
6	-9.131060	-0.165153	-0.405705
6	-10.259841	0.499136	-1.003412
6	-10.915591	0.001273	-2.163882
1	-10.555157	-0.910042	-2.626731
6	-11.987146	0.669155	-2.715540
1	-12.464602	0.274149	-3.607647
6	-12.468408	1.868040	-2.136575
1	-13.316937	2.380022	-2.580770
6	-11.849689	2.386489	-1.021775
1	-12.197906	3.314493	-0.575657
6	-10.732372	1.731089	-0.435400

6	-10.060291	2.289718	0.685321
1	-10.435007	3.211361	1.120941
6	-8.922668	1.701285	1.180411
1	-8.369978	2.130370	2.008630
6	-8.456944	0.499467	0.606157
6	-4.345464	2.037661	0.409395
1	-3.475895	1.937405	-0.248412
6	-4.479223	3.501004	0.794688
6	-3.349177	4.325700	0.743645
1	-2.408198	3.923255	0.376287
6	-3.421402	5.659652	1.152933
1	-2.537528	6.289938	1.099395
6	-4.629058	6.182399	1.619946
1	-4.692686	7.222365	1.927488
6	-5.758075	5.358610	1.686749
1	-6.703280	5.759160	2.042741
6	-5.680374	4.026139	1.285875
1	-6.561794	3.395180	1.308350
6	-4.090902	1.230695	1.694764
1	-4.846156	1.521440	2.435655
1	-3.129220	1.533692	2.111887
6	-5.851346	1.915907	-1.689169
1	-6.709416	1.311991	-1.980335
6	-6.320023	3.363303	-1.753660
6	-7.675308	3.635094	-1.531301
1	-8.355308	2.811640	-1.343467
6	-8.157419	4.943962	-1.539939
1	-9.212871	5.130450	-1.360139
6	-7.283810	6.006417	-1.785454
1	-7.651586	7.028748	-1.788952
6	-5.934698	5.744749	-2.038152
1	-5.248907	6.563868	-2.235720
6	-5.459112	4.432178	-2.030150
1	-4.406439	4.249913	-2.217050
6	-4.716799	1.588847	-2.667699
1	-4.525778	0.512819	-2.668453
1	-3.784830	2.105667	-2.426314
1	-5.006847	1.887374	-3.679864
6	-3.037761	-1.080624	-0.376645
1	-3.250356	-2.010803	-0.903345
1	-3.087164	-0.209065	-1.026858
6	-1.984389	-1.105518	0.609651
1	-1.588149	-2.058477	0.936665
6	-1.304706	0.055352	1.014936
1	-1.665432	0.999067	0.627751
6	-5.355750	-1.009332	3.368924
1	-5.874425	-0.059149	3.466968
6	-3.980141	-1.004088	3.690594
1	-3.560276	-0.059059	4.035427
6	-3.157283	-2.218362	4.088608
1	-3.287247	-2.422849	5.162474
1	-2.103019	-1.955203	3.952852
6	-3.466178	-3.489944	3.270072
1	-4.279888	-4.054185	3.734456
1	-2.590283	-4.146401	3.293166
6	-3.819448	-3.212938	1.811765
1	-3.066339	-3.501265	1.083016
6	-5.110879	-3.051851	1.328960
1	-5.266572	-3.239446	0.270670
6	-6.370373	-3.061186	2.171244
1	-7.185337	-2.666713	1.560383
1	-6.633552	-4.103002	2.405119
6	-6.266219	-2.234389	3.472491
1	-5.920150	-2.865608	4.296711
1	-7.269243	-1.896164	3.748739
6	-0.423209	0.153847	2.164323
6	0.190956	-0.969778	2.757292
6	-0.198213	1.423973	2.733367
6	0.990330	-0.824057	3.887410
1	0.051263	-1.953761	2.324037
6	0.578047	1.562088	3.881018
1	-0.649202	2.297584	2.271117
6	1.177606	0.439613	4.458778
1	1.474135	-1.692758	4.324302
1	0.733247	2.544433	4.314785
1	1.798768	0.546885	5.341817
26	6.182655	4.443637	-1.331342
15	4.813475	0.900663	2.229912
15	4.756076	-0.116499	-1.412197
6	5.924551	2.827050	-0.026656
6	5.288438	2.580247	-1.300279
6	4.306299	3.595846	-1.500767
1	3.667186	3.693252	-2.367563
6	4.348928	4.486628	-0.389097
1	3.752940	5.380879	-0.267624
6	5.347345	4.020444	0.513389
1	5.632775	4.486764	1.444599
6	7.804480	4.453376	-2.625421
1	8.258833	3.566263	-3.046045
6	6.716421	5.187950	-3.189295
1	6.197197	4.951456	-4.108485
6	6.401779	6.262154	-2.302183
1	5.601844	6.979220	-2.431923
6	7.296340	6.194415	-1.191038
1	7.293580	6.849928	-0.330173
6	8.164057	5.080245	-1.391604
1	8.937161	4.753802	-0.709786
6	6.926451	1.926641	0.615918
6	8.235968	1.882156	0.115661
1	8.486421	2.528081	-0.716152
6	9.199158	1.022607	0.643357
1	10.194829	0.993768	0.213130
6	8.865845	0.192000	1.710186
1	9.602504	-0.484701	2.132527
6	7.568772	0.215485	2.225078
1	7.323067	-0.445760	3.048463
6	6.581271	1.053817	1.684943
6	5.592384	1.404758	-2.187844
1	6.659145	1.207138	-2.082992
6	5.312956	1.642793	-3.674790
1	5.558061	0.758184	-4.268888
1	4.270127	1.901548	-3.870563
1	5.932302	2.475941	-4.019818
6	4.832566	-0.341420	3.590852
6	4.982076	-1.692853	3.234217
1	5.154299	-1.956329	2.196432
6	4.925585	-2.697515	4.199229
1	5.059960	-3.732836	3.904035
6	4.693236	-2.366047	5.537861
1	4.636775	-3.147090	6.290717
6	4.536101	-1.027543	5.901859
1	4.356510	-0.762363	6.940056
6	4.611110	-0.018733	4.937015
1	4.484713	1.014691	5.238777
6	4.476299	2.496678	3.068280
6	5.423281	3.105152	3.907920
1	6.374780	2.616378	4.098643
6	5.151979	4.346145	4.484839
1	5.888353	4.814377	5.131856
6	3.935081	4.987469	4.225671
1	3.728014	5.956514	4.671261
6	2.991291	4.383776	3.391554
1	2.049578	4.884174	3.182256
6	3.259576	3.141808	2.810831
1	2.547905	2.684885	2.131796
6	6.128990	-1.322825	-1.131467
6	5.826478	-2.456672	-0.364250
1	4.807677	-2.632814	-0.044362
6	6.824244	-3.357184	0.008806
6	8.151655	-3.135562	-0.350068
1	8.932326	-3.815841	-0.027884
6	8.455763	-2.010062	-1.114552
6	7.459706	-1.123004	-1.520511
1	7.750484	-0.272111	-2.120345
6	3.720982	-0.910581	-2.712345
6	2.643019	-0.169266	-3.225360
1	2.493700	0.860122	-2.922970
6	1.740703	-0.755385	-4.108772
6	1.852598	-2.101908	-4.460003
1	1.134019	-2.562042	-5.128793

6	2.903508	-2.843656	-3.928025
6	3.840846	-2.256425	-3.074861
1	4.652923	-2.864304	-2.694553
29	3.478791	0.287427	0.508578
6	2.971086	-4.322740	-4.187502
6	0.566128	0.029074	-4.620566
6	6.457123	-4.587657	0.791600
6	9.898203	-1.746514	-1.454179
9	10.659046	-1.675956	-0.334110
9	10.070351	-0.586200	-2.124887
9	10.424146	-2.733441	-2.215285
9	5.388490	-4.367756	1.598683
9	6.122872	-5.616422	-0.020799
9	7.471253	-5.012830	1.574262
9	4.232457	-4.799503	-4.107389
9	2.235026	-5.010097	-3.275891
9	2.485976	-4.650737	-5.404812
9	0.321670	-0.218033	-5.924952
9	0.740385	1.364091	-4.485193
9	-0.578905	-0.284780	-3.952431
6	2.356620	-2.512084	0.583757
6	0.967546	-1.038396	-0.593572
6	1.741845	-3.619834	0.027717
1	3.149185	-2.620661	1.314884
6	0.345298	-2.159338	-1.221581
6	0.728888	-3.449304	-0.923198
1	-0.431922	-1.980638	-1.955736
6	0.396240	0.245862	-0.838233
6	0.914031	1.530791	-0.468855
8	1.983153	1.704604	0.187551
7	2.009585	-1.249411	0.268601
1	-0.399330	0.226632	-1.565823
7	0.169645	2.648404	-0.800301
6	0.727213	3.975139	-0.561924
1	1.136639	4.408406	-1.485448
1	-0.057007	4.642527	-0.188565
1	1.526033	3.907564	0.172572
6	-0.942249	2.592833	-1.745971
1	-1.674453	1.837856	-1.454604
1	-1.448073	3.559864	-1.745668
1	-0.607981	2.377763	-2.767387
1	0.262844	-4.297558	-1.411398
35	2.293185	-5.420096	0.559052



Cu-enolate

Conformer_1

Number of imaginary frequencies : 0
The smallest frequency is : 10.4515 cm(-1)
Electronic energy=-4521.7087243
Zero-point correction= 0.853656
(Hartree/Particle)
Thermal correction to Energy= 0.923577
Thermal correction to Enthalpy= 0.924522
Thermal correction to Gibbs Free Energy= 0.740626
Sum of electronic and zero-point Energies= -4520.855069
Sum of electronic and thermal Energies= -4520.785147
Sum of electronic and thermal Enthalpies= -4520.784203
Sum of electronic and thermal Free Energies= -4520.968098

.....

Cartesian Coordinates

.....

26	-4.337304	1.278695	-2.024816
15	-1.786114	-1.971117	1.052194
15	0.251350	0.672356	-0.889879
6	-3.167803	-0.194116	-1.108795
6	-2.372501	0.955442	-1.458104
6	-2.912546	2.083650	-0.766055
1	-2.537351	3.096425	-0.824103
6	-4.042255	1.649549	-0.013941
1	-4.688193	2.279447	0.582874
6	-4.203706	0.250009	-0.226239
1	-4.980335	-0.376180	0.189051
6	-4.550142	1.261739	-4.091546
1	-3.802772	0.897337	-4.783889
6	-4.651652	2.596591	-3.592623
1	-3.992820	3.418985	-3.837426
6	-5.749775	2.644358	-2.680257
1	-6.061543	3.507437	-2.106840
6	-6.326926	1.339369	-2.614495
1	-7.154955	1.040437	-1.985255
6	-5.587389	0.485739	-3.486688
1	-5.762549	-0.571185	-3.635466
6	-2.883863	-1.592547	-1.530571
6	-3.119845	-1.987608	-2.855357
1	-3.510050	-1.252277	-3.547971
6	-2.864014	-3.289785	-3.286105
1	-3.046734	-3.563730	-4.321235
6	-2.382688	-4.232260	-2.379737
1	-2.189717	-5.253271	-2.694692
6	-2.121273	-3.854236	-1.062345
1	-1.721320	-4.592575	-0.377511
6	-2.333719	-2.537111	-0.625323
6	-1.083351	0.898866	-2.226859
1	-1.063252	-0.035158	-2.795616
6	-0.867923	2.065095	-3.193680
1	0.076752	1.964174	-3.735435
1	-0.862627	3.028700	-2.677120
1	-1.683778	2.077819	-3.922790
6	-0.843379	-3.401707	1.726084
6	0.320474	-3.805586	1.047409
1	0.580709	-3.345030	0.100249
6	1.132826	-4.812677	1.563101
1	2.018850	-5.120011	1.015147
6	0.810222	-5.414935	2.783242
1	1.447857	-6.193185	3.192915
6	-0.335446	-5.011503	3.471394
1	-0.593307	-5.475810	4.419303
6	-1.163455	-4.015035	2.945448
1	-2.054878	-3.718577	3.489001
6	-3.333697	-1.927589	2.039236
6	-4.354646	-2.876022	1.872939
1	-4.239045	-3.678801	1.150002
6	-5.525737	-2.782087	2.625920
1	-6.315230	-3.516355	2.491287
6	-5.683436	-1.743554	3.550358
1	-6.597963	-1.670774	4.132543
6	-4.667813	-0.799583	3.720602
1	-4.790222	0.012775	4.431816
6	-3.495269	-0.887382	2.966354
1	-2.718604	-0.134072	3.061396
6	1.493787	-0.463231	-1.635063
6	2.876771	-0.262901	-1.507560
1	3.266684	0.652634	-1.079693
6	3.772897	-1.254524	-1.906573
6	3.320487	-2.468460	-2.422507
1	4.021852	-3.238295	-2.720748
6	1.946468	-2.675595	-2.532614
6	1.037572	-1.690235	-2.143145
1	-0.025671	-1.899687	-2.211893
6	1.091662	2.303587	-0.750509
6	0.822027	3.027991	0.416390
1	0.154456	2.607520	1.161594
6	1.401757	4.282574	0.616740
6	2.259565	4.830554	-0.333246
1	2.716910	5.799471	-0.171157
6	2.525355	4.107546	-1.498949
6	1.945706	2.857329	-1.715159
1	2.174176	2.317001	-2.626789
29	-0.472046	-0.133068	1.129753

6	3.397484	4.709921	-2.566184
6	1.126803	4.997862	1.911251
6	5.252940	-0.992287	-1.830461
6	1.414870	-4.001919	-3.003340
9	0.946383	-4.743152	-1.965185
9	0.383740	-3.853420	-3.865993
9	2.356654	-4.744902	-3.621723
9	5.563416	-0.097276	-0.868695
9	5.725208	-0.490331	-2.999325
9	5.954818	-2.121164	-1.583737
9	2.667056	5.410540	-3.468667
9	4.070397	3.764695	-3.261329
9	4.310189	5.564804	-2.054813
9	1.445559	6.309207	1.853760
9	-0.180501	4.913722	2.258324
9	1.829963	4.463751	2.939843
6	2.223036	-1.091574	1.850512
6	1.499044	0.522387	3.410540
6	3.441334	-1.244700	2.477152
1	1.978267	-1.657713	0.961047
6	2.759103	0.375026	4.083010
6	3.724365	-0.493999	3.629368
1	2.948200	0.972155	4.970154
6	0.561392	1.449142	3.935083
6	-0.705054	1.810484	3.418232
8	-1.214484	1.369486	2.324927
7	1.273044	-0.245149	2.291487
1	0.895361	1.947476	4.834380
7	-1.489903	2.718072	4.121031
6	-2.685339	3.241914	3.470501
1	-2.458350	4.079305	2.794178
1	-3.383726	3.594637	4.235028
1	-3.163765	2.456393	2.887593
6	-0.926738	3.525718	5.195529
1	-0.099455	4.159573	4.848988
1	-0.563974	2.898118	6.015756
1	-1.708378	4.172686	5.599084
1	4.673240	-0.591963	4.146680
35	4.759327	-2.498923	1.741425

Conformer_2

Number of imaginary frequencies : 0
The smallest frequency is : 14.9561 cm(-1)
Electronic energy : HF=-4521.7138307
Zero-point correction= 0.854728
(Hartree/Particle)
Thermal correction to Energy= 0.924099
Thermal correction to Enthalpy= 0.925044
Thermal correction to Gibbs Free Energy= 0.744563
Sum of electronic and zero-point Energies= -4520.859102
Sum of electronic and thermal Energies= -4520.789731
Sum of electronic and thermal Enthalpies= -4520.788787
Sum of electronic and thermal Free Energies= -4520.969268

.....

Cartesian Coordinates

.....

26	-3.560983	-1.209726	-2.713418
15	-1.139370	-1.582697	1.924464
15	0.658137	0.064658	-0.920207
6	-2.336719	-1.538462	-1.043363
6	-1.845501	-0.443897	-1.848875
6	-2.865995	0.553835	-1.901284
1	-2.806982	1.490563	-2.437989
6	-3.994239	0.078799	-1.168492
1	-4.939469	0.591455	-1.056699
6	-3.670889	-1.206242	-0.642642
1	-4.326663	-1.835584	-0.060865
6	-3.126653	-2.158465	-4.509579
1	-2.129468	-2.416451	-4.841425
6	-3.796518	-0.919936	-4.750861
1	-3.393865	-0.073814	-5.291615
6	-5.072241	-0.975225	-4.110545
1	-5.800997	-0.176068	-4.076766
6	-5.191383	-2.247564	-3.472426
1	-6.027690	-2.582909	-2.873282
6	-3.991318	-2.978934	-3.719755
1	-3.765473	-3.967537	-3.343618
6	-1.515668	-2.727922	-0.670425
6	-1.179305	-3.658437	-1.666308
1	-1.585098	-3.511774	-2.659305
6	-0.325071	-4.731880	-1.416790
1	-0.058429	-5.412442	-2.219397
6	0.201559	-4.905477	-0.139218
1	0.878502	-5.727653	0.070538
6	-0.122785	-3.998673	0.869748
1	0.310192	-4.137644	1.853735
6	-0.963695	-2.899229	0.628994
6	-0.450042	-0.353189	-2.404243
1	-0.157359	-1.357671	-2.715801
6	-0.310501	0.586261	-3.604537
1	0.712451	0.577659	-3.991369
1	-0.563519	1.619458	-3.351433
1	-0.986563	0.259000	-4.400757
6	-0.242516	-2.256977	3.387172
6	1.022189	-1.724104	3.681001
1	1.421240	-0.917235	3.075155
6	1.755779	-2.210033	4.766574
1	2.735982	-1.794833	4.979297
6	1.230253	-3.221257	5.572191
1	1.799412	-3.594940	6.418951
6	-0.034557	-3.748522	5.292267
1	-0.450240	-4.531847	5.920113
6	-0.767998	-3.270725	4.206357
1	-1.749168	-3.687102	4.001048
6	-2.896428	-1.664477	2.456124
6	-3.686254	-2.816427	2.317966
1	-3.268184	-3.711035	1.865550
6	-5.017966	-2.809421	2.737061
1	-5.624150	-3.703671	2.621597
6	-5.570573	-1.654974	3.300611
1	-6.608848	-1.649350	3.620033
6	-4.785057	-0.509581	3.453739
1	-5.208410	0.389181	3.893219
6	-3.453606	-0.513920	3.033226
1	-2.845655	0.379721	3.142619
6	1.960028	-1.235860	-0.854886
6	2.137127	-2.258344	-1.793188
1	1.532515	-2.306841	-2.689513
6	3.096961	-3.248465	-1.576711
6	3.920192	-3.219738	-0.450932
1	4.669910	-3.987225	-0.294917
6	3.753599	-2.189474	0.473508
6	2.771515	-1.216852	0.289947
1	2.617062	-0.436620	1.030692
6	1.592959	1.591393	-1.344512
6	0.878285	2.797897	-1.271193
1	-0.182111	2.786530	-1.047400
6	1.535509	4.014662	-1.421851
6	2.918599	4.061524	-1.607171
1	3.433543	5.012861	-1.678112
6	3.630013	2.865497	-1.650568
6	2.975804	1.635464	-1.543388
1	3.559328	0.723171	-1.573759
29	-0.307080	0.377506	1.179366
6	5.125655	2.895790	-1.798332
6	0.788620	5.307640	-1.251390
6	3.221859	-4.404855	-2.529279
6	4.670379	-2.075120	1.659522
9	5.647676	-1.158219	1.443341
9	4.010848	-1.671498	2.773225
9	5.282319	-3.241124	1.955215
9	2.706966	-5.544873	-2.000344
9	4.513782	-4.673949	-2.827291
9	2.573694	-4.187859	-3.694993
9	5.516187	2.907034	-3.094458
9	5.708809	1.816453	-1.223845
9	5.664790	3.995576	-1.218779
9	1.111971	6.203309	-2.213821
9	-0.550224	5.141797	-1.283475

9	1.086532	5.900366	-0.065211
6	1.812729	2.347376	2.029694
6	0.859350	3.399281	2.098343
6	-0.526318	3.352928	1.830206
1	1.231606	4.390094	2.319710
7	3.154777	2.677467	1.979169
6	4.177772	1.654659	2.131158
1	4.985496	2.034226	2.768283
1	3.756744	0.767980	2.598798
1	4.615408	1.371063	1.164674
6	3.653261	4.028395	1.771103
1	2.933955	4.629684	1.216311
1	3.886188	4.537484	2.718064
1	4.569549	3.982096	1.173972
8	1.523249	1.097910	2.021357
6	-1.276608	4.576678	1.923648
6	-2.615428	4.631531	1.623192
1	-0.756039	5.480563	2.224070
6	-3.246258	3.440890	1.221095
6	-2.515910	2.276381	1.140608
1	-2.977028	1.344699	0.838207
7	-1.198270	2.216520	1.428568
1	-3.164230	5.565194	1.691658
35	-5.162335	3.423250	0.780462

Conformer_3

Number of imaginary frequencies : 0
The smallest frequency is : 6.7926 cm(-1)
Electronic energy : HF=-4521.7141035
Zero-point correction= 0.854617
(Hartree/Particle)
Thermal correction to Energy= 0.924059
Thermal correction to Enthalpy= 0.925003
Thermal correction to Gibbs Free Energy= 0.743694
Sum of electronic and zero-point Energies= -4520.859486
Sum of electronic and thermal Energies= -4520.790045
Sum of electronic and thermal Enthalpies= -4520.789101
Sum of electronic and thermal Free Energies= -4520.970410

.....

Cartesian Coordinates

.....

26	-3.417808	-1.167275	-2.827133
15	-1.016607	-1.727843	1.778315
15	0.692692	0.242161	-0.871092
6	-2.190875	-1.556902	-1.174311
6	-1.759094	-0.371412	-1.879982
6	-2.839039	0.563333	-1.862890
1	-2.833751	1.543976	-2.318600
6	-3.941847	-0.037883	-1.186967
1	-4.917596	0.406059	-1.046043
6	-3.545775	-1.340339	-0.764921
1	-4.166088	-2.054541	-0.245542
6	-2.915636	-1.946039	-4.686635
1	-1.904436	-2.126435	-5.026897
6	-3.648434	-0.728938	-4.838605
1	-3.285372	0.177639	-5.304210
6	-4.925334	-0.902048	-4.222345
1	-5.695750	-0.147325	-4.134599
6	-4.982810	-2.226138	-3.689664
1	-5.806560	-2.653674	-3.133368
6	-3.743253	-2.871514	-3.977491
1	-3.470192	-3.875030	-3.680542
6	-1.293428	-2.713496	-0.885331
6	-0.903933	-3.549066	-1.943453
1	-1.341651	-3.373701	-2.918026
6	0.043064	-4.558615	-1.776391
1	0.344231	-5.167088	-2.623349
6	0.622506	-4.753078	-0.524927
1	1.382571	-5.515072	-0.382436
6	0.243351	-3.943647	0.546090
1	0.731004	-4.086544	1.502902
6	-0.708914	-2.922415	0.393973
6	-0.365140	-0.148115	-2.403289
1	0.005019	-1.106786	-2.771936
6	-0.275754	0.878006	-3.535568
1	0.750437	0.970208	-3.902212
1	-0.607005	1.870887	-3.219482
1	-0.914548	0.559781	-4.365446
6	-0.095508	-2.410930	3.223351
6	0.942963	-1.641012	3.768407
1	1.186218	-0.674754	3.336414
6	1.660608	-2.109479	4.872855
1	2.469785	-1.509197	5.278489
6	1.346935	-3.343125	5.442320
1	1.906741	-3.707272	6.299410
6	0.305223	-4.111360	4.910354
1	0.052785	-5.070099	5.354997
6	-0.415521	-3.647462	3.811135
1	-1.226382	-4.248432	3.410756
6	-2.764268	-2.021164	2.271571
6	-3.436515	-3.231305	2.043178
1	-2.931438	-4.046223	1.533151
6	-4.764854	-3.382675	2.445293
1	-5.280609	-4.320841	2.259662
6	-5.430968	-2.330095	3.081160
1	-6.466598	-2.448260	3.387203
6	-4.762267	-1.127165	3.323046
1	-5.273846	-0.306979	3.818924
6	-3.434579	-0.973293	2.919399
1	-2.915687	-0.035628	3.098566
6	2.015545	-1.041748	-0.841237
6	2.397543	-1.823030	-1.937716
1	1.982225	-1.647568	-2.922643
6	3.317133	-2.860228	-1.771753
6	3.881994	-3.125561	-0.525507
1	4.584053	-3.942746	-0.400861
6	3.520214	-2.329175	0.560119
6	2.592822	-1.299173	0.411867
1	2.304843	-0.690713	1.262990
6	1.602366	1.801157	-1.207407
6	0.859592	2.990159	-1.130108
1	-0.208783	2.951357	-0.950631
6	1.496111	4.223212	-1.227995
6	2.883811	4.301275	-1.358739
1	3.381568	5.263892	-1.389593
6	3.622579	3.121430	-1.399105
6	2.991614	1.875931	-1.344197
1	3.592682	0.974247	-1.367850
29	-0.381384	0.354409	1.186763
6	5.121071	3.192235	-1.486222
6	0.716164	5.494773	-1.047519
6	3.641131	-3.780424	-2.914989
6	4.028156	-2.683881	1.929483
9	5.280450	-3.193080	1.892916
9	4.048578	-1.621368	2.766257
9	3.242990	-3.626967	2.510465
9	3.050485	-4.993268	-2.751274
9	4.969633	-4.014284	-3.015665
9	3.223039	-3.297432	-4.104691
9	5.559735	3.280102	-2.764049
9	5.709602	2.098800	-0.944831
9	5.609757	4.273163	-0.831483
9	1.083180	6.440315	-1.943538
9	-0.614684	5.309835	-1.173108
9	0.925152	6.034189	0.183061
6	1.624693	2.370404	2.177221
6	0.634255	3.389161	2.212260
6	-0.746083	3.284577	1.929025
1	0.964365	4.397979	2.416401
7	2.957400	2.742567	2.159545
6	4.010090	1.754407	2.329371
1	4.687853	2.058086	3.138380
1	3.577898	0.789262	2.578118
1	4.604201	1.651054	1.411101
6	3.416487	4.118818	2.056569
1	2.721822	4.722549	1.473609
1	3.554675	4.588142	3.042049
1	4.378189	4.133027	1.534135
8	1.373067	1.113961	2.158722

6	-1.543252	4.480214	1.993884
6	-2.886115	4.474289	1.704402
1	-1.056752	5.411456	2.266563
6	-3.472207	3.249772	1.338992
6	-2.693642	2.116065	1.268103
1	-3.118271	1.162218	0.981142
7	-1.371577	2.116648	1.540747
1	-3.471440	5.386784	1.754392
35	-5.390942	3.140939	0.924243

Conformer_4

Number of imaginary frequencies : 0
The smallest frequency is : 6.6983 cm(-1)
Electronic energy : HF=-4521.7141039
Zero-point correction= 0.854618
(Hartree/Particle)
Thermal correction to Energy= 0.924059
Thermal correction to Enthalpy= 0.925003
Thermal correction to Gibbs Free Energy= 0.743682
Sum of electronic and zero-point Energies= -4520.859486
Sum of electronic and thermal Energies= -4520.790045
Sum of electronic and thermal Enthalpies= -4520.789101
Sum of electronic and thermal Free Energies= -4520.970422

Cartesian Coordinates

26	-3.418052	-1.167058	-2.826987
15	-1.016815	-1.727736	1.778448
15	0.692570	0.242170	-0.870990
6	-2.191064	-1.556720	-1.174205
6	-1.759262	-0.371265	-1.879913
6	-2.839177	0.563521	-1.862778
1	-2.833864	1.544165	-2.318485
6	-3.941985	-0.037643	-1.186809
1	-4.917712	0.406336	-1.045852
6	-3.545942	-1.340108	-0.764770
1	-4.166258	-2.054287	-0.245362
6	-2.915987	-1.945793	-4.686532
1	-1.904806	-2.126175	-5.026858
6	-3.648808	-0.728696	-4.838440
1	-3.285783	0.177891	-5.304057
6	-4.925666	-0.901827	-4.222101
1	-5.696090	-0.147117	-4.134312
6	-4.983095	-2.225926	-3.689434
1	-5.806801	-2.653479	-3.133088
6	-3.743549	-2.871286	-3.977348
1	-3.470452	-3.874800	-3.680425
6	-1.293681	-2.713353	-0.885206
6	-0.904168	-3.548890	-1.943349
1	-1.341831	-3.373458	-2.917937
6	0.042761	-4.558501	-1.776281
1	0.343954	-5.166943	-2.623250
6	0.622112	-4.753064	-0.524792
1	1.382106	-5.515130	-0.382286
6	0.242960	-3.943646	0.546238
1	0.730575	-4.086601	1.503059
6	-0.709226	-2.922341	0.394110
6	-0.365315	-0.147917	-2.403215
1	0.004834	-1.106540	-2.772001
6	-0.275956	0.878364	-3.535350
1	0.750213	0.970566	-3.902054
1	-0.607130	1.871217	-3.219100
1	-0.914827	0.560295	-4.365229
6	-0.095730	-2.410907	3.223457
6	0.942872	-1.641112	3.768441
1	1.186215	-0.674879	3.336441
6	1.660549	-2.109671	4.872830
1	2.469819	-1.509480	5.278413
6	1.346783	-3.343287	5.442307
1	1.906616	-3.707508	6.299347
6	0.304942	-4.111398	4.910414
1	0.052430	-5.070114	5.355066
6	-0.415837	-3.647406	3.811257
1	-1.226790	-4.248287	3.410931
6	-2.764502	-2.020903	2.271702
6	-3.436814	-3.231027	2.043411
1	-2.931767	-4.046021	1.533476
6	-4.765176	-3.382274	2.445498
1	-5.280982	-4.320428	2.259949
6	-5.431248	-2.329584	3.081227
1	-6.466896	-2.447655	3.387247
6	-4.762487	-1.126663	3.322996
1	-5.274038	-0.306390	3.818759
6	-3.434776	-0.972915	2.919377
1	-2.915838	-0.035254	3.098433
6	2.015228	-1.041940	-0.841249
6	2.397226	-1.823025	-1.937871
1	1.982008	-1.647319	-2.922796
6	3.316718	-2.860332	-1.772061
6	3.881501	-3.125958	-0.525842
1	4.583483	-3.943228	-0.401327
6	3.519756	-2.329743	0.559918
6	2.592456	-1.299631	0.411821
1	2.304535	-0.691274	1.263037
6	1.602558	1.800993	-1.207253
6	0.860039	2.990155	-1.130009
1	-0.208359	2.951588	-0.950616
6	1.496835	4.223072	-1.227850
6	2.884557	4.300831	-1.358527
1	3.382533	5.263337	-1.389377
6	3.623070	3.120823	-1.398845
6	2.991837	1.875465	-1.343934
1	3.592716	0.973654	-1.367508
29	-0.381433	0.354460	1.186953
6	5.121569	3.191373	-1.486006
6	0.717156	5.494805	-1.047439
6	3.640689	-3.780312	-2.915477
6	4.027586	-2.684766	1.929240
9	5.279731	-3.194325	1.892626
9	4.048297	-1.622365	2.766145
9	3.242140	-3.627699	2.510102
9	3.049815	-4.993094	-2.752119
9	4.969160	-4.014371	-3.016064
9	3.222805	-3.296963	-4.105107
9	5.560155	3.279802	-2.763825
9	5.709952	2.097584	-0.945191
9	5.610477	4.271915	-0.830789
9	1.084426	6.440251	-1.943454
9	-0.613725	5.310161	-1.173100
9	0.926191	6.034195	0.183146
6	1.624924	2.370211	2.177300
6	0.634621	3.389100	2.212364
6	-0.745721	3.284718	1.929064
1	0.964870	4.397875	2.416495
7	2.957679	2.742193	2.159626
6	4.010238	1.753871	2.329311
1	4.687977	2.057270	3.138447
1	3.577914	0.788714	2.577792
1	4.604402	1.650664	1.411059
6	3.416941	4.118398	2.056782
1	2.722409	4.722246	1.473784
1	3.555080	4.587647	3.042305
1	4.378697	4.132520	1.534449
8	1.373130	1.113803	2.158758
6	-1.542705	4.480482	1.993839
6	-2.885535	4.474777	1.704203
1	-1.056079	5.411649	2.266549
6	-3.471788	3.250352	1.338746
6	-2.693412	2.116507	1.267997
1	-3.118177	1.162722	0.981034
7	-1.371375	2.116876	1.540779
1	-3.470712	5.387372	1.754106
35	-5.390480	3.141847	0.923712

Conformer_5

Number of imaginary frequencies : 0
The smallest frequency is : 6.6441 cm(-1)
Electronic energy : HF=-4521.7141033

Zero-point correction= 0.854615
(Hartree/Particle)
Thermal correction to Energy= 0.924057
Thermal correction to Enthalpy= 0.925001
Thermal correction to Gibbs Free Energy= 0.743664
Sum of electronic and zero-point Energies= -4520.859488
Sum of electronic and thermal Energies= -4520.790046
Sum of electronic and thermal Enthalpies= -4520.789102
Sum of electronic and thermal Free Energies= -4520.970439

Cartesian Coordinates

26	3.417990	-1.167671	2.826815
15	1.016548	-1.727956	-1.778626
15	-0.692451	0.242166	0.870878
6	2.190953	-1.557160	1.174025
6	1.759359	-0.371609	1.879704
6	2.839444	0.562983	1.862549
1	2.834313	1.543642	2.318227
6	3.942148	-0.038402	1.186604
1	4.917955	0.405395	1.045631
6	3.545872	-1.340806	0.764598
1	4.166059	-2.055112	0.245209
6	2.915750	-1.946343	4.686339
1	1.904536	-2.126609	5.026628
6	3.648698	-0.729327	4.838278
1	3.285748	0.177301	5.303871
6	4.925567	-0.902604	4.221999
1	5.696076	-0.147978	4.134238
6	4.982872	-2.226711	3.689338
1	5.806556	-2.654360	3.133032
6	3.743239	-2.871931	3.977193
1	3.470041	-3.875414	3.680260
6	1.293354	-2.713628	0.885035
6	0.903725	-3.549103	1.943184
1	1.341472	-3.373763	2.917751
6	-0.043411	-4.558525	1.776150
1	-0.344696	-5.166908	2.623127
6	-0.622855	-4.752958	0.524685
1	-1.383001	-5.514876	0.382193
6	-0.243585	-3.943609	-0.546354
1	-0.731253	-4.086471	-1.503161
6	0.708814	-2.922496	-0.394263
6	0.365459	-0.148052	2.403044
1	-0.004805	-1.106633	2.771826
6	0.276273	0.878214	3.535204
1	-0.749874	0.970548	3.901938
1	0.607572	1.871029	3.218962
1	0.915125	0.560038	4.365056
6	0.095337	-2.411041	-3.223597
6	-0.943262	-1.641175	-3.768487
1	-1.186486	-0.674922	-3.336465
6	-1.661088	-2.109688	-4.872797
1	-2.470355	-1.509441	-5.278303
6	-1.347461	-3.343327	-5.442303
1	-1.907405	-3.707512	-6.299286
6	-0.305616	-4.111504	-4.910516
1	-0.053213	-5.070237	-5.355192
6	0.415300	-3.647563	-3.811425
1	1.226243	-4.248507	-3.411172
6	2.764200	-2.021295	-2.271880
6	3.436354	-3.231532	-2.043716
1	2.931198	-4.046532	-1.533898
6	4.764711	-3.382893	-2.445773
1	5.280395	-4.321133	-2.260323
6	5.430938	-2.330203	-3.081343
1	6.466583	-2.448364	-3.387337
6	4.762337	-1.127169	-3.322982
1	5.274010	-0.306894	-3.818617
6	3.434631	-0.973307	-2.919393
1	2.915818	-0.035556	-3.098337
6	-2.015366	-1.041684	0.841316
6	-2.397487	-1.822584	1.938027
1	-1.982184	-1.646863	2.922916
6	-3.317234	-2.859690	1.772360
6	-3.882139	-3.125293	0.526188
1	-4.584325	-3.942403	0.401777
6	-3.520264	-2.329254	-0.559657
6	-2.592721	-1.299342	-0.411698
1	-2.304723	-0.691109	-1.262976
6	-1.602071	1.801196	1.207144
6	-0.859299	2.990193	1.129801
1	0.209073	2.951389	0.950305
6	-1.495820	4.223250	1.227675
6	-2.883508	4.301313	1.358506
1	-3.381268	5.263930	1.389398
6	-3.622274	3.121465	1.398943
6	-2.991319	1.875971	1.343978
1	-3.592381	0.974286	1.367653
29	0.381394	0.354306	-1.187174
6	-5.120743	3.192372	1.486329
6	-0.715877	5.494806	1.047151
6	-3.641312	-3.779505	2.915882
6	-4.028262	-2.684209	-1.928934
9	-5.280438	-3.193675	-1.892219
9	-4.048972	-1.621779	-2.765810
9	-3.242931	-3.627172	-2.509902
9	-3.050149	-4.992206	2.752945
9	-4.969761	-4.013814	3.016169
9	-3.223832	-3.295823	4.105518
9	-5.559076	3.281370	2.764197
9	-5.709471	2.098530	0.946008
9	-5.609525	4.272795	0.830818
9	-1.082891	6.440377	1.943139
9	0.614972	5.309877	1.172744
9	-0.924872	6.034171	-0.183448
6	-1.624779	2.370267	-2.177475
6	-0.634328	3.389007	-2.212775
6	0.745985	3.284518	-1.929376
1	-0.964455	4.397788	-2.417077
7	-2.957467	2.742467	-2.159758
6	-4.010209	1.754270	-2.329037
1	-4.688325	2.057880	-3.137770
1	-3.578108	0.789111	-2.577902
1	-4.603920	1.650956	-1.410498
6	-3.416486	4.118752	-2.056865
1	-2.721812	4.722470	-1.473895
1	-3.554592	4.588044	-3.042370
1	-4.378211	4.133037	-1.534482
8	-1.373187	1.113819	-2.158762
6	1.543084	4.480202	-1.994210
6	2.885864	4.474426	-1.704348
1	1.056579	5.411376	-2.267110
6	3.471959	3.249998	-1.338643
6	2.693494	2.116212	-1.267942
1	3.118147	1.162417	-0.980854
7	1.371498	2.116656	-1.540930
1	3.471121	5.386969	-1.754256
35	5.390550	3.141423	-0.923165

Conformer_6

Number of imaginary frequencies : 0
The smallest frequency is : 14.2033 cm(-1)
Electronic energy : HF=-4521.7143606
Zero-point correction= 0.854526
(Hartree/Particle)
Thermal correction to Energy= 0.923890
Thermal correction to Enthalpy= 0.924834
Thermal correction to Gibbs Free Energy= 0.745303
Sum of electronic and zero-point Energies= -4520.859834
Sum of electronic and thermal Energies= -4520.790471
Sum of electronic and thermal Enthalpies= -4520.789526
Sum of electronic and thermal Free Energies= -4520.969057

Cartesian Coordinates

26	-3.571972	-1.118214	-2.718328
15	-1.130748	-1.605321	1.892634
15	0.668341	0.090975	-0.918947

6	-2.343800	-1.496104	-1.062270
6	-1.844897	-0.388435	-1.844202
6	-2.856089	0.619851	-1.869558
1	-2.789830	1.568050	-2.384912
6	-3.985770	0.139219	-1.142866
1	-4.925005	0.658870	-1.014412
6	-3.672787	-1.160380	-0.647657
1	-4.331453	-1.796551	-0.076619
6	-3.155293	-2.035631	-4.534460
1	-2.162749	-2.301482	-4.873904
6	-3.807181	-0.782639	-4.748695
1	-3.392868	0.068649	-5.272191
6	-5.082278	-0.832119	-4.106776
1	-5.798616	-0.022802	-4.054187
6	-5.219434	-2.115667	-3.495369
1	-6.059595	-2.451031	-2.901651
6	-4.030946	-2.859600	-3.760511
1	-3.819518	-3.859410	-3.406101
6	-1.538297	-2.704273	-0.717035
6	-1.228445	-3.628109	-1.727233
1	-1.634659	-3.458817	-2.716374
6	-0.401494	-4.726922	-1.495315
1	-0.157800	-5.403827	-2.308118
6	0.127211	-4.930214	-0.223207
1	0.784037	-5.771910	-0.027838
6	-0.167776	-4.027483	0.798777
1	0.267087	-4.189422	1.778405
6	-0.982791	-2.905211	0.576668
6	-0.450914	-0.297137	-2.402954
1	-0.165718	-1.297929	-2.731469
6	-0.309358	0.660541	-3.588614
1	0.711806	0.650637	-3.979979
1	-0.553578	1.691273	-3.317572
1	-0.991010	0.351328	-4.387208
6	-0.221753	-2.310749	3.333281
6	1.060327	-1.809689	3.607745
1	1.466380	-1.006569	3.001977
6	1.801764	-2.321399	4.675939
1	2.794881	-1.930901	4.874299
6	1.267240	-3.326183	5.483863
1	1.842755	-3.719222	6.317464
6	-0.014240	-3.821742	5.223247
1	-0.436854	-4.600027	5.852729
6	-0.755599	-3.318586	4.154204
1	-1.749581	-3.710698	3.963391
6	-2.881444	-1.681878	2.445549
6	-3.686486	-2.820934	2.290381
1	-3.284930	-3.709161	1.811234
6	-5.011908	-2.809293	2.729048
1	-5.630101	-3.693452	2.600283
6	-5.542753	-1.663266	3.329413
1	-6.576192	-1.653902	3.664065
6	-4.741619	-0.531175	3.499978
1	-5.147994	0.360800	3.968365
6	-3.416608	-0.540053	3.059751
1	-2.796254	0.343338	3.182517
6	1.952988	-1.226766	-0.870150
6	2.073913	-2.279299	-1.784721
1	1.441061	-2.339662	-2.660339
6	3.003691	-3.295017	-1.562220
6	3.860902	-3.260145	-0.461946
1	4.585952	-4.050275	-0.301182
6	3.754220	-2.198506	0.434929
6	2.795442	-1.202120	0.251728
1	2.675840	-0.405850	0.982098
6	1.620745	1.608891	-1.336054
6	0.923342	2.824237	-1.235281
1	-0.131891	2.824127	-0.987831
6	1.589245	4.033481	-1.402913
6	2.966058	4.065176	-1.636692
1	3.488527	5.009747	-1.735304
6	3.658821	2.861041	-1.718060
6	2.995535	1.637197	-1.583776
1	3.565551	0.717659	-1.651690
29	-0.298424	0.369183	1.182119
6	5.155545	2.861693	-1.842365
6	0.859761	5.333392	-1.212167
6	3.079512	-4.477867	-2.486964
6	4.702532	-2.081679	1.595511
9	5.675111	-1.167551	1.349038
9	4.073626	-1.671284	2.724662
9	5.319345	-3.247291	1.881334
9	2.837641	-5.637586	-1.825402
9	4.307077	-4.605241	-3.043683
9	2.185776	-4.406320	-3.498267
9	5.602627	1.847780	-2.616579
9	5.748434	2.705931	-0.625878
9	5.632234	4.012993	-2.361223
9	1.175462	6.231059	-2.174993
9	-0.481210	5.181898	-1.221558
9	1.184200	5.915959	-0.027626
6	1.816453	2.319511	2.058409
6	0.872970	3.381014	2.103157
6	-0.514840	3.340675	1.844456
1	1.253164	4.371891	2.310009
7	3.161838	2.637757	2.022831
6	4.172096	1.617076	2.256644
1	4.934480	2.002655	2.944840
1	3.717160	0.736033	2.702152
1	4.674905	1.323314	1.326761
6	3.670430	3.987632	1.834794
1	2.993113	4.578327	1.218341
1	3.829117	4.512855	2.788724
1	4.629106	3.931348	1.311246
8	1.517195	1.072016	2.057274
6	-1.257707	4.569115	1.932089
6	-2.601087	4.625766	1.652166
1	-0.728785	5.474341	2.213386
6	-3.242657	3.432841	1.275298
6	-2.517359	2.265152	1.193301
1	-2.986681	1.332864	0.906199
7	-1.195372	2.203669	1.459613
1	-3.145206	5.562372	1.717746
35	-5.166425	3.416350	0.869340

Conformer_7

Number of imaginary frequencies : 0
The smallest frequency is : 13.2622 cm(-1)
Electronic energy : HF=-4521.7138804
Zero-point correction= 0.854510
(Hartree/Particle)
Thermal correction to Energy= 0.923920
Thermal correction to Enthalpy= 0.924864
Thermal correction to Gibbs Free Energy= 0.744401
Sum of electronic and zero-point Energies= -4520.859371
Sum of electronic and thermal Energies= -4520.789960
Sum of electronic and thermal Enthalpies= -4520.789016
Sum of electronic and thermal Free Energies= -4520.969480

Cartesian Coordinates

26	-3.598204	-1.129862	-2.692285
15	-1.125875	-1.576421	1.911722
15	0.662679	0.066215	-0.938195
6	-2.360109	-1.491858	-1.039700
6	-1.858735	-0.400131	-1.842537
6	-2.862344	0.615400	-1.876299
1	-2.793095	1.554987	-2.406788
6	-3.990085	0.154949	-1.133625
1	-4.924562	0.683363	-1.006612
6	-3.683184	-1.139069	-0.620388
1	-4.342826	-1.761004	-0.034962
6	-3.205720	-2.086556	-4.493928
1	-2.219308	-2.371572	-4.835923
6	-3.843014	-0.829559	-4.727355
1	-3.421849	0.006000	-5.270365
6	-5.114184	-0.850771	-4.076124
1	-5.819977	-0.031616	-4.034173
6	-5.263128	-2.120552	-3.439293

1	-6.103280	-2.433815	-2.833574
6	-4.085789	-2.884322	-3.697922
1	-3.883799	-3.879520	-3.325435
6	-1.560707	-2.701226	-0.683368
6	-1.263819	-3.638848	-1.684951
1	-1.677224	-3.478814	-2.672615
6	-0.440806	-4.739268	-1.447157
1	-0.207821	-5.427084	-2.254003
6	0.097098	-4.930622	-0.177064
1	0.751865	-5.772865	0.022648
6	-0.185746	-4.015011	0.836803
1	0.255803	-4.168317	1.814846
6	-0.996901	-2.891019	0.608638
6	-0.467663	-0.327166	-2.411325
1	-0.193040	-1.334158	-2.729576
6	-0.325434	0.615016	-3.609099
1	0.693033	0.591016	-4.006909
1	-0.558425	1.651135	-3.349163
1	-1.015420	0.302346	-4.399142
6	-0.216923	-2.273093	3.356371
6	1.065919	-1.771449	3.625788
1	1.473544	-0.975184	3.011648
6	1.807158	-2.274566	4.698205
1	2.800977	-1.883753	4.892539
6	1.271488	-3.271488	5.515028
1	1.846727	-3.657986	6.351864
6	-0.010744	-3.767783	5.259182
1	-0.434022	-4.539978	5.895678
6	-0.751917	-3.273027	4.186159
1	-1.746601	-3.665206	3.999092
6	-2.874819	-1.630634	2.472810
6	-3.689951	-2.764681	2.333906
1	-3.297826	-3.661758	1.863586
6	-5.013832	-2.736492	2.776366
1	-5.639930	-3.616811	2.660118
6	-5.533100	-1.578740	3.364235
1	-6.565434	-1.556474	3.701693
6	-4.721964	-0.451439	3.518428
1	-5.119488	0.449696	3.976732
6	-3.398424	-0.476810	3.074437
1	-2.770640	0.403024	3.184124
6	1.940635	-1.258259	-0.885011
6	2.784134	-1.232748	0.236104
1	2.672278	-0.429473	0.959766
6	3.735693	-2.234601	0.425813
6	3.833077	-3.303951	-0.462798
1	4.551817	-4.098808	-0.297013
6	2.974267	-3.340132	-1.561879
6	2.052382	-2.318708	-1.791680
1	1.418291	-2.380920	-2.666316
6	1.614232	1.582493	-1.361689
6	0.913110	2.796462	-1.278925
1	-0.146205	2.795820	-1.049554
6	1.582488	4.006760	-1.427622
6	2.965123	4.039679	-1.619362
1	3.489795	4.985919	-1.687838
6	3.663250	2.836190	-1.672051
6	2.996274	1.612684	-1.568206
1	3.569916	0.694531	-1.606747
29	-0.276418	0.379466	1.172958
6	5.158573	2.851578	-1.825904
6	0.850001	5.307010	-1.249935
6	4.685406	-2.114435	1.584928
6	3.036715	-4.533024	-2.474467
9	2.767822	-5.681536	-1.803451
9	2.152949	-4.455663	-3.494060
9	4.266540	-4.688430	-3.018812
9	5.664368	-1.209618	1.330144
9	5.293429	-3.281988	1.881329
9	4.059802	-1.688557	2.710477
9	5.543940	2.871962	-3.123450
9	5.732539	1.760364	-1.264703
9	5.711987	3.939623	-1.237607
9	1.173805	6.199634	-2.215047
9	-0.490668	5.154681	-1.270397
9	1.164037	5.896555	-0.066315
6	1.867798	2.331385	2.008043
6	0.921994	3.389104	2.090132
6	-0.466708	3.354285	1.836531
1	1.303316	4.376267	2.312140
7	3.211613	2.654590	1.952260
6	4.230020	1.626509	2.098968
1	5.037789	1.997578	2.741171
1	3.803858	0.738163	2.558573
1	4.668902	1.348417	1.131474
6	3.716054	4.004838	1.754827
1	3.001451	4.612414	1.200757
1	3.947166	4.507440	2.705762
1	4.634483	3.958278	1.161151
8	1.571587	1.083607	1.990879
6	-1.205726	4.584205	1.939238
6	-2.548252	4.649551	1.657969
1	-0.673788	5.484109	2.231625
6	-3.194112	3.463642	1.266081
6	-2.473895	2.293660	1.174496
1	-2.946976	1.365818	0.879203
7	-1.152578	2.223542	1.442727
1	-3.088644	5.587572	1.733581
35	-5.117007	3.460200	0.855823

Conformer_8

Number of imaginary frequencies : 0
The smallest frequency is : 13.1635 cm(-1)
Electronic energy : HF=-4521.713881
Zero-point correction= 0.854513
(Hartree/Particle)
Thermal correction to Energy= 0.923922
Thermal correction to Enthalpy= 0.924866
Thermal correction to Gibbs Free Energy= 0.744386
Sum of electronic and zero-point Energies= -4520.859368
Sum of electronic and thermal Energies= -4520.789959
Sum of electronic and thermal Enthalpies= -4520.789015
Sum of electronic and thermal Free Energies= -4520.969495

Cartesian Coordinates

26	-3.599567	-1.130466	-2.691043
15	-1.125634	-1.574536	1.912621
15	0.662416	0.065006	-0.939422
6	-2.360927	-1.491429	-1.038626
6	-1.859321	-0.400764	-1.842766
6	-2.862432	0.615242	-1.877151
1	-2.792925	1.554272	-2.408591
6	-3.990099	0.156120	-1.133551
1	-4.924255	0.685124	-1.006681
6	-3.683629	-1.137513	-0.619094
1	-4.343355	-1.758512	-0.032763
6	-3.208711	-2.090064	-4.491528
1	-2.222766	-2.376660	-4.833562
6	-3.844716	-0.832701	-4.726472
1	-3.422849	0.001624	-5.270831
6	-5.115688	-0.851652	-4.074780
1	-5.820590	-0.031684	-4.033718
6	-5.265775	-2.120384	-3.436131
1	-6.106059	-2.431908	-2.829697
6	-4.089332	-2.885771	-3.694080
1	-3.888226	-3.880646	-3.320249
6	-1.562113	-2.700980	-0.681529
6	-1.266099	-3.639558	-1.682485
1	-1.679685	-3.479999	-2.670148
6	-0.443768	-4.740354	-1.444092
1	-0.211454	-5.428921	-2.250493
6	0.094299	-4.931148	-0.173985
1	0.748518	-5.773702	0.026208
6	-0.187655	-4.014582	0.839260
1	0.254033	-4.167482	1.817302
6	-0.998098	-2.890194	0.610484
6	-0.468368	-0.328865	-2.411994
1	-0.194252	-1.336201	-2.729562

6	-0.325964	0.612382	-3.610478
1	0.692372	0.587493	-4.008569
1	-0.558269	1.648826	-3.351214
1	-1.016375	0.299540	-4.400083
6	-0.216411	-2.270684	3.357345
6	1.067082	-1.769980	3.625409
1	1.475018	-0.974682	3.010215
6	1.808585	-2.272771	4.697792
1	2.802902	-1.882718	4.891084
6	1.272512	-3.268398	5.515937
1	1.847952	-3.654630	6.352759
6	-0.010356	-3.763737	5.261440
1	-0.433922	-4.534922	5.898968
6	-0.751784	-3.269328	4.188430
1	-1.746945	-3.660773	4.002350
6	-2.874305	-1.627141	2.474689
6	-3.690441	-2.760569	2.336626
1	-3.299322	-3.658121	1.866377
6	-5.014036	-2.731154	2.779866
1	-5.640927	-3.610994	2.664273
6	-5.531996	-1.572794	3.367692
1	-6.564108	-1.549578	3.705766
6	-4.719848	-0.446104	3.521041
1	-5.116369	0.455496	3.979296
6	-3.396600	-0.472686	3.076256
1	-2.768038	0.406679	3.185258
6	1.940101	-1.259728	-0.885721
6	2.784334	-1.233130	0.234812
1	2.673240	-0.428896	0.957515
6	3.735641	-2.235081	0.425202
6	3.832066	-3.305607	-0.462088
1	4.550624	-4.100513	-0.295769
6	2.972551	-3.342843	-1.560588
6	2.050873	-2.321387	-1.791105
1	1.416238	-2.384556	-2.665279
6	1.614357	1.580901	-1.363460
6	0.913724	2.795145	-1.280857
1	-0.145618	2.794916	-1.051619
6	1.583630	4.005172	-1.429490
6	2.966337	4.037553	-1.620813
1	3.491409	4.983592	-1.689155
6	3.663971	2.833753	-1.673287
6	2.996453	1.610547	-1.569718
1	3.569747	0.692194	-1.608242
29	-0.275183	0.380268	1.172060
6	5.159388	2.848663	-1.826368
6	0.851551	5.305737	-1.252352
6	4.686043	-2.113717	1.583624
6	3.034078	-4.536879	-2.471736
9	2.764648	-5.684418	-1.799277
9	2.150148	-4.460244	-3.491242
9	4.263702	-4.693674	-3.016140
9	5.664500	-1.208723	1.327579
9	5.294648	-3.280825	1.880540
9	4.060964	-1.687202	2.709243
9	5.545426	2.872443	-3.123648
9	5.732523	1.755645	-1.267804
9	5.713071	3.934866	-1.234881
9	1.175746	6.197850	-2.217811
9	-0.489162	5.153845	-1.272899
9	1.165634	5.895700	-0.068952
6	1.869042	2.332627	2.005732
6	0.922975	3.390078	2.088314
6	-0.465828	3.355084	1.835220
1	1.304177	4.377318	2.310144
7	3.212699	2.656338	1.949589
6	4.231615	1.628459	2.094261
1	5.039574	1.998845	2.736608
1	3.806059	0.739310	2.552852
1	4.670060	1.351994	1.126088
6	3.716135	4.007280	1.754201
1	3.002655	4.614109	1.197820
1	3.943362	4.510037	2.705995
1	4.636635	3.961881	1.163725
8	1.573197	1.084755	1.988095
6	-1.204856	4.584988	1.938066
6	-2.547357	4.650294	1.656660
1	-0.672967	5.484931	2.230428
6	-3.193187	3.464399	1.264682
6	-2.472975	2.294406	1.173268
1	-2.946050	1.366521	0.878109
7	-1.151686	2.224256	1.441639
1	-3.087771	5.588307	1.732251
35	-5.116040	3.461025	0.854246

Conformer_9

Number of imaginary frequencies : 0
The smallest frequency is : 13.2755 cm(-1)
Electronic energy : HF=-4521.7138802
Zero-point correction= 0.854513
(Hartree/Particle)
Thermal correction to Energy= 0.923921
Thermal correction to Enthalpy= 0.924866
Thermal correction to Gibbs Free Energy= 0.744415
Sum of electronic and zero-point Energies= -4520.859368
Sum of electronic and thermal Energies= -4520.789959
Sum of electronic and thermal Enthalpies= -4520.789015
Sum of electronic and thermal Free Energies= -4520.969465

Cartesian Coordinates

26	-3.597999	-1.129357	-2.692651
15	-1.126052	-1.576745	1.911428
15	0.662697	0.066459	-0.937906
6	-2.360079	-1.491728	-1.040028
6	-1.858641	-0.399802	-1.842546
6	-2.862262	0.615723	-1.876157
1	-2.792971	1.555438	-2.406417
6	-3.990069	0.155068	-1.133707
1	-4.924565	0.683440	-1.006652
6	-3.683204	-1.139076	-0.620766
1	-4.342882	-1.761168	-0.035550
6	-3.205194	-2.085261	-4.494625
1	-2.218685	-2.369904	-4.836647
6	-3.842771	-0.828324	-4.727606
1	-3.421755	0.007555	-5.270238
6	-5.113973	-0.850080	-4.076459
1	-5.819959	-0.031105	-4.034235
6	-5.262668	-2.120147	-3.440142
1	-6.102785	-2.433839	-2.834597
6	-4.085141	-2.883546	-3.699001
1	-3.882968	-3.878856	-3.326910
6	-1.560657	-2.701136	-0.683887
6	-1.263652	-3.638567	-1.685612
1	-1.676963	-3.478378	-2.673290
6	-0.440619	-4.738998	-1.447938
1	-0.207546	-5.426671	-2.254882
6	0.097214	-4.930541	-0.177844
1	0.752006	-5.772789	0.021769
6	-0.185725	-4.015106	0.836156
1	0.255777	-4.168544	1.814198
6	-0.996915	-2.891113	0.608120
6	-0.467518	-0.326717	-2.411188
1	-0.192817	-1.333657	-2.729526
6	-0.325198	0.615599	-3.608848
1	0.693317	0.591702	-4.006541
1	-0.558289	1.651676	-3.348841
1	-1.015066	0.302968	-4.399009
6	-0.217246	-2.273676	3.356052
6	1.065525	-1.772008	3.625764
1	1.473196	-0.975581	3.011869
6	1.806643	-2.275305	4.698179
1	2.800409	-1.884464	4.892730
6	1.270925	-3.272431	5.514719
1	1.846069	-3.659065	6.351557
6	-0.011238	-3.768755	5.258583
1	-0.434560	-4.541113	5.894853
6	-0.752290	-3.273819	4.185559
1	-1.746923	-3.666026	3.998281

6	-2.875055	-1.631101	2.472315
6	-3.690110	-2.765179	2.333220
1	-3.297889	-3.662186	1.862845
6	-5.014032	-2.737116	2.775563
1	-5.640067	-3.617461	2.659164
6	-5.533424	-1.579456	3.363506
1	-6.565788	-1.557288	3.700875
6	-4.722367	-0.452125	3.517888
1	-5.119982	0.448940	3.976252
6	-3.398786	-0.477372	3.074011
1	-2.771068	0.402490	3.183849
6	1.940567	-1.258102	-0.884796
6	2.783926	-1.232808	0.236428
1	2.671979	-0.429672	0.960232
6	3.735480	-2.234681	0.426049
6	3.832995	-3.303844	-0.462774
1	4.551740	-4.098716	-0.297073
6	2.974319	-3.339814	-1.561968
6	2.052436	-2.318366	-1.791668
1	1.418437	-2.380433	-2.666383
6	1.614417	1.582672	-1.361266
6	0.913376	2.796706	-1.278696
1	-0.145975	2.796179	-1.049472
6	1.582859	4.006934	-1.427490
6	2.965511	4.039734	-1.619103
1	3.490256	4.985927	-1.687628
6	3.663555	2.836192	-1.671598
6	2.996480	1.612748	-1.567649
1	3.570063	0.694550	-1.606038
29	-0.276569	0.379361	1.173231
6	5.158884	2.851402	-1.825399
6	0.850437	5.307245	-1.250030
6	4.685083	-2.114711	1.585272
6	3.036920	-4.532497	-2.474820
9	2.768093	-5.681182	-1.804074
9	2.153205	-4.454984	-3.494446
9	4.266787	-4.687678	-3.019134
9	5.664172	-1.209986	1.330650
9	5.292949	-3.282354	1.881647
9	4.059417	-1.688841	2.710789
9	5.544307	2.870672	-3.122945
9	5.732758	1.760590	-1.263300
9	5.712334	3.939878	-1.237955
9	1.175009	6.200012	-2.214744
9	-0.490238	5.155100	-1.271437
9	1.163738	5.896498	-0.066066
6	1.867631	2.331178	2.008493
6	0.921819	3.388885	2.090599
6	-0.466901	3.354068	1.837098
1	1.303143	4.376051	2.312582
7	3.211439	2.654412	1.952502
6	4.229950	1.626485	2.099552
1	5.037310	1.997544	2.742291
1	3.803683	0.737960	2.558706
1	4.669409	1.348725	1.132229
6	3.715849	4.004658	1.755022
1	3.001123	4.612295	1.201182
1	3.947242	4.507183	2.705931
1	4.634122	3.958112	1.161093
8	1.571429	1.083392	1.991488
6	-1.205946	4.583954	1.940035
6	-2.548476	4.649323	1.658786
1	-0.674030	5.483816	2.232595
6	-3.194312	3.463474	1.266683
6	-2.474077	2.293517	1.174913
1	-2.947143	1.365726	0.879437
7	-1.152765	2.223370	1.443153
1	-3.088888	5.587319	1.734582
35	-5.117183	3.460078	0.856318

---

*Conformer*_10

Number of imaginary frequencies : 0
The smallest frequency is : 9.3144 cm(-1)
Electronic energy : HF=-4521.7140753
Zero-point correction= 0.854509
(Hartree/Particle)
Thermal correction to Energy= 0.923958
Thermal correction to Enthalpy= 0.924902
Thermal correction to Gibbs Free Energy= 0.743994
Sum of electronic and zero-point Energies= -4520.859567
Sum of electronic and thermal Energies= -4520.790118
Sum of electronic and thermal Enthalpies= -4520.789173
Sum of electronic and thermal Free Energies= -4520.970081

Cartesian Coordinates

26	-3.396779	-1.177541	-2.850045
15	-1.034088	-1.734788	1.777324
15	0.696493	0.237149	-0.861382
6	-2.182110	-1.563207	-1.186699
6	-1.744441	-0.379956	-1.892531
6	-2.824196	0.555233	-1.886360
1	-2.814951	1.534596	-2.344706
6	-3.932337	-0.043513	-1.217016
1	-4.908991	0.401131	-1.084844
6	-3.540016	-1.344958	-0.788328
1	-4.164693	-2.057388	-0.271740
6	-2.882470	-1.960871	-4.704539
1	-1.868932	-2.142144	-5.037300
6	-3.614048	-0.743983	-4.863990
1	-3.247817	0.161524	-5.329205
6	-4.894998	-0.915578	-4.255740
1	-5.665944	-0.160642	-4.174795
6	-4.956098	-2.238444	-3.720452
1	-5.783602	-2.664739	-3.168785
6	-3.714810	-2.884633	-3.998780
1	-3.443950	-3.887515	-3.697753
6	-1.287612	-2.719746	-0.888820
6	-0.890776	-3.556570	-1.943014
1	-1.321534	-3.382381	-2.920870
6	0.053539	-4.567202	-1.767833
1	0.357622	-5.177915	-2.611726
6	0.625283	-4.759352	-0.512467
1	1.381795	-5.523690	-0.361964
6	0.238519	-3.948595	0.554940
1	0.718954	-4.090501	1.515446
6	-0.713205	-2.928160	0.395140
6	-0.345912	-0.156297	-2.403491
1	0.031130	-1.114675	-2.766389
6	-0.247203	0.868621	-3.536091
1	0.782314	0.961944	-3.893093
1	-0.582684	1.861458	-3.224168
1	-0.877592	0.548762	-4.371791
6	-0.124962	-2.420036	3.228965
6	0.911233	-1.652773	3.782093
1	1.157786	-0.685373	3.354431
6	1.622753	-2.125634	4.888646
1	2.430382	-1.527490	5.300475
6	1.304876	-3.360795	5.452481
1	1.860055	-3.728396	6.311105
6	0.264723	-4.125927	4.913055
1	0.008796	-5.085691	5.353473
6	-0.449700	-3.657796	3.811529
1	-1.258828	-4.256814	3.404792
6	-2.786124	-2.028705	2.254065
6	-3.463202	-0.980561	2.894358
1	-2.946429	-0.042503	3.077580
6	-4.794795	-1.134555	3.284847
1	-5.311503	-0.314196	3.775081
6	-5.460716	-2.337836	3.037080
1	-6.499312	-2.456107	3.332860
6	-4.788083	-3.390578	2.408353
1	-5.301793	-4.328906	2.217934
6	-3.455825	-3.239088	2.019467
1	-2.945605	-4.053971	1.514519
6	2.026410	-1.039262	-0.828061
6	2.444881	-1.788554	-1.932701
1	2.051170	-1.593492	-2.923452
6	3.380844	-2.813453	-1.770848

6	3.919424	-3.101057	-0.518687
1	4.634683	-3.906686	-0.398502
6	3.520146	-2.335555	0.576873
6	2.581707	-1.316116	0.431104
1	2.271497	-0.727305	1.287862
6	1.601846	1.800706	-1.188758
6	0.853798	2.986486	-1.113091
1	-0.215354	2.942731	-0.939341
6	1.485781	4.222289	-1.204921
6	2.873826	4.306290	-1.328367
1	3.367797	5.270965	-1.354524
6	3.617591	3.129610	-1.367370
6	2.991452	1.881379	-1.318065
1	3.596562	0.982395	-1.340482
29	-0.393426	0.345696	1.188494
6	5.116242	3.205963	-1.446187
6	0.699993	5.490285	-1.024882
6	3.735856	-3.687519	-2.940752
6	4.007436	-2.705756	1.949602
9	5.258019	-3.219394	1.925818
9	4.020404	-1.650212	2.795706
9	3.210362	-3.649909	2.512383
9	2.934056	-4.782670	-3.001488
9	5.005960	-4.143575	-2.868790
9	3.600785	-3.042225	-4.120799
9	5.562156	3.287937	-2.721878
9	5.705592	2.117616	-0.895207
9	5.597123	4.292180	-0.794647
9	1.068117	6.440011	-1.916047
9	-0.629447	5.300643	-1.158154
9	0.900510	6.026511	0.208418
6	1.604602	2.357069	2.198215
6	0.614238	3.375980	2.232680
6	-0.764026	3.273239	1.938755
1	0.943281	4.383670	2.444050
7	2.937414	2.729283	2.185312
6	3.990063	1.741783	2.359021
1	4.651475	2.032477	3.186410
1	3.556269	0.770932	2.581567
1	4.601765	1.657463	1.450571
6	3.395548	4.106423	2.090798
1	2.703879	4.711428	1.505436
1	3.526641	4.572286	3.078906
1	4.360692	4.123736	1.574867
8	1.352569	1.100857	2.175645
6	-1.561854	4.468276	2.005997
6	-2.901856	4.464827	1.703612
1	-1.078009	5.397262	2.290781
6	-3.484467	3.243307	1.322923
6	-2.705526	2.109889	1.251490
1	-3.127615	1.158234	0.953714
7	-1.386142	2.108124	1.536816
1	-3.487552	5.376993	1.755106
35	-5.398914	3.138368	0.887795

---

*Conformer*_11

Number of imaginary frequencies : 0
The smallest frequency is : 9.2302 cm(-1)
Electronic energy : HF=-4521.7140754
Zero-point correction= 0.854510
(Hartree/Particle)
Thermal correction to Energy= 0.923958
Thermal correction to Enthalpy= 0.924903
Thermal correction to Gibbs Free Energy= 0.743990
Sum of electronic and zero-point Energies= -4520.859566
Sum of electronic and thermal Energies= -4520.790117
Sum of electronic and thermal Enthalpies= -4520.789173
Sum of electronic and thermal Free Energies= -4520.970085

Cartesian Coordinates

26	3.397355	-1.177171	2.849504
15	1.033948	-1.734894	-1.777429
15	-0.696279	0.237179	0.861372
6	2.182436	-1.563059	1.186401
6	1.744856	-0.379729	1.892157
6	2.824595	0.555474	1.885687
1	2.815413	1.534903	2.343896
6	3.932639	-0.043345	1.216244
1	4.909254	0.401311	1.083836
6	3.540271	-1.344849	0.787782
1	4.164859	-2.057347	0.271179
6	2.883297	-1.960232	4.704168
1	1.869809	-2.141449	5.037107
6	3.614918	-0.743336	4.863358
1	3.248761	0.162240	5.328498
6	4.895779	-0.915027	4.254949
1	5.666725	-0.160112	4.173800
6	4.956788	-2.237967	3.719832
1	5.784208	-2.664344	3.168102
6	3.715529	-2.884102	3.998419
1	3.444610	-3.887019	3.697561
6	1.287923	-2.719643	0.888769
6	0.891243	-3.556369	1.943098
1	1.322087	-3.382054	2.920893
6	-0.053030	-4.567075	1.768126
1	-0.356996	-5.177706	2.612119
6	-0.624867	-4.759415	0.512832
1	-1.381320	-5.523840	0.362477
6	-0.238273	-3.948743	-0.554700
1	-0.718793	-4.090811	-1.515140
6	0.713383	-2.928211	-0.395105
6	0.346402	-0.156087	2.403336
1	-0.030530	-1.114468	2.766343
6	0.247825	0.868885	3.535894
1	-0.781640	0.962178	3.893050
1	0.583213	1.861717	3.223865
1	0.878358	0.549099	4.371513
6	0.124485	-2.420235	-3.228822
6	-0.911916	-1.653054	-3.781680
1	-1.158408	-0.685650	-3.353988
6	-1.623719	-2.125983	-4.888021
1	-2.431508	-1.527901	-5.299624
6	-1.305914	-3.361128	-5.451928
1	-1.861310	-3.728784	-6.310388
6	-0.265545	-4.126170	-4.912793
1	-0.009665	-5.085916	-5.353276
6	0.449156	-3.657974	-3.811472
1	1.258462	-4.256918	-3.404978
6	2.785885	-2.028808	-2.254547
6	3.462890	-0.980696	-2.894968
1	2.946148	-0.042599	-3.078071
6	4.794394	-1.134759	-3.285736
1	5.311044	-0.314422	-3.776069
6	5.460308	-2.338071	-3.038112
1	6.498837	-2.456392	-3.334108
6	4.787753	-3.390780	-2.409246
1	5.301455	-4.329135	-2.218936
6	3.455583	-3.239225	-2.020086
1	2.945433	-4.054092	-1.515043
6	-2.026095	-1.039348	0.828377
6	-2.444355	-1.788558	1.933155
1	-2.050469	-1.593406	2.923821
6	-3.380355	-2.813466	1.771556
6	-3.919166	-3.101158	0.519517
1	-4.634473	-3.906776	0.399531
6	-3.520085	-2.335754	-0.576182
6	-2.581608	-1.316316	-0.430667
1	-2.271536	-0.727583	-1.287526
6	-1.601745	1.800674	1.188750
6	-0.853792	2.986515	1.113043
1	0.215370	2.942848	0.939326
6	-1.485880	4.222269	1.204782
6	-2.873937	4.306162	1.328183
1	-3.367983	5.270797	1.354284
6	-3.617604	3.129425	1.367230
6	-2.991362	1.881241	1.318000
1	-3.596400	0.982207	1.340427
29	0.393283	0.345617	-1.188678

6	-5.116264	3.205633	1.446052
6	-0.700197	5.490324	1.024702
6	-3.735201	-3.687410	2.941604
6	-4.007673	-2.706050	-1.948780
9	-5.258283	-3.219609	-1.924702
9	-4.020738	-1.650584	-2.794984
9	-3.210768	-3.650309	-2.511622
9	-2.933339	-4.782511	3.002404
9	-5.005285	-4.143548	2.869819
9	-3.600060	-3.041953	4.121555
9	-5.562204	3.287132	2.721763
9	-5.705512	2.117408	0.894706
9	-5.597242	4.292012	0.794859
9	-1.068405	6.440049	1.915833
9	0.629257	5.300800	1.157983
9	-0.900756	6.026496	-0.208616
6	-1.604950	2.356980	-2.198151
6	-0.614593	3.375893	-2.232750
6	0.763682	3.273206	-1.938854
1	-0.943675	4.383580	-2.444068
7	-2.937770	2.729198	-2.185139
6	-3.990416	1.741719	-2.358989
1	-4.651338	2.032029	-3.186915
1	-3.556587	0.770709	-2.580768
1	-4.602633	1.657945	-1.450846
6	-3.395881	4.106357	-2.090825
1	-2.704213	4.711420	-1.505522
1	-3.526950	4.572100	-3.078995
1	-4.361033	4.123756	-1.574911
8	-1.352925	1.100771	-2.175481
6	1.561414	4.468320	-2.005875
6	2.901401	4.464935	-1.703421
1	1.077493	5.397321	-2.290480
6	3.484105	3.243392	-1.322947
6	2.705272	2.109881	-1.251807
1	3.127436	1.158197	-0.954234
7	1.385894	2.108062	-1.537169
1	3.487015	5.377167	-1.754696
35	5.398509	3.138575	-0.887596

---

*Conformer*_12

Number of imaginary frequencies : 0
The smallest frequency is : 13.2444 cm(-1)
Electronic energy : HF=-4521.7138803
Zero-point correction= 0.854508
(Hartree/Particle)
Thermal correction to Energy= 0.923919
Thermal correction to Enthalpy= 0.924863
Thermal correction to Gibbs Free Energy= 0.744393
Sum of electronic and zero-point Energies= -4520.859373
Sum of electronic and thermal Energies= -4520.789961
Sum of electronic and thermal Enthalpies= -4520.789017
Sum of electronic and thermal Free Energies= -4520.969488

.....

Cartesian Coordinates

.....

26	-3.598034	-1.129679	-2.692613
15	-1.126135	-1.576365	1.911678
15	0.662736	0.066266	-0.938142
6	-2.360153	-1.491731	-1.039886
6	-1.858673	-0.399969	-1.842602
6	-2.862285	0.615558	-1.876461
1	-2.792968	1.555173	-2.406893
6	-3.990125	0.155075	-1.133955
1	-4.924620	0.683481	-1.007044
6	-3.683291	-1.138964	-0.620738
1	-4.343004	-1.760940	-0.035427
6	-3.205300	-2.086270	-4.494262
1	-2.218834	-2.371244	-4.836135
6	-3.842592	-0.829274	-4.727703
1	-3.421378	0.006325	-5.270611
6	-5.113844	-0.850551	-4.076635
1	-5.819671	-0.031421	-4.034746
6	-5.262845	-2.120372	-3.439900
1	-6.103070	-2.433692	-2.834313
6	-4.085457	-2.884101	-3.698421
1	-3.883509	-3.879324	-3.325978
6	-1.560841	-2.701138	-0.683478
6	-1.263928	-3.638793	-1.685019
1	-1.677175	-3.478712	-2.672740
6	-0.441064	-4.739301	-1.447119
1	-0.208041	-5.427138	-2.253937
6	0.096650	-4.930710	-0.176956
1	0.751292	-5.773026	0.022852
6	-0.186223	-4.015061	0.836868
1	0.255179	-4.168423	1.814966
6	-0.997242	-2.890986	0.608610
6	-0.467566	-0.327042	-2.411314
1	-0.192951	-1.334039	-2.729550
6	-0.325226	0.615135	-3.609082
1	0.693270	0.591105	-4.006815
1	-0.558209	1.651260	-3.349166
1	-1.015157	0.302484	-4.399178
6	-0.217310	-2.273197	3.356357
6	-0.752346	-3.273146	4.186101
1	-1.747050	-3.665265	3.999038
6	-0.011189	-3.768009	5.259085
1	-0.434513	-4.540215	5.895540
6	1.271081	-3.271819	5.514944
1	1.846303	-3.658403	6.351753
6	1.806801	-2.274892	4.698166
1	2.800650	-1.884154	4.892501
6	1.065575	-1.771669	3.625789
1	1.473249	-0.975396	3.011699
6	-2.875116	-1.630359	2.472763
6	-3.398463	-0.476509	3.074576
1	-2.770499	0.403186	3.184346
6	-4.721948	-0.450941	3.518711
1	-5.119246	0.450214	3.977170
6	-5.533311	-1.578071	3.364476
1	-6.565603	-1.555658	3.702055
6	-5.014320	-2.735840	2.776403
1	-5.640594	-3.616028	2.660108
6	-3.690491	-2.764226	2.333792
1	-3.298605	-3.661336	1.863335
6	1.940615	-1.258286	-0.884933
6	2.784155	-1.232759	0.236152
1	2.672374	-0.429442	0.959782
6	3.735639	-2.234675	0.425909
6	3.832926	-3.304090	-0.462630
1	4.551615	-4.098985	-0.296807
6	2.974086	-3.340280	-1.561689
6	2.052254	-2.318815	-1.791525
1	1.418129	-2.381059	-2.666135
6	1.614434	1.582461	-1.361622
6	0.913406	2.796488	-1.278915
1	-0.145922	2.795929	-1.049590
6	1.582886	4.006728	-1.427635
6	2.965526	4.039536	-1.619347
1	3.490276	4.985733	-1.687814
6	3.663555	2.835990	-1.671997
6	2.996481	1.612540	-1.568117
1	3.570059	0.694346	-1.606643
29	-0.276394	0.379467	1.172980
6	5.158875	2.851219	-1.825865
6	0.850489	5.307031	-1.249995
6	4.685299	-2.114525	1.585069
6	3.036440	-4.533233	-2.474205
9	2.767360	-5.681675	-1.803145
9	2.152751	-4.455821	-3.493862
9	4.266282	-4.688829	-3.018460
9	5.664144	-1.209539	1.330443
9	5.293469	-3.282032	1.881348
9	4.059583	-1.688878	2.710641
9	5.544238	2.871037	-3.123420
9	5.732753	1.760179	-1.264231
9	5.712364	3.939457	-1.238009
9	1.174694	6.199752	-2.214880
9	-0.490187	5.154849	-1.270914

9	1.164204	5.896369	-0.066184
6	1.867769	2.331306	2.008206
6	0.921982	3.389036	2.090351
6	-0.466729	3.354235	1.836784
1	1.303313	4.376180	2.312426
7	3.211592	2.654478	1.952409
6	4.229975	1.626374	2.099108
1	5.037778	1.997447	2.741269
1	3.803809	0.738052	2.558759
1	4.668819	1.348242	1.131610
6	3.716087	4.004687	1.754849
1	3.001400	4.612320	1.200952
1	3.947478	4.507268	2.705727
1	4.634371	3.958057	1.160947
8	1.571537	1.083531	1.991038
6	-1.205772	4.584123	1.939701
6	-2.548281	4.649503	1.658360
1	-0.673864	5.483977	2.232299
6	-3.194100	3.463665	1.266192
6	-2.473870	2.293699	1.174469
1	-2.946917	1.365904	0.878979
7	-1.152574	2.223544	1.442788
1	-3.088691	5.587503	1.734119
35	-5.116937	3.460324	0.855669

---

*Conformer*_13

Number of imaginary frequencies : 0
The smallest frequency is : 13.3028 cm(-1)
Electronic energy : HF=-4521.7138802
Zero-point correction= 0.854510
(Hartree/Particle)
Thermal correction to Energy= 0.923920
Thermal correction to Enthalpy= 0.924864
Thermal correction to Gibbs Free Energy= 0.744407
Sum of electronic and zero-point Energies= -4520.859370
Sum of electronic and thermal Energies= -4520.789960
Sum of electronic and thermal Enthalpies= -4520.789016
Sum of electronic and thermal Free Energies= -4520.969473

Cartesian Coordinates

26	-3.597906	-1.129440	-2.692820
15	-1.126175	-1.576374	1.911453
15	0.662824	0.066321	-0.938138
6	-2.360078	-1.491628	-1.040074
6	-1.858517	-0.399887	-1.842774
6	-2.862047	0.615719	-1.876610
1	-2.792652	1.555334	-2.407031
6	-3.989929	0.155297	-1.134134
1	-4.924390	0.683770	-1.007241
6	-3.683194	-1.138777	-0.620938
1	-4.342959	-1.760702	-0.035639
6	-3.205184	-2.085854	-4.494557
1	-2.218714	-2.370772	-4.836464
6	-3.842507	-0.828849	-4.727868
1	-3.421314	0.006816	-5.270692
6	-5.113748	-0.850211	-4.076779
1	-5.819581	-0.031092	-4.034789
6	-5.262712	-2.120095	-3.440159
1	-6.102917	-2.433484	-2.834580
6	-4.085317	-2.883779	-3.698779
1	-3.883343	-3.879032	-3.326431
6	-1.560821	-2.701079	-0.683698
6	-1.263912	-3.638705	-1.685268
1	-1.677166	-3.478603	-2.672983
6	-0.441061	-4.739229	-1.447392
1	-0.208048	-5.427050	-2.254226
6	0.096650	-4.930687	-0.177234
1	0.751277	-5.773022	0.022547
6	-0.186211	-4.015066	0.836619
1	0.255178	-4.168460	1.814720
6	-0.997193	-2.890967	0.608371
6	-0.467370	-0.326995	-2.411388
1	-0.192745	-1.334004	-2.729579
6	-0.324939	0.615154	-3.609166
1	0.693580	0.591101	-4.006840
1	-0.557925	1.651288	-3.349287
1	-1.014829	0.302494	-4.399296
6	-0.217383	-2.273107	3.356173
6	-0.752444	-3.273184	4.185748
1	-1.747084	-3.665384	3.998484
6	-0.011396	-3.768058	5.258803
1	-0.434725	-4.540368	5.895126
6	1.270775	-3.271735	5.514898
1	1.845919	-3.658329	6.351755
6	1.806502	-2.274658	4.698303
1	2.800269	-1.883816	4.892845
6	1.065391	-1.771424	3.625851
1	1.473042	-0.975020	3.011909
6	-2.875147	-1.630426	2.472504
6	-3.398547	-0.476675	3.074463
1	-2.770624	0.403034	3.184363
6	-4.722055	-0.451211	3.518538
1	-5.119406	0.449869	3.977100
6	-5.533380	-1.578343	3.364098
1	-6.565690	-1.556004	3.701624
6	-5.014325	-2.736020	2.775897
1	-5.640564	-3.616214	2.659459
6	-3.690471	-2.764305	2.333360
1	-3.298504	-3.661338	1.862824
6	1.940619	-1.258306	-0.884796
6	2.784020	-1.232833	0.236392
1	2.672172	-0.429526	0.960019
6	3.735463	-2.234768	0.426236
6	3.832835	-3.304158	-0.462328
1	4.551493	-4.099070	-0.296445
6	2.974121	-3.340302	-1.561486
6	2.052346	-2.318805	-1.791410
1	1.418323	-2.381010	-2.666098
6	1.614630	1.582457	-1.361592
6	0.913645	2.796519	-1.279017
1	-0.145705	2.796023	-1.049786
6	1.583187	4.006721	-1.427779
6	2.965843	4.039458	-1.619375
1	3.490637	4.985627	-1.687882
6	3.663830	2.835881	-1.671866
6	2.996698	1.612466	-1.567960
1	3.570243	0.694247	-1.606375
29	-0.276481	0.379497	1.172879
6	5.159167	2.851056	-1.825570
6	0.850833	5.307067	-1.250285
6	4.685052	-2.114633	1.585455
6	3.036569	-4.533217	-2.474046
9	2.767668	-5.681713	-1.803008
9	2.152811	-4.455875	-3.493650
9	4.266396	-4.688641	-3.018382
9	5.664106	-1.209895	1.330749
9	5.292955	-3.282218	1.881972
9	4.059344	-1.688661	2.710910
9	5.544669	2.870927	-3.123083
9	5.732943	1.759969	-1.263926
9	5.712631	3.939247	-1.237602
9	1.175257	6.199753	-2.215127
9	-0.489848	5.154964	-1.271431
9	1.164376	5.896405	-0.066427
6	1.867570	2.331327	2.008273
6	0.921785	3.389077	2.090216
6	-0.466934	3.354226	1.836697
1	1.303106	4.376255	2.312154
7	3.211394	2.654493	1.952439
6	4.229804	1.626450	2.099398
1	5.037412	1.997547	2.741793
1	3.803562	0.738093	2.558903
1	4.668925	1.348378	1.132007
6	3.715861	4.004725	1.754966
1	3.001313	4.612278	1.200802
1	3.946909	4.507380	2.705889
1	4.634344	3.958115	1.161371
8	1.571317	1.083551	1.991314

6	-1.206022	4.584089	1.939585
6	-2.548572	4.649380	1.658413
1	-0.674126	5.483989	2.232068
6	-3.194382	3.463481	1.266416
6	-2.474090	2.293558	1.174628
1	-2.947121	1.365730	0.879211
7	-1.152758	2.223493	1.442784
1	-3.089023	5.587355	1.734189
35	-5.117296	3.459970	0.856249

---

*Conformer*_14

Number of imaginary frequencies : 0
The smallest frequency is : 13.2433 cm(-1)
Electronic energy : HF=-4521.7138804
Zero-point correction= 0.854507
(Hartree/Particle)
Thermal correction to Energy= 0.923919
Thermal correction to Enthalpy= 0.924863
Thermal correction to Gibbs Free Energy= 0.744389
Sum of electronic and zero-point Energies= -4520.859373
Sum of electronic and thermal Energies= -4520.789961
Sum of electronic and thermal Enthalpies= -4520.789017
Sum of electronic and thermal Free Energies= -4520.969492

Cartesian Coordinates

26	-3.598294	-1.128994	-2.692458
15	-1.126176	-1.576370	1.911506
15	0.662753	0.066265	-0.938174
6	-2.360251	-1.491322	-1.039917
6	-1.858664	-0.399652	-1.842692
6	-2.862072	0.616079	-1.876385
1	-2.792636	1.555685	-2.406817
6	-3.989897	0.155811	-1.133726
1	-4.924268	0.684406	-1.006679
6	-3.683247	-1.138294	-0.620557
1	-4.342994	-1.760127	-0.035136
6	-3.206042	-2.085668	-4.494163
1	-2.219698	-2.370870	-4.836196
6	-3.843082	-0.828526	-4.727506
1	-3.421752	0.006979	-5.270471
6	-5.114243	-0.849514	-4.076250
1	-5.819866	-0.030215	-4.034237
6	-5.263438	-2.119302	-3.439493
1	-6.103643	-2.432427	-2.833778
6	-4.086261	-2.883300	-3.698189
1	-3.884472	-3.878564	-3.325768
6	-1.561142	-2.700902	-0.683666
6	-1.264502	-3.638571	-1.685275
1	-1.677792	-3.478368	-2.672959
6	-0.441891	-4.739288	-1.447463
1	-0.209097	-5.427159	-2.254318
6	0.095854	-4.930892	-0.177340
1	0.750285	-5.773390	0.022391
6	-0.186710	-4.015206	0.836537
1	0.254704	-4.168709	1.814609
6	-0.997442	-2.890916	0.608350
6	-0.467547	-0.326880	-2.411395
1	-0.193008	-1.333890	-2.729647
6	-0.325103	0.615312	-3.609136
1	0.693385	0.591178	-4.006882
1	-0.557969	1.651457	-3.349193
1	-1.015080	0.302756	-4.399233
6	-0.217171	-2.273271	3.356014
6	-0.752245	-3.273208	4.185749
1	-1.746972	-3.665282	3.998673
6	-0.011071	-3.768165	5.258679
1	-0.434412	-4.540367	5.895125
6	1.271247	-3.272075	5.514477
1	1.846492	-3.658727	6.351238
6	1.807007	-2.275170	4.697693
1	2.800900	-1.884530	4.891988
6	1.065769	-1.771849	3.625370
1	1.473475	-0.975599	3.011264
6	-2.875100	-1.630518	2.472682
6	-3.398617	-0.476761	3.074503
1	-2.770769	0.402998	3.184370
6	-4.722161	-0.451356	3.518479
1	-5.119611	0.449733	3.976940
6	-5.533400	-1.578551	3.364054
1	-6.565736	-1.556256	3.701504
6	-5.014237	-2.736224	2.775940
1	-5.640421	-3.616454	2.659477
6	-3.690351	-2.764440	2.333496
1	-3.298307	-3.661414	1.862918
6	1.940425	-1.258492	-0.884931
6	2.784086	-1.232937	0.236064
1	2.672481	-0.429514	0.959600
6	3.735485	-2.234931	0.425830
6	3.832566	-3.304452	-0.462606
1	4.551205	-4.099393	-0.296788
6	2.973592	-3.340679	-1.561557
6	2.051833	-2.319151	-1.791402
1	1.417578	-2.381487	-2.665912
6	1.614680	1.582332	-1.361613
6	0.913794	2.796447	-1.278962
1	-0.145544	2.796030	-1.049683
6	1.583420	4.006605	-1.427706
6	2.966070	4.039243	-1.619362
1	3.490934	4.985375	-1.687852
6	3.663960	2.835613	-1.671936
6	2.996739	1.612245	-1.568052
1	3.570213	0.693985	-1.606530
29	-0.276482	0.379521	1.172922
6	5.159293	2.850675	-1.825693
6	0.851166	5.307000	-1.250140
6	4.685367	-2.114732	1.584802
6	3.035795	-4.533692	-2.474006
9	2.766836	-5.682097	-1.802839
9	2.151948	-4.456343	-3.493532
9	4.265552	-4.689305	-3.018451
9	5.664359	-1.210010	1.329801
9	5.293339	-3.282303	1.881226
9	4.059954	-1.688698	2.710399
9	5.544755	2.870527	-3.123219
9	5.733004	1.759538	-1.264078
9	5.712865	3.938816	-1.237734
9	1.175577	6.199675	-2.214996
9	-0.489528	5.154986	-1.271186
9	1.164835	5.896305	-0.066299
6	1.867929	2.331192	2.008126
6	0.922244	3.389017	2.090226
6	-0.466479	3.354329	1.836726
1	1.303670	4.376134	2.312248
7	3.211781	2.654264	1.952314
6	4.230097	1.626134	2.099300
1	5.037719	1.997161	2.741719
1	3.803756	0.737821	2.558799
1	4.669225	1.348009	1.131928
6	3.716356	4.004463	1.754914
1	3.001849	4.612104	1.200792
1	3.947459	4.507050	2.705861
1	4.634826	3.957811	1.161302
8	1.571587	1.083445	1.990982
6	-1.205418	4.584281	1.939645
6	-2.547968	4.649737	1.658519
1	-0.673402	5.484115	2.232110
6	-3.193925	3.463917	1.266526
6	-2.473771	2.293914	1.174693
1	-2.946921	1.366159	0.879256
7	-1.152439	2.223677	1.442813
1	-3.088305	5.587776	1.734315
35	-5.116858	3.460617	0.856446

---

*Conformer*_15

Number of imaginary frequencies : 0
The smallest frequency is : 14.9981 cm(-1)
Electronic energy : HF=-4521.7138308

Zero-point correction= 0.854732
(Hartree/Particle)
Thermal correction to Energy= 0.924102
Thermal correction to Enthalpy= 0.925046
Thermal correction to Gibbs Free Energy= 0.744578
Sum of electronic and zero-point Energies= -4520.859099
Sum of electronic and thermal Energies= -4520.789729
Sum of electronic and thermal Enthalpies= -4520.788785
Sum of electronic and thermal Free Energies= -4520.969253

Cartesian Coordinates

26	-3.560932	-1.210145	-2.713212
15	-1.138777	-1.582976	1.924634
15	0.658129	0.064715	-0.920201
6	-2.336431	-1.538587	-1.043172
6	-1.845404	-0.444149	-1.848955
6	-2.865945	0.553539	-1.901384
1	-2.807047	1.490194	-2.438231
6	-3.994062	0.078558	-1.168377
1	-4.939294	0.591196	-1.056503
6	-3.670561	-1.206359	-0.642334
1	-4.326236	-1.835603	-0.060344
6	-3.126773	-2.158882	-4.509413
1	-2.129605	-2.416674	-4.841460
6	-3.796935	-0.920494	-4.750606
1	-3.394545	-0.074308	-5.291459
6	-5.072518	-0.976001	-4.110021
1	-5.801400	-0.176965	-4.076074
6	-5.191277	-2.248338	-3.471824
1	-6.027430	-2.583852	-2.872560
6	-3.991118	-2.979484	-3.719375
1	-3.765010	-3.968028	-3.343243
6	-1.515217	-2.727980	-0.670348
6	-1.178747	-3.658328	-1.666352
1	-1.584661	-3.511629	-2.659295
6	-0.324242	-4.731598	-1.417085
1	-0.057563	-5.411975	-2.219834
6	0.202562	-4.905260	-0.139594
1	0.879736	-5.727289	0.069988
6	-0.121918	-3.998661	0.869507
1	0.311228	-4.137612	1.853424
6	-0.963058	-2.899337	0.628986
6	-0.449941	-0.353334	-2.404260
1	-0.157110	-1.357774	-2.715806
6	-0.310492	0.586097	-3.604585
1	0.712468	0.577629	-3.991399
1	-0.563666	1.619269	-3.351525
1	-0.986495	0.258708	-4.400806
6	-0.241941	-2.257270	3.387335
6	1.022618	-1.724116	3.681301
1	1.421579	-0.917183	3.075483
6	1.756214	-2.209896	4.766935
1	2.736316	-1.794493	4.979747
6	1.230798	-3.221199	5.572524
1	1.799941	-3.594756	6.419351
6	-0.033897	-3.748698	5.292505
1	-0.449501	-4.532069	5.920347
6	-0.767319	-3.271077	4.206506
1	-1.748411	-3.687605	4.001109
6	-2.895871	-1.664792	2.456101
6	-3.685744	-2.816712	2.318032
1	-3.267721	-3.711388	1.865712
6	-5.017485	-2.809565	2.737031
1	-5.623725	-3.703783	2.621615
6	-5.570051	-1.655022	3.300429
1	-6.608351	-1.649298	3.619770
6	-4.784471	-0.509668	3.453516
1	-5.207800	0.389164	3.892875
6	-3.452995	-0.514139	3.033081
1	-2.844950	0.379448	3.142434
6	1.960244	-1.235577	-0.854954
6	2.771729	-1.216582	0.289878
1	2.617162	-0.436395	1.030648
6	3.753961	-2.189075	0.473332
6	3.920686	-3.219201	-0.451240
1	4.670562	-3.986567	-0.295365
6	3.097409	-3.247967	-1.576987
6	2.137399	-2.257988	-1.793330
1	1.532742	-2.306486	-2.689628
6	1.592660	1.591633	-1.344507
6	0.877769	2.798005	-1.271158
1	-0.182619	2.786445	-1.047349
6	1.534761	4.014897	-1.421804
6	2.917842	4.062010	-1.607130
1	3.432628	5.013431	-1.678067
6	3.629474	2.866114	-1.650563
6	2.975495	1.635956	-1.543409
1	3.559174	0.723760	-1.573817
29	-0.306958	0.377363	1.179446
6	5.125104	2.896718	-1.798369
6	0.787620	5.307733	-1.251349
6	4.670772	-2.074636	1.659310
6	3.222450	-4.404259	-2.529644
9	2.707780	-5.544417	-2.000782
9	2.574208	-4.187272	-3.695314
9	4.514414	-4.673120	-2.827704
9	5.647905	-1.157560	1.443090
9	5.282920	-3.240551	1.954922
9	4.011256	-1.671148	2.773061
9	5.515595	2.908179	-3.094508
9	5.708496	1.817446	-1.224009
9	5.664035	3.996561	-1.218727
9	1.110679	6.203418	-2.213865
9	-0.551192	5.141605	-1.283277
9	1.085536	5.900596	-0.065238
6	1.812370	2.347615	2.029743
6	0.858720	3.399265	2.098478
6	-0.526942	3.352605	1.830319
1	1.230744	4.390165	2.319850
7	3.154337	2.678018	1.979289
6	4.177544	1.655376	2.131009
1	4.985307	2.035046	2.768018
1	3.756766	0.768581	2.598664
1	4.615046	1.371938	1.164419
6	3.652516	4.029064	1.771250
1	2.933072	4.630202	1.216470
1	3.885320	4.538189	2.718222
1	4.568817	3.982986	1.174123
8	1.523209	1.098074	2.021271
6	-1.277470	4.576211	1.923715
6	-2.616282	4.630813	1.623180
1	-0.757088	5.480201	2.224148
6	-3.246878	3.440043	1.221102
6	-2.516326	2.275657	1.140716
1	-2.977285	1.343879	0.838375
7	-1.198681	2.216051	1.428724
1	-3.165253	5.564381	1.691584
35	-5.162928	3.422066	0.780349

---

*Conformer*_16

Number of imaginary frequencies : 0
The smallest frequency is : 13.2538 cm(-1)
Electronic energy : HF=-4521.7138804
Zero-point correction= 0.854519
(Hartree/Particle)
Thermal correction to Energy= 0.923926
Thermal correction to Enthalpy= 0.924871
Thermal correction to Gibbs Free Energy= 0.744439
Sum of electronic and zero-point Energies= -4520.859361
Sum of electronic and thermal Energies= -4520.789954
Sum of electronic and thermal Enthalpies= -4520.789010
Sum of electronic and thermal Free Energies= -4520.969442

Cartesian Coordinates

26	-3.598708	-1.128678	-2.691959
15	-1.125589	-1.577395	1.911490
15	0.662446	0.066819	-0.937563

6	-2.360738	-1.491599	-1.039473
6	-1.859194	-0.399485	-1.841668
6	-2.862752	0.616113	-1.875041
1	-2.793410	1.555966	-2.405050
6	-3.990570	0.155358	-1.132671
1	-4.924992	0.683800	-1.005375
6	-3.683791	-1.138948	-0.620088
1	-4.343445	-1.760949	-0.034777
6	-3.206151	-2.084051	-4.494305
1	-2.219715	-2.368774	-4.836463
6	-3.843490	-0.826908	-4.726815
1	-3.422340	0.009080	-5.269172
6	-5.114674	-0.848644	-4.075633
1	-5.820483	-0.029532	-4.033101
6	-5.263599	-2.118899	-3.439759
1	-6.103751	-2.432642	-2.834290
6	-4.086238	-2.882442	-3.698945
1	-3.884289	-3.877938	-3.327237
6	-1.561268	-2.701134	-0.683855
6	-1.264734	-3.638345	-1.685942
1	-1.678647	-3.478027	-2.673338
6	-0.441421	-4.738726	-1.448981
1	-0.208751	-5.426213	-2.256203
6	0.097182	-4.930468	-0.179242
1	0.752172	-5.772689	0.019832
6	-0.185274	-4.015245	0.835082
1	0.256763	-4.168772	1.812860
6	-0.996647	-2.891282	0.607680
6	-0.468166	-0.326504	-2.410550
1	-0.193661	-1.333556	-2.728714
6	-0.325976	0.615521	-3.608450
1	0.692485	0.591473	-4.006276
1	-0.558953	1.651679	-3.348636
1	-1.015974	0.302757	-4.398439
6	-0.216414	-2.274779	3.355695
6	-0.750842	-3.275801	4.184566
1	-1.745198	-3.668643	3.997078
6	-0.009597	-3.770845	5.257401
1	-0.432472	-4.543890	5.893132
6	1.272159	-3.273740	5.514068
1	1.847444	-3.660450	6.350774
6	1.807249	-2.275721	4.698223
1	2.800679	-1.884218	4.893179
6	1.065950	-1.772347	3.625964
1	1.473251	-0.975285	3.012640
6	-2.874653	-1.631966	2.472202
6	-3.398836	-0.478276	3.073513
1	-2.771445	0.401803	3.183072
6	-4.722479	-0.453347	3.517247
1	-5.120414	0.447701	3.975369
6	-5.533166	-1.580963	3.363031
1	-6.565560	-1.559058	3.700325
6	-5.013377	-2.738553	2.775283
1	-5.639151	-3.619081	2.658887
6	-3.689397	-2.766288	2.333122
1	-3.296881	-3.663186	1.862724
6	1.940395	-1.257692	-0.884991
6	2.783755	-1.232975	0.236237
1	2.671878	-0.430168	0.960413
6	3.735227	-2.235011	0.425393
6	3.832629	-3.303796	-0.463899
1	4.551280	-4.098821	-0.298522
6	2.973953	-3.339198	-1.563115
6	2.052198	-2.317534	-1.792359
1	1.418206	-2.379037	-2.667116
6	1.613947	1.583069	-1.361189
6	0.912982	2.797119	-1.278234
1	-0.146313	2.796614	-1.048755
6	1.582501	4.007339	-1.426960
6	2.965106	4.040099	-1.618932
1	3.489890	4.986276	-1.687397
6	3.663072	2.836530	-1.671854
6	2.995963	1.613107	-1.567935
1	3.569467	0.694872	-1.606652
29	-0.276342	0.379082	1.174119
6	5.158358	2.851679	-1.826044
6	0.850229	5.307660	-1.248940
6	4.684897	-2.115620	1.584627
6	3.036436	-4.531452	-2.476541
9	2.768320	-5.680519	-1.806174
9	2.152160	-4.453739	-3.495663
9	4.266055	-4.686006	-3.021601
9	5.664305	-1.211190	1.330135
9	5.292365	-3.283539	1.880743
9	4.059441	-1.689747	2.710244
9	5.543442	2.871211	-3.123688
9	5.732307	1.760726	-1.264315
9	5.712025	3.940011	-1.238531
9	1.174536	6.200640	-2.213547
9	-0.490465	5.155621	-1.269920
9	1.163993	5.896593	-0.064939
6	1.868269	2.330517	2.008928
6	0.922684	3.388406	2.091373
6	-0.466061	3.353854	1.837970
1	1.304221	4.375473	2.313441
7	3.212136	2.653420	1.952731
6	4.230354	1.625074	2.098931
1	5.038597	1.996009	2.740613
1	3.804241	0.736877	2.558876
1	4.668596	1.346767	1.131206
6	3.716863	4.003508	1.754920
1	3.001934	4.611399	1.201622
1	3.949098	4.505912	2.705683
1	4.634695	3.956702	1.160331
8	1.571776	1.082802	1.991851
6	-1.204883	4.583870	1.940967
6	-2.547374	4.649524	1.659607
1	-0.672803	5.483610	2.233603
6	-3.193408	3.463827	1.267362
6	-2.473411	2.293716	1.175651
1	-2.946652	1.366039	0.880096
7	-1.152137	2.223285	1.444017
1	-3.087604	5.587625	1.735402
35	-5.116221	3.460847	0.856698

---

*Conformer*_17

Number of imaginary frequencies : 0
The smallest frequency is : 13.2979 cm(-1)
Electronic energy : HF=-4521.7138803
Zero-point correction= 0.854510
(Hartree/Particle)
Thermal correction to Energy= 0.923920
Thermal correction to Enthalpy= 0.924864
Thermal correction to Gibbs Free Energy= 0.744404
Sum of electronic and zero-point Energies= -4520.859371
Sum of electronic and thermal Energies= -4520.789961
Sum of electronic and thermal Enthalpies= -4520.789016
Sum of electronic and thermal Free Energies= -4520.969476

.....

Cartesian Coordinates

.....

26	-3.597981	-1.129408	-2.692757
15	-1.126147	-1.576253	1.911509
15	0.662837	0.066230	-0.938193
6	-2.360124	-1.491531	-1.040009
6	-1.858509	-0.399888	-1.842809
6	-2.861980	0.615773	-1.876720
1	-2.792531	1.555338	-2.407223
6	-3.989874	0.155489	-1.134180
1	-4.924302	0.684030	-1.007331
6	-3.683205	-1.138559	-0.620872
1	-4.342995	-1.760393	-0.035500
6	-3.205488	-2.086310	-4.494303
1	-2.219096	-2.371563	-4.836159
6	-3.842469	-0.829185	-4.727884
1	-3.421047	0.006248	-5.270888
6	-5.113723	-0.850069	-4.076804
1	-5.819335	-0.030751	-4.034994
6	-5.263031	-2.119776	-3.439912

1	-6.103323	-2.432805	-2.834267
6	-4.085831	-2.883826	-3.698350
1	-3.884107	-3.879047	-3.325776
6	-1.560969	-2.701037	-0.683588
6	-1.264190	-3.638748	-1.685120
1	-1.677506	-3.478681	-2.672814
6	-0.441389	-4.739307	-1.447237
1	-0.208483	-5.427195	-2.254046
6	0.096406	-4.930716	-0.177107
1	0.751009	-5.773068	0.022677
6	-0.186340	-4.015020	0.836711
1	0.255113	-4.168381	1.814787
6	-0.997278	-2.890889	0.608457
6	-0.467362	-0.327082	-2.411434
1	-0.192779	-1.334111	-2.729591
6	-0.324887	0.615035	-3.609232
1	0.693618	0.590884	-4.006935
1	-0.557771	1.651193	-3.349360
1	-1.014830	0.302421	-4.399335
6	-0.217393	-2.273051	3.356217
6	1.065429	-1.771476	3.625847
1	1.473156	-0.975166	3.011835
6	1.806510	-2.274727	4.698312
1	2.800319	-1.883972	4.892815
6	1.270697	-3.271708	5.514967
1	1.845816	-3.658310	6.351839
6	-0.011520	-3.767933	5.258910
1	-0.434907	-4.540178	5.895273
6	-0.752535	-3.273042	4.185842
1	-1.747209	-3.665164	3.998588
6	-2.875112	-1.630276	2.472534
6	-3.398524	-0.476531	3.074481
1	-2.770615	0.403187	3.184391
6	-4.722041	-0.451089	3.518538
1	-5.119411	0.449983	3.977099
6	-5.533359	-1.578219	3.364061
1	-6.565677	-1.555886	3.701563
6	-5.014287	-2.735890	2.775858
1	-5.640523	-3.616083	2.659390
6	-3.690423	-2.764160	2.333356
1	-3.298446	-3.661179	1.862791
6	1.940620	-1.258409	-0.884830
6	2.784066	-1.232875	0.236324
1	2.672270	-0.429505	0.959891
6	3.735488	-2.234822	0.426208
6	3.832791	-3.304289	-0.462271
1	4.551433	-4.099208	-0.296358
6	2.974032	-3.340492	-1.561393
6	2.052277	-2.318987	-1.791363
1	1.418223	-2.381264	-2.666024
6	1.614641	1.582368	-1.361651
6	0.913662	2.796430	-1.279010
1	-0.145677	2.795928	-1.049729
6	1.583200	4.006636	-1.427768
6	2.965846	4.039374	-1.619431
1	3.490638	4.985544	-1.687937
6	3.663827	2.835796	-1.671996
6	2.996698	1.612379	-1.568094
1	3.570237	0.694159	-1.606564
29	-0.276409	0.379545	1.172837
6	5.159157	2.850970	-1.825779
6	0.850857	5.306980	-1.250209
6	4.685125	-2.114622	1.585382
6	3.036423	-4.533473	-2.473869
9	2.767510	-5.681913	-1.802742
9	2.152644	-4.456182	-3.493459
9	4.266234	-4.688964	-3.018225
9	5.664134	-1.209854	1.330610
9	5.293084	-3.282177	1.881903
9	4.059454	-1.688644	2.710857
9	5.544589	2.870842	-3.123313
9	5.732958	1.759879	-1.264169
9	5.712657	3.939157	-1.237840
9	1.175230	6.199681	-2.215054
9	-0.489825	5.154878	-1.271282
9	1.164464	5.896303	-0.066360
6	1.867718	2.331366	2.008141
6	0.921919	3.389092	2.090216
6	-0.466803	3.354263	1.836707
1	1.303240	4.376251	2.312237
7	3.211535	2.654558	1.952311
6	4.229953	1.626505	2.099145
1	5.037649	1.997608	2.741423
1	3.803769	0.738158	2.558726
1	4.668942	1.348410	1.131700
6	3.715984	4.004796	1.754843
1	3.001384	4.612366	1.200766
1	3.947120	4.507417	2.705763
1	4.634410	3.958208	1.161158
8	1.571499	1.083584	1.991050
6	-1.205876	4.584129	1.939669
6	-2.548419	4.649456	1.658480
1	-0.673972	5.484004	2.232212
6	-3.194245	3.463592	1.266403
6	-2.473976	2.293657	1.174572
1	-2.947016	1.365845	0.879112
7	-1.152646	2.223560	1.442742
1	-3.088854	5.587436	1.734301
35	-5.117151	3.460184	0.856180

---

*Conformer*_18

Number of imaginary frequencies : 0
The smallest frequency is : 13.2386 cm(-1)
Electronic energy : HF=-4521.7138803
Zero-point correction= 0.854508
(Hartree/Particle)
Thermal correction to Energy= 0.923919
Thermal correction to Enthalpy= 0.924863
Thermal correction to Gibbs Free Energy= 0.744396
Sum of electronic and zero-point Energies= -4520.859372
Sum of electronic and thermal Energies= -4520.789961
Sum of electronic and thermal Enthalpies= -4520.789017
Sum of electronic and thermal Free Energies= -4520.969484

Cartesian Coordinates

26	-3.598109	-1.129640	-2.692546
15	-1.126140	-1.576301	1.911642
15	0.662697	0.066235	-0.938135
6	-2.360172	-1.491685	-1.039859
6	-1.858689	-0.399975	-1.842649
6	-2.862257	0.615596	-1.876487
1	-2.792925	1.555183	-2.406965
6	-3.990077	0.155183	-1.133910
1	-4.924547	0.683631	-1.006984
6	-3.683269	-1.138851	-0.620658
1	-4.342982	-1.760763	-0.035286
6	-3.205487	-2.086335	-4.494161
1	-2.219047	-2.371377	-4.836053
6	-3.842713	-0.829313	-4.727637
1	-3.421456	0.006238	-5.270587
6	-5.113946	-0.850482	-4.076527
1	-5.819713	-0.031302	-4.034640
6	-5.263001	-2.120265	-3.439727
1	-6.103223	-2.433501	-2.834091
6	-4.085665	-2.884076	-3.698251
1	-3.883749	-3.879289	-3.325761
6	-1.560849	-2.701090	-0.683474
6	-1.263942	-3.638731	-1.685032
1	-1.677266	-3.478681	-2.672726
6	-0.441003	-4.739192	-1.447176
1	-0.207994	-5.427021	-2.254005
6	0.096803	-4.930571	-0.177046
1	0.751509	-5.772849	0.022717
6	-0.186063	-4.014941	0.836797
1	0.255405	-4.168270	1.814871
6	-0.997143	-2.890907	0.608570
6	-0.467575	-0.327075	-2.411345
1	-0.192988	-1.334079	-2.729593

6	-0.325218	0.615112	-3.609103
1	0.693275	0.591068	-4.006841
1	-0.558185	1.651238	-3.349179
1	-1.015160	0.302481	-4.399200
6	-0.217310	-2.273030	3.356346
6	1.065518	-1.771417	3.625885
1	1.473201	-0.975126	3.011817
6	1.806674	-2.274601	4.698328
1	2.800485	-1.883813	4.892752
6	1.270934	-3.271559	5.515060
1	1.846110	-3.658112	6.351914
6	-0.011288	-3.767819	5.259099
1	-0.434623	-4.540043	5.895522
6	-0.752378	-3.272995	4.186050
1	-1.747054	-3.665154	3.998891
6	-2.875105	-1.630423	2.472694
6	-3.398609	-0.476647	3.074505
1	-2.770787	0.403153	3.184257
6	-4.722104	-0.451281	3.518631
1	-5.119542	0.449806	3.977103
6	-5.533310	-1.578520	3.364354
1	-6.565608	-1.556256	3.701924
6	-5.014157	-2.736207	2.776258
1	-5.640308	-3.616478	2.659937
6	-3.690312	-2.764402	2.333691
1	-3.298254	-3.661448	1.863255
6	1.940537	-1.258349	-0.884868
6	2.783974	-1.232907	0.236296
1	2.672144	-0.429632	0.959962
6	3.735462	-2.234820	0.426042
6	3.832833	-3.304163	-0.462580
1	4.551518	-4.099063	-0.296765
6	2.974084	-3.340274	-1.561712
6	2.052279	-2.318786	-1.791549
1	1.418244	-2.380926	-2.666227
6	1.614461	1.582389	-1.361621
6	0.913480	2.796447	-1.278947
1	-0.145853	2.795938	-1.049648
6	1.583014	4.006656	-1.427668
6	2.965658	4.039404	-1.619346
1	3.490446	4.985581	-1.687803
6	3.663640	2.835830	-1.671967
6	2.996513	1.612409	-1.568089
1	3.570050	0.694188	-1.606594
29	-0.276479	0.379545	1.172984
6	5.158965	2.851003	-1.825779
6	0.850680	5.307002	-1.250104
6	4.685112	-2.114713	1.585214
6	3.036509	-4.533153	-2.474320
9	2.767571	-5.681668	-1.803326
9	2.152757	-4.455751	-3.493924
9	4.266334	-4.688592	-3.018654
9	5.664132	-1.209942	1.330493
9	5.293061	-3.282297	1.881645
9	4.059462	-1.688807	2.710727
9	5.544375	2.870836	-3.123322
9	5.732778	1.759928	-1.264149
9	5.712478	3.939207	-1.237882
9	1.174679	6.199532	-2.215235
9	-0.490003	5.154846	-1.270688
9	1.164688	5.896561	-0.066478
6	1.867779	2.331339	2.008161
6	0.922026	3.389102	2.090303
6	-0.466690	3.354327	1.836756
1	1.303387	4.376240	2.312354
7	3.211610	2.654469	1.952337
6	4.229964	1.626334	2.099036
1	5.037777	1.997380	2.741198
1	3.803770	0.738025	2.558687
1	4.668796	1.348186	1.131536
6	3.716125	4.004679	1.754841
1	3.001517	4.612298	1.200824
1	3.947362	4.507278	2.705748
1	4.634502	3.958046	1.161086
8	1.571505	1.083573	1.991011
6	-1.205725	4.584218	1.939693
6	-2.548236	4.649614	1.658362
1	-0.673809	5.484064	2.232305
6	-3.194069	3.463786	1.266185
6	-2.473852	2.293813	1.174456
1	-2.946912	1.366022	0.878969
7	-1.152553	2.223646	1.442764
1	-3.088638	5.587617	1.734141
35	-5.116903	3.460462	0.855641

---

*Conformer_*19

Number of imaginary frequencies : 0
The smallest frequency is : 13.2488 cm(-1)
Electronic energy : HF=-4521.7138804
Zero-point correction= 0.854508
(Hartree/Particle)
Thermal correction to Energy= 0.923919
Thermal correction to Enthalpy= 0.924863
Thermal correction to Gibbs Free Energy= 0.744393
Sum of electronic and zero-point Energies= -4520.859372
Sum of electronic and thermal Energies= -4520.789961
Sum of electronic and thermal Enthalpies= -4520.789017
Sum of electronic and thermal Free Energies= -4520.969488

Cartesian Coordinates

26	-3.598057	-1.129958	-2.692555
15	-1.126008	-1.576199	1.911708
15	0.662743	0.066136	-0.938266
6	-2.360119	-1.491835	-1.039816
6	-1.858661	-0.400176	-1.842691
6	-2.862262	0.615360	-1.876626
1	-2.792951	1.554909	-2.407174
6	-3.990082	0.154973	-1.134031
1	-4.924574	0.683395	-1.007163
6	-3.683238	-1.139011	-0.620675
1	-4.342939	-1.760903	-0.035267
6	-3.205432	-2.086835	-4.494079
1	-2.218996	-2.371923	-4.835943
6	-3.842644	-0.829830	-4.727682
1	-3.421385	0.005662	-5.270722
6	-5.113881	-0.850926	-4.076576
1	-5.819644	-0.031737	-4.034775
6	-5.262949	-2.120644	-3.439650
1	-6.103175	-2.433815	-2.833988
6	-4.085619	-2.884490	-3.698093
1	-3.883718	-3.879667	-3.325501
6	-1.560833	-2.701224	-0.683298
6	-1.263965	-3.638984	-1.684756
1	-1.677219	-3.478979	-2.672486
6	-0.441172	-4.739521	-1.446752
1	-0.208198	-5.427451	-2.253505
6	0.096523	-4.930857	-0.176569
1	0.751095	-5.773209	0.023319
6	-0.186275	-4.015089	0.837168
1	0.255116	-4.168386	1.815281
6	-0.997195	-2.890969	0.608791
6	-0.467553	-0.327259	-2.411405
1	-0.192915	-1.334263	-2.729592
6	-0.325239	0.614866	-3.609216
1	0.693241	0.590801	-4.006987
1	-0.558194	1.651006	-3.349335
1	-1.015209	0.302192	-4.399272
6	-0.217098	-2.272801	3.356421
6	1.065841	-1.771328	3.625694
1	1.473536	-0.975182	3.011446
6	1.807085	-2.274460	4.698100
1	2.800978	-1.883783	4.892324
6	1.271324	-3.271225	5.515055
1	1.846571	-3.657740	6.351878
6	-0.011005	-3.767343	5.259358
1	-0.434354	-4.539416	5.895955
6	-0.752182	-3.272572	4.186343
1	-1.746940	-3.664615	3.999386

6	-2.874920	-1.629991	2.472952
6	-3.398117	-0.476095	3.074801
1	-2.770093	0.403570	3.184450
6	-4.721552	-0.450437	3.519080
1	-5.118750	0.450749	3.977563
6	-5.533005	-1.577519	3.364950
1	-6.565257	-1.555032	3.702643
6	-5.014158	-2.735333	2.776836
1	-5.640502	-3.615482	2.660625
6	-3.690376	-2.763809	2.334094
1	-3.298580	-3.660940	1.863620
6	1.940606	-1.258429	-0.884937
6	2.784211	-1.232699	0.236094
1	2.672473	-0.429239	0.959569
6	3.735705	-2.234577	0.425987
6	3.832942	-3.304156	-0.462364
1	4.551651	-4.099014	-0.296450
6	2.974027	-3.340556	-1.561356
6	2.052173	-2.319140	-1.791329
1	1.417978	-2.381591	-2.665876
6	1.614411	1.582334	-1.361806
6	0.913340	2.796339	-1.279102
1	-0.145981	2.795745	-1.049744
6	1.582771	4.006601	-1.427862
6	2.965405	4.039452	-1.619607
1	3.490120	4.985666	-1.688106
6	3.663477	2.835930	-1.672247
6	2.996450	1.612456	-1.568338
1	3.570059	0.694281	-1.606864
29	-0.276360	0.379565	1.172821
6	5.158797	2.851223	-1.826110
6	0.850332	5.306887	-1.250258
6	4.685488	-2.114191	1.585022
6	3.036354	-4.533669	-2.473664
9	2.767297	-5.681995	-1.802398
9	2.152638	-4.456438	-3.493313
9	4.266182	-4.689352	-3.017923
9	5.664375	-1.209349	1.330050
9	5.293596	-3.281664	1.881554
9	4.059927	-1.688185	2.710551
9	5.544164	2.871138	-3.123663
9	5.732715	1.760172	-1.264539
9	5.712245	3.939446	-1.238187
9	1.174380	6.199526	-2.215273
9	-0.490340	5.154641	-1.270998
9	1.164161	5.896366	-0.066547
6	1.867741	2.331564	2.007923
6	0.921887	3.389234	2.090105
6	-0.466824	3.354346	1.836557
1	1.303159	4.376397	2.312195
7	3.211539	2.654833	1.952075
6	4.230002	1.626809	2.098786
1	5.037772	1.997945	2.740952
1	3.803899	0.738459	2.558436
1	4.668874	1.348707	1.131290
6	3.715920	4.005093	1.754576
1	3.001227	4.612657	1.200611
1	3.947165	4.507694	2.705479
1	4.634269	3.958551	1.160769
8	1.571595	1.083770	1.990759
6	-1.205962	4.584172	1.939538
6	-2.548484	4.649459	1.658237
1	-0.674118	5.484054	2.232165
6	-3.194220	3.463585	1.266040
6	-2.473897	2.293684	1.174239
1	-2.946877	1.365874	0.878696
7	-1.152590	2.223620	1.442522
1	-3.088966	5.587413	1.734056
35	-5.117073	3.460078	0.855596

---

*Conformer*_20

Number of imaginary frequencies : 0
The smallest frequency is : 15.0427 cm(-1)
Electronic energy : HF=-4521.713831

Zero-point correction= 0.854735
(Hartree/Particle)
Thermal correction to Energy= 0.924103
Thermal correction to Enthalpy= 0.925047
Thermal correction to Gibbs Free Energy= 0.744598
Sum of electronic and zero-point Energies= -4520.859096
Sum of electronic and thermal Energies= -4520.789728
Sum of electronic and thermal Enthalpies= -4520.788784
Sum of electronic and thermal Free Energies= -4520.969233

Cartesian Coordinates

26	-3.560730	-1.211117	-2.713246
15	-1.139101	-1.582565	1.924984
15	0.658045	0.064578	-0.920077
6	-2.336466	-1.539148	-1.042933
6	-1.845496	-0.444722	-1.848768
6	-2.866204	0.552782	-1.901480
1	-2.807379	1.489377	-2.438437
6	-3.994372	0.077683	-1.168623
1	-4.939728	0.590149	-1.057015
6	-3.670739	-1.207133	-0.642406
1	-4.326406	-1.836484	-0.060518
6	-3.126103	-2.160180	-4.509168
1	-2.128840	-2.417992	-4.840915
6	-3.796268	-0.921873	-4.750762
1	-3.393801	-0.075773	-5.291692
6	-5.071998	-0.977314	-4.110464
1	-5.800935	-0.178313	-4.076864
6	-5.190849	-2.249534	-3.472050
1	-6.027127	-2.584971	-2.872918
6	-3.990597	-2.980669	-3.719177
1	-3.764533	-3.969130	-3.342802
6	-1.515134	-2.728331	-0.669712
6	-1.178505	-3.658951	-1.665397
1	-1.584312	-3.512571	-2.658433
6	-0.323997	-4.732121	-1.415698
1	-0.057214	-5.412736	-2.218205
6	0.202689	-4.905356	-0.138101
1	0.879864	-5.727303	0.071819
6	-0.121961	-3.998473	0.870697
1	0.311074	-4.137121	1.854704
6	-0.963135	-2.899267	0.629740
6	-0.450023	-0.353795	-2.404031
1	-0.157053	-1.358236	-2.715461
6	-0.310659	0.585528	-3.604457
1	0.712307	0.577117	-3.991258
1	-0.563926	1.618702	-3.351499
1	-0.986618	0.258001	-4.400656
6	-0.242222	-2.256450	3.387847
6	1.022575	-1.723620	3.681370
1	1.421646	-0.916995	3.075220
6	1.756237	-2.209300	4.767002
1	2.736514	-1.794150	4.979484
6	1.230677	-3.220201	5.573008
1	1.799894	-3.593688	6.419816
6	-0.034241	-3.747380	5.293422
1	-0.449955	-4.530438	5.921581
6	-0.767748	-3.269846	4.207438
1	-1.748991	-3.686155	4.002347
6	-2.896226	-1.664372	2.456353
6	-3.453684	-0.513623	3.032806
1	-2.845853	0.380132	3.141933
6	-4.785254	-0.509250	3.452945
1	-5.208846	0.389664	3.891883
6	-5.570592	-1.654804	3.300110
1	-6.608960	-1.649154	3.619231
6	-5.017691	-2.809452	2.737259
1	-5.623735	-3.703830	2.622057
6	-3.685866	-2.816490	2.318532
1	-3.267549	-3.711294	1.866720
6	1.960278	-1.235597	-0.854760
6	2.771646	-1.216574	0.290160
1	2.616915	-0.436444	1.030953
6	3.754015	-2.188926	0.473621

6	3.920978	-3.218952	-0.451022
1	4.670959	-3.986211	-0.295148
6	3.097849	-3.247728	-1.576872
6	2.137701	-2.257878	-1.793230
1	1.533184	-2.306365	-2.689631
6	1.592504	1.591476	-1.344615
6	0.877611	2.797846	-1.271277
1	-0.182765	2.786283	-1.047413
6	1.534595	4.014735	-1.421970
6	2.917667	4.061849	-1.607360
1	3.432449	5.013270	-1.678329
6	3.629300	2.865953	-1.650810
6	2.975330	1.635796	-1.543588
1	3.559009	0.723598	-1.573981
29	-0.307185	0.377595	1.179427
6	5.124924	2.896546	-1.798673
6	0.787461	5.307573	-1.251498
6	4.670747	-2.074482	1.659659
6	3.223130	-4.403905	-2.529629
9	2.707711	-5.543959	-2.001264
9	2.575736	-4.186503	-3.695689
9	4.515191	-4.673162	-2.826899
9	5.647944	-1.157466	1.443466
9	5.282823	-3.240416	1.955346
9	4.011190	-1.670923	2.773356
9	5.515368	2.907917	-3.094826
9	5.708331	1.817313	-1.224258
9	5.663880	3.996427	-1.219125
9	1.110429	6.203225	-2.214076
9	-0.551353	5.141434	-1.283306
9	1.085479	5.900479	-0.065436
6	1.812261	2.347722	2.029680
6	0.858700	3.399464	2.098388
6	-0.526934	3.352923	1.830111
1	1.230793	4.390320	2.319846
7	3.154250	2.678017	1.979135
6	4.177369	1.655287	2.130833
1	4.985318	2.034999	2.767579
1	3.756590	0.768644	2.598770
1	4.614630	1.371582	1.164209
6	3.652529	4.028995	1.770886
1	2.933033	4.630165	1.216211
1	3.885581	4.538165	2.717772
1	4.568700	3.982781	1.173569
8	1.522985	1.098211	2.021346
6	-1.277414	4.576554	1.923568
6	-2.616167	4.631279	1.622794
1	-0.757031	5.480468	2.224232
6	-3.246747	3.440610	1.220381
6	-2.516253	2.276190	1.139989
1	-2.977184	1.344470	0.837424
7	-1.198681	2.216455	1.428284
1	-3.165101	5.564865	1.691242
35	-5.162693	3.422809	0.779180

---

*Conformer*_21

Number of imaginary frequencies : 0
The smallest frequency is : 13.2479 cm(-1)
Electronic energy : HF=-4521.7138804
Zero-point correction= 0.854510
(Hartree/Particle)
Thermal correction to Energy= 0.923920
Thermal correction to Enthalpy= 0.924865
Thermal correction to Gibbs Free Energy= 0.744403
Sum of electronic and zero-point Energies= -4520.859370
Sum of electronic and thermal Energies= -4520.789960
Sum of electronic and thermal Enthalpies= -4520.789016
Sum of electronic and thermal Free Energies= -4520.969478

Cartesian Coordinates

26	-3.598254	-1.129946	-2.692206
15	-1.125885	-1.576382	1.911808
15	0.662600	0.066133	-0.938115
6	-2.360176	-1.491914	-1.039594
6	-1.858792	-0.400212	-1.842454
6	-2.862392	0.615326	-1.876256
1	-2.793123	1.554900	-2.406766
6	-3.990146	0.154904	-1.133581
1	-4.924629	0.683314	-1.006592
6	-3.683263	-1.139109	-0.620325
1	-4.342941	-1.761045	-0.034941
6	-3.205777	-2.086766	-4.493789
1	-2.219372	-2.371848	-4.835751
6	-3.843011	-0.829756	-4.727304
1	-3.421802	0.005749	-5.270361
6	-5.114195	-0.850874	-4.076095
1	-5.819953	-0.031687	-4.034208
6	-5.263206	-2.120610	-3.439191
1	-6.103382	-2.433800	-2.833468
6	-4.085894	-2.884446	-3.697749
1	-3.883951	-3.879630	-3.325196
6	-1.560782	-2.701279	-0.683212
6	-1.263902	-3.638939	-1.684762
1	-1.677311	-3.478942	-2.672431
6	-0.440885	-4.739348	-1.446933
1	-0.207892	-5.427187	-2.253760
6	0.097030	-4.930662	-0.176840
1	0.751804	-5.772894	0.022893
6	-0.185802	-4.015017	0.836997
1	0.255767	-4.168273	1.815038
6	-0.996956	-2.891032	0.608795
6	-0.467722	-0.327292	-2.411244
1	-0.193122	-1.334309	-2.729433
6	-0.325465	0.614805	-3.609081
1	0.693010	0.590771	-4.006868
1	-0.558458	1.650945	-3.349225
1	-1.015436	0.302080	-4.399115
6	-0.216758	-2.272866	3.356445
6	1.065961	-1.770936	3.625926
1	1.473509	-0.974678	3.011728
6	1.807190	-2.273740	4.698497
1	2.800920	-1.882710	4.892851
6	1.271623	-3.270601	5.515460
1	1.846848	-3.656834	6.352429
6	-0.010494	-3.767170	5.259578
1	-0.433705	-4.539322	5.896169
6	-0.751628	-3.272753	4.186373
1	-1.746220	-3.665176	3.999270
6	-2.874823	-1.630491	2.472928
6	-3.690080	-2.764442	2.333986
1	-3.298007	-3.661574	1.863744
6	-5.014028	-2.736062	2.776237
1	-5.640215	-3.616311	2.659943
6	-5.533244	-1.578210	3.363947
1	-6.565627	-1.555792	3.701245
6	-4.721991	-0.450998	3.518182
1	-5.119473	0.450220	3.976360
6	-3.398391	-0.476557	3.074392
1	-2.770545	0.403228	3.184113
6	1.940523	-1.258381	-0.884910
6	2.784058	-1.232824	0.236179
1	2.672246	-0.429509	0.959802
6	3.735623	-2.234663	0.425910
6	3.832991	-3.304052	-0.462657
1	4.551746	-4.098894	-0.296864
6	2.974155	-3.340277	-1.561718
6	2.052252	-2.318870	-1.791533
1	1.418150	-2.381122	-2.666159
6	1.614236	1.582336	-1.361708
6	0.913185	2.796355	-1.279061
1	-0.146138	2.795798	-1.049706
6	1.582636	4.006599	-1.427899
6	2.965268	4.039421	-1.619648
1	3.489998	4.985622	-1.688210
6	3.663322	2.835886	-1.672234
6	2.996276	1.612432	-1.568259
1	3.569863	0.694243	-1.606751
29	-0.276349	0.379523	1.173168

6	5.158637	2.851156	-1.826140
6	0.850210	5.306903	-1.250380
6	4.685359	-2.114423	1.584999
6	3.036590	-4.533201	-2.474264
9	2.767463	-5.681667	-1.803260
9	2.152978	-4.455764	-3.493986
9	4.266475	-4.688772	-3.018424
9	5.664313	-1.209618	1.330140
9	5.293394	-3.281956	1.881456
9	4.059778	-1.688476	2.710534
9	5.543965	2.871086	-3.123706
9	5.732559	1.760091	-1.264603
9	5.712119	3.939368	-1.238224
9	1.174494	6.199583	-2.215278
9	-0.490463	5.154707	-1.271416
9	1.163810	5.896305	-0.066571
6	1.867853	2.331615	2.007908
6	0.921985	3.389260	2.090164
6	-0.466733	3.354361	1.836640
1	1.303262	4.376433	2.312205
7	3.211641	2.654895	1.951995
6	4.230110	1.626853	2.098544
1	5.038006	1.997997	2.740543
1	3.804080	0.738525	2.558310
1	4.668789	1.348704	1.130975
6	3.715992	4.005159	1.754443
1	3.001247	4.612708	1.200526
1	3.947300	4.507773	2.705324
1	4.634293	3.958624	1.160565
8	1.571738	1.083811	1.990736
6	-1.205847	4.584205	1.939541
6	-2.548363	4.649497	1.658214
1	-0.673991	5.484098	2.232112
6	-3.194121	3.463609	1.266098
6	-2.473834	2.293673	1.174430
1	-2.946829	1.365824	0.879040
7	-1.152527	2.223614	1.442713
1	-3.088827	5.587468	1.733953
35	-5.116963	3.460147	0.855599

Conformer_22

Number of imaginary frequencies : 0
The smallest frequency is : 13.2641 cm(-1)
Electronic energy : HF=-4521.7138803
Zero-point correction= 0.854506
(Hartree/Particle)
Thermal correction to Energy= 0.923917
Thermal correction to Enthalpy= 0.924861
Thermal correction to Gibbs Free Energy= 0.744391
Sum of electronic and zero-point Energies= -4520.859374
Sum of electronic and thermal Energies= -4520.789963
Sum of electronic and thermal Enthalpies= -4520.789019
Sum of electronic and thermal Free Energies= -4520.969489

.....

Cartesian Coordinates

.....

26	-3.598107	-1.129979	-2.692357
15	-1.125952	-1.576019	1.911885
15	0.662785	0.066022	-0.938391
6	-2.359937	-1.491581	-1.039729
6	-1.858479	-0.400176	-1.842955
6	-2.861970	0.615470	-1.876974
1	-2.792626	1.554876	-2.407771
6	-3.989738	0.155389	-1.134115
1	-4.924160	0.683943	-1.007270
6	-3.682973	-1.138501	-0.620467
1	-4.342759	-1.760247	-0.035005
6	-3.206058	-2.087466	-4.493690
1	-2.219767	-2.372789	-4.835781
6	-3.843214	-0.830473	-4.727523
1	-3.422022	0.004797	-5.270958
6	-5.114273	-0.851244	-4.076063
1	-5.819938	-0.031968	-4.034313
6	-5.263280	-2.120740	-3.438679
1	-6.103366	-2.433636	-2.832679
6	-4.086093	-2.884778	-3.697194
1	-3.884158	-3.879844	-3.324321
6	-1.560692	-2.700988	-0.683100
6	-1.263823	-3.638746	-1.684568
1	-1.677143	-3.478753	-2.672273
6	-0.440991	-4.739270	-1.446622
1	-0.208027	-5.427177	-2.253397
6	0.096772	-4.930599	-0.176465
1	0.751392	-5.772923	0.023390
6	-0.186029	-4.014843	0.837286
1	0.255392	-4.168119	1.815394
6	-0.996978	-2.890749	0.608943
6	-0.467350	-0.327354	-2.411665
1	-0.192732	-1.334378	-2.729812
6	-0.324946	0.614745	-3.609480
1	0.693538	0.590600	-4.007237
1	-0.557834	1.650904	-3.349613
1	-1.014928	0.302106	-4.399537
6	-0.217226	-2.272468	3.356740
6	1.065724	-1.771060	3.626084
1	1.473541	-0.975027	3.011768
6	1.806783	-2.274098	4.698662
1	2.800694	-1.883500	4.892950
6	1.270811	-3.270667	5.515720
1	1.845914	-3.657095	6.352682
6	-0.011540	-3.766694	5.259959
1	-0.435046	-4.538606	5.896647
6	-0.752532	-3.272036	4.186765
1	-1.747308	-3.664003	3.999726
6	-2.875038	-1.630282	2.472583
6	-3.398822	-0.476490	3.074116
1	-2.771038	0.403309	3.184111
6	-4.722522	-0.451086	3.517602
1	-5.120181	0.450041	3.975807
6	-5.533649	-1.578340	3.363015
1	-6.566122	-1.556039	3.700043
6	-5.014185	-2.736103	2.775349
1	-5.640263	-3.616406	2.658873
6	-3.690123	-2.764334	2.333417
1	-3.297818	-3.661438	1.863321
6	1.940648	-1.258533	-0.884876
6	2.784066	-1.232860	0.236300
1	2.672186	-0.429445	0.959802
6	3.735574	-2.234715	0.426251
6	3.832989	-3.304218	-0.462177
1	4.551693	-4.099068	-0.296198
6	2.974272	-3.340545	-1.561324
6	2.052441	-2.319126	-1.791369
1	1.418438	-2.381490	-2.666058
6	1.614556	1.582182	-1.361889
6	0.913560	2.796228	-1.279253
1	-0.145776	2.795699	-1.049967
6	1.583072	4.006448	-1.428008
6	2.965720	4.039205	-1.619658
1	3.490499	4.985381	-1.688174
6	3.663724	2.835641	-1.672210
6	2.996616	1.612213	-1.568320
1	3.570163	0.693996	-1.606773
29	-0.276576	0.379715	1.172530
6	5.159056	2.850863	-1.825955
6	0.850685	5.306778	-1.250510
6	4.685219	-2.114396	1.585407
6	3.036787	-4.533562	-2.473745
9	2.767999	-5.682000	-1.802568
9	2.152992	-4.456410	-3.493332
9	4.266610	-4.688946	-3.018103
9	5.664239	-1.209669	1.330538
9	5.293168	-3.281931	1.882037
9	4.059569	-1.688305	2.710851
9	5.544529	2.870919	-3.123474
9	5.732866	1.759710	-1.264474
9	5.712520	3.938985	-1.237851
9	1.175021	6.199440	-2.215407
9	-0.489990	5.154617	-1.271564

9	1.164278	5.896180	-0.066701
6	1.867690	2.331622	2.007839
6	0.921850	3.389304	2.090048
6	-0.466864	3.354469	1.836518
1	1.303153	4.376454	2.312150
7	3.211491	2.654893	1.952013
6	4.229943	1.626849	2.098676
1	5.037762	1.997981	2.740780
1	3.803855	0.738520	2.558385
1	4.668734	1.348708	1.131157
6	3.715861	4.005179	1.754655
1	3.001252	4.612734	1.200568
1	3.946894	4.507765	2.705619
1	4.634329	3.958689	1.161033
8	1.571534	1.083834	1.990630
6	-1.205931	4.584336	1.939512
6	-2.548449	4.649707	1.658231
1	-0.674031	5.484188	2.232132
6	-3.194271	3.463870	1.266064
6	-2.474033	2.293915	1.174286
1	-2.947101	1.366111	0.878847
7	-1.152713	2.223774	1.442529
1	-3.088871	5.587695	1.734051
35	-5.117138	3.460535	0.855667

Conformer_23

Number of imaginary frequencies : 0
The smallest frequency is : 13.2967 cm(-1)
Electronic energy : HF=-4521.7138801
Zero-point correction= 0.854511
(Hartree/Particle)
Thermal correction to Energy= 0.923921
Thermal correction to Enthalpy= 0.924865
Thermal correction to Gibbs Free Energy= 0.744416
Sum of electronic and zero-point Energies= -4520.859369
Sum of electronic and thermal Energies= -4520.789960
Sum of electronic and thermal Enthalpies= -4520.789015
Sum of electronic and thermal Free Energies= -4520.969464

Cartesian Coordinates

26	-3.597807	-1.130067	-2.692668
15	-1.125919	-1.576613	1.911561
15	0.662729	0.066411	-0.937955
6	-2.359934	-1.492131	-1.039922
6	-1.858543	-0.400272	-1.842570
6	-2.862234	0.615172	-1.876377
1	-2.792984	1.554817	-2.406764
6	-3.990046	0.154536	-1.133924
1	-4.924594	0.682852	-1.007007
6	-3.683112	-1.139517	-0.620790
1	-4.342788	-1.761573	-0.035534
6	-3.204938	-2.086411	-4.494416
1	-2.218431	-2.371228	-4.836301
6	-3.842374	-0.829463	-4.727720
1	-3.421243	0.006250	-5.270518
6	-5.113632	-0.850957	-4.076668
1	-5.819537	-0.031901	-4.034674
6	-5.262492	-2.120867	-3.440075
1	-6.102684	-2.434344	-2.834523
6	-4.085015	-2.884434	-3.698675
1	-3.882954	-3.879676	-3.326342
6	-1.560389	-2.701408	-0.683589
6	-1.263301	-3.638948	-1.685189
1	-1.676737	-3.478986	-2.672853
6	-0.440004	-4.739164	-1.447427
1	-0.206856	-5.426907	-2.254290
6	0.097994	-4.930390	-0.177355
1	0.753012	-5.772448	0.022315
6	-0.185089	-4.014888	0.836546
1	0.256526	-4.168096	1.814574
6	-0.996555	-2.891112	0.608417
6	-0.467414	-0.327198	-2.411191
1	-0.192693	-1.334209	-2.729316
6	-0.325123	0.614894	-3.609029
1	0.693405	0.590979	-4.006690
1	-0.558273	1.651009	-3.349215
1	-1.014954	0.302079	-4.399149
6	-0.217187	-2.273313	3.356330
6	1.065510	-1.771510	3.626138
1	1.473166	-0.975081	3.012235
6	1.806548	-2.274669	4.698678
1	2.800248	-1.883719	4.893335
6	1.270833	-3.271800	5.515213
1	1.845920	-3.658324	6.352142
6	-0.011247	-3.768276	5.258957
1	-0.434558	-4.540648	5.895217
6	-0.752224	-3.273470	4.185824
1	-1.746788	-3.665800	3.998429
6	-2.874955	-1.631066	2.472357
6	-3.689935	-2.765202	2.333289
1	-3.297639	-3.662210	1.862977
6	-5.013877	-2.737200	2.775577
1	-5.639850	-3.617590	2.659201
6	-5.533363	-1.579542	3.363440
1	-6.565742	-1.557419	3.700768
6	-4.722381	-0.452155	3.517801
1	-5.120072	0.448907	3.976106
6	-3.398779	-0.477341	3.073981
1	-2.771114	0.402561	3.183809
6	1.940820	-1.257925	-0.884677
6	2.784059	-1.232581	0.236636
1	2.671974	-0.429473	0.960445
6	3.735702	-2.234365	0.426293
6	3.833379	-3.303507	-0.462541
1	4.552156	-4.098334	-0.296764
6	2.974828	-3.339516	-1.561828
6	2.052929	-2.318102	-1.791608
1	1.419105	-2.380061	-2.666454
6	1.614212	1.582727	-1.361473
6	0.913042	2.796675	-1.278788
1	-0.146286	2.796000	-1.049466
6	1.582386	4.006987	-1.427523
6	2.965019	4.039945	-1.619259
1	3.489663	4.986194	-1.687749
6	3.663190	2.836483	-1.671886
6	2.996259	1.612960	-1.567948
1	3.569938	0.694823	-1.606406
29	-0.276619	0.379466	1.173131
6	5.158506	2.851842	-1.825791
6	0.849869	5.307213	-1.249816
6	4.685247	-2.114341	1.585561
6	3.037554	-4.532194	-2.474675
9	2.768944	-5.680910	-1.803897
9	2.153745	-4.454819	-3.494230
9	4.267401	-4.687195	-3.019086
9	5.664404	-1.209695	1.330913
9	5.293035	-3.281995	1.882063
9	4.059554	-1.688348	2.711007
9	5.543839	2.871021	-3.123366
9	5.732526	1.761153	-1.263617
9	5.711880	3.940444	-1.238506
9	1.173959	6.200002	-2.214677
9	-0.490794	5.154904	-1.270680
9	1.163576	5.896538	-0.065994
6	1.867337	2.331433	2.008396
6	0.921472	3.389102	2.090447
6	-0.467232	3.354190	1.836859
1	1.302731	4.376284	2.312477
7	3.211141	2.654679	1.952567
6	4.229578	1.626658	2.099487
1	5.037370	1.997935	2.741543
1	3.803465	0.738425	2.559358
1	4.668423	1.348317	1.132048
6	3.715608	4.004860	1.754762
1	3.000732	4.612503	1.201128
1	3.947388	4.507453	2.705539
1	4.633663	3.958186	1.160500
8	1.571183	1.083638	1.991359

6	-1.206365	4.584029	1.939718
6	-2.548880	4.649300	1.658386
1	-0.674520	5.483935	2.232272
6	-3.194615	3.463399	1.266270
6	-2.474299	2.293485	1.174575
1	-2.947283	1.365649	0.879105
7	-1.152997	2.223435	1.442895
1	-3.089359	5.587263	1.734116
35	-5.117467	3.459890	0.855803

Conformer_24

Number of imaginary frequencies : 0
The smallest frequency is : 14.4527 cm(-1)
Electronic energy : HF=-4521.7142872
Zero-point correction= 0.854354
(Hartree/Particle)
Thermal correction to Energy= 0.923813
Thermal correction to Enthalpy= 0.924757
Thermal correction to Gibbs Free Energy= 0.744829
Sum of electronic and zero-point Energies= -4520.859933
Sum of electronic and thermal Energies= -4520.790474
Sum of electronic and thermal Enthalpies= -4520.789530
Sum of electronic and thermal Free Energies= -4520.969458

Cartesian Coordinates

26	-3.560698	-1.115072	-2.732050
15	-1.138262	-1.606845	1.888657
15	0.670509	0.093662	-0.911215
6	-2.339905	-1.495191	-1.070741
6	-1.838590	-0.385418	-1.848037
6	-2.850777	0.621823	-1.876105
1	-2.782978	1.571190	-2.389108
6	-3.983425	0.138354	-1.155870
1	-4.923871	0.656692	-1.030848
6	-3.671333	-1.161974	-0.661957
1	-4.331876	-1.800056	-0.095224
6	-3.134425	-2.027323	-4.548601
1	-2.139981	-2.291407	-4.883771
6	-3.786407	-0.774342	-4.762623
1	-3.370291	0.078781	-5.281679
6	-5.064508	-0.826632	-4.126941
1	-5.781743	-0.018036	-4.075564
6	-5.203502	-2.111971	-3.519725
1	-6.046249	-2.449718	-2.931055
6	-4.013162	-2.854184	-3.781267
1	-3.802728	-3.854876	-3.428766
6	-1.534329	-2.702892	-0.724056
6	-1.220459	-3.625514	-1.734098
1	-1.624069	-3.455986	-2.724265
6	-0.392755	-4.723447	-1.500660
1	-0.146612	-5.399922	-2.313154
6	0.133053	-4.926815	-0.227356
1	0.791040	-5.767319	-0.030937
6	-0.166316	-4.025484	0.794592
1	0.265982	-4.187623	1.775319
6	-0.982637	-2.904395	0.571183
6	-0.442307	-0.291881	-2.400721
1	-0.155016	-1.291639	-2.730638
6	-0.296201	0.669407	-3.582949
1	0.726449	0.660634	-3.970435
1	-0.541257	1.699317	-3.309434
1	-0.974735	0.362937	-4.385258
6	-0.235191	-2.313237	3.332505
6	1.043448	-1.808342	3.615805
1	1.450071	-1.001963	3.014756
6	1.780687	-2.320495	4.686699
1	2.771259	-1.926939	4.891792
6	1.245271	-3.329611	5.488582
1	1.817477	-3.723096	6.324247
6	-0.032958	-3.828945	5.219270
1	-0.456331	-4.610576	5.844079
6	-0.770097	-3.325290	4.147556
1	-1.761604	-3.720352	3.950008
6	-2.891599	-1.686842	2.432732
6	-3.693569	-2.827484	2.273339
1	-3.287821	-3.714810	1.796044
6	-5.021180	-2.818613	2.705372
1	-5.636910	-3.704018	2.573383
6	-5.557359	-1.673769	3.303258
1	-6.592462	-1.666583	3.632785
6	-4.759400	-0.540077	3.477941
1	-5.169890	0.351045	3.944363
6	-3.432187	-0.546199	3.044346
1	-2.814330	0.338458	3.170347
6	1.954284	-1.224883	-0.859196
6	2.791484	-1.202850	0.266624
1	2.667710	-0.409120	0.998935
6	3.750526	-2.198656	0.451341
6	3.862513	-3.257507	-0.448202
1	4.587780	-4.047296	-0.286618
6	3.010131	-3.290143	-1.552276
6	2.080230	-2.274776	-1.776095
1	1.451267	-2.333413	-2.654682
6	1.626286	1.610566	-1.324149
6	0.933128	2.827639	-1.215516
1	-0.120485	2.829737	-0.961657
6	1.601304	4.035315	-1.385788
6	2.976386	4.063369	-1.630113
1	3.500764	5.006635	-1.731281
6	3.664971	2.857393	-1.719326
6	2.999088	1.635160	-1.582497
1	3.565355	0.713798	-1.657574
29	-0.305303	0.370252	1.185403
6	5.160373	2.853264	-1.858712
6	0.876121	5.337377	-1.192229
6	4.693242	-2.083847	1.616691
6	3.089546	-4.471452	-2.478653
9	2.833563	-5.631119	-1.822125
9	2.207284	-4.392702	-3.499499
9	4.322424	-4.604901	-3.021939
9	5.668113	-1.170550	1.375775
9	5.307370	-3.250374	1.904565
9	4.059249	-1.673419	2.742903
9	5.595620	1.841548	-2.642509
9	5.764844	2.688759	-0.649058
9	5.636320	4.005295	-2.376386
9	1.176073	6.227326	-2.167266
9	-0.464923	5.187247	-1.177541
9	1.221395	5.929219	-0.018142
6	1.806721	2.320496	2.075396
6	0.859142	3.378856	2.128110
6	-0.526801	3.338157	1.861123
1	1.234597	4.367615	2.352982
7	3.151671	2.640869	2.049247
6	4.161428	1.612957	2.247367
1	4.957873	2.001828	2.893271
1	3.721199	0.741141	2.725232
1	4.619081	1.302653	1.299287
6	3.668229	3.982234	1.824398
1	2.941713	4.592118	1.289801
1	3.932867	4.489076	2.764367
1	4.568463	3.916004	1.205649
8	1.510779	1.072563	2.063716
6	-1.271848	4.565177	1.953332
6	-2.613538	4.622229	1.666047
1	-0.745358	5.469082	2.243604
6	-3.251292	3.431332	1.275992
6	-2.524091	2.265235	1.189696
1	-2.990362	1.334642	0.892417
7	-1.203748	2.203008	1.464215
1	-3.159178	5.557710	1.735086
35	-5.172198	3.415892	0.856491

Conformer_25

Number of imaginary frequencies : 0
The smallest frequency is : 13.2528 cm(-1)
Electronic energy : HF=-4521.7138804

Zero-point correction= 0.854509
(Hartree/Particle)
Thermal correction to Energy= 0.923919
Thermal correction to Enthalpy= 0.924864
Thermal correction to Gibbs Free Energy= 0.744397
Sum of electronic and zero-point Energies= -4520.859372
Sum of electronic and thermal Energies= -4520.789961
Sum of electronic and thermal Enthalpies= -4520.789017
Sum of electronic and thermal Free Energies= -4520.969483

Cartesian Coordinates

26	-3.598188	-1.129391	-2.692538
15	-1.126093	-1.576268	1.911578
15	0.662733	0.066227	-0.938236
6	-2.360203	-1.491521	-1.039893
6	-1.858673	-0.399855	-1.842713
6	-2.862167	0.615791	-1.876519
1	-2.792781	1.555373	-2.407000
6	-3.989994	0.155468	-1.133899
1	-4.924421	0.683981	-1.006937
6	-3.683261	-1.138583	-0.620649
1	-4.342999	-1.760441	-0.035250
6	-3.205749	-2.086090	-4.494190
1	-2.219354	-2.371189	-4.836164
6	-3.842926	-0.829032	-4.727609
1	-3.421671	0.006501	-5.270588
6	-5.114111	-0.850142	-4.076404
1	-5.819833	-0.030926	-4.034456
6	-5.263185	-2.119924	-3.439604
1	-6.103378	-2.433125	-2.833912
6	-4.085910	-2.883795	-3.698225
1	-3.884024	-3.879022	-3.325759
6	-1.560998	-2.701008	-0.683518
6	-1.264215	-3.638686	-1.685079
1	-1.677499	-3.478567	-2.672779
6	-0.441460	-4.739282	-1.447211
1	-0.208546	-5.427144	-2.254039
6	0.096275	-4.930767	-0.177067
1	0.750818	-5.773168	0.022713
6	-0.186449	-4.015089	0.836772
1	0.254968	-4.168499	1.814858
6	-0.997322	-2.890910	0.608529
6	-0.467563	-0.327018	-2.411429
1	-0.192995	-1.334027	-2.729669
6	-0.325171	0.615164	-3.609186
1	0.693311	0.591049	-4.006949
1	-0.558056	1.651306	-3.349249
1	-1.015154	0.302586	-4.399268
6	-0.217300	-2.273025	3.356293
6	-0.752390	-3.273027	4.185936
1	-1.747012	-3.665261	3.998655
6	-0.011400	-3.767772	5.259090
1	-0.434746	-4.540031	5.895464
6	1.270737	-3.271381	5.515220
1	1.845834	-3.657862	6.352162
6	1.806498	-2.274389	4.698542
1	2.800251	-1.883515	4.893096
6	1.065446	-1.771288	3.625989
1	1.473157	-0.975005	3.011926
6	-2.875029	-1.630151	2.472726
6	-3.690462	-2.763964	2.333688
1	-3.298610	-3.661055	1.863164
6	-5.014281	-2.735536	2.776321
1	-5.640615	-3.615673	2.659968
6	-5.533177	-1.577784	3.364520
1	-6.565457	-1.555337	3.702131
6	-4.721737	-0.450720	3.518849
1	-5.118967	0.450412	3.977414
6	-3.398269	-0.476322	3.074662
1	-2.770255	0.403336	3.184456
6	1.940446	-1.258482	-0.884938
6	2.783925	-1.233031	0.236193
1	2.672195	-0.429688	0.959800
6	3.735303	-2.235033	0.426009
6	3.832549	-3.304457	-0.462527
1	4.551166	-4.099410	-0.296668
6	2.973762	-3.340573	-1.561630
6	2.052031	-2.319028	-1.791516
1	1.417928	-2.381234	-2.666145
6	1.614613	1.582308	-1.361718
6	0.913717	2.796413	-1.279035
1	-0.145617	2.795974	-1.049733
6	1.583334	4.006578	-1.427756
6	2.965981	4.039230	-1.619434
1	3.490838	4.985368	-1.687904
6	3.663880	2.835604	-1.672054
6	2.996668	1.612231	-1.568184
1	3.570144	0.693973	-1.606696
29	-0.276378	0.379537	1.172872
6	5.159209	2.850700	-1.825853
6	0.851080	5.306969	-1.250165
6	4.684905	-2.114956	1.585223
6	3.036079	-4.533518	-2.474159
9	2.767038	-5.681966	-1.803095
9	2.152341	-4.456103	-3.493775
9	4.265894	-4.689097	-3.018477
9	5.663910	-1.210143	1.330594
9	5.292873	-3.282537	1.881628
9	4.059177	-1.689125	2.710721
9	5.544626	2.870882	-3.123387
9	5.732947	1.759432	-1.264524
9	5.712791	3.938704	-1.237647
9	1.175353	6.199598	-2.215112
9	-0.489612	5.154932	-1.271034
9	1.164894	5.896345	-0.066398
6	1.867910	2.331284	2.008078
6	0.922187	3.389075	2.090188
6	-0.466534	3.354328	1.836662
1	1.303576	4.376212	2.312191
7	3.211753	2.654370	1.952271
6	4.230080	1.626211	2.099006
1	5.037826	1.997192	2.741292
1	3.803825	0.737868	2.558534
1	4.669019	1.348144	1.131530
6	3.716306	4.004579	1.754867
1	3.001793	4.612203	1.200732
1	3.947386	4.507177	2.705813
1	4.634783	3.957939	1.161268
8	1.571599	1.083528	1.990923
6	-1.205528	4.584250	1.939527
6	-2.548052	4.649659	1.658255
1	-0.673574	5.484104	2.232041
6	-3.193937	3.463818	1.266208
6	-2.473750	2.293824	1.174513
1	-2.946846	1.366028	0.879102
7	-1.152441	2.223643	1.442758
1	-3.088423	5.587684	1.733982
35	-5.116804	3.460494	0.855805

Conformer_26

Number of imaginary frequencies : 0
The smallest frequency is : 13.2912 cm(-1)
Electronic energy : HF=-4521.7138804
Zero-point correction= 0.854508
(Hartree/Particle)
Thermal correction to Energy= 0.923919
Thermal correction to Enthalpy= 0.924863
Thermal correction to Gibbs Free Energy= 0.744401
Sum of electronic and zero-point Energies= -4520.859372
Sum of electronic and thermal Energies= -4520.789962
Sum of electronic and thermal Enthalpies= -4520.789017
Sum of electronic and thermal Free Energies= -4520.969479

Cartesian Coordinates

26	-3.598124	-1.129599	-2.692571
15	-1.126024	-1.576161	1.911562
15	0.662800	0.066132	-0.938353

6	-2.360113	-1.491620	-1.039921
6	-1.858554	-0.400042	-1.842843
6	-2.862014	0.615630	-1.876743
1	-2.792606	1.555152	-2.407325
6	-3.989844	0.155422	-1.134055
1	-4.924252	0.683984	-1.007146
6	-3.683147	-1.138589	-0.620674
1	-4.342896	-1.760367	-0.035199
6	-3.205830	-2.086731	-4.494036
1	-2.219493	-2.372115	-4.835942
6	-3.842731	-0.829583	-4.727716
1	-3.421287	0.005750	-5.270855
6	-5.113941	-0.850299	-4.076544
1	-5.819488	-0.030924	-4.034769
6	-5.263297	-2.119922	-3.439494
1	-6.103574	-2.432824	-2.833762
6	-4.086172	-2.884090	-3.697927
1	-3.884489	-3.879282	-3.325254
6	-1.560915	-2.701086	-0.683457
6	-1.264187	-3.638855	-1.684950
1	-1.677561	-3.478839	-2.672631
6	-0.441381	-4.739405	-1.447042
1	-0.208518	-5.427345	-2.253819
6	0.096483	-4.930731	-0.176929
1	0.751096	-5.773071	0.022870
6	-0.186202	-4.014972	0.836849
1	0.255324	-4.168258	1.814904
6	-0.997161	-2.890862	0.608575
6	-0.467436	-0.327292	-2.411545
1	-0.192881	-1.334346	-2.729661
6	-0.325005	0.614748	-3.609408
1	0.693495	0.590598	-4.007126
1	-0.557912	1.650919	-3.349603
1	-1.014954	0.302064	-4.399478
6	-0.217077	-2.272799	3.356237
6	-0.752079	-3.272862	4.185865
1	-1.746749	-3.665034	3.998694
6	-0.010977	-3.767687	5.258905
1	-0.434261	-4.539986	5.895270
6	1.271197	-3.271335	5.514930
1	1.846378	-3.657889	6.351780
6	1.806874	-2.274275	4.698282
1	2.800653	-1.883424	4.892751
6	1.065696	-1.771066	3.625863
1	1.473319	-0.974661	3.011898
6	-2.874958	-1.630302	2.472695
6	-3.690133	-2.764317	2.333769
1	-3.298059	-3.661383	1.863386
6	-5.013987	-2.736119	2.776309
1	-5.640118	-3.616412	2.660042
6	-5.533181	-1.578392	3.364295
1	-6.565491	-1.556118	3.701824
6	-4.721999	-0.451128	3.518514
1	-5.119470	0.449985	3.976907
6	-3.398490	-0.476501	3.074429
1	-2.770674	0.403306	3.184149
6	1.940645	-1.258442	-0.884908
6	2.784167	-1.232741	0.236189
1	2.672383	-0.429288	0.959663
6	3.735628	-2.234645	0.426126
6	3.832896	-3.304218	-0.462231
1	4.551565	-4.099100	-0.296264
6	2.974067	-3.340576	-1.561291
6	2.052259	-2.319130	-1.791312
1	1.418145	-2.381517	-2.665920
6	1.614533	1.582297	-1.361873
6	0.913500	2.796327	-1.279239
1	-0.145838	2.795772	-1.049962
6	1.582985	4.006566	-1.427943
6	2.965637	4.039364	-1.619565
1	3.490398	4.985553	-1.688030
6	3.663674	2.835820	-1.672127
6	2.996597	1.612370	-1.568264
1	3.570175	0.694170	-1.606701
29	-0.276428	0.379606	1.172673
6	5.159009	2.851068	-1.825846
6	0.850579	5.306876	-1.250370
6	4.685332	-2.114328	1.585236
6	3.036434	-4.533662	-2.473628
9	2.767375	-5.682012	-1.802406
9	2.152744	-4.456408	-3.493297
9	4.266278	-4.689311	-3.017863
9	5.664286	-1.209529	1.330360
9	5.293363	-3.281843	1.881770
9	4.059714	-1.688333	2.710729
9	5.544503	2.870812	-3.123365
9	5.732853	1.760075	-1.264088
9	5.712422	3.939353	-1.238003
9	1.174818	6.199569	-2.215271
9	-0.490096	5.154689	-1.271322
9	1.164252	5.896258	-0.066570
6	1.867754	2.331533	2.007814
6	0.921923	3.389217	2.090010
6	-0.466802	3.354361	1.836526
1	1.303221	4.376366	2.312123
7	3.211562	2.654762	1.952005
6	4.229988	1.626719	2.098850
1	5.037673	1.997834	2.741133
1	3.803800	0.738376	2.558440
1	4.668986	1.348614	1.131414
6	3.715995	4.005013	1.754590
1	3.001343	4.612628	1.200630
1	3.947224	4.507560	2.705527
1	4.634363	3.958466	1.160812
8	1.571576	1.083747	1.990599
6	-1.205906	4.584199	1.939595
6	-2.548467	4.649504	1.658486
1	-0.674012	5.484071	2.232163
6	-3.194274	3.463641	1.266375
6	-2.473971	2.293738	1.174426
1	-2.947007	1.365929	0.878960
7	-1.152622	2.223660	1.442510
1	-3.088928	5.587461	1.734396
35	-5.117215	3.460154	0.856322

Conformer_27

Number of imaginary frequencies : 0
The smallest frequency is : 13.2559 cm(-1)
Electronic energy : HF=-4521.7138804
Zero-point correction= 0.854508
(Hartree/Particle)
Thermal correction to Energy= 0.923919
Thermal correction to Enthalpy= 0.924863
Thermal correction to Gibbs Free Energy= 0.744393
Sum of electronic and zero-point Energies= -4520.859372
Sum of electronic and thermal Energies= -4520.789961
Sum of electronic and thermal Enthalpies= -4520.789017
Sum of electronic and thermal Free Energies= -4520.969487

Cartesian Coordinates

26	-3.598230	-1.129615	-2.692417
15	-1.125955	-1.576320	1.911651
15	0.662711	0.066192	-0.938236
6	-2.360189	-1.491652	-1.039795
6	-1.858706	-0.399994	-1.842659
6	-2.862234	0.615616	-1.876482
1	-2.792893	1.555181	-2.406998
6	-3.990029	0.155284	-1.133816
1	-4.924469	0.683775	-1.006845
6	-3.683242	-1.138739	-0.620523
1	-4.342946	-1.760595	-0.035082
6	-3.205852	-2.086507	-4.493990
1	-2.219479	-2.371710	-4.835942
6	-3.842933	-0.829423	-4.727522
1	-3.421616	0.006029	-5.270576
6	-5.114123	-0.850382	-4.076320
1	-5.819784	-0.031109	-4.034447
6	-5.263291	-2.120093	-3.439403

1	-6.103509	-2.433175	-2.833682
6	-4.086068	-2.884073	-3.697947
1	-3.884247	-3.879279	-3.325388
6	-1.560922	-2.701102	-0.683432
6	-1.264167	-3.638779	-1.685004
1	-1.677553	-3.478701	-2.672667
6	-0.441312	-4.739313	-1.447201
1	-0.208422	-5.427170	-2.254040
6	0.096568	-4.930725	-0.177109
1	0.751212	-5.773058	0.022620
6	-0.186133	-4.015054	0.836741
1	0.255416	-4.168419	1.814772
6	-0.997134	-2.890950	0.608575
6	-0.467603	-0.327138	-2.411394
1	-0.193010	-1.334152	-2.729591
6	-0.325257	0.614988	-3.609200
1	0.693226	0.590902	-4.006964
1	-0.558193	1.651132	-3.349319
1	-1.015228	0.302330	-4.399261
6	-0.216979	-2.273029	3.356262
6	-0.752072	-3.272823	4.186151
1	-1.746833	-3.664847	3.999162
6	-0.010872	-3.767682	5.259111
1	-0.434230	-4.539767	5.895687
6	1.271502	-3.271658	5.514761
1	1.846773	-3.658252	6.351531
6	1.807282	-2.274884	4.697825
1	2.801211	-1.884280	4.892014
6	1.065999	-1.771635	3.625504
1	1.473710	-0.975472	3.011290
6	-2.874883	-1.630370	2.472810
6	-3.690181	-2.764287	2.333823
1	-3.298211	-3.661367	1.863379
6	-5.014023	-2.735978	2.776394
1	-5.640249	-3.616198	2.660080
6	-5.533082	-1.578239	3.364472
1	-6.565383	-1.555880	3.702026
6	-4.721777	-0.451071	3.518755
1	-5.119136	0.450052	3.977226
6	-3.398282	-0.476557	3.074640
1	-2.770374	0.403179	3.184402
6	1.940561	-1.258387	-0.884964
6	2.784152	-1.232741	0.236081
1	2.672400	-0.429347	0.959629
6	3.735668	-2.234616	0.425886
6	3.832933	-3.304112	-0.462561
1	4.551657	-4.098969	-0.296712
6	2.974027	-3.340432	-1.561564
6	2.052162	-2.319008	-1.791453
1	1.417986	-2.381370	-2.666019
6	1.614417	1.582376	-1.361743
6	0.913370	2.796396	-1.279081
1	-0.145963	2.795830	-1.049775
6	1.582832	4.006643	-1.427828
6	2.965476	4.039466	-1.619509
1	3.490214	4.985667	-1.688004
6	3.663524	2.835928	-1.672100
6	2.996468	1.612471	-1.568208
1	3.570062	0.694285	-1.606697
29	-0.276360	0.379518	1.172900
6	5.158850	2.851194	-1.825896
6	0.850410	5.306942	-1.250263
6	4.685459	-2.114299	1.584922
6	3.036377	-4.533457	-2.473986
9	2.767361	-5.681857	-1.802830
9	2.152645	-4.456150	-3.493615
9	4.266202	-4.689056	-3.018277
9	5.664278	-1.209356	1.330044
9	5.293657	-3.281764	1.881303
9	4.059888	-1.688478	2.710515
9	5.544275	2.871085	-3.123432
9	5.732727	1.760140	-1.264287
9	5.712287	3.939417	-1.237962
9	1.174659	6.199637	-2.215157
9	-0.490264	5.154744	-1.271251
9	1.164050	5.896323	-0.066453
6	1.867808	2.331418	2.008006
6	0.921986	3.389112	2.090231
6	-0.466736	3.354267	1.836739
1	1.303296	4.376265	2.312303
7	3.211612	2.654657	1.952154
6	4.230056	1.626614	2.098873
1	5.037794	1.997707	2.741105
1	3.803915	0.738247	2.558455
1	4.668977	1.348553	1.131389
6	3.716008	4.004921	1.754723
1	3.001372	4.612485	1.200680
1	3.947141	4.507521	2.705655
1	4.634425	3.958388	1.161022
8	1.571630	1.083631	1.990806
6	-1.205830	4.584119	1.939724
6	-2.548366	4.649438	1.658490
1	-0.673945	5.483994	2.232301
6	-3.194158	3.463573	1.266362
6	-2.473877	2.293646	1.174560
1	-2.946904	1.365832	0.879097
7	-1.152558	2.223553	1.442771
1	-3.088817	5.587409	1.734312
35	-5.117032	3.460121	0.856008

---

*Conformer_*28

Number of imaginary frequencies : 0
The smallest frequency is : 13.3063 cm(-1)
Electronic energy : HF=-4521.7138803
Zero-point correction= 0.854508
(Hartree/Particle)
Thermal correction to Energy= 0.923919
Thermal correction to Enthalpy= 0.924863
Thermal correction to Gibbs Free Energy= 0.744396
Sum of electronic and zero-point Energies= -4520.859372
Sum of electronic and thermal Energies= -4520.789961
Sum of electronic and thermal Enthalpies= -4520.789017
Sum of electronic and thermal Free Energies= -4520.969484

.....

Cartesian Coordinates

.....

26	-3.597887	-1.129199	-2.692939
15	-1.126429	-1.576097	1.911481
15	0.662960	0.066110	-0.938260
6	-2.360065	-1.491272	-1.040171
6	-1.858354	-0.399748	-1.843068
6	-2.861732	0.616005	-1.877060
1	-2.792195	1.555523	-2.407636
6	-3.989667	0.155888	-1.134483
1	-4.924047	0.684522	-1.007668
6	-3.683115	-1.138139	-0.621061
1	-4.342968	-1.759861	-0.035647
6	-3.205443	-2.086171	-4.494446
1	-2.219061	-2.371404	-4.836344
6	-3.842493	-0.829085	-4.728063
1	-3.421132	0.006336	-5.271131
6	-5.113713	-0.849993	-4.076920
1	-5.819362	-0.030707	-4.035115
6	-5.262935	-2.119676	-3.439959
1	-6.103185	-2.432719	-2.834265
6	-4.085715	-2.883688	-3.698416
1	-3.883931	-3.878882	-3.325805
6	-1.561093	-2.700864	-0.683640
6	-1.264242	-3.638624	-1.685103
1	-1.677252	-3.478465	-2.672912
6	-0.441757	-4.739371	-1.446992
1	-0.208757	-5.427289	-2.253746
6	0.095594	-4.930954	-0.176697
1	0.749885	-5.773504	0.023275
6	-0.187194	-4.015188	0.837044
1	0.253889	-4.168667	1.815272
6	-0.997741	-2.890830	0.608532
6	-0.467160	-0.327078	-2.411591
1	-0.192622	-1.334126	-2.729718

6	-0.324506	0.615014	-3.609385
1	0.694025	0.590764	-4.007015
1	-0.557313	1.651195	-3.349543
1	-1.014421	0.302462	-4.399540
6	-0.217741	-2.272996	3.356193
6	1.065273	-1.771752	3.625572
1	1.473128	-0.975637	3.011395
6	1.806339	-2.275013	4.698036
1	2.800280	-1.884510	4.892354
6	1.270312	-3.271661	5.514964
1	1.845411	-3.658265	6.351848
6	-0.012088	-3.767530	5.259169
1	-0.435643	-4.539500	5.895756
6	-0.753095	-3.272633	4.186091
1	-1.747912	-3.664478	3.999081
6	-2.875396	-1.629845	2.472548
6	-3.690955	-2.763540	2.333276
1	-3.299174	-3.660610	1.862659
6	-5.014805	-2.735024	2.775813
1	-5.641230	-3.615073	2.659280
6	-5.533617	-1.577300	3.364137
1	-6.565922	-1.554779	3.701664
6	-4.722054	-0.450357	3.518705
1	-5.119218	0.450756	3.977362
6	-3.398551	-0.476047	3.074624
1	-2.770452	0.403525	3.184612
6	1.940642	-1.258631	-0.884834
6	2.784223	-1.232937	0.236215
1	2.672575	-0.429396	0.959614
6	3.735557	-2.234945	0.426226
6	3.832651	-3.304618	-0.462025
1	4.551241	-4.099568	-0.296039
6	2.973772	-3.340970	-1.561049
6	2.052077	-2.319437	-1.791135
1	1.417920	-2.381876	-2.665711
6	1.614874	1.582197	-1.361656
6	0.913924	2.796278	-1.279050
1	-0.145423	2.795801	-1.049803
6	1.583493	4.006466	-1.427798
6	2.966147	4.039167	-1.619421
1	3.490966	4.985324	-1.687915
6	3.664097	2.835570	-1.671957
6	2.996934	1.612170	-1.568068
1	3.570453	0.693938	-1.606531
29	-0.276389	0.379569	1.172763
6	5.159432	2.850704	-1.825698
6	0.851172	5.306835	-1.250322
6	4.685304	-2.114593	1.585294
6	3.035944	-4.534172	-2.473252
9	2.766331	-5.682358	-1.801968
9	2.152519	-4.456728	-3.493137
9	4.265865	-4.690304	-3.017171
9	5.664182	-1.209727	1.330387
9	5.293412	-3.282066	1.881816
9	4.059701	-1.688619	2.710818
9	5.544904	2.870588	-3.123220
9	5.733190	1.759588	-1.264089
9	5.712945	3.938866	-1.237724
9	1.175397	6.199391	-2.215353
9	-0.489512	5.154729	-1.271171
9	1.164956	5.896343	-0.066611
6	1.867841	2.331364	2.007973
6	0.922068	3.389116	2.090062
6	-0.466652	3.354325	1.836548
1	1.303418	4.376265	2.312081
7	3.211667	2.654530	1.952200
6	4.230061	1.626450	2.098985
1	5.037731	1.997475	2.741341
1	3.803840	0.738067	2.558459
1	4.669092	1.348449	1.131533
6	3.716162	4.004767	1.754841
1	3.001620	4.612387	1.200745
1	3.947243	4.507330	2.705805
1	4.634631	3.958181	1.161224
8	1.571594	1.083590	1.990812
6	-1.205701	4.584208	1.939497
6	-2.548256	4.649552	1.658366
1	-0.673770	5.484083	2.231994
6	-3.194117	3.463687	1.266346
6	-2.473863	2.293747	1.174493
1	-2.946927	1.365943	0.879057
7	-1.152525	2.223630	1.442612
1	-3.088674	5.587543	1.734190
35	-5.117046	3.460252	0.856249

---

*Conformer_*29

Number of imaginary frequencies : 0
The smallest frequency is : 14.3747 cm(-1)
Electronic energy : HF=-4521.714362
Zero-point correction= 0.854529
(Hartree/Particle)
Thermal correction to Energy= 0.923892
Thermal correction to Enthalpy= 0.924836
Thermal correction to Gibbs Free Energy= 0.745317
Sum of electronic and zero-point Energies= -4520.859833
Sum of electronic and thermal Energies= -4520.790470
Sum of electronic and thermal Enthalpies= -4520.789526
Sum of electronic and thermal Free Energies= -4520.969045

Cartesian Coordinates

26	-3.571758	-1.120290	-2.717824
15	-1.129064	-1.605498	1.892829
15	0.668524	0.090540	-0.919325
6	-2.343301	-1.497543	-1.061738
6	-1.844687	-0.389988	-1.844021
6	-2.856074	0.618091	-1.869572
1	-2.790066	1.566157	-2.385205
6	-3.985593	0.137427	-1.142631
1	-4.924934	0.656909	-1.014220
6	-3.672314	-1.161987	-0.647103
1	-4.330794	-1.798126	-0.075813
6	-3.155289	-2.038342	-4.533721
1	-2.162798	-2.304472	-4.873103
6	-3.806937	-0.785288	-4.748294
1	-3.392481	0.065764	-5.272057
6	-5.082029	-0.834337	-4.106337
1	-5.798199	-0.024857	-4.053961
6	-5.219415	-2.117675	-3.494544
1	-6.059627	-2.452694	-2.900705
6	-4.031079	-2.861915	-3.759502
1	-3.819856	-3.861671	-3.404817
6	-1.537215	-2.705323	-0.716387
6	-1.227863	-3.629556	-1.726381
1	-1.635420	-3.461200	-2.715123
6	-0.399738	-4.727557	-1.494783
1	-0.157229	-5.405294	-2.307320
6	0.131027	-4.929453	-0.223295
1	0.789414	-5.769982	-0.028355
6	-0.163809	-4.026554	0.798575
1	0.272398	-4.187505	1.777766
6	-0.980421	-2.905319	0.576894
6	-0.450789	-0.298750	-2.403017
1	-0.165464	-1.299725	-2.730904
6	-0.309531	0.658239	-3.589263
1	0.711628	0.648366	-3.980648
1	-0.553995	1.689071	-3.318804
1	-0.991127	0.348382	-4.387648
6	-0.219525	-2.310361	3.333390
6	1.062179	-1.808325	3.607806
1	1.467556	-1.004857	3.002037
6	1.804091	-2.319543	4.675909
1	2.796912	-1.928282	4.874248
6	1.270408	-3.324823	5.483770
1	1.846284	-3.717488	6.317298
6	-0.010693	-3.821378	5.223181
1	-0.432645	-4.600061	5.852616
6	-0.752528	-3.318707	4.154242
1	-1.746208	-3.711612	3.963482

6	-2.879741	-1.683323	2.445668
6	-3.683871	-2.823048	2.290669
1	-3.281557	-3.711076	1.811792
6	-5.009384	-2.812320	2.729086
1	-5.626863	-3.696997	2.600442
6	-5.541240	-1.666543	3.329034
1	-6.574751	-1.657894	3.663484
6	-4.741024	-0.533778	3.499425
1	-5.148184	0.358025	3.967461
6	-3.415926	-0.541747	3.059440
1	-2.796300	0.342172	3.182035
6	1.954145	-1.226260	-0.870283
6	2.796739	-1.200833	0.251478
1	2.676604	-0.404545	0.981730
6	3.756271	-2.196489	0.434761
6	3.863679	-3.258118	-0.462040
1	4.589430	-4.047657	-0.301511
6	3.006448	-3.293704	-1.562248
6	2.075743	-2.278844	-1.784723
1	1.442874	-2.339791	-2.660297
6	1.619367	1.609326	-1.336792
6	0.920727	2.823924	-1.235529
1	-0.134369	2.822657	-0.987528
6	1.585245	4.033901	-1.403282
6	2.961892	4.067077	-1.637797
1	3.483332	5.012201	-1.736600
6	3.655898	2.863687	-1.719683
6	2.994000	1.639107	-1.585215
1	3.564965	0.720174	-1.653483
29	-0.298208	0.369413	1.181759
6	5.152575	2.866107	-1.844526
6	0.854535	5.333053	-1.211973
6	4.704583	-2.078958	1.595278
6	3.081720	-4.477598	-2.485637
9	2.826206	-5.635192	-1.825289
9	2.196709	-4.400512	-3.504194
9	4.312929	-4.613977	-3.031973
9	5.676757	-1.164450	1.348576
9	5.321920	-3.244249	1.881289
9	4.075575	-1.668598	2.724364
9	5.600662	1.852188	-2.618150
9	5.746074	2.712013	-0.628145
9	5.627630	4.017618	-2.364423
9	1.168016	6.230803	-2.175463
9	-0.486270	5.180050	-1.219586
9	1.179879	5.916320	-0.028039
6	1.815997	2.320925	2.057673
6	0.871684	3.381657	2.103493
6	-0.516145	3.340492	1.845070
1	1.251196	4.372662	2.311011
7	3.161090	2.640287	2.022063
6	4.172155	1.619950	2.253868
1	4.935995	2.006026	2.940122
1	3.718530	0.738941	2.700814
1	4.672921	1.325908	1.322951
6	3.668495	3.990639	1.834106
1	2.990410	4.580886	1.218046
1	3.827083	4.515804	2.788077
1	4.626997	3.935319	1.310159
8	1.517774	1.073196	2.055683
6	-1.259874	4.568337	1.933794
6	-2.603307	4.624300	1.654036
1	-0.731541	5.473702	2.215748
6	-3.244098	3.431216	1.276314
6	-2.518048	2.264063	1.193493
1	-2.986802	1.331647	0.905904
7	-1.195974	2.203271	1.459597
1	-3.148053	5.560488	1.720377
35	-5.167854	3.413756	0.870336

---

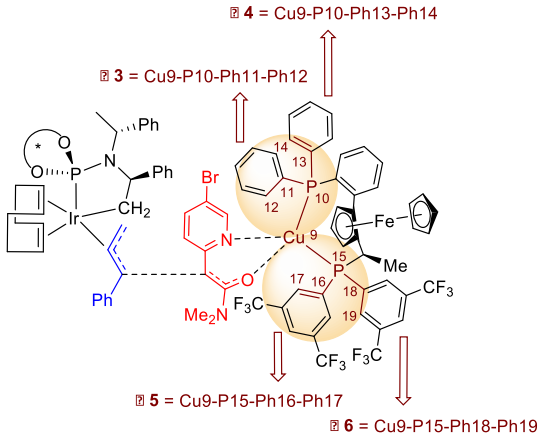
*Conformer*_30

Number of imaginary frequencies : 0
The smallest frequency is : 13.1870 cm(-1)
Electronic energy : HF=-4521.7138805
Zero-point correction= 0.854507
(Hartree/Particle)
Thermal correction to Energy= 0.923919
Thermal correction to Enthalpy= 0.924863
Thermal correction to Gibbs Free Energy= 0.744385
Sum of electronic and zero-point Energies= -4520.859373
Sum of electronic and thermal Energies= -4520.789961
Sum of electronic and thermal Enthalpies= -4520.789017
Sum of electronic and thermal Free Energies= -4520.969496

Cartesian Coordinates

26	-3.598383	-1.129884	-2.692084
15	-1.125989	-1.576165	1.911979
15	0.662576	0.066124	-0.938094
6	-2.360319	-1.491814	-1.039471
6	-1.858922	-0.400110	-1.842329
6	-2.862534	0.615414	-1.876165
1	-2.793268	1.554980	-2.406690
6	-3.990288	0.154998	-1.133486
1	-4.924766	0.683420	-1.006501
6	-3.683402	-1.139002	-0.620199
1	-4.343056	-1.760907	-0.034755
6	-3.205899	-2.086790	-4.493619
1	-2.219494	-2.371925	-4.835536
6	-3.843063	-0.829757	-4.727200
1	-3.421788	0.005710	-5.270264
6	-5.114266	-0.850783	-4.076027
1	-5.819978	-0.031553	-4.034187
6	-5.263364	-2.120488	-3.439084
1	-6.103571	-2.433611	-2.833370
6	-4.086084	-2.884396	-3.697582
1	-3.884206	-3.879581	-3.324996
6	-1.560936	-2.701176	-0.683050
6	-1.264156	-3.638958	-1.684515
1	-1.677637	-3.479078	-2.672172
6	-0.441131	-4.739349	-1.446622
1	-0.208246	-5.427303	-2.253380
6	0.096936	-4.930489	-0.176566
1	0.751747	-5.772687	0.023193
6	-0.185799	-4.014716	0.837187
1	0.255880	-4.167827	1.815201
6	-0.997005	-2.890788	0.608927
6	-0.467865	-0.327189	-2.411159
1	-0.193301	-1.334187	-2.729424
6	-0.325628	0.614982	-3.608942
1	0.692824	0.590929	-4.006784
1	-0.558565	1.651111	-3.349007
1	-1.015652	0.302342	-4.398963
6	-0.216929	-2.272905	3.356531
6	-0.751984	-3.272573	4.186592
1	-1.746787	-3.664568	3.999788
6	-0.010722	-3.767313	5.259564
1	-0.434062	-4.539302	5.896270
6	1.271662	-3.271260	5.515095
1	1.846965	-3.657729	6.351901
6	1.807411	-2.274616	4.697985
1	2.801356	-1.884002	4.892061
6	1.066104	-1.771529	3.625602
1	1.473836	-0.975471	3.011254
6	-2.874993	-1.630486	2.472886
6	-3.689927	-2.764698	2.334128
1	-3.297599	-3.661822	1.864067
6	-5.013877	-2.736624	2.776384
1	-5.639811	-3.617075	2.660251
6	-5.533426	-1.578817	3.363899
1	-6.565812	-1.556642	3.701201
6	-4.722498	-0.451348	3.517941
1	-5.120238	0.449834	3.975966
6	-3.398886	-0.476606	3.074156
1	-2.771280	0.403366	3.183737
6	1.940449	-1.258441	-0.884993
6	2.784121	-1.232859	0.235991
1	2.672377	-0.429533	0.959617
6	3.735732	-2.234683	0.425604

6	3.832989	-3.304084	-0.462956
1	4.551778	-4.098915	-0.297257
6	2.973997	-3.340346	-1.561892
6	2.052066	-2.318948	-1.791616
1	1.417854	-2.381248	-2.666159
6	1.614254	1.582308	-1.361676
6	0.913235	2.796340	-1.278947
1	-0.146080	2.795793	-1.049565
6	1.582713	4.006576	-1.427706
6	2.965341	4.039376	-1.619505
1	3.490091	4.985571	-1.688005
6	3.663359	2.835825	-1.672198
6	2.996288	1.612380	-1.568261
1	3.569858	0.694183	-1.606816
29	-0.276379	0.379630	1.173066
6	5.158670	2.851064	-1.826161
6	0.850337	5.306892	-1.250068
6	4.685643	-2.114418	1.584545
6	3.036292	-4.533318	-2.474387
9	2.767354	-5.681752	-1.803251
9	2.152461	-4.455979	-3.493925
9	4.266068	-4.688870	-3.018798
9	5.664380	-1.209395	1.329632
9	5.293947	-3.281872	1.880752
9	4.060174	-1.688737	2.710240
9	5.543946	2.871089	-3.123739
9	5.732583	1.759939	-1.264732
9	5.712205	3.939212	-1.238178
9	1.174306	6.199483	-2.215154
9	-0.490342	5.154697	-1.270656
9	1.164325	5.896399	-0.066414
6	1.867939	2.331404	2.008093
6	0.922189	3.389160	2.090400
6	-0.466523	3.354426	1.836849
1	1.303567	4.376274	2.312527
7	3.211761	2.654554	1.952172
6	4.230126	1.626412	2.098724
1	5.038046	1.997462	2.740748
1	3.803990	0.738121	2.558463
1	4.668800	1.348231	1.131162
6	3.716252	4.004758	1.754571
1	3.001532	4.612387	1.200709
1	3.947698	4.507350	2.705430
1	4.634499	3.958116	1.160617
8	1.571678	1.083640	1.990891
6	-1.205530	4.584332	1.939825
6	-2.548010	4.649794	1.658371
1	-0.673606	5.484142	2.232530
6	-3.193846	3.464015	1.266047
6	-2.473666	2.294019	1.174335
1	-2.946723	1.366267	0.878723
7	-1.152403	2.223778	1.442791
1	-3.088385	5.587812	1.734157
35	-5.116629	3.460793	0.855265



Conformer_1

Number of imaginary frequencies : 1
The smallest frequency is : -247.7050 cm(-1)
Electronic energy : HF=-7222.6348461
Zero-point correction= 1.755699
(Hartree/Particle)
Thermal correction to Energy= 1.874114
Thermal correction to Enthalpy= 1.875058
Thermal correction to Gibbs Free Energy= 1.593069
Sum of electronic and zero-point Energies= -7220.879147
Sum of electronic and thermal Energies= -7220.760732
Sum of electronic and thermal Enthalpies= -7220.759788
Sum of electronic and thermal Free Energies= -7221.041777

Cartesian Coordinates

26	4.295483	4.787309	1.873229
15	2.562756	1.624351	-1.886440
15	4.540846	0.128139	0.933294
6	3.967410	3.424777	0.318854
6	4.154545	2.746011	1.580203
6	3.132457	3.194330	2.473117
1	3.010044	2.884449	3.501783
6	2.335062	4.162702	1.791781
1	1.509022	4.715925	2.216611
6	2.848836	4.307262	0.470055
1	2.478789	4.983235	-0.285769
6	6.237819	5.325975	2.375695
1	7.098923	4.677221	2.283117
6	5.382659	5.426340	3.515800
1	5.479489	4.864930	4.435514
6	4.350475	6.365732	3.212751
1	3.525333	6.633260	3.859560
6	4.567421	6.847172	1.885647
1	3.938500	7.546977	1.351295
6	5.733290	6.207213	1.369562
1	6.141305	6.344961	0.377594
6	4.764225	3.153541	-0.913015
6	6.097254	3.584398	-0.982741
1	6.500731	4.139446	-0.145405
6	6.905965	3.300484	-2.083113
1	7.941472	3.625280	-2.093003
6	6.383442	2.576975	-3.152563
1	7.003929	2.337237	-4.010062
6	5.061419	2.133590	-3.105883
1	4.672171	1.556787	-3.937886
6	4.241745	2.397541	-1.997457
6	5.179891	1.672429	1.830628
1	6.093248	1.961759	1.307923
6	5.519720	1.464613	3.309098
1	6.298475	0.706859	3.429748
1	4.650907	1.149113	3.892963
1	5.882077	2.407481	3.730094
6	2.354388	0.721764	-3.482108
6	2.616264	-0.657954	-3.490658
1	2.930154	-1.152676	-2.579085
6	2.435238	-1.405079	-4.656781
1	2.642253	-2.470144	-4.648914
6	1.979091	-0.786424	-5.822565
1	1.823954	-1.370497	-6.725154
6	1.718981	0.586581	-5.822737
1	1.363344	1.074348	-6.725869
6	1.908484	1.338355	-4.662346
1	1.691997	2.400842	-4.679702
6	1.403612	3.038197	-2.070606
6	1.740478	4.197636	-2.788318
1	2.733170	4.302579	-3.215953
6	0.806347	5.222726	-2.947869
1	1.077352	6.116575	-3.502627
6	-0.475294	5.095166	-2.402505
1	-1.208148	5.886371	-2.532928
6	-0.814345	3.945094	-1.686943
1	-1.807520	3.839153	-1.267558
6	0.124931	2.927395	-1.509458
1	-0.137151	2.044722	-0.936863

6	5.833965	-0.351382	-0.288271
6	5.486637	-1.402383	-1.149489
1	4.518877	-1.879209	-1.036718
6	6.371537	-1.830052	-2.138412
6	7.598093	-1.194248	-2.319539
1	8.275671	-1.510998	-3.104292
6	7.930518	-0.131841	-1.478494
6	7.072175	0.277465	-0.457524
1	7.378611	1.096731	0.178092
6	4.568674	-1.271479	2.131350
6	3.559625	-1.295138	3.107554
1	2.867800	-0.465444	3.195734
6	3.410590	-2.401818	3.940533
6	4.233786	-3.519362	3.797948
1	4.087853	-4.396385	4.418590
6	5.223241	-3.501172	2.818331
6	5.409653	-2.382703	2.004934
1	6.188576	-2.406568	1.253329
29	2.440299	0.234709	-0.102205
6	6.092016	-4.714936	2.637202
6	2.273267	-2.466890	4.920951
6	5.996979	-3.025825	-2.969177
6	9.225013	0.593122	-1.726107
9	9.227801	1.197511	-2.941072
9	9.466965	1.553228	-0.806824
9	10.282529	-0.251083	-1.717675
9	6.178599	-4.182051	-2.282737
9	6.720536	-3.118143	-4.102531
9	4.686637	-3.002365	-3.326882
9	7.068756	-4.789663	3.569521
9	6.695649	-4.731981	1.427069
9	5.369588	-5.858161	2.739730
9	2.645063	-3.031461	6.090473
9	1.757680	-1.251357	5.200159
9	1.250890	-3.226951	4.437751
6	1.975914	-2.751405	0.404028
6	0.812416	-2.465320	1.213732
6	0.453925	-1.190375	1.765525
1	0.409664	-3.292603	1.779811
77	-3.400074	-1.296233	-1.446980
15	-5.267027	-0.538266	-0.377852
8	-5.260491	0.604631	0.820512
8	-6.330099	0.174126	-1.442024
7	-5.966526	-1.799001	0.479468
6	-4.982081	1.930148	0.525376
6	-3.757901	2.439120	1.010815
1	-3.119048	1.782006	1.589915
6	-3.415991	3.740399	0.740454
1	-2.486837	4.152949	1.120483
6	-4.248689	4.546670	-0.083515
6	-3.843378	5.851233	-0.476680
1	-2.895203	6.232436	-0.106490
6	-4.622828	6.608497	-1.322249
1	-4.300209	7.600847	-1.623443
6	-5.844896	6.086321	-1.809648
1	-6.447900	6.678260	-2.492075
6	-6.275844	4.832853	-1.431460
1	-7.211239	4.445808	-1.818835
6	-5.501762	4.025514	-0.552471
6	-5.909913	2.701982	-0.155776
6	-7.269153	2.156923	-0.436138
6	-8.460122	2.845551	-0.001838
6	-8.420922	4.023133	0.797125
1	-7.464264	4.422269	1.111009
6	-9.579472	4.655891	1.193107
1	-9.518953	5.549253	1.808116
6	-10.845803	4.150782	0.814696
1	-11.749912	4.664885	1.127401
6	-10.923669	2.997890	0.067028
1	-11.888658	2.583673	-0.213172
6	-9.748677	2.311574	-0.344045
6	-9.832613	1.090652	-1.066154
1	-10.811116	0.699023	-1.329281
6	-8.695439	0.398840	-1.398472
1	-8.734297	-0.551501	-1.920336
6	-7.430849	0.928239	-1.059933
6	-5.328328	-3.110859	0.181070
1	-4.591384	-3.316281	0.967104
6	-6.342514	-4.240822	0.175232
6	-6.026794	-5.466224	0.773531
1	-5.072330	-5.581289	1.282463
6	-6.925372	-6.535557	0.723178
1	-6.667715	-7.480489	1.193710
6	-8.155359	-6.385423	0.079323
1	-8.858545	-7.212789	0.045222
6	-8.480066	-5.162146	-0.516900
1	-9.437497	-5.037600	-1.015602
6	-7.578935	-4.098583	-0.471284
1	-7.831509	-3.144332	-0.925449
6	-4.594867	-3.051751	-1.163480
1	-5.333941	-3.113043	-1.971274
1	-3.953584	-3.933841	-1.249441
6	-6.667696	-1.732628	1.808093
1	-7.141346	-2.714901	1.886829
6	-5.678261	-1.640576	2.970994
6	-5.126373	-2.826177	3.482772
1	-5.452940	-3.781296	3.080077
6	-4.182113	-2.800245	4.512528
1	-3.769070	-3.731663	4.890271
6	-3.790207	-1.580870	5.068553
1	-3.063943	-1.554835	5.876380
6	-4.357194	-0.394942	4.591645
1	-4.076226	0.558106	5.032405
6	-5.290609	-0.424605	3.553769
1	-5.716280	0.505726	3.199603
6	-7.806795	-0.715831	1.852940
1	-8.514404	-0.911719	1.044168
1	-7.468521	0.315854	1.765928
1	-8.334929	-0.822792	2.805420
6	-2.525395	-1.128371	0.544898
1	-1.882648	-0.253616	0.590751
1	-3.221247	-1.183612	1.377390
6	-1.992538	-2.367425	0.062609
1	-2.496844	-3.272189	0.385435
6	-0.734615	-2.534737	-0.568679
1	-0.209016	-1.652817	-0.907203
6	-4.223093	-1.143940	-3.492962
1	-5.215254	-1.589616	-3.481799
6	-3.126537	-2.048714	-3.521705
1	-3.365293	-3.111875	-3.550763
6	-1.762002	-1.710558	-4.097524
1	-1.805768	-1.728915	-5.197661
1	-1.073460	-2.507913	-3.807452
6	-1.196672	-0.358791	-3.615743
1	-1.429506	0.434494	-4.332715
1	-0.107368	-0.422413	-3.582549
6	-1.691505	0.068016	-2.237555
1	-0.934684	0.084613	-1.459702
6	-2.806519	0.873812	-2.021990
1	-2.816421	1.461192	-1.109578
6	-3.753045	1.359085	-3.101152
1	-4.645288	1.750094	-2.607258
1	-3.289392	2.204813	-3.630447
6	-4.170809	0.260288	-4.102468
1	-3.492715	0.252276	-4.962250
1	-5.160721	0.506491	-4.498797
6	-0.336566	-3.784974	-1.225126
6	-0.870963	-5.040132	-0.873228
6	0.627007	-3.732217	-2.250687
6	-0.457009	-6.196849	-1.530564
1	-1.601347	-5.116504	-0.074064
6	1.036626	-4.889362	-2.910012
1	1.058507	-2.774554	-2.516059
6	0.497790	-6.127654	-2.551971
1	-0.876991	-7.156881	-1.244167
1	1.782713	-4.824630	-3.697145
1	0.817686	-7.031973	-3.061444
7	2.527339	-3.998361	0.475398
6	3.530290	-4.417758	-0.497346
1	3.343419	-5.458902	-0.776638

1	3.460343	-3.806109	-1.391327
1	4.542644	-4.343808	-0.084271
6	2.172743	-5.004943	1.472710
1	1.857227	-4.544834	2.407757
1	1.379527	-5.669548	1.108107
1	3.059627	-5.605133	1.688322
8	2.451443	-1.919445	-0.431559
6	-0.453472	-1.173945	2.861558
6	-0.885294	0.012322	3.418718
1	-0.794683	-2.114310	3.277100
6	-0.417688	1.201489	2.853870
6	0.455996	1.160372	1.781911
1	0.835564	2.067885	1.329476
7	0.890413	0.000895	1.248320
1	-1.574561	0.013211	4.253996
35	-0.962268	2.928027	3.596277

Conformer_2

Number of imaginary frequencies : 1
The smallest frequency is : -247.7139 cm(-1)
Electronic energy : HF=-7222.6348455
Zero-point correction= 1.755698
(Hartree/Particle)
Thermal correction to Energy= 1.874114
Thermal correction to Enthalpy= 1.875058
Thermal correction to Gibbs Free Energy= 1.593085
Sum of electronic and zero-point Energies= -7220.879148
Sum of electronic and thermal Energies= -7220.760732
Sum of electronic and thermal Enthalpies= -7220.759787
Sum of electronic and thermal Free Energies= -7221.041761

Cartesian Coordinates

26	4.295623	4.787492	1.872387
15	2.562609	1.624222	-1.886844
15	4.540942	0.128231	0.932826
6	3.967468	3.424838	0.318135
6	4.154660	2.746165	1.579531
6	3.132618	3.194562	2.472457
1	3.010250	2.884760	3.501152
6	2.335195	4.162887	1.791087
1	1.509183	4.716156	2.215916
6	2.848907	4.307341	0.469326
1	2.478825	4.983257	-0.286531
6	6.237972	5.326169	2.374774
1	7.099054	4.677377	2.282263
6	5.382824	5.426685	3.514875
1	5.479641	4.865370	4.434649
6	4.350661	6.366067	3.211730
1	3.525532	6.633686	3.858517
6	4.567609	6.847354	1.884570
1	3.938705	7.547120	1.350145
6	5.733457	6.207309	1.368546
1	6.141468	6.344950	0.376563
6	4.764183	3.153482	-0.913770
6	6.097215	3.584303	-0.983641
1	6.500756	4.139439	-0.146393
6	6.905840	3.300240	-2.084038
1	7.941353	3.625012	-2.094043
6	6.383227	2.576602	-3.153357
1	7.003653	2.336732	-4.010864
6	5.061193	2.133262	-3.106537
1	4.671877	1.556352	-3.938434
6	4.241599	2.397379	-1.998091
6	5.180015	1.672596	1.830007
1	6.093364	1.961882	1.307264
6	5.519883	1.464899	3.308487
1	6.298650	0.707164	3.429174
1	4.651091	1.149433	3.892406
1	5.882244	2.407806	3.729394
6	2.354062	0.721529	-3.482428
6	2.615782	-0.658219	-3.490882
1	2.929657	-1.152901	-2.579284
6	2.434583	-1.405420	-4.656930
1	2.641470	-2.470510	-4.648989
6	1.978419	-0.786810	-5.822730
1	1.823142	-1.370941	-6.725257
6	1.718464	0.586225	-5.822998
1	1.362811	1.073956	-6.726142
6	1.908138	1.338073	-4.662683
1	1.691750	2.400580	-4.680106
6	1.403399	3.038015	-2.070967
6	1.740109	4.197411	-2.788820
1	2.732744	4.302372	-3.216587
6	0.805900	5.222436	-2.948334
1	1.076782	6.116255	-3.503200
6	-0.475666	5.094848	-2.402797
1	-1.208582	5.885999	-2.533197
6	-0.814561	3.944820	-1.687091
1	-1.807678	3.838848	-1.267574
6	0.124798	2.927192	-1.509640
1	-0.137151	2.044552	-0.936934
6	5.833938	-0.351367	-0.288838
6	5.486480	-1.402366	-1.150004
1	4.518701	-1.879129	-1.037136
6	6.371280	-1.830115	-2.138981
6	7.597866	-1.194396	-2.320209
1	8.275368	-1.511209	-3.105003
6	7.930409	-0.131974	-1.479227
6	7.072167	0.277407	-0.458200
1	7.378693	1.096672	0.177374
6	4.568902	-1.271331	2.130945
6	3.559919	-1.294997	3.107218
1	2.868059	-0.465336	3.195416
6	3.410979	-2.401658	3.940242
6	4.234190	-3.519186	3.797623
1	4.088322	-4.396198	4.418296
6	5.223581	-3.500989	2.817940
6	5.409909	-2.382533	2.004508
1	6.188789	-2.406394	1.252857
29	2.440313	0.234733	-0.102469
6	6.092378	-4.714728	2.636762
6	2.273746	-2.466725	4.920768
6	5.996575	-3.025872	-2.969706
6	9.224913	0.592926	-1.726976
9	9.227679	1.197136	-2.942030
9	9.466905	1.553165	-0.807841
9	10.282414	-0.251294	-1.718444
9	6.178280	-4.182112	-2.283313
9	6.719959	-3.118181	-4.103173
9	4.686184	-3.002385	-3.327216
9	7.069189	-4.789413	3.569010
9	6.695920	-4.731765	1.426585
9	5.369994	-5.857976	2.739356
9	2.645663	-3.031272	6.090263
9	1.758173	-1.251193	5.200007
9	1.251330	-3.226804	4.437680
6	1.975938	-2.751414	0.403912
6	0.812506	-2.465310	1.213713
6	0.454112	-1.190336	1.765512
1	0.409808	-3.292570	1.779866
77	-3.400234	-1.296174	-1.446510
15	-5.267086	-0.538255	-0.377160
8	-5.260470	0.604660	0.821190
8	-6.330314	0.174058	-1.441230
7	-5.966438	-1.799016	0.480245
6	-4.982086	1.930171	0.525982
6	-3.757872	2.439171	1.011303
1	-3.119001	1.782107	1.590437
6	-3.415949	3.740415	0.740790
1	-2.486755	4.152976	1.120707
6	-4.248687	4.546626	-0.083197
6	-3.843371	5.851138	-0.476529
1	-2.895150	6.232347	-0.106463
6	-4.622876	6.608340	-1.322102
1	-4.300251	7.600649	-1.623428
6	-5.845004	6.086154	-1.809338
1	-6.448053	6.678045	-2.491767
6	-6.275955	4.832736	-1.430989

1	-7.211396	4.445681	-1.818245
6	-5.501815	4.025460	-0.551994
6	-5.909961	2.701970	-0.155150
6	-7.269236	2.156915	-0.435348
6	-8.460149	2.845592	-0.000970
6	-8.420846	4.023231	0.797902
1	-7.464150	4.422372	1.111661
6	-9.579345	4.656040	1.193954
1	-9.518747	5.549448	1.808889
6	-10.845723	4.150924	0.815712
1	-11.749792	4.665065	1.128472
6	-10.923686	2.997979	0.068135
1	-11.888710	2.583757	-0.211936
6	-9.748747	2.311615	-0.343011
6	-9.832777	1.090649	-1.065035
1	-10.811314	0.699024	-1.328042
6	-8.695649	0.398798	-1.397428
1	-8.734578	-0.551571	-1.919234
6	-7.431015	0.928198	-1.059053
6	-5.328274	-3.110862	0.181718
1	-4.591216	-3.316322	0.967637
6	-6.342464	-4.240823	0.175982
6	-6.026689	-5.466228	0.774243
1	-5.072166	-5.581302	1.283064
6	-6.925278	-6.535556	0.723982
1	-6.667575	-7.480491	1.194482
6	-8.155332	-6.385413	0.080258
1	-8.858525	-7.212776	0.046225
6	-8.480097	-5.162130	-0.515923
1	-9.437582	-5.037577	-1.014521
6	-7.578957	-4.098572	-0.470395
1	-7.831576	-3.144314	-0.924523
6	-4.594997	-3.051697	-1.162929
1	-5.334177	-3.112961	-1.970627
1	-3.953725	-3.933785	-1.249007
6	-6.667450	-1.732679	1.808953
1	-7.141101	-2.714949	1.887719
6	-5.677859	-1.640676	2.971724
6	-5.125934	-2.826302	3.483404
1	-5.452590	-3.781408	3.080746
6	-4.181513	-2.800411	4.513015
1	-3.768443	-3.731847	4.890684
6	-3.789470	-1.581054	5.068985
1	-3.063075	-1.555052	5.876694
6	-4.356494	-0.395103	4.592179
1	-4.075423	0.557933	5.032900
6	-5.290074	-0.424724	3.554450
1	-5.715768	0.505623	3.200356
6	-7.806535	-0.715873	1.853966
1	-8.514244	-0.911732	1.045272
1	-7.468267	0.315812	1.766939
1	-8.334557	-0.822858	2.806506
6	-2.525330	-1.128326	0.545249
1	-1.882521	-0.253615	0.591033
1	-3.221098	-1.183503	1.377814
6	-1.992585	-2.367429	0.062946
1	-2.496920	-3.272146	0.385869
6	-0.734736	-2.534814	-0.568473
1	-0.209166	-1.652923	-0.907126
6	-4.223446	-1.143893	-3.492437
1	-5.215604	-1.589573	-3.481180
6	-3.126887	-2.048656	-3.521275
1	-3.365632	-3.111820	-3.550308
6	-1.762395	-1.710482	-4.097188
1	-1.806237	-1.728822	-5.197322
1	-1.073826	-2.507836	-3.807175
6	-1.197049	-0.358716	-3.615417
1	-1.429926	0.434583	-4.332360
1	-0.107745	-0.422327	-3.582268
6	-1.691816	0.068050	-2.237190
1	-0.934936	0.084645	-1.459396
6	-2.806808	0.873864	-2.021551
1	-2.816638	1.461267	-1.109154
6	-3.753409	1.359134	-3.100648
1	-4.645627	1.750118	-2.606691
1	-3.289805	2.204874	-3.629966
6	-4.171213	0.260335	-4.101946
1	-3.493158	0.252329	-4.961759
1	-5.161147	0.506527	-4.498227
6	-0.336805	-3.785097	-1.224912
6	-0.871252	-5.040215	-0.872944
6	0.626705	-3.732429	-2.250537
6	-0.457389	-6.196979	-1.530256
1	-1.601609	-5.116522	-0.073750
6	1.036239	-4.889622	-2.909832
1	1.058229	-2.774799	-2.515983
6	0.497368	-6.127874	-2.551707
1	-0.877411	-7.156977	-1.243805
1	1.782285	-4.824960	-3.697009
1	0.817197	-7.032230	-3.061157
7	2.527397	-3.998354	0.475280
6	3.530277	-4.417740	-0.497543
1	3.343464	-5.458919	-0.776739
1	3.460179	-3.806158	-1.391558
1	4.542672	-4.343676	-0.084589
6	2.172939	-5.004906	1.472669
1	1.857476	-4.544767	2.407720
1	1.379726	-5.669570	1.108166
1	3.059874	-5.605038	1.688239
8	2.451366	-1.919479	-0.431755
6	-0.453161	-1.173844	2.861646
6	-0.884894	0.012454	3.418815
1	-0.794345	-2.114184	3.277264
6	-0.417329	1.201587	2.853865
6	0.456225	1.160407	1.781803
1	0.835742	2.067896	1.329277
7	0.890569	0.000905	1.248214
1	-1.574064	0.013389	4.254175
35	-0.961760	2.928178	3.596240

Conformer_3

Number of imaginary frequencies : 1
The smallest frequency is : -247.6851 cm(-1)
Electronic energy : HF=-7222.6348466
Zero-point correction= 1.755697
(Hartree/Particle)
Thermal correction to Energy= 1.874112
Thermal correction to Enthalpy= 1.875056
Thermal correction to Gibbs Free Energy= 1.593051
Sum of electronic and zero-point Energies= -7220.879150
Sum of electronic and thermal Energies= -7220.760735
Sum of electronic and thermal Enthalpies= -7220.759790
Sum of electronic and thermal Free Energies= -7221.041796

.....

Cartesian Coordinates

.....

26	4.294958	4.787330	1.873779
15	2.562885	1.624402	-1.886218
15	4.540623	0.128186	0.933775
6	3.967157	3.424827	0.319317
6	4.154106	2.746036	1.580680
6	3.131870	3.194315	2.473442
1	3.009300	2.884410	3.502081
6	2.334563	4.162687	1.792003
1	1.508442	4.715879	2.216717
6	2.848545	4.307291	0.470363
1	2.478603	4.983273	-0.285504
6	6.237185	5.325973	2.376683
1	7.098302	4.677205	2.284305
6	5.381765	5.426356	3.516591
1	5.478367	4.864942	4.436327
6	4.349662	6.365758	3.213300
1	3.524376	6.633302	3.859918
6	4.566920	6.847188	1.886243
1	3.938132	7.547000	1.351741
6	5.732900	6.207214	1.370430
1	6.141151	6.344956	0.378559
6	4.764171	3.153624	-0.912430
6	6.097214	3.584475	-0.981923

1	6.500558	4.139492	-0.144503
6	6.906105	3.300581	-2.082167
1	7.941618	3.625362	-2.091874
6	6.383752	2.577108	-3.151724
1	7.004379	2.337393	-4.009129
6	5.061719	2.133727	-3.105275
1	4.672605	1.556947	-3.937355
6	4.241868	2.397646	-1.996972
6	5.179449	1.672485	1.831247
1	6.092875	1.961865	1.308696
6	5.519036	1.464650	3.309769
1	6.297820	0.706942	3.430532
1	4.650144	1.149075	3.893474
1	5.881260	2.407529	3.730854
6	2.354751	0.721876	-3.481954
6	2.616715	-0.657825	-3.490535
1	2.930536	-1.152566	-2.578949
6	2.435866	-1.404912	-4.656709
1	2.642955	-2.469964	-4.648863
6	1.979804	-0.786238	-5.822516
1	1.824805	-1.370282	-6.725147
6	1.719603	0.586750	-5.822657
1	1.364032	1.074533	-6.725805
6	1.908934	1.338487	-4.662213
1	1.692385	2.400963	-4.679551
6	1.403723	3.038220	-2.070468
6	1.740632	4.197680	-2.788125
1	2.733362	4.302653	-3.215666
6	0.806494	5.222753	-2.947743
1	1.077530	6.116620	-3.502457
6	-0.475194	5.095154	-2.402498
1	-1.208052	5.886348	-2.532968
6	-0.814287	3.945060	-1.686992
1	-1.807496	3.839092	-1.267696
6	0.124994	2.927377	-1.509441
1	-0.137115	2.044688	-0.936884
6	5.833958	-0.351192	-0.287616
6	5.486806	-1.402125	-1.148990
1	4.519031	-1.878974	-1.036443
6	6.371917	-1.829723	-2.137754
6	7.598521	-1.193918	-2.318565
1	8.276267	-1.510620	-3.103191
6	7.930777	-0.131587	-1.477359
6	7.072211	0.277652	-0.456548
1	7.378523	1.096853	0.179209
6	4.568405	-1.271487	2.131768
6	3.559253	-1.295272	3.107862
1	2.867355	-0.465634	3.196010
6	3.410223	-2.402002	3.940776
6	4.233523	-3.519474	3.798226
1	4.087597	-4.396538	4.418812
6	5.223071	-3.501165	2.818705
6	5.409479	-2.382643	2.005380
1	6.188478	-2.406418	1.253851
29	2.440234	0.234668	-0.102059
6	6.091955	-4.714855	2.637605
6	2.272794	-2.467220	4.921060
6	5.997555	-3.025447	-2.968678
6	9.225336	0.593380	-1.724623
9	9.228344	1.197998	-2.939474
9	9.467170	1.553307	-0.805121
9	10.282818	-0.250865	-1.716178
9	6.179155	-4.181721	-2.282314
9	6.721289	-3.117617	-4.101932
9	4.687264	-3.002046	-3.326574
9	7.068643	-4.789525	3.569983
9	6.695666	-4.731826	1.427509
9	5.369611	-5.858140	2.740061
9	2.644496	-3.031834	6.090591
9	1.757085	-1.251741	5.200282
9	1.250530	-3.227328	4.437695
6	1.975987	-2.751479	0.404006
6	0.812394	-2.465505	1.213612
6	0.453769	-1.190609	1.765429
1	0.409643	-3.292839	1.779616
77	-3.399949	-1.296318	-1.447397
15	-5.266925	-0.538237	-0.378408
8	-5.260414	0.604596	0.820015
8	-6.329826	0.174291	-1.442661
7	-5.966617	-1.798955	0.478771
6	-4.981987	1.930136	0.524989
6	-3.757844	2.439078	1.010553
1	-3.119024	1.781930	1.589650
6	-3.415919	3.740378	0.740319
1	-2.486791	4.152895	1.120446
6	-4.248559	4.546714	-0.083645
6	-3.843220	5.851306	-0.476684
1	-2.895072	6.232481	-0.106398
6	-4.622612	6.608632	-1.322251
1	-4.299973	7.601005	-1.623348
6	-5.844644	6.086491	-1.809775
1	-6.447601	6.678480	-2.492200
6	-6.275617	4.832993	-1.431712
1	-7.210984	4.445977	-1.819185
6	-5.501595	4.025589	-0.552731
6	-5.909771	2.702024	-0.156169
6	-7.268986	2.156991	-0.436698
6	-8.459996	2.845579	-0.002451
6	-8.420872	4.023080	0.796634
1	-7.464243	4.422181	1.110652
6	-9.579460	4.655801	1.192564
1	-9.519002	5.549100	1.807670
6	-10.845754	4.150733	0.813972
1	-11.749894	4.664807	1.126637
6	-10.923548	2.997917	0.066178
1	-11.888511	2.583735	-0.214163
6	-9.748516	2.311639	-0.344844
6	-9.832381	1.090790	-1.067085
1	-10.810859	0.699191	-1.330353
6	-8.695175	0.399007	-1.399355
1	-8.733981	-0.551281	-1.921319
6	-7.430620	0.928369	-1.060628
6	-5.328537	-3.110859	0.180333
1	-4.591710	-3.316429	0.966435
6	-6.342864	-4.240697	0.174294
6	-6.027401	-5.466162	0.772599
1	-5.073024	-5.581375	1.281661
6	-6.926122	-6.535367	0.722088
1	-6.668663	-7.480350	1.192627
6	-8.155998	-6.385041	0.078065
1	-8.859296	-7.212306	0.043841
6	-8.480448	-5.161700	-0.518169
1	-9.437791	-5.037005	-1.017004
6	-7.579174	-4.098266	-0.472393
1	-7.831548	-3.143964	-0.926565
6	-4.594914	-3.051733	-1.164129
1	-5.333900	-3.112909	-1.972013
1	-3.953705	-3.933881	-1.250066
6	-6.667910	-1.732617	1.807334
1	-7.141656	-2.714853	1.885947
6	-5.678581	-1.640743	2.970338
6	-5.126858	-2.826430	3.482094
1	-5.453476	-3.781494	3.079308
6	-4.182695	-2.800655	4.511944
1	-3.769777	-3.732136	4.889666
6	-3.790726	-1.581353	5.068086
1	-3.064538	-1.555440	5.875985
6	-4.357553	-0.395341	4.591198
1	-4.076539	0.557653	5.032048
6	-5.290867	-0.424847	3.553228
1	-5.716414	0.505547	3.199079
6	-7.806921	-0.715722	1.852157
1	-8.514477	-0.911484	1.043308
1	-7.468547	0.315939	1.765255
1	-8.335148	-0.822710	2.804584
6	-2.525478	-1.128834	0.544591
1	-1.882771	-0.254063	0.590686
1	-3.221423	-1.184265	1.376996
6	-1.992482	-2.367782	0.062158
1	-2.496764	-3.272643	0.384755

6	-0.734470	-2.534926	-0.568990
1	-0.208889	-1.652937	-0.907357
6	-4.222766	-1.143785	-3.493461
1	-5.214958	-1.589400	-3.482439
6	-3.126270	-2.048629	-3.522160
1	-3.365101	-3.111771	-3.551335
6	-1.761641	-1.710517	-4.097784
1	-1.805264	-1.728805	-5.197928
1	-1.073186	-2.507930	-3.807666
6	-1.196282	-0.358810	-3.615857
1	-1.429011	0.434533	-4.332799
1	-0.106983	-0.422492	-3.582572
6	-1.691220	0.067941	-2.237687
1	-0.934483	0.084433	-1.459751
6	-2.806213	0.873769	-2.022172
1	-2.816183	1.461068	-1.109709
6	-3.752604	1.359180	-3.101388
1	-4.644873	1.750201	-2.607555
1	-3.288844	2.204923	-3.630567
6	-4.170329	0.260491	-4.102840
1	-3.492142	0.252508	-4.962549
1	-5.160183	0.506790	-4.499253
6	-0.336216	-3.785072	-1.225482
6	-0.870450	-5.040323	-0.873671
6	0.627417	-3.732126	-2.250976
6	-0.456288	-6.196949	-1.531035
1	-1.600859	-5.116835	-0.074543
6	1.037240	-4.889180	-2.910334
1	1.058799	-2.774389	-2.516269
6	0.498560	-6.127566	-2.552384
1	-0.876143	-7.157056	-1.244703
1	1.783365	-4.824305	-3.697418
1	0.818618	-7.031816	-3.061879
7	2.527494	-3.998398	0.475385
6	3.530581	-4.417691	-0.497265
1	3.343786	-5.458825	-0.776645
1	3.460718	-3.805989	-1.391217
1	4.542879	-4.343724	-0.084058
6	2.172855	-5.005047	1.472615
1	1.857223	-4.545000	2.407654
1	1.379711	-5.669678	1.107903
1	3.059751	-5.605201	1.688282
8	2.451543	-1.919452	-0.431500
6	-0.453691	-1.174294	2.861410
6	-0.885590	0.011917	3.418628
1	-0.794881	-2.114701	3.276873
6	-0.418003	1.201144	2.853890
6	0.455721	1.160138	1.781958
1	0.835270	2.067699	1.329601
7	0.890210	0.000715	1.248307
1	-1.574897	0.012721	4.253873
35	-0.962660	2.927600	3.596441

---

*Conformer_*4

Number of imaginary frequencies : 1
The smallest frequency is : -252.7213 cm(-1)
Electronic energy : HF=-7222.6349087
Zero-point correction= 1.756167
(Hartree/Particle)
Thermal correction to Energy= 1.874507
Thermal correction to Enthalpy= 1.875451
Thermal correction to Gibbs Free Energy= 1.594964
Sum of electronic and zero-point Energies= -7220.878742
Sum of electronic and thermal Energies= -7220.760402
Sum of electronic and thermal Enthalpies= -7220.759457
Sum of electronic and thermal Free Energies= -7221.039945

Cartesian Coordinates

26	4.279443	4.714743	1.902900
15	2.584093	1.561554	-1.887574
15	4.512562	0.053563	0.959528
6	3.962428	3.356736	0.340511
6	4.115765	2.675469	1.606312
6	3.082682	3.138934	2.478415
1	2.935092	2.831405	3.504439
6	2.312697	4.118418	1.781568
1	1.485939	4.682808	2.190160
6	2.854697	4.255518	0.470325
1	2.508408	4.935806	-0.292841
6	6.217270	5.218765	2.453717
1	7.068151	4.553981	2.382973
6	5.335442	5.335381	3.571771
1	5.397471	4.771862	4.493205
6	4.328455	6.293043	3.242430
1	3.492240	6.575861	3.868204
6	4.587634	6.769771	1.921197
1	3.985461	7.480781	1.371063
6	5.754520	6.108458	1.434979
1	6.190645	6.238793	0.454008
6	4.782276	3.065903	-0.871988
6	6.127074	3.463383	-0.902595
1	6.513237	4.026288	-0.062347
6	6.969482	3.130395	-1.962470
1	8.012839	3.427349	-1.940330
6	6.470726	2.387139	-3.029722
1	7.118678	2.102944	-3.853186
6	5.135404	1.982792	-3.026248
1	4.769243	1.378405	-3.848754
6	4.278849	2.303740	-1.961194
6	5.128276	1.595390	1.882334
1	6.055243	1.880944	1.382341
6	5.427540	1.383871	3.368701
1	6.201683	0.624441	3.508340
1	4.543326	1.067400	3.928582
1	5.780022	2.324843	3.802246
6	2.379352	0.668740	-3.490959
6	2.507679	-0.729138	-3.486238
1	2.714660	-1.248673	-2.558664
6	2.329809	-1.462964	-4.661081
1	2.446030	-2.542062	-4.639743
6	2.000971	-0.811244	-5.850157
1	1.848683	-1.381558	-6.761981
6	1.865461	0.580436	-5.863451
1	1.607695	1.094005	-6.785375
6	2.058223	1.317841	-4.694824
1	1.943671	2.395948	-4.723637
6	1.445516	2.990630	-2.078621
6	1.797616	4.146836	-2.793846
1	2.793699	4.241772	-3.216081
6	0.875848	5.183006	-2.953635
1	1.158344	6.074645	-3.506217
6	-0.408078	5.070117	-2.410159
1	-1.131020	5.870400	-2.540484
6	-0.761816	3.923694	-1.695707
1	-1.756350	3.829015	-1.276618
6	0.165212	2.894915	-1.518344
1	-0.106135	2.015368	-0.945227
6	5.839277	-0.369948	-0.248826
6	5.448174	-1.173274	-1.329906
1	4.434633	-1.553073	-1.364871
6	6.351295	-1.480806	-2.345488
6	7.654149	-0.985862	-2.311800
1	8.349880	-1.205863	-3.114245
6	8.044493	-0.194689	-1.232937
6	7.153561	0.108243	-0.201896
1	7.499244	0.721549	0.620871
6	4.535120	-1.365383	2.128618
6	3.530442	-1.407681	3.108620
1	2.841248	-0.578098	3.217310
6	3.383115	-2.532634	3.916747
6	4.205853	-3.646855	3.746908
1	4.063975	-4.535117	4.352527
6	5.187769	-3.611238	2.759924
6	5.367220	-2.478307	1.964792
1	6.133228	-2.487944	1.199219
29	2.425119	0.190344	-0.099040
6	6.052324	-4.823978	2.553574
6	2.246514	-2.620873	4.895952

6	5.885245	-2.239265	-3.556692
6	9.425626	0.400355	-1.248975
9	9.545134	1.333709	-2.228470
9	9.742972	1.007139	-0.085268
9	10.373249	-0.532574	-1.493889
9	6.856309	-3.022900	-4.073291
9	5.498556	-1.393685	-4.544421
9	4.822122	-3.036271	-3.288578
9	7.014733	-4.932838	3.497261
9	6.673731	-4.809056	1.352095
9	5.322509	-5.965893	2.610606
9	2.618694	-3.211071	6.052469
9	1.729012	-1.412721	5.202072
9	1.225001	-3.371228	4.395068
6	1.958396	-2.789158	0.365403
6	0.794800	-2.517053	1.182390
6	0.441405	-1.247219	1.752365
1	0.402266	-3.349501	1.747949
77	-3.411373	-1.270432	-1.453762
15	-5.265342	-0.498284	-0.370937
8	-5.239470	0.633901	0.837985
8	-6.323099	0.237507	-1.425117
7	-5.979199	-1.757030	0.476674
6	-4.940948	1.957127	0.550977
6	-3.705874	2.443028	1.032161
1	-3.074976	1.772168	1.603804
6	-3.343053	3.739565	0.766199
1	-2.404078	4.133532	1.141913
6	-4.167333	4.564871	-0.047309
6	-3.743032	5.865092	-0.435020
1	-2.786094	6.227965	-0.068930
6	-4.515618	6.640696	-1.270206
1	-4.178624	7.629518	-1.567237
6	-5.749465	6.142019	-1.752533
1	-6.347276	6.748400	-2.426796
6	-6.198490	4.893340	-1.379635
1	-7.142692	4.524443	-1.763349
6	-5.432030	4.067582	-0.511121
6	-5.859265	2.748237	-0.120676
6	-7.227697	2.226182	-0.399437
6	-8.405996	2.929267	0.045752
6	-8.345023	4.098302	0.855760
1	-7.380882	4.479415	1.169223
6	-9.491918	4.744990	1.263019
1	-9.414951	5.631144	1.886552
6	-10.767510	4.263340	0.885090
1	-11.662240	4.788127	1.206896
6	-10.866452	3.119504	0.126076
1	-11.838955	2.723254	-0.154231
6	-9.704006	2.419042	-0.296678
6	-9.809575	1.206982	-1.030762
1	-10.795042	0.833839	-1.294847
6	-8.684626	0.500264	-1.373390
1	-8.740566	-0.444079	-1.904511
6	-7.410556	1.005756	-1.033457
6	-5.363707	-3.075860	0.162961
1	-4.634784	-3.305735	0.949423
6	-6.399136	-4.186587	0.138795
6	-6.109952	-5.424735	0.724192
1	-5.160076	-5.563892	1.235829
6	-7.028645	-6.475895	0.657410
1	-6.791339	-7.431036	1.117935
6	-8.252464	-6.294674	0.009811
1	-8.971213	-7.107909	-0.037262
6	-8.550786	-5.058482	-0.573461
1	-9.503269	-4.909791	-1.075045
6	-7.629649	-4.013040	-0.511332
1	-7.861742	-3.048813	-0.955340
6	-4.624352	-3.014716	-1.178447
1	-5.361360	-3.064071	-1.988868
1	-3.991613	-3.902693	-1.267493
6	-6.679162	-1.695426	1.805877
1	-7.171428	-2.669443	1.871404
6	-5.687805	-1.638299	2.969429
6	-5.164092	-2.841459	3.469855
1	-5.511241	-3.784801	3.056632
6	-4.221344	-2.847542	4.501305
1	-3.830344	-3.792019	4.869973
6	-3.802725	-1.643230	5.070518
1	-3.077672	-1.641979	5.879847
6	-4.341214	-0.439847	4.604502
1	-4.039137	0.502086	5.055194
6	-5.272760	-0.437397	3.564485
1	-5.675988	0.505913	3.218466
6	-7.799131	-0.658375	1.866349
1	-8.511250	-0.829743	1.055943
1	-7.442229	0.368069	1.793485
1	-8.328066	-0.769259	2.817928
6	-2.522744	-1.109980	0.533199
1	-1.863615	-0.247375	0.569963
1	-3.215320	-1.146255	1.369288
6	-2.017129	-2.362489	0.058122
1	-2.540575	-3.252212	0.391740
6	-0.765301	-2.565525	-0.576229
1	-0.222763	-1.700377	-0.932512
6	-4.241411	-1.100126	-3.494009
1	-5.236794	-1.538726	-3.481979
6	-3.153606	-2.016023	-3.533997
1	-3.405053	-3.076131	-3.569257
6	-1.785335	-1.691684	-4.109343
1	-1.823648	-1.723164	-5.209449
1	-1.101475	-2.488315	-3.805038
6	-1.219700	-0.337200	-3.639353
1	-1.475438	0.455139	-4.349202
1	-0.129527	-0.390382	-3.630479
6	-1.692064	0.077354	-2.249743
1	-0.927489	0.072675	-1.479117
6	-2.795992	0.894192	-2.018268
1	-2.793932	1.475870	-1.102333
6	-3.742430	1.397672	-3.089519
1	-4.624609	1.800924	-2.587722
1	-3.269365	2.237705	-3.619492
6	-4.186045	0.309148	-4.092352
1	-3.523882	0.302331	-4.964380
1	-5.180709	0.566750	-4.468937
6	-0.407947	-3.834304	-1.222803
6	-0.985060	-5.068523	-0.863212
6	0.557746	-3.822777	-2.247296
6	-0.609787	-6.243482	-1.511471
1	-1.720021	-5.115346	-0.066048
6	0.929718	-4.998046	-2.897119
1	1.017885	-2.881606	-2.521838
6	0.348832	-6.214833	-2.531087
1	-1.063717	-7.186218	-1.219440
1	1.676637	-4.964184	-3.685390
1	0.638014	-7.133128	-3.033866
7	2.526019	-4.029143	0.429151
6	3.532636	-4.437266	-0.543013
1	3.243040	-5.395601	-0.987554
1	3.610981	-3.695479	-1.330836
1	4.510537	-4.555895	-0.062086
6	2.137220	-5.066963	1.380596
1	1.835474	-4.638752	2.335405
1	1.324199	-5.689303	0.986652
1	3.004940	-5.703280	1.568065
8	2.421561	-1.943783	-0.462058
6	-0.457564	-1.242659	2.854911
6	-0.882433	-0.062124	3.430219
1	-0.797498	-2.187182	3.262036
6	-0.418197	1.133163	2.876199
6	0.444755	1.103502	1.795077
1	0.819598	2.015208	1.347446
7	0.873893	-0.050268	1.245628
1	-1.564955	-0.070435	4.270811
35	-0.951533	2.851643	3.645191

Conformer_5

Number of imaginary frequencies : 1
The smallest frequency is : -247.7157 cm(-1)

Electronic energy : HF=-7222.634846
Zero-point correction= 1.755699
(Hartree/Particle)
Thermal correction to Energy= 1.874114
Thermal correction to Enthalpy= 1.875059
Thermal correction to Gibbs Free Energy= 1.593069
Sum of electronic and zero-point Energies= -7220.879147
Sum of electronic and thermal Energies= -7220.760732
Sum of electronic and thermal Enthalpies= -7220.759787
Sum of electronic and thermal Free Energies= -7221.041777

Cartesian Coordinates

26	4.295578	4.787372	1.872975
15	2.562747	1.624284	-1.886532
15	4.540877	0.128166	0.933214
6	3.967464	3.424790	0.318652
6	4.154607	2.746067	1.580024
6	3.132537	3.194431	2.472935
1	3.010134	2.884590	3.501615
6	2.335146	4.162790	1.791576
1	1.509121	4.716042	2.216398
6	2.848905	4.307296	0.469838
1	2.478856	4.983247	-0.286005
6	6.237932	5.326028	2.375384
1	7.099025	4.677259	2.282806
6	5.382798	5.426437	3.515504
1	5.479641	4.865052	4.435232
6	4.350619	6.365833	3.212451
1	3.525495	6.633390	3.859270
6	4.567543	6.847233	1.885329
1	3.938620	7.547031	1.350970
6	5.733392	6.207244	1.369236
1	6.141387	6.344961	0.377256
6	4.764251	3.153497	-0.913222
6	6.097280	3.584345	-0.982998
1	6.500776	4.139432	-0.145696
6	6.905965	3.300378	-2.083376
1	7.941472	3.625169	-2.093305
6	6.383415	2.576818	-3.152778
1	7.003883	2.337034	-4.010279
6	5.061390	2.133443	-3.106049
1	4.672122	1.556600	-3.938015
6	4.241742	2.397452	-1.997619
6	5.179947	1.672484	1.830478
1	6.093302	1.961785	1.307754
6	5.519791	1.464722	3.308953
1	6.298542	0.706966	3.429623
1	4.650983	1.149251	3.892842
1	5.882162	2.407603	3.729907
6	2.354335	0.721630	-3.482156
6	2.616162	-0.658098	-3.490644
1	2.930042	-1.152788	-2.579051
6	2.435092	-1.405271	-4.656730
1	2.642068	-2.470344	-4.648816
6	1.978951	-0.786654	-5.822536
1	1.823779	-1.370764	-6.725095
6	1.718889	0.586360	-5.822770
1	1.363256	1.074097	-6.725919
6	1.908435	1.338181	-4.662416
1	1.691981	2.400675	-4.679817
6	1.403602	3.038125	-2.070729
6	1.740452	4.197538	-2.788490
1	2.733137	4.302470	-3.216144
6	0.806313	5.222618	-2.948065
1	1.077305	6.116447	-3.502860
6	-0.475319	5.095071	-2.402678
1	-1.208180	5.886267	-2.533120
6	-0.814355	3.945024	-1.687067
1	-1.807523	3.839093	-1.267664
6	0.124930	2.927338	-1.509558
1	-0.137137	2.044684	-0.936926
6	5.833960	-0.351414	-0.288366
6	5.486597	-1.402444	-1.149534
1	4.518834	-1.879252	-1.036718
6	6.371467	-1.830163	-2.138462
6	7.598025	-1.194380	-2.319647
1	8.275579	-1.511167	-3.104405
6	7.930482	-0.131940	-1.478655
6	7.072172	0.277414	-0.457677
1	7.378632	1.096703	0.177898
6	4.568723	-1.271414	2.131317
6	3.559692	-1.295038	3.107541
1	2.867872	-0.465339	3.195712
6	3.410664	-2.401694	3.940554
6	4.233847	-3.519249	3.797983
1	4.087918	-4.396255	4.418651
6	5.223286	-3.501093	2.818349
6	5.409693	-2.382647	2.004919
1	6.188603	-2.406538	1.253301
29	2.440312	0.234719	-0.102233
6	6.092050	-4.714867	2.637234
6	2.273362	-2.466727	4.921000
6	5.996870	-3.025962	-2.969173
6	9.224975	0.593002	-1.726338
9	9.227747	1.197305	-2.941345
9	9.466942	1.553174	-0.807125
9	10.282490	-0.251203	-1.717860
9	6.178481	-4.182165	-2.282692
9	6.720402	-3.118338	-4.102538
9	4.686522	-3.002490	-3.326853
9	7.068807	-4.789575	3.569536
9	6.695659	-4.731946	1.427090
9	5.369617	-5.858086	2.739806
9	2.645178	-3.031276	6.090526
9	1.757799	-1.251179	5.200191
9	1.250963	-3.226783	4.437841
6	1.975895	-2.751381	0.404109
6	0.812414	-2.465256	1.213827
6	0.453953	-1.190285	1.765583
1	0.409668	-3.292514	1.779947
77	-3.400098	-1.296252	-1.446855
15	-5.267051	-0.538277	-0.377729
8	-5.260519	0.604662	0.820594
8	-6.330148	0.174060	-1.441914
7	-5.966521	-1.798994	0.479642
6	-4.982104	1.930166	0.525403
6	-3.757919	2.439152	1.010814
1	-3.119070	1.782058	1.589942
6	-3.415999	3.740414	0.740388
1	-2.486839	4.152975	1.120389
6	-4.248696	4.546653	-0.083616
6	-3.843377	5.851194	-0.476845
1	-2.895196	6.232406	-0.106679
6	-4.622826	6.608424	-1.322444
1	-4.300200	7.600757	-1.623687
6	-5.844902	6.086236	-1.809810
1	-6.447906	6.678147	-2.492261
6	-6.275857	4.832789	-1.431560
1	-7.211259	4.445733	-1.818911
6	-5.501776	4.025485	-0.552539
6	-5.909935	2.701975	-0.155779
6	-7.269179	2.156909	-0.436107
6	-8.460141	2.845564	-0.001828
6	-8.420928	4.023184	0.797077
1	-7.464265	4.422330	1.110934
6	-9.579470	4.655970	1.193037
1	-9.518941	5.549363	1.808000
6	-10.845807	4.150849	0.814662
1	-11.749911	4.664973	1.127349
6	-10.923687	2.997920	0.067052
1	-11.888681	2.583694	-0.213118
6	-9.748702	2.311577	-0.343997
6	-9.832651	1.090621	-1.066047
1	-10.811159	0.698985	-1.329145
6	-8.695485	0.398787	-1.398343
1	-8.734353	-0.551578	-1.920161
6	-7.430888	0.928196	-1.059843
6	-5.328309	-3.110854	0.181280
1	-4.591355	-3.316242	0.967314

6	-6.342481	-4.240830	0.175492
6	-6.026739	-5.466207	0.773829
1	-5.072268	-5.581243	1.282753
6	-6.925304	-6.535553	0.723523
1	-6.667630	-7.480466	1.194085
6	-8.155300	-6.385457	0.079676
1	-8.858476	-7.212833	0.045611
6	-8.480029	-5.162204	-0.516585
1	-9.437468	-5.037687	-1.015281
6	-7.578912	-4.098629	-0.471015
1	-7.831502	-3.144396	-0.925209
6	-4.594862	-3.051782	-1.163280
1	-5.333943	-3.113115	-1.971063
1	-3.953566	-3.933866	-1.249215
6	-6.667675	-1.732584	1.808274
1	-7.141313	-2.714860	1.887051
6	-5.678221	-1.640482	2.971156
6	-5.126316	-2.826061	3.482965
1	-5.452887	-3.781197	3.080314
6	-4.182030	-2.800085	4.512698
1	-3.768973	-3.731486	4.890466
6	-3.790114	-1.580687	5.068665
1	-3.063829	-1.554618	5.876472
6	-4.357121	-0.394780	4.591728
1	-4.076148	0.558286	5.032445
6	-5.290563	-0.424488	3.553877
1	-5.716249	0.505827	3.199689
6	-7.806783	-0.715797	1.853099
1	-8.514400	-0.911720	1.044342
1	-7.468521	0.315888	1.766047
1	-8.334906	-0.822731	2.805589
6	-2.525384	-1.128264	0.545000
1	-1.882626	-0.253514	0.590782
1	-3.221221	-1.183439	1.377508
6	-1.992557	-2.367356	0.062782
1	-2.496871	-3.272090	0.385681
6	-0.734651	-2.534724	-0.568529
1	-0.209051	-1.652829	-0.907117
6	-4.223151	-1.144048	-3.492827
1	-5.215305	-1.589738	-3.481631
6	-3.126581	-2.048806	-3.521558
1	-3.365319	-3.111972	-3.550572
6	-1.762062	-1.710648	-4.097414
1	-1.805850	-1.729039	-5.197550
1	-1.073503	-2.507984	-3.807331
6	-1.196746	-0.358858	-3.615683
1	-1.429600	0.434403	-4.332675
1	-0.107441	-0.422462	-3.582496
6	-1.691570	0.067980	-2.237501
1	-0.934736	0.084612	-1.459661
6	-2.806589	0.873776	-2.021950
1	-2.816483	1.461191	-1.109561
6	-3.753132	1.359000	-3.101118
1	-4.645372	1.750018	-2.607228
1	-3.289493	2.204711	-3.630453
6	-4.170898	0.260158	-4.102386
1	-3.492817	0.252123	-4.962178
1	-5.160819	0.506332	-4.498709
6	-0.336650	-3.785000	-1.224934
6	-0.871081	-5.040128	-0.872981
6	0.626908	-3.732312	-2.250512
6	-0.457172	-6.196883	-1.530279
1	-1.601459	-5.116448	-0.073807
6	1.036483	-4.889495	-2.909798
1	1.058431	-2.774673	-2.515930
6	0.497616	-6.127757	-2.551701
1	-0.877181	-7.156891	-1.243840
1	1.782560	-4.824817	-3.696945
1	0.817477	-7.032106	-3.061143
7	2.527311	-3.998339	0.475507
6	3.530239	-4.417769	-0.497246
1	3.343366	-5.458924	-0.776493
1	3.460266	-3.806154	-1.391249
1	4.542604	-4.343797	-0.084201
6	2.172733	-5.004887	1.472858
1	1.857229	-4.544748	2.407894
1	1.379514	-5.669507	1.108289
1	3.059623	-5.605067	1.688478
8	2.451412	-1.919452	-0.431516
6	-0.453421	-1.173801	2.861633
6	-0.885227	0.012494	3.418749
1	-0.794630	-2.114145	3.277223
6	-0.417624	1.201632	2.853839
6	0.456042	1.160461	1.781867
1	0.835606	2.067952	1.329385
7	0.890443	0.000959	1.248321
1	-1.574477	0.013424	4.254042
35	-0.962181	2.928210	3.596165

---

*Conformer_*6

Number of imaginary frequencies : 1
The smallest frequency is : -247.7023 cm(-1)
Electronic energy : HF=-7222.6348463
Zero-point correction= 1.755700
(Hartree/Particle)
Thermal correction to Energy= 1.874114
Thermal correction to Enthalpy= 1.875058
Thermal correction to Gibbs Free Energy= 1.593073
Sum of electronic and zero-point Energies= -7220.879147
Sum of electronic and thermal Energies= -7220.760732
Sum of electronic and thermal Enthalpies= -7220.759788
Sum of electronic and thermal Free Energies= -7221.041773

Cartesian Coordinates

26	4.295336	4.787275	1.873550
15	2.562844	1.624410	-1.886305
15	4.540754	0.128128	0.933530
6	3.967358	3.424788	0.319114
6	4.154391	2.745989	1.580461
6	3.132243	3.194299	2.473309
1	3.009751	2.884396	3.501959
6	2.334912	4.162700	1.791939
1	1.508847	4.715922	2.216722
6	2.848787	4.307286	0.470255
1	2.478803	4.983280	-0.285581
6	6.237636	5.325868	2.376228
1	7.098728	4.677085	2.283727
6	5.382360	5.426240	3.516244
1	5.479070	4.864805	4.435956
6	4.350238	6.365670	3.213105
1	3.525037	6.633213	3.859832
6	4.567340	6.847129	1.886033
1	3.938499	7.546966	1.351627
6	5.733242	6.207143	1.370059
1	6.141370	6.344900	0.378138
6	4.764258	3.153566	-0.912703
6	6.097302	3.584394	-0.982319
1	6.500729	4.139412	-0.144938
6	6.906090	3.300485	-2.082635
1	7.941606	3.625252	-2.092438
6	6.383630	2.577013	-3.152141
1	7.004176	2.337280	-4.009599
6	5.061592	2.133657	-3.105571
1	4.672394	1.556880	-3.937615
6	4.241843	2.397599	-1.997199
6	5.179719	1.672402	1.830944
1	6.093114	1.961746	1.308317
6	5.519427	1.464557	3.309437
1	6.298184	0.706811	3.430134
1	4.650571	1.149028	3.893221
1	5.881735	2.407420	3.730485
6	2.354563	0.721873	-3.482015
6	2.616435	-0.657846	-3.490592
1	2.930268	-1.152596	-2.579015
6	2.435479	-1.404934	-4.656750
1	2.642493	-2.469999	-4.648902
6	1.979405	-0.786241	-5.822542
1	1.824324	-1.370284	-6.725159

6	1.719297	0.586765	-5.822687
1	1.363717	1.074561	-6.725824
6	1.908732	1.338502	-4.662260
1	1.692251	2.400991	-4.679598
6	1.403705	3.038257	-2.070491
6	1.740606	4.197716	-2.788154
1	2.733321	4.302673	-3.215734
6	0.806479	5.222807	-2.947729
1	1.077509	6.116671	-3.502449
6	-0.475190	5.095226	-2.402437
1	-1.208041	5.886432	-2.532878
6	-0.814276	3.945133	-1.686925
1	-1.807472	3.839179	-1.267594
6	0.124995	2.927434	-1.509416
1	-0.137112	2.044744	-0.936857
6	5.833962	-0.351335	-0.287962
6	5.486692	-1.402281	-1.149271
1	4.518914	-1.879098	-1.036609
6	6.371678	-1.829918	-2.138130
6	7.598269	-1.194137	-2.319101
1	8.275916	-1.510865	-3.103803
6	7.930640	-0.131787	-1.477963
6	7.072205	0.277488	-0.457058
1	7.378601	1.096706	0.178638
6	4.568535	-1.271529	2.131542
6	3.559431	-1.295242	3.107688
1	2.867581	-0.465566	3.195855
6	3.410379	-2.401951	3.940626
6	4.233609	-3.519471	3.798052
1	4.087663	-4.396517	4.418659
6	5.223113	-3.501230	2.818485
6	5.409543	-2.382731	2.005133
1	6.188505	-2.406558	1.253567
29	2.440286	0.234713	-0.102117
6	6.091922	-4.714970	2.637361
6	2.272998	-2.467083	4.920974
6	5.997181	-3.025644	-2.968991
6	9.225179	0.593156	-1.725406
9	9.228083	1.197661	-2.940313
9	9.467091	1.553168	-0.806012
9	10.282664	-0.251087	-1.716970
9	6.178786	-4.181910	-2.282617
9	6.720802	-3.117875	-4.102312
9	4.686858	-3.002184	-3.326764
9	7.068630	-4.789695	3.569713
9	6.695598	-4.731976	1.427249
9	5.369515	-5.858214	2.739839
9	2.644734	-3.031693	6.090496
9	1.757374	-1.251569	5.200198
9	1.250664	-3.227143	4.437681
6	1.975913	-2.751417	0.404002
6	0.812373	-2.465370	1.213659
6	0.453836	-1.190447	1.765472
1	0.409606	-3.292675	1.779695
77	-3.400018	-1.296220	-1.447199
15	-5.266998	-0.538254	-0.378120
8	-5.260494	0.604608	0.820277
8	-6.330016	0.174183	-1.442317
7	-5.966549	-1.799003	0.479135
6	-4.982072	1.930135	0.525191
6	-3.757907	2.439090	1.010687
1	-3.119073	1.781959	1.589787
6	-3.415987	3.740377	0.740380
1	-2.486845	4.152911	1.120453
6	-4.248656	4.546677	-0.083591
6	-3.843329	5.851251	-0.476701
1	-2.895166	6.232440	-0.106466
6	-4.622750	6.608543	-1.322271
1	-4.300119	7.600903	-1.623423
6	-5.844802	6.086385	-1.809727
1	-6.447783	6.678347	-2.492155
6	-6.275765	4.832906	-1.431594
1	-7.211148	4.445875	-1.819013
6	-5.501713	4.025537	-0.552606
6	-5.909880	2.701993	-0.155967
6	-7.269109	2.156945	-0.436402
6	-8.460095	2.845561	-0.002128
6	-8.420926	4.023111	0.796883
1	-7.464280	4.422231	1.110825
6	-9.579491	4.655858	1.192839
1	-9.518996	5.549196	1.807886
6	-10.845806	4.150768	0.814351
1	-11.749928	4.664863	1.127035
6	-10.923644	2.997906	0.066633
1	-11.888623	2.583705	-0.213626
6	-9.748636	2.311601	-0.344413
6	-9.832544	1.090708	-1.066574
1	-10.811037	0.699093	-1.329761
6	-8.695358	0.398904	-1.398867
1	-8.734196	-0.551416	-1.920771
6	-7.430782	0.928286	-1.060250
6	-5.328363	-3.110863	0.180722
1	-4.591461	-3.316326	0.966783
6	-6.342574	-4.240804	0.174800
6	-6.026918	-5.466228	0.773087
1	-5.072484	-5.581329	1.282066
6	-6.925522	-6.535536	0.722665
1	-6.667914	-7.480485	1.193190
6	-8.155472	-6.385355	0.078751
1	-8.858679	-7.212701	0.044595
6	-8.480115	-5.162056	-0.517464
1	-9.437517	-5.037474	-1.016213
6	-7.578958	-4.098519	-0.471778
1	-7.831482	-3.144250	-0.925936
6	-4.594840	-3.051726	-1.163792
1	-5.333878	-3.112987	-1.971621
1	-3.953564	-3.933823	-1.249747
6	-6.667778	-1.732663	1.807731
1	-7.141447	-2.714931	1.886412
6	-5.678395	-1.640666	2.970680
6	-5.126553	-2.826292	3.482448
1	-5.453117	-3.781394	3.079709
6	-4.182343	-2.800409	4.512252
1	-3.769335	-3.731846	4.889986
6	-3.790444	-1.581058	5.068336
1	-3.064221	-1.555062	5.876200
6	-4.357387	-0.395106	4.591436
1	-4.076426	0.557924	5.032241
6	-5.290750	-0.424720	3.553512
1	-5.716387	0.505629	3.199354
6	-7.806862	-0.715849	1.852562
1	-8.514440	-0.911698	1.043753
1	-7.468568	0.315834	1.765599
1	-8.335039	-0.822834	2.805016
6	-2.525423	-1.128453	0.544722
1	-1.882685	-0.253696	0.590649
1	-3.221311	-1.183744	1.377181
6	-1.992530	-2.367480	0.062398
1	-2.496838	-3.272266	0.385161
6	-0.734576	-2.534752	-0.568836
1	-0.208969	-1.652813	-0.907300
6	-4.222955	-1.143859	-3.493210
1	-5.215119	-1.589531	-3.482104
6	-3.126405	-2.048642	-3.521932
1	-3.365173	-3.111799	-3.551035
6	-1.761839	-1.710484	-4.097678
1	-1.805546	-1.728829	-5.197817
1	-1.073316	-2.507845	-3.807575
6	-1.196527	-0.358724	-3.615853
1	-1.429346	0.434573	-4.332816
1	-0.107223	-0.422342	-3.582632
6	-1.691403	0.068053	-2.237671
1	-0.934613	0.084618	-1.459787
6	-2.806422	0.873845	-2.022124
1	-2.816359	1.461196	-1.109695
6	-3.752905	1.359153	-3.101308
1	-4.645163	1.750154	-2.607437
1	-3.289226	2.204892	-3.630563
6	-4.170640	0.260387	-4.102672
1	-3.492515	0.252396	-4.962430

1	-5.160537	0.506609	-4.499028
6	-0.336471	-3.784960	-1.225302
6	-0.870854	-5.040141	-0.873463
6	0.627149	-3.732152	-2.250815
6	-0.456842	-6.196830	-1.530812
1	-1.601272	-5.116552	-0.074334
6	1.036825	-4.889268	-2.910154
1	1.058639	-2.774471	-2.516138
6	0.498002	-6.127583	-2.552173
1	-0.876814	-7.156879	-1.244460
1	1.782947	-4.824498	-3.697251
1	0.817943	-7.031880	-3.061656
7	2.527359	-3.998364	0.475368
6	3.530366	-4.417721	-0.497336
1	3.343512	-5.458854	-0.776679
1	3.460470	-3.806037	-1.391298
1	4.542695	-4.343785	-0.084198
6	2.172719	-5.004983	1.472626
1	1.857152	-4.544910	2.407674
1	1.379527	-5.669582	1.107960
1	3.059597	-5.605175	1.688262
8	2.451468	-1.919427	-0.431541
6	-0.453606	-1.174065	2.861467
6	-0.885461	0.012178	3.418653
1	-0.794826	-2.114447	3.276962
6	-0.417839	1.201371	2.853871
6	0.455884	1.160300	1.781942
1	0.835465	2.067834	1.329557
7	0.890328	0.000846	1.248323
1	-1.574762	0.013031	4.253902
35	-0.962456	2.927873	3.596338

Conformer_7

Number of imaginary frequencies : 1
The smallest frequency is : -247.6951 cm(-1)
Electronic energy : HF=-7222.6348457
Zero-point correction= 1.755696
(Hartree/Particle)
Thermal correction to Energy= 1.874112
Thermal correction to Enthalpy= 1.875056
Thermal correction to Gibbs Free Energy= 1.593068
Sum of electronic and zero-point Energies= -7220.879150
Sum of electronic and thermal Energies= -7220.760734
Sum of electronic and thermal Enthalpies= -7220.759789
Sum of electronic and thermal Free Energies= -7221.041778

Cartesian Coordinates

26	4.295435	4.787495	1.872566
15	2.562609	1.624221	-1.886776
15	4.540837	0.128255	0.932967
6	3.967333	3.424868	0.318278
6	4.154465	2.746181	1.579673
6	3.132385	3.194574	2.472558
1	3.009967	2.884764	3.501245
6	2.335001	4.162913	1.791163
1	1.508972	4.716180	2.215962
6	2.848776	4.307382	0.469428
1	2.478733	4.983307	-0.286440
6	6.237781	5.326139	2.375006
1	7.098864	4.677351	2.282472
6	5.382618	5.426599	3.515100
1	5.479424	4.865240	4.434848
6	4.350462	6.366001	3.211990
1	3.525325	6.633590	3.858778
6	4.567430	6.847355	1.884858
1	3.938533	7.547148	1.350459
6	5.733282	6.207332	1.368817
1	6.141308	6.345018	0.376845
6	4.764110	3.153521	-0.913590
6	6.097136	3.584372	-0.983402
1	6.500631	4.139515	-0.146137
6	6.905815	3.300330	-2.083765
1	7.941322	3.625123	-2.093723
6	6.383263	2.576689	-3.153112
1	7.003730	2.336842	-4.010596
6	5.061237	2.133318	-3.106349
1	4.671968	1.556409	-3.938269
6	4.241592	2.397407	-1.997935
6	5.179827	1.672631	1.830186
1	6.093188	1.961945	1.307479
6	5.519640	1.464934	3.308678
1	6.298416	0.707212	3.429395
1	4.650829	1.149450	3.892557
1	5.881965	2.407845	3.729606
6	2.354153	0.721543	-3.482381
6	1.908192	1.338068	-4.662631
1	1.691717	2.400557	-4.680041
6	1.718596	0.586222	-5.822961
1	1.362912	1.073937	-6.726101
6	1.978670	-0.786790	-5.822713
1	1.823458	-1.370919	-6.725253
6	2.434875	-1.405380	-4.656918
1	2.641860	-2.470451	-4.648992
6	2.615993	-0.658182	-3.490856
1	2.929908	-1.152852	-2.579265
6	1.403412	3.038022	-2.070936
6	1.740161	4.197411	-2.788781
1	2.732807	4.302354	-3.216526
6	0.805976	5.222455	-2.948318
1	1.076889	6.116268	-3.503177
6	-0.475603	5.094893	-2.402806
1	-1.208500	5.886060	-2.533219
6	-0.814537	3.944870	-1.687110
1	-1.807664	3.838922	-1.267611
6	0.124796	2.927221	-1.509641
1	-0.137188	2.044587	-0.936943
6	5.833922	-0.351281	-0.288629
6	5.486559	-1.402285	-1.149827
1	4.518788	-1.879085	-1.037033
6	6.371447	-1.830005	-2.138738
6	7.598028	-1.194249	-2.319871
1	8.275599	-1.511042	-3.104613
6	7.930482	-0.131830	-1.478852
6	7.072149	0.277524	-0.457892
1	7.378609	1.096790	0.177713
6	4.568805	-1.271311	2.131083
6	3.559810	-1.295002	3.107342
1	2.867938	-0.465350	3.195538
6	3.410883	-2.401669	3.940359
6	4.234127	-3.519175	3.797755
1	4.088273	-4.396190	4.418426
6	5.223531	-3.500953	2.818086
6	5.409841	-2.382493	2.004655
1	6.188730	-2.406334	1.253015
29	2.440256	0.234688	-0.102444
6	6.092365	-4.714670	2.636932
6	2.273629	-2.466774	4.920856
6	5.996852	-3.025779	-2.969486
6	9.224991	0.593101	-1.726488
9	9.227796	1.197431	-2.941483
9	9.466948	1.553251	-0.807251
9	10.282494	-0.251117	-1.718005
9	6.178545	-4.182008	-2.283071
9	6.720333	-3.118071	-4.102893
9	4.686488	-3.002342	-3.327102
9	7.069158	-4.789325	3.569201
9	6.695934	-4.731700	1.426768
9	5.370008	-5.857936	2.739517
9	2.645532	-3.031312	6.090361
9	1.758008	-1.251260	5.200084
9	1.251252	-3.226887	4.437738
6	1.975986	-2.751445	0.403928
6	0.812531	-2.465379	1.213706
6	0.454070	-1.190423	1.765496
1	0.409850	-3.292656	1.779845
77	-3.400184	-1.296268	-1.446648
15	-5.267035	-0.538250	-0.377380
8	-5.260409	0.604666	0.820965

8	-6.330181	0.174116	-1.441497
7	-5.966489	-1.798971	0.479997
6	-4.982037	1.930184	0.525781
6	-3.757834	2.439186	1.011130
1	-3.118953	1.782112	1.590243
6	-3.415933	3.740447	0.740675
1	-2.486752	4.153010	1.120623
6	-4.248675	4.546676	-0.083290
6	-3.843379	5.851211	-0.476563
1	-2.895173	6.232426	-0.106465
6	-4.622884	6.608431	-1.322121
1	-4.300275	7.600759	-1.623401
6	-5.844992	6.086239	-1.809400
1	-6.448041	6.678143	-2.491817
6	-6.275924	4.832797	-1.431107
1	-7.211351	4.445738	-1.818394
6	-5.501784	4.025502	-0.552129
6	-5.909914	2.701991	-0.155341
6	-7.269173	2.156924	-0.435590
6	-8.460111	2.845563	-0.001223
6	-8.420855	4.023173	0.797693
1	-7.464174	4.422323	1.111491
6	-9.579377	4.655942	1.193739
1	-9.518815	5.549327	1.808710
6	-10.845734	4.150813	0.815444
1	-11.749823	4.664923	1.128199
6	-10.923653	2.997895	0.067821
1	-11.888662	2.583664	-0.212291
6	-9.748689	2.311570	-0.343318
6	-9.832674	1.090627	-1.065387
1	-10.811196	0.698989	-1.328431
6	-8.695523	0.398810	-1.397772
1	-8.734417	-0.551544	-1.919608
6	-7.430911	0.928225	-1.059342
6	-5.328379	-3.110850	0.181499
1	-4.591365	-3.316337	0.967450
6	-6.342625	-4.240760	0.175728
6	-6.026938	-5.466175	0.774016
1	-5.072445	-5.581292	1.282881
6	-6.925581	-6.535457	0.723729
1	-6.667948	-7.480400	1.194251
6	-8.155600	-6.385257	0.079951
1	-8.858835	-7.212584	0.045899
6	-8.480276	-5.161964	-0.516258
1	-9.437733	-5.037366	-1.014899
6	-7.579082	-4.098452	-0.470705
1	-7.831632	-3.144187	-0.924855
6	-4.595042	-3.051729	-1.163119
1	-5.334191	-3.112957	-1.970849
1	-3.953813	-3.933851	-1.249166
6	-6.667540	-1.732602	1.808684
1	-7.141229	-2.714854	1.887437
6	-5.677990	-1.640629	2.971492
6	-5.126128	-2.826272	3.483201
1	-5.452798	-3.781367	3.080531
6	-4.181753	-2.800410	4.512855
1	-3.768732	-3.731858	4.890546
6	-3.789698	-1.581065	5.068841
1	-3.063341	-1.555084	5.876586
6	-4.356657	-0.395095	4.592004
1	-4.075573	0.557932	5.032735
6	-5.290189	-0.424688	3.554231
1	-5.715834	0.505673	3.200115
6	-7.806590	-0.715754	1.853663
1	-8.514283	-0.911588	1.044950
1	-7.468280	0.315918	1.766646
1	-8.334640	-0.822719	2.806189
6	-2.525373	-1.128572	0.545163
1	-1.882601	-0.253838	0.591045
1	-3.221180	-1.183848	1.377692
6	-1.992544	-2.367616	0.062794
1	-2.496848	-3.272391	0.385602
6	-0.734654	-2.534905	-0.568565
1	-0.209101	-1.652978	-0.907142
6	-4.223321	-1.143899	-3.492602
1	-5.215499	-1.589537	-3.481387
6	-3.126800	-2.048706	-3.521420
1	-3.365590	-3.111859	-3.550483
6	-1.762275	-1.710574	-4.097278
1	-1.806082	-1.728887	-5.197413
1	-1.073749	-2.507964	-3.807261
6	-1.196880	-0.358842	-3.615465
1	-1.429700	0.434477	-4.332405
1	-0.107579	-0.422506	-3.582293
6	-1.691663	0.067938	-2.237249
1	-0.934811	0.084496	-1.459427
6	-2.806636	0.873776	-2.021628
1	-2.816480	1.461148	-1.109211
6	-3.753188	1.359102	-3.100741
1	-4.645404	1.750115	-2.606804
1	-3.289532	2.204833	-3.630028
6	-4.171009	0.260342	-4.102075
1	-3.492930	0.252328	-4.961868
1	-5.160922	0.506586	-4.498378
6	-0.336612	-3.785144	-1.225017
6	-0.870930	-5.040314	-0.873043
6	0.626886	-3.732377	-2.250647
6	-0.456966	-6.197035	-1.530368
1	-1.601257	-5.116693	-0.073828
6	1.036518	-4.889526	-2.909957
1	1.058322	-2.774705	-2.516085
6	0.497766	-6.127831	-2.551836
1	-0.876886	-7.157076	-1.243911
1	1.782548	-4.824788	-3.697144
1	0.817673	-7.032154	-3.061296
7	2.527478	-3.998370	0.475303
6	3.530397	-4.417731	-0.497489
1	3.343600	-5.458906	-0.776712
1	3.460332	-3.806133	-1.391496
1	4.542775	-4.343668	-0.084491
6	2.173018	-5.004933	1.472682
1	1.857522	-4.544804	2.407727
1	1.379830	-5.669614	1.108158
1	3.059960	-5.605046	1.688271
8	2.451413	-1.919492	-0.431723
6	-0.453211	-1.173973	2.861624
6	-0.884982	0.012304	3.418804
1	-0.794364	-2.114329	3.277231
6	-0.417452	1.201460	2.853870
6	0.456104	1.160322	1.781808
1	0.835598	2.067827	1.329296
7	0.890482	0.000838	1.248205
1	-1.574152	0.013209	4.254163
35	-0.961938	2.928020	3.596285

---

*Conformer_*8

Number of imaginary frequencies : 1
The smallest frequency is : -247.6994 cm(-1)
Electronic energy : HF=-7222.6348461
Zero-point correction= 1.755697
(Hartree/Particle)
Thermal correction to Energy= 1.874113
Thermal correction to Enthalpy= 1.875057
Thermal correction to Gibbs Free Energy= 1.593060
Sum of electronic and zero-point Energies= -7220.879149
Sum of electronic and thermal Energies= -7220.760734
Sum of electronic and thermal Enthalpies= -7220.759789
Sum of electronic and thermal Free Energies= -7221.041786

.....

Cartesian Coordinates

.....

26	4.295245	4.787336	1.873320
15	2.562727	1.624358	-1.886421
15	4.540791	0.128175	0.933353
6	3.967263	3.424792	0.318939
6	4.154394	2.746028	1.580291
6	3.132271	3.194307	2.473183
1	3.009845	2.884417	3.501845
6	2.334853	4.162650	1.791832

1	1.508781	4.715839	2.216645
6	2.848651	4.307232	0.470117
1	2.478598	4.983198	-0.285710
6	6.237545	5.326095	2.375829
1	7.098682	4.677379	2.283279
6	5.382354	5.426435	3.515912
1	5.479187	4.865038	4.435634
6	4.350134	6.365775	3.212828
1	3.524965	6.633273	3.859614
6	4.567090	6.847210	1.885723
1	3.938149	7.546980	1.351348
6	5.733000	6.207299	1.369673
1	6.141033	6.345052	0.377713
6	4.764124	3.153592	-0.912908
6	6.097146	3.584480	-0.982583
1	6.500583	4.139525	-0.145226
6	6.905900	3.300600	-2.082931
1	7.941400	3.625417	-2.092781
6	6.383429	2.577096	-3.152410
1	7.003950	2.337385	-4.009892
6	5.061414	2.133680	-3.105781
1	4.672206	1.556881	-3.937805
6	4.241699	2.397594	-1.997377
6	5.179764	1.672472	1.830729
1	6.093126	1.961835	1.308053
6	5.519556	1.464645	3.309205
1	6.298333	0.706915	3.429868
1	4.650736	1.149107	3.893039
1	5.881869	2.407519	3.730227
6	2.354428	0.721799	-3.482115
6	1.908498	1.338390	-4.662342
1	1.691950	2.400866	-4.679678
6	1.719046	0.586631	-5.822752
1	1.363388	1.074399	-6.725875
6	1.979236	-0.786358	-5.822609
1	1.824140	-1.370420	-6.725212
6	2.435411	-1.405013	-4.656836
1	2.642490	-2.470066	-4.648990
6	2.616384	-0.657904	-3.490695
1	2.930294	-1.152628	-2.579130
6	1.403558	3.038183	-2.070585
6	1.740407	4.197626	-2.788297
1	2.733096	4.302580	-3.215940
6	0.806265	5.222708	-2.947839
1	1.077256	6.116561	-3.502597
6	-0.475370	5.095134	-2.402463
1	-1.208233	5.886333	-2.532876
6	-0.814404	3.945057	-1.686901
1	-1.807572	3.839106	-1.267505
6	0.124883	2.927367	-1.509427
1	-0.137183	2.044692	-0.936828
6	5.833964	-0.351279	-0.288182
6	5.486699	-1.402269	-1.149439
1	4.518948	-1.879126	-1.036717
6	6.371654	-1.829896	-2.138330
6	7.598205	-1.194062	-2.319387
1	8.275826	-1.510782	-3.104115
6	7.930569	-0.131668	-1.478302
6	7.072168	0.277598	-0.457364
1	7.378559	1.096854	0.178287
6	4.568642	-1.271466	2.131383
6	3.559576	-1.295180	3.107569
1	2.867721	-0.465511	3.195754
6	3.410569	-2.401881	3.940525
6	4.233808	-3.519392	3.797932
1	4.087897	-4.396433	4.418556
6	5.223278	-3.501149	2.818331
6	5.409663	-2.382657	2.004959
1	6.188599	-2.406481	1.253366
29	2.440265	0.234673	-0.102217
6	6.092100	-4.714878	2.637194
6	2.273233	-2.467018	4.920922
6	5.997167	-3.025664	-2.969135
6	9.225060	0.593328	-1.725836
9	9.227875	1.197788	-2.940766
9	9.466972	1.553386	-0.806491
9	10.282587	-0.250862	-1.717422
9	6.178808	-4.181899	-2.282716
9	6.720767	-3.117929	-4.102466
9	4.686836	-3.002245	-3.326885
9	7.068833	-4.789582	3.569521
9	6.695745	-4.731885	1.427066
9	5.369712	-5.858132	2.739699
9	2.645032	-3.031594	6.090441
9	1.757591	-1.251510	5.200143
9	1.250897	-3.227113	4.437690
6	1.975980	-2.751462	0.403953
6	0.812459	-2.465437	1.213644
6	0.453923	-1.190519	1.765468
1	0.409725	-3.292748	1.779694
77	-3.400055	-1.296266	-1.447053
15	-5.266979	-0.538251	-0.377916
8	-5.260415	0.604610	0.820481
8	-6.330012	0.174205	-1.442085
7	-5.966536	-1.798985	0.479354
6	-4.982021	1.930143	0.525395
6	-3.757849	2.439111	1.010859
1	-3.118990	1.781987	1.589941
6	-3.415952	3.740403	0.740552
1	-2.486803	4.152945	1.120603
6	-4.248653	4.546700	-0.083389
6	-3.843350	5.851279	-0.476506
1	-2.895180	6.232476	-0.106300
6	-4.622804	6.608567	-1.322050
1	-4.300192	7.600931	-1.623209
6	-5.844866	6.086399	-1.809471
1	-6.447874	6.678357	-2.491878
6	-6.275805	4.832914	-1.431329
1	-7.211196	4.445876	-1.818722
6	-5.501719	4.025549	-0.552369
6	-5.909859	2.701998	-0.155726
6	-7.269094	2.156944	-0.436121
6	-8.460071	2.845544	-0.001800
6	-8.420886	4.023086	0.797220
1	-7.464233	4.422214	1.111132
6	-9.579444	4.655817	1.193223
1	-9.518937	5.549150	1.808276
6	-10.845767	4.150718	0.814775
1	-11.749883	4.664800	1.127496
6	-10.923619	2.997862	0.067048
1	-11.888603	2.583654	-0.213182
6	-9.748618	2.311574	-0.344047
6	-9.832539	1.090687	-1.066217
1	-10.811037	0.699065	-1.329373
6	-8.695357	0.398898	-1.398557
1	-8.734203	-0.551417	-1.920468
6	-7.430775	0.928290	-1.059977
6	-5.328407	-3.110862	0.180895
1	-4.591474	-3.316360	0.966919
6	-6.342657	-4.240768	0.175001
6	-6.027025	-5.466205	0.773274
1	-5.072578	-5.581342	1.282221
6	-6.925669	-6.535481	0.722875
1	-6.668080	-7.480441	1.193387
6	-8.155633	-6.385254	0.078999
1	-8.858869	-7.212576	0.044861
6	-8.480252	-5.161941	-0.517199
1	-9.437665	-5.037322	-1.015918
6	-7.579057	-4.098435	-0.471536
1	-7.831562	-3.144155	-0.925680
6	-4.594939	-3.051727	-1.163650
1	-5.334012	-3.112940	-1.971451
1	-3.953704	-3.933849	-1.249650
6	-6.667712	-1.732641	1.807978
1	-7.141406	-2.714896	1.886665
6	-5.678281	-1.640687	2.970889
6	-5.126455	-2.826336	3.482622
1	-5.453062	-3.781424	3.079885
6	-4.182203	-2.800491	4.512389
1	-3.769208	-3.731944	4.890097

6	-3.790243	-1.581158	5.068468
1	-3.063986	-1.555191	5.876303
6	-4.357168	-0.395183	4.591602
1	-4.076157	0.557834	5.032402
6	-5.290573	-0.424759	3.553715
1	-5.716195	0.505607	3.199581
6	-7.806766	-0.715796	1.852869
1	-8.514383	-0.911614	1.044087
1	-7.468447	0.315878	1.765907
1	-8.334906	-0.822780	2.805344
6	-2.525414	-1.128651	0.544850
1	-1.882683	-0.253892	0.590832
1	-3.221287	-1.184009	1.377319
6	-1.992503	-2.367642	0.062441
1	-2.496794	-3.272461	0.385143
6	-0.734552	-2.534855	-0.568814
1	-0.208977	-1.652893	-0.907263
6	-4.223037	-1.143824	-3.493053
1	-5.215218	-1.589457	-3.481931
6	-3.126521	-2.048642	-3.521816
1	-3.365324	-3.111792	-3.550934
6	-1.761954	-1.710512	-4.097576
1	-1.805687	-1.728807	-5.197714
1	-1.073455	-2.507911	-3.807525
6	-1.196576	-0.358792	-3.615709
1	-1.429354	0.434539	-4.332649
1	-0.107276	-0.422466	-3.582489
6	-1.691426	0.067976	-2.237514
1	-0.934626	0.084511	-1.459640
6	-2.806416	0.873798	-2.021935
1	-2.816320	1.461130	-1.109493
6	-3.752902	1.359160	-3.101091
1	-4.645144	1.750169	-2.607197
1	-3.289208	2.204903	-3.630327
6	-4.170676	0.260434	-4.102481
1	-3.492551	0.252441	-4.962238
1	-5.160564	0.506699	-4.498831
6	-0.336411	-3.785037	-1.225308
6	-0.870703	-5.040249	-0.873446
6	0.627159	-3.732168	-2.250865
6	-0.456655	-6.196912	-1.530817
1	-1.601074	-5.116704	-0.074277
6	1.036871	-4.889260	-2.910227
1	1.058583	-2.774463	-2.516205
6	0.498136	-6.127606	-2.552224
1	-0.876555	-7.156987	-1.244446
1	1.782952	-4.824443	-3.697359
1	0.818107	-7.031884	-3.061724
7	2.527448	-3.998400	0.475308
6	3.530436	-4.417742	-0.497422
1	3.343605	-5.458885	-0.776743
1	3.460490	-3.806075	-1.391391
1	4.542777	-4.343767	-0.084320
6	2.172872	-5.005010	1.472598
1	1.857333	-4.544926	2.407651
1	1.379679	-5.669633	1.107977
1	3.059772	-5.605178	1.688208
8	2.451497	-1.919466	-0.431606
6	-0.453470	-1.174150	2.861504
6	-0.885311	0.012087	3.418713
1	-0.794659	-2.114537	3.277012
6	-0.417733	1.201285	2.853907
6	0.455935	1.160227	1.781933
1	0.835476	2.067766	1.329526
7	0.890373	0.000779	1.248295
1	-1.574570	0.012930	4.253997
35	-0.962330	2.927780	3.596405

Conformer_9

Number of imaginary frequencies : 1
The smallest frequency is : -247.7215 cm(-1)
Electronic energy : HF=-7222.6348462
Zero-point correction= 1.755701
(Hartree/Particle)
Thermal correction to Energy= 1.874116
Thermal correction to Enthalpy= 1.875060
Thermal correction to Gibbs Free Energy= 1.593080
Sum of electronic and zero-point Energies= -7220.879145
Sum of electronic and thermal Energies= -7220.760731
Sum of electronic and thermal Enthalpies= -7220.759786
Sum of electronic and thermal Free Energies= -7221.041767

Cartesian Coordinates

26	4.295540	4.787317	1.873314
15	2.562877	1.624340	-1.886366
15	4.540811	0.128129	0.933481
6	3.967490	3.424777	0.318941
6	4.154538	2.746024	1.580311
6	3.132422	3.194394	2.473167
1	3.009949	2.884537	3.501833
6	2.335097	4.162787	1.791777
1	1.509058	4.716049	2.216559
6	2.848943	4.307307	0.470074
1	2.478957	4.983280	-0.285779
6	6.237875	5.325898	2.375873
1	7.098954	4.677102	2.283341
6	5.382663	5.426307	3.515934
1	5.479419	4.864894	4.435655
6	4.350536	6.365743	3.212830
1	3.525375	6.633311	3.859597
6	4.567571	6.847168	1.885735
1	3.938708	7.547000	1.351348
6	5.733436	6.207154	1.369710
1	6.141509	6.344881	0.377763
6	4.764350	3.153490	-0.912888
6	6.097397	3.584297	-0.982563
1	6.500855	4.139349	-0.145221
6	6.906147	3.300327	-2.082892
1	7.941667	3.625082	-2.092742
6	6.383646	2.576813	-3.152349
1	7.004164	2.337031	-4.009814
6	5.061603	2.133480	-3.105721
1	4.672372	1.556671	-3.937727
6	4.241889	2.397486	-1.997337
6	5.179844	1.672421	1.830813
1	6.093235	1.961720	1.308151
6	5.519588	1.464627	3.309305
1	6.298325	0.706862	3.430012
1	4.650738	1.149148	3.893128
1	5.881936	2.407496	3.730305
6	2.354537	0.721721	-3.482021
6	1.908740	1.338311	-4.662300
1	1.692327	2.400813	-4.679697
6	1.719254	0.586520	-5.822683
1	1.363702	1.074287	-6.725848
6	1.979271	-0.786503	-5.822458
1	1.824147	-1.370589	-6.725041
6	2.435308	-1.405158	-4.656632
1	2.642249	-2.470238	-4.648723
6	2.616318	-0.658014	-3.490518
1	2.930121	-1.152732	-2.578913
6	1.403757	3.038197	-2.070601
6	1.740667	4.197630	-2.788299
1	2.733384	4.302568	-3.215878
6	0.806547	5.222721	-2.947911
1	1.077585	6.116567	-3.502658
6	-0.475126	5.095166	-2.402622
1	-1.207972	5.886370	-2.533093
6	-0.814222	3.945098	-1.687074
1	-1.807423	3.839162	-1.267748
6	0.125042	2.927399	-1.509527
1	-0.137071	2.044728	-0.936943
6	5.833967	-0.351431	-0.288030
6	5.486639	-1.402416	-1.149267
1	4.518854	-1.879203	-1.036543
6	6.371575	-1.830125	-2.138140
6	7.598171	-1.194377	-2.319198
1	8.275778	-1.511159	-3.103912

6	7.930596	-0.131984	-1.478135
6	7.072213	0.277361	-0.457213
1	7.378651	1.096611	0.178422
6	4.568575	-1.271479	2.131549
6	3.559489	-1.295123	3.107715
1	2.867667	-0.465422	3.195864
6	3.410411	-2.401796	3.940695
6	4.233598	-3.519351	3.798147
1	4.087632	-4.396370	4.418786
6	5.223089	-3.501178	2.818564
6	5.409545	-2.382714	2.005169
1	6.188495	-2.406595	1.253592
29	2.440322	0.234743	-0.102100
6	6.091854	-4.714953	2.637468
6	2.273046	-2.466849	4.921067
6	5.997013	-3.025885	-2.968923
6	9.225136	0.592923	-1.725677
9	9.228011	1.197325	-2.940635
9	9.467086	1.553009	-0.806372
9	10.282612	-0.251331	-1.717202
9	6.178578	-4.182118	-2.282481
9	6.720611	-3.118218	-4.102250
9	4.686686	-3.002388	-3.326675
9	7.068574	-4.789680	3.569807
9	6.695511	-4.732019	1.427347
9	5.369411	-5.858170	2.739994
9	2.644781	-3.031436	6.090601
9	1.757477	-1.251304	5.200261
9	1.250670	-3.226880	4.437821
6	1.975847	-2.751355	0.404153
6	0.812329	-2.465232	1.213816
6	0.453839	-1.190268	1.765570
1	0.409546	-3.292495	1.779903
77	-3.400033	-1.296222	-1.447085
15	-5.267046	-0.538279	-0.378041
8	-5.260577	0.604647	0.820297
8	-6.330097	0.174070	-1.442264
7	-5.966545	-1.799009	0.479287
6	-4.982131	1.930149	0.525132
6	-3.757960	2.439114	1.010600
1	-3.119140	1.782003	1.589740
6	-3.416017	3.740377	0.740208
1	-2.486869	4.152924	1.120254
6	-4.248672	4.546637	-0.083818
6	-3.843326	5.851182	-0.477005
1	-2.895159	6.232380	-0.106790
6	-4.622732	6.608433	-1.322625
1	-4.300086	7.600770	-1.623836
6	-5.844789	6.086262	-1.810056
1	-6.447759	6.678191	-2.492522
6	-6.275771	4.832812	-1.431847
1	-7.211158	4.445771	-1.819247
6	-5.501736	4.025487	-0.552805
6	-5.909924	2.701974	-0.156083
6	-7.269158	2.156921	-0.436483
6	-8.460136	2.845583	-0.002257
6	-8.420953	4.023192	0.796666
1	-7.464302	4.422322	1.110580
6	-9.579509	4.655984	1.192573
1	-9.519002	5.549368	1.807552
6	-10.845832	4.150883	0.814123
1	-11.749946	4.665014	1.126768
6	-10.923684	2.997965	0.066495
1	-11.888668	2.583754	-0.213733
6	-9.748685	2.311614	-0.344501
6	-9.832609	1.090668	-1.066570
1	-10.811107	0.699045	-1.329725
6	-8.695432	0.398826	-1.398814
1	-8.734283	-0.551532	-1.920646
6	-7.430847	0.928216	-1.060240
6	-5.328293	-3.110859	0.180965
1	-4.591386	-3.316233	0.967045
6	-6.342446	-4.240853	0.175114
6	-6.026715	-5.466229	0.773460
1	-5.072269	-5.581252	1.282435
6	-6.925260	-6.535589	0.723101
1	-6.667595	-7.480501	1.193670
6	-8.155225	-6.385509	0.079192
1	-8.858386	-7.212896	0.045086
6	-8.479943	-5.162258	-0.517080
1	-9.437357	-5.037754	-1.015825
6	-7.578844	-4.098668	-0.471457
1	-7.831426	-3.144437	-0.925661
6	-4.594767	-3.051779	-1.163550
1	-5.333799	-3.113137	-1.971376
1	-3.953444	-3.933848	-1.249442
6	-6.667775	-1.732612	1.807879
1	-7.141403	-2.714894	1.886628
6	-5.678392	-1.640495	2.970820
6	-5.126496	-2.826065	3.482660
1	-5.453026	-3.781205	3.079986
6	-4.182275	-2.800077	4.512451
1	-3.769224	-3.731472	4.890241
6	-3.790419	-1.580673	5.068450
1	-3.064186	-1.554594	5.876303
6	-4.357419	-0.394775	4.591482
1	-4.076494	0.558294	5.032224
6	-5.290794	-0.424496	3.553572
1	-5.716477	0.505813	3.199363
6	-7.806901	-0.715841	1.852638
1	-8.514468	-0.911775	1.043839
1	-7.468648	0.315849	1.765606
1	-8.335078	-0.822782	2.805097
6	-2.525406	-1.128159	0.544810
1	-1.882652	-0.253405	0.590587
1	-3.221276	-1.183307	1.377292
6	-1.992571	-2.367262	0.062642
1	-2.496897	-3.271984	0.385554
6	-0.734643	-2.534654	-0.568619
1	-0.209013	-1.652766	-0.907184
6	-4.223001	-1.144052	-3.493083
1	-5.215144	-1.589767	-3.481931
6	-3.126408	-2.048789	-3.521764
1	-3.365127	-3.111959	-3.550786
6	-1.761873	-1.710613	-4.097571
1	-1.805611	-1.729037	-5.197708
1	-1.073307	-2.507923	-3.807433
6	-1.196613	-0.358796	-3.615851
1	-1.429484	0.434444	-4.332861
1	-0.107306	-0.422360	-3.582645
6	-1.691484	0.068041	-2.237687
1	-0.934677	0.084685	-1.459821
6	-2.806527	0.873814	-2.022177
1	-2.816466	1.461231	-1.109789
6	-3.753043	1.359011	-3.101383
1	-4.645304	1.750022	-2.607526
1	-3.289400	2.204723	-3.630712
6	-4.170762	0.260151	-4.102652
1	-3.492662	0.252124	-4.962429
1	-5.160680	0.506301	-4.498998
6	-0.336638	-3.784936	-1.225009
6	-0.871132	-5.040051	-0.873106
6	0.626986	-3.732266	-2.250527
6	-0.457219	-6.196811	-1.530393
1	-1.601565	-5.116357	-0.073981
6	1.036563	-4.889454	-2.909803
1	1.058555	-2.774637	-2.515905
6	0.497633	-6.127703	-2.551755
1	-0.877279	-7.156808	-1.243993
1	1.782690	-4.824790	-3.696903
1	0.817496	-7.032055	-3.061190
7	2.527250	-3.998319	0.475558
6	3.530226	-4.417743	-0.497150
1	3.343345	-5.458887	-0.776438
1	3.460319	-3.806102	-1.391140
1	4.542567	-4.343807	-0.084042
6	2.172597	-5.004890	1.472859
1	1.857049	-4.544772	2.407891
1	1.379387	-5.669485	1.108226
1	3.059464	-5.605093	1.688510

8	2.451414	-1.919418	-0.431435
6	-0.453600	-1.173799	2.861566
6	-0.885435	0.012489	3.418674
1	-0.794837	-2.114148	3.277122
6	-0.417791	1.201636	2.853815
6	0.455940	1.160479	1.781896
1	0.835541	2.067976	1.329456
7	0.890364	0.000983	1.248355
1	-1.574738	0.013408	4.253923
35	-0.962390	2.928201	3.596146

---

*Conformer*_10

Number of imaginary frequencies : 1
The smallest frequency is : -247.7141 cm(-1)
Electronic energy : HF=-7222.6348463
Zero-point correction= 1.755701
(Hartree/Particle)
Thermal correction to Energy= 1.874115
Thermal correction to Enthalpy= 1.875059
Thermal correction to Gibbs Free Energy= 1.593081
Sum of electronic and zero-point Energies= -7220.879146
Sum of electronic and thermal Energies= -7220.760731
Sum of electronic and thermal Enthalpies= -7220.759787
Sum of electronic and thermal Free Energies= -7221.041765

Cartesian Coordinates

26	4.295523	4.787283	1.873415
15	2.562859	1.624389	-1.886344
15	4.540779	0.128116	0.933480
6	3.967467	3.424790	0.318999
6	4.154487	2.746003	1.580354
6	3.132366	3.194366	2.473206
1	3.009873	2.884484	3.501862
6	2.335068	4.162790	1.791831
1	1.509031	4.716054	2.216616
6	2.848935	4.307338	0.470140
1	2.478968	4.983332	-0.285704
6	6.237859	5.325784	2.376050
1	7.098917	4.676959	2.283529
6	5.382612	5.426193	3.516086
1	5.479316	4.864752	4.435795
6	4.350528	6.365674	3.212972
1	3.525355	6.633254	3.859719
6	4.567624	6.847126	1.885897
1	3.938804	7.546994	1.351507
6	5.733484	6.207085	1.369894
1	6.141595	6.344828	0.377965
6	4.764335	3.153514	-0.912827
6	6.097389	3.584304	-0.982483
1	6.500846	4.139335	-0.145127
6	6.906147	3.300340	-2.082807
1	7.941671	3.625079	-2.092641
6	6.383646	2.576849	-3.152280
1	7.004169	2.337072	-4.009743
6	5.061597	2.133532	-3.105672
1	4.672367	1.556740	-3.937690
6	4.241875	2.397531	-1.997292
6	5.179790	1.672394	1.830849
1	6.093188	1.961706	1.308207
6	5.519512	1.464574	3.309343
1	6.298249	0.706809	3.430047
1	4.650655	1.149083	3.893147
1	5.881852	2.407437	3.730364
6	2.354520	0.721816	-3.482025
6	1.908698	1.338433	-4.662281
1	1.692262	2.400931	-4.679642
6	1.719216	0.586674	-5.822685
1	1.363644	1.074462	-6.725831
6	1.979265	-0.786343	-5.822507
1	1.824145	-1.370404	-6.725107
6	2.435327	-1.405025	-4.656705
1	2.642293	-2.470100	-4.648832
6	2.616331	-0.657914	-3.490569
1	2.930153	-1.152654	-2.578983
6	1.403740	3.038250	-2.070541
6	1.740649	4.197698	-2.788216
1	2.733367	4.302644	-3.215793
6	0.806529	5.222792	-2.947806
1	1.077566	6.116649	-3.502535
6	-0.475144	5.095225	-2.402520
1	-1.207990	5.886432	-2.532974
6	-0.814239	3.945142	-1.686995
1	-1.807439	3.839196	-1.267670
6	0.125025	2.927440	-1.509470
1	-0.137089	2.044756	-0.936905
6	5.833953	-0.351407	-0.288025
6	5.486635	-1.402359	-1.149307
1	4.518845	-1.879143	-1.036618
6	6.371590	-1.830042	-2.138174
6	7.598198	-1.194303	-2.319180
1	8.275821	-1.511066	-3.103888
6	7.930614	-0.131943	-1.478071
6	7.072210	0.277377	-0.457157
1	7.378641	1.096600	0.178516
6	4.568549	-1.271515	2.131522
6	3.559458	-1.295186	3.107682
1	2.867626	-0.465495	3.195841
6	3.410391	-2.401874	3.940645
6	4.233594	-3.519415	3.798083
1	4.087636	-4.396446	4.418709
6	5.223087	-3.501216	2.818504
6	5.409531	-2.382738	2.005126
1	6.188483	-2.406598	1.253550
29	2.440300	0.234739	-0.102121
6	6.091867	-4.714978	2.637393
6	2.273022	-2.466957	4.921009
6	5.997038	-3.025770	-2.969008
6	9.225167	0.592959	-1.725555
9	9.228067	1.197427	-2.940480
9	9.467118	1.552993	-0.806194
9	10.282632	-0.251309	-1.717111
9	6.178623	-4.182032	-2.282621
9	6.720629	-3.118040	-4.102345
9	4.686707	-3.002276	-3.326751
9	7.068584	-4.789707	3.569735
9	6.695530	-4.732018	1.427274
9	5.369438	-5.858205	2.739898
9	2.644757	-3.031557	6.090536
9	1.757434	-1.251424	5.200219
9	1.250659	-3.226996	4.437745
6	1.975859	-2.751371	0.404067
6	0.812338	-2.465278	1.213737
6	0.453834	-1.190330	1.765518
1	0.409561	-3.292558	1.779802
77	-3.400038	-1.296205	-1.447131
15	-5.267035	-0.538264	-0.378057
8	-5.260548	0.604631	0.820310
8	-6.330084	0.174120	-1.442259
7	-5.966543	-1.799009	0.479241
6	-4.982113	1.930144	0.525179
6	-3.757942	2.439104	1.010653
1	-3.119114	1.781985	1.589774
6	-3.416010	3.740377	0.740294
1	-2.486862	4.152919	1.120347
6	-4.248674	4.546654	-0.083704
6	-3.843337	5.851211	-0.476862
1	-2.895170	6.232405	-0.106643
6	-4.622754	6.608480	-1.322457
1	-4.300115	7.600826	-1.623645
6	-5.844812	6.086314	-1.809892
1	-6.447789	6.678257	-2.492339
6	-6.275784	4.832852	-1.431712
1	-7.211172	4.445816	-1.819115
6	-5.501738	4.025509	-0.552697
6	-5.909915	2.701983	-0.156008
6	-7.269150	2.156934	-0.436413
6	-8.460127	2.845576	-0.002156
6	-8.420942	4.023159	0.796804

1	-7.464290	4.422285	1.110722
6	-9.579498	4.655933	1.192743
1	-9.518991	5.549296	1.807751
6	-10.845821	4.150837	0.814288
1	-11.749936	4.664952	1.126958
6	-10.923674	2.997943	0.066621
1	-11.888658	2.583737	-0.213613
6	-9.748675	2.311612	-0.344407
6	-9.832599	1.090689	-1.066516
1	-10.811098	0.699071	-1.329677
6	-8.695422	0.398863	-1.398790
1	-8.734272	-0.551479	-1.920653
6	-7.430837	0.928248	-1.060208
6	-5.328312	-3.110858	0.180874
1	-4.591396	-3.316264	0.966938
6	-6.342479	-4.240839	0.175002
6	-6.026759	-5.466233	0.773317
1	-5.072312	-5.581280	1.282283
6	-6.925318	-6.535581	0.722938
1	-6.667662	-7.480507	1.193483
6	-8.155285	-6.385470	0.079039
1	-8.858456	-7.212848	0.044917
6	-8.479991	-5.162201	-0.517202
1	-9.437406	-5.037673	-1.015939
6	-7.578879	-4.098624	-0.471559
1	-7.831451	-3.144378	-0.925738
6	-4.594801	-3.051746	-1.163648
1	-5.333845	-3.113062	-1.971468
1	-3.953496	-3.933823	-1.249577
6	-6.667766	-1.732642	1.807839
1	-7.141405	-2.714922	1.886560
6	-5.678377	-1.640571	2.970778
6	-5.126490	-2.826162	3.482580
1	-5.453026	-3.781288	3.079875
6	-4.182269	-2.800213	4.512372
1	-3.769224	-3.731623	4.890132
6	-3.790405	-1.580831	5.068411
1	-3.064173	-1.554783	5.876266
6	-4.357395	-0.394913	4.591479
1	-4.076462	0.558140	5.032251
6	-5.290769	-0.424594	3.553567
1	-5.716443	0.505730	3.199385
6	-7.806880	-0.715860	1.852635
1	-8.514455	-0.911763	1.043836
1	-7.468617	0.315829	1.765630
1	-8.335051	-0.822823	2.805095
6	-2.525418	-1.128266	0.544773
1	-1.882671	-0.253511	0.590612
1	-3.221292	-1.183476	1.377248
6	-1.992563	-2.367337	0.062535
1	-2.496883	-3.272084	0.385387
6	-0.734629	-2.534681	-0.568722
1	-0.209007	-1.652774	-0.907247
6	-4.223001	-1.143956	-3.493131
1	-5.215152	-1.589654	-3.481995
6	-3.126424	-2.048709	-3.521833
1	-3.365159	-3.111875	-3.550887
6	-1.761880	-1.710535	-4.097621
1	-1.805614	-1.728919	-5.197759
1	-1.073329	-2.507867	-3.807509
6	-1.196596	-0.358744	-3.615853
1	-1.429442	0.434522	-4.332842
1	-0.107291	-0.422334	-3.582638
6	-1.691470	0.068067	-2.237681
1	-0.934667	0.084682	-1.459810
6	-2.806505	0.873845	-2.022154
1	-2.816442	1.461236	-1.109749
6	-3.753013	1.359085	-3.101347
1	-4.645274	1.750084	-2.607480
1	-3.289362	2.204813	-3.630644
6	-4.170732	0.260264	-4.102657
1	-3.492619	0.252254	-4.962423
1	-5.160640	0.506441	-4.499011
6	-0.336590	-3.784934	-1.225145
6	-0.871041	-5.040074	-0.873265
6	0.627028	-3.732212	-2.250665
6	-0.457095	-6.196807	-1.530578
1	-1.601464	-5.116421	-0.074135
6	1.036639	-4.889373	-2.909968
1	1.058567	-2.774563	-2.516023
6	0.497750	-6.127646	-2.551945
1	-0.877121	-7.156824	-1.244196
1	1.782761	-4.824668	-3.697070
1	0.817639	-7.031978	-3.061400
7	2.527278	-3.998329	0.475452
6	3.530260	-4.417727	-0.497261
1	3.343383	-5.458864	-0.776575
1	3.460356	-3.806064	-1.391236
1	4.542598	-4.343798	-0.084145
6	2.172633	-5.004921	1.472735
1	1.857080	-4.544823	2.407776
1	1.379429	-5.669517	1.108090
1	3.059505	-5.605121	1.688376
8	2.451415	-1.919413	-0.431506
6	-0.453604	-1.173896	2.861516
6	-0.885440	0.012374	3.418660
1	-0.794838	-2.114258	3.277044
6	-0.417800	1.201539	2.853837
6	0.455926	1.160417	1.781912
1	0.835523	2.067929	1.329498
7	0.890350	0.000937	1.248334
1	-1.574741	0.013267	4.253910
35	-0.962394	2.928080	3.596228

---

*Conformer_*11

Number of imaginary frequencies : 1
The smallest frequency is : -247.7126 cm(-1)
Eectronic energy : HF=-7222.6348461
Zero-point correction= 1.755699
(Hartree/Particle)
Thermal correction to Energy= 1.874114
Thermal correction to Enthalpy= 1.875059
Thermal correction to Gibbs Free Energy= 1.593073
Sum of electronic and zero-point Energies= -7220.879147
Sum of electronic and thermal Energies= -7220.760732
Sum of electronic and thermal Enthalpies= -7220.759788
Sum of electronic and thermal Free Energies= -7221.041773

Cartesian Coordinates

26	4.295529	4.787371	1.873113
15	2.562813	1.624303	-1.886472
15	4.540798	0.128166	0.933365
6	3.967455	3.424815	0.318756
6	4.154497	2.746078	1.580136
6	3.132386	3.194474	2.472985
1	3.009909	2.884634	3.501656
6	2.335074	4.162868	1.791584
1	1.509043	4.716147	2.216359
6	2.848922	4.307364	0.469879
1	2.478941	4.983328	-0.285986
6	6.237873	5.325909	2.375676
1	7.098935	4.677091	2.283153
6	5.382657	5.426347	3.515732
1	5.479393	4.864939	4.435457
6	4.350555	6.365808	3.212617
1	3.525397	6.633400	3.859377
6	4.567609	6.847218	1.885520
1	3.938767	7.547062	1.351124
6	5.733461	6.207172	1.369505
1	6.141543	6.344887	0.377561
6	4.764298	3.153492	-0.913075
6	6.097343	3.584301	-0.982785
1	6.500810	4.139382	-0.145466
6	6.906078	3.300295	-2.083116
1	7.941597	3.625053	-2.092993
6	6.383563	2.576739	-3.152538
1	7.004070	2.336927	-4.010002
6	5.061522	2.133405	-3.105876

1	4.672282	1.556563	-3.937854
6	4.241823	2.397450	-1.997491
6	5.179809	1.672485	1.830661
1	6.093200	1.961782	1.307998
6	5.519552	1.464728	3.309160
1	6.298296	0.706973	3.429884
1	4.650705	1.149256	3.892990
1	5.881893	2.407611	3.730136
6	2.354444	0.721661	-3.482109
6	1.908594	1.338225	-4.662382
1	1.692156	2.400722	-4.679785
6	1.719079	0.586413	-5.822746
1	1.363484	1.074160	-6.725905
6	1.979123	-0.786605	-5.822511
1	1.823976	-1.370708	-6.725079
6	2.435214	-1.405234	-4.656692
1	2.642175	-2.470310	-4.648775
6	2.616251	-0.658070	-3.490596
1	2.930089	-1.152769	-2.578993
6	1.403678	3.038147	-2.070698
6	1.740551	4.197565	-2.788440
1	2.733253	4.302501	-3.216056
6	0.806415	5.222642	-2.948045
1	1.077424	6.116476	-3.502825
6	-0.475238	5.095088	-2.402707
1	-1.208096	5.886282	-2.533173
6	-0.814296	3.945036	-1.687115
1	-1.807481	3.839100	-1.267751
6	0.124985	2.927352	-1.509576
1	-0.137100	2.044693	-0.936959
6	5.833945	-0.351393	-0.288156
6	5.486613	-1.402385	-1.149382
1	4.518830	-1.879172	-1.036647
6	6.371547	-1.830105	-2.138252
6	7.598144	-1.194362	-2.319318
1	8.275750	-1.511153	-3.104030
6	7.930571	-0.131960	-1.478267
6	7.072191	0.277396	-0.457347
1	7.378631	1.096651	0.178280
6	4.568615	-1.271424	2.131455
6	3.559551	-1.295077	3.107643
1	2.867713	-0.465390	3.195799
6	3.410515	-2.401743	3.940641
6	4.233721	-3.519283	3.798087
1	4.087786	-4.396298	4.418740
6	5.223190	-3.501101	2.818483
6	5.409605	-2.382644	2.005071
1	6.188541	-2.406517	1.253479
29	2.440294	0.234726	-0.102187
6	6.091978	-4.714859	2.637382
6	2.273177	-2.466806	4.921043
6	5.996982	-3.025872	-2.969025
6	9.225109	0.592946	-1.725822
9	9.227982	1.197326	-2.940791
9	9.467056	1.553051	-0.806534
9	10.282588	-0.251303	-1.717331
9	6.178575	-4.182102	-2.282586
9	6.720558	-3.118197	-4.102368
9	4.686648	-3.002391	-3.326752
9	7.068719	-4.789554	3.569702
9	6.695611	-4.731924	1.427249
9	5.369563	-5.858091	2.739934
9	2.644953	-3.031376	6.090572
9	1.757592	-1.251269	5.200239
9	1.250802	-3.226862	4.437830
6	1.975877	-2.751375	0.404118
6	0.812375	-2.465264	1.213808
6	0.453887	-1.190298	1.765560
1	0.409620	-3.292527	1.779915
77	-3.400070	-1.296252	-1.446977
15	-5.267042	-0.538269	-0.377894
8	-5.260533	0.604661	0.820439
8	-6.330105	0.174083	-1.442103
7	-5.966543	-1.798987	0.479449
6	-4.982105	1.930166	0.525264
6	-3.757929	2.439144	1.010706
1	-3.119096	1.782045	1.589845
6	-3.415995	3.740405	0.740292
1	-2.486840	4.152958	1.120316
6	-4.248668	4.546653	-0.083725
6	-3.843333	5.851193	-0.476939
1	-2.895158	6.232398	-0.106751
6	-4.622760	6.608433	-1.322551
1	-4.300122	7.600766	-1.623782
6	-5.844828	6.086254	-1.809946
1	-6.447814	6.678172	-2.492406
6	-6.275799	4.832807	-1.431713
1	-7.211194	4.445759	-1.819086
6	-5.501741	4.025494	-0.552679
6	-5.909916	2.701984	-0.155936
6	-7.269155	2.156926	-0.436303
6	-8.460126	2.845583	-0.002050
6	-8.420928	4.023194	0.796868
1	-7.464271	4.422331	1.110756
6	-9.579478	4.655982	1.192802
1	-9.518961	5.549368	1.807776
6	-10.845807	4.150873	0.814385
1	-11.749917	4.664999	1.127052
6	-10.923672	2.997952	0.066761
1	-11.888660	2.583735	-0.213442
6	-9.748679	2.311607	-0.344262
6	-9.832615	1.090659	-1.066328
1	-10.811117	0.699032	-1.329460
6	-8.695442	0.398823	-1.398599
1	-8.734301	-0.551536	-1.920430
6	-7.430853	0.928221	-1.060056
6	-5.328337	-3.110851	0.181092
1	-4.591409	-3.316256	0.967144
6	-6.342523	-4.240815	0.175262
6	-6.026821	-5.466197	0.773609
1	-5.072368	-5.581248	1.282566
6	-6.925400	-6.535530	0.723271
1	-6.667757	-7.480447	1.193840
6	-8.155371	-6.385414	0.079382
1	-8.858559	-7.212779	0.045292
6	-8.480061	-5.162156	-0.516890
1	-9.437480	-5.037624	-1.015620
6	-7.578929	-4.098594	-0.471288
1	-7.831489	-3.144357	-0.925491
6	-4.594850	-3.051773	-1.163446
1	-5.333907	-3.113096	-1.971252
1	-3.953558	-3.933862	-1.249368
6	-6.667735	-1.732586	1.808062
1	-7.141384	-2.714858	1.886814
6	-5.678314	-1.640505	2.970973
6	-5.126434	-2.826093	3.482788
1	-5.453003	-3.781223	3.080119
6	-4.182176	-2.800135	4.512546
1	-3.769138	-3.731544	4.890317
6	-3.790265	-1.580745	5.068537
1	-3.064002	-1.554691	5.876363
6	-4.357249	-0.394830	4.591595
1	-4.076281	0.558230	5.032329
6	-5.290662	-0.424519	3.553717
1	-5.716330	0.505803	3.199525
6	-7.806836	-0.715789	1.852865
1	-8.514432	-0.911699	1.044086
1	-7.468562	0.315894	1.765832
1	-8.334985	-0.822727	2.805340
6	-2.525412	-1.128298	0.544905
1	-1.882660	-0.253545	0.590721
1	-3.221273	-1.183491	1.377392
6	-1.992565	-2.367380	0.062683
1	-2.496881	-3.272122	0.385555
6	-0.734642	-2.534735	-0.568595
1	-0.209035	-1.652834	-0.907161
6	-4.223068	-1.144028	-3.492971
1	-5.215223	-1.589716	-3.481808
6	-3.126499	-2.048789	-3.521677
1	-3.365240	-3.111953	-3.550709

6	-1.761962	-1.710629	-4.097490
1	-1.805713	-1.729018	-5.197627
1	-1.073412	-2.507966	-3.807385
6	-1.196658	-0.358840	-3.615738
1	-1.429496	0.434423	-4.332733
1	-0.107354	-0.422443	-3.582525
6	-1.691518	0.067991	-2.237567
1	-0.934706	0.084614	-1.459705
6	-2.806541	0.873785	-2.022040
1	-2.816461	1.461193	-1.109647
6	-3.753056	1.359017	-3.101231
1	-4.645309	1.750032	-2.607362
1	-3.289402	2.204731	-3.630547
6	-4.170794	0.260183	-4.102519
1	-3.492687	0.252152	-4.962291
1	-5.160703	0.506361	-4.498869
6	-0.336613	-3.785004	-1.224996
6	-0.871041	-5.040139	-0.873062
6	0.626972	-3.732303	-2.250548
6	-0.457102	-6.196888	-1.530352
1	-1.601439	-5.116469	-0.073907
6	1.036576	-4.889480	-2.909827
1	1.058493	-2.774658	-2.515949
6	0.497712	-6.127748	-2.551748
1	-0.877109	-7.156900	-1.243928
1	1.782673	-4.824791	-3.696954
1	0.817596	-7.032092	-3.061185
7	2.527307	-3.998327	0.475526
6	3.530271	-4.417740	-0.497199
1	3.343410	-5.458892	-0.776467
1	3.460327	-3.806113	-1.391196
1	4.542620	-4.343770	-0.084117
6	2.172707	-5.004889	1.472854
1	1.857166	-4.544763	2.407885
1	1.379507	-5.669514	1.108252
1	3.059596	-5.605062	1.688497
8	2.451405	-1.919439	-0.431494
6	-0.453510	-1.173827	2.861591
6	-0.885329	0.012463	3.418710
1	-0.794723	-2.114175	3.277168
6	-0.417717	1.201608	2.853821
6	0.455968	1.160449	1.781864
1	0.835540	2.067945	1.329399
7	0.890380	0.000952	1.248315
1	-1.574596	0.013384	4.253988
35	-0.962283	2.928177	3.596162

---

*Conformer*_12

Number of imaginary frequencies : 1
The smallest frequency is : -247.7381 cm(-1)
Electronic energy : HF=-7222.6348463
Zero-point correction= 1.755705
(Hartree/Particle)
Thermal correction to Energy= 1.874118
Thermal correction to Enthalpy= 1.875062
Thermal correction to Gibbs Free Energy= 1.593102
Sum of electronic and zero-point Energies= -7220.879141
Sum of electronic and thermal Energies= -7220.760728
Sum of electronic and thermal Enthalpies= -7220.759784
Sum of electronic and thermal Free Energies= -7221.041744

Cartesian Coordinates

26	4.295840	4.787191	1.873517
15	2.562936	1.624433	-1.886248
15	4.540873	0.128032	0.933513
6	3.967682	3.424716	0.319109
6	4.154744	2.745915	1.580451
6	3.132675	3.194295	2.473355
1	3.010226	2.884407	3.502015
6	2.335368	4.162744	1.792024
1	1.509366	4.716025	2.216851
6	2.849175	4.307286	0.470308
1	2.479190	4.983298	-0.285512
6	6.238211	5.325654	2.376061
1	7.099252	4.676813	2.283505
6	5.383019	5.426088	3.516135
1	5.479755	4.864652	4.435844
6	4.350940	6.365588	3.213063
1	3.525802	6.633189	3.859846
6	4.567985	6.847028	1.885975
1	3.939154	7.546905	1.351610
6	5.733808	6.206960	1.369923
1	6.141875	6.344685	0.377973
6	4.764499	3.153440	-0.912750
6	6.097570	3.584175	-0.982432
1	6.501077	4.139163	-0.145071
6	6.906284	3.300213	-2.082789
1	7.941822	3.624910	-2.092643
6	6.383722	2.576779	-3.152270
1	7.004209	2.337003	-4.009759
6	5.061656	2.133515	-3.105636
1	4.672377	1.556767	-3.937662
6	4.241978	2.397512	-1.997223
6	5.180012	1.672259	1.830880
1	6.093398	1.961534	1.308197
6	5.519798	1.464396	3.309353
1	6.298500	0.706588	3.430005
1	4.650952	1.148942	3.893195
1	5.882209	2.407233	3.730373
6	2.354531	0.721870	-3.481925
6	2.616239	-0.657880	-3.490466
1	2.930017	-1.152644	-2.578878
6	2.435195	-1.404974	-4.656607
1	2.642079	-2.470065	-4.648734
6	1.979202	-0.786254	-5.822416
1	1.824055	-1.370301	-6.725020
6	1.719257	0.586783	-5.822595
1	1.363740	1.074600	-6.725747
6	1.908775	1.338524	-4.662186
1	1.692424	2.401039	-4.679548
6	1.403865	3.038338	-2.070432
6	1.740834	4.197802	-2.788054
1	2.733569	4.302734	-3.215592
6	0.806747	5.222927	-2.947647
1	1.077831	6.116794	-3.502336
6	-0.474950	5.095375	-2.402416
1	-1.207771	5.886606	-2.532875
6	-0.814105	3.945277	-1.686945
1	-1.807326	3.839346	-1.267665
6	0.125125	2.927543	-1.509415
1	-0.137039	2.044845	-0.936894
6	5.833981	-0.351575	-0.288029
6	5.486580	-1.402521	-1.149284
1	4.518775	-1.879263	-1.036548
6	6.371466	-1.830242	-2.138196
6	7.598084	-1.194543	-2.319277
1	8.275652	-1.511333	-3.104022
6	7.930583	-0.132188	-1.478195
6	7.072250	0.277167	-0.457235
1	7.378742	1.096389	0.178411
6	4.568555	-1.271600	2.131554
6	3.559461	-1.295196	3.107713
1	2.867686	-0.465457	3.195864
6	3.410313	-2.401870	3.940679
6	4.233439	-3.519469	3.798124
1	4.087419	-4.396487	4.418753
6	5.222937	-3.501342	2.818548
6	5.409461	-2.382882	2.005164
1	6.188410	-2.406798	1.253587
29	2.440369	0.234799	-0.102018
6	6.091632	-4.715167	2.637445
6	2.272933	-2.466866	4.921037
6	5.996820	-3.025958	-2.969004
6	9.225145	0.592671	-1.725759
9	9.228005	1.197109	-2.940699
9	9.467166	1.552721	-0.806433
9	10.282586	-0.251626	-1.717343
9	6.178356	-4.182222	-2.282607

9	6.720371	-3.118287	-4.102362
9	4.686480	-3.002390	-3.326708
9	7.068336	-4.789964	3.569796
9	6.695303	-4.732252	1.427331
9	5.369120	-5.858342	2.739946
9	2.644623	-3.031480	6.090572
9	1.757429	-1.251294	5.200231
9	1.250519	-3.226836	4.437775
6	1.975746	-2.751283	0.404165
6	0.812237	-2.465111	1.213824
6	0.453788	-1.190138	1.765586
1	0.409406	-3.292362	1.779894
77	-3.400029	-1.296117	-1.447162
15	-5.267098	-0.538292	-0.378116
8	-5.260678	0.604628	0.820229
8	-6.330194	0.174020	-1.442320
7	-5.966522	-1.799062	0.479218
6	-4.982207	1.930123	0.525061
6	-3.758030	2.439071	1.010534
1	-3.119220	1.781943	1.589666
6	-3.416077	3.740332	0.740146
1	-2.486929	4.152874	1.120199
6	-4.248722	4.546600	-0.083881
6	-3.843367	5.851147	-0.477054
1	-2.895203	6.232340	-0.106826
6	-4.622760	6.608408	-1.322677
1	-4.300107	7.600746	-1.623876
6	-5.844814	6.086246	-1.810126
1	-6.447772	6.678181	-2.492596
6	-6.275806	4.832795	-1.431931
1	-7.211191	4.445760	-1.819341
6	-5.501785	4.025461	-0.552884
6	-5.909987	2.701952	-0.156166
6	-7.269225	2.156906	-0.436563
6	-8.460196	2.845585	-0.002345
6	-8.421000	4.023203	0.796565
1	-7.464346	4.422327	1.110476
6	-9.579549	4.656013	1.192465
1	-9.519032	5.549403	1.807435
6	-10.845878	4.150922	0.814022
1	-11.749987	4.665067	1.126661
6	-10.923742	2.997995	0.066407
1	-11.888731	2.583791	-0.213815
6	-9.748751	2.311627	-0.344580
6	-9.832690	1.090670	-1.066630
1	-10.811192	0.699055	-1.329779
6	-8.695521	0.398811	-1.398863
1	-8.734383	-0.551555	-1.920679
6	-7.430928	0.928191	-1.060299
6	-5.328157	-3.110867	0.180947
1	-4.591238	-3.316151	0.967040
6	-6.342203	-4.240956	0.175121
6	-6.026330	-5.466304	0.773450
1	-5.071863	-5.581232	1.282406
6	-6.924765	-6.535758	0.723102
1	-6.666992	-7.480646	1.193657
6	-8.154760	-6.385800	0.079221
1	-8.857836	-7.213260	0.045124
6	-8.479619	-5.162578	-0.517034
1	-9.437057	-5.038169	-1.015757
6	-7.578629	-4.098896	-0.471424
1	-7.831318	-3.144688	-0.925616
6	-4.594631	-3.051768	-1.163566
1	-5.333659	-3.113207	-1.971389
1	-3.953234	-3.933784	-1.249436
6	-6.667775	-1.732679	1.807799
1	-7.141333	-2.714994	1.886569
6	-5.678417	-1.640456	2.970754
6	-5.126428	-2.825972	3.482622
1	-5.452867	-3.781145	3.079951
6	-4.182236	-2.799890	4.512436
1	-3.769111	-3.731244	4.890246
6	-3.790506	-1.580446	5.068435
1	-3.064298	-1.554294	5.876309
6	-4.357598	-0.394603	4.591440
1	-4.076772	0.558495	5.032182
6	-5.290943	-0.424418	3.553505
1	-5.716700	0.505850	3.199277
6	-7.806973	-0.715987	1.852506
1	-8.514510	-0.911996	1.043700
1	-7.468790	0.315725	1.765449
1	-8.335161	-0.822935	2.804958
6	-2.525386	-1.127790	0.544722
1	-1.882619	-0.253039	0.590377
1	-3.221241	-1.182825	1.377221
6	-1.992613	-2.366952	0.062665
1	-2.496962	-3.271616	0.385698
6	-0.734709	-2.534447	-0.568618
1	-0.209033	-1.652600	-0.907221
6	-4.223013	-1.144094	-3.493141
1	-5.215129	-1.589869	-3.481965
6	-3.126364	-2.048769	-3.521799
1	-3.365020	-3.111954	-3.550775
6	-1.761865	-1.710544	-4.097661
1	-1.805635	-1.729022	-5.197796
1	-1.073244	-2.507800	-3.807507
6	-1.196675	-0.358674	-3.616017
1	-1.429613	0.434520	-4.333055
1	-0.107364	-0.422171	-3.582835
6	-1.691540	0.068186	-2.237859
1	-0.934715	0.084899	-1.460011
6	-2.806624	0.873910	-2.022358
1	-2.816575	1.461365	-1.109995
6	-3.753188	1.359012	-3.101568
1	-4.645460	1.749996	-2.607707
1	-3.289605	2.204727	-3.630945
6	-4.170871	0.260085	-4.102777
1	-3.492797	0.252060	-4.962575
1	-5.160814	0.506160	-4.499106
6	-0.336806	-3.784774	-1.224986
6	-0.871455	-5.039831	-0.873108
6	0.626857	-3.732210	-2.250472
6	-0.457651	-6.196635	-1.530387
1	-1.601932	-5.116060	-0.074017
6	1.036327	-4.889441	-2.909739
1	1.058542	-2.774627	-2.515834
6	0.497244	-6.127631	-2.551716
1	-0.877832	-7.156585	-1.244009
1	1.782489	-4.824858	-3.696813
1	0.817021	-7.032017	-3.061146
7	2.527083	-3.998277	0.475554
6	3.530030	-4.417748	-0.497163
1	3.343079	-5.458873	-0.776472
1	3.460165	-3.806084	-1.391140
1	4.542376	-4.343889	-0.084053
6	2.172359	-5.004850	1.472828
1	1.856833	-4.544734	2.407869
1	1.379109	-5.669386	1.108173
1	3.059186	-5.605114	1.688471
8	2.451358	-1.919359	-0.431410
6	-0.453705	-1.173643	2.861536
6	-0.885532	0.012658	3.418625
1	-0.795000	-2.113983	3.277067
6	-0.417814	1.201791	2.853801
6	0.455986	1.160610	1.781938
1	0.835653	2.068097	1.329532
7	0.890393	0.001100	1.248412
1	-1.574887	0.013594	4.253832
35	-0.962417	2.928371	3.596094

---

*Conformer_*13

Number of imaginary frequencies : 1
The smallest frequency is : -247.7265 cm(-1)
Electronic energy : HF=-7222.6348462
Zero-point correction= 1.755703
(Hartree/Particle)
Thermal correction to Energy= 1.874117
Thermal correction to Enthalpy= 1.875061
Thermal correction to Gibbs Free Energy= 1.593091

Sum of electronic and zero-point Energies= -7220.879143
Sum of electronic and thermal Energies= -7220.760729
Sum of electronic and thermal Enthalpies= -7220.759785
Sum of electronic and thermal Free Energies= -7221.041755

Cartesian Coordinates

26	4.295686	4.787218	1.873484
15	2.562882	1.624418	-1.886287
15	4.540861	0.128064	0.933464
6	3.967576	3.424733	0.319076
6	4.154664	2.745935	1.580415
6	3.132583	3.194277	2.473323
1	3.010146	2.884381	3.501982
6	2.335239	4.162698	1.791996
1	1.509217	4.715948	2.216826
6	2.849036	4.307261	0.470279
1	2.479027	4.983263	-0.285537
6	6.238038	5.325774	2.376005
1	7.099110	4.676976	2.283435
6	5.382857	5.426162	3.516092
1	5.479634	4.864727	4.435797
6	4.350728	6.365612	3.213037
1	3.525586	6.633171	3.859832
6	4.567731	6.847067	1.885948
1	3.938858	7.546915	1.351594
6	5.733578	6.207057	1.369877
1	6.141624	6.344803	0.377922
6	4.764400	3.153488	-0.912786
6	6.097453	3.584275	-0.982472
1	6.500942	4.139279	-0.145113
6	6.906173	3.300347	-2.082834
1	7.941698	3.625085	-2.092692
6	6.383634	2.576895	-3.152315
1	7.004127	2.337147	-4.009807
6	5.061586	2.133581	-3.105675
1	4.672325	1.556821	-3.937702
6	4.241903	2.397543	-1.997259
6	5.179963	1.672306	1.830835
1	6.093339	1.961607	1.308148
6	5.519762	1.464447	3.309306
1	6.298485	0.706658	3.429952
1	4.650927	1.148969	3.893151
1	5.882151	2.407291	3.730327
6	2.354504	0.721857	-3.481969
6	2.616279	-0.657880	-3.490522
1	2.930094	-1.152635	-2.578941
6	2.435253	-1.404977	-4.656664
1	2.642189	-2.470058	-4.648799
6	1.979210	-0.786274	-5.822462
1	1.824075	-1.370323	-6.725066
6	1.719199	0.586751	-5.822630
1	1.363643	1.074555	-6.725773
6	1.908700	1.338495	-4.662220
1	1.692297	2.401000	-4.679573
6	1.403785	3.038302	-2.070464
6	1.740725	4.197763	-2.788106
1	2.733448	4.302702	-3.215670
6	0.806624	5.222878	-2.947683
1	1.077685	6.116743	-3.502387
6	-0.475057	5.095320	-2.402416
1	-1.207888	5.886543	-2.532862
6	-0.814182	3.945225	-1.686925
1	-1.807390	3.839288	-1.267617
6	0.125062	2.927502	-1.509412
1	-0.137078	2.044808	-0.936873
6	5.833980	-0.351502	-0.288083
6	5.486614	-1.402466	-1.149331
1	4.518828	-1.879244	-1.036588
6	6.371511	-1.830157	-2.138246
6	7.598103	-1.194412	-2.319337
1	8.275679	-1.511180	-3.104084
6	7.930567	-0.132041	-1.478261
6	7.072224	0.277287	-0.457299
1	7.378689	1.096523	0.178341
6	4.568586	-1.271572	2.131500
6	3.559502	-1.295196	3.107668
1	2.867709	-0.465473	3.195831
6	3.410389	-2.401877	3.940632
6	4.233540	-3.519456	3.798065
1	4.087547	-4.396480	4.418692
6	5.223028	-3.501302	2.818479
6	5.409518	-2.382833	2.005099
1	6.188462	-2.406727	1.253516
29	2.440346	0.234767	-0.102067
6	6.091752	-4.715104	2.637365
6	2.273022	-2.466906	4.921003
6	5.996907	-3.025893	-2.969045
6	9.225102	0.592863	-1.725833
9	9.227936	1.197297	-2.940775
9	9.467094	1.552924	-0.806512
9	10.282573	-0.251397	-1.717420
9	6.178469	-4.182144	-2.282633
9	6.720471	-3.118214	-4.102395
9	4.686569	-3.002366	-3.326761
9	7.068463	-4.789883	3.569709
9	6.695416	-4.732169	1.427248
9	5.369267	-5.858297	2.739865
9	2.644742	-3.031511	6.090533
9	1.757485	-1.251350	5.200204
9	1.250625	-3.226908	4.437752
6	1.975807	-2.751330	0.404110
6	0.812296	-2.465194	1.213779
6	0.453827	-1.190236	1.765558
1	0.409490	-3.292461	1.779843
77	-3.400034	-1.296155	-1.447131
15	-5.267067	-0.538283	-0.378061
8	-5.260610	0.604623	0.820296
8	-6.330148	0.174064	-1.442256
7	-5.966522	-1.799044	0.479259
6	-4.982159	1.930127	0.525147
6	-3.757984	2.439081	1.010618
1	-3.119160	1.781954	1.589736
6	-3.416046	3.740351	0.740252
1	-2.486899	4.152894	1.120304
6	-4.248707	4.546626	-0.083752
6	-3.843366	5.851182	-0.476910
1	-2.895201	6.232376	-0.106687
6	-4.622776	6.608450	-1.322512
1	-4.300134	7.600795	-1.623700
6	-5.844831	6.086284	-1.809955
1	-6.447802	6.678226	-2.492409
6	-6.275808	4.832824	-1.431774
1	-7.211194	4.445788	-1.819181
6	-5.501770	4.025483	-0.552750
6	-5.909955	2.701963	-0.156051
6	-7.269192	2.156913	-0.436447
6	-8.460165	2.845572	-0.002202
6	-8.420972	4.023172	0.796735
1	-7.464318	4.422297	1.110645
6	-9.579523	4.655961	1.192661
1	-9.519009	5.549337	1.807652
6	-10.845850	4.150867	0.814218
1	-11.749961	4.664996	1.126878
6	-10.923712	2.997958	0.066576
1	-11.888699	2.583752	-0.213647
6	-9.748718	2.311610	-0.344439
6	-9.832652	1.090670	-1.066518
1	-10.811153	0.699052	-1.329667
6	-8.695480	0.398829	-1.398778
1	-8.734337	-0.551525	-1.920618
6	-7.430890	0.928213	-1.060212
6	-5.328213	-3.110866	0.180943
1	-4.591289	-3.316200	0.967018
6	-6.342307	-4.240912	0.175104
6	-6.026489	-5.466281	0.773418
1	-5.072025	-5.581259	1.282369
6	-6.924973	-6.535693	0.723060
1	-6.667241	-7.480599	1.193604
6	-8.154962	-6.385673	0.079184

1	-8.858076	-7.213100	0.045079
6	-8.479767	-5.162429	-0.517056
1	-9.437200	-5.037971	-1.015775
6	-7.578729	-4.098788	-0.471436
1	-7.831377	-3.144563	-0.925616
6	-4.594704	-3.051759	-1.163580
1	-5.333745	-3.113144	-1.971396
1	-3.953347	-3.933802	-1.249482
6	-6.667755	-1.732669	1.807851
1	-7.141345	-2.714970	1.886602
6	-5.678379	-1.640510	2.970794
6	-5.126429	-2.826057	3.482630
1	-5.452907	-3.781209	3.079944
6	-4.182223	-2.800031	4.512434
1	-3.769129	-3.731409	4.890220
6	-3.790438	-1.580613	5.068452
1	-3.064219	-1.554506	5.876316
6	-4.357489	-0.394739	4.591486
1	-4.076619	0.558340	5.032241
6	-5.290849	-0.424497	3.553562
1	-5.716573	0.505794	3.199356
6	-7.806919	-0.715940	1.852603
1	-8.514476	-0.911904	1.043803
1	-7.468703	0.315762	1.765567
1	-8.335094	-0.822897	2.805061
6	-2.525389	-1.128000	0.544757
1	-1.882631	-0.253247	0.590490
1	-3.221247	-1.183113	1.377250
6	-1.992583	-2.367120	0.062613
1	-2.496918	-3.271821	0.385566
6	-0.734668	-2.534547	-0.568665
1	-0.209017	-1.652671	-0.907230
6	-4.223020	-1.144029	-3.493114
1	-5.215152	-1.589769	-3.481949
6	-3.126404	-2.048740	-3.521800
1	-3.365096	-3.111916	-3.550810
6	-1.761889	-1.710538	-4.097640
1	-1.805653	-1.728971	-5.197775
1	-1.073298	-2.507830	-3.807513
6	-1.196651	-0.358705	-3.615942
1	-1.429551	0.434523	-4.332955
1	-0.107343	-0.422247	-3.582752
6	-1.691510	0.068133	-2.237774
1	-0.934689	0.084802	-1.459920
6	-2.806571	0.873881	-2.022251
1	-2.816508	1.461305	-1.109869
6	-3.753117	1.359047	-3.101446
1	-4.645380	1.750038	-2.607576
1	-3.289507	2.204768	-3.630790
6	-4.170825	0.260169	-4.102699
1	-3.492740	0.252152	-4.962489
1	-5.160756	0.506292	-4.499031
6	-0.336709	-3.784837	-1.225066
6	-0.871271	-5.039932	-0.873193
6	0.626930	-3.732198	-2.250571
6	-0.457410	-6.196701	-1.530497
1	-1.601721	-5.116217	-0.074081
6	1.036456	-4.889395	-2.909864
1	1.058552	-2.774585	-2.515927
6	0.497457	-6.127622	-2.551847
1	-0.877524	-7.156682	-1.244122
1	1.782596	-4.824754	-3.696954
1	0.817279	-7.031982	-3.061296
7	2.527174	-3.998311	0.475487
6	3.530129	-4.417751	-0.497235
1	3.343205	-5.458879	-0.776548
1	3.460242	-3.806085	-1.391210
1	4.542475	-4.343865	-0.084130
6	2.172487	-5.004893	1.472765
1	1.856961	-4.544787	2.407810
1	1.379249	-5.669449	1.108119
1	3.059331	-5.605136	1.688397
8	2.451396	-1.919387	-0.431460
6	-0.453641	-1.173774	2.861530
6	-0.885473	0.012510	3.418650
1	-0.794908	-2.114126	3.277055
6	-0.417792	1.201660	2.853830
6	0.455975	1.160512	1.781939
1	0.835609	2.068012	1.329533
7	0.890392	0.001018	1.248385
1	-1.574803	0.013422	4.253876
35	-0.962399	2.928218	3.596174

---

*Conformer*_14

Number of imaginary frequencies : 1
The smallest frequency is : -247.7215 cm(-1)
Electronic energy : HF=-7222.6348463
Zero-point correction= 1.755703
(Hartree/Particle)
Thermal correction to Energy= 1.874117
Thermal correction to Enthalpy= 1.875061
Thermal correction to Gibbs Free Energy= 1.593090
Sum of electronic and zero-point Energies= -7220.879144
Sum of electronic and thermal Energies= -7220.760730
Sum of electronic and thermal Enthalpies= -7220.759786
Sum of electronic and thermal Free Energies= -7221.041756

Cartesian Coordinates

26	4.295613	4.787192	1.873604
15	2.562875	1.624453	-1.886248
15	4.540844	0.128057	0.933494
6	3.967530	3.424730	0.319171
6	4.154619	2.745911	1.580498
6	3.132526	3.194225	2.473408
1	3.010086	2.884308	3.502060
6	2.335174	4.162648	1.792093
1	1.509142	4.715879	2.216927
6	2.848979	4.307241	0.470382
1	2.478966	4.983253	-0.285424
6	6.237952	5.325765	2.376154
1	7.099034	4.676979	2.283585
6	5.382757	5.426129	3.516232
1	5.479531	4.864685	4.435931
6	4.350620	6.365571	3.213177
1	3.525467	6.633112	3.859966
6	4.567632	6.847044	1.886096
1	3.938757	7.546891	1.351743
6	5.733493	6.207055	1.370030
1	6.141549	6.344817	0.378081
6	4.764369	3.153519	-0.912689
6	6.097421	3.584316	-0.982350
1	6.500898	4.139301	-0.144973
6	6.906155	3.300420	-2.082709
1	7.941678	3.625164	-2.092548
6	6.383632	2.576992	-3.152214
1	7.004135	2.337270	-4.009706
6	5.061586	2.133667	-3.105600
1	4.672338	1.556926	-3.937645
6	4.241890	2.397596	-1.997185
6	5.179925	1.672286	1.830903
1	6.093302	1.961606	1.308228
6	5.519714	1.464399	3.309372
1	6.298443	0.706616	3.430008
1	4.650877	1.148900	3.893202
1	5.882090	2.407238	3.730416
6	2.354522	0.721929	-3.481954
6	2.616329	-0.657802	-3.490544
1	2.930153	-1.152574	-2.578975
6	2.435326	-1.404872	-4.656706
1	2.642289	-2.469948	-4.648869
6	1.979274	-0.786149	-5.822490
1	1.824159	-1.370178	-6.725110
6	1.719231	0.586869	-5.822623
1	1.363668	1.074690	-6.725754
6	1.908709	1.338588	-4.662191
1	1.692282	2.401088	-4.679519
6	1.403772	3.038334	-2.070403
6	1.740710	4.197808	-2.788024

1	2.733434	4.302757	-3.215584
6	0.806609	5.222924	-2.947584
1	1.077669	6.116800	-3.502272
6	-0.475074	5.095354	-2.402322
1	-1.207906	5.886578	-2.532754
6	-0.814198	3.945246	-1.686853
1	-1.807406	3.839300	-1.267547
6	0.125047	2.927521	-1.509356
1	-0.137092	2.044817	-0.936833
6	5.833982	-0.351470	-0.288049
6	5.486638	-1.402417	-1.149325
1	4.518855	-1.879209	-1.036605
6	6.371551	-1.830077	-2.138239
6	7.598140	-1.194317	-2.319299
1	8.275729	-1.511060	-3.104044
6	7.930583	-0.131963	-1.478193
6	7.072223	0.277334	-0.457233
1	7.378672	1.096558	0.178430
6	4.568570	-1.271602	2.131502
6	3.559476	-1.295253	3.107661
1	2.867675	-0.465538	3.195830
6	3.410368	-2.401950	3.940604
6	4.233532	-3.519518	3.798025
1	4.087543	-4.396554	4.418636
6	5.223029	-3.501337	2.818448
6	5.409514	-2.382852	2.005088
1	6.188464	-2.406726	1.253511
29	2.440337	0.234757	-0.102062
6	6.091765	-4.715128	2.637321
6	2.272992	-2.467010	4.920962
6	5.996971	-3.025798	-2.969069
6	9.225117	0.592957	-1.725728
9	9.227958	1.197435	-2.940648
9	9.467095	1.552986	-0.806370
9	10.282592	-0.251298	-1.717336
9	6.178546	-4.182063	-2.282684
9	6.720546	-3.118081	-4.102415
9	4.686636	-3.002283	-3.326795
9	7.068469	-4.789913	3.569673
9	6.695440	-4.732168	1.427209
9	5.369291	-5.858329	2.739796
9	2.644708	-3.031626	6.090488
9	1.757436	-1.251465	5.200176
9	1.250612	-3.227019	4.437689
6	1.975830	-2.751352	0.404049
6	0.812309	-2.465246	1.213714
6	0.453821	-1.190305	1.765519
1	0.409505	-3.292531	1.779754
77	-3.400025	-1.296147	-1.447187
15	-5.267049	-0.538273	-0.378105
8	-5.260583	0.604606	0.820278
8	-6.330118	0.174108	-1.442288
7	-5.966521	-1.799044	0.479185
6	-4.982139	1.930120	0.525162
6	-3.757968	2.439068	1.010647
1	-3.119140	1.781932	1.589750
6	-3.416039	3.740348	0.740318
1	-2.486894	4.152886	1.120384
6	-4.248703	4.546641	-0.083665
6	-3.843369	5.851209	-0.476789
1	-2.895207	6.232399	-0.106555
6	-4.622783	6.608494	-1.322372
1	-4.300147	7.600849	-1.623534
6	-5.844835	6.086335	-1.809829
1	-6.447809	6.678291	-2.492267
6	-6.275805	4.832862	-1.431681
1	-7.211189	4.445831	-1.819098
6	-5.501762	4.025503	-0.552677
6	-5.909940	2.701969	-0.156015
6	-7.269175	2.156923	-0.436426
6	-8.460151	2.845564	-0.002165
6	-8.420964	4.023139	0.796808
1	-7.464312	4.422260	1.110731
6	-9.579519	4.655912	1.192752
1	-9.519010	5.549269	1.807770
6	-10.845843	4.150824	0.814291
1	-11.749957	4.664938	1.126965
6	-10.923698	2.997937	0.066613
1	-11.888684	2.583736	-0.213624
6	-9.748701	2.311606	-0.344420
6	-9.832628	1.090688	-1.066536
1	-10.811127	0.699074	-1.329699
6	-8.695452	0.398861	-1.398814
1	-8.734304	-0.551477	-1.920682
6	-7.430866	0.928240	-1.060228
6	-5.328232	-3.110868	0.180835
1	-4.591310	-3.316233	0.966905
6	-6.342343	-4.240899	0.174966
6	-6.026548	-5.466286	0.773255
1	-5.072088	-5.581290	1.282207
6	-6.925049	-6.535682	0.722869
1	-6.667335	-7.480603	1.193394
6	-8.155033	-6.385627	0.078991
1	-8.858161	-7.213042	0.044866
6	-8.479815	-5.162365	-0.517223
1	-9.437245	-5.037880	-1.015943
6	-7.578760	-4.098740	-0.471575
1	-7.831390	-3.144501	-0.925735
6	-4.594723	-3.051737	-1.163686
1	-5.333765	-3.113086	-1.971504
1	-3.953380	-3.933787	-1.249612
6	-6.667757	-1.732695	1.807777
1	-7.141361	-2.714991	1.886500
6	-5.678384	-1.640580	2.970726
6	-5.126454	-2.826147	3.482535
1	-5.452942	-3.781286	3.079822
6	-4.182256	-2.800161	4.512347
1	-3.769177	-3.731554	4.890113
6	-3.790459	-1.580763	5.068400
1	-3.064247	-1.554686	5.876272
6	-4.357490	-0.394869	4.591459
1	-4.076610	0.558195	5.032241
6	-5.290841	-0.424587	3.553527
1	-5.716549	0.505719	3.199340
6	-7.806908	-0.715953	1.852554
1	-8.514467	-0.911885	1.043749
1	-7.468679	0.315748	1.765548
1	-8.335085	-0.822929	2.805009
6	-2.525393	-1.128096	0.544711
1	-1.882641	-0.253342	0.590498
1	-3.221259	-1.183261	1.377195
6	-1.992568	-2.367189	0.062510
1	-2.496898	-3.271913	0.385410
6	-0.734643	-2.534573	-0.568756
1	-0.208998	-1.652680	-0.907281
6	-4.222998	-1.143952	-3.493175
1	-5.215135	-1.589679	-3.482029
6	-3.126395	-2.048677	-3.521875
1	-3.365103	-3.111849	-3.550916
6	-1.761869	-1.710479	-4.097691
1	-1.805620	-1.728885	-5.197828
1	-1.073291	-2.507788	-3.807577
6	-1.196616	-0.358666	-3.615956
1	-1.429499	0.434582	-4.332952
1	-0.107308	-0.422224	-3.582762
6	-1.691477	0.068148	-2.237781
1	-0.934664	0.084789	-1.459920
6	-2.806531	0.873900	-2.022245
1	-2.816470	1.461300	-1.109847
6	-3.753066	1.359106	-3.101432
1	-4.645329	1.750091	-2.607557
1	-3.289445	2.204838	-3.630748
6	-4.170778	0.260262	-4.102721
1	-3.492684	0.252260	-4.962503
1	-5.160701	0.506408	-4.499056
6	-0.336649	-3.784837	-1.225187
6	-0.871179	-5.039955	-0.873344
6	0.626993	-3.732147	-2.250686
6	-0.457283	-6.196697	-1.530673
1	-1.601627	-5.116277	-0.074235

6	1.036553	-4.889317	-2.910004
1	1.058591	-2.774517	-2.516016
6	0.497586	-6.127568	-2.552019
1	-0.877371	-7.156696	-1.244321
1	1.782695	-4.824637	-3.697089
1	0.817434	-7.031906	-3.061488
7	2.527209	-3.998329	0.475409
6	3.530177	-4.417743	-0.497311
1	3.343262	-5.458867	-0.776649
1	3.460298	-3.806059	-1.391274
1	4.542518	-4.343861	-0.084192
6	2.172521	-5.004933	1.472665
1	1.856988	-4.544845	2.407718
1	1.379288	-5.669485	1.108003
1	3.059367	-5.605176	1.688290
8	2.451419	-1.919387	-0.431498
6	-0.453653	-1.173880	2.861486
6	-0.885495	0.012386	3.418636
1	-0.794917	-2.114245	3.276983
6	-0.417819	1.201555	2.853853
6	0.455952	1.160443	1.781964
1	0.835582	2.067958	1.329584
7	0.890378	0.000967	1.248378
1	-1.574830	0.013270	4.253859
35	-0.962438	2.928086	3.596251

---

*Conformer*_15

Number of imaginary frequencies : 1
The smallest frequency is : -247.7358 cm(-1)
Electronic energy : HF=-7222.6348463
Zero-point correction= 1.755702
(Hartree/Particle)
Thermal correction to Energy= 1.874116
Thermal correction to Enthalpy= 1.875060
Thermal correction to Gibbs Free Energy= 1.593081
Sum of electronic and zero-point Energies= -7220.879144
Sum of electronic and thermal Energies= -7220.760730
Sum of electronic and thermal Enthalpies= -7220.759786
Sum of electronic and thermal Free Energies= -7221.041766

Cartesian Coordinates

26	4.295574	4.787382	1.873216
15	2.562959	1.624264	-1.886363
15	4.540792	0.128152	0.933596
6	3.967542	3.424784	0.318890
6	4.154535	2.746081	1.580296
6	3.132400	3.194512	2.473099
1	3.009886	2.884705	3.501775
6	2.335118	4.162892	1.791643
1	1.509079	4.716194	2.216374
6	2.849010	4.307345	0.469951
1	2.479065	4.983294	-0.285945
6	6.237919	5.325962	2.375738
1	7.098994	4.677163	2.283195
6	5.382728	5.426383	3.515813
1	5.479502	4.864978	4.435537
6	4.350599	6.365819	3.212720
1	3.525449	6.633393	3.859500
6	4.567611	6.847232	1.885616
1	3.938738	7.547061	1.351237
6	5.733464	6.207210	1.369576
1	6.141517	6.344924	0.377618
6	4.764429	3.153431	-0.912907
6	6.097481	3.584227	-0.982576
1	6.500922	4.139322	-0.145254
6	6.906253	3.300194	-2.082872
1	7.941775	3.624941	-2.092717
6	6.383769	2.576628	-3.152303
1	7.004305	2.336796	-4.009741
6	5.061721	2.133311	-3.105684
1	4.672503	1.556463	-3.937669
6	4.241984	2.397382	-1.997333
6	5.179816	1.672471	1.830881
1	6.093230	1.961735	1.308239
6	5.519505	1.464734	3.309395
1	6.298226	0.706963	3.430158
1	4.650631	1.149293	3.893201
1	5.881855	2.407616	3.730366
6	2.354635	0.721569	-3.481977
6	2.616353	-0.658179	-3.490390
1	2.930101	-1.152861	-2.578747
6	2.435343	-1.405378	-4.656469
1	2.642232	-2.470467	-4.648496
6	1.979371	-0.786765	-5.822343
1	1.824246	-1.370893	-6.724898
6	1.719416	0.586270	-5.822650
1	1.363914	1.074004	-6.725852
6	1.908902	1.338116	-4.662303
1	1.692537	2.400626	-4.679763
6	1.403852	3.038119	-2.070688
6	1.740783	4.197526	-2.788419
1	2.733515	4.302451	-3.215967
6	0.806664	5.222608	-2.948102
1	1.077718	6.116433	-3.502873
6	-0.475027	5.095068	-2.402853
1	-1.207872	5.886265	-2.533380
6	-0.814144	3.945027	-1.687271
1	-1.807359	3.839103	-1.267977
6	0.125119	2.927339	-1.509652
1	-0.137009	2.044688	-0.937043
6	5.833966	-0.351467	-0.287872
6	5.486642	-1.402478	-1.149078
1	4.518847	-1.879246	-1.036357
6	6.371598	-1.830243	-2.137909
6	7.598209	-1.194522	-2.318960
1	8.275834	-1.511348	-3.103641
6	7.930630	-0.132102	-1.477929
6	7.072228	0.277296	-0.457046
1	7.378663	1.096565	0.178567
6	4.568523	-1.271422	2.131708
6	3.559417	-1.295034	3.107855
1	2.867598	-0.465329	3.195972
6	3.410312	-2.401687	3.940858
6	4.233491	-3.519253	3.798350
1	4.087503	-4.396258	4.419005
6	5.223000	-3.501112	2.818787
6	5.409485	-2.382669	2.005372
1	6.188450	-2.406575	1.253811
29	2.440337	0.234755	-0.102031
6	6.091758	-4.714899	2.637730
6	2.272927	-2.466703	4.921209
6	5.997037	-3.026030	-2.968653
6	9.225191	0.592770	-1.725464
9	9.228115	1.197117	-2.940448
9	9.467132	1.552893	-0.806193
9	10.282650	-0.251503	-1.716918
9	6.178541	-4.182237	-2.282149
9	6.720680	-3.118437	-4.101946
9	4.686726	-3.002513	-3.326461
9	7.068482	-4.789597	3.570067
9	6.695410	-4.732009	1.427607
9	5.369310	-5.858108	2.740299
9	2.644629	-3.031279	6.090759
9	1.757376	-1.251145	5.200374
9	1.250545	-3.226722	4.437956
6	1.975795	-2.751320	0.404315
6	0.812267	-2.465150	1.213949
6	0.453785	-1.190158	1.765646
1	0.409467	-3.292385	1.780066
77	-3.400008	-1.296253	-1.447098
15	-5.267064	-0.538294	-0.378136
8	-5.260639	0.604679	0.820157
8	-6.330093	0.174003	-1.442415
7	-5.966569	-1.798999	0.479225
6	-4.982155	1.930162	0.524942
6	-3.757987	2.439123	1.010423
1	-3.119200	1.782023	1.589611
6	-3.416008	3.740366	0.739976

1	-2.486861	4.152911	1.120027
6	-4.248621	4.546603	-0.084112
6	-3.843237	5.851123	-0.477346
1	-2.895074	6.232319	-0.107119
6	-4.622602	6.608352	-1.323024
1	-4.299927	7.600668	-1.624270
6	-5.844654	6.086182	-1.810470
1	-6.447590	6.678092	-2.492983
6	-6.275673	4.832758	-1.432219
1	-7.211055	4.445718	-1.819631
6	-5.501681	4.025458	-0.553115
6	-5.909909	2.701972	-0.156343
6	-7.269144	2.156929	-0.436760
6	-8.460123	2.845636	-0.002609
6	-8.420941	4.023284	0.796257
1	-7.464294	4.422408	1.110188
6	-9.579498	4.656124	1.192088
1	-9.518994	5.549537	1.807024
6	-10.845818	4.151033	0.813616
1	-11.749933	4.665201	1.126200
6	-10.923669	2.998078	0.066044
1	-11.888652	2.583874	-0.214199
6	-9.748670	2.311680	-0.344873
6	-9.832595	1.090699	-1.066884
1	-10.811093	0.699086	-1.330056
6	-8.695422	0.398816	-1.399053
1	-8.734276	-0.551567	-1.920839
6	-7.430837	0.928195	-1.060462
6	-5.328287	-3.110853	0.180986
1	-4.591412	-3.316182	0.967107
6	-6.342426	-4.240860	0.175147
6	-6.026704	-5.466204	0.773563
1	-5.072276	-5.581193	1.282579
6	-6.925236	-6.535576	0.723221
1	-6.667580	-7.480463	1.193845
6	-8.155179	-6.385539	0.079258
1	-8.858331	-7.212935	0.045166
6	-8.479886	-5.162321	-0.517086
1	-9.437282	-5.037850	-1.015874
6	-7.578801	-4.098720	-0.471479
1	-7.831373	-3.144513	-0.925739
6	-4.594706	-3.051828	-1.163502
1	-5.333704	-3.113251	-1.971353
1	-3.953357	-3.933886	-1.249319
6	-6.667845	-1.732550	1.807790
1	-7.141462	-2.714835	1.886568
6	-5.678498	-1.640365	2.970757
6	-5.126601	-2.825904	3.482668
1	-5.453114	-3.781068	3.080033
6	-4.182402	-2.799856	4.512477
1	-3.769348	-3.731228	4.890320
6	-3.790569	-1.580421	5.068425
1	-3.064352	-1.554295	5.876290
6	-4.357577	-0.394553	4.591391
1	-4.076675	0.558540	5.032094
6	-5.290931	-0.424335	3.553463
1	-5.716620	0.505952	3.199204
6	-7.806985	-0.715791	1.852459
1	-8.514520	-0.911774	1.043644
1	-7.468741	0.315899	1.765387
1	-8.335195	-0.822691	2.804905
6	-2.525418	-1.127996	0.544805
1	-1.882657	-0.253243	0.590503
1	-3.221301	-1.183053	1.377282
6	-1.992601	-2.367149	0.062759
1	-2.496944	-3.271831	0.385756
6	-0.734673	-2.534618	-0.568485
1	-0.209022	-1.652764	-0.907107
6	-4.222941	-1.144214	-3.493111
1	-5.215075	-1.589950	-3.481956
6	-3.126325	-2.048925	-3.521729
1	-3.365015	-3.112103	-3.550699
6	-1.761793	-1.710745	-4.097542
1	-1.805523	-1.729220	-5.197678
1	-1.073211	-2.508026	-3.807362
6	-1.196569	-0.358894	-3.615877
1	-1.429439	0.434307	-4.332930
1	-0.107262	-0.422434	-3.582641
6	-1.691481	0.067998	-2.237744
1	-0.934686	0.084697	-1.459867
6	-2.806542	0.873764	-2.022298
1	-2.816507	1.461231	-1.109943
6	-3.753046	1.358883	-3.101550
1	-4.645324	1.749906	-2.607732
1	-3.289407	2.204572	-3.630919
6	-4.170723	0.259956	-4.102762
1	-3.492607	0.251893	-4.962526
1	-5.160639	0.506061	-4.499141
6	-0.336708	-3.784949	-1.224807
6	-0.871273	-5.040024	-0.872865
6	0.626940	-3.732370	-2.250306
6	-0.457399	-6.196832	-1.530091
1	-1.601733	-5.116262	-0.073758
6	1.036479	-4.889606	-2.909521
1	1.058558	-2.774772	-2.515716
6	0.497482	-6.127814	-2.551433
1	-0.877513	-7.156797	-1.243662
1	1.782626	-4.825012	-3.696609
1	0.817313	-7.032204	-3.060822
7	2.527182	-3.998287	0.475769
6	3.530168	-4.417751	-0.496911
1	3.343282	-5.458901	-0.776170
1	3.460282	-3.806135	-1.390920
1	4.542503	-4.343810	-0.083791
6	2.172498	-5.004828	1.473089
1	1.856933	-4.544683	2.408101
1	1.379291	-5.669427	1.108456
1	3.059356	-5.605032	1.688776
8	2.451385	-1.919417	-0.431295
6	-0.453674	-1.173629	2.861625
6	-0.885511	0.012690	3.418669
1	-0.794925	-2.113956	3.277220
6	-0.417845	1.201805	2.853763
6	0.455908	1.160590	1.781864
1	0.835527	2.068063	1.329389
7	0.890333	0.001065	1.248386
1	-1.574829	0.013654	4.253906
35	-0.962440	2.928412	3.595999

---

*Conformer*_16

Number of imaginary frequencies : 1
The smallest frequency is : -247.6887 cm(-1)
Electronic energy : HF=-7222.6348464
Zero-point correction= 1.755698
(Hartree/Particle)
Thermal correction to Energy= 1.874113
Thermal correction to Enthalpy= 1.875057
Thermal correction to Gibbs Free Energy= 1.593067
Sum of electronic and zero-point Energies= -7220.879148
Sum of electronic and thermal Energies= -7220.760733
Sum of electronic and thermal Enthalpies= -7220.759789
Sum of electronic and thermal Free Energies= -7221.041779

.....

Cartesian Coordinates

.....

26	4.295208	4.787275	1.873634
15	2.562826	1.624424	-1.886287
15	4.540717	0.128141	0.933561
6	3.967274	3.424801	0.319177
6	4.154296	2.745989	1.580519
6	3.132127	3.194275	2.473356
1	3.009622	2.884359	3.502000
6	2.334793	4.162672	1.791983
1	1.508713	4.715877	2.216759
6	2.848688	4.307282	0.470310
1	2.478708	4.983279	-0.285524
6	6.237494	5.325896	2.376333
1	7.098599	4.677132	2.283826
6	5.382209	5.426231	3.516346

1	5.478925	4.864783	4.436049
6	4.350071	6.365647	3.213217
1	3.524862	6.633163	3.859944
6	4.567172	6.847133	1.886155
1	3.938319	7.546967	1.351758
6	5.733089	6.207178	1.370176
1	6.141220	6.344958	0.378260
6	4.764199	3.153605	-0.912629
6	6.097237	3.584458	-0.982219
1	6.500642	4.139472	-0.144826
6	6.906047	3.300574	-2.082525
1	7.941558	3.625359	-2.092308
6	6.383616	2.577108	-3.152049
1	7.004180	2.337397	-4.009500
6	5.061585	2.133729	-3.105505
1	4.672410	1.556957	-3.937563
6	4.241814	2.397642	-1.997142
6	5.179636	1.672416	1.831005
1	6.093035	1.961783	1.308397
6	5.519323	1.464559	3.309502
1	6.298090	0.706824	3.430203
1	4.650462	1.149009	3.893267
1	5.881608	2.407423	3.730568
6	2.354585	0.721912	-3.482015
6	2.616517	-0.657795	-3.490620
1	2.930372	-1.152550	-2.579054
6	2.435594	-1.404868	-4.656793
1	2.642657	-2.469924	-4.648966
6	1.979492	-0.786172	-5.822572
1	1.824437	-1.370205	-6.725201
6	1.719324	0.586821	-5.822690
1	1.363722	1.074621	-6.725818
6	1.908727	1.338544	-4.662248
1	1.692200	2.401025	-4.679566
6	1.403674	3.038261	-2.070464
6	1.740566	4.197726	-2.788121
1	2.733279	4.302692	-3.215703
6	0.806433	5.222813	-2.947686
1	1.077456	6.116682	-3.502401
6	-0.475234	5.095222	-2.402390
1	-1.208089	5.886424	-2.532823
6	-0.814310	3.945122	-1.686884
1	-1.807504	3.839160	-1.267550
6	0.124966	2.927427	-1.509385
1	-0.137133	2.044733	-0.936831
6	5.833959	-0.351275	-0.287914
6	5.486730	-1.402216	-1.149245
1	4.518961	-1.879057	-1.036612
6	6.371749	-1.829822	-2.138088
6	7.598333	-1.194016	-2.319020
1	8.276006	-1.510721	-3.103709
6	7.930664	-0.131672	-1.477858
6	7.072194	0.277573	-0.456969
1	7.378560	1.096787	0.178746
6	4.568512	-1.271532	2.131554
6	3.559400	-1.295279	3.107691
1	2.867533	-0.465618	3.195862
6	3.410364	-2.402001	3.940614
6	4.233620	-3.519502	3.798033
1	4.087689	-4.396559	4.418628
6	5.223132	-3.501228	2.818474
6	5.409545	-2.382715	2.005138
1	6.188513	-2.406516	1.253578
29	2.440262	0.234690	-0.102128
6	6.091968	-4.714948	2.637344
6	2.272977	-2.467173	4.920949
6	5.997298	-3.025545	-2.968974
6	9.225197	0.593296	-1.725254
9	9.228112	1.197847	-2.940138
9	9.467084	1.553276	-0.805821
9	10.282692	-0.250934	-1.716835
9	6.178913	-4.181816	-2.282610
9	6.720948	-3.117746	-4.102279
9	4.686982	-3.002111	-3.326778
9	7.068672	-4.789661	3.569701
9	6.695653	-4.731928	1.427235
9	5.369585	-5.858208	2.739804
9	2.644715	-3.031788	6.090469
9	1.757320	-1.251675	5.200183
9	1.250667	-3.227252	4.437638
6	1.975952	-2.751452	0.403946
6	0.812400	-2.465443	1.213598
6	0.453834	-1.190537	1.765432
1	0.409642	-3.292766	1.779613
77	-3.400009	-1.296237	-1.447248
15	-5.266971	-0.538242	-0.378163
8	-5.260448	0.604596	0.820257
8	-6.329965	0.174236	-1.442355
7	-5.966557	-1.798992	0.479062
6	-4.982038	1.930132	0.525204
6	-3.757879	2.439086	1.010715
1	-3.119039	1.781948	1.589802
6	-3.415968	3.740382	0.740444
1	-2.486829	4.152912	1.120531
6	-4.248641	4.546698	-0.083506
6	-3.843322	5.851285	-0.476585
1	-2.895161	6.232471	-0.106340
6	-4.622747	6.608592	-1.322137
1	-4.300123	7.600961	-1.623265
6	-5.844796	6.086438	-1.809607
1	-6.447780	6.678413	-2.492020
6	-6.275751	4.832946	-1.431504
1	-7.211131	4.445920	-1.818934
6	-5.501694	4.025561	-0.552536
6	-5.909851	2.702003	-0.155933
6	-7.269077	2.156958	-0.436386
6	-8.460069	2.845553	-0.002096
6	-8.420909	4.023078	0.796952
1	-7.464267	4.422194	1.110909
6	-9.579480	4.655805	1.192924
1	-9.518993	5.549123	1.807999
6	-10.845791	4.150719	0.814415
1	-11.749917	4.664799	1.127112
6	-10.923618	2.997881	0.066659
1	-11.888594	2.583684	-0.213618
6	-9.748605	2.311597	-0.344405
6	-9.832502	1.090726	-1.066605
1	-10.810992	0.699114	-1.329809
6	-8.695311	0.398939	-1.398916
1	-8.734140	-0.551364	-1.920850
6	-7.430740	0.928318	-1.060274
6	-5.328412	-3.110863	0.180610
1	-4.591513	-3.316370	0.966663
6	-6.342659	-4.240772	0.174656
6	-6.027050	-5.466217	0.772924
1	-5.072623	-5.581360	1.281909
6	-6.925690	-6.535493	0.722475
1	-6.668118	-7.480460	1.192984
6	-8.155629	-6.385259	0.078553
1	-8.858864	-7.212580	0.044377
6	-8.480226	-5.161938	-0.517642
1	-9.437619	-5.037314	-1.016397
6	-7.579033	-4.098432	-0.471929
1	-7.831520	-3.144146	-0.926070
6	-4.594888	-3.051708	-1.163903
1	-5.333929	-3.112918	-1.971734
1	-3.953644	-3.933825	-1.249886
6	-6.667788	-1.732671	1.807657
1	-7.141483	-2.714928	1.886308
6	-5.678407	-1.640734	2.970613
6	-5.126600	-2.826389	3.482352
1	-5.453186	-3.781471	3.079584
6	-4.182396	-2.800558	4.512162
1	-3.769414	-3.732016	4.889873
6	-3.790468	-1.581233	5.068281
1	-3.064249	-1.555277	5.876151
6	-4.357374	-0.395252	4.591408
1	-4.076390	0.557758	5.032240
6	-5.290731	-0.424814	3.553478
1	-5.716340	0.505557	3.199340

6	-7.806846	-0.715829	1.852518
1	-8.514429	-0.911636	1.043703
1	-7.468526	0.315847	1.765585
1	-8.335025	-0.822828	2.804969
6	-2.525439	-1.128634	0.544690
1	-1.882714	-0.253873	0.590703
1	-3.221340	-1.184006	1.377135
6	-1.992510	-2.367617	0.062283
1	-2.496805	-3.272441	0.384961
6	-0.734538	-2.534820	-0.568931
1	-0.208947	-1.652852	-0.907342
6	-4.222924	-1.143779	-3.493271
1	-5.215102	-1.589422	-3.482190
6	-3.126400	-2.048590	-3.522007
1	-3.365197	-3.111740	-3.551147
6	-1.761815	-1.710448	-4.097717
1	-1.805506	-1.728746	-5.197857
1	-1.073320	-2.507840	-3.807636
6	-1.196466	-0.358722	-3.615832
1	-1.429241	0.434607	-4.332774
1	-0.107165	-0.422381	-3.582590
6	-1.691355	0.068033	-2.237647
1	-0.934579	0.084562	-1.459749
6	-2.806359	0.873840	-2.022092
1	-2.816297	1.461161	-1.109643
6	-3.752818	1.359205	-3.101271
1	-4.645077	1.750202	-2.607398
1	-3.289116	2.204957	-3.630486
6	-4.170556	0.260486	-4.102684
1	-3.492408	0.252506	-4.962423
1	-5.160435	0.506748	-4.499058
6	-0.336371	-3.784990	-1.225432
6	-0.870682	-5.040208	-0.873617
6	0.627245	-3.732103	-2.250945
6	-0.456607	-6.196858	-1.530993
1	-1.601088	-5.116676	-0.074483
6	1.036983	-4.889182	-2.910312
1	1.058683	-2.774393	-2.516246
6	0.498229	-6.127535	-2.552357
1	-0.876522	-7.156938	-1.244660
1	1.783099	-4.824352	-3.697409
1	0.818220	-7.031803	-3.061861
7	2.527421	-3.998390	0.475299
6	3.530450	-4.417712	-0.497396
1	3.343619	-5.458845	-0.776760
1	3.460556	-3.806016	-1.391350
1	4.542772	-4.343765	-0.084242
6	2.172795	-5.005027	1.472545
1	1.857213	-4.544970	2.407596
1	1.379617	-5.669637	1.107867
1	3.059683	-5.605204	1.688178
8	2.451500	-1.919439	-0.431579
6	-0.453607	-1.174195	2.861429
6	-0.885472	0.012028	3.418647
1	-0.794812	-2.114593	3.276901
6	-0.417868	1.201241	2.853894
6	0.455847	1.160210	1.781957
1	0.835412	2.067759	1.329591
7	0.890303	0.000774	1.248306
1	-1.574769	0.012851	4.253900
35	-0.962496	2.927716	3.596420

---

*Conformer*_17

Number of imaginary frequencies : 1
The smallest frequency is : -247.6882 cm(-1)
Electronic energy : HF=-7222.6348457
Zero-point correction= 1.755694
(Hartree/Particle)
Thermal correction to Energy= 1.874111
Thermal correction to Enthalpy= 1.875055
Thermal correction to Gibbs Free Energy= 1.593060
Sum of electronic and zero-point Energies= -7220.879152
Sum of electronic and thermal Energies= -7220.760734
Sum of electronic and thermal Enthalpies= -7220.759790
Sum of electronic and thermal Free Energies= -7221.041786

Cartesian Coordinates

26	4.295363	4.787509	1.872529
15	2.562566	1.624211	-1.886802
15	4.540844	0.128272	0.932918
6	3.967277	3.424873	0.318246
6	4.154439	2.746190	1.579638
6	3.132360	3.194559	2.472537
1	3.009963	2.884745	3.501225
6	2.334945	4.162879	1.791151
1	1.508908	4.716126	2.215959
6	2.848700	4.307360	0.469410
1	2.478634	4.983279	-0.286453
6	6.237702	5.326212	2.374939
1	7.098804	4.677450	2.282395
6	5.382553	5.426650	3.515046
1	5.479391	4.865296	4.434794
6	4.350365	6.366020	3.211949
1	3.525229	6.633586	3.858749
6	4.567298	6.847376	1.884812
1	3.938372	7.547149	1.350421
6	5.733162	6.207387	1.368755
1	6.141167	6.345081	0.376776
6	4.764047	3.153548	-0.913631
6	6.097061	3.584434	-0.983459
1	6.500554	4.139582	-0.146196
6	6.905732	3.300421	-2.083835
1	7.941230	3.625242	-2.093806
6	6.383184	2.576774	-3.153179
1	7.003645	2.336950	-4.010674
6	5.061171	2.133366	-3.106400
1	4.671905	1.556454	-3.938319
6	4.241535	2.397427	-1.997973
6	5.179823	1.672655	1.830135
1	6.093173	1.961984	1.307418
6	5.519655	1.464959	3.308622
1	6.298443	0.707247	3.429328
1	4.650856	1.149462	3.892510
1	5.881973	2.407873	3.729549
6	2.354118	0.721534	-3.482409
6	2.616006	-0.658182	-3.490895
1	2.929955	-1.152845	-2.579312
6	2.434895	-1.405380	-4.656958
1	2.641918	-2.470444	-4.649040
6	1.978647	-0.786802	-5.822742
1	1.823439	-1.370933	-6.725281
6	1.718524	0.586201	-5.822978
1	1.362807	1.073908	-6.726111
6	1.908114	1.338048	-4.662649
1	1.691601	2.400529	-4.680051
6	1.403351	3.037998	-2.070951
6	1.740078	4.197386	-2.788811
1	2.732714	4.302333	-3.216577
6	0.805883	5.222423	-2.948333
1	1.076778	6.116234	-3.503204
6	-0.475684	5.094857	-2.402793
1	-1.208588	5.886018	-2.533194
6	-0.814594	3.944836	-1.687082
1	-1.807711	3.838884	-1.267560
6	0.124749	2.927194	-1.509627
1	-0.137217	2.044562	-0.936917
6	5.833924	-0.351243	-0.288692
6	5.486577	-1.402266	-1.149874
1	4.518822	-1.879093	-1.037060
6	6.371459	-1.829967	-2.138799
6	7.598016	-1.194175	-2.319962
1	8.275581	-1.510952	-3.104715
6	7.930454	-0.131738	-1.478959
6	7.072129	0.277598	-0.457985
1	7.378576	1.096880	0.177606
6	4.568841	-1.271296	2.131032
6	3.559856	-1.294998	3.107301
1	2.867977	-0.465353	3.195505

6	3.410950	-2.401666	3.940320
6	4.234205	-3.519163	3.797707
1	4.088368	-4.396179	4.418381
6	5.223600	-3.500930	2.818030
6	5.409888	-2.382467	2.004597
1	6.188771	-2.406299	1.252949
29	2.440246	0.234668	-0.102474
6	6.092447	-4.714636	2.636869
6	2.273708	-2.466785	4.920831
6	5.996883	-3.025760	-2.969529
6	9.224937	0.593228	-1.726626
9	9.227710	1.197532	-2.941633
9	9.466876	1.553404	-0.807411
9	10.282467	-0.250958	-1.718138
9	6.178593	-4.181976	-2.283096
9	6.720365	-3.118057	-4.102934
9	4.686518	-3.002348	-3.327145
9	7.069249	-4.789279	3.569129
9	6.696006	-4.731659	1.426699
9	5.370105	-5.857911	2.739460
9	2.645634	-3.031313	6.090332
9	1.758073	-1.251277	5.200061
9	1.251338	-3.226915	4.437727
6	1.976024	-2.751473	0.403897
6	0.812572	-2.465427	1.213684
6	0.454101	-1.190479	1.765486
1	0.409904	-3.292713	1.779821
77	-3.400191	-1.296293	-1.446609
15	-5.267019	-0.538246	-0.377325
8	-5.260369	0.604663	0.821026
8	-6.330157	0.174140	-1.441436
7	-5.966491	-1.798959	0.480047
6	-4.982011	1.930187	0.525853
6	-3.757809	2.439194	1.011200
1	-3.118919	1.782121	1.590304
6	-3.415920	3.740461	0.740758
1	-2.486739	4.153026	1.120705
6	-4.248673	4.546693	-0.083194
6	-3.843387	5.851233	-0.476458
1	-2.895181	6.232451	-0.106363
6	-4.622902	6.608456	-1.322004
1	-4.300302	7.600789	-1.623278
6	-5.845011	6.086261	-1.809278
1	-6.448069	6.678168	-2.491686
6	-6.275933	4.832813	-1.430993
1	-7.211360	4.445752	-1.818278
6	-5.501781	4.025515	-0.552029
6	-5.909899	2.701996	-0.155251
6	-7.269158	2.156926	-0.435499
6	-8.460097	2.845553	-0.001116
6	-8.420843	4.023152	0.797815
1	-7.464163	4.422304	1.111612
6	-9.579367	4.655908	1.193877
1	-9.518807	5.549286	1.808859
6	-10.845723	4.150777	0.815582
1	-11.749813	4.664877	1.128349
6	-10.923639	2.997868	0.067944
1	-11.888647	2.583635	-0.212169
6	-9.748674	2.311556	-0.343212
6	-9.832655	1.090623	-1.065296
1	-10.811176	0.698982	-1.328340
6	-8.695502	0.398817	-1.397697
1	-8.734393	-0.551530	-1.919546
6	-7.430891	0.928236	-1.059267
6	-5.328414	-3.110849	0.181524
1	-4.591395	-3.316363	0.967464
6	-6.342687	-4.240734	0.175750
6	-6.027028	-5.466161	0.774028
1	-5.072534	-5.581306	1.282886
6	-6.925698	-6.535420	0.723739
1	-6.668086	-7.480373	1.194252
6	-8.155717	-6.385185	0.079969
1	-8.858973	-7.212494	0.045915
6	-8.480366	-5.161880	-0.516230
1	-9.437822	-5.037255	-1.014864
6	-7.579145	-4.098391	-0.470674
1	-7.831674	-3.144116	-0.924815
6	-4.595090	-3.051726	-1.163102
1	-5.334249	-3.112922	-1.970825
1	-3.953886	-3.933864	-1.249168
6	-6.667528	-1.732592	1.808742
1	-7.141236	-2.714836	1.887487
6	-5.677965	-1.640654	2.971541
6	-5.126125	-2.826315	3.483232
1	-5.452820	-3.781399	3.080556
6	-4.181740	-2.800484	4.512878
1	-3.768737	-3.731946	4.890556
6	-3.789651	-1.581153	5.068872
1	-3.063285	-1.555198	5.876609
6	-4.356587	-0.395166	4.592051
1	-4.075475	0.557851	5.032787
6	-5.290130	-0.424728	3.554287
1	-5.715757	0.505646	3.200183
6	-7.806557	-0.715723	1.853746
1	-8.514263	-0.911532	1.045039
1	-7.468229	0.315943	1.766740
1	-8.334600	-0.822691	2.806277
6	-2.525373	-1.128708	0.545200
1	-1.882607	-0.253972	0.591132
1	-3.221178	-1.184036	1.377727
6	-1.992522	-2.367724	0.062771
1	-2.496812	-3.272525	0.385527
6	-0.734626	-2.534965	-0.568588
1	-0.209091	-1.653018	-0.907140
6	-4.223337	-1.143861	-3.492563
1	-5.215525	-1.589478	-3.481351
6	-3.126837	-2.048690	-3.521402
1	-3.365649	-3.111838	-3.550484
6	-1.762304	-1.710572	-4.097252
1	-1.806113	-1.728855	-5.197388
1	-1.073796	-2.507986	-3.807257
6	-1.196877	-0.358865	-3.615406
1	-1.429672	0.434477	-4.332329
1	-0.107578	-0.422558	-3.582231
6	-1.691652	0.067903	-2.237182
1	-0.934801	0.084436	-1.459359
6	-2.806610	0.873755	-2.021545
1	-2.816443	1.461109	-1.109117
6	-3.753155	1.359121	-3.100647
1	-4.645364	1.750139	-2.606702
1	-3.289484	2.204855	-3.629915
6	-4.170995	0.260391	-4.102006
1	-3.492912	0.252381	-4.961796
1	-5.160900	0.506664	-4.498308
6	-0.336546	-3.785178	-1.225063
6	-0.870804	-5.040375	-0.873092
6	0.626933	-3.732360	-2.250709
6	-0.456802	-6.197072	-1.530435
1	-1.601110	-5.116793	-0.073861
6	1.036602	-4.889485	-2.910038
1	1.058325	-2.774667	-2.516143
6	0.497909	-6.127816	-2.551919
1	-0.876674	-7.157134	-1.243979
1	1.782616	-4.824707	-3.697236
1	0.817846	-7.032120	-3.061394
7	2.527533	-3.998391	0.475266
6	3.530451	-4.417738	-0.497534
1	3.343664	-5.458915	-0.776758
1	3.460372	-3.806139	-1.391539
1	4.542830	-4.343664	-0.084543
6	2.173098	-5.004957	1.472651
1	1.857606	-4.544830	2.407698
1	1.379914	-5.669649	1.108137
1	3.060051	-5.605057	1.688231
8	2.451436	-1.919511	-0.431754
6	-0.453164	-1.174047	2.861627
6	-0.884938	0.012220	3.418824
1	-0.794302	-2.114410	3.277230
6	-0.417429	1.201386	2.853893
6	0.456109	1.160265	1.781816

1	0.835586	2.067778	1.329305
7	0.890492	0.000791	1.248196
1	-1.574095	0.013111	4.254193
35	-0.961919	2.927933	3.596334

---

*Conformer*_18

Number of imaginary frequencies : 1
The smallest frequency is : -247.7054 cm(-1)
Electronic energy : HF=-7222.634846
Zero-point correction= 1.755698
(Hartree/Particle)
Thermal correction to Energy= 1.874114
Thermal correction to Enthalpy= 1.875058
Thermal correction to Gibbs Free Energy= 1.593067
Sum of electronic and zero-point Energies= -7220.879148
Sum of electronic and thermal Energies= -7220.760732
Sum of electronic and thermal Enthalpies= -7220.759788
Sum of electronic and thermal Free Energies= -7221.041779

Cartesian Coordinates

26	4.295495	4.787381	1.873007
15	2.562742	1.624291	-1.886535
15	4.540843	0.128178	0.933233
6	3.967414	3.424808	0.318668
6	4.154532	2.746077	1.580040
6	3.132443	3.194436	2.472932
1	3.010018	2.884589	3.501607
6	2.335065	4.162798	1.791562
1	1.509030	4.716046	2.216370
6	2.848852	4.307313	0.469835
1	2.478817	4.983266	-0.286012
6	6.237836	5.326025	2.375473
1	7.098929	4.677252	2.282915
6	5.382671	5.426430	3.515569
1	5.479484	4.865037	4.435296
6	4.350505	6.365833	3.212494
1	3.525364	6.633389	3.859292
6	4.567469	6.847240	1.885381
1	3.938564	7.547046	1.351009
6	5.733329	6.207251	1.369317
1	6.141354	6.344973	0.377350
6	4.764222	3.153519	-0.913194
6	6.097251	3.584371	-0.982947
1	6.500731	4.139459	-0.145639
6	6.905955	3.300404	-2.083311
1	7.941462	3.625198	-2.093224
6	6.383425	2.576842	-3.152722
1	7.003908	2.337058	-4.010211
6	5.061400	2.133463	-3.106015
1	4.672147	1.556618	-3.937986
6	4.241732	2.397472	-1.997598
6	5.179875	1.672502	1.830513
1	6.093239	1.961814	1.307810
6	5.519688	1.464741	3.308995
1	6.298446	0.706994	3.429680
1	4.650871	1.149257	3.892863
1	5.882038	2.407626	3.729960
6	2.354351	0.721649	-3.482169
6	2.616197	-0.658075	-3.490668
1	2.930080	-1.152768	-2.579077
6	2.435143	-1.405241	-4.656761
1	2.642135	-2.470310	-4.648854
6	1.978997	-0.786621	-5.822563
1	1.823837	-1.370725	-6.725128
6	1.718916	0.586390	-5.822786
1	1.363278	1.074130	-6.725932
6	1.908447	1.338204	-4.662425
1	1.691977	2.400694	-4.679819
6	1.403585	3.038123	-2.070729
6	1.740425	4.197539	-2.788490
1	2.733109	4.302478	-3.216146
6	0.806278	5.222612	-2.948062
1	1.077262	6.116444	-3.502857
6	-0.475352	5.095055	-2.402671
1	-1.208219	5.886246	-2.533111
6	-0.814377	3.945006	-1.687061
1	-1.807543	3.839066	-1.267655
6	0.124916	2.927326	-1.509554
1	-0.137142	2.044670	-0.936922
6	5.833953	-0.351372	-0.288332
6	5.486613	-1.402389	-1.149525
1	4.518849	-1.879203	-1.036738
6	6.371508	-1.830092	-2.138436
6	7.598072	-1.194307	-2.319579
1	8.275647	-1.511084	-3.104323
6	7.930507	-0.131880	-1.478562
6	7.072168	0.277459	-0.457600
1	7.378612	1.096737	0.177996
6	4.568702	-1.271410	2.131324
6	3.559664	-1.295062	3.107540
1	2.867828	-0.465377	3.195713
6	3.410652	-2.401728	3.940543
6	4.233857	-3.519266	3.797969
1	4.087940	-4.396279	4.418629
6	5.223302	-3.501083	2.818341
6	5.409693	-2.382627	2.004922
1	6.188609	-2.406498	1.253310
29	2.440294	0.234709	-0.102249
6	6.092089	-4.714839	2.637221
6	2.273345	-2.466791	4.920981
6	5.996936	-3.025881	-2.969174
6	9.225006	0.593066	-1.726198
9	9.227806	1.197400	-2.941190
9	9.466955	1.553215	-0.806956
9	10.282519	-0.251142	-1.717718
9	6.178559	-4.182094	-2.282714
9	6.720482	-3.118223	-4.102534
9	4.686591	-3.002422	-3.326867
9	7.068845	-4.789536	3.569525
9	6.695702	-4.731900	1.427078
9	5.369677	-5.858073	2.739783
9	2.645163	-3.031346	6.090504
9	1.757758	-1.251256	5.200182
9	1.250963	-3.226861	4.437807
6	1.975918	-2.751402	0.404067
6	0.812431	-2.465303	1.213783
6	0.453952	-1.190342	1.765552
1	0.409693	-3.292572	1.779893
77	-3.400097	-1.296260	-1.446879
15	-5.267035	-0.538268	-0.377745
8	-5.260491	0.604656	0.820593
8	-6.330119	0.174094	-1.441925
7	-5.966525	-1.798986	0.479607
6	-4.982083	1.930167	0.525422
6	-3.757900	2.439152	1.010840
1	-3.119049	1.782056	1.589963
6	-3.415984	3.740418	0.740430
1	-2.486824	4.152976	1.120436
6	-4.248682	4.546665	-0.083564
6	-3.843365	5.851210	-0.476780
1	-2.895184	6.232420	-0.106612
6	-4.622818	6.608448	-1.322370
1	-4.300194	7.600785	-1.623604
6	-5.844893	6.086263	-1.809739
1	-6.447900	6.678181	-2.492182
6	-6.275846	4.832811	-1.431502
1	-7.211248	4.445759	-1.818856
6	-5.501762	4.025499	-0.552492
6	-5.909917	2.701983	-0.155748
6	-7.269160	2.156919	-0.436085
6	-8.460124	2.845564	-0.001795
6	-8.420914	4.023170	0.797131
1	-7.464252	4.422312	1.110996
6	-9.579458	4.655945	1.193101
1	-9.518932	5.549327	1.808081
6	-10.845793	4.150828	0.814716
1	-11.749899	4.664944	1.127412
6	-10.923669	2.997912	0.067085

1	-11.888662	2.583690	-0.213095
6	-9.748682	2.311580	-0.343976
6	-9.832628	1.090638	-1.066049
1	-10.811135	0.699005	-1.329157
6	-8.695459	0.398813	-1.398357
1	-8.734324	-0.551542	-1.920194
6	-7.430865	0.928219	-1.059844
6	-5.328343	-3.110853	0.181213
1	-4.591391	-3.316276	0.967238
6	-6.342543	-4.240805	0.175401
6	-6.026838	-5.466197	0.773726
1	-5.072372	-5.581265	1.282654
6	-6.925431	-6.535519	0.723402
1	-6.667785	-7.480444	1.193953
6	-8.155419	-6.385383	0.079549
1	-8.858616	-7.212739	0.045469
6	-8.480112	-5.162114	-0.516700
1	-9.437543	-5.037565	-1.015401
6	-7.578966	-4.098562	-0.471111
1	-7.831528	-3.144317	-0.925295
6	-4.594898	-3.051766	-1.163347
1	-5.333981	-3.113063	-1.971132
1	-3.953623	-3.933863	-1.249304
6	-6.667677	-1.732592	1.808240
1	-7.141335	-2.714860	1.886995
6	-5.678221	-1.640536	2.971123
6	-5.126341	-2.826137	3.482909
1	-5.452933	-3.781258	3.080239
6	-4.182054	-2.800201	4.512641
1	-3.769017	-3.731619	4.890391
6	-3.790111	-1.580822	5.068632
1	-3.063825	-1.554784	5.876438
6	-4.357092	-0.394894	4.591717
1	-4.076097	0.558158	5.032451
6	-5.290535	-0.424561	3.553867
1	-5.716200	0.505770	3.199695
6	-7.806766	-0.715784	1.853091
1	-8.514389	-0.911675	1.044331
1	-7.468485	0.315897	1.766061
1	-8.334888	-0.822730	2.805580
6	-2.525395	-1.128381	0.544984
1	-1.882641	-0.253631	0.590820
1	-3.221239	-1.183605	1.377483
6	-1.992547	-2.367447	0.062713
1	-2.496855	-3.272204	0.385561
6	-0.734632	-2.534775	-0.568587
1	-0.209042	-1.652862	-0.907147
6	-4.223137	-1.143990	-3.492859
1	-5.215299	-1.589662	-3.481680
6	-3.126583	-2.048766	-3.521601
1	-3.365340	-3.111927	-3.550642
6	-1.762051	-1.710616	-4.097432
1	-1.805824	-1.728980	-5.197568
1	-1.073509	-2.507971	-3.807358
6	-1.196716	-0.358846	-3.615662
1	-1.429548	0.434435	-4.332639
1	-0.107413	-0.422470	-3.582465
6	-1.691548	0.067972	-2.237476
1	-0.934723	0.084576	-1.459628
6	-2.806556	0.873778	-2.021917
1	-2.816451	1.461173	-1.109515
6	-3.753084	1.359040	-3.101082
1	-4.645324	1.750057	-2.607191
1	-3.289429	2.204759	-3.630390
6	-4.170852	0.260230	-4.102383
1	-3.492758	0.252205	-4.962165
1	-5.160764	0.506430	-4.498715
6	-0.336594	-3.785028	-1.225012
6	-0.870983	-5.040178	-0.873074
6	0.626961	-3.732295	-2.250590
6	-0.457036	-6.196912	-1.530386
1	-1.601355	-5.116531	-0.073897
6	1.036574	-4.889457	-2.909890
1	1.058453	-2.774639	-2.515996
6	0.497749	-6.127741	-2.551807
1	-0.877011	-7.156937	-1.243957
1	1.782648	-4.824745	-3.697038
1	0.817640	-7.032073	-3.061260
7	2.527355	-3.998351	0.475459
6	3.530298	-4.417757	-0.497290
1	3.343443	-5.458912	-0.776549
1	3.460322	-3.806134	-1.391288
1	4.542658	-4.343773	-0.084236
6	2.172789	-5.004913	1.472801
1	1.857273	-4.544785	2.407839
1	1.379583	-5.669544	1.108225
1	3.059688	-5.605079	1.688421
8	2.451426	-1.919459	-0.431549
6	-0.453416	-1.173882	2.861607
6	-0.885226	0.012401	3.418745
1	-0.794614	-2.114235	3.277186
6	-0.417636	1.201552	2.853849
6	0.456018	1.160404	1.781867
1	0.835569	2.067905	1.329394
7	0.890425	0.000913	1.248301
1	-1.574470	0.013313	4.254043
35	-0.962192	2.928114	3.596214

C2-P2 *si-si* conf1

Number of imaginary frequencies : 1
The smallest frequency is : -247.7047 cm(-1)
Electronic energy : HF=-7222.6348462
Zero-point correction= 1.755700
(Hartree/Particle)
Thermal correction to Energy= 1.874115
Thermal correction to Enthalpy= 1.875059
Thermal correction to Gibbs Free Energy= 1.593083
Sum of electronic and zero-point Energies= -7220.879146
Sum of electronic and thermal Energies= -7220.760731
Sum of electronic and thermal Enthalpies= -7220.759787
Sum of electronic and thermal Free Energies= -7221.041763

Cartesian Coordinates

26	-4.295437	4.787355	1.873202
15	-2.562805	1.624327	-1.886450
15	-4.540775	0.128166	0.933392
6	-3.967400	3.424797	0.318842
6	-4.154449	2.746058	1.580220
6	-3.132327	3.194430	2.473067
1	-3.009849	2.884580	3.501734
6	-2.334999	4.162811	1.791665
1	-1.508954	4.716069	2.216440
6	-2.848848	4.307323	0.469963
1	-2.478862	4.983288	-0.285896
6	-6.237760	5.325940	2.375800
1	-7.098839	4.677139	2.283312
6	-5.382516	5.426388	3.515834
1	-5.479243	4.865002	4.435574
6	-4.350403	6.365820	3.212671
1	-3.525224	6.633413	3.859406
6	-4.567478	6.847204	1.885567
1	-3.938634	7.547022	1.351141
6	-5.733355	6.207169	1.369596
1	-6.141457	6.344865	0.377657
6	-4.764269	3.153492	-0.912977
6	-6.097323	3.584280	-0.982639
1	-6.500778	4.139337	-0.145298
6	-6.906087	3.300278	-2.082949
1	-7.941613	3.625013	-2.092786
6	-6.383592	2.576754	-3.152403
1	-7.004122	2.336950	-4.009854
6	-5.061542	2.133443	-3.105789
1	-4.672316	1.556624	-3.937792
6	-4.241815	2.397477	-1.997422
6	-5.179769	1.672470	1.830733
1	-6.093160	1.961786	1.308082
6	-5.519495	1.464681	3.309230
1	-6.298243	0.706930	3.429948

1	-4.650642	1.149189	3.893039
1	-5.881822	2.407557	3.730235
6	-2.354461	0.721721	-3.482111
6	-2.616243	-0.658015	-3.490617
1	-2.930053	-1.152734	-2.579016
6	-2.435227	-1.405154	-4.656733
1	-2.642167	-2.470234	-4.648829
6	-1.979184	-0.786494	-5.822554
1	-1.824055	-1.370575	-6.725138
6	-1.719168	0.586530	-5.822771
1	-1.363613	1.074301	-6.725932
6	-1.908661	1.338316	-4.662386
1	-1.692248	2.400819	-4.679778
6	-1.403676	3.038178	-2.070656
6	-1.740556	4.197606	-2.788378
1	-2.733256	4.302541	-3.215998
6	-0.806428	5.222696	-2.947956
1	-1.077442	6.116537	-3.502721
6	0.475220	5.095145	-2.402608
1	1.208071	5.886350	-2.533051
6	0.814284	3.945084	-1.687034
1	1.807464	3.839152	-1.267659
6	-0.124988	2.927386	-1.509523
1	0.137097	2.044720	-0.936918
6	-5.833954	-0.351351	-0.288109
6	-5.486642	-1.402292	-1.149405
1	-4.518843	-1.879066	-1.036746
6	-6.371623	-1.829989	-2.138243
6	-7.598250	-1.194274	-2.319206
1	-8.275893	-1.511055	-3.103890
6	-7.930661	-0.131925	-1.478082
6	-7.072228	0.277409	-0.457198
1	-7.378658	1.096619	0.178492
6	-4.568586	-1.271452	2.131450
6	-3.559513	-1.295134	3.107628
1	-2.867673	-0.465451	3.195798
6	-3.410474	-2.401824	3.940594
6	-4.233691	-3.519354	3.798021
1	-4.087756	-4.396385	4.418651
6	-5.223171	-3.501141	2.818428
6	-5.409585	-2.382662	2.005045
1	-6.188526	-2.406511	1.253458
29	-2.440281	0.234724	-0.102190
6	-6.091969	-4.714890	2.637310
6	-2.273122	-2.466927	4.920975
6	-5.997085	-3.025715	-2.969085
6	-9.225234	0.592960	-1.725516
9	-9.228151	1.197511	-2.940401
9	-9.467207	1.552928	-0.806092
9	-10.282676	-0.251335	-1.717126
9	-6.178690	-4.181980	-2.282707
9	-6.720677	-3.117967	-4.102424
9	-4.686754	-3.002237	-3.326825
9	-7.068699	-4.789599	3.569641
9	-6.695617	-4.731925	1.427184
9	-5.369560	-5.858128	2.739829
9	-2.644887	-3.031518	6.090498
9	-1.757515	-1.251404	5.200191
9	-1.250767	-3.226987	4.437728
6	-1.975894	-2.751384	0.404035
6	-0.812390	-2.465302	1.213731
6	-0.453886	-1.190357	1.765515
1	-0.409642	-3.292585	1.779814
77	3.400058	-1.296214	-1.447055
15	5.267032	-0.538264	-0.377953
8	5.260515	0.604632	0.820413
8	6.330094	0.174129	-1.442135
7	5.966540	-1.799001	0.479356
6	4.982080	1.930143	0.525274
6	3.757894	2.439098	1.010716
1	3.119051	1.781975	1.589817
6	3.415964	3.740371	0.740351
1	2.486805	4.152909	1.120380
6	4.248649	4.546652	-0.083622
6	3.843320	5.851210	-0.476787
1	2.895142	6.232401	-0.106594
6	4.622758	6.608483	-1.322358
1	4.300125	7.600830	-1.623550
6	5.844831	6.086323	-1.809761
1	6.447826	6.678270	-2.492188
6	6.275796	4.832860	-1.431574
1	7.211195	4.445828	-1.818952
6	5.501727	4.025512	-0.552583
6	5.909897	2.701986	-0.155887
6	7.269139	2.156938	-0.436261
6	8.460106	2.845577	-0.001972
6	8.420903	4.023158	0.796991
1	7.464244	4.422286	1.110883
6	9.579451	4.655925	1.192965
1	9.518930	5.549286	1.807975
6	10.845783	4.150826	0.814544
1	11.749891	4.664936	1.127243
6	10.923652	2.997935	0.066874
1	11.888643	2.583726	-0.213333
6	9.748662	2.311610	-0.344190
6	9.832602	1.090689	-1.066300
1	10.811106	0.699068	-1.329435
6	8.695431	0.398867	-1.398607
1	8.734292	-0.551473	-1.920471
6	7.430840	0.928255	-1.060056
6	5.328337	-3.110858	0.180972
1	4.591423	-3.316290	0.967031
6	6.342526	-4.240820	0.175098
6	6.026818	-5.466230	0.773385
1	5.072363	-5.581304	1.282332
6	6.925397	-6.535560	0.723005
1	6.667750	-7.480499	1.193528
6	8.155374	-6.385415	0.079134
1	8.858562	-7.212779	0.045011
6	8.480070	-5.162129	-0.517078
1	9.437494	-5.037574	-1.015792
6	7.578937	-4.098569	-0.471435
1	7.831501	-3.144311	-0.925590
6	4.594830	-3.051752	-1.163554
1	5.333876	-3.113068	-1.971371
1	3.953525	-3.933830	-1.249482
6	6.667729	-1.732629	1.807972
1	7.141378	-2.714903	1.886702
6	5.678308	-1.640575	2.970885
6	5.126431	-2.826175	3.482675
1	5.452995	-3.781295	3.079979
6	4.182184	-2.800242	4.512444
1	3.769148	-3.731660	4.890196
6	3.790282	-1.580866	5.068470
1	3.064029	-1.554831	5.876307
6	4.357260	-0.394938	4.591550
1	4.076297	0.558110	5.032312
6	5.290662	-0.424603	3.553663
1	5.716327	0.505727	3.199489
6	7.806830	-0.715833	1.852804
1	8.514428	-0.911722	1.044022
1	7.468556	0.315852	1.765797
1	8.334977	-0.822796	2.805277
6	2.525378	-1.128243	0.544821
1	1.882608	-0.253504	0.590611
1	3.221230	-1.183407	1.377318
6	1.992560	-2.367340	0.062609
1	2.496886	-3.272067	0.385508
6	0.734650	-2.534722	-0.568683
1	0.209022	-1.652832	-0.907242
6	4.223052	-1.143972	-3.493042
1	5.215202	-1.589672	-3.481890
6	3.126479	-2.048729	-3.521760
1	3.365222	-3.111893	-3.550807
6	1.761944	-1.710569	-4.097577
1	1.805699	-1.728966	-5.197714
1	1.073388	-2.507899	-3.807469
6	1.196652	-0.358774	-3.615835
1	1.429525	0.434488	-4.332820
1	0.107346	-0.422356	-3.582652

6	1.691489	0.068035	-2.237650
1	0.934668	0.084646	-1.459797
6	2.806514	0.873821	-2.022098
1	2.816425	1.461214	-1.109695
6	3.753039	1.359069	-3.101273
1	4.645283	1.750086	-2.607389
1	3.289387	2.204787	-3.630586
6	4.170800	0.260249	-4.102568
1	3.492722	0.252237	-4.962362
1	5.160724	0.506430	-4.498882
6	0.336645	-3.784997	-1.225085
6	0.871124	-5.040118	-0.873180
6	-0.626971	-3.732315	-2.250610
6	0.457207	-6.196872	-1.530475
1	1.601547	-5.116434	-0.074047
6	-1.036553	-4.889497	-2.909893
1	-1.058532	-2.774681	-2.515986
6	-0.497635	-6.127752	-2.551846
1	0.877255	-7.156874	-1.244075
1	-1.782672	-4.824824	-3.697000
1	-0.817501	-7.032100	-3.061287
7	-2.527335	-3.998332	0.475409
6	-3.530308	-4.417710	-0.497322
1	-3.343462	-5.458859	-0.776613
1	-3.460363	-3.806065	-1.391307
1	-4.542655	-4.343739	-0.084232
6	-2.172731	-5.004927	1.472704
1	-1.857177	-4.544831	2.407745
1	-1.379541	-5.669547	1.108073
1	-3.059622	-5.605100	1.688340
8	-2.451419	-1.919421	-0.431553
6	0.453527	-1.173928	2.861533
6	0.885357	0.012338	3.418690
1	0.794742	-2.114293	3.277071
6	0.417740	1.201507	2.853854
6	-0.455954	1.160391	1.781903
1	-0.835530	2.067905	1.329475
7	-0.890375	0.000915	1.248314
1	1.574634	0.013224	4.253959
35	0.962326	2.928041	3.596268

C2-P2 *re-si* conf1

Number of imaginary frequencies : 1
The smallest frequency is : -207.6432 cm(-1)
Electronic energy : HF=-7222.6226241
Zero-point correction= 1.754801
(Hartree/Particle)
Thermal correction to Energy= 1.873691
Thermal correction to Enthalpy= 1.874635
Thermal correction to Gibbs Free Energy= 1.591070
Sum of electronic and zero-point Energies= -7220.867823
Sum of electronic and thermal Energies= -7220.748933
Sum of electronic and thermal Enthalpies= -7220.747989
Sum of electronic and thermal Free Energies= -7221.031554

.....

Cartesian Coordinates

.....

26	-3.537559	4.933678	2.365887
15	-2.430775	1.875807	-1.665330
15	-4.905493	0.554700	1.039527
6	-3.429227	3.780081	0.619380
6	-4.030930	3.035572	1.696227
6	-3.078478	2.960040	2.760166
1	-3.236207	2.472982	3.713164
6	-1.906457	3.668378	2.361093
1	-1.023868	3.829111	2.965776
6	-2.124278	4.180751	1.048957
1	-1.433778	4.779267	0.472552
6	-5.226402	6.096288	2.712956
1	-6.222867	5.856508	2.366250
6	-4.645625	5.680501	3.950010
1	-5.121395	5.062442	4.699766
6	-3.309717	6.183300	4.000569
1	-2.594658	6.009075	4.793896
6	-3.064627	6.909198	2.795041
1	-2.133867	7.385865	2.517082
6	-4.248422	6.856829	2.000515
1	-4.368959	7.289547	1.016704
6	-4.054965	3.999464	-0.713703
6	-5.099945	4.924240	-0.851466
1	-5.417968	5.471254	0.026979
6	-5.728715	5.142413	-2.077845
1	-6.542167	5.858646	-2.149143
6	-5.304417	4.439891	-3.203170
1	-5.778730	4.600162	-4.166453
6	-4.276812	3.503235	-3.086551
1	-3.975055	2.948696	-3.967044
6	-3.657427	3.251235	-1.852439
6	-5.345107	2.315403	1.597922
1	-5.895256	2.730304	0.747999
6	-6.227529	2.414701	2.844478
1	-7.176422	1.890035	2.701335
1	-5.735577	1.999638	3.728511
1	-6.446755	3.467535	3.042745
6	-2.391338	1.092887	-3.332333
6	-3.507054	0.326948	-3.714362
1	-4.378408	0.285580	-3.070463
6	-3.523078	-0.356459	-4.928375
1	-4.398868	-0.934860	-5.208336
6	-2.411772	-0.299652	-5.775985
1	-2.415471	-0.840972	-6.717503
6	-1.298533	0.457033	-5.406221
1	-0.432020	0.507170	-6.059319
6	-1.288060	1.155219	-4.194790
1	-0.416130	1.741368	-3.926972
6	-0.821357	2.743792	-1.509722
6	-0.499895	3.859966	-2.297940
1	-1.203277	4.220662	-3.043107
6	0.720276	4.513852	-2.121386
1	0.966645	5.373972	-2.737444
6	1.620643	4.066426	-1.148682
1	2.570886	4.573649	-1.015495
6	1.297192	2.964945	-0.353680
1	1.992309	2.616367	0.403092
6	0.083017	2.299438	-0.534314
1	-0.182698	1.454867	0.094702
6	-6.293799	0.064811	-0.065657
6	-6.960642	-1.165479	0.020071
1	-6.765570	-1.846434	0.839220
6	-7.864569	-1.546509	-0.972241
6	-8.116221	-0.726633	-2.071256
1	-8.809893	-1.035511	-2.843436
6	-7.438380	0.487649	-2.166800
6	-6.533986	0.883633	-1.180464
1	-5.999009	1.821470	-1.298940
6	-5.057403	-0.507350	2.534476
6	-3.860544	-1.028522	3.037527
1	-2.924592	-0.778098	2.550358
6	-3.868006	-1.864717	4.156400
6	-5.061056	-2.191017	4.793940
1	-5.067263	-2.851295	5.652848
6	-6.254839	-1.660486	4.299044
6	-6.260726	-0.824539	3.183111
1	-7.205553	-0.440327	2.816814
29	-2.903091	0.325791	-0.082593
6	-7.552954	-1.950421	5.003010
6	-2.559615	-2.451160	4.607937
6	-8.610223	-2.846017	-0.825761
6	-7.612303	1.370148	-3.373227
9	-6.488334	1.382427	-4.136914
9	-7.853824	2.654152	-3.023934
9	-8.625305	0.968745	-4.167670
9	-7.881874	-3.773729	-0.165950
9	-9.758568	-2.681039	-0.124801
9	-8.955130	-3.371586	-2.022036
9	-7.861216	-0.978438	5.895487
9	-8.587481	-2.024083	4.135013
9	-7.511463	-3.114038	5.686928
9	-2.666246	-3.146959	5.757204

9	-1.620683	-1.492507	4.801179
9	-2.056466	-3.297205	3.671727
6	-3.928713	-2.124015	-1.402345
6	-2.015091	-2.667492	-0.167948
6	-4.113810	-3.435447	-1.798819
1	-4.608779	-1.345105	-1.717953
6	-2.191444	-4.030893	-0.536374
6	-3.229056	-4.423284	-1.359430
1	-1.485060	-4.768909	-0.172994
6	-0.853930	-2.324108	0.603451
6	-0.674063	-1.140536	1.400386
8	-1.299026	-0.049094	1.194626
7	-2.905959	-1.737101	-0.620815
1	-0.261572	-3.184943	0.877316
7	0.251755	-1.153567	2.407642
6	0.606222	0.087336	3.083678
1	0.164225	0.121637	4.087243
1	1.693910	0.147711	3.184867
1	0.242410	0.939027	2.513169
6	0.863160	-2.350847	2.972582
1	0.252655	-3.232761	2.791335
1	1.872361	-2.515991	2.580924
1	0.937626	-2.223208	4.055264
77	3.863156	-1.086179	-1.381528
15	5.660694	-0.580324	-0.078168
8	5.764089	0.699321	0.970763
8	6.994161	-0.288662	-1.032086
7	5.940295	-1.833221	0.996289
6	6.023332	1.989752	0.524749
6	4.982236	2.927151	0.699716
1	4.070876	2.596501	1.185279
6	5.155612	4.221412	0.276660
1	4.372862	4.959210	0.427031
6	6.351918	4.606615	-0.387009
6	6.506081	5.915526	-0.918754
1	5.694320	6.626445	-0.787958
6	7.648784	6.272747	-1.598019
1	7.753676	7.273583	-2.006419
6	8.685425	5.325937	-1.777275
1	9.576029	5.602894	-2.334010
6	8.575038	4.054329	-1.257603
1	9.375763	3.340798	-1.411988
6	7.416561	3.654500	-0.534672
6	7.266996	2.330411	0.013692
6	8.389006	1.349658	0.034046
6	9.651965	1.646237	0.660397
6	9.883795	2.841636	1.397450
1	9.083810	3.564312	1.503616
6	11.102911	3.086672	1.991477
1	11.250782	4.003801	2.554477
6	12.161850	2.154315	1.881543
1	13.119209	2.364828	2.349166
6	11.966485	0.976865	1.196084
1	12.763594	0.241918	1.119630
6	10.716413	0.684867	0.585522
6	10.498919	-0.555040	-0.074825
1	11.315085	-1.269218	-0.137580
6	9.265665	-0.860971	-0.594493
1	9.061650	-1.814821	-1.069605
6	8.221940	0.085857	-0.507502
6	5.148494	-3.050361	0.667266
1	4.274257	-3.076900	1.332119
6	5.952390	-4.320737	0.883090
6	5.363304	-5.428237	1.503569
1	4.345521	-5.351860	1.879360
6	6.073078	-6.623823	1.649178
1	5.603174	-7.475081	2.134108
6	7.385453	-6.719331	1.182243
1	7.941236	-7.645164	1.300535
6	7.983683	-5.614065	0.567314
1	9.006904	-5.679937	0.207361
6	7.271194	-4.424888	0.416038
1	7.737621	-3.560843	-0.049895
6	4.668892	-2.983773	-0.788970
1	5.514834	-3.228570	-1.441948
1	3.919481	-3.764315	-0.945969
6	6.466387	-1.803597	2.400550
1	6.834796	-2.821696	2.550373
6	5.354566	-1.598058	3.427242
6	4.813040	-2.718634	4.074407
1	5.182605	-3.708342	3.818319
6	3.822834	-2.578556	5.050816
1	3.419601	-3.459926	5.541945
6	3.360748	-1.308146	5.398238
1	2.595761	-1.192598	6.160886
6	3.890203	-0.183843	4.757231
1	3.540262	0.809085	5.026517
6	4.875696	-0.326617	3.778253
1	5.280152	0.553372	3.293144
6	7.677613	-0.898516	2.632618
1	8.480922	-1.151682	1.938827
1	7.453995	0.161838	2.531777
1	8.039494	-1.074507	3.650323
6	2.631299	-0.764792	0.388900
1	2.128352	0.199897	0.350129
1	3.124181	-0.949664	1.340076
6	1.997034	-1.875979	-0.260801
1	2.272389	-2.873770	0.060821
6	0.841397	-1.762637	-1.071611
1	0.438422	-0.765154	-1.216620
6	5.101135	-1.217233	-3.236439
1	5.980052	-1.803700	-2.984296
6	3.900060	-1.932990	-3.457096
1	3.942798	-3.018770	-3.376505
6	2.756579	-1.417307	-4.312387
1	3.025622	-1.507390	-5.376257
1	1.898401	-2.075686	-4.160284
6	2.338351	0.037730	-4.001485
1	2.829440	0.731607	-4.692108
1	1.266187	0.133308	-4.185037
6	2.613605	0.498739	-2.572049
1	1.736100	0.712050	-1.972295
6	3.790272	1.115759	-2.160972
1	3.725881	1.760556	-1.289438
6	5.003718	1.352505	-3.039129
1	5.838780	1.631439	-2.392722
1	4.808522	2.219146	-3.688235
6	5.411623	0.130254	-3.891019
1	4.924819	0.172242	-4.870717
1	6.487289	0.183527	-4.083905
6	0.393054	-2.748970	-2.047445
6	0.905429	-4.060459	-2.105855
6	-0.580355	-2.365351	-2.990852
6	0.466008	-4.948210	-3.084969
1	1.657338	-4.383180	-1.392787
6	-1.017984	-3.255759	-3.969447
1	-0.986841	-1.359952	-2.955231
6	-0.494723	-4.550225	-4.022320
1	0.874943	-5.954068	-3.120554
1	-1.764446	-2.933662	-4.688414
1	-0.831715	-5.245333	-4.785899
1	-3.345944	-5.460889	-1.652616
35	-5.605669	-3.870390	-2.983613

C2-P2 *re-re* conf1

Number of imaginary frequencies : 1
The smallest frequency is : -153.7490 cm(-1)
Electronic energy : HF=-7222.6206504
Zero-point correction= 1.754801
(Hartree/Particle)
Thermal correction to Energy= 1.873746
Thermal correction to Enthalpy= 1.874690
Thermal correction to Gibbs Free Energy= 1.591401
Sum of electronic and zero-point Energies= -7220.865850
Sum of electronic and thermal Energies= -7220.746904
Sum of electronic and thermal Enthalpies= -7220.745960
Sum of electronic and thermal Free Energies= -7221.029250

.....

Cartesian Coordinates

.....			
26	-3.848815	4.474038	3.163571
15	-1.178196	2.281163	-0.762619
15	-4.500735	0.586678	0.479637
6	-3.024899	3.723646	1.383359
6	-3.993749	2.811162	1.934884
6	-3.547074	2.432492	3.239977
1	-4.065125	1.762936	3.913485
6	-2.327904	3.122425	3.509484
1	-1.763928	3.081824	4.431821
6	-2.013816	3.927019	2.375719
1	-1.163357	4.585570	2.281329
6	-5.547678	5.667846	3.062478
1	-6.305508	5.590952	2.294592
6	-5.522980	4.940855	4.291703
1	-6.255351	4.213774	4.615529
6	-4.335308	5.306043	4.996047
1	-4.009366	4.900646	5.944925
6	-3.625250	6.257669	4.202055
1	-2.669105	6.702386	4.444690
6	-4.374341	6.482383	3.008691
1	-4.082891	7.128999	2.192228
6	-3.093660	4.259107	-0.006428
6	-4.022763	5.264815	-0.310069
1	-4.632675	5.654343	0.494407
6	-4.183964	5.753562	-1.606999
1	-4.919114	6.527997	-1.805896
6	-3.399995	5.239397	-2.635937
1	-3.512157	5.602520	-3.652811
6	-2.472360	4.233875	-2.360348
1	-1.882781	3.835751	-3.176872
6	-2.311541	3.720787	-1.063363
6	-5.144042	2.234635	1.164052
1	-5.296655	2.843947	0.267845
6	-6.465569	2.166542	1.932385
1	-7.256091	1.716614	1.324572
1	-6.372459	1.589336	2.855956
1	-6.774958	3.180889	2.199178
6	-0.393806	2.041237	-2.411425
6	-1.067586	1.203547	-3.315764
1	-1.980172	0.709364	-3.000198
6	-0.596199	1.033860	-4.617521
1	-1.136267	0.393218	-5.308890
6	0.568838	1.689520	-5.027015
1	0.942708	1.555005	-6.037694
6	1.257600	2.507392	-4.128354
1	2.172798	3.006321	-4.434356
6	0.779130	2.685885	-2.828666
1	1.326732	3.322496	-2.144992
6	0.125625	3.020655	0.301035
6	0.593189	2.270094	1.388423
1	0.219855	1.263219	1.539828
6	1.487399	2.836209	2.298789
1	1.831309	2.247395	3.141354
6	1.927402	4.150313	2.127637
1	2.621316	4.591014	2.837972
6	1.472402	4.901078	1.038012
1	1.812584	5.923383	0.900178
6	0.571297	4.342086	0.130308
1	0.190964	4.944910	-0.689166
6	-5.435537	0.398634	-1.092956
6	-6.286910	-0.660847	-1.430276
1	-6.507661	-1.449004	-0.722168
6	-6.846374	-0.729863	-2.707556
6	-6.547295	0.223174	-3.680227
1	-6.969846	0.148552	-4.674646
6	-5.669387	1.255628	-3.355214
6	-5.123109	1.350992	-2.075786
1	-4.428766	2.157069	-1.853612
6	-5.123842	-0.668699	1.669124
6	-4.155195	-1.205260	2.527467
1	-3.124080	-0.891268	2.423723
6	-4.512586	-2.123313	3.515007
6	-5.836875	-2.533597	3.658500
1	-6.114379	-3.252783	4.419869
6	-6.803057	-1.994975	2.808349
6	-6.459847	-1.060188	1.829654
1	-7.241192	-0.641463	1.206850
29	-2.216633	0.413509	0.037266
6	-8.252356	-2.363175	2.977041
6	-3.437891	-2.713807	4.385625
6	-7.829741	-1.824940	-3.022557
6	-5.253989	2.275056	-4.380508
9	-3.903318	2.292336	-4.532239
9	-5.614490	3.528138	-4.017635
9	-5.788076	2.037435	-5.595171
9	-7.806155	-2.171272	-4.328782
9	-7.596066	-2.941334	-2.297754
9	-9.099940	-1.439115	-2.745267
9	-8.874275	-2.494767	1.782384
9	-8.411508	-3.523133	3.648435
9	-8.929436	-1.410381	3.663059
9	-3.919686	-3.145366	5.570564
9	-2.453997	-1.821131	4.646779
9	-2.842248	-3.782257	3.793898
6	-3.022076	-1.777692	-1.904706
6	-2.167523	-2.715210	0.063567
6	-3.602389	-2.973499	-2.286588
1	-3.122605	-0.893822	-2.522858
6	-2.824287	-3.936930	-0.260382
6	-3.536480	-4.078617	-1.434278
1	-2.729286	-4.779147	0.416711
6	-1.270084	-2.718815	1.177994
6	-0.781542	-1.577089	1.893775
8	-1.078883	-0.377610	1.590708
7	-2.330323	-1.630305	-0.759229
1	-1.212009	-3.671856	1.683712
7	0.061431	-1.764290	2.958049
6	0.414954	-0.627611	3.802938
1	-0.248955	0.209716	3.597411
1	0.315969	-0.909920	4.855133
1	1.449552	-0.315441	3.628521
6	0.448599	-3.070399	3.475583
1	0.628499	-3.786038	2.672937
1	1.379684	-2.958743	4.036294
1	-0.317685	-3.481829	4.144105
77	3.324811	-1.621256	-1.294941
15	4.944766	-0.732630	0.043854
8	4.932245	0.801502	0.679756
8	6.379665	-0.682495	-0.807385
7	5.080214	-1.627383	1.451612
6	5.100838	1.896575	-0.167456
6	3.964235	2.704101	-0.389256
1	3.040795	2.450732	0.116040
6	4.056707	3.784010	-1.231606
1	3.197319	4.427611	-1.389014
6	5.263702	4.053917	-1.929924
6	5.336925	5.103715	-2.885262
1	4.455271	5.718571	-3.046830
6	6.490004	5.327817	-3.602766
1	6.533677	6.128024	-4.335789
6	7.618439	4.499258	-3.394996
1	8.518939	4.660584	-3.980560
6	7.585904	3.485363	-2.461972
1	8.457290	2.856171	-2.326920
6	6.419077	3.237573	-1.685893
6	6.344408	2.175751	-0.713059
6	7.542586	1.375698	-0.335797
6	8.743531	1.995997	0.164634
6	8.814779	3.380647	0.485518
1	7.935058	4.000756	0.360325
6	9.977994	3.940962	0.967788
1	10.002459	4.998912	1.213003
6	11.138276	3.152282	1.152900
1	12.049693	3.609327	1.526916
6	11.100024	1.805214	0.872124
1	11.977294	1.182364	1.026578
6	9.911774	1.192526	0.389816
6	9.856604	-0.206691	0.146074
1	10.751065	-0.804453	0.297176

6	8.680610	-0.800107	-0.237672
1	8.601088	-1.871379	-0.389816
6	7.528643	-0.006530	-0.436996
6	4.212014	-2.840196	1.444922
1	3.276873	-2.596094	1.966660
6	4.851920	-4.024925	2.148608
6	4.095539	-4.801663	3.033718
1	3.071960	-4.511962	3.258111
6	4.644722	-5.940405	3.630441
1	4.045129	-6.533053	4.315980
6	5.962397	-6.309191	3.352890
1	6.393802	-7.189344	3.821095
6	6.726421	-5.535923	2.471974
1	7.753905	-5.814785	2.254706
6	6.173321	-4.405679	1.870770
1	6.767864	-3.798736	1.192831
6	3.910916	-3.232060	-0.005204
1	4.821703	-3.673642	-0.427915
1	3.159548	-4.022976	-0.015008
6	5.650712	-1.249653	2.781851
1	5.949852	-2.208256	3.210562
6	4.639131	-0.661463	3.766330
6	4.098088	-1.498204	4.754998
1	4.330772	-2.559683	4.735497
6	3.302029	-0.982936	5.781079
1	2.902687	-1.649006	6.541054
6	3.038774	0.386632	5.837928
1	2.436971	0.796838	6.643903
6	3.554812	1.226927	4.847461
1	3.362003	2.295375	4.890236
6	4.337319	0.707763	3.812668
1	4.736629	1.375023	3.057162
6	6.934130	-0.420856	2.715089
1	7.699123	-0.947687	2.142923
1	6.788751	0.565660	2.276511
1	7.306909	-0.286089	3.734718
6	1.821838	-0.703978	-0.028123
1	1.635621	0.332736	-0.295925
1	1.996199	-0.841426	1.037346
6	1.037369	-1.703501	-0.709668
1	0.457764	-1.410292	-1.575978
6	0.824305	-2.989951	-0.189307
1	1.320596	-3.219461	0.745023
6	4.850463	-2.360752	-2.784668
1	5.639243	-2.831294	-2.204316
6	3.665032	-3.103617	-2.959079
1	3.634376	-4.099957	-2.518856
6	2.672642	-2.900151	-4.089186
1	3.057071	-3.370951	-5.007206
1	1.763747	-3.446973	-3.826480
6	2.312991	-1.424482	-4.364393
1	2.961366	-1.011535	-5.144122
1	1.295404	-1.374193	-4.763490
6	2.385797	-0.517547	-3.139691
1	1.437332	-0.119822	-2.796214
6	3.514431	0.199931	-2.769956
1	3.352193	1.095514	-2.180559
6	4.853958	0.129482	-3.472526
1	5.589780	0.629686	-2.843537
1	4.791951	0.712250	-4.403690
6	5.339124	-1.305301	-3.775909
1	5.035379	-1.603521	-4.784789
1	6.433030	-1.309260	-3.773348
6	0.353554	-4.139609	-0.950390
6	-0.199482	-4.025599	-2.240705
6	0.458892	-5.422511	-0.377161
6	-0.612432	-5.157345	-2.938996
1	-0.318525	-3.047913	-2.693548
6	0.043634	-6.554039	-1.076074
1	0.871623	-5.522964	0.623680
6	-0.490027	-6.425734	-2.362749
1	-1.039111	-5.048856	-3.931915
1	0.137091	-7.535417	-0.620051
1	-0.813350	-7.306753	-2.909456
1	-4.006063	-5.021744	-1.691069
35	-4.469991	-3.113521	-4.032577

C2-P2 *si-re* conf1

Number of imaginary frequencies : 1
The smallest frequency is : -68.1152 cm(-1)
Electronic energy : HF=-7222.6318937
Zero-point correction= 1.754510
(Hartree/Particle)
Thermal correction to Energy= 1.873363
Thermal correction to Enthalpy= 1.874307
Thermal correction to Gibbs Free Energy= 1.591959
Sum of electronic and zero-point Energies= -7220.877384
Sum of electronic and thermal Energies= -7220.758531
Sum of electronic and thermal Enthalpies= -7220.757587
Sum of electronic and thermal Free Energies= -7221.039934

Cartesian Coordinates

26	4.418781	-3.967516	3.287034
15	1.345940	-2.104493	-0.575991
15	4.499202	-0.254366	0.279287
6	3.472727	-3.243735	1.557490
6	4.283628	-2.221959	2.175827
6	3.794937	-2.019844	3.502876
1	4.199355	-1.326740	4.227183
6	2.706899	-2.919562	3.720973
1	2.150878	-3.029909	4.641044
6	2.510178	-3.672610	2.526699
1	1.777261	-4.451744	2.378378
6	6.312883	-4.812526	3.147372
1	7.061892	-4.531699	2.418971
6	6.127850	-4.214662	4.431453
1	6.704607	-3.396176	4.841416
6	5.017383	-4.855476	5.060638
1	4.602786	-4.603468	6.027871
6	4.514442	-5.847925	4.165137
1	3.654572	-6.482088	4.336296
6	5.315310	-5.823449	2.984809
1	5.168102	-6.440757	2.109241
6	3.623348	-3.699034	0.145642
6	4.750051	-4.462437	-0.198902
1	5.452121	-4.714621	0.584907
6	4.992324	-4.878896	-1.506599
1	5.890254	-5.441924	-1.740604
6	4.080835	-4.550345	-2.506199
1	4.248951	-4.864034	-3.531496
6	2.957298	-3.786612	-2.191249
1	2.272691	-3.528540	-2.989427
6	2.715530	-3.330322	-0.883805
6	5.369427	-1.455682	1.468028
1	5.893169	-2.161949	0.822150
6	6.396073	-0.809492	2.402503
1	7.185170	-0.310891	1.833055
1	5.943192	-0.067982	3.066402
1	6.854376	-1.583819	3.025889
6	0.561395	-2.000206	-2.239975
6	1.113160	-1.078150	-3.146919
1	1.866005	-0.376916	-2.803853
6	0.705139	-1.072152	-4.482226
1	1.157886	-0.375823	-5.179042
6	-0.287952	-1.955251	-4.915305
1	-0.610979	-1.944120	-5.952146
6	-0.876433	-2.838878	-4.007965
1	-1.665217	-3.511795	-4.332186
6	-0.447184	-2.869571	-2.679772
1	-0.894202	-3.578943	-1.994031
6	0.138044	-3.018860	0.464544
6	-0.078478	-4.399032	0.319065
1	0.466006	-4.956762	-0.437383
6	-0.973130	-5.064219	1.158823
1	-1.135458	-6.131368	1.037740
6	-1.653849	-4.359003	2.155901
1	-2.346492	-4.877579	2.812249
6	-1.443782	-2.986477	2.307753

1	-1.975312	-2.441528	3.080317
6	-0.553015	-2.316772	1.464619
1	-0.384221	-1.251267	1.585545
6	5.172531	-0.606971	-1.398930
6	4.577280	0.111799	-2.446567
1	3.810150	0.844614	-2.214141
6	4.949751	-0.126253	-3.769431
6	5.882260	-1.113351	-4.081387
1	6.151524	-1.315952	-5.111969
6	6.454350	-1.844330	-3.039718
6	6.125606	-1.584282	-1.709147
1	6.610315	-2.165928	-0.936776
6	5.136008	1.433273	0.649911
6	4.622990	2.058211	1.798895
1	3.949544	1.520562	2.455358
6	4.948619	3.380391	2.085880
6	5.767353	4.117808	1.228523
1	6.002437	5.153522	1.444355
6	6.269225	3.500052	0.086782
6	5.967805	2.166254	-0.202332
1	6.376930	1.716453	-1.099421
29	2.135023	-0.147348	0.195349
6	7.067165	4.301904	-0.902577
6	4.324814	4.072632	3.265137
6	4.357153	0.732136	-4.851081
6	7.407042	-2.954921	-3.387911
9	6.787602	-3.934660	-4.093363
9	7.948594	-3.537193	-2.295656
9	8.427630	-2.515828	-4.160220
9	3.028584	0.951692	-4.651756
9	4.934699	1.958339	-4.887026
9	4.490601	0.190207	-6.077438
9	6.263556	4.822544	-1.871078
9	7.703307	5.343847	-0.326937
9	7.995430	3.553544	-1.537111
9	5.193275	4.906514	3.879205
9	3.868907	3.202998	4.191955
9	3.265289	4.835928	2.883629
6	2.121940	2.779617	-0.546991
6	1.424998	3.138601	0.653835
6	1.201471	2.316626	1.788570
1	1.290909	4.193318	0.844249
77	-3.275841	1.440895	-1.593606
15	-4.791212	0.444226	-0.228461
8	-4.587711	-1.062127	0.433044
8	-6.218559	0.217334	-1.054598
7	-5.022124	1.361968	1.146053
6	-4.774125	-2.217913	-0.323971
6	-3.619422	-2.990132	-0.578489
1	-2.674349	-2.659468	-0.166047
6	-3.720554	-4.134008	-1.330011
1	-2.844040	-4.747802	-1.513354
6	-4.963531	-4.513531	-1.902925
6	-5.059395	-5.639854	-2.764312
1	-4.162852	-6.224765	-2.953274
6	-6.253834	-5.973619	-3.361380
1	-6.314948	-6.831601	-4.024410
6	-7.403747	-5.184056	-3.121670
1	-8.339561	-5.434474	-3.613025
6	-7.348424	-4.096913	-2.276430
1	-8.238450	-3.500989	-2.113662
6	-6.135990	-3.732614	-1.626195
6	-6.040895	-2.595126	-0.745702
6	-7.245961	-1.828192	-0.322607
6	-8.361151	-2.455494	0.338690
6	-8.346235	-3.819554	0.744539
1	-7.461450	-4.417818	0.563170
6	-9.431983	-4.386390	1.375928
1	-9.391715	-5.428107	1.681031
6	-10.595688	-3.624550	1.637809
1	-11.446217	-4.087300	2.129648
6	-10.635918	-2.295376	1.283103
1	-11.514270	-1.691860	1.496661
6	-9.527609	-1.675237	0.644417
6	-9.549342	-0.289734	0.328012
1	-10.439967	0.289364	0.554724
6	-8.447807	0.316175	-0.223261
1	-8.422725	1.379302	-0.437747
6	-7.304597	-0.458152	-0.517899
6	-4.307367	2.672629	1.078443
1	-3.346309	2.558167	1.595131
6	-5.079514	3.791440	1.756262
6	-4.426869	4.642347	2.655113
1	-3.386687	4.452219	2.908666
6	-5.103826	5.718372	3.235868
1	-4.584399	6.370534	3.932659
6	-6.447403	5.946317	2.931104
1	-6.977722	6.777314	3.387533
6	-7.109508	5.095110	2.039757
1	-8.156775	5.263135	1.803577
6	-6.428715	4.028415	1.453529
1	-6.945468	3.360772	0.768697
6	-4.054637	3.039405	-0.383470
1	-5.005084	3.359625	-0.825623
1	-3.394804	3.907268	-0.422824
6	-5.495280	0.999169	2.517517
1	-6.155302	1.821509	2.806719
6	-4.334529	0.989196	3.501884
6	-4.402813	1.776589	4.655766
1	-5.267649	2.415341	4.814910
6	-3.368893	1.754171	5.594901
1	-3.434827	2.368884	6.488434
6	-2.250011	0.950139	5.377917
1	-1.442888	0.932295	6.102073
6	-2.169570	0.168412	4.220521
1	-1.293440	-0.446904	4.044583
6	-3.207172	0.184466	3.288505
1	-3.149049	-0.428088	2.394176
6	-6.327428	-0.278511	2.663395
1	-7.211318	-0.257439	2.027576
1	-5.755538	-1.181969	2.456323
1	-6.667033	-0.321334	3.702826
6	-1.673501	0.729173	-0.303906
1	-1.382740	-0.298374	-0.512578
1	-1.852870	0.910182	0.754814
6	-0.981065	1.757161	-1.047879
1	-0.378167	1.482467	-1.903166
6	-0.960281	3.083626	-0.622425
1	-1.425051	3.294534	0.336233
6	-4.851767	1.956470	-3.139691
1	-5.683319	2.389772	-2.591196
6	-3.729848	2.784653	-3.336558
1	-3.791117	3.800179	-2.946569
6	-2.686995	2.606277	-4.424955
1	-3.064218	3.026681	-5.369746
1	-1.821843	3.213350	-4.145850
6	-2.228248	1.148258	-4.638083
1	-2.844865	0.658089	-5.398078
1	-1.208070	1.150982	-5.033950
6	-2.240312	0.300956	-3.371422
1	-1.269598	0.009492	-2.992585
6	-3.308775	-0.479719	-2.961883
1	-3.078787	-1.316908	-2.312739
6	-4.642030	-0.564897	-3.671138
1	-5.340570	-1.087290	-3.017616
1	-4.519501	-1.194329	-4.564790
6	-5.239936	0.804173	-4.064657
1	-4.953288	1.064155	-5.088712
1	-6.330225	0.718228	-4.065884
6	-0.598397	4.252507	-1.406878
6	0.043722	4.172304	-2.659309
6	-0.931765	5.526802	-0.902930
6	0.332159	5.326776	-3.381275
1	0.331312	3.205486	-3.056771
6	-0.649026	6.680487	-1.630581
1	-1.419700	5.600640	0.065789
6	-0.014637	6.584476	-2.873239
1	0.831754	5.247481	-4.342270
1	-0.919363	7.652807	-1.229287
1	0.210939	7.482034	-3.441650

8	2.144666	1.599978	-1.036539
6	0.775231	2.944499	3.003374
6	0.766473	2.262196	4.197674
1	0.526244	4.000365	2.984276
6	1.142883	0.910417	4.176814
6	1.417044	0.295567	2.973769
1	1.639408	-0.761238	2.921061
7	1.441055	0.963699	1.801133
6	3.296696	3.510836	-2.573943
1	2.772739	2.674554	-3.028014
1	4.368467	3.286493	-2.541395
1	3.150525	4.395372	-3.200612
6	2.975536	5.122915	-0.733873
1	3.086957	5.119367	0.350378
1	2.154699	5.795902	-1.011876
1	3.904052	5.511013	-1.159466
7	2.762666	3.772993	-1.244464
1	0.491303	2.758577	5.121643
35	1.287166	-0.113618	5.841433

C2-P2 *si-si* conf2

Number of imaginary frequencies : 1
The smallest frequency is : -255.0249 cm(-1)
Electronic energy : HF=-7222.6284099
Zero-point correction= 1.754397
(Hartree/Particle)
Thermal correction to Energy= 1.873023
Thermal correction to Enthalpy= 1.873967
Thermal correction to Gibbs Free Energy= 1.592763
Sum of electronic and zero-point Energies= -7220.874013
Sum of electronic and thermal Energies= -7220.755387
Sum of electronic and thermal Enthalpies= -7220.754443
Sum of electronic and thermal Free Energies= -7221.035647

Cartesian Coordinates

26	-4.735526	4.665373	1.791059
15	-2.779367	1.496281	-1.852960
15	-4.720730	-0.025239	0.973444
6	-4.311830	3.285601	0.276525
6	-4.472359	2.629466	1.554048
6	-3.486915	3.159103	2.443532
1	-3.358205	2.884261	3.481404
6	-2.740405	4.154872	1.744466
1	-1.953665	4.767635	2.162197
6	-3.248231	4.235351	0.415148
1	-2.909530	4.911371	-0.355130
6	-6.713017	5.103259	2.249197
1	-7.535475	4.405793	2.160640
6	-5.885277	5.281187	3.399995
1	-5.965963	4.738366	4.332357
6	-4.904017	6.271220	3.089588
1	-4.108014	6.603472	3.742961
6	-5.124981	6.706369	1.747414
1	-4.528228	7.428088	1.205344
6	-6.242843	5.987421	1.229001
1	-6.640157	6.077598	0.227411
6	-5.073820	2.936500	-0.957512
6	-6.426326	3.293695	-1.059997
1	-6.869819	3.852934	-0.245983
6	-7.201644	2.932676	-2.161712
1	-8.252417	3.201907	-2.196849
6	-6.625285	2.202715	-3.198624
1	-7.219168	1.901770	-4.055735
6	-5.282261	1.833211	-3.119552
1	-4.850080	1.249785	-3.925041
6	-4.494213	2.178012	-2.010374
6	-5.440781	1.509428	1.827072
1	-6.364961	1.737946	1.293901
6	-5.782674	1.323878	3.308429
1	-6.521497	0.529364	3.443000
1	-4.905246	1.071489	3.910403
1	-6.199325	2.257376	3.699168
6	-2.495996	0.578242	-3.427521
6	-2.670034	-0.815179	-3.410733
1	-2.964176	-1.310709	-2.493184
6	-2.423001	-1.572857	-4.557826
1	-2.561924	-2.648635	-4.530662
6	-1.987294	-0.949870	-5.729031
1	-1.779998	-1.540871	-6.616525
6	-1.814474	0.436749	-5.754383
1	-1.474843	0.927516	-6.662039
6	-2.070288	1.198311	-4.613325
1	-1.918188	2.271451	-4.648716
6	-1.681790	2.957877	-2.032004
6	-2.044603	4.089834	-2.779855
1	-3.025906	4.143487	-3.242056
6	-1.152673	5.154441	-2.921353
1	-1.443243	6.027389	-3.498989
6	0.112075	5.094453	-2.326491
1	0.811369	5.917856	-2.440284
6	0.477247	3.971249	-1.581665
1	1.457157	3.918282	-1.122299
6	-0.420394	2.913401	-1.424697
1	-0.140133	2.049927	-0.831957
6	-5.971124	-0.590150	-0.256777
6	-5.553733	-1.626509	-1.104533
1	-4.561892	-2.045965	-0.974635
6	-6.401191	-2.111789	-2.099807
6	-7.659553	-1.547997	-2.300452
1	-8.307977	-1.907293	-3.091693
6	-8.062892	-0.501393	-1.470966
6	-7.242612	-0.037181	-0.442451
1	-7.604743	0.765705	0.184817
6	-4.702302	-1.400594	2.197640
6	-3.709971	-1.360019	3.190275
1	-3.061790	-0.495164	3.278111
6	-3.522024	-2.446938	4.041308
6	-4.285565	-3.606469	3.900975
1	-4.105550	-4.466124	4.536707
6	-5.258689	-3.650572	2.906048
6	-5.486475	-2.553167	2.074761
1	-6.251910	-2.624563	1.312407
29	-2.608735	0.155127	-0.035102
6	-6.064137	-4.907704	2.727220
6	-2.402696	-2.444343	5.043711
6	-5.953504	-3.292743	-2.915088
6	-9.394006	0.145557	-1.738945
9	-9.430300	0.702638	-2.975386
9	-9.682326	1.125983	-0.854966
9	-10.407037	-0.750338	-1.693726
9	-6.096681	-4.452319	-2.225093
9	-6.647804	-3.424782	-4.062928
9	-4.638879	-3.210841	-3.245950
9	-7.051453	-5.017477	3.644513
9	-6.645932	-4.969422	1.507798
9	-5.289128	-6.013279	2.856471
9	-2.771955	-3.007066	6.214919
9	-1.947789	-1.202758	5.312811
9	-1.339078	-3.165744	4.591268
6	-2.009369	-2.804850	0.520170
6	-0.863612	-2.457614	1.334614
6	-0.587109	-1.161505	1.886983
1	-0.431043	-3.259570	1.915526
77	3.322569	-1.086486	-1.263050
15	5.180741	-0.221194	-0.276149
8	5.130757	0.890244	0.963923
8	6.128459	0.604470	-1.364928
7	6.047339	-1.433883	0.500206
6	4.741712	2.196245	0.704864
6	3.488507	2.600376	1.216391
1	2.907855	1.886198	1.789858
6	3.040148	3.874567	0.972245
1	2.085956	4.205411	1.369188
6	3.795509	4.760745	0.156365
6	3.284723	6.038795	-0.199861
1	2.316988	6.337337	0.194465
6	3.988936	6.871655	-1.040248
1	3.586993	7.843070	-1.312803

6	5.237076	6.453475	-1.560775
1	5.780352	7.103308	-2.240706
6	5.768671	5.228690	-1.218812
1	6.721951	4.923226	-1.633623
6	5.076044	4.346825	-0.343142
6	5.590202	3.050337	0.018394
6	6.972214	2.613912	-0.328902
6	8.128302	3.381795	0.060715
6	8.044062	4.517649	0.914261
1	7.079512	4.819878	1.304138
6	9.170487	5.229288	1.266405
1	9.078365	6.087293	1.926158
6	10.446157	4.849798	0.785302
1	11.323988	5.424105	1.066542
6	10.568758	3.743595	-0.024268
1	11.543515	3.427171	-0.386280
6	9.429233	2.978431	-0.394004
6	9.561412	1.808487	-1.189123
1	10.546593	1.519094	-1.543806
6	8.465405	1.033140	-1.475985
1	8.547038	0.115855	-2.049028
6	7.190066	1.428541	-1.015903
6	5.443179	-2.781188	0.301000
1	4.791015	-2.998342	1.156202
6	6.472510	-3.893633	0.199725
6	6.274210	-5.090809	0.894106
1	5.410989	-5.192606	1.548527
6	7.182564	-6.146133	0.768659
1	7.019315	-7.068528	1.319535
6	8.303110	-6.008564	-0.051823
1	9.018483	-6.821322	-0.141013
6	8.503197	-4.815683	-0.756428
1	9.377369	-4.698884	-1.390861
6	7.589067	-3.771403	-0.638611
1	7.754758	-2.836396	-1.164828
6	4.593058	-2.785249	-0.980933
1	5.270320	-2.851573	-1.840027
1	3.984656	-3.694162	-0.987294
6	6.810086	-1.156700	1.767601
1	7.023418	-0.087767	1.739527
6	8.169315	-1.849982	1.808068
6	9.227120	-1.293359	1.078221
1	9.059692	-0.381573	0.515124
6	10.485575	-1.894168	1.061251
1	11.290126	-1.445032	0.484810
6	10.709626	-3.065644	1.789361
1	11.686576	-3.540892	1.777055
6	9.668898	-3.616782	2.540092
1	9.831973	-4.525851	3.112228
6	8.411694	-3.008795	2.554683
1	7.615255	-3.461519	3.133926
6	5.942712	-1.411640	3.006174
1	5.035929	-0.803817	2.954446
1	5.648667	-2.459589	3.108112
1	6.494729	-1.131815	3.908537
6	2.423892	-0.942271	0.713536
1	1.733221	-0.103765	0.748461
1	3.113803	-0.949706	1.552422
6	1.959118	-2.216212	0.248250
1	2.509451	-3.086056	0.591079
6	0.718412	-2.463313	-0.395676
1	0.157912	-1.616940	-0.767815
6	4.132562	-0.907031	-3.324345
1	5.147583	-1.297966	-3.310764
6	3.087754	-1.867375	-3.343002
1	3.379352	-2.917284	-3.360400
6	1.703481	-1.602724	-3.907970
1	1.738961	-1.624301	-5.008285
1	1.060746	-2.433661	-3.608181
6	1.071785	-0.279427	-3.428077
1	1.253715	0.520325	-4.152656
1	-0.011319	-0.402410	-3.384116
6	1.553657	0.184547	-2.056986
1	0.802214	0.170750	-1.273978
6	2.623611	1.052942	-1.860648
1	2.612674	1.651102	-0.955295
6	3.526156	1.575835	-2.958708
1	4.395580	2.033549	-2.483435
1	3.001121	2.378148	-3.498149
6	4.001859	0.486921	-3.945952
1	3.321991	0.429744	-4.802419
1	4.975598	0.781614	-4.348699
6	0.402899	-3.745088	-1.038908
6	1.009774	-4.961164	-0.667729
6	-0.556184	-3.764833	-2.069909
6	0.668558	-6.149779	-1.310239
1	1.741888	-4.983459	0.133170
6	-0.894512	-4.953758	-2.712918
1	-1.041721	-2.838417	-2.352446
6	-0.284986	-6.152660	-2.334881
1	1.145326	-7.078409	-1.009525
1	-1.639499	-4.944708	-3.503696
1	-0.548365	-7.081673	-2.832138
7	-2.504675	-4.073995	0.599919
6	-3.479229	-4.544784	-0.378568
1	-3.254481	-5.584254	-0.634568
1	-3.416757	-3.947610	-1.282943
1	-4.499417	-4.496580	0.018440
6	-2.122847	-5.051000	1.616548
1	-1.837670	-4.564269	2.548136
1	-1.299424	-5.688620	1.271567
1	-2.987954	-5.682567	1.831190
8	-2.516461	-2.003190	-0.325657
6	0.286472	-1.090641	3.007860
6	0.634528	0.119535	3.573574
1	0.657762	-2.011226	3.441329
6	0.116064	1.278655	2.989075
6	-0.718021	1.183704	1.889292
1	-1.130629	2.067056	1.418394
7	-1.071701	0.000661	1.348813
1	1.285951	0.163052	4.439853
35	0.516986	3.037621	3.743411

C2-P2 *re-si* conf2

Number of imaginary frequencies : 1
The smallest frequency is : -216.8088 cm(-1)
Electronic energy : HF=-7222.6176097
Zero-point correction= 1.754258
(Hartree/Particle)
Thermal correction to Energy= 1.873240
Thermal correction to Enthalpy= 1.874184
Thermal correction to Gibbs Free Energy= 1.589712
Sum of electronic and zero-point Energies= -7220.863352
Sum of electronic and thermal Energies= -7220.744369
Sum of electronic and thermal Enthalpies= -7220.743425
Sum of electronic and thermal Free Energies= -7221.027898

Cartesian Coordinates

26	-3.751073	4.706004	2.839634
15	-2.590871	1.976120	-1.414747
15	-5.010192	0.394924	1.200239
6	-3.620888	3.680124	1.019391
6	-4.188951	2.841943	2.044171
6	-3.226776	2.723733	3.094967
1	-3.363400	2.170661	4.014529
6	-2.081347	3.496316	2.740173
1	-1.199599	3.642823	3.349587
6	-2.325683	4.092038	1.468420
1	-1.657964	4.750164	0.931297
6	-5.469358	5.801223	3.255929
1	-6.458124	5.562305	2.887453
6	-4.884835	5.317391	4.465972
1	-5.348323	4.638281	5.168862
6	-3.561812	5.846961	4.558718
1	-2.847305	5.638679	5.344324
6	-3.328870	6.658415	3.406776
1	-2.408191	7.173955	3.166807
6	-4.506572	6.630737	2.602318

1	-4.632577	7.126218	1.649375
6	-4.264866	3.978616	-0.289369
6	-5.340876	4.875934	-0.351368
1	-5.674287	5.339422	0.568029
6	-5.981356	5.170980	-1.555234
1	-6.818555	5.862848	-1.567468
6	-5.537393	4.576642	-2.734017
1	-6.019379	4.798521	-3.681114
6	-4.481361	3.666050	-2.693064
1	-4.166721	3.193099	-3.615471
6	-3.849524	3.335221	-1.483675
6	-5.483723	2.092680	1.907476
1	-6.059566	2.559394	1.102636
6	-6.343566	2.073070	3.173575
1	-7.289992	1.551775	3.006294
1	-5.829853	1.592549	4.010651
1	-6.568743	3.103056	3.463729
6	-2.563170	1.346159	-3.143306
6	-3.655102	0.556909	-3.546052
1	-4.483885	0.401820	-2.864129
6	-3.699821	-0.001787	-4.821352
1	-4.556534	-0.599669	-5.117885
6	-2.640442	0.205346	-5.710905
1	-2.665818	-0.238256	-6.701857
6	-1.551742	0.986605	-5.320387
1	-0.726921	1.153883	-6.007058
6	-1.513758	1.561270	-4.046016
1	-0.662554	2.170128	-3.763065
6	-0.997666	2.855443	-1.170792
6	-0.676543	4.036867	-1.856945
1	-1.360528	4.438020	-2.599331
6	0.514336	4.708722	-1.574507
1	0.760172	5.620585	-2.111221
6	1.381860	4.217113	-0.592860
1	2.304505	4.744656	-0.372579
6	1.059992	3.047090	0.098072
1	1.721861	2.665496	0.869728
6	-0.120628	2.361939	-0.193696
1	-0.388540	1.466474	0.358343
6	-6.402601	-0.039012	0.075946
6	-7.045743	-1.285096	0.079880
1	-6.828537	-2.020060	0.845048
6	-7.958317	-1.610717	-0.924096
6	-8.236329	-0.721384	-1.960948
1	-8.933056	-0.987920	-2.745966
6	-7.580258	0.508168	-1.978452
6	-6.673676	0.852189	-0.974755
1	-6.160254	1.807386	-1.035321
6	-5.124265	-0.793778	2.599171
6	-3.916950	-1.351470	3.034081
1	-2.988864	-1.053041	2.559096
6	-3.904218	-2.286428	4.071335
6	-5.086535	-2.675735	4.694698
1	-5.076258	-3.409265	5.492204
6	-6.290004	-2.109823	4.268205
6	-6.316214	-1.175389	3.233135
1	-7.267203	-0.765949	2.912543
29	-3.025412	0.278329	0.036066
6	-7.577864	-2.467329	4.960123
6	-2.590167	-2.913776	4.444332
6	-8.684891	-2.927683	-0.857230
6	-7.775141	1.465982	-3.122472
9	-6.654398	1.546948	-3.886887
9	-8.036089	2.719821	-2.688038
9	-8.784788	1.100960	-3.938537
9	-7.938747	-3.886637	-0.265652
9	-9.829363	-2.824230	-0.138282
9	-9.033840	-3.378549	-2.082505
9	-7.901575	-1.552956	5.906290
9	-8.615080	-2.512499	4.092971
9	-7.510148	-3.666286	5.576818
9	-2.651102	-3.607767	5.597933
9	-1.612107	-1.985991	4.578342
9	-2.168245	-3.776665	3.481457
6	-4.049175	-2.089442	-1.454655
6	-2.090797	-2.680569	-0.317761
6	-4.210990	-3.368778	-1.953269
1	-4.759072	-1.308506	-1.690380
6	-2.243621	-4.014033	-0.790050
6	-3.292751	-4.365737	-1.616481
1	-1.510822	-4.760360	-0.504530
6	-0.912549	-2.370385	0.442902
6	-0.730679	-1.257918	1.337533
8	-1.395580	-0.173633	1.268476
7	-3.014696	-1.739160	-0.670109
1	-0.293217	-3.236036	0.628905
7	0.246219	-1.348552	2.291811
6	0.582328	-0.187670	3.105816
1	0.175924	-0.288549	4.119572
1	1.671280	-0.091788	3.174989
1	0.169301	0.712060	2.654622
6	0.877956	-2.609003	2.678339
1	0.137793	-3.404908	2.780525
1	1.648122	-2.922084	1.965969
1	1.351463	-2.470585	3.652094
77	3.683484	-0.732043	-1.549594
15	5.455104	-0.250026	-0.211656
8	5.522295	0.981458	0.900597
8	6.806198	0.093143	-1.122734
7	5.748516	-1.550620	0.814325
6	5.890401	2.277136	0.555093
6	4.889503	3.263828	0.692393
1	3.915934	2.961726	1.059824
6	5.168888	4.568230	0.371546
1	4.413062	5.338897	0.491685
6	6.442317	4.924797	-0.146738
6	6.714966	6.256182	-0.562612
1	5.933738	7.003414	-0.449661
6	7.932524	6.590886	-1.110021
1	8.129145	7.609851	-1.430121
6	8.925369	5.595737	-1.272480
1	9.875664	5.854203	-1.730744
6	8.698383	4.299537	-0.863007
1	9.469227	3.552797	-1.008746
6	7.461413	3.921029	-0.268829
6	7.189991	2.574029	0.170486
6	8.247205	1.523930	0.160216
6	9.508998	1.687730	0.835259
6	9.769974	2.768234	1.723478
1	8.992299	3.499194	1.911522
6	10.987264	2.888929	2.357869
1	11.158021	3.717933	3.038665
6	12.015004	1.940567	2.138066
1	12.970730	2.052357	2.641541
6	11.792672	0.873757	1.297338
1	12.566347	0.128754	1.130908
6	10.543787	0.710956	0.637674
6	10.295388	-0.416112	-0.191665
1	11.088795	-1.140667	-0.349835
6	9.055240	-0.612969	-0.746329
1	8.830704	-1.483941	-1.351481
6	8.039255	0.343496	-0.535315
6	5.042474	-2.781200	0.366018
1	4.141882	-2.906006	0.979552
6	5.877488	-4.042494	0.495429
6	5.294910	-5.211065	0.996125
1	4.262507	-5.189699	1.339239
6	6.032816	-6.395169	1.082126
1	5.569582	-7.292970	1.482468
6	7.366035	-6.418310	0.669057
1	7.946882	-7.333004	0.747388
6	7.951588	-5.254763	0.157206
1	8.991152	-5.262546	-0.158627
6	7.209347	-4.079828	0.062391
1	7.670501	-3.169804	-0.305597
6	4.609324	-2.613560	-1.103893
1	5.488934	-2.746347	-1.746792
1	3.919997	-3.424826	-1.354332
6	6.097375	-1.380472	2.266505
1	6.470220	-0.360721	2.345387

6	7.246331	-2.276329	2.714887
6	8.556772	-1.839316	2.487061
1	8.716470	-0.875939	2.016677
6	9.651055	-2.623532	2.852142
1	10.658809	-2.264337	2.661697
6	9.446426	-3.860082	3.469249
1	10.294104	-4.477511	3.753561
6	8.143422	-4.292671	3.729662
1	7.974250	-5.249824	4.215089
6	7.052692	-3.502657	3.362005
1	6.048995	-3.861246	3.560845
6	4.856259	-1.474872	3.163211
1	4.138042	-0.696877	2.890865
1	4.355756	-2.444252	3.096129
1	5.145266	-1.322213	4.207351
6	2.439592	-0.677393	0.229737
1	1.883257	0.254737	0.309045
1	2.943382	-0.948691	1.150702
6	1.851459	-1.739485	-0.537035
1	2.183832	-2.752085	-0.341302
6	0.649194	-1.604807	-1.272609
1	0.195869	-0.618138	-1.299752
6	4.905820	-0.606117	-3.420242
1	5.816126	-1.170797	-3.236525
6	3.740432	-1.358389	-3.696690
1	3.848597	-2.442498	-3.730655
6	2.537736	-0.833601	-4.460667
1	2.751186	-0.841030	-5.540803
1	1.715888	-1.536803	-4.305291
6	2.075934	0.574642	-4.028159
1	2.548069	1.341604	-4.650632
1	1.002617	0.653104	-4.210188
6	2.332979	0.904639	-2.560966
1	1.452844	0.991458	-1.933541
6	3.481543	1.528448	-2.089574
1	3.393951	2.064024	-1.149479
6	4.676555	1.918176	-2.938584
1	5.501547	2.162955	-2.265194
1	4.438677	2.841915	-3.486811
6	5.140999	0.819957	-3.921892
1	4.648580	0.944766	-4.891519
1	6.211525	0.950670	-4.106405
6	0.201837	-2.515282	-2.319449
6	0.762290	-3.794389	-2.512783
6	-0.822913	-2.092018	-3.188639
6	0.319222	-4.611873	-3.548943
1	1.553829	-4.145157	-1.858163
6	-1.264399	-2.912869	-4.224721
1	-1.267904	-1.112295	-3.049182
6	-0.694214	-4.174608	-4.410456
1	0.765121	-5.592651	-3.688127
1	-2.051799	-2.562726	-4.884133
1	-1.035124	-4.814461	-5.219298
1	-3.392658	-5.378833	-1.989913
35	-5.715334	-3.747842	-3.140755

C2-P2 *re-re* conf2

Number of imaginary frequencies : 1
The smallest frequency is : -121.0242 cm(-1)
Electronic energy : HF=-7222.6230214
Zero-point correction= 1.755800
(Hartree/Particle)
Thermal correction to Energy= 1.874307
Thermal correction to Enthalpy= 1.875251
Thermal correction to Gibbs Free Energy= 1.593527
Sum of electronic and zero-point Energies= -7220.867221
Sum of electronic and thermal Energies= -7220.748715
Sum of electronic and thermal Enthalpies= -7220.747770
Sum of electronic and thermal Free Energies= -7221.029495

.....

Cartesian Coordinates

.....

26	-3.531492	3.834999	4.070237
15	-1.204385	2.333391	-0.336032
15	-4.538932	0.592510	0.723575
6	-2.848457	3.413977	2.131598
6	-3.845501	2.462046	2.549815
6	-3.360637	1.807680	3.725074
1	-3.886234	1.044435	4.283171
6	-2.086765	2.361897	4.048883
1	-1.481630	2.105100	4.908151
6	-1.774455	3.356377	3.075980
1	-0.887552	3.972726	3.055945
6	-5.133669	5.140507	4.294799
1	-5.914251	5.287591	3.560340
6	-5.138258	4.164092	5.336999
1	-5.916651	3.436139	5.521696
6	-3.909631	4.280577	6.055909
1	-3.595414	3.655739	6.881622
6	-3.144672	5.327983	5.457496
1	-2.150207	5.637195	5.751199
6	-3.900933	5.860505	4.370650
1	-3.578813	6.646511	3.701138
6	-2.954776	4.218717	0.881744
6	-3.817665	5.322976	0.839076
1	-4.346532	5.593019	1.743552
6	-4.013950	6.059095	-0.330145
1	-4.696396	6.904149	-0.328977
6	-3.335414	5.698588	-1.491018
1	-3.481139	6.252966	-2.412784
6	-2.472715	4.601703	-1.474009
1	-1.965313	4.326066	-2.390167
6	-2.278062	3.844194	-0.308653
6	-5.059794	2.107437	1.742246
1	-5.203585	2.885813	0.986926
6	-6.351803	1.963344	2.548366
1	-7.196778	1.701110	1.904877
1	-6.264777	1.202089	3.328317
1	-6.575832	2.917783	3.033552
6	-0.605187	2.303140	-2.081003
6	-1.386018	1.590088	-3.005213
1	-2.272631	1.071333	-2.659142
6	-1.051976	1.569285	-4.359449
1	-1.674595	1.021487	-5.061168
6	0.082191	2.252954	-4.806667
1	0.350730	2.233502	-5.858777
6	0.870128	2.959603	-3.894762
1	1.756657	3.487855	-4.233791
6	0.526870	2.990579	-2.541603
1	1.138063	3.558697	-1.851959
6	0.239457	2.893392	0.661662
6	0.685026	4.225929	0.631041
1	0.195802	4.949665	-0.013768
6	1.742281	4.633665	1.445297
1	2.082555	5.664539	1.411533
6	2.361547	3.716926	2.300653
1	3.184635	4.034926	2.934112
6	1.916770	2.393943	2.342300
1	2.386671	1.685112	3.016202
6	0.856838	1.981739	1.530517
1	0.475579	0.968476	1.592968
6	-5.513666	0.768644	-0.832464
6	-6.404137	-0.181231	-1.353578
1	-6.629864	-1.090978	-0.813107
6	-7.003666	0.024557	-2.596237
6	-6.703723	1.149207	-3.365214
1	-7.159471	1.290869	-4.337787
6	-5.791006	2.074261	-2.864916
6	-5.206379	1.896059	-1.610378
1	-4.491357	2.631601	-1.254308
6	-5.237355	-0.846606	1.634163
6	-4.308727	-1.642738	2.317280
1	-3.257596	-1.386138	2.277964
6	-4.731340	-2.749286	3.054128
6	-6.081189	-3.092212	3.114813
1	-6.407036	-3.958480	3.678356
6	-7.007874	-2.289976	2.449923
6	-6.598048	-1.168927	1.725869
1	-7.348350	-0.552485	1.245676

29	-2.244787	0.393514	0.262345
6	-8.470759	-2.642510	2.455539
6	-3.704757	-3.612675	3.733489
6	-8.034122	-0.946624	-3.107855
6	-5.386769	3.278450	-3.670971
9	-4.044630	3.300098	-3.878062
9	-5.696535	4.432646	-3.035494
9	-5.977311	3.315014	-4.882614
9	-7.911559	-1.155065	-4.439618
9	-7.960667	-2.147468	-2.496628
9	-9.290684	-0.478206	-2.906294
9	-8.844594	-3.202721	1.279392
9	-8.786995	-3.518004	3.432138
9	-9.246728	-1.546404	2.623675
9	-4.211668	-4.267394	4.799269
9	-2.647114	-2.885702	4.170163
9	-3.204795	-4.556725	2.895740
6	-3.205686	-1.527663	-1.867108
6	-2.205759	-2.725324	-0.123677
6	-3.792158	-2.665837	-2.388565
1	-3.364641	-0.565015	-2.335352
6	-2.847115	-3.906713	-0.599066
6	-3.637822	-3.889236	-1.729161
1	-2.688845	-4.838406	-0.066331
6	-1.275955	-2.865293	0.951660
6	-0.804221	-1.831906	1.820954
8	-1.124408	-0.606321	1.713349
7	-2.436952	-1.534497	-0.761305
1	-1.175508	-3.880124	1.304127
7	0.050102	-2.165798	2.857597
6	0.148977	-1.226058	3.974838
1	-0.729309	-1.294560	4.631928
1	1.040713	-1.459052	4.559198
1	0.222208	-0.205120	3.606026
6	0.354158	-3.556379	3.181326
1	0.651562	-4.109343	2.288345
1	1.191659	-3.577505	3.881993
1	-0.497986	-4.071292	3.643495
77	3.072523	-1.482067	-1.762259
15	4.593017	-0.536388	-0.363487
8	4.502152	0.999769	0.242329
8	6.085709	-0.476398	-1.100183
7	4.654660	-1.387404	1.081199
6	4.845274	2.106467	-0.525428
6	3.785910	2.969572	-0.873613
1	2.794503	2.733561	-0.508281
6	4.039569	4.075601	-1.644550
1	3.236204	4.757703	-1.908940
6	5.351045	4.329203	-2.129627
6	5.610642	5.423522	-2.998638
1	4.785727	6.079637	-3.264306
6	6.871656	5.641488	-3.505446
1	7.057620	6.477431	-4.173366
6	7.926892	4.761656	-3.166128
1	8.915711	4.920313	-3.586694
6	7.712510	3.701110	-2.312342
1	8.532002	3.034112	-2.072887
6	6.427784	3.456833	-1.751125
6	6.167418	2.353462	-0.860006
6	7.255938	1.482953	-0.334198
6	8.391157	2.018356	0.373801
6	8.476676	3.382885	0.769780
1	7.659562	4.055471	0.537305
6	9.571448	3.856670	1.459746
1	9.606527	4.900177	1.759344
6	10.646507	2.997111	1.789393
1	11.505319	3.386489	2.328146
6	10.589955	1.667174	1.438501
1	11.399041	0.990254	1.700093
6	9.467514	1.141786	0.741739
6	9.378166	-0.243845	0.441834
1	10.199994	-0.897634	0.718558
6	8.247662	-0.758718	-0.140257
1	8.136842	-1.818987	-0.338912
6	7.192065	0.106991	-0.496913
6	4.014210	-2.721951	0.966406
1	3.021473	-2.664961	1.427028
6	4.800652	-3.818560	1.659715
6	4.146928	-4.726092	2.499890
1	3.081727	-4.611201	2.685892
6	4.854585	-5.764551	3.113160
1	4.336556	-6.457548	3.770637
6	6.225486	-5.903995	2.887547
1	6.779531	-6.704869	3.368982
6	6.883107	-5.004124	2.041237
1	7.951489	-5.101013	1.868851
6	6.174653	-3.971254	1.431252
1	6.689752	-3.251649	0.802408
6	3.835335	-3.078667	-0.516376
1	4.805388	-3.389817	-0.920576
1	3.184986	-3.952822	-0.588457
6	4.764888	-0.740720	2.433597
1	4.836852	0.325708	2.229592
6	6.031192	-1.100313	3.208690
6	7.163389	-0.290813	3.050790
1	7.124545	0.549550	2.364963
6	8.339950	-0.547086	3.757392
1	9.203007	0.096005	3.611079
6	8.399285	-1.621806	4.646368
1	9.312147	-1.826509	5.199242
6	7.272696	-2.429608	4.824113
1	7.306109	-3.269182	5.513109
6	6.098908	-2.166854	4.116501
1	5.241756	-2.813580	4.262570
6	3.482950	-0.948661	3.247645
1	2.610891	-0.627871	2.673601
1	3.330173	-1.989597	3.541560
1	3.537127	-0.351248	4.162354
6	1.536525	-0.659593	-0.465404
1	1.264995	0.357011	-0.735547
1	1.737925	-0.779387	0.596011
6	0.825932	-1.726175	-1.120392
1	0.199617	-1.507489	-1.975864
6	0.769596	-3.011739	-0.564728
1	1.314767	-3.158435	0.358684
6	4.587814	-2.077999	-3.304566
1	5.414749	-2.541833	-2.773581
6	3.430371	-2.870847	-3.480559
1	3.464148	-3.887291	-3.089254
6	2.387237	-2.664396	-4.566415
1	2.744592	-3.098951	-5.512725
1	1.502962	-3.241964	-4.281952
6	1.977873	-1.191168	-4.782645
1	2.605200	-0.728456	-5.550859
1	0.954460	-1.159146	-5.170183
6	2.035127	-0.337858	-3.519244
1	1.076260	-0.002497	-3.137606
6	3.140361	0.406229	-3.124232
1	2.945417	1.258788	-2.483072
6	4.473617	0.441221	-3.841827
1	5.198079	0.919992	-3.180503
1	4.382228	1.088835	-4.726344
6	5.003883	-0.950466	-4.250491
1	4.679375	-1.198846	-5.265901
1	6.096777	-0.911165	-4.282039
6	0.363186	-4.228522	-1.248620
6	-0.274984	-4.226665	-2.504901
6	0.632705	-5.468420	-0.633835
6	-0.608046	-5.424998	-3.132050
1	-0.512988	-3.286786	-2.990956
6	0.292959	-6.665230	-1.259127
1	1.115247	-5.481073	0.340406
6	-0.325687	-6.647292	-2.514108
1	-1.096809	-5.405318	-4.101853
1	0.511619	-7.611107	-0.772140
1	-0.589276	-7.579420	-3.005276
1	-4.104807	-4.796132	-2.097680
35	-4.823869	-2.546664	-4.044691

C2-P2 *si-re* conf2

Number of imaginary frequencies : 1
The smallest frequency is : -148.7219 cm(-1)
Electronic energy : HF=-7222.6391298
Zero-point correction= 1.757111
(Hartree/Particle)
Thermal correction to Energy= 1.874979
Thermal correction to Enthalpy= 1.875924
Thermal correction to Gibbs Free Energy= 1.598885
Sum of electronic and zero-point Energies= -7220.882019
Sum of electronic and thermal Energies= -7220.764150
Sum of electronic and thermal Enthalpies= -7220.763206
Sum of electronic and thermal Free Energies= -7221.040245

Cartesian Coordinates

26	3.653893	-4.360826	3.266689
15	1.382999	-2.053270	-0.847744
15	4.440964	-0.458015	0.640385
6	3.076074	-3.463491	1.464424
6	3.810097	-2.538835	2.296451
6	3.093824	-2.394632	3.524797
1	3.392602	-1.779650	4.362411
6	1.942298	-3.237188	3.474287
1	1.222278	-3.375347	4.268911
6	1.932735	-3.896080	2.210667
1	1.202476	-4.616865	1.874351
6	5.489987	-5.330068	3.367006
1	6.365897	-5.057110	2.793124
6	5.132873	-4.809750	4.648634
1	5.684491	-4.066921	5.209638
6	3.895876	-5.406790	5.038855
1	3.344405	-5.191963	5.944727
6	3.487630	-6.296577	3.999021
1	2.573988	-6.875940	3.979829
6	4.471801	-6.250351	2.967111
1	4.433286	-6.792498	2.032068
6	3.440014	-3.817872	0.062562
6	4.561088	-4.629496	-0.165344
1	5.108779	-4.991673	0.694951
6	4.985116	-4.958247	-1.452268
1	5.872545	-5.566848	-1.593075
6	4.273986	-4.481027	-2.550446
1	4.592472	-4.720826	-3.559817
6	3.159533	-3.666093	-2.350354
1	2.628547	-3.288829	-3.216568
6	2.733106	-3.309425	-1.060830
6	5.038307	-1.781532	1.865854
1	5.661407	-2.462038	1.283003
6	5.878292	-1.243189	3.027833
1	6.779414	-0.743841	2.661611
1	5.323813	-0.527678	3.640986
1	6.179354	-2.075157	3.672036
6	0.864009	-1.690642	-2.582495
6	1.483220	-0.606492	-3.228944
1	2.176354	0.022435	-2.681425
6	1.200541	-0.328202	-4.568118
1	1.697660	0.499900	-5.061540
6	0.275664	-1.107378	-5.267928
1	0.049511	-0.883022	-6.306365
6	-0.363551	-2.170065	-4.625039
1	-1.091756	-2.773791	-5.159086
6	-0.064748	-2.467303	-3.293907
1	-0.553725	-3.311061	-2.820366
6	-0.016291	-3.013086	-0.145487
6	-0.245248	-4.360914	-0.468802
1	0.419578	-4.876030	-1.155950
6	-1.314305	-5.048639	0.106653
1	-1.487117	-6.089698	-0.150652
6	-2.158461	-4.401109	1.014980
1	-2.989071	-4.938582	1.463032
6	-1.932693	-3.063482	1.345060
1	-2.584752	-2.558164	2.048829
6	-0.865901	-2.372628	0.766969
1	-0.684247	-1.336218	1.026933
6	5.348522	-0.750570	-0.935296
6	4.990268	0.084493	-2.003995
1	4.245550	0.857943	-1.843612
6	5.573049	-0.086616	-3.259835
6	6.489670	-1.110910	-3.489036
1	6.926983	-1.252512	-4.470891
6	6.825586	-1.955006	-2.430494
6	6.278027	-1.772016	-1.160854
1	6.572417	-2.448166	-0.370367
6	5.098980	1.163508	1.212392
6	4.422668	1.766076	2.285380
1	3.619229	1.237008	2.783566
6	4.748027	3.057437	2.688805
6	5.730865	3.789013	2.018661
1	5.962504	4.806003	2.314077
6	6.396982	3.192320	0.951640
6	6.098326	1.886074	0.554221
1	6.636994	1.453129	-0.280165
29	2.137728	-0.227137	0.246146
6	7.370728	3.998091	0.138431
6	3.961409	3.727591	3.780360
6	5.231075	0.890267	-4.349352
6	7.765218	-3.099036	-2.698256
9	7.223213	-3.994761	-3.561381
9	8.087761	-3.779352	-1.575768
9	8.920903	-2.677625	-3.261803
9	3.896862	1.146050	-4.397957
9	5.835161	2.088198	-4.148377
9	5.599010	0.458274	-5.571408
9	6.743291	4.614369	-0.902693
9	7.965219	4.969842	0.861174
9	8.343619	3.232274	-0.400909
9	4.755413	4.437840	4.611750
9	3.267038	2.846929	4.531695
9	3.057658	4.608126	3.269484
6	2.379755	2.744893	-0.332962
6	1.531224	3.067185	0.783596
6	1.065175	2.192012	1.808382
1	1.459646	4.110665	1.050290
77	-2.905918	1.854984	-1.750265
15	-4.264534	0.521607	-0.508885
8	-4.048164	-1.105561	-0.291959
8	-5.810395	0.537706	-1.122586
7	-4.240999	1.015847	1.096297
6	-4.414767	-2.026434	-1.266267
6	-3.357500	-2.719432	-1.892901
1	-2.346524	-2.516884	-1.564591
6	-3.634232	-3.628301	-2.881748
1	-2.828907	-4.175026	-3.364093
6	-4.973402	-3.844113	-3.306137
6	-5.266797	-4.721332	-4.385045
1	-4.443796	-5.246508	-4.862928
6	-6.559040	-4.892245	-4.827521
1	-6.771294	-5.560798	-5.656684
6	-7.613202	-4.178846	-4.209163
1	-8.628702	-4.293863	-4.577083
6	-7.364747	-3.333623	-3.149202
1	-8.184601	-2.788708	-2.696837
6	-6.045588	-3.150512	-2.647938
6	-5.750841	-2.269578	-1.544794
6	-6.824445	-1.611743	-0.747555
6	-7.869758	-2.362775	-0.100075
6	-7.864184	-3.784446	-0.030168
1	-7.044228	-4.334613	-0.476493
6	-8.874047	-4.469544	0.609981
1	-8.840346	-5.554244	0.657428
6	-9.950348	-3.775415	1.212560
1	-10.741876	-4.329402	1.708542
6	-9.979880	-2.399544	1.179661
1	-10.790010	-1.851598	1.653640
6	-8.945383	-1.660923	0.542716
6	-8.939296	-0.240737	0.571887
1	-9.758102	0.280349	1.059097
6	-7.885763	0.461790	0.044062
1	-7.832195	1.543728	0.099143

6	-6.834070	-0.233995	-0.588970
6	-3.595405	2.346698	1.256321
1	-2.561062	2.193151	1.583512
6	-4.280180	3.221572	2.288242
6	-3.517678	3.849058	3.279838
1	-2.445902	3.666560	3.322994
6	-4.125130	4.685828	4.220814
1	-3.523864	5.160116	4.991785
6	-5.503747	4.903580	4.173619
1	-5.980174	5.547457	4.907530
6	-6.269691	4.286209	3.178433
1	-7.343769	4.445985	3.142291
6	-5.661301	3.452466	2.242108
1	-6.259182	2.946729	1.489369
6	-3.568991	3.064998	-0.098803
1	-4.583202	3.415170	-0.324100
1	-2.955814	3.963582	-0.006981
6	-4.242269	0.055917	2.254323
1	-4.338198	-0.927631	1.799624
6	-5.435865	0.187614	3.198260
6	-6.562151	-0.609859	2.958613
1	-6.570422	-1.270977	2.097901
6	-7.670736	-0.572113	3.806272
1	-8.530813	-1.199945	3.590954
6	-7.665293	0.265954	4.922688
1	-8.524505	0.300197	5.587121
6	-6.540990	1.054010	5.184643
1	-6.523153	1.708590	6.051783
6	-5.435301	1.010442	4.333943
1	-4.579636	1.637962	4.553705
6	-2.899729	0.071366	2.987868
1	-2.077674	-0.105372	2.290606
1	-2.706079	1.012749	3.504126
1	-2.888724	-0.721797	3.739012
6	-1.251841	0.867068	-0.741771
1	-0.992107	-0.092142	-1.180659
1	-1.365287	0.820291	0.337983
6	-0.601085	2.023977	-1.296140
1	-0.036050	1.907165	-2.211018
6	-0.505486	3.248233	-0.614953
1	-1.006443	3.316014	0.341183
6	-4.578105	2.719336	-2.955338
1	-5.358854	3.012516	-2.258116
6	-3.458717	3.581261	-3.043018
1	-3.474054	4.475720	-2.420944
6	-2.527591	3.684986	-4.239784
1	-2.981874	4.325927	-5.011151
1	-1.624167	4.203876	-3.905775
6	-2.126661	2.326139	-4.854627
1	-2.828852	2.042711	-5.644397
1	-1.151396	2.432068	-5.341476
6	-2.031866	1.187838	-3.844480
1	-1.032472	0.824659	-3.636325
6	-3.067782	0.319862	-3.537987
1	-2.790593	-0.646085	-3.130195
6	-4.474727	0.403866	-4.091325
1	-5.111192	-0.241496	-3.483650
1	-4.481435	-0.017018	-5.107599
6	-5.066197	1.830486	-4.100966
1	-4.849557	2.325629	-5.052648
1	-6.155811	1.753839	-4.039220
6	-0.134202	4.526861	-1.213322
6	0.533717	4.632663	-2.449327
6	-0.453695	5.710924	-0.519107
6	0.865298	5.881567	-2.969599
1	0.805047	3.738690	-2.999573
6	-0.129134	6.959486	-1.045082
1	-0.960154	5.640274	0.440445
6	0.534882	7.049262	-2.272620
1	1.384143	5.945983	-3.921714
1	-0.389352	7.861053	-0.498054
1	0.794158	8.020596	-2.683491
8	2.412353	1.597754	-0.884598
6	0.414283	2.778366	2.936902
6	0.020584	2.016207	4.015713
1	0.270264	3.853469	2.956399
6	0.262151	0.637412	3.959083
6	0.831023	0.086946	2.827649
1	0.994359	-0.979294	2.743927
7	1.221125	0.830724	1.771828
6	3.774136	3.568279	-2.175722
1	3.305195	2.749858	-2.715282
1	4.842999	3.357988	-2.062262
1	3.666992	4.484837	-2.764518
6	3.344534	5.055497	-0.261934
1	3.300421	4.985072	0.824045
1	2.615607	5.797619	-0.609695
1	4.347756	5.398517	-0.527548
7	3.126084	3.753428	-0.884087
1	-0.450669	2.473582	4.878830
35	-0.211994	-0.518593	5.463298

P2-C1 *re-si* conf1

Number of imaginary frequencies : 1
The smallest frequency is : -255.8618 cm(-1)
Electronic energy : HF=-7222.6359279
Zero-point correction= 1.754830
(Hartree/Particle)
Thermal correction to Energy= 1.873567
Thermal correction to Enthalpy= 1.874511
Thermal correction to Gibbs Free Energy= 1.591721
Sum of electronic and zero-point Energies= -7220.881098
Sum of electronic and thermal Energies= -7220.762361
Sum of electronic and thermal Enthalpies= -7220.761417
Sum of electronic and thermal Free Energies= -7221.044207

Cartesian Coordinates

26	-8.013585	0.343897	-1.088066
15	-2.922532	1.119765	-2.182064
15	-3.990229	0.789981	1.429510
6	-6.009727	0.919138	-1.309794
6	-6.234266	0.288003	-0.031298
6	-6.714893	-1.035525	-0.275536
1	-6.991852	-1.757614	0.480056
6	-6.821167	-1.218896	-1.687297
1	-7.193866	-2.102310	-2.185261
6	-6.384704	-0.020045	-2.323710
1	-6.365875	0.166428	-3.387146
6	-9.369801	1.645924	-0.202897
1	-9.121733	2.363341	0.567879
6	-9.768064	0.290874	0.011963
1	-9.868212	-0.198103	0.971781
6	-9.968867	-0.318377	-1.263998
1	-10.240037	-1.351161	-1.439402
6	-9.694377	0.659312	-2.268013
1	-9.724054	0.498671	-3.337631
6	-9.326245	1.872438	-1.613604
1	-9.033500	2.790205	-2.104997
6	-5.448299	2.287370	-1.493808
6	-6.228200	3.396000	-1.127490
1	-7.220695	3.213810	-0.736441
6	-5.757374	4.702772	-1.243501
1	-6.378555	5.534264	-0.925750
6	-4.484610	4.926807	-1.762333
1	-4.101643	5.936520	-1.869047
6	-3.685297	3.841621	-2.119483
1	-2.690234	4.036899	-2.499706
6	-4.129307	2.516357	-1.968797
6	-5.879962	0.906477	1.293815
1	-6.095716	1.973722	1.226218
6	-6.650607	0.334890	2.486675
1	-6.373280	0.846161	3.412751
1	-6.465570	-0.733535	2.626049
1	-7.723876	0.471584	2.321711
6	-1.372942	2.004486	-2.636755
6	-0.596619	2.521408	-1.588057
1	-0.871447	2.306826	-0.562153
6	0.516855	3.315024	-1.857986

1	1.097015	3.719966	-1.039079
6	0.894043	3.567458	-3.179151
1	1.768850	4.177171	-3.386267
6	0.150596	3.022693	-4.228866
1	0.444707	3.205400	-5.258558
6	-0.984828	2.253225	-3.961556
1	-1.567529	1.858243	-4.786949
6	-3.388234	0.262077	-3.734089
6	-4.120953	0.871566	-4.763020
1	-4.466335	1.895325	-4.651753
6	-4.416914	0.159295	-5.927190
1	-4.989510	0.634668	-6.718488
6	-3.977008	-1.159910	-6.076442
1	-4.211704	-1.711110	-6.982506
6	-3.236075	-1.768112	-5.059595
1	-2.890969	-2.792220	-5.170375
6	-2.946676	-1.059899	-3.892315
1	-2.386229	-1.532306	-3.091901
6	-3.365067	2.493353	1.742100
6	-1.969775	2.608751	1.822245
1	-1.363782	1.711991	1.747155
6	-1.366465	3.859593	1.950376
6	-2.134041	5.022455	1.965849
1	-1.664559	5.996572	2.043932
6	-3.521414	4.906831	1.862576
6	-4.139376	3.659304	1.767062
1	-5.217730	3.623620	1.691951
6	-3.620326	-0.110043	2.992437
6	-3.817723	-1.500192	2.965952
1	-4.221766	-1.973060	2.078184
6	-3.469084	-2.282548	4.063264
6	-2.887458	-1.707057	5.193904
1	-2.597672	-2.320527	6.039191
6	-2.675268	-0.331111	5.211879
6	-3.047389	0.469972	4.128846
1	-2.871896	1.538234	4.177447
29	-2.774266	-0.168179	-0.329656
6	-1.945819	0.286375	6.372373
6	-3.605167	-3.777839	4.000112
6	0.129155	3.921549	2.091867
6	-4.340426	6.168202	1.808339
9	-4.074819	6.881200	0.686067
9	-5.669524	5.925061	1.817700
9	-4.070787	6.984207	2.853582
9	0.749568	3.062411	1.232615
9	0.537272	3.564982	3.331985
9	0.626428	5.150700	1.840889
9	-2.296359	1.574532	6.571417
9	-0.598981	0.279052	6.162938
9	-2.158141	-0.380955	7.525952
9	-4.008173	-4.298975	5.179179
9	-4.481473	-4.176891	3.054785
9	-2.412686	-4.368264	3.707710
6	-0.684270	-1.248018	1.603274
6	-0.979343	-2.614031	1.228778
6	-2.125789	-3.069664	0.497687
1	-0.548422	-3.383922	1.852395
77	3.285994	-1.400841	-1.340864
15	5.130050	-0.468749	-0.389346
8	5.129980	0.850851	0.608671
8	6.198061	0.045254	-1.559467
7	5.836775	-1.580625	0.647523
6	4.988865	2.141733	0.117587
6	3.809202	2.825907	0.484014
1	3.095744	2.325615	1.128465
6	3.598915	4.102882	0.026441
1	2.713554	4.653171	0.328165
6	4.521105	4.706591	-0.870386
6	4.255578	5.977447	-1.448944
1	3.340923	6.493310	-1.168274
6	5.126170	6.536262	-2.357599
1	4.909479	7.503637	-2.801145
6	6.302575	5.840109	-2.725166
1	6.976644	6.273494	-3.458403
6	6.599625	4.615603	-2.166711
1	7.500876	4.093093	-2.465823
6	5.729997	4.013015	-1.215613
6	6.002414	2.727491	-0.626094
6	7.311827	2.035310	-0.793625
6	8.554317	2.660744	-0.415695
6	8.613518	3.927716	0.230415
1	7.693760	4.451075	0.461742
6	9.820338	4.493587	0.580772
1	9.835357	5.458598	1.079266
6	11.038694	3.828579	0.305626
1	11.982209	4.290564	0.580991
6	11.019193	2.590539	-0.295379
1	11.945164	2.057694	-0.495514
6	9.791362	1.971174	-0.655083
6	9.770946	0.669846	-1.225856
1	10.712231	0.161365	-1.414815
6	8.578302	0.050053	-1.503615
1	8.533575	-0.955622	-1.907759
6	7.365993	0.731728	-1.260776
6	5.257581	-2.943055	0.493732
1	4.516197	-3.087677	1.290022
6	6.315481	-4.022913	0.632083
6	6.025570	-5.193709	1.342471
1	5.058859	-5.295613	1.830990
6	6.964063	-6.225820	1.428305
1	6.725267	-7.128468	1.984138
6	8.208923	-6.091871	0.809744
1	8.942888	-6.889639	0.880865
6	8.508546	-4.921993	0.103573
1	9.477716	-4.808921	-0.374839
6	7.567748	-3.896147	0.013387
1	7.802952	-2.981983	-0.524445
6	4.544156	-3.068651	-0.859606
1	5.297704	-3.190653	-1.647305
1	3.944224	-3.983004	-0.850979
6	6.497243	-1.329322	1.973705
1	6.976835	-2.286640	2.194633
6	5.476687	-1.096454	3.088429
6	4.933107	-2.208517	3.751555
1	5.273828	-3.205540	3.484266
6	3.981754	-2.053968	4.763393
1	3.576546	-2.930020	5.262337
6	3.568680	-0.775393	5.143393
1	2.831533	-0.647594	5.931251
6	4.119314	0.341204	4.507372
1	3.815321	1.341034	4.805624
6	5.062545	0.182258	3.490057
1	5.477042	1.060834	3.011866
6	7.628632	-0.303576	1.924271
1	8.357645	-0.587921	1.162658
1	7.287443	0.707665	1.708018
1	8.132257	-0.292434	2.895927
6	2.348044	-1.109401	0.602813
1	1.665523	-0.267453	0.545778
1	3.012226	-1.072223	1.463453
6	1.876670	-2.401500	0.201076
1	2.397768	-3.262137	0.607984
6	0.652580	-2.660400	-0.467897
1	0.109245	-1.817138	-0.872079
6	4.157221	-1.403955	-3.385837
1	5.163595	-1.804488	-3.299028
6	3.092997	-2.339778	-3.364876
1	3.354414	-3.394594	-3.286062
6	1.731807	-2.083852	-3.989331
1	1.804121	-2.178119	-5.084213
1	1.066468	-2.883897	-3.659208
6	1.103537	-0.720021	-3.622120
1	1.306962	0.020496	-4.402154
1	0.014181	-0.826433	-3.595175
6	1.559941	-0.148565	-2.280616
1	0.786661	-0.057986	-1.523445
6	2.654492	0.696163	-2.123149
1	2.636668	1.358649	-1.263653
6	3.612026	1.106893	-3.223777
1	4.486996	1.559363	-2.753048

1	3.137817	1.890867	-3.830470
6	4.071021	-0.063061	-4.118574
1	3.399358	-0.169034	-4.976699
1	5.056618	0.175249	-4.530032
6	0.336898	-3.958646	-1.072350
6	0.921475	-5.168588	-0.650994
6	-0.608250	-4.004979	-2.114296
6	0.581260	-6.373009	-1.264333
1	1.638155	-5.172316	0.164094
6	-0.944076	-5.207961	-2.732054
1	-1.079183	-3.082027	-2.434736
6	-0.348895	-6.398983	-2.309381
1	1.042200	-7.296397	-0.925188
1	-1.672913	-5.216163	-3.537420
1	-0.609116	-7.339972	-2.785251
6	-2.451669	-4.452802	0.569606
6	-3.474498	-4.987257	-0.184695
1	-1.880098	-5.091581	1.231937
6	-4.184930	-4.119330	-1.019837
6	-3.867688	-2.774891	-1.048114
1	-4.408674	-2.080890	-1.677058
7	-2.868225	-2.251627	-0.308050
8	-0.967651	-0.249167	0.867839
7	0.021726	-1.033130	2.752665
6	0.543942	0.295018	3.057710
1	1.541339	0.198552	3.492484
1	-0.098617	0.816994	3.774276
1	0.616692	0.884610	2.149455
6	0.302200	-2.062226	3.751766
1	1.249953	-2.575782	3.550132
1	-0.503026	-2.793752	3.802617
1	0.372604	-1.582198	4.729720
1	-3.710164	-6.044566	-0.133593
35	-5.605909	-4.807716	-2.176937

P2-C1 *si-si* conf1

Number of imaginary frequencies : 1
The smallest frequency is : -265.7217 cm(-1)
Electronic energy : HF=-7222.6279167
Zero-point correction= 1.756220
(Hartree/Particle)
Thermal correction to Energy= 1.874726
Thermal correction to Enthalpy= 1.875671
Thermal correction to Gibbs Free Energy= 1.594484
Sum of electronic and zero-point Energies= -7220.871696
Sum of electronic and thermal Energies= -7220.753190
Sum of electronic and thermal Enthalpies= -7220.752246
Sum of electronic and thermal Free Energies= -7221.033432

.....

Cartesian Coordinates

.....

26	-7.446044	-1.994494	-1.432371
15	-2.804950	0.143088	-2.396528
15	-4.203109	0.516716	1.047348
6	-5.747914	-0.813568	-1.748292
6	-5.882726	-1.165584	-0.355363
6	-5.849050	-2.589418	-0.263148
1	-5.934535	-3.164080	0.648204
6	-5.727533	-3.122546	-1.578879
1	-5.718781	-4.171674	-1.841401
6	-5.668578	-2.032931	-2.493508
1	-5.587293	-2.102442	-3.568512
6	-9.252220	-1.048363	-1.025935
1	-9.352218	-0.090783	-0.532183
6	-9.205148	-2.322816	-0.382560
1	-9.254811	-2.499891	0.683494
6	-9.038339	-3.320495	-1.390670
1	-8.931335	-4.383728	-1.220351
6	-8.983960	-2.663530	-2.657679
1	-8.829995	-3.140891	-3.616514
6	-9.117520	-1.260977	-2.433216
1	-9.087675	-0.494236	-3.195470
6	-5.621999	0.571472	-2.281292
6	-6.757307	1.389503	-2.371197
1	-7.707429	0.983335	-2.048889
6	-6.685108	2.696897	-2.850800
1	-7.578574	3.311338	-2.885909
6	-5.457933	3.210072	-3.263944
1	-5.384107	4.225799	-3.639454
6	-4.312361	2.418467	-3.174661
1	-3.363445	2.836736	-3.489659
6	-4.366319	1.108805	-2.672054
6	-5.956553	-0.177670	0.777243
1	-6.548166	0.669756	0.429730
6	-6.629559	-0.724864	2.040262
1	-6.686009	0.040193	2.819342
1	-6.100690	-1.587148	2.453888
1	-7.645943	-1.043673	1.790931
6	-1.487041	1.296524	-2.960167
6	-1.109569	2.308575	-2.060583
1	-1.610314	2.385381	-1.099675
6	-0.119866	3.227778	-2.401179
1	0.144987	4.012078	-1.705292
6	0.527714	3.135162	-3.636364
1	1.312095	3.842316	-3.889593
6	0.164586	2.128526	-4.532462
1	0.663203	2.048413	-5.494149
6	-0.841744	1.216534	-4.201431
1	-1.109436	0.440922	-4.909535
6	-2.861782	-1.184534	-3.657816
6	-3.298512	-0.966106	-4.973336
1	-3.620201	0.024148	-5.283107
6	-3.331096	-2.024897	-5.882485
1	-3.668357	-1.852378	-6.900543
6	-2.933351	-3.305989	-5.483693
1	-2.960535	-4.127218	-6.194326
6	-2.513045	-3.530270	-4.170420
1	-2.216585	-4.526117	-3.853125
6	-2.484168	-2.473774	-3.258524
1	-2.213633	-2.642363	-2.221235
6	-4.348849	2.351175	0.875952
6	-3.169297	3.098664	1.005255
1	-2.260813	2.621492	1.342477
6	-3.139340	4.457900	0.694463
6	-4.289658	5.115354	0.266391
1	-4.263460	6.168201	0.008473
6	-5.472183	4.383030	0.164358
6	-5.507908	3.020472	0.458456
1	-6.444536	2.497795	0.330791
6	-3.807646	0.223484	2.816342
6	-3.513278	-1.109823	3.144628
1	-3.555803	-1.874530	2.376686
6	-3.157207	-1.454231	4.444657
6	-3.028718	-0.473998	5.430895
1	-2.733988	-0.740213	6.439490
6	-3.293767	0.852703	5.096000
6	-3.698219	1.205245	3.804507
1	-3.917066	2.243870	3.582765
29	-2.513651	-0.501220	-0.231243
6	-3.077099	1.938411	6.115120
6	-2.836308	-2.887883	4.766774
6	-1.838007	5.200874	0.824593
6	-6.711796	5.100955	-0.298180
9	-6.537839	5.653900	-1.522893
9	-7.787634	4.287733	-0.375703
9	-7.034223	6.114539	0.538308
9	-0.791232	4.416825	0.440551
9	-1.587458	5.576626	2.098416
9	-1.798984	6.311577	0.063049
9	-3.921634	2.978261	5.933632
9	-1.819216	2.440377	6.037026
9	-3.243272	1.494344	7.379928
9	-3.197567	-3.217582	6.024826
9	-3.458011	-3.745259	3.924082
9	-1.505448	-3.146589	4.666306
6	-0.469370	0.806528	1.480102
6	-0.454674	-1.490388	1.908432
6	0.205455	1.083661	2.656755
1	-0.723520	1.595311	0.784173

6	0.309157	-1.247762	3.081496
6	0.617118	0.036005	3.482922
6	-0.709586	-2.861920	1.552949
6	-1.877914	-3.314470	0.833054
8	-2.536509	-2.573405	0.038962
7	-0.829135	-0.440287	1.117159
1	-0.285698	-3.561034	2.259382
77	3.381035	-1.624164	-1.235990
15	5.087347	-0.367642	-0.417419
8	4.888227	0.976658	0.526153
8	6.016392	0.279243	-1.636951
7	5.991633	-1.292386	0.653223
6	4.361369	2.143310	-0.002330
6	3.080734	2.516895	0.459481
1	2.594630	1.883158	1.191648
6	2.500661	3.665615	-0.016327
1	1.530579	3.983523	0.348483
6	3.146844	4.429288	-1.026428
6	2.510477	5.562165	-1.603278
1	1.537536	5.859761	-1.220101
6	3.104275	6.258441	-2.632397
1	2.605528	7.116426	-3.073468
6	4.366266	5.846293	-3.124430
1	4.821335	6.382280	-3.952317
6	5.024960	4.773437	-2.562765
1	5.992008	4.473086	-2.949769
6	4.449081	4.039267	-1.489201
6	5.109265	2.912505	-0.879280
6	6.542923	2.583650	-1.124844
6	7.580814	3.565625	-0.914700
6	7.323066	4.855998	-0.370709
1	6.313460	5.121787	-0.083367
6	8.338065	5.769947	-0.185972
1	8.110598	6.744085	0.237540
6	9.671945	5.450874	-0.532807
1	10.460182	6.184109	-0.389451
6	9.964632	4.202130	-1.031860
1	10.987432	3.931237	-1.280672
6	8.943865	3.230847	-1.218816
6	9.259327	1.923192	-1.676044
1	10.291336	1.681268	-1.913784
6	8.279549	0.969539	-1.783217
1	8.499451	-0.045557	-2.096510
6	6.939771	1.302639	-1.484173
6	5.555086	-2.715488	0.684967
1	4.859778	-2.837853	1.524549
6	6.723534	-3.661216	0.896774
6	6.581554	-4.763091	1.748565
1	5.648647	-4.900494	2.291035
6	7.622962	-5.681904	1.904918
1	7.498775	-6.531378	2.570961
6	8.823712	-5.501488	1.215110
1	9.637540	-6.210096	1.340398
6	8.974876	-4.400622	0.365284
1	9.908307	-4.252340	-0.171063
6	7.931444	-3.488723	0.205452
1	8.049292	-2.628004	-0.447050
6	4.816873	-3.076028	-0.609576
1	5.554688	-3.209580	-1.410053
1	4.320248	-4.041046	-0.470628
6	6.687144	-0.820372	1.900070
1	7.304621	-1.677850	2.180686
6	5.708752	-0.599119	3.056181
6	5.322093	-1.701802	3.835227
1	5.765438	-2.674077	3.637555
6	4.396331	-1.566532	4.873279
1	4.114139	-2.435558	5.461670
6	3.854562	-0.313291	5.165571
1	3.142771	-0.199885	5.978863
6	4.254530	0.799018	4.418977
1	3.853841	1.782272	4.649988
6	5.173338	0.657220	3.377678
1	5.470451	1.532803	2.814330
6	7.659685	0.331102	1.650978
1	8.373334	0.052732	0.871982
1	7.166296	1.253049	1.345094
1	8.215429	0.531048	2.572242
6	2.452207	-1.181895	0.686477
1	1.713838	-0.400637	0.548203
1	3.134608	-0.982242	1.508629
6	2.100657	-2.552783	0.469627
1	2.717120	-3.278232	0.988707
6	0.903254	-3.061023	-0.105510
1	0.268341	-2.382314	-0.659922
6	4.172185	-1.837046	-3.290237
1	5.211824	-2.147287	-3.213561
6	3.198676	-2.852511	-3.075322
1	3.570877	-3.856545	-2.870240
6	1.790596	-2.825968	-3.645304
1	1.806681	-3.136735	-4.701947
1	1.207177	-3.581885	-3.113141
6	1.083331	-1.462430	-3.511302
1	1.253695	-0.852629	-4.402620
1	0.003855	-1.625622	-3.467458
6	1.497153	-0.658300	-2.283643
1	0.743315	-0.554863	-1.507221
6	2.505240	0.295932	-2.290322
1	2.446241	1.075217	-1.537933
6	3.394406	0.616464	-3.474781
1	4.227392	1.220703	-3.110241
1	2.829981	1.248368	-4.173938
6	3.950369	-0.626693	-4.202224
1	3.285690	-0.914928	-5.023533
1	4.905749	-0.360551	-4.665147
6	0.774866	-4.484594	-0.457120
6	1.629415	-5.480426	0.059293
6	-0.234923	-4.882465	-1.352812
6	1.476539	-6.814711	-0.310915
1	2.414923	-5.216339	0.758855
6	-0.388035	-6.216974	-1.724388
1	-0.902373	-4.132516	-1.758563
6	0.466544	-7.191393	-1.203141
1	2.146912	-7.564718	0.099175
1	-1.175488	-6.495093	-2.419006
1	0.350017	-8.232701	-1.488848
7	-2.268113	-4.615425	0.977785
6	-3.309758	-5.166752	0.120480
1	-4.215880	-5.384135	0.699985
1	-2.955687	-6.097873	-0.334786
1	-3.553604	-4.450484	-0.659128
6	-1.655765	-5.548460	1.920821
1	-0.693704	-5.923014	1.554922
1	-2.330276	-6.397675	2.047013
1	-1.519495	-5.088848	2.900639
1	1.172250	0.218686	4.394973
1	0.621810	-2.088751	3.688999
35	0.523342	2.932769	3.188581

P2-C1 *re-re* conf1

Number of imaginary frequencies : 1
The smallest frequency is : -129.6199 cm(-1)
Electronic energy : HF=-7222.6324643
Zero-point correction= 1.754828
(Hartree/Particle)
Thermal correction to Energy= 1.873410
Thermal correction to Enthalpy= 1.874354
Thermal correction to Gibbs Free Energy= 1.592590
Sum of electronic and zero-point Energies= -7220.877637
Sum of electronic and thermal Energies= -7220.759054
Sum of electronic and thermal Enthalpies= -7220.758110
Sum of electronic and thermal Free Energies= -7221.039874

.....

Cartesian Coordinates

.....

26	-8.003890	0.535566	-0.858794
15	-2.937988	1.172384	-2.105429
15	-3.903793	0.834210	1.536138
6	-5.990347	1.055563	-1.115708
6	-6.207648	0.424180	0.164300

6	-6.729963	-0.884036	-0.076119
1	-7.012639	-1.601361	0.681993
6	-6.868040	-1.058283	-1.486177
1	-7.273277	-1.929953	-1.980245
6	-6.410565	0.131149	-2.126277
1	-6.407013	0.320672	-3.189396
6	-9.301507	1.883611	0.045256
1	-9.014316	2.596080	0.807040
6	-9.738124	0.543182	0.275880
1	-9.835801	0.063437	1.240657
6	-9.982438	-0.066493	-0.992189
1	-10.289443	-1.091121	-1.155838
6	-9.695783	0.896155	-2.007336
1	-9.749415	0.730002	-3.075186
6	-9.276435	2.100579	-1.367427
1	-8.961294	3.005025	-1.869508
6	-5.392609	2.409612	-1.299378
6	-6.133043	3.535728	-0.904898
1	-7.122845	3.377599	-0.497121
6	-5.628771	4.830260	-1.016791
1	-6.222067	5.674824	-0.680954
6	-4.358914	5.025010	-1.553914
1	-3.949256	6.024757	-1.653976
6	-3.597294	3.922174	-1.938852
1	-2.604470	4.094589	-2.335989
6	-4.077699	2.608912	-1.800000
6	-5.792712	1.016022	1.484079
1	-5.982368	2.089455	1.442124
6	-6.534867	0.445288	2.695471
1	-6.206978	0.929446	3.619615
1	-6.378539	-0.630937	2.806653
1	-7.609044	0.618500	2.575339
6	-1.365084	2.011567	-2.575314
6	-0.536934	2.457240	-1.531021
1	-0.782039	2.203854	-0.506001
6	0.586182	3.237088	-1.805196
1	1.204690	3.590108	-0.990616
6	0.923816	3.543122	-3.125953
1	1.808134	4.138311	-3.335526
6	0.132947	3.064127	-4.172045
1	0.397336	3.284584	-5.202323
6	-1.012603	2.310695	-3.900001
1	-1.635356	1.973547	-4.722064
6	-3.531091	0.436053	-3.679490
6	-4.233159	1.176010	-4.643879
1	-4.443656	2.227942	-4.475262
6	-4.676108	0.558584	-5.814982
1	-5.222360	1.136239	-6.555264
6	-4.422340	-0.799447	-6.033291
1	-4.776719	-1.279233	-6.941087
6	-3.715673	-1.538401	-5.081356
1	-3.523036	-2.594971	-5.242819
6	-3.270681	-0.921861	-3.910648
1	-2.735752	-1.497083	-3.163707
6	-3.203815	2.503927	1.868286
6	-1.803611	2.563888	1.922557
1	-1.236118	1.643447	1.834558
6	-1.148962	3.790224	2.034938
6	-1.868441	4.982606	2.066686
1	-1.359302	5.937613	2.131572
6	-3.261061	4.922266	1.993397
6	-3.929960	3.700669	1.907468
1	-5.009462	3.709763	1.846349
6	-3.500589	-0.138279	3.045923
6	-3.727933	-1.520681	2.955165
1	-4.171269	-1.936818	2.057899
6	-3.351204	-2.367602	3.993031
6	-2.712721	-1.863475	5.127957
1	-2.398448	-2.526595	5.925894
6	-2.471183	-0.494005	5.208861
6	-2.870839	0.370616	4.185713
1	-2.670480	1.431386	4.280891
29	-2.787150	-0.157308	-0.283877
6	-1.683282	0.045914	6.370248
6	-3.524710	-3.854620	3.853161
6	0.350981	3.792703	2.129852
6	-4.026792	6.217386	1.965405
9	-3.731786	6.942228	0.857819
9	-5.364877	6.031830	1.973323
9	-3.720977	7.000060	3.026524
9	0.904734	2.912419	1.246604
9	0.787025	3.414231	3.353145
9	0.890289	5.001200	1.864338
9	-1.964132	1.341726	6.622703
9	-0.343271	-0.019432	6.128443
9	-1.901361	-0.651043	7.505477
9	-3.955865	-4.422762	5.000824
9	-4.400600	-4.182316	2.880021
9	-2.347092	-4.464357	3.543223
6	-0.664618	-1.343779	1.568125
6	-0.978067	-2.683055	1.144436
6	-2.105648	-3.099675	0.371665
1	-0.534831	-3.488568	1.711424
77	3.317360	-1.168261	-1.663083
15	5.086051	-0.635548	-0.337471
8	5.147114	0.646869	0.712297
8	6.419382	-0.301638	-1.273955
7	5.382708	-1.872892	0.752307
6	5.093938	1.941340	0.214706
6	3.922669	2.675242	0.499373
1	3.159375	2.211649	1.111422
6	3.785653	3.947113	0.002123
1	2.908543	4.538430	0.245215
6	4.776293	4.488919	-0.861866
6	4.587239	5.747248	-1.495212
1	3.677494	6.302471	-1.281546
6	5.523394	6.245101	-2.373624
1	5.363959	7.202950	-2.860077
6	6.692360	5.498157	-2.654394
1	7.418263	5.882659	-3.365069
6	6.917166	4.285452	-2.039016
1	7.814683	3.723395	-2.270132
6	5.978206	3.745382	-1.117032
6	6.173879	2.470569	-0.473410
6	7.473496	1.741497	-0.517906
6	8.698688	2.375843	-0.089723
6	8.729461	3.667587	0.507785
1	7.801889	4.202851	0.668885
6	9.917447	4.244819	0.902321
1	9.907776	5.229156	1.361672
6	11.146448	3.567788	0.722654
1	12.075404	4.038674	1.030497
6	11.153327	2.305334	0.174465
1	12.085789	1.760982	0.049612
6	9.944378	1.675075	-0.226614
6	9.950186	0.349627	-0.738300
1	10.897883	-0.169175	-0.851536
6	8.772557	-0.278082	-1.052212
1	8.745614	-1.302187	-1.409395
6	7.547319	0.412849	-0.911950
6	4.478865	-3.038698	0.557847
1	3.622325	-2.931166	1.237613
6	5.160225	-4.360359	0.866996
6	4.476101	-5.342630	1.592576
1	3.485519	-5.122596	1.984952
6	5.055329	-6.594453	1.818986
1	4.512542	-7.347034	2.384430
6	6.332526	-6.872698	1.327951
1	6.788051	-7.842213	1.508564
6	7.025434	-5.894084	0.607110
1	8.021626	-6.102745	0.226598
6	6.441547	-4.648920	0.374838
1	6.979722	-3.884697	-0.180005
6	3.981610	-3.056184	-0.891386
1	4.810426	-3.394618	-1.525733
1	3.196513	-3.808029	-0.987752
6	6.060015	-1.787521	2.086950
1	6.349542	-2.821694	2.288701
6	5.113751	-1.387694	3.220964
6	4.455679	-2.398772	3.938012

1	4.621061	-3.437361	3.663530
6	3.611561	-2.093375	5.008966
1	3.114559	-2.894232	5.549218
6	3.412058	-0.764114	5.385051
1	2.747936	-0.520000	6.209711
6	4.068313	0.252366	4.684259
1	3.926018	1.290361	4.972860
6	4.911577	-0.055917	3.614710
1	5.416562	0.745463	3.090342
6	7.366059	-0.993532	2.066696
1	8.037607	-1.391153	1.302667
1	7.225259	0.070737	1.879485
1	7.854068	-1.102902	3.039908
6	2.037822	-0.563759	-0.021653
1	1.867713	0.509758	-0.005942
1	2.339479	-0.958567	0.946512
6	1.126730	-1.359133	-0.802591
1	0.457311	-0.854996	-1.487689
6	0.890079	-2.720818	-0.540821
1	1.492548	-3.178405	0.236813
6	4.591862	-1.533292	-3.475866
1	5.426017	-2.154432	-3.158489
6	3.355285	-2.194074	-3.655959
1	3.341394	-3.269576	-3.479775
6	2.221618	-1.710671	-4.542860
1	2.429265	-1.974615	-5.591614
1	1.325087	-2.270086	-4.259044
6	1.930652	-0.200554	-4.426890
1	2.514331	0.358217	-5.165222
1	0.879790	-0.018640	-4.672220
6	2.200958	0.382911	-3.042860
1	1.321846	0.684430	-2.485682
6	3.398028	0.973716	-2.666098
1	3.358076	1.692024	-1.853416
6	4.635510	1.051792	-3.535880
1	5.470005	1.367339	-2.908603
1	4.490378	1.848229	-4.281138
6	5.002847	-0.273467	-4.240052
1	4.558562	-0.307561	-5.240192
1	6.086551	-0.297610	-4.388563
6	0.253048	-3.644818	-1.466985
6	-0.551408	-3.206530	-2.538361
6	0.447676	-5.029189	-1.298871
6	-1.130086	-4.121177	-3.412224
1	-0.726742	-2.146634	-2.678783
6	-0.124863	-5.944817	-2.182095
1	1.056937	-5.381590	-0.470229
6	-0.916524	-5.494688	-3.241414
1	-1.746639	-3.763945	-4.231734
1	0.043494	-7.008489	-2.040384
1	-1.366453	-6.205604	-3.928249
6	-2.375532	-4.497008	0.298040
6	-3.405259	-4.991793	-0.472884
1	-1.751333	-5.179032	0.863015
6	-4.191349	-4.068646	-1.170036
6	-3.927347	-2.717494	-1.060514
1	-4.529179	-1.983958	-1.579772
7	-2.910818	-2.233947	-0.318995
8	-1.010437	-0.304093	0.925976
7	0.123647	-1.187449	2.678108
6	0.677401	0.121984	3.001388
1	1.694729	0.002151	3.380026
1	0.083392	0.630983	3.768268
1	0.710999	0.735585	2.107635
6	0.433338	-2.264960	3.611711
1	1.335075	-2.818157	3.319425
1	-0.401576	-2.959606	3.701103
1	0.610287	-1.829356	4.596274
1	-3.594101	-6.058022	-0.533278
35	-5.659027	-4.674031	-2.315731

P2-C1 *si-re* conf1

Number of imaginary frequencies : 1
The smallest frequency is : -132.9607 cm(-1)

Electronic energy : HF=-7222.6148776
Zero-point correction= 1.754242
(Hartree/Particle)
Thermal correction to Energy= 1.873142
Thermal correction to Enthalpy= 1.874086
Thermal correction to Gibbs Free Energy= 1.589201
Sum of electronic and zero-point Energies= -7220.860636
Sum of electronic and thermal Energies= -7220.741736
Sum of electronic and thermal Enthalpies= -7220.740791
Sum of electronic and thermal Free Energies= -7221.025677

Cartesian Coordinates

77	-4.332396	-0.374629	-1.603431
15	-6.025750	0.348253	-0.273900
8	-6.544391	-0.442426	1.085853
8	-7.452148	0.436447	-1.130948
7	-5.630408	1.837402	0.383436
6	-7.404842	-1.534014	1.018542
6	-6.870200	-2.775879	1.425842
1	-5.847254	-2.805383	1.786433
6	-7.648829	-3.904255	1.357368
1	-7.252601	-4.865284	1.672470
6	-8.971623	-3.836502	0.842834
6	-9.756983	-5.010419	0.684014
1	-9.331298	-5.963224	0.987590
6	-11.021358	-4.947369	0.143451
1	-11.610485	-5.851316	0.019907
6	-11.549151	-3.700160	-0.267815
1	-12.537704	-3.656312	-0.715803
6	-10.820523	-2.540978	-0.110980
1	-11.237540	-1.596890	-0.440850
6	-9.518059	-2.564841	0.461554
6	-8.725103	-1.373626	0.626852
6	-9.276406	-0.014953	0.364525
6	-10.442101	0.484438	1.046144
6	-11.083222	-0.229751	2.097135
1	-10.682692	-1.186344	2.410760
6	-12.194677	0.282497	2.730439
1	-12.661434	-0.279839	3.534059
6	-12.730814	1.535990	2.350071
1	-13.611743	1.923086	2.853633
6	-12.122640	2.265270	1.353828
1	-12.511373	3.237822	1.063215
6	-10.965422	1.773674	0.690608
6	-10.309336	2.547756	-0.304550
1	-10.723091	3.513625	-0.580065
6	-9.153135	2.095002	-0.890820
1	-8.621576	2.677890	-1.634862
6	-8.638216	0.832171	-0.525981
6	-4.473202	2.462424	-0.310995
1	-3.588658	2.322733	0.322535
6	-4.655760	3.953650	-0.538056
6	-3.539685	4.797784	-0.479353
1	-2.570385	4.383320	-0.215657
6	-3.661243	6.160184	-0.762446
1	-2.785919	6.802278	-0.711671
6	-4.905957	6.696658	-1.101082
1	-5.004377	7.757290	-1.314332
6	-6.025382	5.860726	-1.159122
1	-6.997962	6.271211	-1.416976
6	-5.899904	4.498332	-0.883901
1	-6.769918	3.849430	-0.915470
6	-4.239226	1.769942	-1.660766
1	-4.999801	2.125685	-2.367627
1	-3.276996	2.095506	-2.060404
6	-5.919074	2.430463	1.727104
1	-5.917368	3.507670	1.539505
6	-4.792885	2.161493	2.722883
6	-4.082311	3.239366	3.266005
1	-4.326163	4.251238	2.951341
6	-3.065153	3.030753	4.202556
1	-2.526899	3.880977	4.612188
6	-2.729035	1.733808	4.593410
1	-1.924223	1.563003	5.301609

6	-3.428765	0.650610	4.053264
1	-3.167690	-0.361708	4.347880
6	-4.457565	0.862301	3.134232
1	-5.002695	0.016739	2.731616
6	-7.295553	2.120943	2.324049
1	-8.091833	2.359130	1.616779
1	-7.398614	1.084453	2.641683
1	-7.423705	2.759140	3.203909
6	-3.162798	-0.687350	0.185106
1	-3.357187	-1.657387	0.642379
1	-3.208281	0.128467	0.902990
6	-2.130595	-0.625976	-0.821616
1	-1.746505	-1.549882	-1.234773
6	-1.417210	0.550553	-1.111116
1	-1.761653	1.465697	-0.647745
6	-5.572529	-0.319746	-3.491331
1	-6.097222	0.632047	-3.487794
6	-4.208452	-0.280733	-3.848576
1	-3.795032	0.692537	-4.111720
6	-3.389898	-1.453872	-4.362016
1	-3.553540	-1.579979	-5.443430
1	-2.333374	-1.191502	-4.241446
6	-3.661411	-2.787008	-3.631675
1	-4.476042	-3.329679	-4.120183
1	-2.776195	-3.424857	-3.722590
6	-3.988902	-2.628396	-2.148659
1	-3.224379	-2.977866	-1.459155
6	-5.274710	-2.522152	-1.634638
1	-5.412421	-2.808339	-0.596587
6	-6.548563	-2.471991	-2.453460
1	-7.353730	-2.136574	-1.797015
1	-6.809180	-3.492988	-2.768310
6	-6.477416	-1.538100	-3.680881
1	-6.145473	-2.093894	-4.563300
1	-7.488193	-1.185584	-3.906788
6	-0.539571	0.718805	-2.256941
6	0.049480	-0.371389	-2.931896
6	-0.295966	2.021280	-2.738852
6	0.848977	-0.161993	-4.052044
1	-0.105626	-1.381169	-2.569131
6	0.477659	2.224115	-3.878663
1	-0.730346	2.868524	-2.215372
6	1.057791	1.134590	-4.534571
1	1.317705	-1.007151	-4.547229
1	0.646583	3.230840	-4.245962
1	1.680333	1.294533	-5.409291
26	6.436005	4.125323	1.552940
15	4.788566	0.969086	-2.212482
15	4.760229	-0.355784	1.288420
6	6.075154	2.650657	0.112248
6	5.529620	2.272533	1.391793
6	4.571111	3.263789	1.765445
1	3.999476	3.273139	2.683413
6	4.539956	4.261994	0.748898
1	3.941690	5.162490	0.761645
6	5.466567	3.889206	-0.266531
1	5.687643	4.442688	-1.167726
6	8.181348	4.016208	2.675849
1	8.692739	3.096320	2.927461
6	7.139714	4.631182	3.436033
1	6.720922	4.257803	4.361001
6	6.716157	5.803004	2.737856
1	5.917868	6.468589	3.039113
6	7.495468	5.913357	1.546196
1	7.392553	6.676581	0.786131
6	8.401884	4.812218	1.508783
1	9.108815	4.603894	0.717369
6	7.027495	1.835287	-0.691129
6	8.384210	1.798518	-0.339825
1	8.702660	2.368055	0.523534
6	9.310617	1.053962	-1.070027
1	10.352428	1.036270	-0.765903
6	8.887562	0.332725	-2.184542
1	9.596209	-0.245877	-2.767539
6	7.538210	0.336223	-2.537883
1	7.220348	-0.243913	-3.396951
6	6.591903	1.060790	-1.797027
6	5.844068	0.986073	2.101867
1	6.873190	0.717856	1.857606
6	5.727521	1.064050	3.627042
1	5.982542	0.107772	4.092229
1	4.719424	1.336996	3.950217
1	6.419089	1.826962	3.996330
6	4.704496	-0.335888	-3.504852
6	4.883674	-1.664064	-3.076371
1	5.128530	-1.863508	-2.036563
6	4.755131	-2.725475	-3.969750
1	4.903708	-3.741618	-3.617714
6	4.427299	-2.473744	-5.306761
1	4.315892	-3.298527	-6.004750
6	4.246011	-1.158931	-5.740526
1	3.995069	-0.957947	-6.778363
6	4.389006	-0.092028	-4.847090
1	4.246410	0.924323	-5.198044
6	4.491816	2.565707	-3.066405
6	5.420651	3.114857	-3.965143
1	6.327042	2.569409	-4.212343
6	5.192234	4.370907	-4.527888
1	5.914128	4.791573	-5.222222
6	4.039945	5.090236	-4.190505
1	3.868907	6.072503	-4.622252
6	3.115352	4.547354	-3.295679
1	2.222806	5.106177	-3.027665
6	3.337872	3.287812	-2.733611
1	2.636787	2.871186	-2.018067
6	5.903843	-1.728206	0.819084
6	5.338711	-2.961397	0.453130
1	4.267887	-3.117777	0.530870
6	6.147964	-4.007963	0.006237
6	7.526621	-3.849476	-0.104770
1	8.150582	-4.668864	-0.441707
6	8.087558	-2.621686	0.240923
6	7.292062	-1.568266	0.690627
1	7.773930	-0.629674	0.929115
6	3.763388	-1.056926	2.671284
6	2.636050	-0.308996	3.043079
1	2.403537	0.610962	2.518671
6	1.805824	-0.747083	4.072732
6	2.057869	-1.953420	4.727743
1	1.401971	-2.301615	5.517020
6	3.174070	-2.698012	4.353289
6	4.032897	-2.252456	3.344285
1	4.904947	-2.846301	3.094511
29	3.441533	0.389311	-0.476643
6	3.442929	-4.032697	4.993580
6	0.574691	0.041776	4.421619
6	5.512433	-5.310821	-0.396109
6	9.577955	-2.456271	0.103152
9	9.952281	-2.346941	-1.194606
9	10.039019	-1.361644	0.745449
9	10.240207	-3.525602	0.602787
9	4.999368	-5.245999	-1.652295
9	4.495981	-5.642538	0.428165
9	6.393231	-6.333670	-0.387911
9	4.765457	-4.237515	5.188454
9	3.003813	-5.050064	4.212155
9	2.830776	-4.161256	6.190030
9	0.262790	-0.043040	5.733331
9	0.714445	1.354588	4.125262
9	-0.516127	-0.402251	3.741355
6	2.053133	-2.250536	-0.860792
6	0.757264	-0.782787	0.428466
6	1.289511	-3.339707	-0.476762
1	2.871062	-2.357170	-1.563455
6	0.029133	-1.900264	0.934877
6	0.280150	-3.177586	0.478766
1	-0.744695	-1.730795	1.673075
6	0.264835	0.521343	0.738458
6	0.910461	1.778108	0.469995
8	2.037492	1.883813	-0.097140

7	1.817135	-1.004201	-0.410820
1	-0.547750	0.523283	1.448591
7	0.243864	2.942370	0.797394
6	0.945503	4.214628	0.661265
1	1.405205	4.522147	1.611591
1	0.234546	4.989540	0.357643
1	1.728742	4.126063	-0.087247
6	-0.892408	2.961566	1.716044
1	-1.661660	2.245609	1.426488
1	-1.345688	3.953535	1.694960
1	-0.590790	2.744341	2.744820
1	-0.295838	-4.022463	0.841445
35	1.597199	-5.089668	-1.291352

P2-C1 *re-si* conf2

Number of imaginary frequencies : 1
The smallest frequency is : -267.9767 cm(-1)
Electronic energy : HF=-7222.6289103
Zero-point correction= 1.754635
(Hartree/Particle)
Thermal correction to Energy= 1.873395
Thermal correction to Enthalpy= 1.874339
Thermal correction to Gibbs Free Energy= 1.590919
Sum of electronic and zero-point Energies= -7220.874275
Sum of electronic and thermal Energies= -7220.755515
Sum of electronic and thermal Enthalpies= -7220.754571
Sum of electronic and thermal Free Energies= -7221.037991

.....

Cartesian Coordinates

.....

26	-8.164627	0.057258	-1.065056
15	-3.103215	1.071739	-2.100875
15	-4.188583	0.684021	1.495427
6	-6.189305	0.736413	-1.267302
6	-6.395438	0.096480	0.009527
6	-6.803895	-1.250638	-0.237111
1	-7.046643	-1.986448	0.517012
6	-6.886909	-1.440226	-1.649618
1	-7.207327	-2.342424	-2.150055
6	-6.506085	-0.221142	-2.283619
1	-6.484707	-0.035891	-3.347268
6	-9.603795	1.270912	-0.185159
1	-9.409258	1.994807	0.595273
6	-9.926972	-0.107268	0.009603
1	-10.010702	-0.613254	0.962148
6	-10.076161	-0.711579	-1.275898
1	-10.286432	-1.755699	-1.466962
6	-9.844918	0.291956	-2.265243
1	-9.852705	0.142690	-3.336881
6	-9.556076	1.516207	-1.592551
1	-9.310740	2.455236	-2.069711
6	-5.687471	2.127783	-1.444822
6	-6.520940	3.200170	-1.089263
1	-7.509097	2.971867	-0.711177
6	-6.106729	4.526498	-1.198552
1	-6.767927	5.329763	-0.889183
6	-4.838039	4.806492	-1.700072
1	-4.498189	5.832040	-1.801561
6	-3.986762	3.757676	-2.046174
1	-2.996266	3.996837	-2.412938
6	-4.373487	2.413945	-1.900997
6	-6.080420	0.732436	1.335960
1	-6.333268	1.791008	1.260490
6	-6.845595	0.140099	2.522346
1	-6.595096	0.662999	3.449630
1	-6.628981	-0.921518	2.667768
1	-7.920604	0.242918	2.344627
6	-1.588256	2.028907	-2.520716
6	-0.854192	2.565279	-1.451744
1	-1.135358	2.319372	-0.434517
6	0.224853	3.414332	-1.691563
1	0.772275	3.834021	-0.857674
6	0.609956	3.704561	-3.002644
1	1.458429	4.357514	-3.186282
6	-0.089245	3.140346	-4.072380
1	0.212843	3.351726	-5.094226
6	-1.190974	2.314111	-3.835221
1	-1.740995	1.903498	-4.675341
6	-3.509487	0.207207	-3.665494
6	-4.242699	0.799502	-4.704237
1	-4.621911	1.811291	-4.593517
6	-4.494589	0.085449	-5.877629
1	-5.067255	0.547452	-6.676739
6	-4.010711	-1.218413	-6.025923
1	-4.211234	-1.771012	-6.939299
6	-3.270233	-1.809574	-4.998783
1	-2.891297	-2.821777	-5.108627
6	-3.024733	-1.099685	-3.822499
1	-2.463757	-1.559055	-3.014833
6	-3.628067	2.407084	1.823032
6	-2.240256	2.573630	1.936669
1	-1.598047	1.701166	1.877043
6	-1.686858	3.846352	2.075416
6	-2.496697	4.980207	2.070209
1	-2.064452	5.970660	2.157203
6	-3.876055	4.813822	1.934770
6	-4.444576	3.544227	1.826131
1	-5.518449	3.466908	1.725256
6	-3.813247	-0.208535	3.060639
6	-3.953177	-1.605412	3.026630
1	-4.319934	-2.091735	2.130204
6	-3.596890	-2.375974	4.129803
6	-3.066368	-1.780576	5.275698
1	-2.771185	-2.384507	6.125832
6	-2.916692	-0.396811	5.303276
6	-3.295856	0.390940	4.212801
1	-3.170008	1.465730	4.269138
29	-2.914389	-0.222419	-0.250930
6	-2.249939	0.256051	6.481960
6	-3.672285	-3.875360	4.060073
6	-0.197558	3.963067	2.247629
6	-4.738377	6.045317	1.864166
9	-4.463300	6.776960	0.756422
9	-6.057682	5.755554	1.830887
9	-4.530439	6.861124	2.923739
9	0.470335	3.133043	1.394911
9	0.198654	3.612299	3.492956
9	0.259078	5.210987	2.013743
9	-2.716304	1.503103	6.706278
9	-0.908081	0.375665	6.278115
9	-2.405996	-0.451977	7.619593
9	-4.076246	-4.416492	5.229632
9	-4.514138	-4.305467	3.097178
9	-2.452208	-4.416622	3.787833
6	-0.794431	-1.230090	1.704803
6	-1.032434	-2.604850	1.318073
6	-2.160810	-3.099280	0.581783
1	-0.578073	-3.361320	1.941823
77	3.150248	-1.209094	-1.279168
15	4.969673	-0.206197	-0.363083
8	4.906103	1.091553	0.671777
8	5.977806	0.396016	-1.542326
7	5.781249	-1.285238	0.636034
6	4.737106	2.390790	0.215375
6	3.534557	3.030063	0.588299
1	2.825818	2.487869	1.203111
6	3.295559	4.317217	0.177371
1	2.390918	4.830795	0.487255
6	4.215290	4.980298	-0.678977
6	3.925776	6.268675	-1.204750
1	2.995146	6.748843	-0.913348
6	4.793704	6.888768	-2.075136
1	4.559551	7.869942	-2.477539
6	5.990066	6.236662	-2.457820
1	6.662314	6.717237	-3.162781
6	6.309535	4.995453	-1.950757
1	7.225643	4.508827	-2.263904
6	5.445243	4.330559	-1.036623
6	5.742922	3.027629	-0.496323

6	7.065426	2.369024	-0.700156
6	8.303484	3.008170	-0.332868
6	8.351307	4.234255	0.388649
1	7.425616	4.710223	0.689592
6	9.554354	4.816360	0.724215
1	9.562232	5.747676	1.283257
6	10.779386	4.210049	0.356587
1	11.719380	4.683912	0.623714
6	10.772150	3.013970	-0.324112
1	11.704305	2.526230	-0.597187
6	9.549171	2.379077	-0.674232
6	9.542772	1.120606	-1.334249
1	10.489076	0.657902	-1.599548
6	8.358714	0.473582	-1.587626
1	8.328875	-0.509454	-2.045150
6	7.139114	1.094955	-1.242775
6	5.288977	-2.680555	0.489171
1	4.625244	-2.904366	1.333081
6	6.406358	-3.709268	0.471281
6	6.247922	-4.922587	1.148004
1	5.344924	-5.096874	1.729607
6	7.245138	-5.900790	1.098804
1	7.112177	-6.835860	1.636321
6	8.414162	-5.670503	0.371596
1	9.197211	-6.423017	0.342538
6	8.574169	-4.462231	-0.316409
1	9.485282	-4.271920	-0.877004
6	7.573663	-3.493785	-0.273904
1	7.708082	-2.543396	-0.781634
6	4.481752	-2.823384	-0.818203
1	5.189316	-2.934270	-1.648145
1	3.915436	-3.757515	-0.765689
6	6.412671	-0.852692	1.931326
1	6.571832	0.218423	1.817575
6	7.794520	-1.452908	2.161222
6	8.903473	-0.808050	1.600233
1	8.755903	0.106445	1.037050
6	10.190381	-1.325304	1.751519
1	11.034508	-0.809937	1.300956
6	10.388724	-2.496572	2.486437
1	11.387626	-2.907417	2.604529
6	9.293547	-3.130036	3.079569
1	9.437447	-4.037735	3.658924
6	8.008772	-2.606538	2.925138
1	7.170992	-3.119755	3.383866
6	5.452989	-1.041281	3.112248
1	4.539112	-0.465571	2.943836
1	5.178459	-2.087017	3.273580
1	5.923841	-0.676867	4.030315
6	2.211349	-0.949093	0.664911
1	1.486568	-0.142814	0.610226
1	2.877946	-0.874836	1.519657
6	1.803542	-2.266255	0.277710
1	2.370507	-3.095565	0.687714
6	0.583919	-2.588666	-0.374943
1	0.002701	-1.773371	-0.784455
6	4.003435	-1.173992	-3.334234
1	5.026108	-1.534114	-3.259055
6	2.980269	-2.154369	-3.305783
1	3.288377	-3.196737	-3.231164
6	1.603539	-1.956038	-3.915390
1	1.666414	-2.055688	-5.010388
1	0.973590	-2.778802	-3.572018
6	0.928652	-0.614885	-3.549963
1	1.105923	0.131550	-4.330499
1	-0.155780	-0.759474	-3.523157
6	1.364575	-0.027204	-2.208830
1	0.591475	0.027085	-1.448133
6	2.424440	0.861223	-2.055503
1	2.387926	1.519427	-1.193202
6	3.353834	1.313672	-3.163631
1	4.210623	1.806001	-2.699853
1	2.839314	2.074057	-3.767211
6	3.858263	0.164662	-4.061951
1	3.188775	0.032729	-4.918127
1	4.831859	0.444521	-4.475569
6	0.332417	-3.902849	-0.976818
6	0.980416	-5.079744	-0.554989
6	-0.609486	-3.999896	-2.018315
6	0.707569	-6.300270	-1.170134
1	1.695585	-5.045282	0.260748
6	-0.878579	-5.218901	-2.637400
1	-1.132495	-3.104430	-2.336763
6	-0.218407	-6.375738	-2.216531
1	1.218099	-7.197441	-0.831647
1	-1.606273	-5.266146	-3.442538
1	-0.425975	-7.328863	-2.694156
6	-2.439914	-4.491991	0.654309
6	-3.434671	-5.063463	-0.110404
1	-1.853719	-5.109753	1.323792
6	-4.162758	-4.222890	-0.957634
6	-3.892060	-2.868232	-0.985269
1	-4.447336	-2.195952	-1.625001
7	-2.921474	-2.308020	-0.233194
8	-1.106842	-0.239353	0.971772
7	-0.110066	-0.996949	2.865573
6	0.376830	0.341672	3.180703
1	1.377473	0.267450	3.618817
1	-0.277053	0.842017	3.902282
1	0.435635	0.940033	2.277296
6	0.169849	-2.010177	3.880411
1	1.149658	-2.480153	3.723726
1	-0.599318	-2.780768	3.897645
1	0.170951	-1.524820	4.859250
1	-3.634474	-6.128068	-0.059188
35	-5.540006	-4.964556	-2.134005

P2-C1 *si-si* conf2

Number of imaginary frequencies : 1
The smallest frequency is : -266.9252 cm(-1)
Electronic energy : HF=-7222.6225041
Zero-point correction= 1.755305
(Hartree/Particle)
Thermal correction to Energy= 1.873789
Thermal correction to Enthalpy= 1.874733
Thermal correction to Gibbs Free Energy= 1.596156
Sum of electronic and zero-point Energies= -7220.867200
Sum of electronic and thermal Energies= -7220.748715
Sum of electronic and thermal Enthalpies= -7220.747771
Sum of electronic and thermal Free Energies= -7221.026348

Cartesian Coordinates

26	-7.587737	-2.030120	-1.503578
15	-2.982145	0.290134	-2.301438
15	-4.408503	0.363313	1.158495
6	-5.910194	-0.797811	-1.737637
6	-6.045487	-1.241406	-0.371125
6	-5.984273	-2.666595	-0.366827
1	-6.061588	-3.298816	0.506460
6	-5.847183	-3.111998	-1.714095
1	-5.816015	-4.141703	-2.043405
6	-5.805672	-1.965233	-2.558266
1	-5.719254	-1.966488	-3.634902
6	-9.411110	-1.164151	-1.007964
1	-9.524467	-0.257497	-0.428184
6	-9.332159	-2.490786	-0.483910
1	-9.370071	-2.765494	0.561692
6	-9.150577	-3.388404	-1.579896
1	-9.020587	-4.460268	-1.508050
6	-9.116668	-2.617626	-2.781714
1	-8.958973	-3.002187	-3.780748
6	-9.278997	-1.244724	-2.429334
1	-9.270492	-0.411021	-3.118186
6	-5.813259	0.628040	-2.160974
6	-6.966849	1.425874	-2.171613
1	-7.906619	0.967310	-1.892626
6	-6.926067	2.776475	-2.516030
1	-7.833657	3.370536	-2.489856

6	-5.711640	3.356397	-2.874325
1	-5.660840	4.406631	-3.143498
6	-4.548595	2.585868	-2.864101
1	-3.610231	3.056927	-3.132745
6	-4.570425	1.231128	-2.495048
6	-6.147653	-0.315184	0.808645
1	-6.710589	0.554532	0.470750
6	-6.880430	-0.900879	2.019068
1	-6.922259	-0.181175	2.841372
1	-6.407743	-1.812402	2.392121
1	-7.903848	-1.152778	1.725778
6	-1.696044	1.506233	-2.806632
6	-1.308245	2.452313	-1.842264
1	-1.780838	2.450113	-0.865178
6	-0.340765	3.411024	-2.134609
1	-0.063706	4.138879	-1.384071
6	0.272839	3.426692	-3.389954
1	1.040171	4.163886	-3.607896
6	-0.102141	2.488160	-4.352854
1	0.369765	2.492138	-5.331237
6	-1.084434	1.535572	-4.067389
1	-1.358886	0.813545	-4.827830
6	-3.024373	-0.958034	-3.641947
6	-3.483239	-0.670641	-4.936489
1	-3.835003	0.327737	-5.180319
6	-3.500509	-1.672787	-5.908177
1	-3.855396	-1.447454	-6.909791
6	-3.064349	-2.964904	-5.593817
1	-3.079468	-3.741132	-6.353684
6	-2.621482	-3.258475	-4.301722
1	-2.294495	-4.263382	-4.049774
6	-2.609322	-2.259187	-3.327461
1	-2.323342	-2.483730	-2.305137
6	-4.586523	2.202559	1.171447
6	-3.406763	2.947169	1.308168
1	-2.486690	2.444570	1.568588
6	-3.392252	4.323874	1.083888
6	-4.559426	4.998675	0.735291
1	-4.544650	6.063574	0.531420
6	-5.743208	4.268481	0.633010
6	-5.765116	2.891021	0.849402
1	-6.707336	2.373713	0.735995
6	-3.984023	-0.127869	2.874739
6	-3.800150	-1.506259	3.073924
1	-3.981371	-2.198174	2.259017
6	-3.351382	-1.985637	4.299730
6	-3.023056	-1.105273	5.331860
1	-2.644004	-1.478063	6.277408
6	-3.175939	0.263913	5.120270
6	-3.668938	0.757962	3.909861
1	-3.786002	1.827315	3.780416
29	-2.671094	-0.489416	-0.185857
6	-2.712818	1.206199	6.197233
6	-3.121335	-3.457736	4.496390
6	-2.092172	5.070769	1.207198
6	-6.996213	5.003425	0.237303
9	-6.842756	5.633724	-0.952664
9	-8.065468	4.186331	0.121469
9	-7.316338	5.959702	1.139242
9	-1.048641	4.307505	0.774004
9	-1.814905	5.412257	2.484499
9	-2.076139	6.203968	0.477696
9	-3.100815	2.479518	5.975162
9	-1.357473	1.211062	6.283723
9	-3.174111	0.845838	7.416237
9	-3.629667	-3.895178	5.668971
9	-3.670476	-4.201419	3.510756
9	-1.793668	-3.755215	4.519455
6	-0.655877	0.743710	1.630039
6	-0.638721	-1.572463	1.927870
6	-0.065667	0.958541	2.864419
1	-0.869166	1.568309	0.961855
6	0.020897	-1.391874	3.172509
6	0.281009	-0.129956	3.668636
6	-0.830053	-2.923155	1.463339
6	-1.981571	-3.354441	0.703627
8	-2.674443	-2.568196	-0.014418
7	-0.983157	-0.482844	1.177981
1	-0.396854	-3.657551	2.127216
77	3.249702	-1.353953	-1.191222
15	4.980383	-0.111354	-0.400278
8	4.786750	1.132620	0.694008
8	5.791872	0.691865	-1.604590
7	6.025333	-1.086679	0.486867
6	4.165387	2.307615	0.299515
6	2.885259	2.561738	0.839178
1	2.460850	1.840555	1.528158
6	2.218962	3.709108	0.488588
1	1.248093	3.929903	0.915264
6	2.775601	4.600843	-0.467735
6	2.052354	5.743244	-0.908393
1	1.083531	5.947966	-0.459549
6	2.558960	6.563232	-1.891720
1	1.995281	7.428200	-2.228564
6	3.815955	6.269698	-2.473442
1	4.201616	6.903069	-3.267098
6	4.557010	5.190135	-2.042460
1	5.517664	4.981791	-2.498886
6	4.074030	4.330988	-1.016403
6	4.821494	3.193713	-0.539746
6	6.247008	2.965437	-0.908242
6	7.249032	3.982496	-0.696563
6	6.982310	5.187734	0.012310
1	5.996154	5.353524	0.428541
6	7.962015	6.139720	0.195545
1	7.731517	7.045817	0.748646
6	9.265030	5.946545	-0.321017
1	10.024430	6.709253	-0.175741
6	9.566726	4.782288	-0.990153
1	10.568243	4.607887	-1.374807
6	8.584255	3.773004	-1.180717
6	8.909765	2.551198	-1.827940
1	9.914821	2.408384	-2.214461
6	7.976183	1.551583	-1.935139
1	8.207728	0.599236	-2.400263
6	6.669172	1.753820	-1.437371
6	5.503862	-2.482518	0.608196
1	4.826803	-2.526032	1.471196
6	6.594349	-3.515506	0.822127
6	6.500817	-4.410780	1.892276
1	5.669207	-4.324837	2.588272
6	7.469792	-5.400752	2.082399
1	7.386643	-6.085136	2.922383
6	8.546678	-5.499720	1.200720
1	9.308449	-6.259650	1.350951
6	8.643363	-4.611633	0.122885
1	9.484150	-4.677443	-0.561974
6	7.670748	-3.633504	-0.068620
1	7.762044	-2.929414	-0.889730
6	4.701377	-2.822897	-0.653531
1	5.400111	-2.951205	-1.488719
1	4.204870	-3.785707	-0.504651
6	6.838547	-0.514542	1.613808
1	6.918846	0.551492	1.391314
6	8.271917	-1.044484	1.628640
6	9.136787	-0.659239	0.596078
1	8.769013	0.004679	-0.177798
6	10.453131	-1.114706	0.548968
1	11.103648	-0.803250	-0.264173
6	10.934077	-1.964616	1.549127
1	11.957839	-2.326918	1.516299
6	10.088629	-2.337583	2.595309
1	10.450863	-2.995556	3.380435
6	8.770401	-1.875485	2.638058
1	8.131015	-2.190353	3.454715
6	6.105061	-0.643980	2.952757
1	5.121362	-0.174050	2.880776
1	5.971500	-1.686373	3.253771
1	6.671785	-0.137031	3.739421
6	2.318315	-1.070200	0.755855

1	1.559398	-0.299935	0.679539
1	3.003253	-0.913907	1.585731
6	1.998348	-2.432440	0.445753
1	2.635957	-3.175261	0.912855
6	0.817255	-2.930609	-0.174793
1	0.168654	-2.225006	-0.676007
6	4.022496	-1.428697	-3.273842
1	5.069154	-1.720004	-3.222733
6	3.074783	-2.474430	-3.115846
1	3.468441	-3.480273	-2.970482
6	1.662516	-2.437511	-3.672419
1	1.680858	-2.665149	-4.749895
1	1.101479	-3.246424	-3.199723
6	0.923776	-1.105375	-3.433387
1	1.067264	-0.431602	-4.282261
1	-0.150876	-1.297224	-3.390687
6	1.332603	-0.373143	-2.159149
1	0.588904	-0.340278	-1.367119
6	2.317779	0.603716	-2.123063
1	2.263352	1.332004	-1.320746
6	3.167382	1.014023	-3.309561
1	3.978624	1.641595	-2.937885
1	2.558247	1.645894	-3.969469
6	3.763633	-0.168918	-4.105441
1	3.109604	-0.426838	-4.945559
1	4.711027	0.153960	-4.547676
6	0.732928	-4.322475	-0.646696
6	1.632388	-5.328497	-0.237527
6	-0.281065	-4.677026	-1.556531
6	1.516381	-6.630094	-0.720953
1	2.426262	-5.100209	0.464569
6	-0.398245	-5.978573	-2.040027
1	-0.980711	-3.918388	-1.884172
6	0.499392	-6.963978	-1.622039
1	2.221314	-7.388102	-0.391630
1	-1.190821	-6.222555	-2.741667
1	0.411355	-7.980124	-1.995193
7	-2.319757	-4.676802	0.726304
6	-3.368129	-5.177616	-0.152904
1	-4.255889	-5.464131	0.425316
1	-3.004638	-6.058515	-0.692500
1	-3.645772	-4.403945	-0.863112
6	-1.663159	-5.672476	1.570751
1	-0.686093	-5.961851	1.171121
1	-2.297112	-6.560357	1.606387
1	-1.545581	-5.312153	2.593206
1	0.731780	0.007933	4.644936
1	0.271878	-2.266163	3.762167
35	0.201993	2.776895	3.513522

P2-C1 *re-re* conf2

Number of imaginary frequencies : 1
The smallest frequency is : -137.3962 cm(-1)
Electronic energy : HF=-7222.6278114
Zero-point correction= 1.754810
(Hartree/Particle)
Thermal correction to Energy= 1.873359
Thermal correction to Enthalpy= 1.874303
Thermal correction to Gibbs Free Energy= 1.591878
Sum of electronic and zero-point Energies= -7220.873001
Sum of electronic and thermal Energies= -7220.754453
Sum of electronic and thermal Enthalpies= -7220.753508
Sum of electronic and thermal Free Energies= -7221.035933

Cartesian Coordinates

26	-8.123830	0.204817	-0.683927
15	-3.132747	1.198590	-1.972785
15	-4.000833	0.629849	1.659803
6	-6.156690	0.873804	-0.966363
6	-6.291582	0.146445	0.273574
6	-6.735904	-1.174737	-0.041560
1	-6.941051	-1.960623	0.672289
6	-6.909847	-1.263180	-1.455847
1	-7.272232	-2.125234	-1.997412
6	-6.552872	-0.005819	-2.024679
1	-6.595405	0.253864	-3.071878
6	-9.466827	1.394445	0.361458
1	-9.192734	2.071904	1.159431
6	-9.802175	0.013870	0.513080
1	-9.819592	-0.538898	1.442826
6	-10.059790	-0.523214	-0.785216
1	-10.303576	-1.553319	-1.009495
6	-9.883652	0.524484	-1.739583
1	-9.973240	0.428638	-2.813632
6	-9.519449	1.708777	-1.032295
1	-9.289638	2.665763	-1.480591
6	-5.636227	2.266554	-1.076882
6	-6.429587	3.328160	-0.614828
1	-7.409802	3.097080	-0.218331
6	-5.987012	4.649856	-0.645487
1	-6.617885	5.442727	-0.256545
6	-4.728217	4.937427	-1.166532
1	-4.365227	5.959493	-1.200712
6	-3.917224	3.898765	-1.623499
1	-2.934798	4.142698	-2.008904
6	-4.335965	2.558612	-1.570007
6	-5.896603	0.683288	1.622884
1	-6.155847	1.743175	1.643569
6	-6.589979	-0.005894	2.801336
1	-6.291410	0.445409	3.751596
1	-6.357697	-1.073434	2.848205
1	-7.673959	0.098343	2.691782
6	-1.620922	2.142911	-2.443869
6	-0.769686	2.550694	-1.402612
1	-0.958555	2.208684	-0.391279
6	0.304277	3.402272	-1.661963
1	0.942535	3.723868	-0.849577
6	0.567313	3.822954	-2.967828
1	1.412791	4.475193	-3.167330
6	-0.246152	3.385154	-4.014705
1	-0.038506	3.695587	-5.034697
6	-1.341324	2.556600	-3.755104
1	-1.981951	2.249119	-4.574863
6	-3.732211	0.499302	-3.560832
6	-4.464886	1.254067	-4.490390
1	-4.700886	2.293347	-4.281471
6	-4.905950	0.667107	-5.677594
1	-5.475059	1.256333	-6.391010
6	-4.621204	-0.675782	-5.946196
1	-4.973197	-1.131797	-6.867066
6	-3.887095	-1.430113	-5.027782
1	-3.670054	-2.475292	-5.228498
6	-3.444029	-0.843807	-3.840577
1	-2.887264	-1.432059	-3.120240
6	-3.415752	2.330194	2.055306
6	-2.023077	2.495509	2.067452
1	-1.387458	1.629709	1.911397
6	-1.460009	3.760121	2.235426
6	-2.265409	4.890007	2.361671
1	-1.826279	5.875922	2.466685
6	-3.651230	4.724875	2.334576
6	-4.227969	3.461500	2.199829
1	-5.306733	3.386918	2.186479
6	-3.510402	-0.363061	3.129032
6	-3.637351	-1.755537	3.002554
1	-4.068750	-2.180391	2.103758
6	-3.176788	-2.599758	4.008590
6	-2.557424	-2.081300	5.147057
1	-2.181401	-2.741917	5.920028
6	-2.419641	-0.700412	5.264888
6	-2.900411	0.159351	4.273648
1	-2.779819	1.228868	4.398918
29	-2.839595	-0.191799	-0.212967
6	-1.651058	-0.137351	6.427414
6	-3.240742	-4.091098	3.829599
6	0.037777	3.866988	2.295458
6	-4.515539	5.952937	2.424933
9	-4.283961	6.798085	1.390200

9	-5.835130	5.662422	2.413714
9	-4.267026	6.655228	3.555005
9	0.627862	3.065410	1.360426
9	0.527756	3.462856	3.490381
9	0.486273	5.118575	2.074983
9	-2.007827	1.132758	6.712831
9	-0.314866	-0.116276	6.163946
9	-1.809224	-0.870708	7.549759
9	-3.569034	-4.723366	4.977487
9	-4.135022	-4.459028	2.888460
9	-2.035524	-4.596975	3.445913
6	-0.596946	-1.310832	1.558812
6	-0.839938	-2.647708	1.083186
6	-1.978417	-3.108230	0.349191
1	-0.324117	-3.444415	1.599846
77	3.154574	-0.810432	-1.893890
15	4.874631	-0.232943	-0.533709
8	4.808648	1.011509	0.566420
8	6.215817	0.219437	-1.404746
7	5.231685	-1.484954	0.535020
6	4.834519	2.332021	0.143781
6	3.650287	3.074423	0.336794
1	2.810277	2.588501	0.815203
6	3.598694	4.385027	-0.066524
1	2.704734	4.976439	0.110955
6	4.705715	4.971979	-0.738501
6	4.630567	6.292194	-1.258949
1	3.711158	6.853533	-1.113492
6	5.689480	6.844826	-1.943540
1	5.618633	7.852547	-2.342226
6	6.870431	6.090141	-2.140267
1	7.695768	6.519839	-2.700607
6	6.983134	4.813735	-1.632341
1	7.892632	4.248179	-1.798522
6	5.916747	4.216388	-0.904455
6	5.999840	2.881927	-0.365520
6	7.272569	2.106319	-0.331999
6	8.464311	2.635319	0.284726
6	8.474198	3.855462	1.017595
1	7.552288	4.411399	1.137394
6	9.632128	4.332606	1.592768
1	9.608321	5.262376	2.153940
6	10.848884	3.620938	1.467984
1	11.754736	4.013078	1.920839
6	10.872338	2.424548	0.788186
1	11.793891	1.854778	0.702214
6	9.692478	1.895856	0.197354
6	9.706403	0.634997	-0.457211
1	10.642210	0.088448	-0.532555
6	8.545828	0.095887	-0.953691
1	8.522875	-0.882628	-1.421316
6	7.339571	0.824000	-0.857761
6	4.400102	-2.691762	0.281417
1	3.515556	-2.648988	0.929480
6	5.112676	-4.002899	0.558555
6	4.455132	-5.008234	1.274712
1	3.464534	-4.815143	1.681844
6	5.065247	-6.247783	1.488390
1	4.545062	-7.017015	2.052858
6	6.345334	-6.489926	0.988217
1	6.828803	-7.447011	1.162775
6	7.006218	-5.490578	0.264330
1	8.006480	-5.669336	-0.120232
6	6.390088	-4.260985	0.043266
1	6.911243	-3.477228	-0.497811
6	3.937040	-2.681577	-1.180741
1	4.794585	-2.948374	-1.809447
1	3.197314	-3.471815	-1.318555
6	5.700064	-1.204269	1.936317
1	6.162363	-0.218192	1.886574
6	6.802579	-2.156978	2.389046
6	8.101540	-1.950218	1.907121
1	8.291516	-1.116026	1.240281
6	9.146060	-2.802795	2.262467
1	10.144605	-2.625236	1.871785
6	8.907226	-3.878177	3.122434
1	9.715622	-4.549031	3.399683
6	7.621965	-4.078644	3.630011
1	7.425330	-4.909013	4.302493
6	6.579986	-3.220121	3.271713
1	5.587813	-3.404039	3.668203
6	4.517388	-1.101523	2.906428
1	3.825162	-0.331123	2.559577
1	3.967779	-2.041876	3.001307
1	4.874820	-0.824035	3.902655
6	1.893470	-0.285061	-0.200998
1	1.666502	0.777440	-0.167093
1	2.242065	-0.673042	0.753858
6	1.006479	-1.118566	-0.963988
1	0.284058	-0.646689	-1.617112
6	0.870653	-2.498851	-0.722995
1	1.538935	-2.932227	0.010376
6	4.420417	-1.061445	-3.710510
1	5.288197	-1.650741	-3.425455
6	3.212461	-1.779803	-3.897356
1	3.256647	-2.859875	-3.758256
6	2.048303	-1.327666	-4.762564
1	2.251803	-1.561639	-5.819201
1	1.179096	-1.928789	-4.477856
6	1.697133	0.166319	-4.609713
1	2.253915	0.767067	-5.335537
1	0.638389	0.312232	-4.845891
6	1.949838	0.721423	-3.210744
1	1.060928	0.960727	-2.639171
6	3.120274	1.354659	-2.816236
1	3.049086	2.046132	-1.982317
6	4.351912	1.520850	-3.682239
1	5.174390	1.839216	-3.038853
1	4.175358	2.341134	-4.393988
6	4.766985	0.239497	-4.439088
1	4.312308	0.221344	-5.434678
1	5.848748	0.266793	-4.601092
6	0.262198	-3.443384	-1.648214
6	-0.595839	-3.035189	-2.688853
6	0.544177	-4.816110	-1.511291
6	-1.150214	-3.968543	-3.558631
1	-0.825637	-1.983994	-2.814789
6	-0.001512	-5.749557	-2.392574
1	1.199047	-5.144362	-0.707909
6	-0.853573	-5.329879	-3.417100
1	-1.811414	-3.634225	-4.352615
1	0.233634	-6.803551	-2.276130
1	-1.283594	-6.055186	-4.101692
6	-2.182133	-4.515505	0.264164
6	-3.216414	-5.049806	-0.473445
1	-1.506797	-5.174110	0.797120
6	-4.072537	-4.157089	-1.125492
6	-3.867160	-2.796496	-1.009406
1	-4.521848	-2.087723	-1.497711
7	-2.846025	-2.273531	-0.300442
8	-1.038046	-0.269545	0.983126
7	0.230638	-1.148996	2.642535
6	0.669024	0.189289	3.023469
1	1.672535	0.128951	3.453752
1	0.002836	0.636616	3.769449
1	0.704748	0.830204	2.147669
6	0.618167	-2.233399	3.540728
1	1.546396	-2.725316	3.219247
1	-0.170166	-2.982179	3.620539
1	0.777517	-1.818695	4.538273
1	-3.356787	-6.122981	-0.541506
35	-5.556135	-4.822422	-2.216132

P2-C1 *si-re* conf2

Number of imaginary frequencies : 1
The smallest frequency is : -133.9792 cm(-1)
Electronic energy : HF=-7222.6089123
Zero-point correction= 1.754200
(Hartree/Particle)

Thermal correction to Energy= 1.873225
Thermal correction to Enthalpy= 1.874170
Thermal correction to Gibbs Free Energy= 1.588051
Sum of electronic and zero-point Energies= -7220.854713
Sum of electronic and thermal Energies= -7220.735687
Sum of electronic and thermal Enthalpies= -7220.734743
Sum of electronic and thermal Free Energies= -7221.020861

Cartesian Coordinates

77	4.163394	-0.905691	1.466574
15	5.888732	-0.077176	0.255889
8	6.427972	-0.741237	-1.163095
8	7.297192	-0.051063	1.141311
7	5.526030	1.472669	-0.289678
6	7.373590	-1.759853	-1.201906
6	6.930404	-3.001340	-1.708319
1	5.902321	-3.086230	-2.044108
6	7.803080	-4.058401	-1.773576
1	7.477209	-5.015994	-2.169464
6	9.135200	-3.923533	-1.298271
6	10.023451	-5.033099	-1.288988
1	9.668713	-5.983292	-1.679548
6	11.298091	-4.914661	-0.783544
1	11.967334	-5.769982	-0.776304
6	11.731230	-3.675381	-0.255291
1	12.728349	-3.589994	0.167011
6	10.900216	-2.575970	-0.264725
1	11.249247	-1.640940	0.156110
6	9.584273	-2.653321	-0.801413
6	8.686878	-1.524912	-0.823998
6	9.131060	-0.165153	-0.405705
6	10.259841	0.499136	-1.003412
6	10.915591	0.001273	-2.163882
1	10.555157	-0.910042	-2.626731
6	11.987146	0.669155	-2.715540
1	12.464602	0.274149	-3.607647
6	12.468408	1.868040	-2.136575
1	13.316937	2.380022	-2.580770
6	11.849689	2.386489	-1.021775
1	12.197906	3.314493	-0.575657
6	10.732372	1.731089	-0.435400
6	10.060291	2.289718	0.685321
1	10.435007	3.211361	1.120941
6	8.922668	1.701285	1.180411
1	8.369978	2.130370	2.008630
6	8.456944	0.499467	0.606157
6	4.345464	2.037661	0.409395
1	3.475895	1.937405	-0.248412
6	4.479223	3.501004	0.794688
6	3.349177	4.325700	0.743645
1	2.408198	3.923255	0.376287
6	3.421402	5.659652	1.152933
1	2.537528	6.289938	1.099395
6	4.629058	6.182399	1.619946
1	4.692686	7.222365	1.927488
6	5.758075	5.358610	1.686749
1	6.703280	5.759160	2.042741
6	5.680374	4.026139	1.285875
1	6.561794	3.395180	1.308350
6	4.090902	1.230695	1.694764
1	4.846156	1.521440	2.435655
1	3.129220	1.533692	2.111887
6	5.851346	1.915907	-1.689169
1	6.709416	1.311991	-1.980335
6	6.320023	3.363303	-1.753660
6	7.675308	3.635094	-1.531301
1	8.355308	2.811640	-1.343467
6	8.157419	4.943962	-1.539939
1	9.212871	5.130450	-1.360139
6	7.283810	6.006417	-1.785454
1	7.651586	7.028748	-1.788952
6	5.934698	5.744749	-2.038152
1	5.248907	6.563868	-2.235720
6	5.459112	4.432178	-2.030150
1	4.406439	4.249913	-2.217050
6	4.716799	1.588847	-2.667699
1	4.525778	0.512819	-2.668453
1	3.784830	2.105667	-2.426314
1	5.006847	1.887374	-3.679864
6	3.037761	-1.080624	-0.376645
1	3.250356	-2.010803	-0.903345
1	3.087164	-0.209065	-1.026858
6	1.984389	-1.105518	0.609651
1	1.588149	-2.058477	0.936665
6	1.304706	0.055352	1.014936
1	1.665432	0.999067	0.627751
6	5.355750	-1.009332	3.368924
1	5.874425	-0.059149	3.466968
6	3.980141	-1.004088	3.690594
1	3.560276	-0.059059	4.035427
6	3.157283	-2.218362	4.088608
1	3.287247	-2.422849	5.162474
1	2.103019	-1.955203	3.952852
6	3.466178	-3.489944	3.270072
1	4.279888	-4.054185	3.734456
1	2.590283	-4.146401	3.293166
6	3.819448	-3.212938	1.811765
1	3.066339	-3.501265	1.083016
6	5.110879	-3.051851	1.328960
1	5.266572	-3.239446	0.270670
6	6.370373	-3.061186	2.171244
1	7.185337	-2.666713	1.560383
1	6.633552	-4.103002	2.405119
6	6.266219	-2.234389	3.472491
1	5.920150	-2.865608	4.296711
1	7.269243	-1.896164	3.748739
6	0.423209	0.153847	2.164323
6	-0.190956	-0.969778	2.757292
6	0.198213	1.423973	2.733367
6	-0.990330	-0.824057	3.887410
1	-0.051263	-1.953761	2.324037
6	-0.578047	1.562088	3.881018
1	0.649202	2.297584	2.271117
6	-1.177606	0.439613	4.458778
1	-1.474135	-1.692758	4.324302
1	-0.733247	2.544433	4.314785
1	-1.798768	0.546885	5.341817
26	-6.182655	4.443637	-1.331342
15	-4.813475	0.900663	2.229912
15	-4.756076	-0.116499	-1.412197
6	-5.924551	2.827050	-0.026656
6	-5.288438	2.580247	-1.300279
6	-4.306299	3.595846	-1.500767
1	-3.667186	3.693252	-2.367563
6	-4.348928	4.486628	-0.389097
1	-3.752940	5.380879	-0.267624
6	-5.347345	4.020444	0.513389
1	-5.632775	4.486764	1.444599
6	-7.804480	4.453376	-2.625421
1	-8.258833	3.566263	-3.046045
6	-6.716421	5.187950	-3.189295
1	-6.197197	4.951456	-4.108485
6	-6.401779	6.262154	-2.302183
1	-5.601844	6.979220	-2.431923
6	-7.296340	6.194415	-1.191038
1	-7.293580	6.849928	-0.330173
6	-8.164057	5.080245	-1.391604
1	-8.937161	4.753802	-0.709786
6	-6.926451	1.926641	0.615918
6	-8.235968	1.882156	0.115661
1	-8.486421	2.528081	-0.716152
6	-9.199158	1.022607	0.643357
1	-10.194829	0.993768	0.213130
6	-8.865845	0.192000	1.710186
1	-9.602504	-0.484701	2.132527
6	-7.568772	0.215485	2.225078
1	-7.323067	-0.445760	3.048463
6	-6.581271	1.053817	1.684943
6	-5.592384	1.404758	-2.187844

1	-6.659145	1.207138	-2.082992
6	-5.312956	1.642793	-3.674790
1	-5.558061	0.758184	-4.268888
1	-4.270127	1.901548	-3.870563
1	-5.932302	2.475941	-4.019818
6	-4.832566	-0.341420	3.590852
6	-4.982076	-1.692853	3.234217
1	-5.154299	-1.956329	2.196432
6	-4.925585	-2.697515	4.199229
1	-5.059960	-3.732836	3.904035
6	-4.693236	-2.366047	5.537861
1	-4.636775	-3.147090	6.290717
6	-4.536101	-1.027543	5.901859
1	-4.356510	-0.762363	6.940056
6	-4.611110	-0.018733	4.937015
1	-4.484713	1.014691	5.238777
6	-4.476299	2.496678	3.068280
6	-5.423281	3.105152	3.907920
1	-6.374780	2.616378	4.098643
6	-5.151979	4.346145	4.484839
1	-5.888353	4.814377	5.131856
6	-3.935081	4.987469	4.225671
1	-3.728014	5.956514	4.671261
6	-2.991291	4.383776	3.391554
1	-2.049578	4.884174	3.182256
6	-3.259576	3.141808	2.810831
1	-2.547905	2.684885	2.131796
6	-6.128990	-1.322825	-1.131467
6	-5.826478	-2.456672	-0.364250
1	-4.807677	-2.632814	-0.044362
6	-6.824244	-3.357184	0.008806
6	-8.151655	-3.135562	-0.350068
1	-8.932326	-3.815841	-0.027884
6	-8.455763	-2.010062	-1.114552
6	-7.459706	-1.123004	-1.520511
1	-7.750484	-0.272111	-2.120345
6	-3.720982	-0.910581	-2.712345
6	-2.643019	-0.169266	-3.225360
1	-2.493700	0.860122	-2.922970
6	-1.740703	-0.755385	-4.108772
6	-1.852598	-2.101908	-4.460003
1	-1.134019	-2.562042	-5.128793
6	-2.903508	-2.843656	-3.928025
6	-3.840846	-2.256425	-3.074861
1	-4.652923	-2.864304	-2.694553
29	-3.478791	0.287427	0.508578
6	-2.971086	-4.322740	-4.187502
6	-0.566128	0.029074	-4.620566
6	-6.457123	-4.587657	0.791600
6	-9.898203	-1.746514	-1.454179
9	-10.659046	-1.675956	-0.334110
9	-10.070351	-0.586200	-2.124887
9	-10.424146	-2.733441	-2.215285
9	-5.388490	-4.367756	1.598683
9	-6.122872	-5.616422	-0.020799
9	-7.471253	-5.012830	1.574262
9	-4.232457	-4.799503	-4.107389
9	-2.235026	-5.010097	-3.275891
9	-2.485976	-4.650737	-5.404812
9	-0.321670	-0.218033	-5.924952
9	-0.740385	1.364091	-4.485193
9	0.578905	-0.284780	-3.952431
6	-2.356620	-2.512084	0.583757
6	-0.967546	-1.038396	-0.593572
6	-1.741845	-3.619834	0.027717
1	-3.149185	-2.620661	1.314884
6	-0.345298	-2.159338	-1.221581
6	-0.728888	-3.449304	-0.923198
1	0.431922	-1.980638	-1.955736
6	-0.396240	0.245862	-0.838233
6	-0.914031	1.530791	-0.468855
8	-1.983153	1.704604	0.187551
7	-2.009585	-1.249411	0.268601
1	0.399330	0.226632	-1.565823
7	-0.169645	2.648404	-0.800301
6	-0.727213	3.975139	-0.561924
1	-1.136639	4.408406	-1.485448
1	0.057007	4.642527	-0.188565
1	-1.526033	3.907564	0.172572
6	0.942249	2.592833	-1.745971
1	1.674453	1.837856	-1.454604
1	1.448073	3.559864	-1.745668
1	0.607981	2.377763	-2.767387
1	-0.262844	-4.297558	-1.411398
35	-2.293185	-5.420096	0.559052

End of Supporting Information