Supporting Information

for

Refined Transition State Models for Proline-Catalyzed Asymmetric Michael Reactions Under Basic and Base-free Conditions

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1. Additional Details on Different Transition State Models

The nomenclature used for different TS is given in Scheme S1. The prochiral faces (*re* or *si*) of enamine and nitrostyrene have been used to distinguish between different diastereomeric TSs for the stereoselective C–C bond formation. Four different TS-models have been considered in the present study as shown in Scheme S2.

The TSs (**1-2**) with two different conformations of the pyrrolidine ring in proline-enamine has been studied (Figure S1a) for first model system. The enamine (**1**) in '*up*' conformation is of lower energy than the '*down*' conformation. Calculations were carried out, first using the '*up*' conformation. For each mode of addition (*re-re*, *si-si*, *si-re*, and *re-si*) two different types of TSs have been located that maintain H-bonding interaction between the –COOH group and $–NO_2$ group. These TSs differ in the interacting O-atom of NO_2 group in the H-bonding (Figure S1b). The optimized geometries of these TSs are given in Figure S2.

In the case of *syn*-face addition, since the electrophile is very close to the COOH group we have also studied the different position of OH in both *si-si* and *si-re* modes of addition. For example, **(1-2)I**$_{syn}$ (*si-si*)$_1$ and **(1-2)I**$_{syn\text{-Conf}}$(*si-si*)$_1$ in Figure S2. Then we have studied the C–C bond formation with '*down*' conformation of proline enamine (**1**). Only the TS for the *re-re* mode of addition is lower in energy in the'*down*' conformation than the '*up*' conformation. Hence, the difference between *re-re* and *si-si* mode further increases. Besides, TSs with different cyclohexane ring conformations, with its C4 pointing away from the incoming electrophile is also considered. Such TSs are found to be of higher energy (Table S2). The stereoselectivity could not be explained by TS **1-2** model (*syn*-face addition) at all levels of theory (Table S1).

The Michael reaction is quite different as compared to an aldol reaction. In Michael addition transition states for the critical C–C bond formation (1) the developing negative charge is stabilized by the NO_2 group, (2) H-transfer occurs after the C–C bond formation and, (3) there are two extra atoms between the site of attack of the nucleophile and the O-atom involved in H-bonding (Scheme S3). Hence, the addition of nitrostyrene can occur from the face *anti* to the COOH group (*anti*-face addition) while still maintaining H-bonding. The *anti*-face addition has been studied mainly with '*down*' conformer, as the two TSs optimized with the '*up*' conformer (*re-re* and *re-si* mode) are of higher energy. In *anti*-face addition, the *re-re* and *re-si* modes of addition are of lower energy than the *syn*-face addition (except in the *re-si* mode at the SMD/mPW1K/6-31+G** level of theory) whereas for the other two modes of addition *syn*-face addition with '*up*' conformer is more preferred. All these different models are

considered toward identifying the lowest energy diastereomer. The stereoselectivity could not be explained (Table S1).

Since, in nitrostyrene the NO_2 group can stabilize the developing negative charge, the TS without H-bonding (**(1-2)'**) has also been studied. It is found to be lower energy than TS (**1-2**) with H-bonding. We have studied different rotameric possibilities along the C–C bond formation named as 60, 180, 300 depending on the dihedral between enamine double bond and the double bond of nitrostyrene. We have first done conformational sampling by optimizing TS in the *re-re* mode (Figure S8, Table S3-S4). The lowest energy TS is considered for further analyses. This model has been found to be successful in rationalizing the experimental stereoselectivity (Table S5).

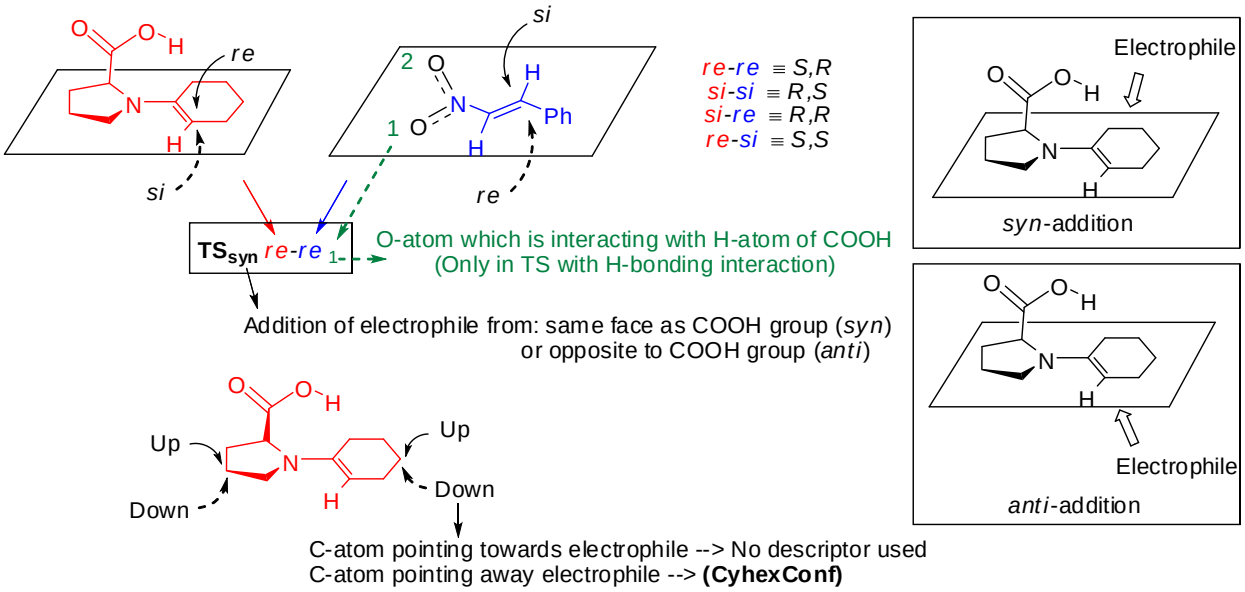
After analyzing the transition state involving enamine carboxylic acid, under base-free reaction conditions, we examined the nature of the transition states with enamine carboxylate, which is the potential intermediate under basic reaction conditions. Two model systems have been considered; one that involves enamine carboxylate and nitrostyrene (TS **3-4**), and the other consisting of enamine carboxylate (**3**) + $DBUH^+$ and nitrostyrene (TS $\mathbf{(3\text{-}4)_{DBU}}$). For the both TS models we have used the insights of conformational details derived from TS **(1-2)'**.

For TS **3-4** we have studied both *anti*- and *syn*-face addition. The TS in *syn*-face addition has been found to be of higher energy as compared to the *anti*-face addition. In *syn*-face addition due to steric interaction of COO^- group with nitrostyrene TSs are higher in energy. However, surprisingly in the gas phase calculation the TS for *re-re* mode (**(3-4)***syn*$(re\text{-}re)_{180}$) for *syn*-addition has the lowest energy (Table S7). Whereas other TSs of *syn*-addition are of higher in energy.

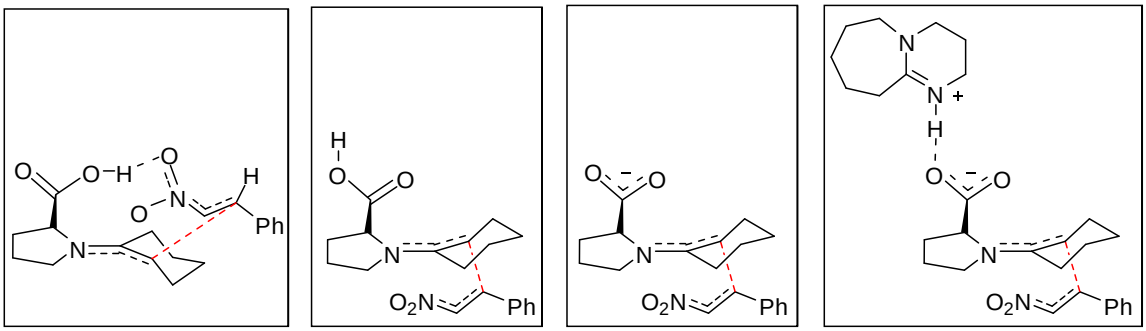
The interaction of DBU with **1** leads to the formation of **3**+$DBUH^+$ ($\mathbf{3_{DBU}}$)**.** In TS $\mathbf{(3\text{-}4)_{DBU}}$**,** $DBUH^+$ can interact with COO^- group of enamine or NO_2 group of nitrostyrene. The interaction of $DBUH^+$ with NO_2 group (instead of COO^-) in the TS of C–C bond formation is higher in energy by ~9 kcal/mol (Figure S14). This TS is higher in energy due to steric interaction between DBU and enamine moieties. Besides this, it also reflects the fact that NO_2 stabilizes the negative charge more effectively than the COO^-. The TS with $DBUH^+$ interacting with COO^- of **3** (TS $\mathbf{(3\text{-}4)_{DBU}}$) has been studied for only *anti*-addition as the *syn*-addition has been found to have higher energy in TS **3-4**.

There is difference between the gas phase and the solvent phase geometries in the case of $\mathbf{3_{DBU}}$ adduct. The proton remains with the COOH group in $\mathbf{3_{DBU}}$ adduct in the gas phase geometry. The TS in the gas phase involves simultaneous formation of C–C bond and transfer of proton from COOH to DBU.

Another conformation of DBU in TS **(3-4)$_{DBU}$** at the SMD$_{THF}$/M06-2X/6-31+G** is located, in which DBU is bent toward the cyclohexane ring of enamine (Figure S17, Table S13). Also at this level of theory the TS **(3-4)$_{DBU2}$** has been lower in energy. Further, for *si-si* mode the TS with dihedral '300' instead of '180' is found to be lower in energy at this level of theory. It is noticed that the energy difference between TS with **3$_{DBU}$**, **3$_{DBU1}$** and **3$_{DBU2}$** conformations at various level of theory is very less. Also the difference between the enthalpy of TS **(3-4)$_{DBU\text{-}anti}$**(*re-re*)$_{60}$ for different enamine-DBU adducts is very small as compared to the Gibbs free energy differences (Table S8). The %ee obtained through the SMD$_{THF}$/M06-2X/6-31+G** level of theory is found to be overestimated as compared to the experimental values while all other levels of theory considered in this study offers lower %ee in line with the experimental observation (Table S14). The comparison of energies of different TS-models has been provided in Table S15-S16.

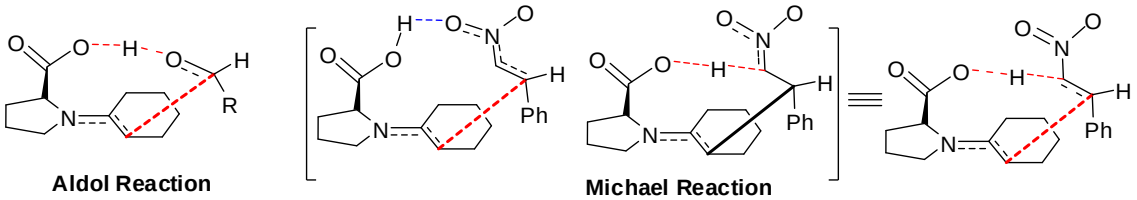


Scheme S1. The TS nomenclature employed in the manuscript.



(1-2) **(1-2)'** **(3-4)** **(3-4)$_{DBU}$**

Scheme S2. Four different TS models examined for the stereoselective bond formation in Michael reaction between the enamine (derived from cyclohexanone and proline) and nitrostyrene. First two are under base-free conditions while the rest are under basic conditions.



Aldol Reaction **Michael Reaction**

Scheme S3. Comparison of TSs for the stereoselective C–C bond formation in aldol and Michael reaction. In Michael reaction the C–C bond formation and H-transfer occurs in two steps. The two steps are also shown together for Michael reaction.

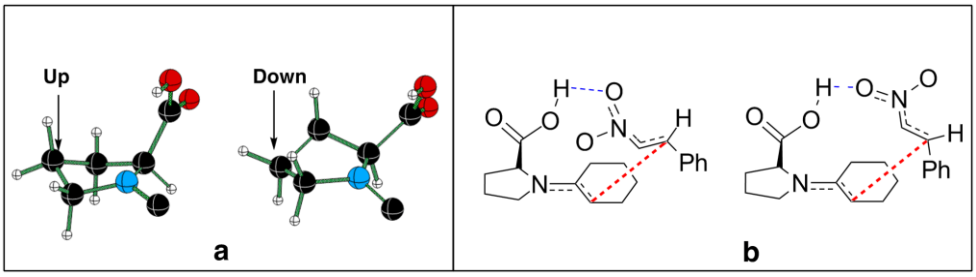
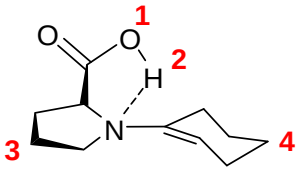
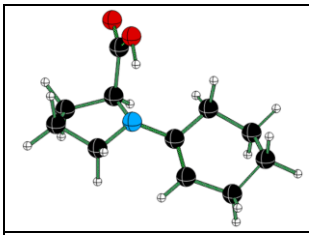
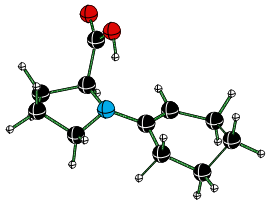
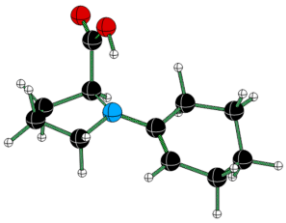
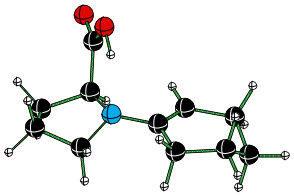


Figure S1. (a) Conformation of pyrrolidine ring in proline-enamine. (b) The TS **1-2** showing different O-atom of NO2 group involved in H-bonding with COOH group.



1 = ∠OCCN ≈ 0 or 180
2 = ∠HOCO ≈ 0 or 180
3 = Towards/Away from COOH
4 = Towards/Away from COOH

Changes in conformation/position of atoms (1, 2, 3, 4) leads to different conformations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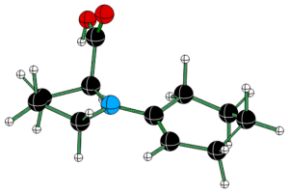	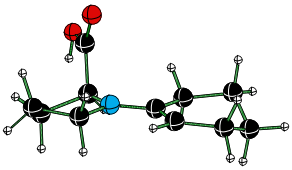	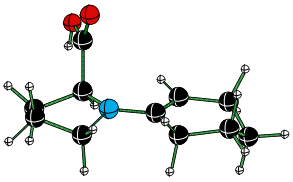	
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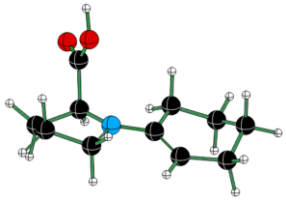	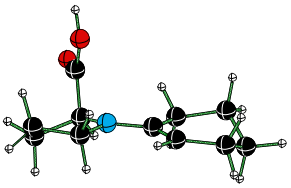	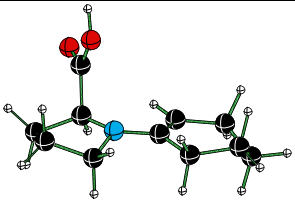	
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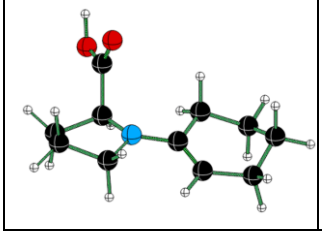	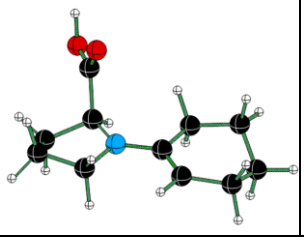	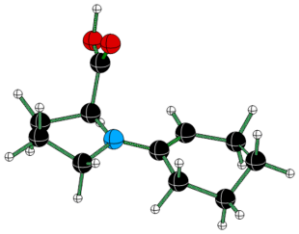	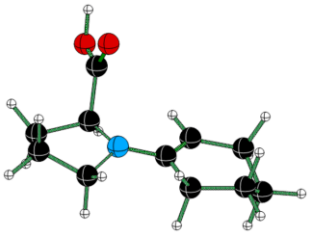

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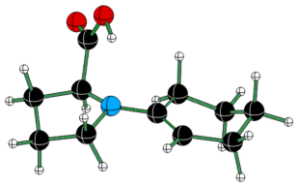	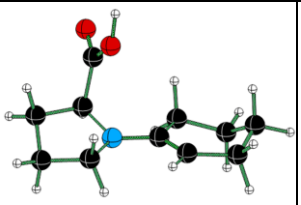	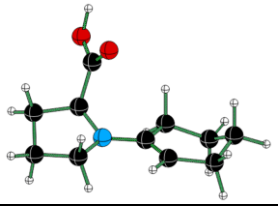	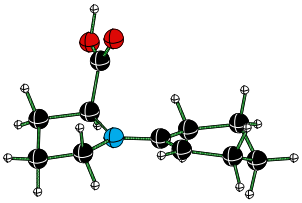
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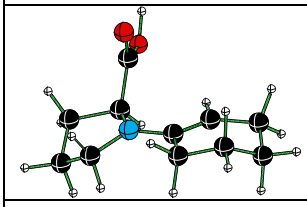			
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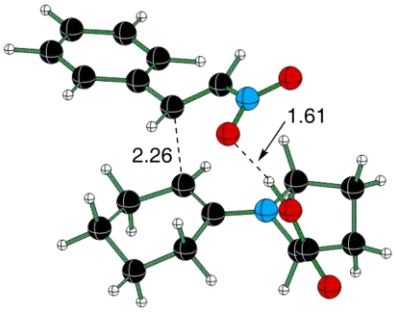
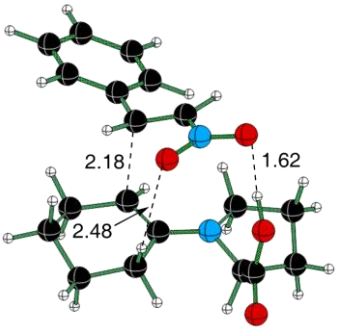
Figure S2. Different conformations of proline-enamine and their relative energies with respect to the lowest energy conformer obtained at the $SMD_{(THF)}$/mPW1K/6-31+G** level of theory.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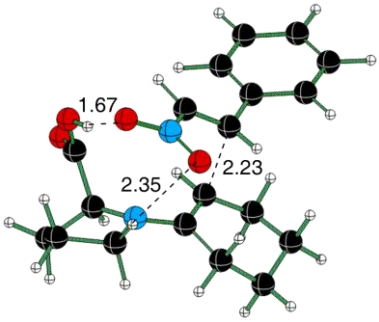	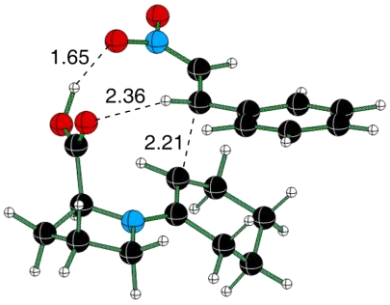
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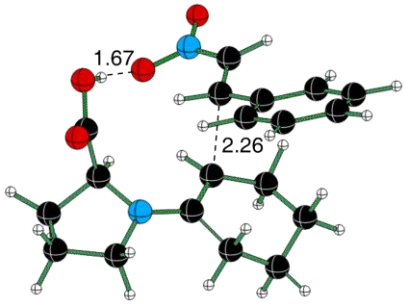
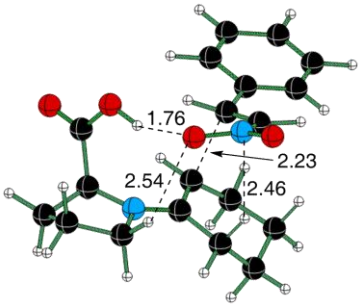
<tr><td> 
</td><td> 
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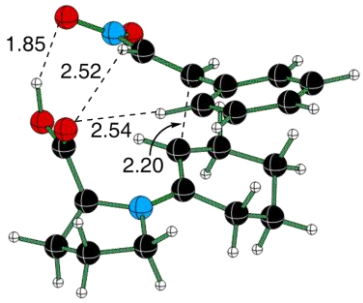
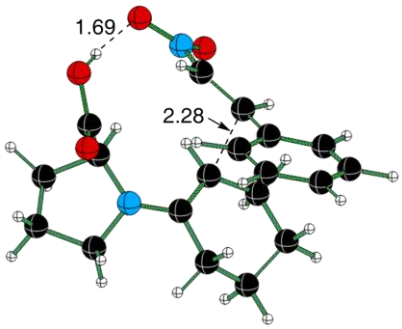
<tr><td> 
</td><td> 
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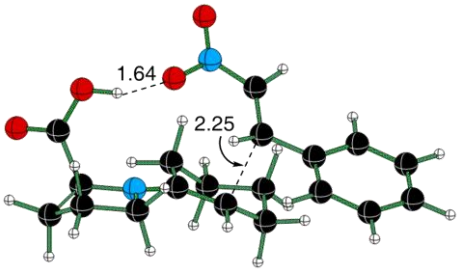
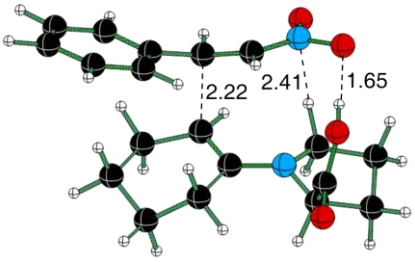
<tr><td> 
</td><td> 
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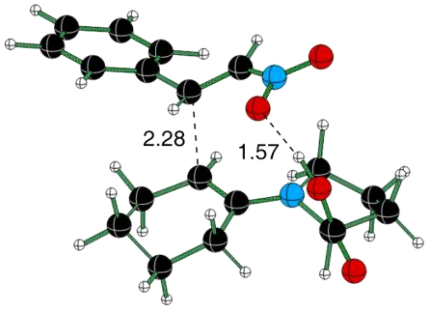
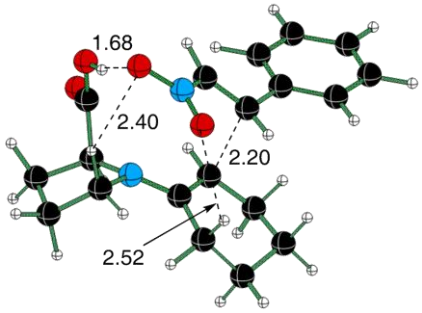
Figure S3. Optimized geometries of TS for C–C bond formation at the SMD_{THF}/mPW1K/6-31+G** level of theory for *syn*-addition having H-Bonding with '*up*' conformation of pyrrolidine.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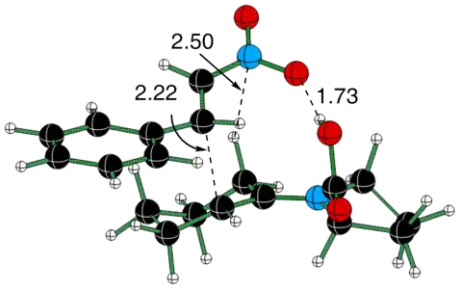
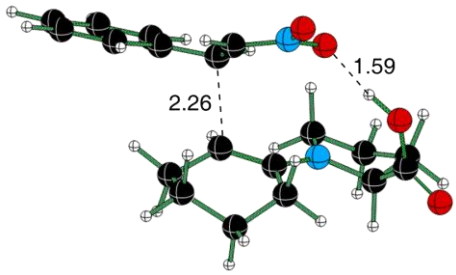
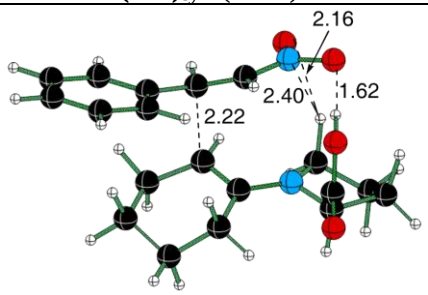
	
(1-2)$_{syn}$ (*si-re*)$_1$	**(1-2)$_{syn}$** (*re-si*)$_1$
	
(1-2)$_{syn}$ (*re-si*)$_2$	

Figure S4. Optimized geometries of TSs for C–C bond formation at the SMD$_{THF}$/mPW1K/6-31+G** level of theory for *syn*-addition having H-Bonding with '*down*' conformation of pyrrolidine.

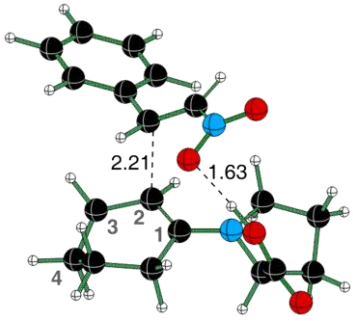
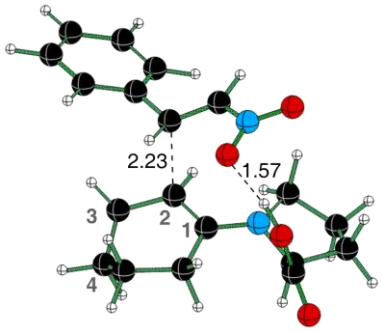
	
(1-2)$_{syn}$ (*re-re*)$_1$ (Cyhex$_{Conf}$) (up)	**(1-2)$_{syn}$** (*re-re*)$_1$ (Cyhex$_{Conf}$) (*down*)

Figure S5. Optimized geometries of TS for C–C bond formation for *re-re* mode of addition having 4th-carbon in cyclohexane pointing away from the incoming electrophile at the SMD$_{THF}$/mPW1K/6-31+G** level of theory for *syn*-addition having H-Bonding.

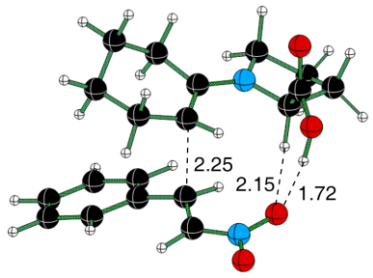
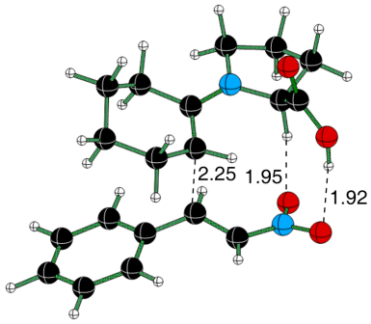
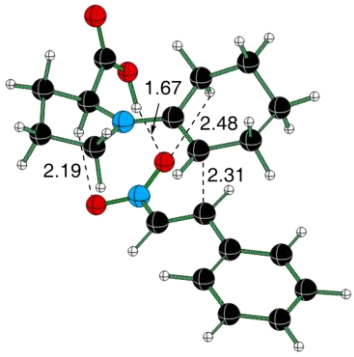
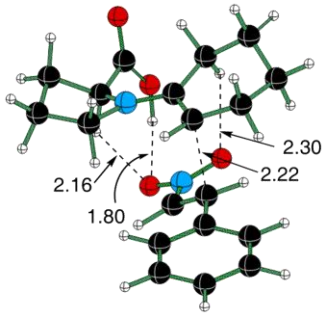
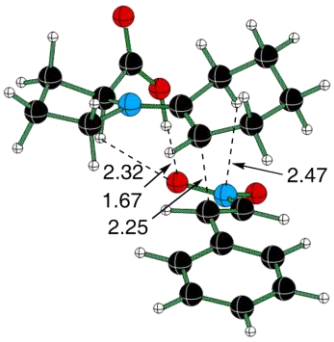
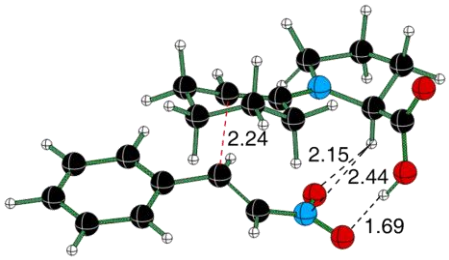
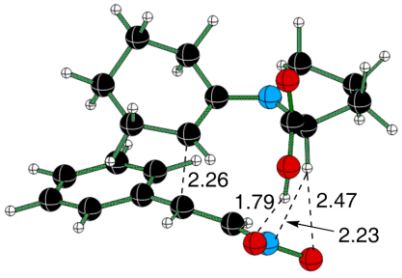
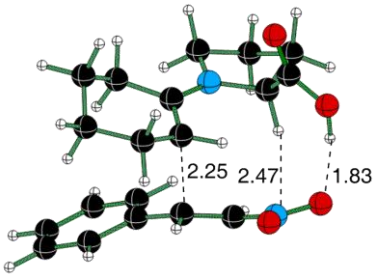
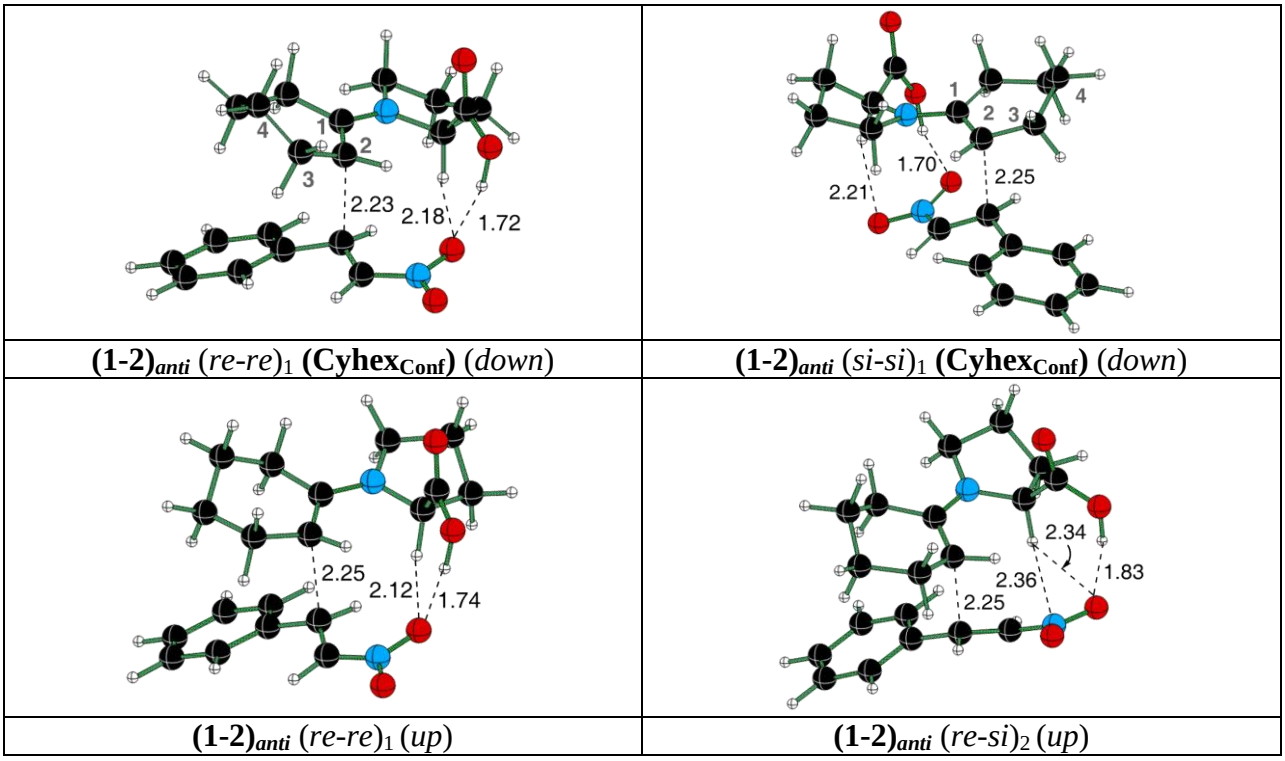
	
(1-2)*anti* (*re-re*)$_1$	**(1-2)*anti*** (*re-re*)$_2$
	
(1-2)*anti* (*si-si*)$_1$	**(1-2)*anti*** (*si-si*)$_2$
	
(1-2)*anti* (*si-re*)$_1$	**(1-2)*anti*** (*si-re*)$_2$
	
(1-2)*anti* (re-si)$_1$	**(1-2)*anti*** (*re-si*)$_2$

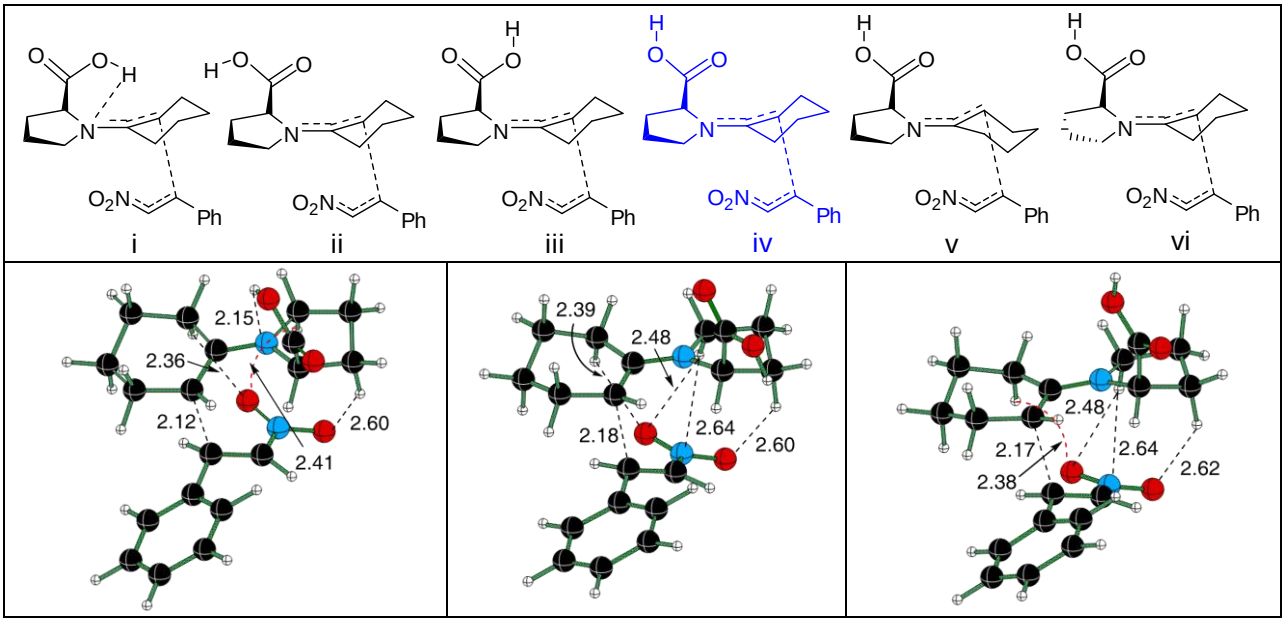
Figure S6. Optimized geometries of TS for C–C bond formation at the SMD$_{(THF)}$/mPW1K/6-31+G** level of theory for *anti*-addition having H-Bonding with '*down*' conformation of pyrrolidine.



(1-2)$_{anti}$ (*re-re*)$_1$ **(Cyhex$_{Conf}$)** (*down*) | **(1-2)**$_{anti}$ (*si-si*)$_1$ **(Cyhex$_{Conf}$)** (*down*)

(1-2)$_{anti}$ (*re-re*)$_1$ (*up*) | **(1-2)**$_{anti}$ (*re-si*)$_2$ (*up*)

Figure S7. Optimized geometries of TS for C–C bond formation at the SMD$_{(THF)}$/mPW1K/6-31+G** level of theory for *anti*-addition having H-Bonding with '*up*' conformation of pyrrolidine and '*down*' conformation of pyrrolidine with different conformation of cyclohexane.



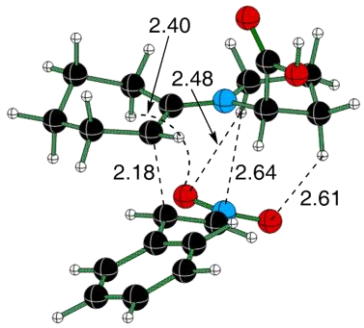
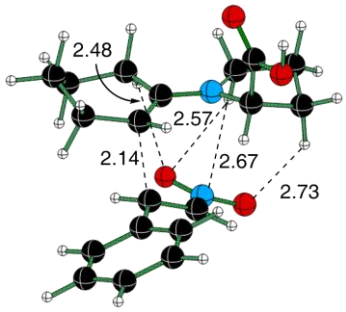
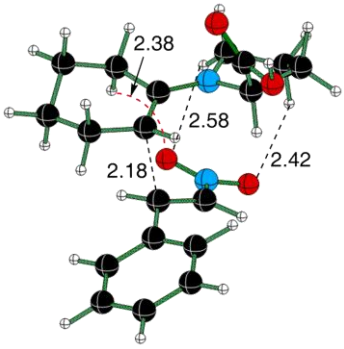
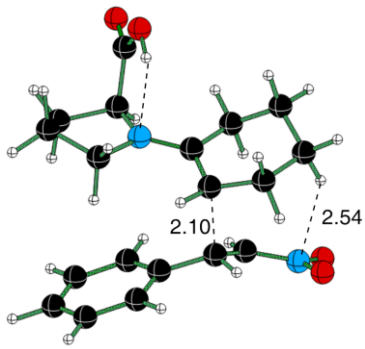
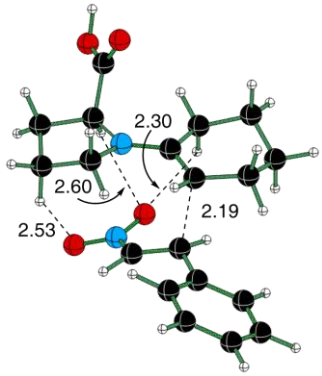
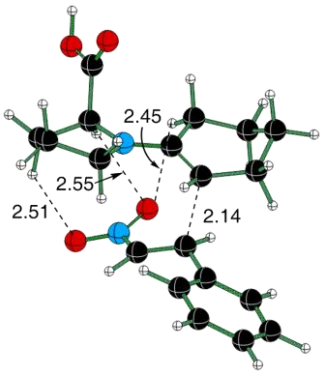
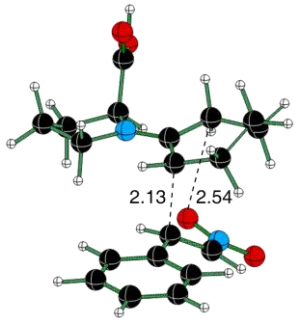
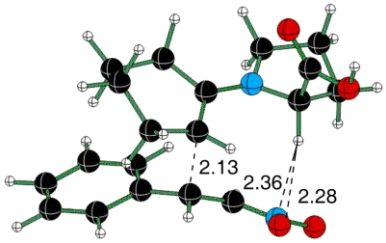
(1-2)'*anti*-(i) (*re-re*)$_{60}$	**(1-2)'*anti*-(ii)** (*re-re*)$_{60}$	**(1-2)'*anti*-(iii)** (*re-re*)$_{60}$
		
(1-2)'*anti*-(iv) (*re-re*)$_{60}$ **Lowest Energy**	**(1-2)'*anti*-(v)** (*re-re*)$_{60}$	**(1-2)'*anti*-(vi)** (*re-re*)$_{60}$
		
(1-2)'*anti*-(i) (*si-si*)$_{60}$	**(1-2)'*anti*-(vi)** (*si-si*)$_{300}$	**(1-2)'*anti*-(v)** (*si-si*)$_{300}$
		
(1-2)'*anti*-(v) (*si-re*)$_{60}$	**(1-2)'I*anti*-(v)** (*re-si*)$_{60}$	

Figure S8. Optimized geometries of TS for C–C bond formation at the SMD$_{(THF)}$/mPW1K/6-31+G** level of theory for *anti*-addition devoid of H-bonding between carboxylic acid group and nitrostyrene with different conformation of pyrrolidine and cyclohexane. Among the different TSs (*re-re*)$_{60}$ (**iv**) is most preferred and used in the main text for discussions and further calculation are done with same conformation (see Table S9).

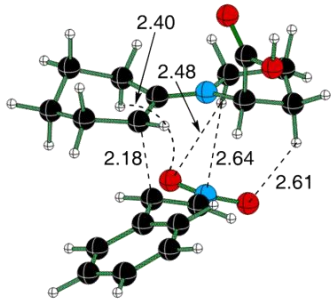
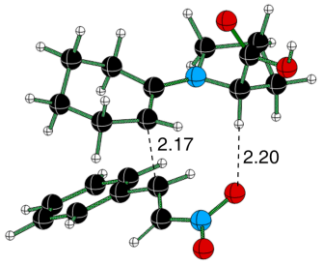
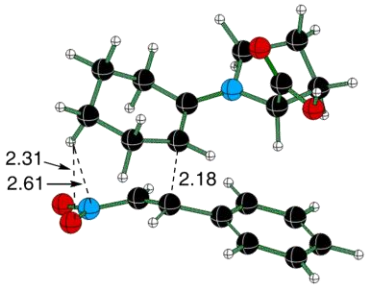
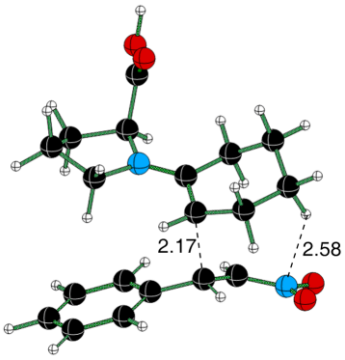
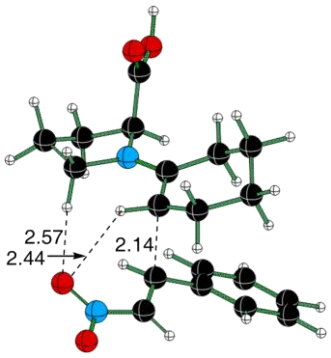
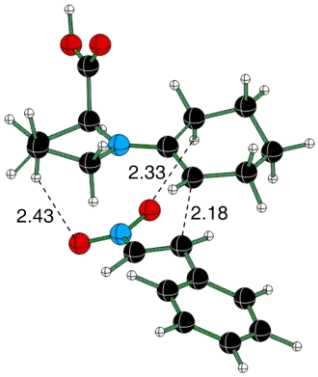
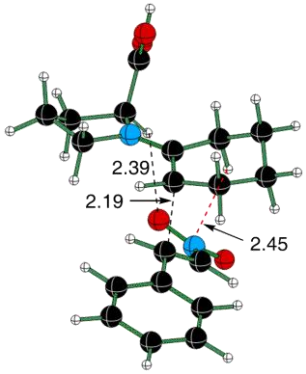
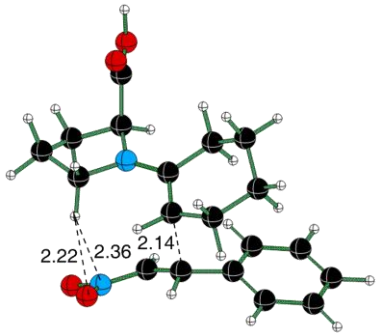
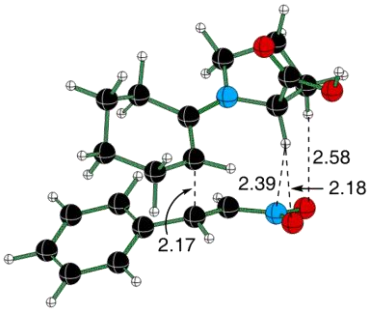
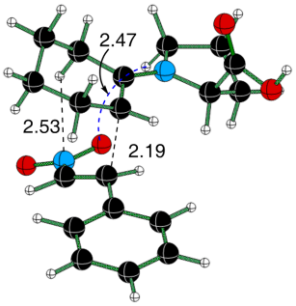
		
(1-2)'*anti* (*re-re*)$_{60}$	**(1-2)'*anti* (*re-re*)$_{180}$**	**(1-2)'*anti* (*re-re*)$_{300}$**
		
(1-2)'*anti* (*si-si*)$_{60}$	**(1-2)'*anti* (*si-si*)$_{180}$**	**(1-2)'*anti* (*si-si*)$_{300}$**
		
(1-2)'*anti* (*si-re*)$_{60}$	**(1-2)'*anti* (*si-re*)$_{300}$**	
		
(1-2)'*anti* (*re-si*)$_{60}$	**(1-2)'*anti* (*re-si*)$_{300}$**	

Figure S9. Optimized geometries of TS for the C–C bond formation at the $SMD_{(THF)}$/mPW1K/6-31+G** level of theory for *anti*-addition devoid of H-bonding between carboxylic acid group and nitrostyrene.

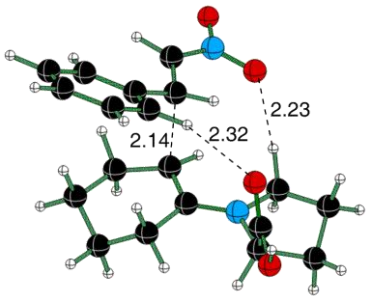
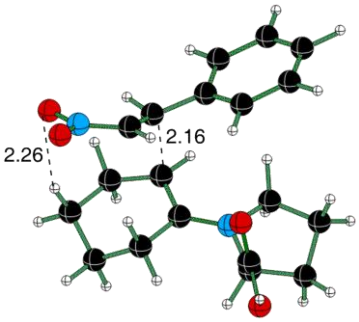
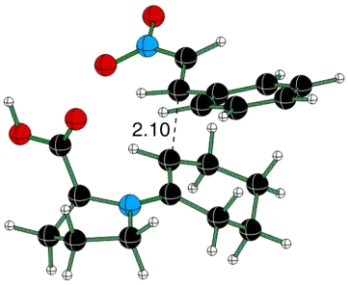
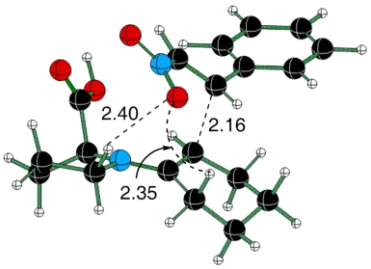
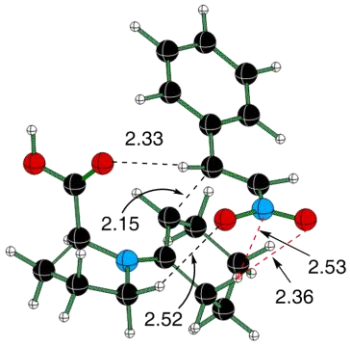
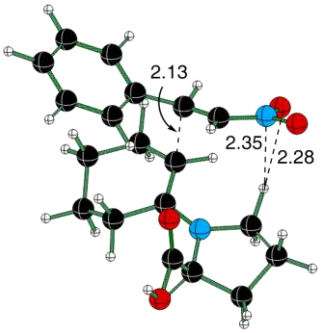
		
(1-2)'$_{syn}$ $(re\text{-}re)_{180}$	**(1-2)'**$_{syn}$ $(re\text{-}re)_{300}$	**(1-2)'**$_{syn}$ $(si\text{-}si)_{180}$
		
(1-2)'$_{syn}$ $(si\text{-}si)_{300}$	**(1-2)'**$_{syn}$ $(si\text{-}re)_{60}$	**(1-2)'**$_{syn}$ $(re\text{-}si)_{60}$

Figure S10. Optimized geometries of TS for C–C bond formation at the $SMD_{(THF)}$/mPW1K/6-31+G** level of theory for *syn*-addition devoid of H-bonding between carboxylic acid group and nitrostyrene with '*up*' conformation of pyrrolidine.

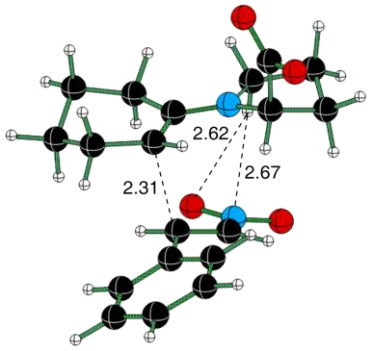
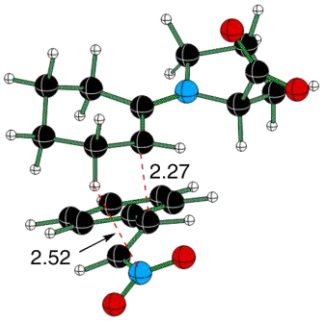
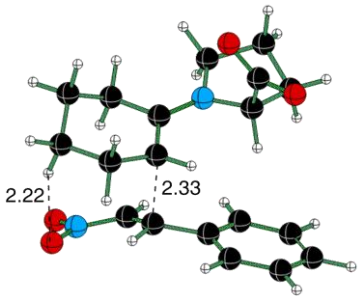
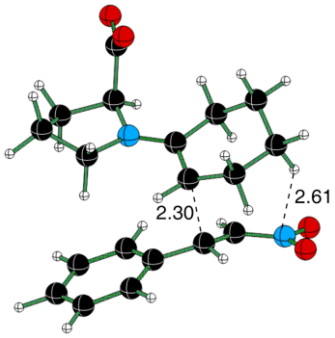
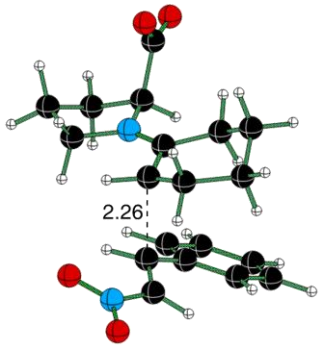
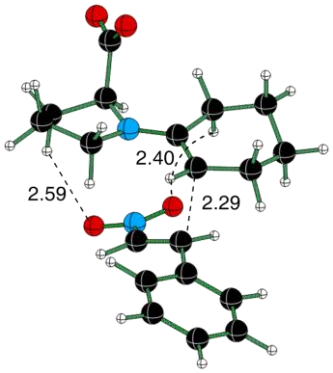
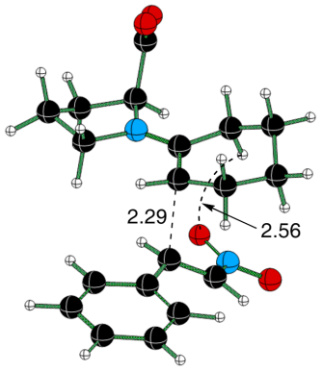
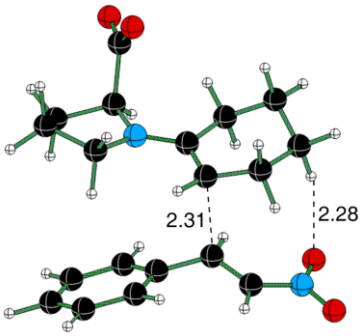
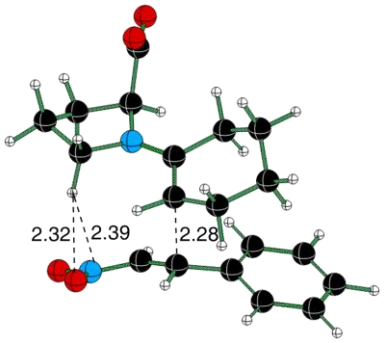
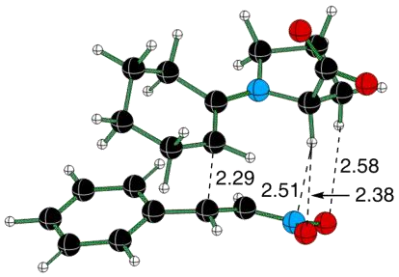
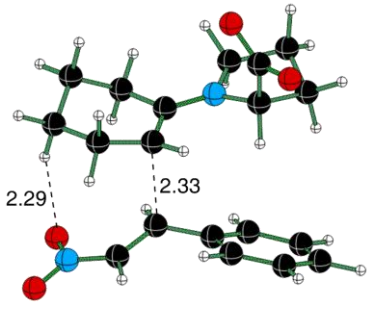
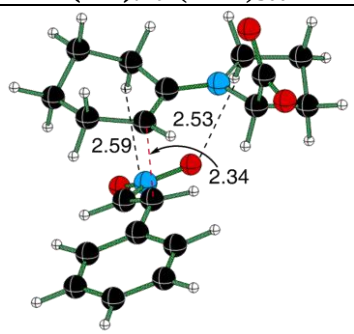
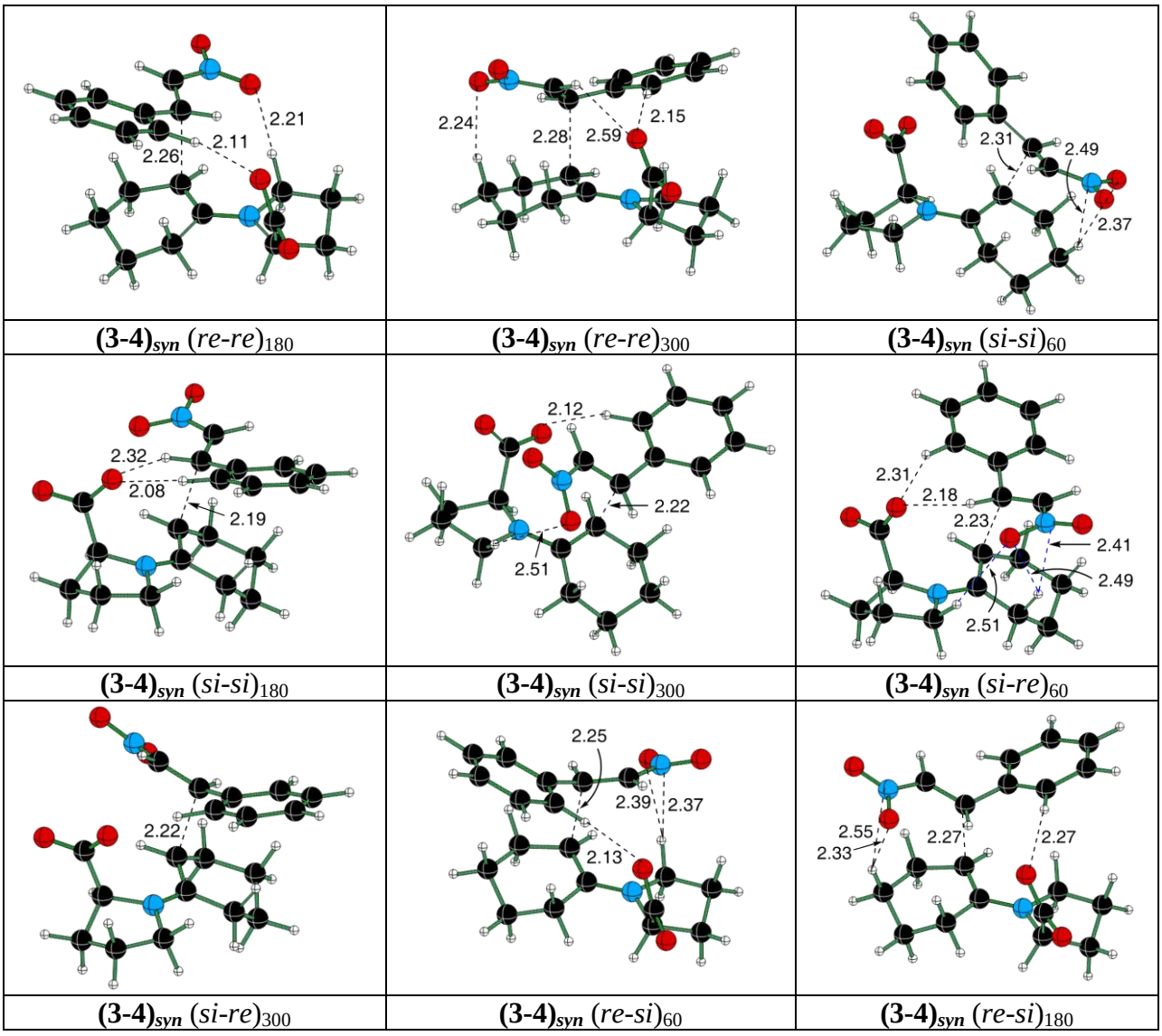
		
(3-4)$_{anti}$ (*re-re*)$_{60}$	**(3-4)**$_{anti}$ (*re-re*)$_{180}$	**(3-4)**$_{anti}$ (*re-re*)$_{300}$
		
(3-4)$_{anti}$ (*si-si*)$_{60}$	**(3-4)**$_{anti}$ (*si-si*)$_{180}$	**(3-4)**$_{anti}$ (*si-si*)$_{300}$
		
(3-4)$_{anti}$ (*si-re*)$_{60}$	**(3-4)**$_{anti}$ (*si-re*)$_{180}$	**(3-4)**$_{anti}$ (*si-re*)$_{300}$
		
(3-4)$_{anti}$ (*re-si*)$_{60}$	**(3-4)**$_{anti}$ (*re-si*)$_{180}$	**(3-4)**$_{anti}$ (*re-si*)$_{300}$

Figure S11. The optimized geometries of TSs at the SMD$_{(THF)}$/mPW1K/6-31+G** level of theory for C–C bond formation by the addition of enamine to nitrostyrene from the face opposite to the carboxylate group (*anti*-face addition) of enamine carboxylate (**3**).



(3-4)$_{syn}$ $(re\text{-}re)_{180}$	**(3-4)**$_{syn}$ $(re\text{-}re)_{300}$	**(3-4)**$_{syn}$ $(si\text{-}si)_{60}$
(3-4)$_{syn}$ $(si\text{-}si)_{180}$	**(3-4)**$_{syn}$ $(si\text{-}si)_{300}$	**(3-4)**$_{syn}$ $(si\text{-}re)_{60}$
(3-4)$_{syn}$ $(si\text{-}re)_{300}$	**(3-4)**$_{syn}$ $(re\text{-}si)_{60}$	**(3-4)**$_{syn}$ $(re\text{-}si)_{180}$

Figure S12. The optimized geometries of TSs at the SMD$_{(THF)}$/mPW1K/6-31+G** level of theory for C–C bond formation by the addition of enamine to nitrostyrene from the same face of the carboxylate (**3**) (*syn*-face addition).

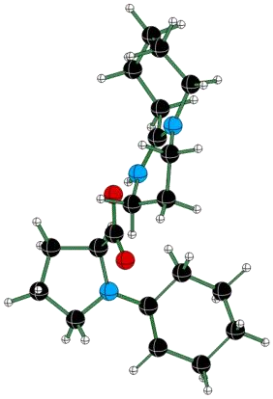
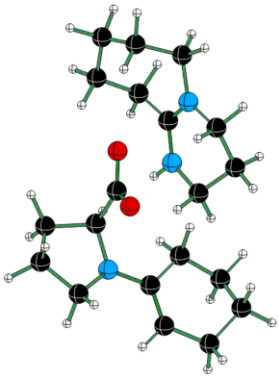
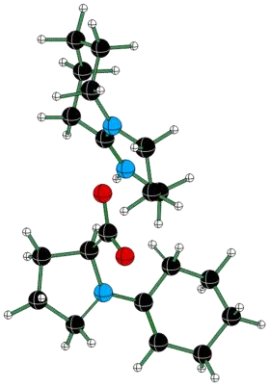
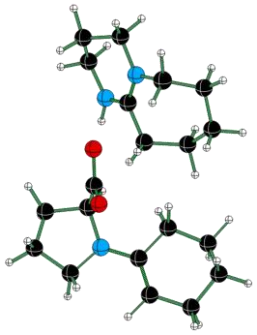
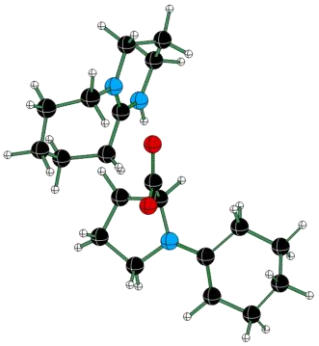
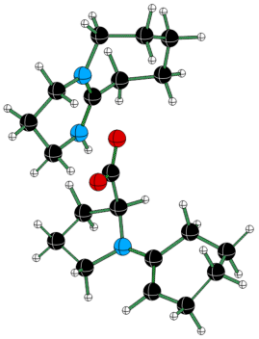
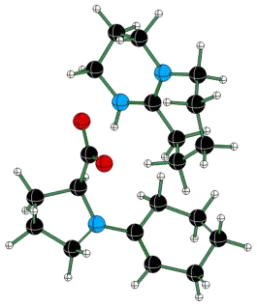
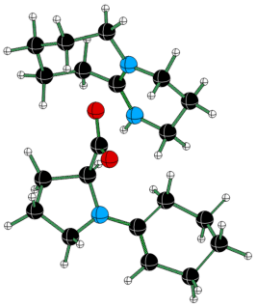
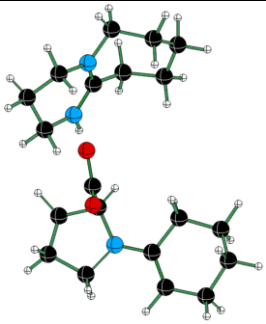
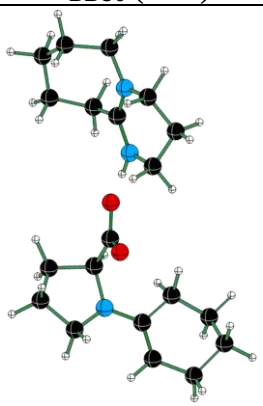
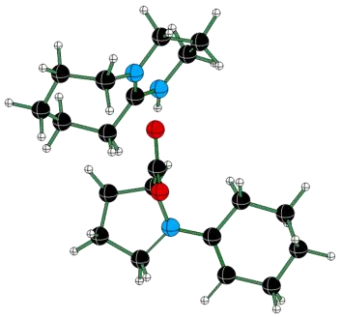
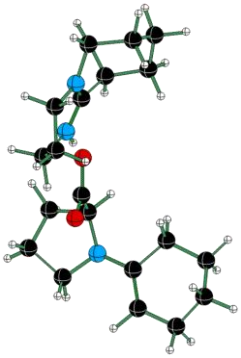
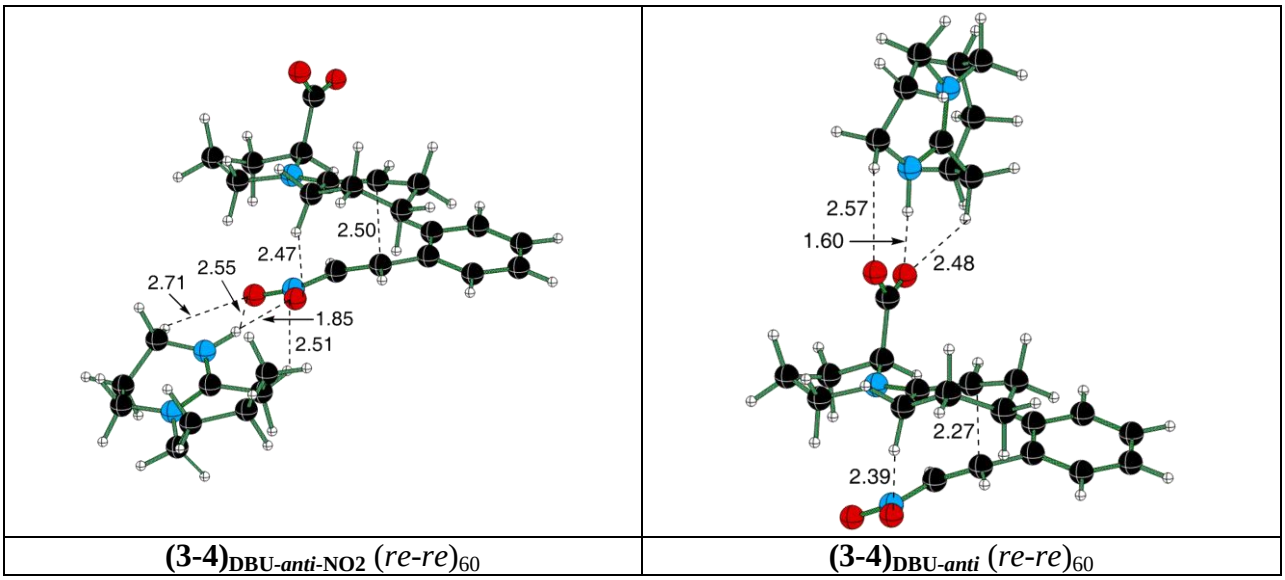
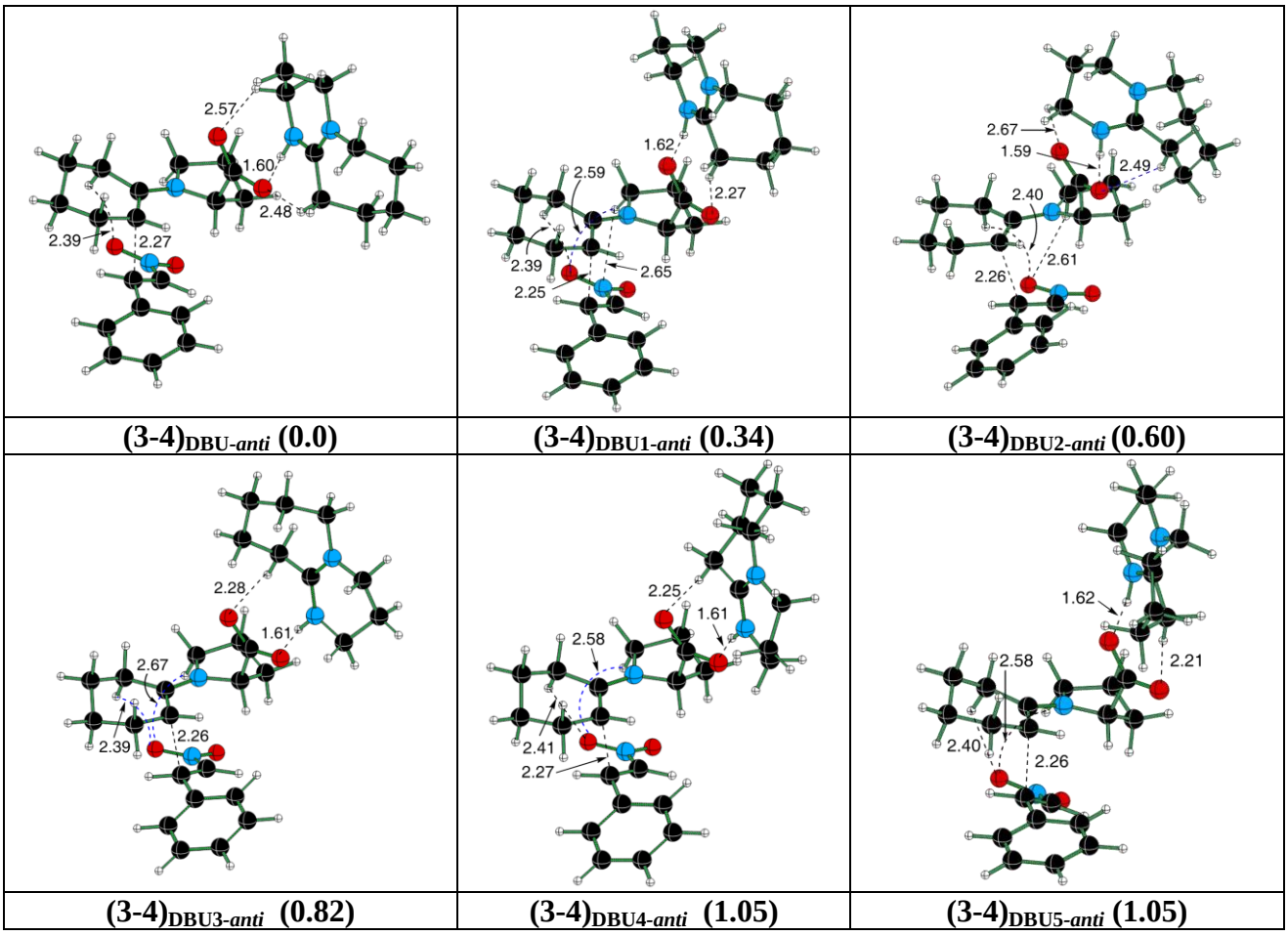
		
3$_{\mathbf{DBU}}$ (0.36)	**3**$_{\mathbf{DBU1}}$ (0.75)	**3**$_{\mathbf{DBU2}}$ 1 (0.0)
		
3$_{\mathbf{DBU3}}$ (0.95)	**3**$_{\mathbf{DBU4}}$ (0.32)	**3**$_{\mathbf{DBU5}}$ (0.77)
		
3$_{\mathbf{DBU6}}$ (0.55)	**3**$_{\mathbf{DBU7}}$ (0.65)	**3**$_{\mathbf{DBU8}}$ (0.97)
		
3$_{\mathbf{DBU9}}$ (1.04)	**3**$_{\mathbf{DBU10}}$ (1.05)	**3**$_{\mathbf{DBU-conf}}$ (0.35)

Figure S13. Different conformations of proline-enamine-DBU adduct obtained at the $SMD_{(THF)}$/mPW1K/6-31+G** level of theory.



(3-4)$_{\text{DBU-}anti\text{-NO2}}$ (*re-re*)$_{60}$ | **(3-4)$_{\text{DBU-}anti}$ (*re-re*)$_{60}$**

Figure S14. The two possible modes of DBU interaction in the C–C bond formation step.



(3-4)$_{\text{DBU-}anti}$ (0.0) | **(3-4)$_{\text{DBU1-}anti}$ (0.34)** | **(3-4)$_{\text{DBU2-}anti}$ (0.60)**

(3-4)$_{\text{DBU3-}anti}$ (0.82) | **(3-4)$_{\text{DBU4-}anti}$ (1.05)** | **(3-4)$_{\text{DBU5-}anti}$ (1.05)**

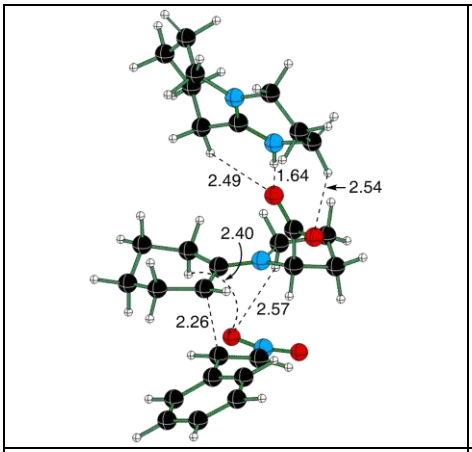
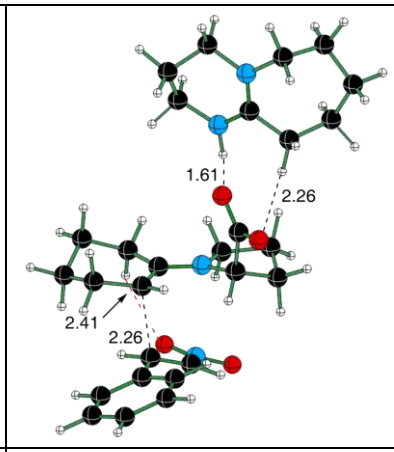
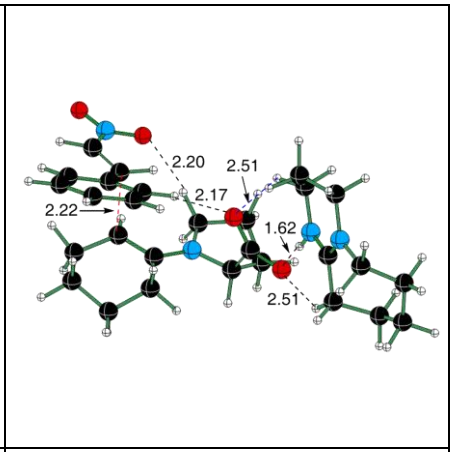
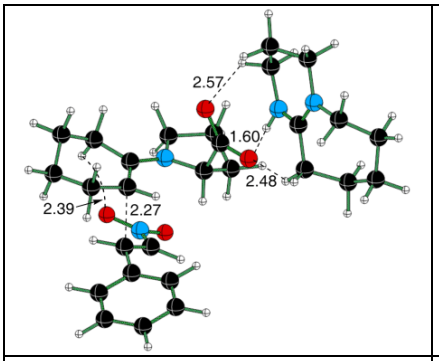
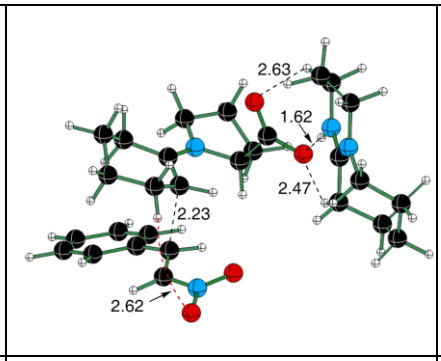
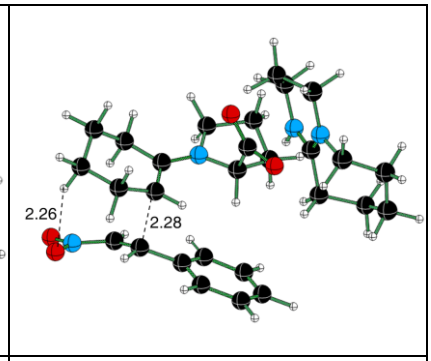
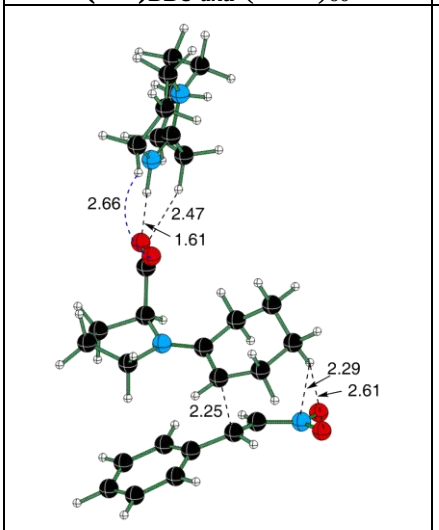
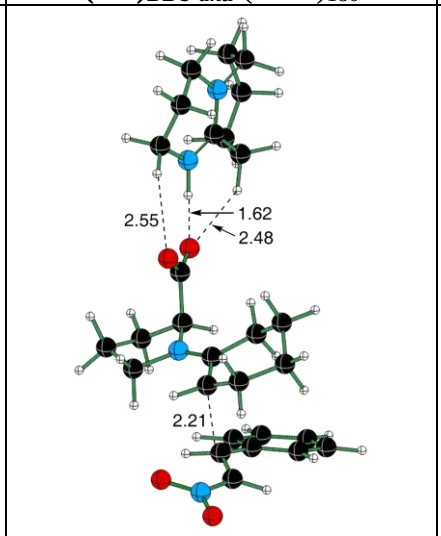
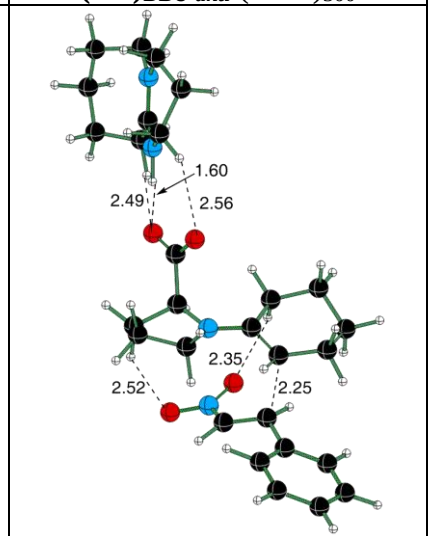
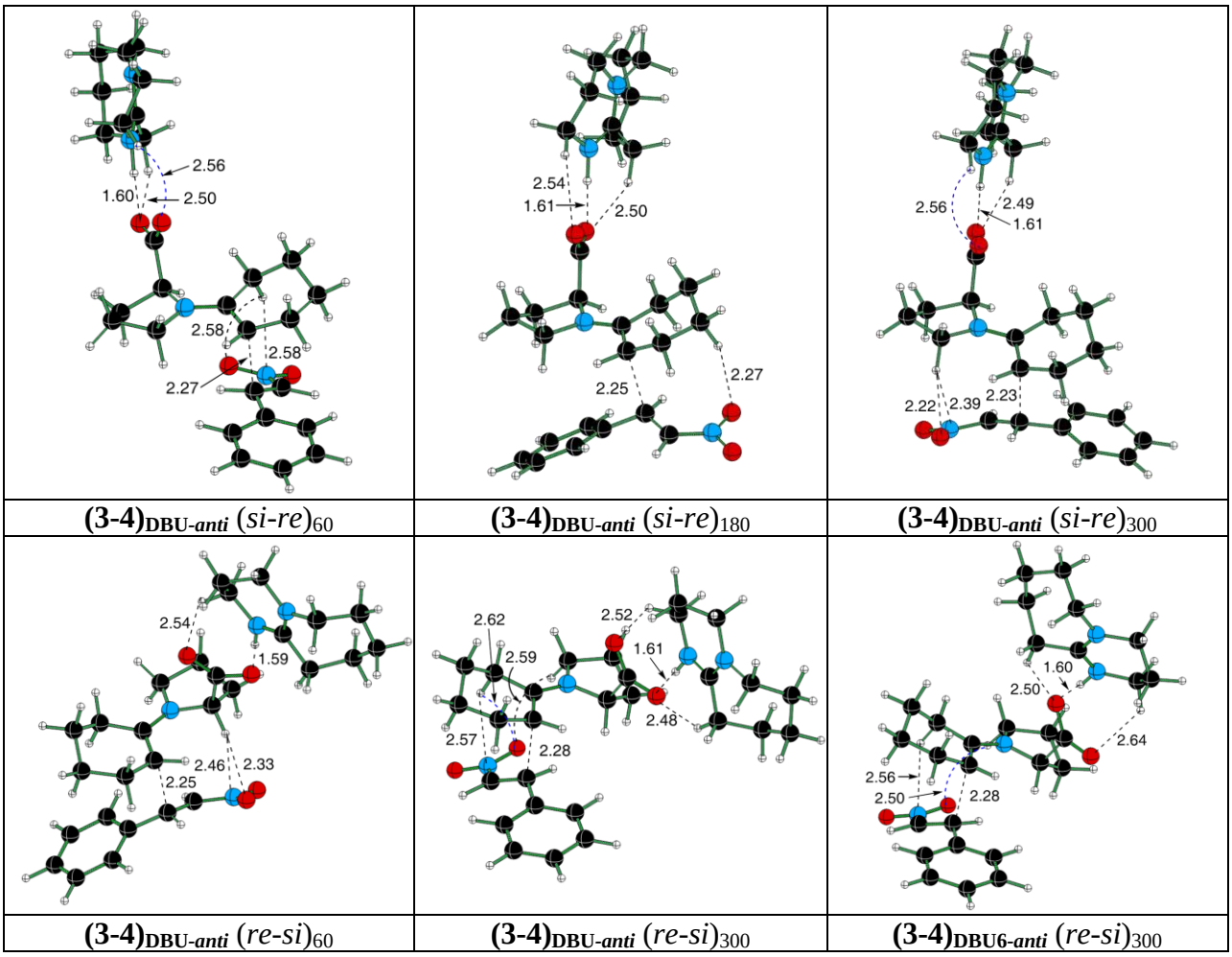
		
(3-4)$_{\text{DBU6-}anti}$ (1.97)	**(3-4)$_{\text{DBU7-}anti}$ (1.45)**	**(3-4)$_{\text{DBU-}syn}$ (3.02)**

Figure S15. The optimized geometries of TS for C–C bond formation in $(re\text{-}re)_{60}$ mode having different orientation of DBU in Enamine-DBU ($\mathbf{3_{DBU}}$) adduct at the $SMD_{(THF)}$/mPW1K/6-31+G** level of theory. The relative Gibbs free energies are provided in parenthesis.

		
(3-4)$_{\text{DBU-}anti}$ $(re\text{-}re)_{60}$	**(3-4)$_{\text{DBU-}anti}$ $(re\text{-}re)_{180}$**	**(3-4)$_{\text{DBU-}anti}$ $(re\text{-}re)_{300}$**
		
(3-4)$_{\text{DBU-}anti}$ $(si\text{-}si)_{60}$	**(3-4)$_{\text{DBU-}anti}$ $(si\text{-}si)_{180}$**	**(3-4)$_{\text{DBU-}anti}$ $(si\text{-}si)_{300}$**



(3-4)$_{\textbf{DBU-}\textit{anti}}$ $(\textit{si-re})_{60}$	**(3-4)**$_{\textbf{DBU-}\textit{anti}}$ $(\textit{si-re})_{180}$	**(3-4)**$_{\textbf{DBU-}\textit{anti}}$ $(\textit{si-re})_{300}$
(3-4)$_{\textbf{DBU-}\textit{anti}}$ $(\textit{re-si})_{60}$	**(3-4)**$_{\textbf{DBU-}\textit{anti}}$ $(\textit{re-si})_{300}$	**(3-4)**$_{\textbf{DBU6-}\textit{anti}}$ $(\textit{re-si})_{300}$

Figure S16. The optimized geometries of TSs at the $SMD_{(THF)}$/mPW1K/6-31+G** level of theory for C–C bond formation by the addition of enamine-DBU adduct to nitrostyrene.

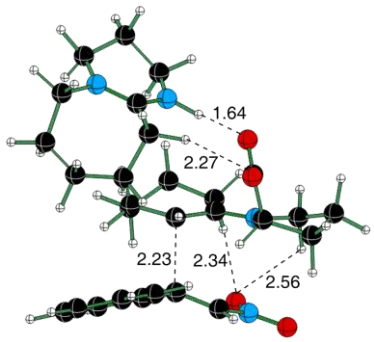
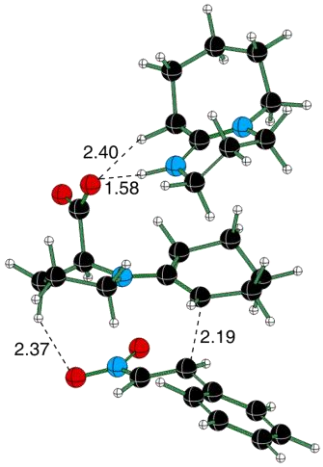
	
(3-4)$_{\textbf{DBU-bent-}\textit{anti}}$ $(re\text{-}re)_{60}$	**(3-4)**$_{\textbf{DBU-bent-}\textit{anti}}$ $(si\text{-}si)_{300}$

Figure S17. The optimized geometries of TS for C–C bond formation at the $SMD_{(THF)}$/M06-2X/6-31+G** level of theory wherein DBU is bent towards the cyclohexane ring in Enamine-DBU adduct.

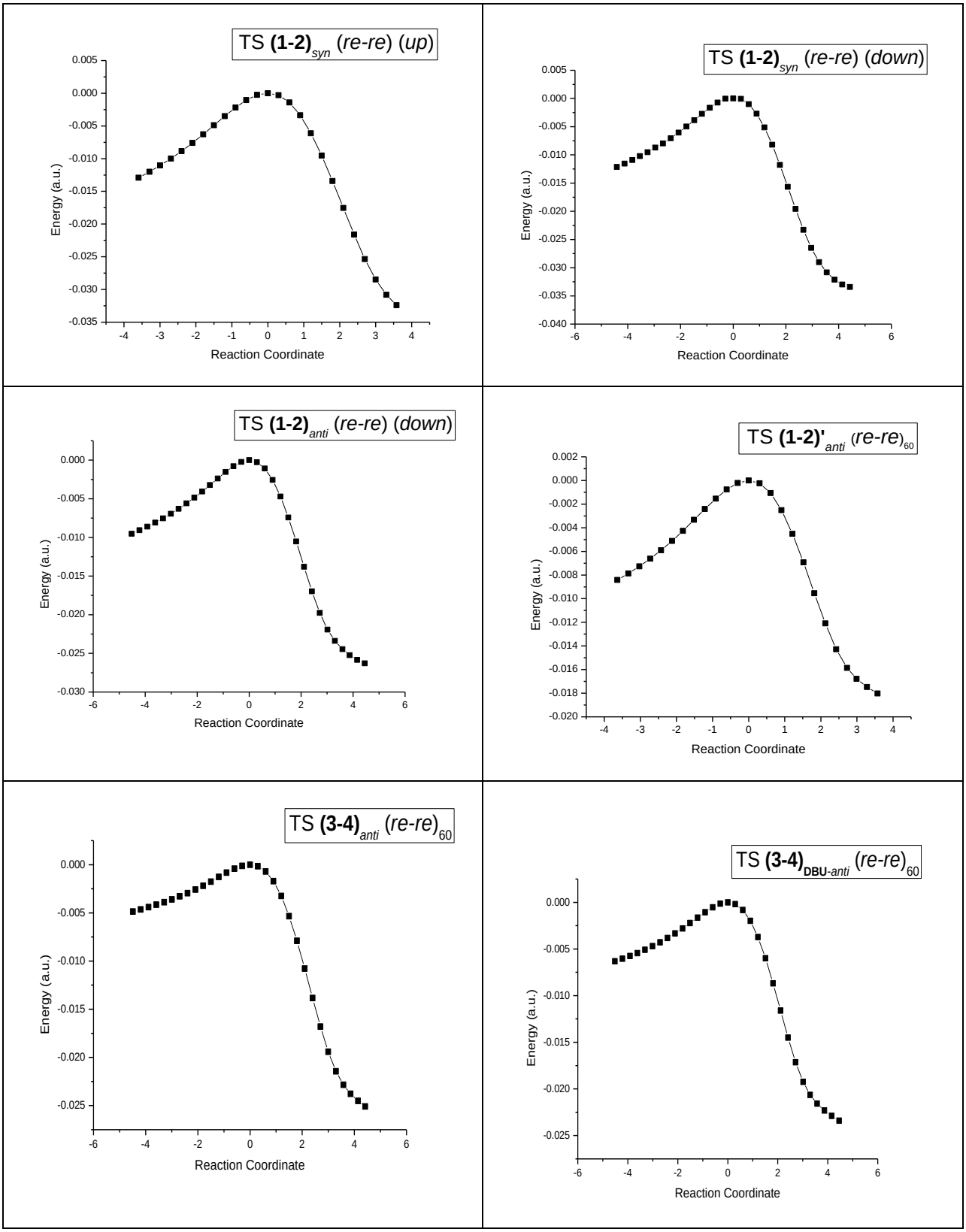

TS (1-2)syn (re-re) (up)
Energy (a.u.)
Reaction Coordinate
TS (1-2)syn (re-re) (down)
Energy (a.u.)
Reaction Coordinate
TS (1-2)anti (re-re) (down)
Energy (a.u.)
Reaction Coordinate
TS (1-2)'anti (re-re)60
Energy (a.u.)
Reaction Coordinate
TS (3-4)anti (re-re)60
Energy (a.u.)
Reaction Coordinate
TS (3-4)DBU-anti (re-re)60
Energy (a.u.)
Reaction Coordinate

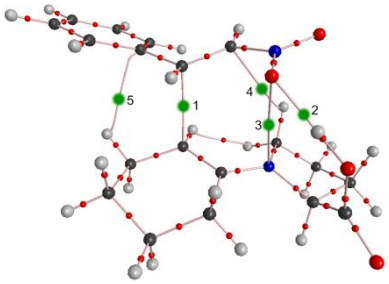
Figure S18. The energy profile along the reaction-coordinate for the different transition states calculated through intrinsic reaction coordinate (IRC) calculations.

2. Atoms-in-Molecules (AIM) Analysis

AIM analysis has been done to analyze the interactions in the TS between proline-enamine and nitrostyrene. The bond critical points for the key interactions between nitrostyrene and proline-enamine are shown in green color balloons along with the electron densities below each topological map (Figure S19-S22). The major stabilizing factor in the TS is H-bonding between COOH of enamine and NO_2 of nitrostyrene, except in those TSs that do not have this kind of interaction. The other interactions include C–H···X (N, O), and C–H···π. Other weak interactions are between the N of enamine with N, O, or C of nitrostyrene, which are the interactions in the TS having no H-bonding.

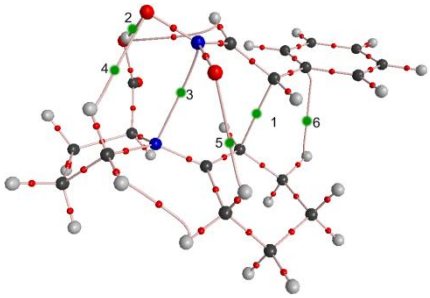
The interaction between N of enamine with C of nitrostyrene is noticed in all lower energy TSs for C–C bond formation having no H-bonding, except for *si-re* mode where N–O interaction is present (Figure S19). In *si-re* and *re-si* mode this interaction is weaker, as evident from the electron density at the bond critical point, than that in *re-re* and *si-si* modes. Also the *si-re* mode has weaker interaction than the other modes of approaches due to which it is higher in energy. In the *re-si* mode, although the interactions are more due to C–H···π interaction, the deformation is noticed to be higher due to the positioning of the phenyl group of nitrostyrene below the cyclohexyl ring, which makes the energy of the TS higher as compared to *re-re* and *si-si* modes. Among the *re-re* and *si-si* modes, a slight variation in energy arises due to small differences in interaction/strain energy or corresponding difference in the entropies. Similar interactions can be noticed for the TS-model involving enamine carboxylate (**3-4**) (Figure S21) and TS-model with explicitly bound DBU in the system ($\mathbf{(3\text{-}4)_{DBU}}$) (Figure S22).

Figure S19. The Summary of AIM Analysis for TS**(1-2)** at the SMD_{THF}/mPW1K/6-31+G** level of theory



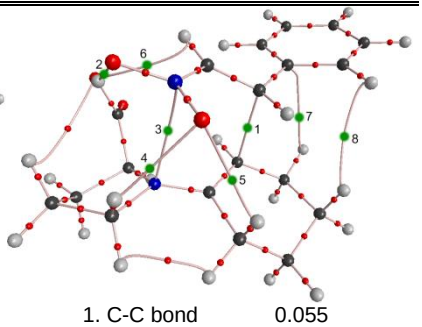
1. C-C bond	0.050
2 OH-O_{Nitro}	0.060
3. α'-CH-C_{Nitro}	0.008
4. N-O_{Nitro}	0.009
5. C_1H_{Cyc}-C_{Nitro}	0.012

(1-2)$_{syn}$ (*re-re*)$_1$ (*down*)



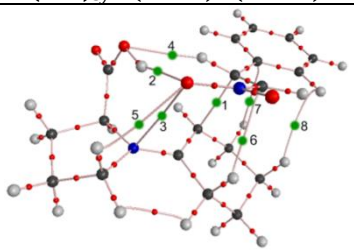
1. C-C bond	0.058
2. OH-O_{Nitro}	0.047
3. N-N	0.015
4. CH_{Prol}-O_{Nitro}	0.012
5. C_3H_{Cyc}-O_{Nitro}	0.009
6. C_2H_{Cyc}-C_{Nitro}	0.011

(1-2)$_{syn}$-Conf(*si-si*)$_2$ (*down*)



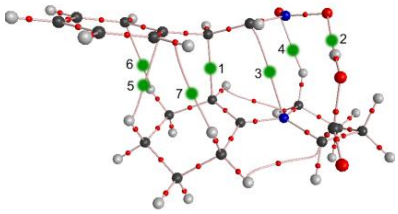
1. C-C bond	0.055
2. OH-O_{Nitro}	0.048
3. N-N	0.013
4. CH_{Prol}-O_{Nitro}	0.013
5. C_3H_{Cyc}-O_{Nitro}	0.010
6. O-H_{Nitro}	0.011
7. C_2H_{Cyc}-C_{Nitro}	0.011
8. C_2H_{Cyc}-C_{Nitro}	0.004

(1-2)$_{syn}$ (*si-si*)$_2$



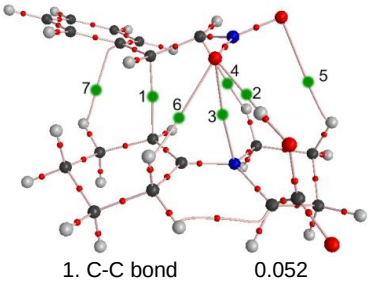
1 C-C bond	0.057
2. OH-O_{Nitro}	0.038
3. N-O	0.010
4. O_{Prol}-CH_{Nitro}	0.015
5. α'CH_{Prol}-C_{Nitro}	0.007
6. C_1H_{Cyc}-C_{Nitro}	0.012
7. C_2H_{Cyc}-C_{Nitro}	0.013
8. H-H	0.006

(1-2)$_{syn}$ (*si-re*)$_1$ (*down*)

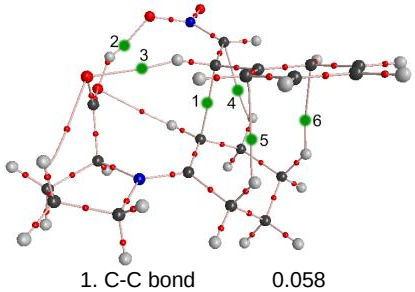


1. C-C bond	0.057
2. OH-O_{Nitro}	0.055
3. N-O	0.012
4. CH_{Prol}-O_{Nitro}	0.018
5. C_3H_{Cyc}-C_{Nitro}	0.009
6. C_2H_{Cyc}-C_{Nitro}	0.010
7. C_1H_{Cyc}-C-H_{Nitro}	0.006

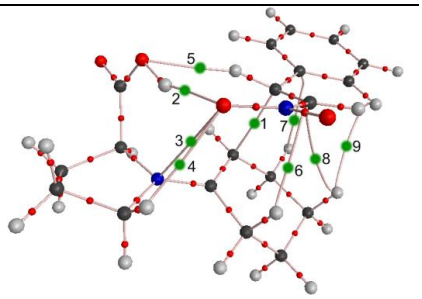
(1-2)$_{syn}$ (*re-si*)$_2$ (*down*)



1. C-C bond	0.052
2. OH-O_{Nitro}	0.054
3. N-O	0.009
4. α'CH_{Prol}-C_{Nitro}	0.010
5. γCH_{Prol}-C_{Nitro}	0.002
6. C_1H_{Cyc}-O_{Nitro}	0.008
7. C_2H_{Cyc}-C_{Nitro}	0.013



1. C-C bond	0.058
2. OH-O_{Nitro}	0.047
3. O_{Enam}-CH_{Nitro}	0.012
4. C_2H_{Cyc}-C_{Nitro}	0.011
5. C_1H_{Cyc}-C_{Nitro}	0.009
6. C_3H_{Cyc}-C_{Nitro}	0.009



1. C-C bond	0.056
2. OH-O_{Nitro}	0.035
3. N-O	0.010
4. α'CH_{Prol}-O_{Nitro}	0.009
5. O_{Prol}-CH_{Nitro}	0.015
6. C_1H_{Cyc}-C_{Nitro}	0.012
7. C_2H_{Cyc}-C_{Nitro}	0.013
8. C3H_{Cyc}-C_{Nitro}	0.006

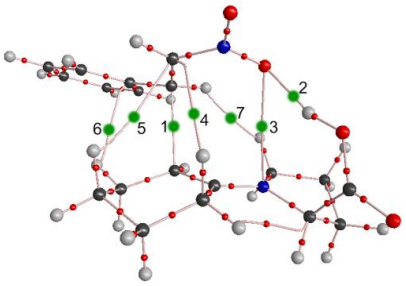
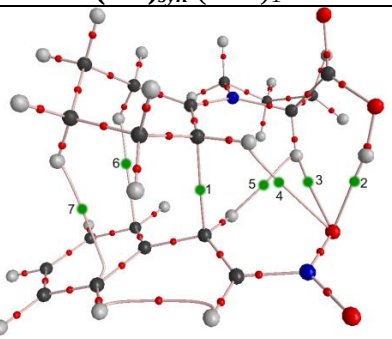
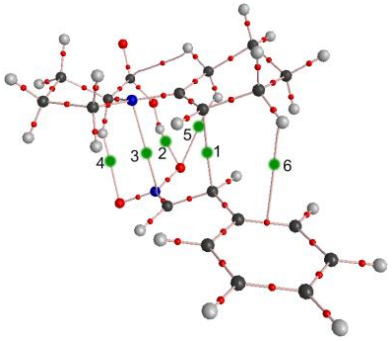
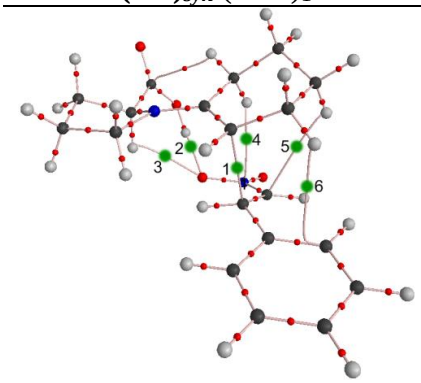
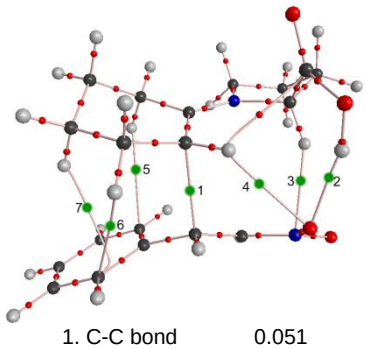
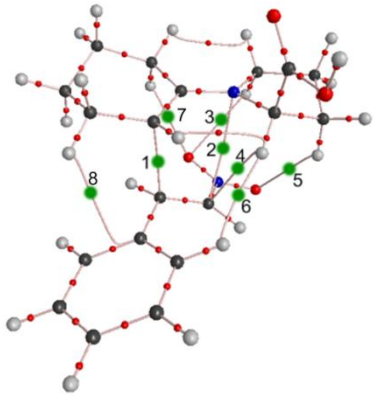
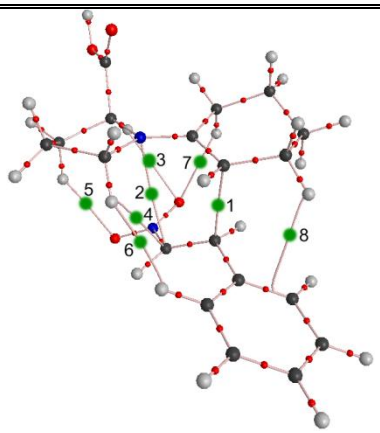
		9. H-H 0.005
(1-2)$_{syn}$ (*re-re*)$_1$	**(1-2)$_{syn}$** (*si-si*)$_1$	**(1-2)$_{syn}$** (*si-re*)$_1$
		
1. C-C bond 0.053 2. OH-O_{Nitro} 0.048 3. N-O 0.009 4. C_1H_{Cyc}-C_{Nitro} 0.007 5. C_3H_{Cyc}-C_{Nitro} 0.005 6. C_2H_{Cyc}-C_{Nitro} 0.013 7. H-H 0.006	1. C-C bond 0.053 2. OH-O_{Nitro} 0.040 3. α-CH-O_{Nitro} 0.019 4. α-CH_{Cyc}-O_{Nitro} 0.008 5. α-CH-CH_{Nitro} 0.009 6. α-C'H-C_{Nitro} 0.006 7. γ-CH-C_{Nitro} 0.008	1. C-C bond 0.047 2. OH-O_{Nitro} 0.046 3. N-N_{Nitro} 0.012 4. α-CH-O_{Nitro} 0.018 5. C_5H_{Cyc}-C_{Nitro} 0.010 6. C_2H_{Cyc}-C_{Nitro} 0.011
(1-2)$_{syn}$ (*re-si*)$_1$	**(1-2)$_{anti}$** (*re-re*)$_1$ (*down*)	**(1-2)$_{anti}$** (*si-si*)$_1$ (*down*)
		
1. C-C bond 0.053 2. OH-O_{Nitro} 0.046 3. α-CH-O_{Nitro} 0.014 4. C_1H_{Cyc}-N_{Nitro} 0.010 5. C_3H_{Cyc}-C_{Nitro} 0.006 6. C_2H_{Cyc}-C=C_{Nitro} 0.011	1. C-C bond 0.051 2. OH-O_{Nitro} 0.033 3. α-CH-N_{Nitro} 0.014 4. CH_{Cyc}-O_{Nitro} 0.013 5. C_1H_{Cyc}-C_{Nitro} 0.006 6. C_2H_{Cyc}-C_{Nitro} 0.006 7. C_3H_{Cyc}-C_{Nitro} 0.008	
(1-2)$_{anti}$ (*si-re*)$_1$ (*down*)	**(1-2)$_{anti}$** (*re-si*)$_1$(*down*)	

Figure S20. The Summary of AIM analysis for (TS **(1-2)'**) at the SMD_{THF}/6-31+G** level of theory



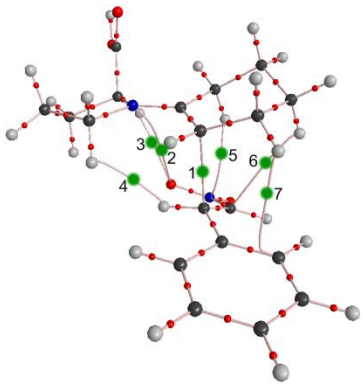
1. C-C bond	0.061
2. N_{Prol}-C_{Nitro}	0.013
3. α-C'H-O_{Nitro}	0.010
4. α-CH-C_{Nitro}	0.010
5. β-CH-O_{Nitro}	0.008
6. CH-CH	0.004
7. α-C'H_{Cyc}-O_{Nitro}	0.011
8. β-CH_{Cyc}-CC_{Nitro}	0.010

(1-2)'*anti* $(re\text{-}re)_{60}$



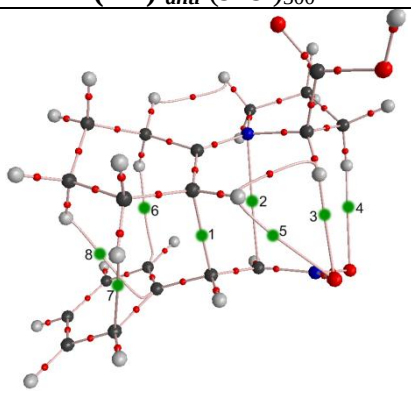
1. C-C bond	0.062
2. N-C_{Nitro}	0.012
3. α-CH-O_{Nitro}	0.007
4. α-C'H-C_{Nitro}	0.010
5. β-CH-O_{Nitro}	0.010
6. H-H	0.004
7. α-C'H_{Cyc}-O_{Nitro}	0.013
8. β-CH_{Cyc}-C_{Nitro}	0.010

(1-2)'*anti* $(si\text{-}si)_{300}$



1. C-C bond	0.060
2. N-O_{Nitro}	0.008
3. α-CH-O_{Nitro}	0.011
4. α-C'H-CH_{Cyc}	0.006
5. α-C'H_{Cyc}-N_{Nitro}	0.010
6. γ-CH_{Cyc}-C_{Nitro}	0.006
7. β-CH_{Cyc}-C_{Nitro}	0.011

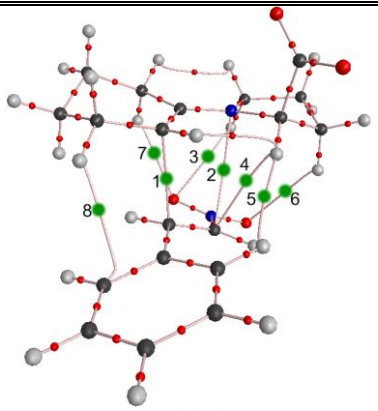
(1-2)'*anti* $(si\text{-}re)_{60}$



1. C-C bond	0.062
2. N_{Prol}-C_{Nitro}	0.009
3. α-CH-O_{Nitro}	0.018
4. β-CH-O_{Nitro}	0.008
5. α-CH_{Cyc}-O_{Nitro}	0.008
6. α-C'H-C_{Nitro}	0.008
7. β-CH-C_{Nitro}	0.007
8. γ-CH-C_{Nitro}	0.009

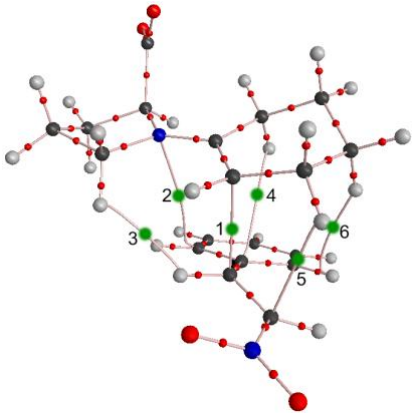
(1-2)'*anti* $(re\text{-}si)_{60}$

Figure S21. The Summary of AIM analysis for (TS **3-4**) at the SMD_{THF}/6-31+G** level of theory



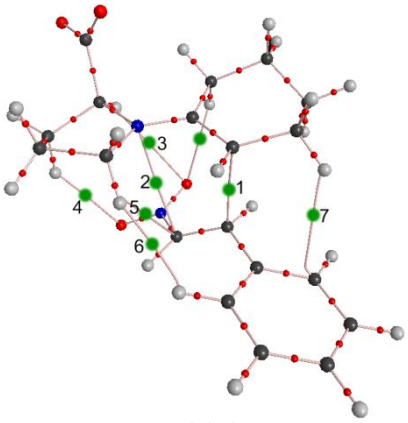
1. 0.048
2. 0.013
3. 0.008
4. 0.009
5. 0.005
6. 0.006
7. 0.011
8. 0.009

(3-4)*anti* $(re\text{-}re)_{60}$



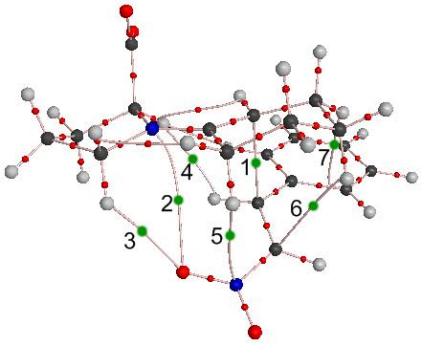
1. 0.053
2. 0.007
3. 0.006
4. 0.007
5. 0.015
6. 0.006

(3-4)*anti* $(si\text{-}si)_{180}$



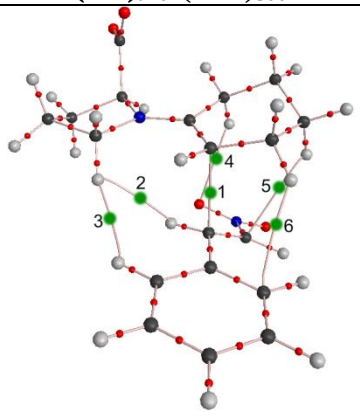
1. 0.050
2. 0.011
3. 0.004
4. 0.008
5. 0.009
6. 0.005
7. 0.009

(3-4)*anti* $(si\text{-}si)_{300}$



1. 0.046
2. 0.006
3. 0.008
4. 0.007
5. 0.007
6. 0.006
7. 0.010

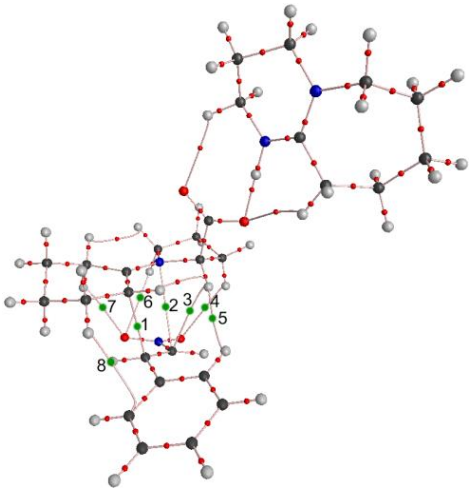
(3-4)*anti* $(re\text{-}si)_{300}$



1. 0.050
2. 0.006
3. 0.006
4. 0.008
5. 0.008
6. 0.009

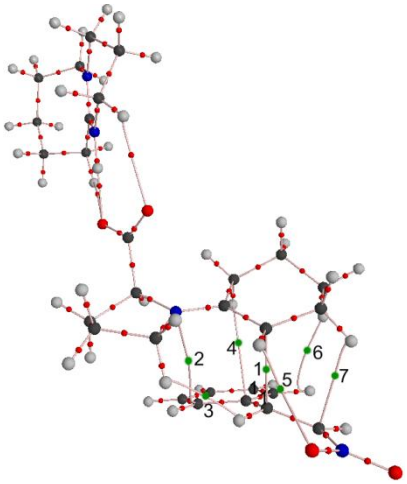
(3-4)*anti* $(si\text{-}re)_{60}$

Figure S22. The summary of AIM analysis for (TS **(3-4)$_{DBU}$**) at the SMD$_{THF}$/6-31+G** level of theory



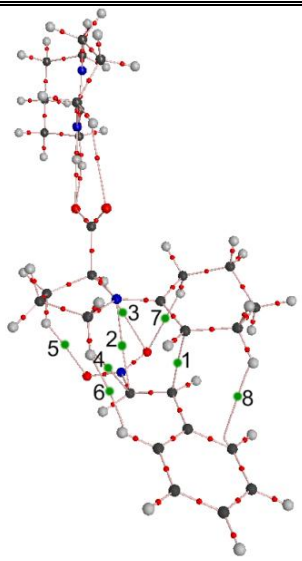
1. 0.052
2. 0.013
3. 0.010
4. 0.006
5. 0.005
6. 0.008
7. 0.011
8. 0.010

(3-4)$_{DBU\text{-}anti}$ (*re-re*)$_{60}$



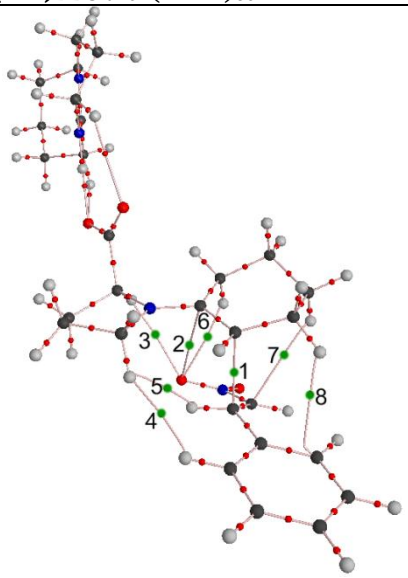
1. 0.058
2. 0.007
3. 0.006
4. 0.007
5. 0.008
6. 0.006
7. 0.016

(3-4)$_{DBU\text{-}anti}$ (*si-si*)$_{180}$



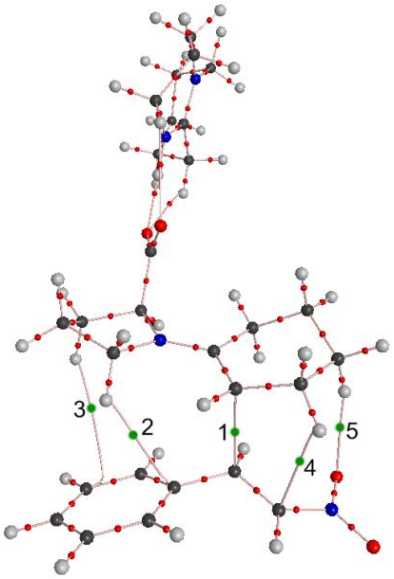
1. 0.054
2. 0.012
3. 0.005
4. 0.009
5. 0.009
6. 0.005
7. 0.012
8. 0.010

(3-4)$_{DBU\text{-}anti}$ (*si-si*)$_{300}$



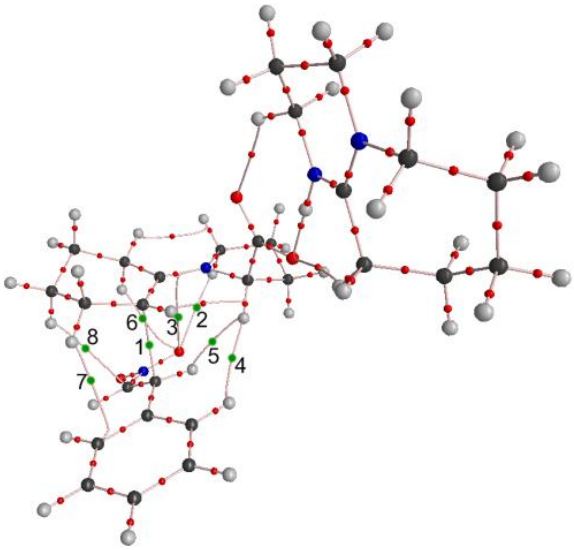
1. 0.052
2. 0.006
3. 0.005
4. 0.004
5. 0.006
6. 0.008
7. 0.007
8. 0.010

(3-4)$_{DBU\text{-}anti}$ (*si-re*)$_{60}$



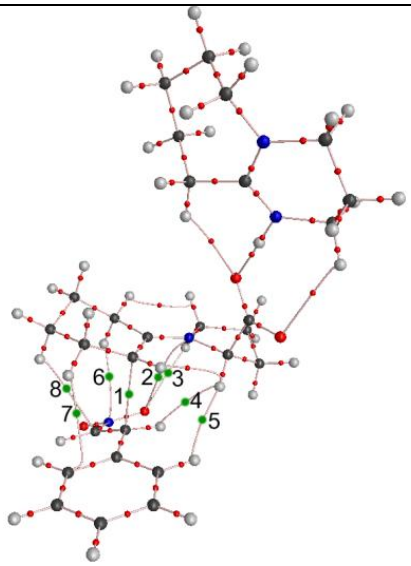
1. 0.054
2. 0.009
3. 0.003
4. 0.014
5. 0.015

(3-4)$_{DBU\text{-}anti}$ (*si-re*)$_{180}$



1. 0.051
2. 0.007
3. 0.006
4. 0.005
5. 0.007
6. 0.008
7. 0.010
8. 0.006

(3-4)$_{\text{DBU-}anti}$ $(re\text{-}si)_{300}$



1. 0.051
2. 0.006
3. 0.009
4. 0.007
5. 0.004
6. 0.008
7. 0.019
8. 0.006

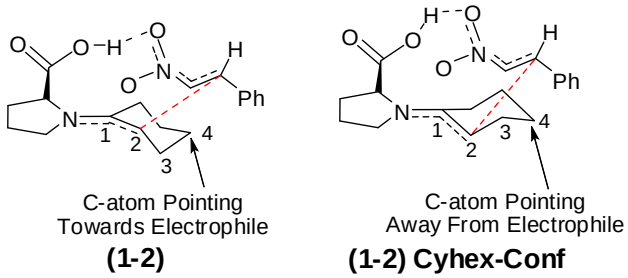
(3-4)$_{\text{DBU6-}anti}$ $(re\text{-}si)_{300}$

Table S1. The Relative Energies[a] (in kcal/mol) of **TS(1-2)** involving Reaction through Enamine Carboxylic Acid having H-bonding Interaction between −COOH and −NO2 groups

	SMD_{THF}/mPW1K		SMD_{THF}/M06-2X		mPW1K		B3LYP	
TS [b]	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH
(1-2)*syn*	*syn*-addition with '*up*' conformation of Pyrrolidine							
re-re$_1$	43.07	25.96	28.40	11.46	41.39	23.99	44.64	27.55
re-re$_2$	45.70	27.57	- [c]	- [c]	- [c]	- [c]	- [c]	- [c]
si-si$_1$	46.65	29.53	- [c]	- [c]	45.30	26.88	49.28	31.06
si-si$_2$	**45.39**	**27.08**	**28.95**	**10.28**	**40.96**	**21.77**	**45.46**	**26.86**
si-si$_{1\text{-Conf}}$	46.69	29.62	- [c]	- [c]	- [c]	- [c]	- [c]	- [c]
si-re$_1$	**43.18**	**25.64**	**28.92**	**11.10**	**41.09**	**22.71**	**45.86**	**27.72**
si-re$_2$	46.06	28.12	- [c]	- [c]	- [c]	- [c]	- [c]	- [c]
si-re$_{2\text{-Conf}}$	50.01	32.80	- [c]	- [c]	- [c]	- [c]	- [c]	- [c]
re-si$_1$	**42.96**	26.63	30.13	13.22	44.84	27.55	47.95	29.14
re-si$_2$	45.82	27.30	- [c]	- [c]	43.55	24.53	- [c]	- [c]
(1-2)*syn*	*syn*-addition with '*down*' conformation of Pyrrolidine							
re-re$_1$	42.76	25.63	28.44	11.19	40.85	23.30	**43.97**	26.76
si-si$_1$	- [c]	- [c]	- [c]	- [c]	46.41	28.48	- [c]	- [c]
si-si$_2$	46.12	28.13	30.51	12.10	42.53	23.40	47.23	28.59
si-re$_1$	45.57	28.28	- [c]	- [c]	43.59	25.48	47.79	30.14
re-si$_1$	43.96	27.00	31.28	14.13	43.13	25.78	46.47	29.14
re-si$_2$	44.69	26.29	- [c]	- [c]	42.33	22.82	46.82	27.57
re-si$_{1\text{-conf}}$	-	-	- [c]	- [c]	44.66	27.95	- [c]	- [c]
(1-2)*anti*	*anti*-addition with '*down*' conformation of Pyrrolidine							
re-re$_1$	**41.45**	**24.10**	**28.24**	**10.67**	**40.09**	**22.06**	44.27	**26.40**
re-re$_2$	48.99	31.81	- [c]	- [c]	- [c]	- [c]	- [c]	- [c]
si-si$_1$	46.40	28.49	31.57	13.09	42.03	23.32	46.07	27.88
si-si$_2$	49.96	32.52	- [c]	- [c]	- [c]	- [c]	- [c]	- [c]
si-re$_1$	49.24	31.70	34.94	17.31	46.63	28.37	50.46	32.64
si-re$_2$	52.49	34.31	- [c]	- [c]	48.41	30.25	52.61	34.82
re-si$_1$	43.86	**26.47**	**28.86**	**11.54**	**41.27**	**22.93**	**45.35**	**27.17**
re-si$_2$	46.15	28.63	- [c]	- [c]	44.80	26.94	- [c]	- [c]
%de (*S*,*R*)	85	85	47	59 (*R*,*S*)	69	47	83	59
%ee (*S*,*R*)	> 99	99	53	33 (*R*,*S*)	64	-25	85	40

[a] Computed with reference to **Proline+Cyclohexanone+Nitrostyrene**, with 6-31+G** basis set. [b] 1 and 2 represents the O-atom of NO_2 group which is interacting with –COOH (See Scheme 1). The lowest energy TS for different modes are in bold font type. [c] Not optimized because corresponding TS at other level of theory are of high energy.

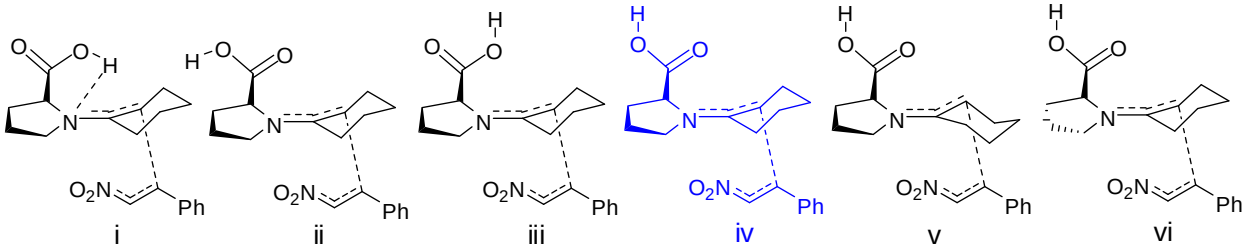
Table S2. Comparison of Energies[a] of Lowest Energy **TS(1-2)** (*re-re* mode) which differs by 4[th]-Carbon of Cyclohexyl Group in Proline Enamine at the SMD_{THF}/mPW1K/6-31+G** Level of Theory



	ΔG (**1-2**)	ΔG **(1-2)Cychex-Conf**	ΔH (**1-2**)	ΔH **(1-2)Cychex-Conf**
I$_{syn}$ *re-re*$_1$	43.07	44.24	25.96	26.69
II$_{syn}$ *re-re*$_1$	42.76	43.35	25.63	26.37
II$_{anti}$ *re-re*$_1$	41.45	42.00	24.10	24.60
II$_{anti}$ *si-si*$_1$	46.40	47.88	28.49	29.87

[a] Computed with reference to **Proline+ Cyclohexanone +Nitrostyrene**.

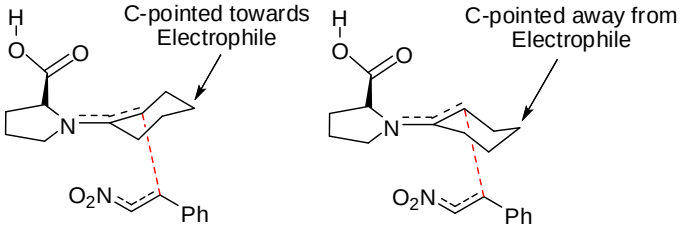
Table S3. The Relative Energies[a] of **TS(1-2)'*re-re*** Mode in different Conformations Obtained at the SMD_{THF}/mPW1K/6-31+G** Level of Theory



TS **(1-2)'**	ΔG	ΔH
(i)	44.4	26.9
(ii)	44.0	27.6
(iii)	41.2	24.7
(iv)	**40.5**	**24.0**
(v)	40.6	24.0
(vi)	41.3	24.6

[a] Computed with reference to **Proline+ Cyclohexanone +Nitrostyrene**.

Table S4. The Relative Energies[a] of **TS(1-2)'** for Different Modes of Addition in Two Different Cyclohexyl Conformations (4^{th}-carbon away or towards the Electrophile) at the SMD_{THF}/mPW1K/6-31+G** Level of Theory



Conf. Cyclohex	TS **(1-2)'**	
(iv) vs (v)	ΔG	ΔH
re-re	**40.5** / 40.6	**24.0** / 24.0
si-si	**41.0** / 41.5	**24.4** / 24.8
si-re	**42.1** / 43.1	**26.3** / 27.6
re-si	**42.7** / 43.1	26.9 / **26.4**

[a] Computed with reference to **Proline+ Cyclohexanone +Nitrostyrene**.

Table S5. The Relative Energies[a] (in kcal/mol) of **TS(1-2)'** involving Reaction Through Enamine Carboxylic Acid having no H-bonding Interaction between −COOH and $-NO_2$ Group

	SMD_{THF}/mPW1K		SMD_{THF}/M06-2X		mPW1K		B3LYP	
TS	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH
(1-2)′*anti*	*anti*-addition							
$(re\text{-}re)_{60}$	**40.47**	**23.98**	**26.03**	**8.71**	**36.63**	**19.64**	**42.06**	**25.52**
$(re\text{-}re)_{180}$	40.77	26.31	-[c]	-[c]	41.57	24.87	47.31	30.57
$(re\text{-}re)_{300}$	45.56	29.57	-[c]	-[c]	46.20	29.29	51.52	35.25
$(si\text{-}si)_{60}$	45.67	29.38	-[c]	-[c]	46.21	29.12	51.89	35.35
$(si\text{-}si)_{180}$	41.99	26.62	29.66	12.59	42.99	26.37	49.37	32.90
$(si\text{-}si)_{300}$	**40.99**	**24.38**	**26.15**	**9.37**	**36.92**	**19.81**	**42.51**	**25.74**
$(si\text{-}re)_{60}$	**42.07**	**26.28**	**28.84**	**12.87**	**39.96**	**23.55**	**45.51**	**29.29**
$(si\text{-}re)_{180}$	-[b]	-[b]	-[c]	-[c]	-[b]	-[b]	-[b]	-[b]
$(si\text{-}re)_{300}$	43.33	27.39	-[c]	-[c]	42.26	25.30	53.94	35.51
$(re\text{-}si)_{60}$	**42.73**	**26.86**	**29.36**	**12.38**	41.24	**23.99**	46.92	**29.96**
$(re\text{-}si)_{180}$	-	-	-[c]	-[c]	-[b]	-[b]	-[b]	-[b]
$(re\text{-}si)_{300}$	43.32	27.05	-[c]	-[c]	**41.09**	24.87	**46.06**	30.09
(1-2)′*syn*	*syn*-addition							
$(re\text{-}re)_{180}$	43.6	27.31	-[c]	-[c]	43.66	26.53	-[b]	-[b]
$(re\text{-}re)_{300}$	47.1	30.81	-[c]	-[c]	47.59	30.45	52.59	36.45
$(si\text{-}si)_{180}$	44.4	28.27	-[c]	-[c]	-[b]	-[b]	-[b]	-[b]
$(si\text{-}si)_{300}$	48.0	31.40	-[c]	-[c]	45.95	28.18	50.70	33.72
$(si\text{-}re)_{60}$	46.6	29.84	-[c]	-[c]	45.83	28.46	51.45	34.56
$(re\text{-}si)_{60}$	45.7	28.79	-[c]	-[c]	44.63	26.58	-[b]	-[b]
%de (*S*,*R*)	87	96	98	>99	>99	>99	>99	>99
%ee (*S*,*R*)	40	33	8	53	25	17	40	17

[a] Computed with reference to **Proline+ Cyclohexanone +Nitrostyrene**, with 6-31+G** basis set. [b] Could not optimize the TS. [c] Only the lowest energy TS are attempted at this level of theory.

Table S6. The Energetics[a] of *Activation-Strain Analysis* for the Lowest Energy TS for **TS(3-4)** calculated at the SMD_{THF}/mPWPW91/6-31+G** Level of Theory

3-4	$\Delta E^{\ddagger}_{strain\text{-}Enamine}$	$\Delta E^{\ddagger}_{strain\text{-}Nitrostyrene}$	$\Delta E^{\ddagger}_{strain}$	$\Delta E^{\ddagger}_{int}$	$\Delta E^{\ddagger}$
		TS **(3-4)'**$_{anti}$ (up)			
re-*re*$_{60}$	6.4	9.0	15.4	-8.6	6.8
si-*si*$_{180}$	5.0	9.9	14.9	-7.9	7.0
si-*si*$_{300}$	4.5	9.7	14.3	-7.3	7.0
si-*re*$_{60}$	4.7	9.3	14.0	-4.7	9.3
re-*si*$_{300}$	6.5	9.1	15.6	-6.1	9.5

[a] The energies given in table are total electronic energy and calculated with respect to the separated lowest energy enamine+nitrostyrene

Table S7. The Relative Energies[a] (in kcal/mol) of **TS(3-4)** involving C−C Bond Formation Through Enamine Carboxylate Intermediate (**3**)

TS	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH
	SMD_{THF}/mPW1K		SMD_{THF}/M06-2X		mPW1K[b]		B3LYP[b]	
3-4	*anti*-addition							
$(re\text{-}re)_{60}$	**42.16**	**25.78**	**29.93**	**12.12**	111.34	94.66	112.17	96.43
$(re\text{-}re)_{180}$	44.86	28.46	-[d]	-[d]	-[c]	-[c]	-[c]	-[c]
$(re\text{-}re)_{300}$	46.87	30.95	-[d]	-[d]	115.34	99.87	116.63	100.98
$(si\text{-}si)_{60}$	45.89	29.38	-[d]	-[d]	113.52	96.76	115.07	98.72
$(si\text{-}si)_{180}$	**42.35**	**25.88**	**30.42**	13.33	**109.60**	**93.43**	**110.89**	**95.45**
$(si\text{-}si)_{300}$	42.72	26.10	30.60	**13.11**	111.96	95.15	113.26	97.24
$(si\text{-}re)_{60}$	**44.11**	28.21	32.52	16.64	-[c]	-[c]	-[c]	-[c]
$(si\text{-}re)_{180}$	44.47	27.85	-[d]	-[d]	**111.93**	**94.98**	**112.77**	**96.85**
$(si\text{-}re)_{300}$	44.25	**27.61**	**31.76**	**14.40**	112.28	95.76	113.31	97.46
$(re\text{-}si)_{60}$	46.71	30.02	-[d]	-[d]	117.27	100.68	119.09	102.54
$(re\text{-}si)_{180}$	45.78	30.03	-[d]	-[d]	114.86	98.92	-[c]	-[c]
$(re\text{-}si)_{300}$	**44.23**	**28.43**	**34.17**	**17.41**	114.08	97.63	**113.80**	98.44
	syn-addition							
$(re\text{-}re)_{60}$	-[c]	-[c]	-[d]	-[d]	-[c]	-[c]	-[c]	-[c]
$(re\text{-}re)_{180}$	43.73	26.69	-[d]	-[d]	**108.38**	**91.45**	**110.88**	**94.23**
$(re\text{-}re)_{300}$	47.94	31.21	-[d]	-[d]	114.38	96.61	115.53	99.37
$(si\text{-}si)_{60}$	58.63	40.72	-[d]	-[d]	-[c]	-[c]	-[c]	-[c]
$(si\text{-}si)_{180}$	47.31	29.53	-[d]	-[d]	116.40	99.38	119.15	102.65
$(si\text{-}si)_{300}$	50.16	32.33	-[d]	-[d]	117.00	98.47	119.90	102.04
$(si\text{-}re)_{60}$	47.38	29.93	-[d]	-[d]	114.37	96.83	117.41	100.57
$(si\text{-}re)_{180}$	-[c]	-[c]	-[d]	-[d]	-[c]	-[c]	-[c]	-[c]
$(si\text{-}re)_{300}$	51.01	33.10	-[d]	-[d]	120.46	103.71	123.09	106.33
$(re\text{-}si)_{60}$	46.31	29.09	-[d]	-[d]	112.49	94.57	114.60	97.57
$(re\text{-}si)_{180}$	45.38	29.57	-[d]	-[d]	**111.99**	**94.39**	114.36	**97.26**
$(re\text{-}si)_{300}$	-[c]	-[c]	-[d]	-[d]	-[c]	-[c]	-[c]	-[c]
%de(*S*,*R*)	93	91	91	96	>99	99	92	98
%ee(*S*,*R*)	17	8	40	69	77	93	0	77

[a] Computed with reference to **Proline+ Cyclohexanone +Nitrostyrene**, with 6-31+G** basis set. [b] The computed energies are very high as the gas phase calculations fails in acid-base reaction; **1**+DBU → **3**+$DBUH^+$. [c] Could not

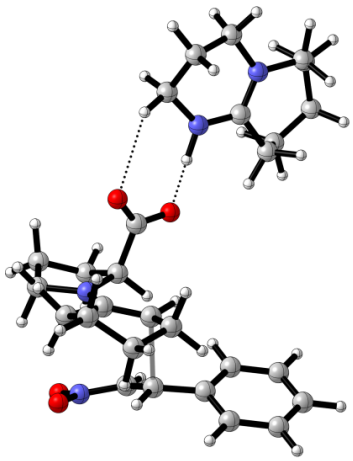
optimize the TS or the TS is less probable due to positioning of COO^- group in *syn*-face addition. [d] Only the lowest energy TS are attempted at this level of theory.

Table S8. The Relative Energies[a] (in kcal/mol) of TS **(3-4)$_{DBU}$**(*re-re*)$_{60}$ having Different Orientation of DBU in **3$_{DBU}$** Adduct at the SMD$_{THF}$/mPW1K/6-31+G** Level of Theory

	(3-4)$_{DBUn\text{-}anti}$ (*re-re*)[b]		**Enamine$_{anti}$-DBU** adduct [c]	
	ΔG	ΔH	ΔG	ΔH
3$_{DBU}$	**33.98 (0.00)**	**7.13 (0.0)**	**0.36**	**-0.06**
3$_{DBU1}$	34.32 (0.34)	7.73 (0.60)	0.75	-0.14
3$_{DBU2}$	34.58 (0.60)	7.26 (0.13)	0.0	0.0
3$_{DBU3}$	34.80 (0.82)	7.43 (0.30)	0.95	0.0
3$_{DBU4}$	35.03 (1.05)	7.26 (0.13)	0.32	0.03
3$_{DBU5}$	35.04 (1.06)	7.40 (0.27)	0.77	-0.01
3$_{DBU6}$	35.96 (1.98)	7.54 (0.41)	0.55	-0.11
3$_{DBU7}$	35.45 (1.47)	7.29 (0.16)	0.65	0.02

[a] Computed with reference to **Proline+ Cyclohexanone +Nitrostyrene**. [b] The energies in parenthesis are energies with respect to lowest energy **3$_{DBU}$** adduct. The *syn*-enamine is involved in this TS. [c]Enamine-DBU adducts involves *anti*-enamine as it is more stable than *syn*-enamine.

Table S9. The Relative Energies[a] (in kcal/mol) for the Lowest Energy TS **(3-4)$_{DBU}$** involving C–C Bond Formation in Presence of DBU



	SMD$_{THF}$/mPW1K		SMD$_{THF}$/M06-2X		mPW1K		B3LYP	
TS	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH
(3-4)$_{DBU}$				*anti*-addition				
(*re-re*)$_{60}$	**33.98**	**7.13**	**19.48**	**-8.74**	**31.43**	**3.60**	**37.23**	**9.80**
(*re-re*)$_{180}$	36.52	9.02	-[c]	-[c]	-[b]	-[b]	-[b]	-[b]
(*re-re*)$_{300}$	41.09	12.13	-[c]	-[c]	39.82	11.88	44.82	17.62
(*si-si*)$_{60}$	38.80	11.39	-[c]	-[c]	39.53	9.83	42.99	16.56

$(si\text{-}si)_{180}$	**34.51**	8.33	22.77	-6.14	-[b]	-[b]	40.92	13.85
$(si\text{-}si)_{300}$	35.53	**7.48**	**20.86**	**-7.82**	**31.68**	**3.82**	**37.22**	**10.18**
$(si\text{-}re)_{60}$	**36.32**	**9.46**	**22.78**	**-4.52**	**34.12**	**7.21**	**39.63**	**13.10**
$(si\text{-}re)_{180}$	36.49	10.11	-[c]	-[c]	37.07	9.96	-[b]	-[b]
$(si\text{-}re)_{300}$	37.95	9.76	-[c]	-[c]	-[b]	-[b]	42.20	14.44
$(re\text{-}si)_{60}$	38.4	10.7	**22.79**	**-4.51**	**34.60**	**7.82**	40.98	13.90
$(re\text{-}si)_{180}$	-[b]	-[b]	-[c]	-[c]	-[b]	-[b]	-[b]	-[b]
$(re\text{-}si)_{300}$	**36.99**	**10.21**	23.18	-3.28	35.64	8.30	**40.70**	**13.50**
				syn-addition				
$(re\text{-}re)_{180}$	37.00	9.19	25.01	-4.30	-[d]	-[d]	-[d]	-[d]
%de (*S*,*R*)	For %*ee* and %*de* see Table S14 which is calculated according to all TS in different conformation							
%ee (*S*,*R*)								

[a] Computed with reference to **Proline+ Cyclohexanone +Nitrostyrene**, with 6-31+G** basis set. [b] Could not optimize TS. [c] Only the lowest energy TS are attempted at this level of theory. [d] not attempted.

Table S10. The Relative Energies[a] (in kcal/mol) for TS **(3-4)$_{DBU}$** involving C−C Bond Formation in Presence of DBU for **3$_{DBU6}$** Conformation

	SMD_{THF}/mPW1K		SMD_{THF}/M06-2X		mPW1K		B3LYP	
TS	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH
(3-4)$_{DBU6}$				*anti*-addition				
$(re\text{-}re)_{60}$	35.96	7.54	-[c]	-[c]	32.34	4.31	38.05	10.60
$(re\text{-}re)_{180}$	36.91	10.04	-[c]	-[c]	35.09	6.35	-[b]	-[b]
$(re\text{-}re)_{300}$	39.80	12.88	-[c]	-[c]	39.72	12.39	44.97	18.21
$(si\text{-}si)_{60}$	38.83	11.74	-[c]	-[c]	39.11	11.13	44.52	17.24
$(si\text{-}si)_{180}$	35.76	8.27	-[c]	-[c]	-[b]	-[b]	-[b]	-[b]
$(si\text{-}si)_{300}$	35.50	7.83	-[c]	-[c]	33.47	5.51	-[b]	-[b]
$(si\text{-}re)_{60}$	36.82	9.97	-[c]	-[c]	38.15	8.26	-[b]	-[b]
$(si\text{-}re)_{180}$	37.88	10.33	-[c]	-[c]	37.46	10.37	-[b]	-[b]
$(si\text{-}re)_{300}$	37.63	9.95	-[c]	-[c]	36.22	8.67	42.79	15.02
$(re\text{-}si)_{60}$	38.50	11.29	-[c]	-[c]	-[b]	-[b]	-[b]	-[b]
$(re\text{-}si)_{180}$	37.96	11.69	-[c]	-[c]	36.18	8.85	-[b]	-[b]
$(re\text{-}si)_{300}$	36.49	10.17	-[c]	-[c]	-[b]	-[b]	40.26	14.15

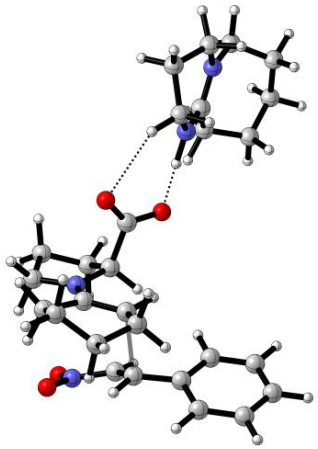
[a] Computed with reference to **Proline+ Cyclohexanone +Nitrostyrene**, with 6-31+G** basis set. [b] Could not optimize the TS. [c] TSs are not attempted as it is higher in energy at other level of theory.

Table S11. The Relative Energies[a] (in kcal/mol) for TS **(3-4)$_{DBU}$** involving C−C Bond Formation in presence of DBU for **3$_{DBU1}$** Conformation at the SMD$_{THF}$/mPW1K/6-31+G** Level of Theory

TS **(3-4)$_{DBU1}$**	ΔG	ΔH
(*re-re*)$_{60}$	34.32	7.73
(*si-si*)$_{300}$	36.01	8.27
(*si-si*)$_{180}$	36.07	8.54

[a] Computed with reference to **Proline+ Cyclohexanone +Nitrostyrene**.

Table S12. The Relative Energies[a] (in kcal/mol) for TS **(3-4)$_{DBU}$** involving C−C Bond Formation in Presence of DBU for **3$_{DBU2}$** Conformation



	anti-addition							
(3-4)$_{DBU2}$	SMD$_{THF}$/mPW1K		SMD$_{THF}$/M06-2X		mPW1K		B3LYP	
	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH
(*re-re*)$_{60}$	34.58	7.26	19.09	-8.98	31.44	3.52	37.19	9.75
(*si-si*)$_{180}$	-[c]	-[c]	-[c]	-[c]	31.99	4.03	38.45	10.32
(*si-si*)$_{300}$	35.29	7.54	20.06	-7.71	35.47	7.96	-[b]	-[b]
(*si-re*)$_{60}$	-[b]	-[b]	-[b]	-[b]	34.49	7.49	39.80	13.36
(*re-si*)$_{300}$	36.85	10.25	24.36	-3.34	35.79	8.31	40.73	13.57

[a] Computed with reference to **Proline+ Cyclohexanone +Nitrostyrene**, with 6-31+G** basis set. [b] Could not optimize the TS. [c] TSs are not attempted as it is higher in energy at other levels of theory.

Table S13. The Relative Energies[a] (in kcal/mol) for TS **(3-4)$_{DBU\text{-}bent}$** involving C−C Bond Formation in Presence of DBU[b] at the SMD$_{THF}$/M06-2X/6-31+G** Level of Theory

(3-4)$_{DBU\text{-}bent}$	ΔG	ΔH
re-re	20.17	-9.59
si-si	21.69	-7.97

[a] Computed with reference to **Proline+ Cyclohexanone +Nitrostyrene**. [b] The 3-DBU adduct involves DBU bent towards cyclohexane carbon of enamine. These are higher in energy in free energy than TS **(3-4)$_{DBU}$** and but lower in enthalpy.

Table S14. The Relative Energies[a] (in kcal/mol) of the Lowest Energy TS for Each Mode from Different **3$_{DBU}$**-adducts and Computed Stereoselectivity

(3-4)$_{DBU}$	SMD$_{THF}$/mPW1K		SMD$_{THF}$/M06-2X		mPW1K		B3LYP	
TS	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH
re-re$_{60}$	33.98	7.13	19.09	-8.98	31.43	3.52	37.19	9.75
si-si$_{300}$	34.51_{180}	7.48_{180}	20.06	-7.82	31.68	3.82	37.22	10.18
si-re$_{60}$	36.32	9.46	22.78	-4.52	34.12	7.21	39.63	13.10
re-si$_{60}$	36.49_{300}	10.17_{300}	22.79	-4.51	34.60	7.82	40.26_{300}	13.50_{300}
	Relative energies of TS with reference to lowest energy TS							
	ΔΔG	ΔΔH	ΔΔG	ΔΔH	ΔΔG	ΔΔH	ΔΔG	ΔΔH
re-re$_{60}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
si-si$_{300}$	0.5	0.4	1.0	1.2	0.2	0.3	0.0	0.4
si-re$_{60}$	2.3	2.3	3.7	4.5	2.7	3.7	2.4	3.3
re-si$_{60}$	2.5	3.0	3.7	4.5	3.2	4.3	3.1	3.8
%de (*S*,*R*)	96	96	> 99	> 99	98	> 99	97	> 99
%ee (*S*,*R*)	40	33	69	77	17	25	0	33

[a] Lowest TS for different modes has been taken from Table S9-S12.

Table S15. Comparison of Relative Energies (in kcal/mol) of the Lowest Energy TS (*re-re* mode) for Different TS-Models with Respect to Proline, Enamine, and Nitrostyrene

(3-4)$_{DBU}$	SMD$_{THF}$/mPW1K		SMD$_{THF}$/M06-2X		mPW1K		B3LYP	
TS	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH
(1-2)$_{anti}$ (*Down*)	41.45	24.10	28.24	10.67	40.09	22.06	43.97[a]	26.76[a]
(1-2)'	40.47	23.98	26.03	8.71	36.63	19.64	42.06	25.52
(3-4)$_{anti}$ (*re-re*)$_{60}$	42.16	25.78	29.93	12.12	108.38[b]	91.45[b]	110.88[b]	94.23[b]
(3-4)$_{DBU\text{-}anti}$ (*re-re*)$_{60}$	33.98	7.13	19.09[c]	-8.98[c]	31.43	3.60	37.19[c]	9.75[c]

[a] TS **(1-2)**$_{syn}$ (*down*) [b] TS **(3-4)***syn*, computed energies are very high as gas phase calculations failed in acid-base reaction; **1**+DBU → **3**+DBUH$^+$. [c] TS(**3-4)$_{DBU2\text{-}anti}$** (*re-re*)$_{60}$. The lowest energy TS chosen on the basis of Gibbs free energy.

Table S16. Comparison of Relative Energy of Lowest Energy TS (*re-re* mode) for Different TS-Models with Respect to Enamine and Nitrostyrene

(3-4)$_{DBU}$	SMD_{THF}/mPW1K		SMD_{THF}/M06-2X		mPW1K		B3LYP	
TS	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG	ΔH
(1-2)	29.21	14.33	20.65	5.14	29.48	13.79	31.22[a]	16.30[a]
(1-2)'	28.24	14.22	18.43	3.18	26.02	11.37	29.30	15.05
(3-4)$_{anti}$ (*re-re*)$_{60}$	22.17	7.51	12.03	-3.14	11.67[b]	-3.87[b]	14.14[b]	-1.34[b]
(3-4)$_{DBU\text{-}anti}$ (*re-re*)$_{60}$	21.75	-2.64	11.50	-14.51	20.82[c]	-4.67[c]	24.43[c]	-0.72[c]

[a] TS **(1-2)**$_{syn}$ (*down*). [b] TS **(3-4)***syn*. [c] TS (**3-4)$_{DBU2\text{-}anti}$** (*re-re*)$_{60}$. TS chosen on basis of lower free energy.

3. The Cartesian coordinates of the optimized geometries of stationary points. Total Electronic Energy (E_0), Zero Point Energy Correction to E_0 (E_{0+ZPE}), Internal Energy (E_{298}), Enthalpy (H_{298}), Free Energy (G_{298}) and Number of Imaginary Frequency (NImag) Obtained at the SMD_{THF}/mPW1K/6-31+G** Level of Theory

Note: To distinguish the pyrrolidine '*up*' and '*down*' conformer, the up conformation has not been mentioned, whereas for the *down* conformation '*down*' is included after the TS name.

H_2O

E_0 = -76.4111824
E_{0+ZPE} = -76.389235
E_{298} = -76.386399
H_{298} = -76.385455
G_{298} = -76.406856
NImag = 0

O	0.000000	0.000000	0.115667
H	0.000000	0.760811	-0.462668
H	0.000000	-0.760811	-0.462668

Proline

E_0 = -401.0919396
E_{0+ZPE} = -400.942287
E_{298} = -400.935270
H_{298} = -400.934326
G_{298} = -400.974413
NImag = 0

N	0.693357	-1.014477	0.563273
C	1.962759	-0.639339	-0.067326
C	1.634605	0.654288	-0.789702
C	0.687299	1.343208	0.182428
C	-0.132666	0.179683	0.747069
C	-1.446946	-0.014550	-0.001675
O	-2.327198	0.808004	-0.028796
O	-1.531138	-1.178861	-0.609607
H	-0.395395	0.342182	1.791011
H	0.062349	2.105894	-0.273352
H	1.251392	1.807764	0.989439
H	2.521601	1.243417	-1.008502
H	1.130091	0.444158	-1.733291
H	2.737534	-0.468018	0.682848
H	2.304318	-1.427681	-0.734549
H	-0.657610	-1.599190	-0.397505
H	0.828594	-1.520076	1.423443

Nitrostyrene

E_0 = -514.0229494
E_{0+ZPE} = -513.881602
E_{298} = -513.872763
H_{298} = -513.871819
G_{298} = -513.916749
NImag = 0

C	0.612965	0.452157	-0.000529
H	0.901332	1.494663	-0.000672
C	-0.812436	0.175146	-0.000321
C	-1.338335	-1.121432	-0.000385
C	-2.705619	-1.318846	-0.000147
C	-3.570694	-0.229478	0.000283
C	-3.061630	1.060454	0.000360
C	-1.691094	1.261162	0.000022
H	-0.678645	-1.976037	-0.000680
H	-3.101948	-2.323431	-0.000193
H	-4.638873	-0.390075	0.000608
H	-3.730124	1.908584	0.000746
H	-1.291978	2.265593	-0.000066
C	1.592067	-0.453227	0.000203
H	1.493612	-1.523782	0.000612
N	2.957363	-0.034304	0.000202
O	3.232527	1.149421	-0.000189
O	3.791689	-0.920797	0.000353

Cyclohexane

E_0 = -309.8478851
E_{0+ZPE} = -309.692903
E_{298} = -309.686546
H_{298} = -309.685602
G_{298} = -309.723202
NImag = 0

C	1.009713	1.251588	-0.280960
C	-0.389639	1.272543	0.332188
C	-1.142582	-0.000011	0.061795
C	-0.389604	-1.272554	0.332153
C	1.009777	-1.251576	-0.280926
C	1.774096	0.000031	0.117317
H	-0.301040	1.361617	1.418845
H	-0.979109	2.114750	-0.022766
H	0.925277	1.292242	-1.369108
H	1.549212	2.147492	0.024697
H	-0.301060	-1.361663	1.418814
H	-0.979050	-2.114757	-0.022849
H	1.549290	-2.147439	0.024824
H	0.925405	-1.292300	-1.369074
H	1.938506	0.000048	1.198075
H	2.758628	0.000050	-0.350928
O	-2.289577	-0.000021	-0.329991

DBU

E_0 = -462.0355954
E_{0+ZPE} = -461.782798
E_{298} = -461.773217
H_{298} = -461.772273
G_{298} = -461.817695
NImag = 0

N	-1.339223	-1.468677	0.063935
C	-2.567253	-0.838264	0.495952
H	-3.398294	-1.493946	0.235936
H	-2.570001	-0.763175	1.588082
C	-2.769890	0.535202	-0.107813
H	-2.933079	0.442370	-1.182474
H	-3.643237	1.026764	0.317937
C	-1.535365	1.368848	0.143328
H	-1.582809	2.298751	-0.421020
H	-1.467027	1.634874	1.202419
C	-0.350688	-0.716904	-0.272774

$DBUH^+$

E_0 = -462.5203667
E_{0+ZPE} = -462.252316
E_{298} = -462.242664
H_{298} = -462.241720
G_{298} = -462.286982
NImag = 0

N	-1.366257	-1.350899	0.059941
C	-2.625125	-0.777063	0.492584
H	-3.422384	-1.438972	0.169006
H	-2.644567	-0.725245	1.580750
C	-2.759387	0.594933	-0.119985
H	-2.918049	0.505052	-1.193795
H	-3.617144	1.110561	0.302719
C	-1.510191	1.400312	0.147733
H	-1.527325	2.322503	-0.424983
H	-1.428484	1.661507	1.202949
C	-0.302186	-0.651155	-0.278978

N	-0.349979	0.644475	-0.274810
C	0.841837	1.425922	-0.547243
H	1.223204	1.197796	-1.544971
H	0.520368	2.463585	-0.574345
C	1.960465	1.276229	0.475283
C	0.921862	-1.407907	-0.681112
H	0.658057	-2.455040	-0.796898
H	1.254893	-1.048006	-1.656821
C	2.061240	-1.278767	0.330333
H	1.669116	-1.441772	1.336165
H	2.767152	-2.088790	0.145002
C	2.817019	0.038279	0.269832
H	1.527722	1.282233	1.477860
H	2.600862	2.157013	0.405644
H	3.307125	0.115803	-0.704732
H	3.615002	0.025133	1.013625
N	-0.310735	0.662757	-0.249040
C	0.889288	1.450178	-0.537461
H	1.232237	1.226848	-1.547340
H	0.564665	2.484800	-0.537333
C	2.012753	1.266953	0.468306
C	0.925015	-1.407067	-0.672855
H	0.646022	-2.451183	-0.789128
H	1.254610	-1.057605	-1.651722
C	2.066015	-1.289864	0.340145
H	1.675592	-1.438118	1.347886
H	2.747727	-2.117165	0.150257
C	2.842582	0.012538	0.255870
H	1.595801	1.289978	1.476657
H	2.666465	2.134706	0.382288
H	3.321686	0.072582	-0.724140
H	3.646762	-0.010891	0.990951
H	-1.287255	-2.350966	0.016519

1

(Lowest energy enamine conformation others given at end)

E_0 = -634.5121219
E_{0+ZPE} = -634.232212
E_{298} = -634.219850
H_{298} = -634.218906
G_{298} = -634.271259
NImag = 0

N	0.429174	0.556919	0.168744
C	0.850716	1.944364	0.339694
C	2.340376	1.912056	0.066273
C	2.438676	0.885663	-1.049497
C	1.406925	-0.170159	-0.640985
C	2.064270	-1.276208	0.174932
O	1.759830	-1.264690	1.460519
C	-0.941911	0.279354	0.042229
C	-1.295427	-1.129760	-0.351401
C	-3.357286	0.916966	0.242995
O	2.815424	-2.087093	-0.299844
H	0.966018	-0.642131	-1.514941
H	3.430182	0.462110	-1.181910
H	2.130320	1.328643	-1.994670
H	2.725562	2.887318	-0.219367
H	2.887764	1.579793	0.948610
H	0.340572	2.586772	-0.384865
H	0.602602	2.300074	1.337789
C	-1.885197	1.193108	0.310012
C	-2.734633	-1.478652	-0.010149
C	-3.674595	-0.382990	-0.475580
H	-3.770649	0.886469	1.256444
H	-3.858733	1.750867	-0.251586
H	-0.623357	-1.833225	0.141166
H	-1.597707	2.187035	0.622183
H	-1.135582	-1.259352	-1.424364
H	1.119188	-0.532801	1.559394
H	-2.992209	-2.434045	-0.466145
H	-3.556375	-0.244538	-1.552792
H	-4.713142	-0.664930	-0.303010
H	-2.832175	-1.604678	1.070323

3

E_0 = -634.0150093
E_{0+ZPE} = -633.749534
E_{298} = -633.736878
H_{298} = -633.735934
G_{298} = -633.789857
NImag = 0

N	0.418982	0.655406	-0.224225
C	0.935142	1.921720	0.232524
C	2.444671	1.804989	0.056914
C	2.599222	0.706644	-0.985279
C	1.464029	-0.256362	-0.640644
C	1.923809	-1.288747	0.419864
O	1.604456	-1.090171	1.605988
C	-0.901535	0.334616	-0.090458
C	-1.295435	-1.036417	-0.572939
C	-3.292624	0.891166	0.480485
O	2.607164	-2.227629	-0.043898
H	1.160170	-0.815283	-1.523991
H	3.570324	0.219315	-0.962149
H	2.444697	1.112162	-1.986331
H	2.900145	2.746748	-0.242988
H	2.902560	1.492609	0.993248
H	0.514853	2.740854	-0.362693
H	0.662560	2.110956	1.274165
C	-1.824648	1.195611	0.397831
C	-2.698575	-1.435222	-0.147881
H	-2.999663	-2.331259	-0.691335
H	-2.694600	-1.696163	0.912970
C	-3.680540	-0.302265	-0.375300
H	-4.698704	-0.620009	-0.146383
H	-3.664070	-0.017925	-1.430858
H	-3.590060	0.695638	1.517710
H	-3.869007	1.767800	0.174487
H	-0.580677	-1.767578	-0.198161
H	-1.509948	2.165348	0.757615
H	-1.215507	-1.063048	-1.663155

(1-2)$_{syn}$ (*re-re*)$_1$

E_0 = -1148.5092603
E_{0+ZPE} = -1148.087470
E_{298} = -1148.065871
H_{298} = -1148.064927
G_{298} = -1148.138874

(1-2)$_{syn}$ (*re-re*)$_2$

E_0 = -1148.5076221
E_{0+ZPE} = -1148.084602
E_{298} = -1148.063300
H_{298} = -1148.062356
G_{298} = -1148.134683

(1-2)$_{syn\text{-}Conf}$ (*re-re*)$_2$

E_0 = -1148.5002159
E_{0+ZPE} = -1148.077992
E_{298} = -1148.056521
H_{298} = -1148.055577
G_{298} = -1148.129008

NImag = 1 (-438.0364)

C	-3.813497	0.296014	-0.934388
C	-2.883936	-0.486468	-0.248838
C	-3.319611	-1.260312	0.828676
C	-4.651651	-1.254845	1.203037
C	-5.572207	-0.481681	0.505014
C	-5.150144	0.291799	-0.565785
C	-1.492052	-0.497152	-0.711464
C	-0.800893	-1.699441	-0.742016
N	0.356835	-1.814679	-1.433583
O	0.953006	-2.894245	-1.463214
O	0.805942	-0.812929	-2.051561
C	-0.611683	0.856369	0.864644
C	0.713336	0.980231	0.460263
C	1.117160	2.107322	-0.447402
C	0.285272	3.365041	-0.252659
C	-1.194753	3.042980	-0.257034
C	-1.513525	2.062763	0.855017
N	1.649847	0.075906	0.812348
C	1.358866	-0.981676	1.785557
C	2.663440	-1.736102	1.883597
C	3.684146	-0.617370	1.809542
C	3.087683	0.361508	0.784403
C	3.831061	0.250131	-0.542630
O	4.976631	0.632906	-0.575751
O	3.271456	-0.257992	-1.607657
H	3.272400	1.381782	1.112793
H	4.678661	-0.942655	1.521836
H	3.760980	-0.116025	2.772296
H	2.734112	-2.313750	2.801128
H	2.769647	-2.416744	1.039770
H	1.094416	-0.529254	2.745980
H	0.530169	-1.595129	1.455441
H	-1.237315	0.228353	-1.468036
H	-2.554844	1.749335	0.803991
H	-1.408721	2.572713	1.817855
H	-1.784269	3.950395	-0.129847
H	-1.471767	2.618195	-1.224390
H	0.551428	3.836448	0.695376
H	0.535065	4.074866	-1.039916
H	-2.613641	-1.860702	1.384083
H	-4.974463	-1.854760	2.041412
H	-6.612014	-0.482135	0.797808
H	-5.859296	0.895373	-1.113233
H	-3.486435	0.899487	-1.769227
H	-0.819574	0.137810	1.643827
H	2.169321	2.346668	-0.326922
H	0.999811	1.747732	-1.472084
H	-1.109387	-2.595944	-0.236264
H	2.310597	-0.497230	-1.584775

NImag = 1 (-446.8747)

C	3.941486	0.482896	0.694672
C	2.880524	-0.360545	0.363237
C	3.139270	-1.485079	-0.424636
C	4.422742	-1.755423	-0.864696
C	5.472887	-0.910848	-0.523289
C	5.229094	0.207353	0.258945
C	1.541597	-0.056259	0.884784
C	0.708441	-1.088497	1.295845
N	-0.444696	-0.783822	1.928563
O	-1.269441	-1.709700	2.171014
O	-0.702169	0.382180	2.239040
C	0.639830	0.951399	-0.862080
C	-0.740467	0.902757	-0.663906
C	-1.522889	2.115180	-0.237552
C	-0.794929	3.425989	-0.492032
C	0.658850	3.341415	-0.076410
C	1.357354	2.272376	-0.894267
N	-1.416986	-0.250276	-0.833356
C	-0.814844	-1.407266	-1.502163
C	-1.878609	-2.470075	-1.378503
C	-3.155509	-1.682295	-1.611757
C	-2.874938	-0.294170	-1.000362
C	-3.767989	-0.080435	0.217284
O	-4.793001	0.541135	0.066595
O	-3.509901	-0.656049	1.363215
H	-3.184115	0.478711	-1.698053
H	-4.034662	-2.152531	-1.179696
H	-3.337188	-1.562575	-2.677275
H	-1.744889	-3.271989	-2.099448
H	-1.860693	-2.900197	-0.378436
H	-0.624750	-1.158768	-2.550821
H	0.122306	-1.679088	-1.037121
H	1.442306	0.878902	1.414494
H	2.385619	2.140285	-0.556883
H	1.433522	2.608891	-1.932481
H	1.155290	4.300586	-0.221108
H	0.724131	3.106487	0.988140
H	-0.846749	3.671670	-1.554696
H	-1.312643	4.221913	0.041056
H	2.333455	-2.149353	-0.702375
H	4.607007	-2.627457	-1.475177
H	6.474341	-1.125766	-0.866572
H	6.039983	0.866551	0.532456
H	3.757662	1.349448	1.313922
H	1.059259	0.180633	-1.491657
H	-2.475219	2.129688	-0.763422
H	-1.757522	2.016045	0.820942
H	0.842804	-2.129407	1.069221
H	-2.622766	-1.065362	1.520944

NImag = 1 (-450.4469)

C	3.990305	0.176659	0.365876
C	2.784494	-0.524267	0.326377
C	2.765498	-1.791093	-0.262798
C	3.920039	-2.336693	-0.795984
C	5.115716	-1.629507	-0.749121
C	5.148129	-0.372996	-0.164055
C	1.587147	0.082571	0.924595
C	0.657896	-0.708300	1.584438
N	-0.327446	-0.094858	2.280801
O	-1.207313	-0.802419	2.842526
O	-0.371987	1.134653	2.344534
C	0.638704	0.997415	-0.810555
C	-0.726079	1.028904	-0.533835
C	-1.449894	2.328595	-0.285856
C	-0.622987	3.579602	-0.559977
C	0.830200	3.409761	-0.174769
C	1.416659	2.271062	-0.983320
N	-1.449301	-0.118615	-0.445643
C	-1.039372	-1.355122	-1.121293
C	-1.916189	-1.415773	-2.380311
C	-3.058230	-0.426820	-2.101858
C	-2.903454	-0.106427	-0.616202
C	-3.669060	-1.121964	0.236239
O	-4.714782	-1.562737	-0.173114
O	-3.239265	-1.458743	1.425214
H	-3.328520	0.851545	-0.338373
H	-4.041501	-0.824496	-2.325049
H	-2.920092	0.491524	-2.668350
H	-1.351615	-1.125159	-3.262781
H	-2.283781	-2.426194	-2.540277
H	0.021890	-1.376437	-1.321799
H	-1.259428	-2.187096	-0.455679
H	1.711544	1.083462	1.310074
H	2.458313	2.095276	-0.713364
H	1.432211	2.549458	-2.041183
H	1.383493	4.329178	-0.363866
H	0.910776	3.195119	0.892250
H	-0.671933	3.816660	-1.624413
H	-1.077834	4.416789	-0.032814
H	1.843843	-2.352572	-0.309831
H	3.888920	-3.316696	-1.249517
H	6.015539	-2.058749	-1.165108
H	6.074452	0.180761	-0.117035
H	4.024112	1.150524	0.833324
H	1.003914	0.159047	-1.381528
H	-2.321365	2.360647	-0.938890
H	-1.824642	2.332525	0.735043
H	0.601331	-1.780186	1.553361
H	-2.402754	-1.070289	1.780888

(1-2)$_{syn}$ $(si\text{-}si)_1$

E_0 = -1148.5040311
E_{0+ZPE} = -1148.081870
E_{298} = -1148.060172
H_{298} = -1148.059228
G_{298} = -1148.133160
NImag = 1 (-399.6916)

C	-3.236013	0.000646	-0.356745
C	-1.917945	0.038424	-0.816632
C	-1.532497	-0.873489	-1.801294
C	-2.429806	-1.801837	-2.304880
C	-3.732123	-1.839118	-1.827821
C	-4.130216	-0.933449	-0.852912
C	-0.943194	1.049600	-0.378925
C	-1.378569	2.267955	0.140639
N	-0.645112	3.407328	0.035219
O	-1.050317	4.431318	0.595112
O	0.397074	3.446340	-0.666258

(1-2)$_{syn\text{-}Conf}$ $(si\text{-}si)_1$

E_0 = -1148.5042453
E_{0+ZPE} = -1148.081805
E_{298} = -1148.060040
H_{298} = -1148.059096
G_{298} = -1148.133110
NImag = 1 (-387.2698)

C	-3.314588	0.303010	-0.491885
C	-1.970874	0.230759	-0.868234
C	-1.594296	-0.707580	-1.832245
C	-2.532637	-1.545798	-2.410633
C	-3.864605	-1.464604	-2.029019
C	-4.250528	-0.538982	-1.067842
C	-0.946998	1.122857	-0.325170
C	-1.289464	2.353452	0.212113
N	-0.345931	3.261428	0.586780
O	-0.702188	4.352577	1.028719
O	0.876587	2.977052	0.518266

(1-2)$_{syn}$ $(si\text{-}si)_2$

E_0 = -1148.5080359
E_{0+ZPE} = -1148.085376
E_{298} = -1148.064082
H_{298} = -1148.063138
G_{298} = -1148.135171
NImag = 1 (-362.5786)

C	-0.396079	0.840425	-0.947527
C	0.792458	1.307585	-0.404490
N	1.873209	0.503925	-0.306239
C	2.168055	-0.514355	-1.319649
C	3.698883	-0.472032	-1.418441
C	4.128464	-0.116890	-0.006434
C	3.090207	0.905177	0.409549
C	1.747851	-1.960287	-1.083282
O	1.927239	-2.529824	0.088133
O	1.378355	-2.618204	-2.024980
H	4.119279	-1.404406	-1.786288

C	-0.173109	-2.345207	1.047917
C	0.640516	-1.101889	0.860052
C	0.134671	0.125197	1.310574
C	-0.839149	0.148777	2.461703
C	-1.687394	-1.105278	2.602860
C	-0.851052	-2.353359	2.412997
N	1.825658	-1.218102	0.257464
C	2.311642	-2.434726	-0.398988
C	3.568440	-1.978463	-1.111686
C	4.112814	-0.903209	-0.186254
C	2.857539	-0.188116	0.310582
C	2.477281	0.986723	-0.572487
O	2.170037	0.870401	-1.732289
O	2.486041	2.126202	0.085814
H	2.963151	0.168787	1.331948
H	4.808439	-0.224299	-0.672168
H	4.619152	-1.352118	0.666447
H	4.267203	-2.796831	-1.262197
H	3.318341	-1.552346	-2.080125
H	2.545329	-3.192596	0.350519
H	1.559466	-2.833139	-1.073311
H	-0.058529	1.097204	-0.994523
H	-1.467037	-3.248088	2.495589
H	-0.089703	-2.418587	3.193061
H	-2.163662	-1.111212	3.583204
H	-2.487148	-1.104866	1.864146
H	-0.261389	0.290196	3.379992
H	-1.473349	1.033601	2.382409
H	-0.522325	-0.841200	-2.184713
H	-2.112605	-2.491135	-3.073999
H	-4.435081	-2.560272	-2.218850
H	-5.145640	-0.947741	-0.484092
H	-3.575235	0.705197	0.387499
H	0.449100	-3.227255	0.935200
H	0.832016	0.950512	1.325764
H	-2.295600	2.409336	0.681034
H	1.858902	2.761453	-0.335426
H	-0.931315	-2.388373	0.262575

C	-0.091232	-2.431142	1.063395
C	0.584977	-1.096807	0.943456
C	-0.043072	0.035911	1.444061
C	-1.172801	-0.064255	2.430626
C	-1.935825	-1.376110	2.373606
C	-0.973784	-2.542226	2.295214
N	1.762874	-1.070794	0.288253
C	2.561344	-2.271671	0.001904
C	3.963939	-1.758146	-0.305810
C	3.983828	-0.350599	0.271285
C	2.549376	0.131293	0.064482
C	2.393339	0.632082	-1.371997
O	2.542786	-0.094601	-2.319960
O	2.149706	1.917317	-1.541894
H	2.284732	0.908152	0.771840
H	4.717684	0.300132	-0.197778
H	4.180872	-0.369323	1.341921
H	4.722071	-2.394387	0.143274
H	4.131503	-1.730627	-1.377325
H	2.575403	-2.910522	0.882179
H	2.136719	-2.835348	-0.825380
H	0.014732	1.032981	-0.793969
H	-1.512266	-3.488593	2.259182
H	-0.346486	-2.567629	3.188791
H	-2.579353	-1.465371	3.248594
H	-2.585430	-1.393377	1.498603
H	-0.762408	0.067432	3.436562
H	-1.852898	0.778990	2.285068
H	-0.558975	-0.765920	-2.137606
H	-2.224640	-2.257716	-3.162418
H	-4.599195	-2.115760	-2.480022
H	-5.286061	-0.471183	-0.767647
H	-3.635967	1.012761	0.255535
H	0.637168	-3.235066	1.057826
H	0.564104	0.922646	1.549330
H	-2.293778	2.673406	0.415256
H	1.777304	2.346991	-0.741928
H	-0.695181	-2.564544	0.159995

H	3.978019	0.320470	-2.110795
H	1.695675	-0.232390	-2.255087
H	1.992749	-1.949540	0.884328
C	-1.205684	0.004044	0.955919
C	-0.264015	-0.900329	1.424793
C	-1.445031	1.787450	-1.456931
H	-1.224887	0.972676	1.432168
H	-0.263529	-1.948011	1.190390
C	-2.495017	-0.473686	0.442068
C	-2.621436	-1.661792	-0.281160
C	-3.863875	-2.089475	-0.714871
C	-5.001408	-1.342533	-0.431259
C	-4.887199	-0.160485	0.284653
C	-3.641575	0.273933	0.711719
H	-1.746444	-2.249812	-0.516989
H	-3.946455	-3.008455	-1.276659
H	-5.969719	-1.680937	-0.770179
H	-5.766136	0.425850	0.509785
H	-3.554978	1.194508	1.271435
N	0.792682	-0.480385	2.166502
O	0.854640	0.667622	2.611276
O	1.724471	-1.300535	2.395934
H	-0.379905	-0.130121	-1.424494
C	0.853833	2.701460	0.157145
H	0.581632	2.661734	1.211896
H	1.872689	3.075458	0.119866
C	-0.065128	3.662755	-0.583890
C	-1.468776	3.105212	-0.705653
H	-1.246192	1.977686	-2.516076
H	-2.421505	1.306279	-1.424469
H	0.336814	3.854374	-1.580890
H	-0.069711	4.616579	-0.057528
H	-1.888763	2.959137	0.291602
H	-2.118965	3.812359	-1.219865
H	5.133377	0.294475	0.034463
H	4.103197	-0.989205	0.643616
H	3.403693	1.898181	0.091860
H	2.894031	0.928787	1.479605

(1-2)*syn* (*si-re*)$_1$

E_0 = -1148.5103668
E_{0+ZPE} = -1148.087948
E_{298} = -1148.066385
H_{298} = -1148.065440
G_{298} = -1148.138698
NImag = 1 (-384.9677)

C	2.588149	1.853941	0.172717
C	2.444557	0.486878	0.418637
C	3.565971	-0.335630	0.292306
C	4.793485	0.197874	-0.064553
C	4.923789	1.559389	-0.302911
C	3.815929	2.387209	-0.181677
C	1.125319	-0.012474	0.826789
C	1.014783	-1.178289	1.580260
N	-0.112285	-1.461839	2.285580
O	-0.120067	-2.438305	3.042917
O	-1.139351	-0.753054	2.167570
C	-0.975806	-2.246830	-0.863065
C	-0.992209	-0.754026	-0.911512
C	0.199734	-0.086244	-1.200362
C	1.213991	-0.741245	-2.101719
C	1.294330	-2.243898	-1.915719
C	-0.091201	-2.855530	-1.943532
N	-2.134445	-0.116623	-0.621752
C	-3.354276	-0.791900	-0.170610
C	-4.351827	0.337832	0.015272
C	-3.889531	1.374825	-0.994260
C	-2.364615	1.290463	-0.890794
C	-1.873373	2.251308	0.182071

(1-2)*syn* (*si-re*)$_2$

E_0 = -1148.5065383
E_{0+ZPE} = -1148.083925
E_{298} = -1148.062430
H_{298} = -1148.061486
G_{298} = -1148.134102
NImag = 1 (-401.1022)

C	-3.089404	0.909040	-0.659696
C	-1.723234	0.750391	-0.890926
C	-1.309674	-0.144283	-1.880666
C	-2.241703	-0.862245	-2.611760
C	-3.600367	-0.694875	-2.374801
C	-4.021580	0.196848	-1.399137
C	-0.762205	1.555615	-0.121725
C	0.330050	2.086195	-0.802496
N	1.150476	2.991908	-0.217029
O	2.190547	3.330120	-0.840371
O	0.906347	3.444648	0.906104
C	-1.357437	-1.697191	1.346802
C	-0.077505	-0.956093	1.103604
C	0.042887	0.365594	1.537834
C	-0.763398	0.842655	2.719820
C	-2.124801	0.181849	2.827682
C	-1.999556	-1.320580	2.676650
N	0.892837	-1.592696	0.436211
C	0.750735	-2.938445	-0.129926
C	2.089219	-3.202357	-0.789268
C	3.057544	-2.435612	0.095246
C	2.286530	-1.160742	0.436977
C	2.553079	-0.083582	-0.599779

(1-2)*syn*-Conf (*si-re*)$_2$

E_0 = - 1148.498735
E_{0+ZPE} = -1148.076647
E_{298} = -1148.054972
H_{298} = -1148.054028
G_{298} = -1148.127817
NImag = 1 (-388.7306)

C	-3.337082	-0.987570	0.110049
C	-1.977015	-1.024433	0.423682
C	-1.578604	-0.736261	1.731628
C	-2.520672	-0.427443	2.697984
C	-3.872303	-0.404467	2.377500
C	-4.278397	-0.686190	1.080705
C	-1.026937	-1.402534	-0.621566
C	0.099131	-2.149514	-0.324995
N	0.913395	-2.583597	-1.328491
O	2.023084	-3.090122	-1.017848
O	0.596067	-2.448665	-2.509216
C	-0.854219	2.458065	-0.145004
C	0.116248	1.391020	-0.566021
C	-0.244947	0.514511	-1.577971
C	-1.339591	0.870699	-2.553916
C	-2.381420	1.830192	-2.008624
C	-1.710842	2.978142	-1.285895
N	1.273914	1.334878	0.126605
C	1.842564	2.504976	0.817575
C	3.347459	2.245047	0.877962
C	3.584245	1.119718	-0.119122
C	2.289937	0.311311	-0.014134
C	2.375873	-0.548885	1.243114

O	-1.817423	3.432633	-0.044829
O	-1.562911	1.779082	1.371644
H	-1.878484	1.587180	-1.817082
H	-4.259189	2.377240	-0.801610
H	-4.185255	1.087424	-2.001669
H	-5.371581	0.005447	-0.157022
H	-4.298887	0.735872	1.027722
H	-3.700002	-1.486254	-0.935966
H	-3.156105	-1.346831	0.744043
H	0.424070	0.768886	1.060340
H	-0.043755	-3.932815	-1.789574
H	-0.548534	-2.694933	-2.921905
H	1.921363	-2.680447	-2.692665
H	1.767590	-2.471308	-0.959395
H	0.938175	-0.520635	-3.137993
H	2.190524	-0.283111	-1.953983
H	3.487570	-1.397587	0.470523
H	5.651383	-0.452232	-0.156194
H	5.882967	1.972320	-0.579402
H	3.908481	3.448689	-0.359373
H	1.729883	2.503978	0.273157
H	-1.979555	-2.654135	-0.921635
H	0.150578	0.990916	-1.295092
H	1.796181	-1.902714	1.710919
H	-1.528485	0.803650	1.449053
H	-0.577010	-2.534120	0.115573
O	2.259674	-0.182161	-1.764344
O	3.162483	0.956488	-0.067710
H	2.547718	-0.771214	1.416701
H	4.011273	-2.226059	-0.382166
H	3.252547	-2.982328	1.016283
H	2.312191	-4.265006	-0.833402
H	2.101141	-2.802533	-1.799972
H	0.573929	-3.658922	0.669912
H	-0.085123	-2.976218	-0.822804
H	-1.184066	2.161259	0.666564
H	-2.975704	-1.800083	2.741641
H	-1.396106	-1.721205	3.493862
H	-2.580026	0.431038	3.785839
H	-2.788609	0.566338	2.053469
H	-0.190121	0.635721	3.628954
H	-0.863036	1.927399	2.679550
H	-0.255476	-0.288499	-2.070190
H	-1.906593	-1.552849	-3.372341
H	-4.324745	-1.253238	-2.949838
H	-5.076159	0.340570	-1.213070
H	-3.423959	1.608462	0.093153
H	-1.187364	-2.768654	1.314088
H	1.020137	0.821916	1.466591
H	0.654196	1.758410	-1.771253
H	3.115576	1.743094	-0.648498
H	-2.042311	-1.467723	0.526616
O	2.103379	-0.118738	2.333928
O	2.879225	-1.762784	1.106815
H	2.122320	-0.301192	-0.892707
H	4.473383	0.531811	0.094905
H	3.662269	1.501476	-1.135531
H	3.911508	3.139264	0.626849
H	3.638518	1.934986	1.877396
H	1.634394	3.399318	0.235960
H	1.411562	2.624597	1.808014
H	-1.435265	-1.511349	-1.614068
H	-2.450146	3.671677	-0.886937
H	-1.087707	3.543789	-1.981859
H	-3.004148	2.196100	-2.824759
H	-3.041252	1.311516	-1.313042
H	-0.868532	1.319307	-3.434281
H	-1.822896	-0.035864	-2.923471
H	-0.530643	-0.737399	1.993338
H	-2.199284	-0.203255	3.704724
H	-4.604349	-0.167380	3.135740
H	-5.327887	-0.672772	0.824941
H	-3.655058	-1.213253	-0.898056
H	-0.346185	3.279663	0.346399
H	0.531200	-0.097294	-2.014017
H	0.443991	-2.369771	0.667515
H	2.712219	-2.180998	0.231310
H	-1.493779	2.002214	0.617708

(1-2)$_{syn}$ (*re-si*)$_1$

E_0 = -1148.5082867
E_{0+ZPE} = -1148.086624
E_{298} = -1148.064798
H_{298} = -1148.063854
G_{298} = -1148.139046
NImag = 1 (-438.9753)

C	3.807977	-0.722045	-0.122601
C	2.840034	0.151731	-0.624094
C	3.222025	1.456532	-0.944614
C	4.530331	1.876546	-0.776744
C	5.483172	0.997702	-0.279126
C	5.116833	-0.301279	0.045947
C	1.450096	-0.248694	-0.858613
C	1.099771	-1.585886	-1.012723
N	-0.069578	-1.907597	-1.619816
O	-0.352423	-3.089196	-1.830029
O	-0.848857	-0.985125	-1.977050
C	0.560056	0.723800	0.963033
C	-0.768974	0.302009	0.963711
C	-1.123994	-0.973029	1.660975
C	-0.311921	-1.221189	2.922873
C	1.168783	-1.061531	2.645920
C	1.455245	0.327392	2.109842
N	-1.732028	0.952194	0.290855
C	-1.450975	2.157287	-0.484254
C	-2.799200	2.547505	-1.052465
C	-3.754298	2.117089	0.045101
C	-3.160361	0.791131	0.535822
C	-3.867731	-0.382477	-0.133206
O	-4.999006	-0.634325	0.203899
O	-3.279579	-1.085340	-1.067555
H	-3.352781	0.666862	1.598273
H	-4.783407	2.003275	-0.280548
H	-3.734729	2.833526	0.864375
H	-2.856411	3.610043	-1.271641
H	-2.997647	2.001486	-1.974101
H	-1.059595	2.936725	0.173876
H	-0.710444	1.949693	-1.250247
H	0.868656	0.440863	-1.446917
H	2.499599	0.413941	1.814032
H	1.318303	1.055774	2.915912

(1-2)$_{syn}$ (*re-si*)$_2$

E_0 = -1148.5079508
E_{0+ZPE} = -1148.084917
E_{298} = -1148.063728
H_{298} = -1148.062784
G_{298} = -1148.134488
NImag = 1 (-386.2723)

C	-2.502911	0.386167	1.475285
C	-2.400638	0.875584	0.169042
C	-3.570838	1.025225	-0.578130
C	-4.802898	0.673505	-0.050189
C	-4.887096	0.167890	1.238704
C	-3.733065	0.032894	2.001014
C	-1.128262	1.296036	-0.425378
C	-0.073072	1.709502	0.387174
N	0.939451	2.448152	-0.110389
O	1.966328	2.615468	0.609110
O	0.889465	2.947574	-1.240896
C	-0.461202	-0.435829	-1.634631
C	0.422731	-1.008306	-0.720242
C	-0.096211	-2.041061	0.228514
C	-1.073938	-2.985838	-0.459611
C	-2.204381	-2.216622	-1.113396
C	-1.674319	-1.193406	-2.104291
N	1.684393	-0.572627	-0.611491
C	2.342547	0.181362	-1.689698
C	3.745750	0.415503	-1.175556
C	4.028470	-0.831758	-0.359680
C	2.676991	-1.183498	0.276625
C	2.623618	-0.757246	1.738621
O	2.787653	-1.589829	2.596950
O	2.474081	0.504707	2.063910
H	2.552762	-2.259964	0.297326
H	4.810901	-0.699982	0.383090
H	4.323243	-1.652348	-1.010640
H	4.453719	0.551805	-1.988469
H	3.770477	1.309678	-0.555692
H	2.341822	-0.436050	-2.589748
H	1.822338	1.107899	-1.906685
H	-1.218209	1.810653	-1.369762
H	-2.463459	-0.495041	-2.383050
H	-1.395962	-1.701108	-3.032868

H	1.748465	-1.236116	3.551972
H	1.481706	-1.812191	1.917977
H	-0.620800	-0.519058	3.699650
H	-0.535470	-2.221000	3.291896
H	2.484128	2.143379	-1.335835
H	4.807538	2.887515	-1.037683
H	6.505241	1.322013	-0.147815
H	5.853113	-0.990852	0.432407
H	3.547475	-1.736674	0.138265
H	0.751214	1.709923	0.563590
H	-2.185403	-1.032260	1.880717
H	-0.911840	-1.776171	0.945229
H	1.689461	-2.432028	-0.715016
H	-2.337430	-0.894525	-1.288462
H	-2.881065	-2.899621	-1.626401
H	-2.786978	-1.719026	-0.339121
H	-0.537221	-3.576476	-1.204818
H	-1.463655	-3.686461	0.277483
H	-3.512639	1.434609	-1.576622
H	-5.696728	0.800308	-0.643494
H	-5.845977	-0.108143	1.652667
H	-3.793015	-0.345343	3.011143
H	-1.622137	0.283833	2.091276
H	-0.027502	0.204981	-2.388126
H	0.706896	-2.608752	0.685185
H	-0.606270	-1.519159	1.043282
H	0.058571	1.406831	1.408762
H	2.315304	1.184225	1.360790

(1-2)$_{syn}$ (*re-re*)$_1$ (*down*)

E_0 = -1148.5099153
E_{0+ZPE} = -1148.088052
E_{298} = -1148.066395
H_{298} = -1148.065451
G_{298} = -1148.139372
NImag = 1 (-406.1622)

C	-3.357497	-1.246922	0.761676
C	-2.889172	-0.471983	-0.301854
C	-3.789968	0.342437	-0.988866
C	-5.130731	0.367917	-0.636676
C	-5.585140	-0.407074	0.419679
C	-4.693263	-1.211440	1.119908
C	-1.494279	-0.509137	-0.747243
C	-0.607807	0.807127	0.886530
C	-1.483450	2.030602	0.918104
C	-0.801265	-1.708114	-0.743043
N	0.367709	-1.830705	-1.413354
O	0.992546	-2.893742	-1.374044
C	0.731110	0.910546	0.526385
C	1.202408	2.095390	-0.271437
N	1.636599	-0.044765	0.824400
C	3.085371	0.157336	0.699991
C	3.681702	-1.102275	1.327661
C	2.703055	-1.401257	2.442698
C	1.361316	-1.114164	1.798600
C	3.723845	0.384271	-0.660928
O	3.190020	-0.090156	-1.753755
O	4.792188	0.948842	-0.691795
O	0.796409	-0.854405	-2.085508
H	2.873004	-0.727085	3.281438
H	2.768791	-2.423275	2.805730
H	3.693627	-1.915339	0.602014
H	4.697976	-0.925925	1.665339
H	3.380268	1.019409	1.298608
H	0.622293	-0.779760	2.520844
H	0.976805	-1.995724	1.292729
H	-1.102832	-2.590400	-0.209244
H	-1.214090	0.211903	-1.498638
H	-3.436856	0.947412	-1.811955
H	-5.817620	0.995719	-1.185185
H	-6.628171	-0.384599	0.699857
H	-5.041818	-1.812357	1.947168
H	-2.674110	-1.871208	1.319086
H	2.267882	-0.461935	-1.718241
H	-0.872891	0.037231	1.594518
H	1.158911	1.822921	-1.327962
H	2.243967	2.312689	-0.050712
C	0.378788	3.352372	-0.037474
C	-1.104561	3.062263	-0.125342
H	-1.406357	2.485166	1.911058
H	-2.527693	1.741162	0.811552
H	-1.347683	2.694228	-1.124563

(1-2)$_{syn}$ (*si-si*)$_2$ (*down*)

E_0 = -1148.5062518
E_{0+ZPE} = -1148.083749
E_{298} = -1148.062402
H_{298} = -1148.061457
G_{298} = -1148.134015
NImag = 1 (-366.2775)

C	-0.346091	0.829095	-0.898262
C	0.847663	1.243040	-0.322191
N	1.869915	0.371641	-0.177300
C	2.183556	-0.612100	-1.221275
C	3.731243	-0.619253	-1.305224
C	4.170688	0.586204	-0.487957
C	3.089281	0.672615	0.565790
C	1.727159	-2.051783	-1.054246
O	1.815412	-2.647521	0.115033
O	1.409546	-2.682402	-2.032839
H	4.169733	1.490579	-1.095755
H	5.162104	0.458564	-0.061375
H	4.129599	-1.530622	-0.862435
H	4.055318	-0.586436	-2.340726
H	1.745164	-0.271783	-2.153961
H	3.024794	1.622844	1.075639
H	3.218973	-0.095533	1.331992
H	1.871839	-2.084408	0.923699
C	-1.237816	0.016727	0.947291
C	-0.349315	-0.938402	1.422724
C	-1.337321	1.818701	-1.440438
H	-1.235829	0.971542	1.451655
H	-0.385702	-1.979566	1.163033
C	-2.534046	-0.403697	0.396645
C	-2.682270	-1.561963	-0.369108
C	-3.929120	-1.938931	-0.836321
C	-5.049422	-1.169490	-0.544580
C	-4.913087	-0.016257	0.213188
C	-3.662660	0.367323	0.673999
H	-1.820086	-2.166555	-0.610999
H	-4.028503	-2.835598	-1.430529
H	-6.021411	-1.468216	-0.909305
H	-5.778566	0.587339	0.444858
H	-3.559469	1.265531	1.266113
N	0.700225	-0.581880	2.205259
O	0.801848	0.553931	2.672226
O	1.582327	-1.452688	2.447927
H	-0.355682	-0.142310	-1.374031
C	0.975596	2.645793	0.208586
H	0.722648	2.647217	1.268788
H	2.009982	2.971708	0.135177
C	0.095070	3.635376	-0.542889
C	-1.326682	3.131551	-0.682030
H	-1.097326	2.004119	-2.491759
H	-2.332796	1.377362	-1.439411
H	0.513311	3.809072	-1.536363

(1-2)$_{syn}$ (*si-re*)$_1$ (*down*)

E_0 = -1148.5063462
E_{0+ZPE} = -1148.083829
E_{298} = -1148.062175
H_{298} = -1148.061231
G_{298} = -1148.134891
NImag = 1 (-381.7990)

C	0.140086	-0.031686	-1.151012
C	-1.037804	-0.726655	-0.851500
C	-0.981778	-2.220116	-0.850236
N	-2.175900	-0.103263	-0.518487
C	-2.401051	1.315847	-0.748060
C	-3.934307	1.491589	-0.662938
C	-4.482474	0.075483	-0.717484
C	-3.400434	-0.730932	-0.033484
C	-1.770542	2.266052	0.250416
O	-1.472838	1.816853	1.452744
O	-1.628466	3.429773	-0.025508
H	-4.592406	-0.258804	-1.748224
H	-5.444154	-0.017406	-0.220241
H	-4.209348	1.959639	0.280878
H	-4.292156	2.130737	-1.463569
H	-2.024687	1.589700	-1.731009
H	-3.438191	-1.784811	-0.271230
H	-3.449380	-0.634239	1.053451
H	-1.462892	0.842212	1.559831
H	-0.554206	-2.525188	0.110889
C	1.138112	-0.023561	0.836736
H	0.474957	0.778134	1.108622
C	1.012030	-1.197553	1.577763
H	0.074674	1.047189	-1.212494
N	-0.098238	-1.453475	2.317657
O	-0.118561	-2.447976	3.051402
O	-1.100051	-0.700822	2.259428
C	2.461446	0.438879	0.397219
C	2.639697	1.803250	0.158527
C	3.871973	2.302583	-0.228184
C	4.950201	1.443091	-0.388819
C	4.785929	0.084308	-0.155979
C	3.553936	-0.415183	0.233132
H	1.804723	2.477776	0.287558
H	3.991023	3.362278	-0.400748
H	5.912735	1.829194	-0.691255
H	5.620726	-0.590588	-0.276903
H	3.450709	-1.475631	0.407063
H	1.768518	-1.954188	1.665281
C	1.131375	-0.635193	-2.112758
H	-1.970694	-2.659220	-0.903270
C	-0.113829	-2.779420	-1.970403
C	1.257470	-2.138805	-1.972203
H	0.807155	-0.394690	-3.130422
H	2.100214	-0.153953	-1.991469
H	1.769024	-2.381386	-1.039609

H	-1.682205	3.973651	0.025961
H	0.678067	4.104692	-0.765821
H	0.608504	3.758031	0.949705
H	0.121532	4.590329	-0.019335
H	-1.764794	2.993497	0.308497
H	-1.943434	3.865147	-1.200169
H	1.866602	-2.538334	-2.782680
H	-0.039789	-3.858782	-1.843378
H	-0.605077	-2.606946	-2.930189

(1-2)$_{syn}$ (*re-si*)$_1$ (*down*)

E_0 = -1148.5077487
E_{0+ZPE} = -1148.085944
E_{298} = -1148.064211
H_{298} = -1148.063267
G_{298} = -1148.137446
NImag = 1 (-422.8741)

C	3.811250	-0.699519	-0.212547
C	2.822384	0.223890	-0.560227
C	3.173590	1.572146	-0.662298
C	4.473610	1.987126	-0.430867
C	5.447166	1.059182	-0.085029
C	5.111423	-0.283512	0.022178
C	1.442288	-0.164994	-0.859470
C	1.122125	-1.461583	-1.241964
N	-0.045711	-1.699583	-1.886093
O	-0.319883	-2.837279	-2.272834
O	-0.834612	-0.738763	-2.099856
C	0.551737	0.427014	1.127758
C	-0.815811	0.177326	1.005065
C	-1.383164	-1.110082	1.525104
C	-0.630895	-1.666827	2.723626
C	0.858076	-1.700671	2.454696
C	1.359393	-0.298315	2.171378
N	-1.654968	1.024714	0.390256
C	-1.235060	2.344647	-0.079873
C	-2.518150	3.149379	-0.142557
C	-3.562622	2.100722	-0.463966
C	-3.112004	0.901933	0.373809
C	-3.762656	-0.353378	-0.183888
O	-4.852107	-0.664986	0.233659
O	-3.205357	-1.026438	-1.157238
H	-3.498318	0.999607	1.388157
H	-3.529608	1.847403	-1.523708
H	-4.576912	2.394724	-0.213396
H	0.832944	0.603593	-1.303768
H	2.408148	-0.319504	1.876902
H	1.329346	0.282727	3.098880
H	1.392598	-2.121074	3.306140
H	1.057276	-2.350501	1.600497
H	-0.830628	-1.046314	3.599358
H	-1.015631	-2.661378	2.944339
H	2.418516	2.296156	-0.935970
H	4.728683	3.032801	-0.523072
H	6.462675	1.379966	0.096358
H	5.865023	-1.010207	0.288259
H	3.571356	-1.748793	-0.128581
H	0.880501	1.434940	0.926368
H	-2.431403	-0.988038	1.784901
H	-1.345900	-1.842030	0.712912
H	1.726870	-2.334421	-1.083762
H	-2.285525	-0.792122	-1.442194
H	-2.724378	3.603106	0.825970
H	-2.468726	3.940017	-0.886183
H	-0.513528	2.778029	0.607992
H	-0.769041	2.258221	-1.060970

(1-2)$_{syn}$ (*re-si*)$_2$ (*down*)

E_0 = -1148.5095408
E_{0+ZPE} = -1148.086568
E_{298} = -1148.065348
H_{298} = -1148.064404
G_{298} = -1148.136284
NImag = 1 (-372.4791)

C	3.577068	-0.960206	-0.724046
C	2.425268	-0.871341	0.060245
C	2.554763	-0.453751	1.389002
C	3.794609	-0.122641	1.905599
C	4.931039	-0.203140	1.109577
C	4.818991	-0.628541	-0.205675
C	1.142670	-1.272059	-0.526019
C	0.123168	-1.757130	0.289857
N	-0.931524	-2.417216	-0.228065
O	-0.951899	-2.797447	-1.403739
O	-1.930106	-2.634615	0.522323
C	0.391108	0.516005	-1.599919
C	1.573011	1.337458	-2.036051
C	-0.506289	1.009792	-0.653912
C	-0.031423	2.015633	0.345507
N	-1.753905	0.530122	-0.569085
C	-2.727463	0.955096	0.445379
C	-4.038307	0.318658	-0.013206
C	-3.896820	0.319148	-1.521345
C	-2.446605	-0.072786	-1.719783
C	-2.414978	0.589806	1.889749
O	-2.146448	-0.657250	2.192966
O	-2.486129	1.430805	2.751961
H	-4.080288	1.316256	-1.919844
H	-4.573963	-0.376590	-2.009145
H	-4.117755	-0.703881	0.353215
H	-4.892725	0.880018	0.352913
H	-2.825251	2.038351	0.427320
H	-2.026409	0.322700	-2.639361
H	-2.324342	-1.154084	-1.726323
H	1.209338	-1.709411	-1.510201
H	0.048762	-1.553045	1.340700
H	1.687184	-0.385166	2.028108
H	3.875732	0.198179	2.933953
H	5.897636	0.055684	1.516644
H	5.698607	-0.708500	-0.827626
H	3.497938	-1.309406	-1.743826
H	-0.024826	-0.115002	-2.372348
H	0.477007	1.485417	1.155758
H	-2.128421	-1.331842	1.460282
H	-0.865846	2.542616	0.797551
C	0.927044	3.015304	-0.291790
C	2.077257	2.310616	-0.983373
H	2.381477	0.682432	-2.360526
H	1.273627	1.894132	-2.929651
H	1.297496	3.687678	0.480796
H	0.377230	3.629012	-1.008237
H	2.741316	3.038153	-1.449353
H	2.666459	1.778488	-0.237610

(1-2)$_{anti}$ (*re-re*)$_1$ (*down*)

E_0 = -1148.5129632
E_{0+ZPE} = -1148.090506
E_{298} = -1148.068835
H_{298} = -1148.067891
G_{298} = -1148.141457

(1-2)$_{anti}$ (*re-re*)$_2$ (*down*)

E_0 = -1148.5007194
E_{0+ZPE} = -1148.078250
E_{298} = -1148.056539
H_{298} = -1148.055595
G_{298} = -1148.129445

(1-2)$_{anti}$ (*si-si*)$_1$ (*down*)

E_0 = -1148.5063521
E_{0+ZPE} = -1148.083262
E_{298} = -1148.061829
H_{298} = -1148.060884
G_{298} = -1148.133562

NImag = 1 (-367.9061)

C	-2.430202	-0.316931	-0.586898
N	-1.482351	-1.366281	-0.249224
C	-1.760624	-2.598026	-0.986582
C	-2.604276	-2.118259	-2.150163
C	-3.421765	-0.996358	-1.535769
C	-0.445715	-1.188275	0.576033
C	-0.107571	0.062870	1.085783
C	0.823131	0.201581	2.256785
C	1.768295	-0.975657	2.431810
C	1.019397	-2.284042	2.289157
C	0.379300	-2.393412	0.913660
C	-3.165944	0.230651	0.632242
O	-3.280870	1.544027	0.695116
O	-3.673423	-0.482424	1.456274
C	0.902696	1.143063	-0.608036
C	0.784895	2.471535	-0.217850
N	-0.393156	3.135188	-0.337562
O	-1.373427	2.569788	-0.892504
C	2.216494	0.506980	-0.719991
C	2.350217	-0.609921	-1.548399
C	3.578169	-1.226682	-1.718318
C	4.697085	-0.738662	-1.057231
C	4.578440	0.372807	-0.233394
C	3.351843	0.993723	-0.067017
O	-0.496468	4.284668	0.093999
H	-1.913580	0.497971	-1.088000
H	-4.250481	-1.409464	-0.963665
H	-3.819633	-0.295367	-2.263483
H	0.153097	0.767704	-1.285577
H	1.385971	1.133171	2.163158
H	0.221043	0.315175	3.163208
H	2.250199	-0.914117	3.407269
H	2.560126	-0.935932	1.683782
H	0.243205	-2.353433	3.053710
H	1.687074	-3.131972	2.436352
H	3.285525	1.857432	0.576967
H	5.446380	0.760756	0.279595
H	5.656638	-1.217472	-1.187706
H	3.663391	-2.084265	-2.369720
H	1.483052	-0.986136	-2.073151
H	-0.861500	0.830779	1.026600
H	-0.241044	-3.284660	0.863006
H	1.156955	-2.507371	0.152849
H	1.551016	3.040205	0.274094
H	-2.678935	2.001138	0.068573
H	-1.963218	-1.735150	-2.943354
H	-3.222236	-2.911230	-2.562518
H	-0.838811	-3.073981	-1.304930
H	-2.315380	-3.296512	-0.357572

NImag = 1 (-362.7945)

C	-2.604238	0.001165	-0.224969
N	-1.741188	-1.141664	-0.472435
C	-2.306832	-2.016621	-1.505488
C	-3.399710	-1.174308	-2.131283
C	-3.898695	-0.343526	-0.964687
C	-0.535385	-1.314067	0.069909
C	0.070121	-0.360267	0.894379
C	1.096288	-0.783684	1.910053
C	1.901151	-2.005355	1.503912
C	0.992448	-3.087211	0.957859
C	0.197774	-2.585991	-0.241019
C	-2.901802	0.236075	1.248305
O	-2.920173	1.492608	1.663791
O	-3.190870	-0.656791	1.998390
C	1.042909	1.093280	-0.518556
C	0.546085	2.280475	0.023957
N	-0.662553	2.727392	-0.382862
O	-1.152440	2.360159	-1.465636
C	2.457782	0.726850	-0.466543
C	2.957075	-0.133800	-1.447918
C	4.298234	-0.475277	-1.478791
C	5.164602	0.030848	-0.519124
C	4.682607	0.891522	0.458323
C	3.343188	1.243398	0.482519
O	-1.328864	3.476785	0.377091
H	-2.166346	0.890596	-0.686097
H	-4.544613	-0.940416	-0.322683
H	-4.434247	0.553035	-1.262857
H	0.521696	0.742868	-1.395778
H	1.761414	0.050085	2.136388
H	0.565687	-0.997717	2.843069
H	2.457963	-2.375369	2.364311
H	2.634254	-1.734778	0.744599
H	0.298360	-3.415831	1.733716
H	1.568478	-3.961543	0.657034
H	2.992307	1.929227	1.239025
H	5.354775	1.297198	1.200402
H	6.211331	-0.235674	-0.537775
H	4.667858	-1.134184	-2.250955
H	2.285086	-0.524366	-2.199263
H	-0.557158	0.441056	1.246574
H	-0.499613	-3.352846	-0.563805
H	0.873545	-2.400318	-1.080070
H	0.908942	2.743864	0.923419
H	-2.534447	2.142745	1.049191
H	-2.983194	-0.530647	-2.904656
H	-4.178528	-1.786270	-2.577843
H	-1.543465	-2.308462	-2.219678
H	-2.716725	-2.915492	-1.043315

NImag = 1 (-283.6481)

C	2.774020	-0.636211	-0.271735
N	1.486485	-0.239120	-0.846919
C	1.148967	-1.187891	-1.920189
C	2.396611	-2.043106	-2.113545
C	3.503804	-1.241879	-1.452498
C	0.706183	0.829330	-0.603124
C	1.244158	2.035046	0.118006
C	0.514907	3.316797	-0.260118
C	-0.985541	3.146742	-0.151673
C	-1.443429	2.061250	-1.105385
C	-0.619344	0.811915	-1.013534
C	3.609247	0.390106	0.485924
O	3.352720	0.496438	1.771945
O	4.518354	0.992395	-0.024142
C	-1.421996	-0.336551	0.822208
C	-0.658124	-1.478991	0.982835
N	0.509820	-1.451837	1.669986
O	1.183288	-2.483856	1.780191
C	-2.814344	-0.431305	0.375544
C	-3.251712	-1.410311	-0.520298
C	-4.583870	-1.482174	-0.886114
C	-5.504686	-0.580685	-0.363599
C	-5.081956	0.396621	0.524189
C	-3.745361	0.474551	0.885454
O	0.908944	-0.378145	2.188210
H	2.570420	-1.442793	0.444650
H	3.872887	-0.447673	-2.098319
H	4.345764	-1.851749	-1.136597
H	-1.182821	0.502450	1.457019
H	0.867944	4.118047	0.387891
H	0.774784	3.598769	-1.282553
H	-1.497703	4.081687	-0.377320
H	-1.248436	2.880272	0.874516
H	-1.387194	2.436155	-2.132514
H	-2.493508	1.819173	-0.942716
H	-3.418624	1.236309	1.579122
H	-5.790355	1.101312	0.934709
H	-6.544298	-0.640767	-0.650935
H	-4.907535	-2.242312	-1.582142
H	-2.546804	-2.113160	-0.940940
H	2.297088	2.159900	-0.114281
H	-0.939852	0.004255	-1.652505
H	-0.909445	-2.445845	0.587549
H	2.514999	0.034889	2.014379
H	2.279939	-3.000543	-1.609554
H	2.584950	-2.240610	-3.165209
H	0.283003	-1.790356	-1.658684
H	0.905604	-0.613088	-2.812795
H	1.163406	1.878184	1.192033

(1-2)$_{anti}$ (*si-si*)$_2$ (*down*)

E_0 = -1148.4998357
E_{0+ZPE} = -1148.077054
E_{298} = -1148.055419
H_{298} = -1148.054475
G_{298} = -1148.127891
NImag = 1 (-346.4158)

C	2.538478	-1.071148	-0.249867
N	1.289851	-0.536422	-0.801829
C	0.638792	-1.628845	-1.540688
C	1.704876	-2.712922	-1.695416
C	3.007854	-2.019401	-1.331927
C	0.760426	0.694052	-0.774704
C	1.633844	1.887524	-0.489267
C	1.022944	3.190242	-0.987406
C	-0.434969	3.306300	-0.593953
C	-1.222852	2.186674	-1.245964
C	-0.607684	0.837585	-1.017117

(1-2)$_{anti}$ (*si-re*)$_1$ (*down*)

E_0 = -1148.5010017
E_{0+ZPE} = -1148.078307
E_{298} = -1148.056717
H_{298} = -1148.055772
G_{298} = -1148.129033
NImag = 1 (-347.9318)

C	2.719625	0.958100	-0.445027
N	1.557300	1.108098	0.432232
C	1.119364	2.503757	0.360133
C	2.302869	3.273396	-0.227974
C	3.446982	2.271646	-0.246169
C	0.774457	0.158540	0.968979
C	1.334860	-1.189483	1.305949
C	0.695922	-1.784518	2.554604
C	-0.812690	-1.803084	2.433643
C	-1.335533	-0.390867	2.253246
C	-0.568644	0.407763	1.240336

(1-2)$_{anti}$ (*si-re*)$_2$ (*down*)

E_0 = -1148.4969086
E_{0+ZPE} = -1148.073859
E_{298} = -1148.052552
H_{298} = -1148.051608
G_{298} = -1148.123853
NImag = 1 (-354.4435)

C	2.875571	-0.415913	-0.199206
N	1.679714	-0.131845	-1.000101
C	1.575697	-1.176799	-2.025035
C	2.942971	-1.855334	-2.067237
C	3.842481	-0.959732	-1.232310
C	0.675286	0.714238	-0.773052
C	0.873160	1.874202	0.147126
C	-0.003886	3.069407	-0.201836
C	-1.451566	2.662731	-0.363637
C	-1.578891	1.615458	-1.451170
C	-0.601307	0.484051	-1.301173

C	3.616458	-0.118088	0.245273
O	3.599906	0.127718	1.539353
O	4.489473	0.311714	-0.461630
C	-1.480158	0.140361	0.902303
C	-0.628603	-0.790744	1.488738
N	0.484357	-0.340980	2.112396
O	1.349025	-1.164479	2.519027
C	-2.819207	-0.249321	0.441974
C	-3.095235	-1.511625	-0.088525
C	-4.378915	-1.846694	-0.480693
C	-5.413310	-0.926668	-0.352394
C	-5.152875	0.329608	0.172504
C	-3.865360	0.666115	0.564067
O	0.684161	0.872892	2.246380
H	2.243958	-1.666316	0.621250
H	3.415059	-1.449833	-2.164903
H	3.770312	-2.703916	-0.970410
H	-1.392731	1.150626	1.270746
H	1.606130	4.019374	-0.589336
H	1.104248	3.240413	-2.075312
H	-0.839604	4.271192	-0.898013
H	-0.525761	3.248383	0.492640
H	-1.288973	2.371423	-2.322414
H	-2.253819	2.177682	-0.890056
H	-3.670680	1.641401	0.987270
H	-5.950950	1.049631	0.280800
H	-6.414766	-1.190777	-0.659543
H	-4.574987	-2.827381	-0.889368
H	-2.300861	-2.234729	-0.200877
H	2.588652	1.734689	-0.984638
H	-1.109420	0.015598	-1.503131
H	-0.718079	-1.859159	1.421557
H	2.833689	-0.284344	1.993015
H	1.516123	-3.530817	-1.002936
H	1.709851	-3.122774	-2.701512
H	-0.236294	-1.992077	-1.009552
H	0.315261	-1.237323	-2.502883
H	1.826630	1.960059	0.576983

C	3.630208	-0.248018	-0.242391
O	3.409075	-1.274439	-1.035029
O	4.553746	-0.240847	0.529934
C	-1.316379	-0.185117	-0.799397
C	-1.016650	-1.496758	-1.159503
N	0.148692	-1.805792	-1.775856
O	0.988294	-0.894421	-2.017173
C	-2.706722	0.223272	-0.563868
C	-3.046962	1.567780	-0.729486
C	-4.351390	1.997453	-0.558284
C	-5.341290	1.089148	-0.206517
C	-5.016073	-0.248975	-0.034040
C	-3.711533	-0.680524	-0.211346
O	0.381462	-2.971445	-2.109433
H	2.342326	0.906728	-1.468805
H	3.974429	2.243389	0.704567
H	4.168344	2.459210	-1.036766
H	-0.677957	0.572395	-1.226973
H	1.089362	-2.789936	2.696914
H	0.991237	-1.200916	3.428756
H	-1.263991	-2.255265	3.316363
H	-1.096749	-2.420702	1.580282
H	-1.281018	0.138478	3.210081
H	-2.392536	-0.399403	1.986016
H	-3.482834	-1.726894	-0.075922
H	-5.781190	-0.961298	0.238049
H	-6.360045	1.421762	-0.070472
H	-4.596640	3.039847	-0.700593
H	-2.279232	2.277838	-1.004376
H	2.406543	-1.124363	1.457053
H	-0.920061	1.419640	1.111257
H	-1.661467	-2.341130	-1.005891
H	2.552613	-1.191468	-1.519378
H	2.071487	3.596898	-1.240340
H	2.536402	4.159030	0.356363
H	0.236748	2.606267	-0.270639
H	0.856082	2.835418	1.362578
H	1.163066	-1.873515	0.473529

C	3.494648	0.703873	0.627423
O	3.248003	0.676228	1.918736
O	4.235533	1.524617	0.150567
C	-1.306800	-0.885240	0.330249
C	-0.609448	-0.675860	1.525495
N	0.532063	-1.353776	1.763043
O	1.285917	-0.955836	2.700839
C	-2.746662	-0.646862	0.204227
C	-3.434467	-1.265790	-0.842849
C	-4.802375	-1.110034	-0.986364
C	-5.509345	-0.325409	-0.085098
C	-4.838644	0.292914	0.961648
C	-3.470617	0.133415	1.108051
O	0.865329	-2.345841	1.096193
H	2.598466	-1.233493	0.476228
H	4.245738	-0.132932	-1.812891
H	4.666825	-1.493878	-0.767911
H	-0.943827	-1.722689	-0.244711
H	0.108575	3.818940	0.580235
H	0.357616	3.521409	-1.127265
H	-2.068898	3.527556	-0.604944
H	-1.823468	2.261022	0.579846
H	-1.412505	2.083849	-2.426892
H	-2.592702	1.218571	-1.485910
H	-2.971827	0.610577	1.938029
H	-5.384253	0.897522	1.671448
H	-6.576902	-0.200951	-0.193831
H	-5.316917	-1.602140	-1.798743
H	-2.886492	-1.876932	-1.546739
H	1.908180	2.193504	0.137087
H	-0.695729	-0.289393	-2.048424
H	-0.829575	0.085179	2.251086
H	2.569335	0.007585	2.177732
H	2.881972	-2.845140	-1.621446
H	3.301179	-1.970322	-3.086359
H	0.792829	-1.885584	-1.763015
H	1.313194	-0.704676	-2.968773
H	0.643662	1.538514	1.163367

(1-2)$_{anti}$ (re-si)$_1$ (*down*)

E_0 = -1148.5095723
E_{0+ZPE} = -1148.086699
E_{298} = -1148.065046
H_{298} = -1148.064102
G_{298} = -1148.137613
NImag = 1 (-332.0332)

C	2.564763	-0.000329	0.279226
N	1.478989	-0.827768	0.793285
C	1.783575	-1.313749	2.142178
C	2.929018	-0.429518	2.587488
C	3.688636	-0.204495	1.293932
C	0.380713	-1.183197	0.111024
C	-0.006872	-0.570006	-1.071901
C	-0.963187	-1.241419	-2.020261
C	-1.886649	-2.250389	-1.357947
C	-1.118796	-3.124280	-0.389410
C	-0.458599	-2.282819	0.692812
C	3.029631	-0.397550	-1.117353
O	3.100206	0.585005	-1.998366
O	3.388366	-1.510336	-1.392244
C	-1.085266	1.324250	-0.471017
C	-0.269880	2.113174	0.326743
N	0.851415	2.684637	-0.179963
O	1.196259	2.437489	-1.362170
C	-2.401413	0.908781	0.017039
C	-2.637672	0.600899	1.359394
C	-3.906774	0.252484	1.787422
C	-4.963018	0.210253	0.885080
C	-4.742004	0.522159	-0.448410

(1-2)$_{anti}$ (re-si)$_2$ (*down*)

E_0 = -1148.5061413
E_{0+ZPE} = -1148.083232
E_{298} = -1148.061614
H_{298} = -1148.060669
G_{298} = -1148.133956
NImag = 1 (-350.3195)

C	-2.221166	-0.457940	-0.664223
N	-1.040360	-1.264260	-0.372895
C	-0.947606	-2.404103	-1.291909
C	-1.894018	-2.037253	-2.414690
C	-2.996562	-1.295412	-1.685690
C	-0.160507	-1.047637	0.615864
C	-0.123175	0.116754	1.374344
C	0.587350	0.160747	2.700848
C	1.726278	-0.834742	2.822825
C	1.290189	-2.194045	2.320330
C	0.853862	-2.126032	0.864454
C	-3.110214	-0.186461	0.539030
O	-3.658340	1.015551	0.573237
O	-3.380156	-1.019559	1.361330
C	0.976611	1.549320	0.032243
C	-0.017187	2.000557	-0.826645
N	-1.088619	2.654176	-0.313027
O	-1.083765	3.083253	0.844248
C	2.182466	0.906261	-0.494778
C	2.182080	0.168112	-1.681043
C	3.355120	-0.383691	-2.167197
C	4.549751	-0.205971	-1.480686
C	4.562744	0.524984	-0.301347

C	-3.470392	0.865491	-0.879503
O	1.556888	3.395173	0.543554
H	2.288848	1.047702	0.283913
H	4.259115	-1.093660	1.030966
H	4.360584	0.648597	1.318808
H	-1.008171	1.478163	-1.536215
H	-1.548852	-0.488748	-2.551846
H	-0.373384	-1.746166	-2.791375
H	-2.369973	-2.858485	-2.122330
H	-2.678751	-1.733378	-0.816433
H	-0.351777	-3.689849	-0.922238
H	-1.778870	-3.851365	0.082155
H	-3.302723	1.114787	-1.917450
H	-5.559313	0.498860	-1.154447
H	-5.952854	-0.061121	1.222132
H	-4.074536	0.013377	2.827571
H	-1.825674	0.629165	2.071462
H	0.701405	0.089368	-1.548905
H	0.150040	-2.918104	1.329619
H	-1.225316	-1.837837	1.332581
H	-0.435929	2.316248	1.368699
H	2.594089	1.368730	-1.707208
H	2.551593	0.514644	2.978145
H	3.533709	-0.902582	3.356375
H	0.909813	-1.234848	2.782654
H	2.095478	-2.358681	2.104698
C	3.388043	1.072335	0.188936
O	-2.130591	2.727375	-1.019866
H	-1.944599	0.483357	-1.127706
H	-3.643890	-2.001195	-1.167463
H	-3.608158	-0.669348	-2.328872
H	1.102443	2.087915	0.958803
H	0.944515	1.173489	2.895014
H	-0.150762	-0.039312	3.483751
H	2.049856	-0.895415	3.861658
H	2.584730	-0.498046	2.241823
H	0.461008	-2.562662	2.927220
H	2.097136	-2.920230	2.411091
H	3.403271	1.648389	1.103319
H	5.488205	0.672273	0.236063
H	5.464423	-0.633420	-1.864894
H	3.338791	-0.951894	-3.085929
H	1.261542	0.018534	-2.225770
H	-0.969632	0.785622	1.327966
H	0.452098	-3.088886	0.562293
H	1.720594	-1.933388	0.225303
H	-0.125139	1.702285	-1.852812
H	-3.247332	1.640123	-0.057132
H	-1.400840	-1.381337	-3.131062
H	-2.254751	-2.913959	-2.945674
H	0.074827	-2.543539	-1.629065
H	-1.277037	-3.316416	-0.792057

(1-2)$_{anti}$ (*re-re*)$_1$

E_0 = -1148.5120821
E_{0+ZPE} = -1148.089532
E_{298} = -1148.067745
H_{298} = -1148.066801
G_{298} = -1148.141151
NImag = -377.3295 24.2072

C	-2.335677	-0.175025	-0.655094
N	-1.525938	-1.313950	-0.270738
C	-1.996006	-2.556014	-0.887548
C	-3.345931	-2.184875	-1.472957
C	-3.200844	-0.708682	-1.799126
C	-0.461140	-1.200927	0.531166
C	-0.063310	0.025526	1.062003
C	0.879170	0.092745	2.231614
C	1.782801	-1.121555	2.369404
C	0.990897	-2.399147	2.187184
C	0.338683	-2.435606	0.814043
C	-3.206540	0.330998	0.490809
O	-3.297180	1.644464	0.601531
O	-3.822469	-0.400883	1.219333
C	0.993273	1.158937	-0.576125
C	0.927077	2.464940	-0.107590
N	-0.224581	3.180445	-0.192701
O	-1.222048	2.687799	-0.784003
C	2.275461	0.469859	-0.725782
C	2.354435	-0.608646	-1.610511
C	3.551954	-1.272174	-1.817119
C	4.693760	-0.871214	-1.136608
C	4.629456	0.202041	-0.257907
C	3.433528	0.870036	-0.054905
O	-0.285075	4.305853	0.304681
H	-1.702201	0.638493	-0.991350
H	-4.150876	-0.187342	-1.882765
H	-2.660616	-0.571393	-2.734410
H	0.233391	0.857591	-1.277299
H	1.475346	1.005973	2.167059
H	0.283957	0.199318	3.143398
H	2.266802	-1.105890	3.345661
H	2.575560	-1.086572	1.622299
H	0.218362	-2.472607	2.955098
H	1.632484	-3.272521	2.297201

(1-2)$_{anti}$ (*re-si*)$_2$

E_0 = -1148.5043884
E_{0+ZPE} = -1148.081770
E_{298} = -1148.059980
H_{298} = -1148.059036
G_{298} = -1148.133042
NImag = 1 (-387.6945)

C	-2.099322	-0.270999	-0.688241
N	-1.109255	-1.283603	-0.360175
C	-1.291457	-2.496043	-1.166464
C	-2.627962	-2.289319	-1.853329
C	-2.729887	-0.781860	-1.987258
C	-0.162419	-1.127499	0.575534
C	-0.045330	0.020585	1.357143
C	0.705503	-0.020448	2.664564
C	1.818907	-1.050657	2.709132
C	1.330214	-2.377623	2.169658
C	0.840794	-2.230725	0.737373
C	-3.168412	-0.099551	0.380897
O	-3.677556	1.117687	0.471716
O	-3.582244	-1.001166	1.059068
C	1.080293	1.537046	0.134875
C	0.110481	2.150470	-0.649126
N	-0.926989	2.785766	-0.046517
O	-0.893361	3.071695	1.152929
C	2.232942	0.883211	-0.491230
C	2.144225	0.225675	-1.720488
C	3.267724	-0.340747	-2.298269
C	4.499812	-0.257181	-1.661844
C	4.600199	0.393365	-0.440474
C	3.474696	0.954029	0.142136
O	-1.969159	2.986030	-0.727393
H	-1.622152	0.679975	-0.865248
H	-3.746732	-0.423734	-2.124942
H	-2.133157	-0.426871	-2.825705
H	-2.672747	-2.799435	-2.811687
H	-3.431807	-2.669407	-1.226916
H	-0.478313	-2.590189	-1.886750
H	-1.299368	-3.381063	-0.537564
H	1.255728	1.961928	1.110945
H	1.097511	0.970129	2.900623
H	-0.015825	-0.239703	3.457727

(1-2)$_{anti}$ (*re-re*)$_1$ (*down* $Cyhex_{Conf}$)

E_0 = -1148.5122525
E_{0+ZPE} = -1148.089708
E_{298} = -1148.068027
H_{298} = -1148.067083
G_{298} = -1148.140584
NImag = -368.3149 33.1307

C	-2.418891	-0.397802	-0.587949
N	-1.422821	-1.389993	-0.211358
C	-1.686732	-2.678670	-0.846094
C	-2.559446	-2.307713	-2.027203
C	-3.398546	-1.166719	-1.479913
C	-0.389252	-1.131115	0.596270
C	-0.125722	0.151511	1.069635
C	0.751309	0.374497	2.273171
C	1.173005	-0.923523	2.942043
C	1.636885	-1.911671	1.891344
C	0.496268	-2.283016	0.957016
C	-3.160682	0.188553	0.609794
O	-3.306632	1.500459	0.614229
O	-3.648773	-0.498416	1.466925
C	0.882236	1.139022	-0.654539
C	0.757133	2.484435	-0.324389
N	-0.429927	3.124954	-0.468846
O	-1.404799	2.518770	-0.991390
C	2.194748	0.495749	-0.736283
C	2.331777	-0.640554	-1.538080
C	3.555575	-1.272722	-1.672332
C	4.667872	-0.781913	-1.000886
C	4.546931	0.348298	-0.204537
C	3.323455	0.985870	-0.074376
O	-0.549454	4.291998	-0.090046
H	-1.941326	0.406678	-1.141969
H	-4.210598	-1.561728	-0.872408
H	-3.821759	-0.526788	-2.248400
H	0.136528	0.738375	-1.322395
H	1.646687	0.938001	1.996869
H	0.212113	1.002573	2.982222
H	3.256709	1.870731	0.540380
H	5.410015	0.739935	0.313772
H	5.624424	-1.273262	-1.103855

H	3.408369	1.704028	0.629524
H	5.515878	0.522793	0.269746
H	5.629647	-1.386900	-1.295300
H	3.595767	-2.098558	-2.511628
H	1.468850	-0.916695	-2.149264
H	-0.798836	0.814546	1.045082
H	-0.284243	-3.319476	0.719822
H	1.110132	-2.517368	0.042299
H	1.710836	2.971584	0.423808
H	-2.621289	2.112372	0.067424
H	-3.586907	-2.785071	-2.346112
H	-4.125569	-2.332366	-0.729435
H	-1.294914	-2.876501	-1.659513
H	-2.078395	-3.348070	-0.149319
H	2.175497	-1.159399	3.733124
H	2.665938	-0.715120	2.110852
H	0.516789	-2.755171	2.792278
H	2.123056	-3.124232	2.195383
H	3.558093	1.466563	1.090031
H	5.555200	0.466635	0.059093
H	5.375639	-0.696527	-2.116675
H	3.182865	-0.848338	-3.248183
H	1.192427	0.146989	-2.224691
H	-0.891082	0.692335	1.381476
H	0.439700	-3.175271	0.387404
H	1.684673	-1.992741	0.082193
H	-0.021668	1.984340	-1.702579
H	-3.163989	1.788821	-0.021435
H	3.643914	-2.145139	-2.303302
H	1.469731	-1.020138	-2.068668
H	-0.907770	0.879866	0.941762
H	-0.137044	-3.043465	1.420075
H	0.893897	-2.735978	0.047832
H	1.517835	3.079533	0.144658
H	-2.710003	1.945834	-0.025467
H	-1.940189	-1.966349	-2.855985
H	-3.162282	-3.143670	-2.371481
H	-0.761774	-3.163110	-1.140227
H	-2.215176	-3.335939	-0.153059
H	0.331669	-1.347025	3.495017
H	1.964963	-0.728888	3.664234
H	2.024278	-2.821211	2.348176
H	2.454132	-1.471159	1.319752

(1-2)*anti* (*si-si*)$_1$ (*down* Cyhex$_{Conf}$)

E_0 = -1148.5041882
E_{0+ZPE} = -1148.081057
E_{298} = -1148.059635
H_{298} = -1148.058691
G_{298} = -1148.131203
NImag = 1 (-308.7150)

C	-2.767993	-0.616209	0.291850
N	-1.476103	-0.210335	0.850902
C	-1.151021	-1.117448	1.964913
C	-2.408880	-1.948708	2.192129
C	-3.505358	-1.161136	1.498241
C	-0.688575	0.835611	0.559981
C	-1.222088	2.016237	-0.198937
C	-0.173636	3.082218	-0.473514
C	0.663155	3.336692	0.761021
C	1.452394	2.083809	1.097905
C	0.638875	0.823289	0.979574
C	-3.592170	0.396134	-0.493932
O	-3.425413	0.364831	-1.802077
O	-4.418266	1.104914	0.016275
C	1.397030	-0.334672	-0.794564
C	0.647166	-1.496692	-0.931574
N	-0.519123	-1.510951	-1.615062
O	-1.176351	-2.558885	-1.694111
C	2.800326	-0.427392	-0.372068
C	3.240103	-1.369785	0.560981
C	4.577287	-1.445427	0.906570
C	5.501790	-0.583836	0.326090
C	5.077561	0.354530	-0.601475
C	3.735495	0.435395	-0.943842
O	-0.942848	-0.460994	-2.164893
H	-2.573934	-1.453931	-0.388522
H	-3.861593	-0.334159	2.109323
H	-4.356366	-1.771665	1.208659
H	1.161401	0.478156	-1.464078
H	1.847188	2.144582	2.112922
H	2.330207	2.027120	0.450438
H	3.409493	1.162760	-1.673778
H	5.788794	1.026223	-1.059710
H	6.545400	-0.645988	0.598117
H	4.902219	-2.177004	1.632013
H	2.532780	-2.042244	1.025438
H	-2.026688	2.447748	0.399875
H	0.944377	0.021167	1.631378
H	0.916885	-2.446559	-0.508445
H	-2.603545	-0.123648	-2.042260
H	-2.303510	-2.926841	1.727075
H	-2.600163	-2.100826	3.250742
H	-0.293704	-1.741400	1.727919
H	-0.900866	-0.508506	2.832519
H	-1.657194	1.706707	-1.141001

(1-2)*syn* (*re-re*)$_1$ (Cyhex$_{Conf}$)

E_0 = -1148.5084315
E_{0+ZPE} = -1148.086206
E_{298} = -1148.064708
H_{298} = -1148.063764
G_{298} = -1148.137012
NImag = 1 (-445.9680)

C	-3.930132	0.272773	-0.851225
C	-2.892947	-0.458745	-0.273716
C	-3.185175	-1.319882	0.786087
C	-4.481624	-1.445330	1.252735
C	-5.509693	-0.716887	0.665150
C	-5.231221	0.139550	-0.388798
C	-1.533640	-0.339112	-0.823533
C	-0.810826	-1.507590	-1.024170
N	0.343128	-1.493162	-1.727491
O	0.954226	-2.544326	-1.940029
O	0.786604	-0.392027	-2.152298
C	-0.638832	0.943541	0.731989
C	0.724320	1.004512	0.444600
C	1.319791	2.194360	-0.247750
C	0.283206	3.186092	-0.738828
C	-0.717604	3.457436	0.364657
C	-1.496085	2.188106	0.667855
N	1.565307	0.019407	0.811850
C	1.136291	-1.063398	1.706073
C	2.406795	-1.840995	1.962324
C	3.447133	-0.739163	2.012112
C	3.017102	0.203367	0.883807
C	3.851068	-0.044875	-0.373142
O	5.051068	0.051112	-0.276923
O	3.301751	-0.320636	-1.526299
H	3.250579	1.231686	1.151571
H	4.468427	-1.078492	1.879447
H	3.383596	-0.208291	2.960350
H	2.351676	-2.418102	2.881203
H	2.608674	-2.525266	1.138789
H	0.752823	-0.630500	2.634244
H	0.351088	-1.654158	1.250571
H	-1.365706	0.465034	-1.523034
H	0.789809	4.098271	-1.049840
H	-0.229370	2.792354	-1.618119
H	-2.391925	-1.884655	1.255429
H	-4.692820	-2.110660	2.077254
H	-6.521516	-0.817308	1.030037
H	-6.025335	0.706031	-0.852881
H	-3.718371	0.934487	-1.679199
H	-0.928495	0.217979	1.476166
H	1.968896	2.698379	0.473668
H	1.962856	1.874199	-1.064390
H	-1.093114	-2.472566	-0.645032
H	2.316208	-0.355800	-1.601033
H	-2.274095	2.077984	-0.090029

(1-2)*syn* (*re-re*)$_1$ (*down* Cyhex$_{Conf}$)

E_0 = -1148.5087312
E_{0+ZPE} = -1148.086919
E_{298} = -1148.065206
H_{298} = -1148.064261
G_{298} = -1148.138432
NImag = 1 (-414.7419)

C	-3.337911	-1.204388	0.788708
C	-2.905967	-0.458869	-0.310744
C	-3.838809	0.302835	-1.014530
C	-5.174503	0.308111	-0.640643
C	-5.591985	-0.436439	0.451593
C	-4.668345	-1.190399	1.166952
C	-1.513064	-0.480182	-0.774067
C	-0.631720	0.867792	0.771653
C	-1.480389	2.117847	0.743605
C	-0.817514	-1.680550	-0.761075
N	0.355669	-1.807813	-1.417880
O	0.981449	-2.871312	-1.365751
C	0.724354	0.921077	0.457275
C	1.294419	2.097103	-0.281662
N	1.591656	-0.051004	0.805178
C	3.045542	0.134340	0.726027
C	3.611987	-1.088019	1.449253
C	2.573238	-1.345130	2.519807
C	1.271393	-1.103896	1.782821
C	3.743504	0.272673	-0.618436
O	3.238719	-0.236417	-1.710803
O	4.832141	0.796781	-0.629031
O	0.795930	-0.832797	-2.086682
H	2.686868	-0.630515	3.334432
H	2.626376	-2.348759	2.932980
H	3.671991	-1.935379	0.766296
H	4.605807	-0.885413	1.835013
H	3.321695	1.031341	1.279783
H	0.476704	-0.773694	2.444641
H	0.945946	-2.006098	1.271581
H	-1.121662	-2.556649	-0.218757
H	-1.257366	0.226465	-1.547987
H	-3.516602	0.878584	-1.870624
H	-5.886197	0.895371	-1.202333
H	-6.630791	-0.430023	0.747890
H	-4.987891	-1.767919	2.022121
H	-2.629331	-1.788271	1.358627
H	2.290705	-0.542590	-1.707476
H	-0.933118	0.125041	1.491928
H	1.820329	1.757741	-1.171409
H	2.046800	2.556151	0.364872
C	0.265227	3.144995	-0.665634
C	-0.684495	3.384759	0.487459
H	-2.014438	2.190004	1.691142
H	-2.255466	2.040029	-0.021308

H	0.006821	3.603279	1.592422	H	-2.027674	2.288548	1.614013	H	-0.113829	3.662498	1.376738
H	1.342098	4.174809	0.609536	H	-0.184973	3.799363	1.255051	H	-1.362118	4.209873	0.271474
H	-0.682223	3.986590	-0.803743	H	-1.407034	4.252227	0.082276	H	0.787129	4.056387	-0.952451
H	0.472969	2.768030	-1.295359					H	-0.298502	2.815528	-1.540321

(1-2)'$_{anti}$ $(re\text{-}re)_{60}$

E_0 = -1148.5133564
E_{0+ZPE} = -1148.091038
E_{298} = -1148.069015
H_{298} = -1148.068070
G_{298} = -1148.143008
NImag = 1 (-366.4135)

C	2.519453	-1.655918	0.145962
C	2.513018	-0.299656	0.476676
C	3.708332	0.412843	0.392257
C	4.882335	-0.215121	0.000199
C	4.876563	-1.563270	-0.322935
C	3.688807	-2.281551	-0.249757
C	1.291630	0.386115	0.939522
C	0.468312	-0.273259	1.843839
N	-0.449914	0.403718	2.593884
O	-1.128140	-0.229317	3.419224
O	-0.592978	1.627131	2.451793
C	0.341905	0.639404	-1.009763
C	-0.922752	1.037462	-0.581289
C	-1.299335	2.491778	-0.544771
C	-0.513125	3.332599	-1.538005
C	0.970351	3.039521	-1.451468
C	1.225630	1.580394	-1.780002
N	-1.800823	0.151763	-0.101986
C	-3.046600	0.507859	0.578756
C	-3.778143	-0.813283	0.753082
C	-2.668968	-1.851557	0.735041
C	-1.681477	-1.280730	-0.283865
C	-2.058195	-1.685711	-1.695455
O	-2.639974	-1.003859	-2.494628
O	-1.680532	-2.936202	-1.945731
H	-0.673555	-1.631984	-0.091772
H	-3.007480	-2.849942	0.473074
H	-2.172806	-1.894690	1.702104
H	-4.351936	-0.835357	1.675119
H	-4.466591	-0.975112	-0.074540
H	-2.801207	0.973507	1.534750
H	-3.626334	1.214349	-0.008436
H	1.374520	1.455460	1.064090
H	2.270141	1.323589	-1.603064
H	1.061177	1.419680	-2.849827
H	1.529125	3.675738	-2.137419
H	1.328418	3.268009	-0.445440
H	-0.862121	3.122592	-2.551046
H	-0.716934	4.385164	-1.344985
H	3.720874	1.462859	0.648622
H	5.800492	0.351869	-0.053230
H	5.788498	-2.052808	-0.632455
H	3.674578	-3.331381	-0.504951
H	1.600179	-2.223570	0.188308
H	0.481487	-0.401985	-1.256235
H	-2.363022	2.590976	-0.747092
H	0.504705	-1.328620	2.042021
H	-1.970485	-3.172179	-2.834020
H	-1.140031	2.855932	0.469728

(1-2)'$_{anti}$ $(si\text{-}si)_{60}$

E_0 = -1148.5047883
E_{0+ZPE} = -1148.082345
E_{298} = -1148.060409
H_{298} = -1148.059465
G_{298} = -1148.134731

(1-2)'$_{anti}$ $(re\text{-}re)_{180}$

E_0 = -1148.5095751
E_{0+ZPE} = -1148.087622
E_{298} = -1148.065304
H_{298} = -1148.064360
G_{298} = -1148.142531
NImag = 1 (-401.7586)

C	3.437854	0.537264	-0.051796
C	2.236341	0.287303	-0.718171
C	2.189629	-0.767455	-1.631169
C	3.307870	-1.549176	-1.876235
C	4.494420	-1.292894	-1.204549
C	4.553547	-0.247324	-0.292031
C	1.037818	1.120198	-0.539663
C	1.174786	2.465132	-0.212689
N	0.108919	3.310135	-0.319533
O	0.254080	4.499941	-0.006019
O	-0.985185	2.880880	-0.726814
C	-0.087370	0.293077	1.115140
C	-0.442919	-0.966914	0.635018
C	0.342443	-2.172371	1.050923
C	0.850332	-2.051487	2.480508
C	1.622898	-0.763047	2.670737
C	0.753594	0.442816	2.352240
N	-1.427196	-1.135434	-0.254948
C	-1.747057	-2.402751	-0.918742
C	-2.991168	-2.098987	-1.743015
C	-2.954615	-0.591534	-1.932266
C	-2.374704	-0.099256	-0.608290
C	-3.443791	0.033608	0.459012
O	-3.562962	-0.669574	1.426002
O	-4.264481	1.041752	0.189969
H	-1.900515	0.875254	-0.717301
H	-3.923570	-0.154308	-2.151996
H	-2.268918	-0.314725	-2.730737
H	-2.993235	-2.641205	-2.684416
H	-3.884835	-2.387326	-1.191798
H	-0.909678	-2.709947	-1.543983
H	-1.935515	-3.188570	-0.191919
H	0.224444	0.875982	-1.206227
H	1.365042	1.344185	2.260394
H	0.083064	0.633370	3.195260
H	1.991501	-0.686166	3.693540
H	2.496733	-0.778741	2.020676
H	0.002236	-2.085204	3.167356
H	1.476310	-2.913901	2.706896
H	1.269889	-0.963567	-2.165057
H	3.253201	-2.354513	-2.594538
H	5.368798	-1.898516	-1.393810
H	5.474445	-0.040512	0.233938
H	3.504990	1.342973	0.663981
H	-0.816133	1.080470	0.984381
H	-0.260775	-3.069034	0.947225
H	2.058671	2.921609	0.191054
H	-4.927234	1.092062	0.887583
H	1.187956	-2.283780	0.365990

(1-2)'$_{anti}$ $(si\text{-}si)_{180}$

E_0 = -1148.5090886
E_{0+ZPE} = -1148.087005
E_{298} = -1148.064817
H_{298} = -1148.063873
G_{298} = -1148.140591

(1-2)'$_{anti}$ $(re\text{-}re)_{300}$

E_0 = -1148.5042057
E_{0+ZPE} = -1148.082215
E_{298} = -1148.060118
H_{298} = -1148.059174
G_{298} = -1148.134908
NImag = 1 (-370.1873)

C	0.235804	2.296547	1.001999
C	-0.329567	1.989051	-0.236249
C	0.224127	2.565429	-1.382010
C	1.309596	3.420807	-1.296391
C	1.867248	3.714701	-0.058780
C	1.323582	3.151936	1.087481
C	-1.512714	1.121944	-0.383186
C	-2.433176	1.029277	0.655303
N	-3.755712	0.762394	0.417168
O	-4.530053	0.742186	1.385720
O	-4.165361	0.566157	-0.734232
C	-0.532001	-0.726196	-0.998621
C	-0.126405	-1.240860	0.234258
C	-1.138142	-1.995473	1.025418
C	-1.913654	-2.976866	0.154468
C	-2.572981	-2.259873	-1.005830
C	-1.559520	-1.471787	-1.818428
N	1.078784	-1.008673	0.763868
C	1.519049	-1.473352	2.083746
C	3.025773	-1.282176	2.065262
C	3.234452	-0.142976	1.083962
C	2.163494	-0.398191	0.021087
C	2.687343	-1.330450	-1.052913
O	2.520929	-2.518969	-1.097382
O	3.408064	-0.663655	-1.948998
H	1.857342	0.530626	-0.449314
H	4.235354	-0.104121	0.663474
H	3.027680	0.815601	1.553879
H	3.416389	-1.059601	3.054283
H	3.512961	-2.187533	1.708209
H	1.044531	-0.877656	2.863107
H	1.252949	-2.514726	2.237180
H	-1.948203	1.115028	-1.371991
H	-2.073618	-0.781404	-2.487306
H	-1.009925	-2.160876	-2.467691
H	-3.076306	-2.975847	-1.655896
H	-3.341261	-1.586568	-0.630767
H	-1.233007	-3.748053	-0.212006
H	-2.660689	-3.478737	0.768273
H	-0.208908	2.342970	-2.347587
H	1.718096	3.861334	-2.194384
H	2.712941	4.383235	0.012036
H	1.745453	3.383071	2.055078
H	-0.174687	1.876837	1.908109
H	0.224101	-0.244065	-1.602856
H	-0.697072	-2.503802	1.874821
H	-2.217996	1.222834	1.689481
H	3.764539	-1.293832	-2.585206
H	-1.834650	-1.245459	1.425511

(1-2)'$_{anti}$ $(si\text{-}si)_{300}$

E_0 = -1148.5127062
E_{0+ZPE} = -1148.090303
E_{298} = -1148.068381
H_{298} = -1148.067437
G_{298} = -1148.142186

NImag = 1 (-381.5208)

C	-0.631972	2.245367	-1.103873
C	-1.369119	1.837826	0.008256
C	-1.526701	2.735167	1.066900
C	-0.958388	3.996970	1.022272
C	-0.213630	4.385610	-0.083987
C	-0.057148	3.506411	-1.146500
C	-2.024488	0.519677	0.093205
C	-2.397299	-0.140366	-1.074802
N	-3.459708	-1.003087	-1.103277
O	-3.757178	-1.526328	-2.188298
O	-4.114083	-1.238738	-0.078953
C	0.158990	-2.093522	-0.329120
C	0.373883	-0.858533	0.476928
C	-0.621879	-0.505067	1.389117
C	-1.422703	-1.584040	2.079694
C	-1.616328	-2.850609	1.262780
C	-0.345512	-3.242930	0.536529
N	1.439226	-0.086731	0.247987
C	1.824972	1.031663	1.114112
C	3.211976	1.420591	0.630413
C	3.214984	0.983246	-0.824759
C	2.427557	-0.328353	-0.783321
C	3.355936	-1.471891	-0.421825
O	3.472580	-1.962479	0.668029
O	4.069887	-1.856216	-1.474079
H	1.966179	-0.546332	-1.742700
H	4.208492	0.857776	-1.245350
H	2.669677	1.692476	-1.443436
H	3.395812	2.484847	0.747477
H	3.975768	0.884136	1.190457
H	1.121890	1.852308	0.998485
H	1.813843	0.711130	2.153943
H	-2.722830	0.414531	0.911341
H	-0.520706	-4.111106	-0.097638
H	0.430515	-3.522389	1.251446
H	-1.938083	-3.658005	1.920824
H	-2.417288	-2.699772	0.542148
H	-0.892779	-1.832716	3.004569
H	-2.390242	-1.189150	2.389403
H	-2.104864	2.437358	1.930883
H	-1.098798	4.678682	1.848618
H	0.231803	5.369116	-0.121880
H	0.509661	3.805412	-2.016577
H	-0.507430	1.582763	-1.946964
H	1.045651	-2.395428	-0.875981
H	-0.419794	0.353678	2.013843
H	-1.945620	0.008224	-2.037723
H	4.672394	-2.556295	-1.198317
H	-0.608300	-1.845748	-1.075545

NImag = 1 (-415.7588)

C	-3.036218	-1.501386	-0.210331
C	-1.985739	-0.802070	-0.807856
C	-1.190121	-1.470077	-1.739877
C	-1.432073	-2.795701	-2.066367
C	-2.475120	-3.480707	-1.460304
C	-3.275255	-2.827209	-0.531808
C	-1.718385	0.620731	-0.537011
C	-2.773955	1.463814	-0.195500
N	-2.606187	2.817552	-0.221264
O	-3.554525	3.544475	0.111325
O	-1.516111	3.300001	-0.572084
C	0.841039	-1.416406	1.193219
C	0.708130	0.003987	0.735685
C	-0.395014	0.760652	1.133409
C	-1.175636	0.389392	2.363233
C	-1.103536	-1.083774	2.729861
C	0.314239	-1.603764	2.609752
N	1.616474	0.503255	-0.106864
C	1.684350	1.924950	-0.460033
C	2.922090	2.038465	-1.336851
C	3.099940	0.636517	-1.896825
C	2.691642	-0.248948	-0.716867
C	3.862579	-0.435028	0.228859
O	4.004650	0.116982	1.285611
O	4.748532	-1.288650	-0.272879
H	2.360370	-1.229940	-1.047722
H	4.106803	0.427852	-2.246084
H	2.409197	0.456140	-2.718213
H	2.799291	2.786544	-2.114788
H	3.786828	2.318882	-0.738200
H	0.781746	2.228270	-0.985477
H	1.757324	2.524627	0.445303
H	-0.960494	1.054941	-1.169969
H	0.360488	-2.661834	2.865008
H	0.967589	-1.078358	3.308824
H	-1.475550	-1.226699	3.744198
H	-1.747503	-1.666414	2.072423
H	-0.796317	0.986158	3.197696
H	-2.214208	0.702620	2.231030
H	-0.384359	-0.936886	-2.225121
H	-0.809639	-3.290539	-2.798011
H	-2.668156	-4.513214	-1.712787
H	-4.092365	-3.351846	-0.058011
H	-3.672056	-1.012413	0.512633
H	1.873735	-1.746947	1.141261
H	-0.325496	1.825369	0.956623
H	-3.731486	1.144275	0.169964
H	5.489203	-1.359688	0.339886
H	0.274929	-2.049646	0.504321

NImag = 1 (-379.1476)

C	-3.077736	-1.246760	-0.899908
C	-2.854179	-0.352265	0.148665
C	-3.921565	0.419898	0.604811
C	-5.182148	0.294343	0.037848
C	-5.392355	-0.599351	-1.000722
C	-4.333634	-1.369203	-1.468326
C	-1.538275	-0.227229	0.805179
C	-0.834429	-1.394137	1.084482
N	0.171887	-1.420204	2.003870
O	0.709421	-2.509329	2.266484
O	0.529756	-0.376371	2.571965
C	1.339117	1.965679	0.619846
C	0.732103	0.909512	-0.260842
C	-0.584847	1.019916	-0.701743
C	-1.301659	2.340850	-0.655964
C	-0.790373	3.261371	0.437485
C	0.722358	3.336066	0.388713
N	1.443203	-0.183006	-0.544530
C	1.069965	-1.140519	-1.589754
C	2.242542	-2.108322	-1.650932
C	2.890854	-1.986281	-0.280723
C	2.727556	-0.497528	0.041237
C	3.854384	0.291598	-0.591322
O	3.801535	0.863906	-1.646990
O	4.950952	0.245757	0.156346
H	2.719903	-0.314900	1.113960
H	3.928839	-2.306260	-0.259259
H	2.339538	-2.551971	0.467231
H	1.918273	-3.122706	-1.866421
H	2.939022	-1.807916	-2.431194
H	0.144907	-1.642552	-1.321153
H	0.913761	-0.612223	-2.529314
H	-1.455474	0.562760	1.536577
H	1.104461	4.024715	1.141268
H	1.036594	3.720610	-0.583740
H	-1.228520	4.252014	0.318980
H	-1.102432	2.893965	1.417716
H	-1.182868	2.835334	-1.624802
H	-2.372675	2.171796	-0.544390
H	-3.766273	1.113222	1.419444
H	-5.998318	0.896944	0.409444
H	-6.371850	-0.695931	-1.446047
H	-4.487719	-2.064679	-2.280725
H	-2.260874	-1.843247	-1.281878
H	2.411763	2.020349	0.451085
H	-0.883977	0.366303	-1.507609
H	-1.045325	-2.349486	0.641100
H	5.656141	0.715691	-0.302767
H	1.198100	1.663091	1.656498

(1-2)'*anti* $(si\text{-}re)_{60}$

E_0 = -1148.5093733
E_{0+ZPE} = -1148.087485
E_{298} = -1148.065353
H_{298} = -1148.064408
G_{298} = -1148.140467
NImag = 1 (-376.8640)

C	3.052266	1.775847	0.327850
C	2.806761	0.402540	0.375401
C	3.845527	-0.469706	0.044773
C	5.090798	0.020173	-0.316467
C	5.322699	1.387971	-0.354555
C	4.297579	2.265825	-0.028587
C	1.475552	-0.064496	0.800098
C	1.333367	-1.309101	1.408565
N	0.264411	-1.574018	2.215204
O	0.230964	-2.656498	2.822078
O	-0.648542	-0.739364	2.340477

(1-2)'*anti* $(si\text{-}re)_{300}$

E_0 = -1148.507895
E_{0+ZPE} = -1148.085616
E_{298} = -1148.063595
H_{298} = -1148.062650
G_{298} = -1148.138462
NImag = 1 (-378.1885)

C	-3.766499	0.371917	0.313983
C	-2.533888	0.481027	-0.331240
C	-2.387937	-0.113999	-1.586945
C	-3.434081	-0.813434	-2.164649
C	-4.651220	-0.926456	-1.504648
C	-4.815672	-0.324897	-0.265656
C	-1.466179	1.274283	0.302530
C	-0.649884	2.061724	-0.510970
N	0.033061	3.120151	0.000966
O	0.682991	3.846403	-0.769458
O	0.014267	3.339848	1.225543

C	-1.223491	-1.578866	-0.817393
C	-0.784579	-0.150371	-0.768617
C	0.517967	0.163153	-1.158664
C	1.248455	-0.710414	-2.141822
C	0.854198	-2.174143	-2.064535
C	-0.653674	-2.317545	-2.020576
N	-1.616442	0.775390	-0.288713
C	-1.313509	2.204089	-0.282550
C	-2.560107	2.840514	0.303872
C	-3.090348	1.761602	1.233216
C	-2.824952	0.474012	0.446419
C	-3.991026	0.168450	-0.469211
O	-4.031492	0.369068	-1.653315
O	-5.010576	-0.341191	0.213888
H	-2.665232	-0.368788	1.116404
H	-4.137573	1.881930	1.494912
H	-2.510828	1.724616	2.153180
H	-2.336939	3.769294	0.821489
H	-3.281762	3.056825	-0.482148
H	-0.443660	2.403522	0.343383
H	-1.091857	2.544070	-1.292185
H	0.829957	0.703938	1.196539
H	-0.941821	-3.366109	-1.956900
H	-1.094456	-1.920558	-2.937065
H	1.265894	-2.712100	-2.918248
H	1.280551	-2.626644	-1.168054
H	1.038771	-0.334901	-3.148376
H	2.323783	-0.596556	-2.006323
H	3.687835	-1.537711	0.068467
H	5.882706	-0.670224	-0.568375
H	6.294927	1.766626	-0.634654
H	4.469086	3.332326	-0.049468
H	2.257993	2.464224	0.582175
H	-2.305465	-1.661890	-0.806111
H	0.761958	1.213465	-1.228596
H	2.041075	-2.114065	1.348026
H	-5.742996	-0.489628	-0.394475
H	-0.861462	-2.064606	0.092646

(1-2)'$_{anti}$ $(re\text{-}si)_{60}$

E_0 = -1148.5088026
E_{0+ZPE} = -1148.086584
E_{298} = -1148.064440
H_{298} = -1148.063495
G_{298} = -1148.139418
NImag = 1 (-364.8104)

C	-3.513433	0.681428	-1.031038
C	-2.466268	0.803602	-0.116506
C	-2.742214	0.616596	1.239822
C	-4.021605	0.298755	1.663321
C	-5.052624	0.167271	0.741308
C	-4.795140	0.365997	-0.607142
C	-1.134079	1.183928	-0.610525
C	-0.350882	2.051418	0.147263
N	0.667861	2.746790	-0.428700
O	1.280384	3.588103	0.248078
O	0.983456	2.521211	-1.611419
C	-0.101755	-0.669417	-1.055756
C	0.360951	-1.055979	0.200928
C	-0.423406	-2.042860	1.011171
C	-1.086353	-3.091238	0.128253
C	-1.922117	-2.438941	-0.953288
C	-1.068564	-1.530317	-1.823198
N	1.457847	-0.515866	0.740716
C	1.876363	-0.704764	2.134561
C	3.273057	-0.104019	2.205647
C	3.327569	0.857155	1.030594
C	2.490140	0.146427	-0.031677
C	3.314681	-0.868888	-0.797697
C	0.139123	-1.966664	-0.016156
C	0.514840	-0.665212	0.621452
C	-0.350766	-0.070249	1.539667
C	-1.343414	-0.904379	2.306504
C	-1.749139	-2.194135	1.609609
C	-0.551136	-2.882725	0.987444
N	1.641204	-0.056868	0.252219
C	2.303683	0.986807	1.044966
C	3.588474	1.286856	0.283036
C	3.302442	0.799136	-1.128716
C	2.449826	-0.447026	-0.883931
C	3.343281	-1.631758	-0.573984
O	3.579736	-2.065105	0.520954
O	3.870430	-2.132541	-1.685617
H	1.833303	-0.694446	-1.743648
H	4.195906	0.587334	-1.708922
H	2.701308	1.523071	-1.674335
H	3.833480	2.344536	0.312466
H	4.424328	0.737436	0.711607
H	1.675294	1.866383	1.138470
H	2.492201	0.605377	2.047150
H	-1.746603	1.727573	1.242126
H	-0.855406	-3.797208	0.479912
H	0.163129	-3.169990	1.761265
H	-2.235676	-2.855344	2.326498
H	-2.479412	-1.984359	0.829151
H	-0.893367	-1.146221	3.273780
H	-2.226875	-0.307519	2.538781
H	-1.453198	-0.029890	-2.121982
H	-3.301089	-1.269159	-3.135383
H	-5.466605	-1.470818	-1.958424
H	-5.762627	-0.393760	0.249996
H	-3.906287	0.850670	1.272690
H	1.011561	-2.466366	-0.425472
H	0.053765	0.761527	2.099034
H	-0.533661	1.933143	-1.570785
H	4.461020	-2.856393	-1.448238
H	-0.534858	-1.772296	-0.853178

(1-2)'$_{anti}$ $(re\text{-}si)_{300}$

E_0 = -1148.5085752
E_{0+ZPE} = -1148.086221
E_{298} = -1148.064135
H_{298} = -1148.063191
G_{298} = -1148.138475
NImag = 1 (-385.9484)

C	2.193162	1.860427	-0.914531
C	2.375343	0.529340	-0.533822
C	3.607043	0.156928	0.006950
C	4.622458	1.088531	0.158876
C	4.428793	2.407123	-0.227449
C	3.208302	2.790367	-0.767629
C	1.276118	-0.427764	-0.751485
C	1.539864	-1.785152	-0.905017
N	0.655537	-2.593840	-1.560493
O	0.960991	-3.784010	-1.739726
O	-0.422715	-2.137519	-1.977063
C	0.146067	0.093394	1.050261
C	-1.031270	-0.606223	0.777026
C	-1.177263	-2.004243	1.291344
C	-0.516335	-2.203736	2.646788
C	0.925642	-1.742731	2.610737
C	0.999423	-0.274397	2.234038
N	-2.006712	-0.107044	0.014509
C	-3.117945	-0.894503	-0.518323
C	-3.970250	0.118388	-1.261407
C	-2.972203	1.176924	-1.695586
C	-1.995145	1.237435	-0.517700
C	-2.447209	2.244944	0.519609

O	3.283509	-2.061021	-0.649617
O	4.116101	-0.267301	-1.669499
H	2.092517	0.853880	-0.753859
H	4.335927	1.071300	0.689093
H	2.842616	1.801439	1.267443
H	3.450990	0.389050	3.157180
H	4.021932	-0.885805	2.090777
H	1.176463	-0.193681	2.793770
H	1.887233	-1.757877	2.400055
H	-1.076606	1.328928	-1.679385
H	-1.704943	-0.900329	-2.446895
H	-0.489599	-2.142099	-2.521682
H	-2.398210	-3.195880	-1.576356
H	-2.722062	-1.866255	-0.484973
H	-0.315685	-3.719910	-0.321870
H	-1.700722	-3.739757	0.751791
H	-1.953734	0.718220	1.971043
H	-4.216303	0.154724	2.716373
H	-6.050186	-0.080606	1.073812
H	-5.592599	0.279022	-1.330941
H	-3.321338	0.848077	-2.081472
H	0.589525	-0.123951	-1.682095
H	0.221124	-2.529994	1.736087
H	-0.506750	2.276831	1.186024
H	4.642886	-0.938771	-2.116793
H	-1.185965	-1.507882	1.582177
O	-3.008638	1.992894	1.550179
O	-2.164918	3.484238	0.128653
H	-1.006423	1.533544	-0.858731
H	-3.422077	2.141458	-1.912583
H	-2.425962	0.850792	-2.577949
H	-4.491860	-0.332811	-2.100761
H	-4.715409	0.547120	-0.593343
H	-2.715164	-1.661346	-1.181820
H	-3.673423	-1.378294	0.279921
H	0.472430	-0.061505	-1.371796
H	2.032232	0.018965	2.043946
H	0.675996	0.330728	3.086769
H	1.404729	-1.898878	3.577135
H	1.473534	-2.343181	1.883442
H	-1.066389	-1.645486	3.407000
H	-0.581705	-3.257143	2.916362
H	3.782685	-0.865133	0.307344
H	5.569647	0.780601	0.577506
H	5.223024	3.130121	-0.111112
H	3.048207	3.813178	-1.076731
H	1.245129	2.166727	-1.335641
H	0.150702	1.150255	0.828466
H	-2.223915	-2.286967	1.339824
H	2.426827	-2.289613	-0.571412
H	-2.500299	4.099172	0.790584
H	-0.709616	-2.671263	0.563047

Other possible conformations

(1-2)'*anti*-(i) (*re-re*)$_{60}$

COOH – NH Interaction

sol-rere-sa-hk-mich-test-smdPCM-NH.log

E_0 = -1148.5091568

E_{0+ZPE} = -1148.086018

E_{298} = -1148.064354

H_{298} = -1148.063410

G_{298} = -1148.136695

NImag = 1 (-408.6458)

C	2.530328	-1.646960	-0.009969
C	2.516250	-0.324368	0.434648
C	3.710378	0.394381	0.434253
C	4.893223	-0.196942	0.013527
C	4.895969	-1.512674	-0.423326
C	3.708983	-2.235496	-0.434975
C	1.282754	0.320871	0.932956
C	0.490176	-0.409394	1.820053
N	-0.437342	0.202663	2.604184
O	-1.093351	-0.481387	3.408421
O	-0.623280	1.427686	2.507219
C	0.343177	0.685102	-0.929274
C	-0.931861	1.059371	-0.501334
C	-1.311095	2.506698	-0.371931
C	-0.526834	3.408988	-1.311865
C	0.956904	3.114874	-1.236855
C	1.220824	1.677623	-1.645059
N	-1.839867	0.139069	-0.141194
C	-3.060699	0.436139	0.623595
C	-3.791032	-0.892864	0.683063
C	-2.670731	-1.916754	0.626341
C	-1.679939	-1.295585	-0.356865
C	-1.982241	-1.722381	-1.789283
O	-1.760122	-2.838358	-2.169672
O	-2.520552	-0.823286	-2.601954
H	-0.667842	-1.623217	-0.150611
H	-2.990754	-2.905362	0.311891
H	-2.185127	-1.997487	1.596468
H	-4.390520	-0.978047	1.584625
H	-4.456954	-1.002862	-0.172791
H	-2.771223	0.791825	1.613748

(1-2)'*anti*-(i) (*si-si*)$_{60}$

COOH – NH Interaction

sol-sisi-aa-hk-mich-test1-conf-smdPCM.log

E_0 = -1148.5000604

E_{0+ZPE} = -1148.077613

E_{298} = -1148.055817

H_{298} = -1148.054873

G_{298} = -1148.129176

NImag = 1 (-411.9596)

C	2.404344	-0.439025	-0.794282
N	1.477572	-0.247627	0.316956
C	1.898899	0.858719	1.189262
C	3.304259	1.179970	0.715386
C	3.257315	0.831479	-0.762864
C	0.319430	-0.909381	0.463491
C	0.027472	-2.088096	-0.397217
C	-0.574900	-3.230640	0.415144
C	-1.822977	-2.772792	1.142344
C	-1.554429	-1.550311	2.004190
C	-0.672674	-0.502416	1.359573
C	3.297689	-1.665515	-0.646600
O	3.347487	-2.245634	0.545168
O	3.961361	-2.074345	-1.558008
C	-1.941836	0.632640	0.133017
C	-2.418580	0.021033	-1.029144
N	-3.575852	-0.707094	-1.028872
O	-4.221159	-0.873809	0.015556
C	-1.183378	1.896237	0.018535
C	-0.413161	2.219301	-1.098315
C	0.253918	3.432948	-1.166995
C	0.159447	4.346432	-0.125920
C	-0.614746	4.040469	0.985524
C	-1.276477	2.825834	1.055788
O	-3.967869	-1.182095	-2.106242
H	1.878919	-0.547062	-1.738405
H	4.233451	0.678326	-1.212871
H	2.741381	1.609332	-1.320852
H	3.558474	2.220864	0.893407
H	4.039886	0.565123	1.233437
H	1.237111	1.709987	1.055564

(1-2)'*anti*-(ii) (*re-re*)$_{60}$

sol-rere-sa-hk-mich-test-t1-smdPCM-conf1.log

E_0 = -1148.5075479

E_{0+ZPE} = -1148.085326

E_{298} = -1148.063245

H_{298} = -1148.062301

G_{298} = -1148.137460

NImag = 1 (-367.5797)

C	2.524049	-1.655078	0.102128
C	2.512235	-0.307905	0.467769
C	3.705212	0.410447	0.403175
C	4.881849	-0.203351	-0.002992
C	4.881285	-1.542805	-0.360224
C	3.695899	-2.266759	-0.307580
C	1.288338	0.361284	0.947621
C	0.466364	-0.325657	1.832475
N	-0.457829	0.325811	2.597917
O	-1.137230	-0.333891	3.401238
O	-0.604914	1.551875	2.490675
C	0.339813	0.671140	-0.994665
C	-0.926088	1.050492	-0.554020
C	-1.310902	2.500814	-0.474628
C	-0.525330	3.377088	-1.437347
C	0.959010	3.086928	-1.356810
C	1.220865	1.640319	-1.732152
N	-1.799664	0.146682	-0.099673
C	-3.051243	0.475871	0.584512
C	-3.779703	-0.852280	0.706886
C	-2.665310	-1.883935	0.667760
C	-1.676354	-1.276824	-0.329882
C	-2.051047	-1.631068	-1.763836
O	-2.606070	-0.896209	-2.528472
O	-1.740636	-2.873158	-2.136897
H	-0.663712	-1.623716	-0.137839
H	-3.004933	-2.876027	0.380756
H	-2.174190	-1.951658	1.635958
H	-4.363319	-0.907681	1.621197
H	-4.456921	-0.990908	-0.133961
H	-2.814013	0.908024	1.558069

H	-3.648342	1.210237	0.138746
H	1.366689	1.377782	1.140590
H	2.266614	1.418801	-1.484278
H	1.053835	1.572449	-2.720716
H	1.515558	3.788748	-1.885611
H	1.311469	3.290190	-0.219114
H	-0.872330	3.262133	-2.337208
H	-0.734709	4.446598	-1.054219
H	3.714573	1.419328	0.777663
H	5.810922	0.373085	0.026121
H	5.814606	-1.973434	-0.756248
H	3.702146	-3.259647	-0.778908
H	1.612597	-2.218329	-0.032162
H	0.470984	-0.334911	-1.260372
H	-2.376617	2.618782	-0.557122
H	0.561268	-1.472023	1.962503
H	-2.611811	0.019096	-2.145174
H	-1.143325	2.803110	0.662926
H	1.853960	0.546343	2.230556
H	-2.643784	0.612585	0.955380
H	-0.804063	-4.056182	-0.256940
H	0.168164	-3.598482	1.125657
H	-2.207322	-3.576477	1.770266
H	-2.603872	-2.546905	0.420059
H	-1.050920	-1.863694	2.923747
H	-2.495654	-1.100174	2.316524
H	-1.879760	2.591986	1.922342
H	-0.706411	4.749927	1.795230
H	0.676747	5.292989	-0.184996
H	0.843985	3.669216	-2.040840
H	-0.333495	1.528407	-1.924578
H	0.896030	-2.432789	-0.949052
H	-0.409072	0.306618	2.027331
H	-1.986145	0.134602	-2.005423
H	2.735238	-1.812919	1.149521
H	-0.711144	-1.752830	-1.138953
H	-3.628765	1.200539	0.017975
H	1.367730	1.427069	1.101223
H	2.266170	1.382480	-1.561550
H	1.058721	1.513234	-2.806696
H	1.516843	3.746978	-2.020639
H	1.314166	3.284138	-0.343176
H	-0.870991	3.199911	-2.457681
H	-0.733711	4.421828	-1.209770
H	3.713853	1.453524	0.686431
H	5.798084	0.367939	-0.040593
H	5.795286	-2.021092	-0.680891
H	3.686256	-3.309667	-0.589906
H	1.606125	-2.225986	0.128319
H	0.482868	-0.360946	-1.276587
H	-2.374087	2.599257	-0.679862
H	0.509656	-1.385186	2.005295
H	-1.292182	-3.355038	-1.436772
H	-1.159317	2.834274	0.551518

(1-2)'$_{\textbf{\textit{anti}-(iii)}}$ $(re\text{-}re)_{60}$

sol-rere-sa-hk-mich-test-t1-smdPCM-conf.log

E_0 = -1148.5122692
E_{0+ZPE} = -1148.089866
E_{298} = -1148.067846
H_{298} = -1148.066901
G_{298} = -1148.141912
NImag = 1 (-378.2625)

C	2.539302	-1.656176	0.056915
C	2.523362	-0.315877	0.447162
C	3.712220	0.410002	0.388631
C	4.889624	-0.189255	-0.036412
C	4.893439	-1.521736	-0.418938
C	3.712234	-2.252848	-0.371985
C	1.299082	0.341174	0.944713
C	0.490097	-0.359985	1.832153
N	-0.429698	0.279412	2.611024
O	-1.098215	-0.389029	3.416625
O	-0.585834	1.506184	2.513456
C	0.336141	0.673214	-0.973568
C	-0.932607	1.036780	-0.524041
C	-1.329916	2.482593	-0.423554
C	-0.553914	3.380576	-1.374123
C	0.932802	3.100199	-1.302740
C	1.204845	1.661640	-1.701157
N	-1.799411	0.119343	-0.086654
C	-3.045068	0.428573	0.618471
C	-3.759610	-0.907865	0.734856
C	-2.635484	-1.927933	0.673298
C	-1.655305	-1.305887	-0.321550
C	-1.986644	-1.726329	-1.740589
O	-1.678628	-2.801758	-2.184325
O	-2.672463	-0.828452	-2.433931
H	-0.643521	-1.645718	-0.132915
H	-2.956246	-2.920566	0.370941
H	-2.137338	-2.000710	1.637610
H	-4.332425	-0.976650	1.655192
H	-4.446934	-1.043913	-0.098468
H	-2.797896	0.849971	1.594332
H	-3.636050	1.156895	0.070420
H	1.377409	1.404686	1.114454
H	2.253072	1.410629	-1.539193
H	1.039546	1.549654	-2.776932
H	1.483485	3.774825	-1.957856
H	1.289778	3.284557	-0.287356
H	-0.901032	3.218479	-2.396639
H	-0.769383	4.419845	-1.128708
H	3.716961	1.447702	0.691280
H	5.802579	0.387647	-0.068916
H	5.807726	-1.988973	-0.754854

(1-2)'$_{\textbf{\textit{anti}-(vi)}}$ $(re\text{-}re)_{60}$

sol-rere-sa-hk-mich-conf-pyr.log

E_0 = -1148.5124766
E_{0+ZPE} = -1148.090000
E_{298} = -1148.068033
H_{298} = -1148.067089
G_{298} = -1148.141707
NImag = 1 (-361.3293)

C	2.552481	-1.537232	0.535350
C	2.473669	-0.143585	0.563600
C	3.627888	0.594191	0.303188
C	4.831589	-0.041082	0.033024
C	4.897463	-1.425535	0.009250
C	3.751720	-2.171291	0.260836
C	1.224842	0.567404	0.894767
C	0.429803	0.066482	1.918681
N	-0.486148	0.854614	2.554026
O	-1.097781	0.387563	3.528564
O	-0.684998	2.016515	2.168633
C	0.276076	0.409950	-1.063879
C	-0.995791	0.857709	-0.719687
C	-1.394603	2.289883	-0.932161
C	-0.641821	2.940284	-2.082382
C	0.848790	2.691548	-1.967269
C	1.132896	1.201232	-2.012371
N	-1.873118	0.049052	-0.120867
C	-3.114460	0.495680	0.502237
C	-3.488629	-0.679818	1.382748
C	-3.056000	-1.883373	0.561759
C	-1.781676	-1.399097	-0.154029
C	-1.774840	-1.937959	-1.567099
O	-2.222906	-1.386926	-2.535025
O	-1.256313	-3.161467	-1.600471
H	-0.890684	-1.750764	0.357956
H	-3.823376	-2.131006	-0.170699
H	-2.860040	-2.769531	1.157302
H	1.266274	1.643160	0.812270
H	2.184770	1.004762	-1.806236
H	0.958498	0.834563	-3.028476
H	1.384623	3.192777	-2.772989
H	1.216197	3.117198	-1.030787
H	-1.003523	2.538310	-3.030932
H	-0.860590	4.007576	-2.087054
H	3.584837	1.674032	0.327047
H	5.716512	0.548178	-0.159493
H	5.832499	-1.922851	-0.204035
H	3.793681	-3.250819	0.241381
H	1.669500	-2.131504	0.723851
H	0.438633	-0.657611	-1.093814
H	-2.466105	2.336053	-1.115779

(1-2)'$_{\textbf{\textit{anti}-(vi)}}$ $(si\text{-}si)_{300}$

sol-sisi-aa-hk-mich-conf-pyr.log

E_0 = -1148.5095881
E_{0+ZPE} = -1148.087222
E_{298} = -1148.065222
H_{298} = -1148.064278
G_{298} = -1148.139401
NImag = 1 (-375.4033)

C	-3.148540	-1.165308	-0.917841
C	-2.847059	-0.323183	0.154597
C	-3.860695	0.478764	0.677605
C	-5.144335	0.434588	0.152190
C	-5.431731	-0.405830	-0.912000
C	-4.427359	-1.205161	-1.445740
C	-1.506632	-0.280608	0.768405
C	-0.831026	-1.480602	0.957766
N	0.199115	-1.595140	1.846826
O	0.698752	-2.716218	2.033447
O	0.611394	-0.600214	2.462399
C	1.329695	1.871100	0.685217
C	0.751260	0.873181	-0.280895
C	-0.561966	1.021296	-0.720286
C	-1.265417	2.346957	-0.620440
C	-0.766875	3.214675	0.519882
C	0.747052	3.263881	0.509226
N	1.465504	-0.207713	-0.608079
C	1.073856	-1.188477	-1.617129
C	1.835216	-2.430289	-1.205251
C	3.149826	-1.885435	-0.670016
C	2.786199	-0.502048	-0.087169
C	3.838072	0.477545	-0.550638
O	3.764134	1.183662	-1.520234
O	4.914342	0.416189	0.224669
H	2.760059	-0.521138	1.001834
H	3.866851	-1.773174	-1.482079
H	3.600720	-2.518086	0.087336
H	-1.368065	0.469520	1.532853
H	1.122784	3.903144	1.307304
H	1.093842	3.693066	-0.432930
H	-1.186586	4.216364	0.431022
H	-1.107393	2.813710	1.477062
H	-1.124411	2.881933	-1.564750
H	-2.339773	2.183713	-0.536544
H	-3.644152	1.131966	1.511232
H	-5.917661	1.059041	0.575663
H	-6.429148	-0.438974	-1.325621
H	-4.642648	-1.859972	-2.277831
H	-2.376487	-1.787436	-1.348716
H	2.409439	1.922132	0.593393
H	-0.871536	0.417637	-1.559344

H	3.705492	-3.290255	-0.673816
H	1.625962	-2.234416	0.077549
H	0.485234	-0.353356	-1.272495
H	-2.394575	2.574557	-0.624830
H	0.537935	-1.421723	1.989862
H	-2.853485	-1.197387	-3.306110
H	-1.179002	2.802203	0.607000

(1-2)'*anti*-(v)$(re\text{-}re)_{60}$

sol-rere-sa-hk-mich-test-smdPCM-cycconf-t1.log

E_0 = -1148.513288

E_{0+ZPE} = -1148.091043

E_{298} = -1148.069054

H_{298} = -1148.068110

G_{298} = -1148.142857

NImag = 1 (-372.4372)

C	2.533558	-1.583755	0.330673
C	2.518697	-0.200032	0.516689
C	3.707800	0.507399	0.348120
C	4.882473	-0.149695	0.008666
C	4.884318	-1.523844	-0.173143
C	3.703706	-2.239265	-0.010005
C	1.291366	0.520765	0.910380
C	0.482102	-0.045984	1.890921
N	-0.473020	0.694714	2.520727
O	-1.166442	0.159940	3.402652
O	-0.636846	1.884599	2.208654
C	0.336880	0.598684	-1.009286
C	-0.951676	0.963579	-0.617215
C	-1.436379	2.377818	-0.726854
C	-0.356214	3.347623	-1.166725
C	0.434559	2.763926	-2.320163
C	1.178343	1.520823	-1.858953
N	-1.792369	0.072520	-0.091524
C	-3.084454	0.424379	0.498952
C	-3.778713	-0.910229	0.712061
C	-2.628426	-1.893588	0.850233
C	-1.606216	-1.362376	-0.155713
C	-1.888208	-1.889466	-1.549075
O	-2.434144	-1.289264	-2.434309
O	-1.469781	-3.145422	-1.673125
H	-0.598005	-1.654231	0.117193
H	-2.905625	-2.925771	0.656904
H	-2.190546	-1.829925	1.844077
H	-4.421173	-0.894250	1.587809
H	-4.392608	-1.160650	-0.151617
H	-2.906446	0.944953	1.441971
H	-3.645205	1.081932	-0.159447
H	1.369809	1.597803	0.923136
H	-0.822531	4.291380	-1.446054
H	0.313427	3.560815	-0.331764
H	3.716445	1.577426	0.500564
H	5.795689	0.414907	-0.112449
H	5.796985	-2.036551	-0.440179
H	3.695658	-3.310274	-0.152595
H	1.620014	-2.150671	0.445560
H	0.514652	-0.452060	-1.173715
H	-2.243541	2.373152	-1.465586
H	0.536797	-1.069104	2.214386
H	-1.697491	-3.459009	-2.555514
H	-1.873654	2.691263	0.216529
H	-0.249488	2.510393	-3.133244
H	1.142830	3.491438	-2.715545
H	2.067005	1.831920	-1.304220
H	1.551354	0.965082	-2.718972

(1-2)'*anti*-(v) $(re\text{-}si)_{60}$

sol-resi-sa-hk-60-cnf-cyc.log

H	0.507423	-0.927010	2.319694
H	-1.333290	-3.503051	-2.498577
H	-1.209245	2.834727	-0.006987
H	-2.928769	-0.628204	2.314276
H	-4.550062	-0.696638	1.615428
H	-2.936772	1.406182	1.067596
H	-3.876541	0.687980	-0.256046

(1-2)'*anti*-(v)$(si\text{-}si)_{300}$

sol-sisi-aa-hk300-cnf-cyc.log

E_0 = -1148.5121134

E_{0+ZPE} = -1148.089628

E_{298} = -1148.067706

H_{298} = -1148.066762

G_{298} = -1148.141380

NImag = 1 (-385.3484)

C	-3.087304	-1.274915	-0.822292
C	-2.866622	-0.337053	0.188189
C	-3.940222	0.437766	0.624022
C	-5.203077	0.276142	0.071019
C	-5.409900	-0.659073	-0.930911
C	-4.345703	-1.435021	-1.375543
C	-1.543285	-0.169466	0.822959
C	-0.837214	-1.320185	1.168424
N	0.206365	-1.262631	2.039752
O	0.785788	-2.315339	2.359667
O	0.563406	-0.167155	2.505214
C	1.393761	1.959753	0.492520
C	0.727496	0.867397	-0.289319
C	-0.597934	0.979395	-0.712370
C	-1.302160	2.314328	-0.720710
C	-0.411761	3.471934	-0.296990
C	0.436083	3.066888	0.892267
N	1.419916	-0.241013	-0.555351
C	1.025147	-1.215925	-1.577022
C	2.216761	-2.154029	-1.679930
C	2.885339	-2.040624	-0.319712
C	2.704142	-0.559877	0.030388
C	3.830981	0.252461	-0.568425
O	3.803500	0.809678	-1.633341
O	4.900634	0.241148	0.218038
H	2.683902	-0.405956	1.107636
H	3.928683	-2.344035	-0.319318
H	2.355650	-2.625609	0.428988
H	1.911776	-3.171438	-1.909011
H	2.891224	-1.821143	-2.466404
H	0.125219	-1.739986	-1.267128
H	0.817182	-0.698040	-2.512046
H	-1.460908	0.659511	1.510502
H	-1.703766	2.494776	-1.717858
H	-2.171018	2.279335	-0.059636
H	-3.789344	1.159911	1.414056
H	-6.024005	0.882262	0.426075
H	-6.391281	-0.783782	-1.365020
H	-4.497276	-2.163945	-2.158584
H	-2.265502	-1.876161	-1.186283
H	2.170119	2.378742	-0.152998
H	-0.912885	0.287877	-1.478248
H	-1.053426	-2.304424	0.796379
H	5.610895	0.721493	-0.222075
H	1.889354	1.549607	1.367435
H	1.011893	3.910539	1.270129
H	-0.204237	2.728592	1.708595
H	0.245000	3.760268	-1.120798
H	-1.025021	4.341086	-0.061224

(1-2)'*anti*-(v) $(si\text{-}re)_{60}$

sol-sire-aa-hk-60-cnf-cyc-t2.log

E_0 = -1148.5076707

E_{0+ZPE} = -1148.085460

E_{298} = -1148.063290

H_{298} = -1148.062346

G_{298} = -1148.138880

NImag = 1 (-427.7885)

C	-2.837731	-0.603991	-0.580172
N	-1.558782	-0.762189	0.078479
C	-1.089881	-2.145989	0.034062
C	-2.260253	-2.917435	-0.549778
C	-2.966008	-1.884098	-1.411585
C	-0.865640	0.241739	0.616628
C	-1.568386	1.559517	0.765589
C	-0.711162	2.643621	1.397127
C	0.090918	2.073294	2.548272
C	1.077451	1.049933	2.012041
C	0.454128	0.063905	1.052851
C	-3.982012	-0.510795	0.407334
O	-5.077296	-0.038488	-0.176234
O	-3.942384	-0.844077	1.561071
C	1.564551	0.230488	-0.757079
C	1.659373	1.547897	-1.201471
N	0.639157	2.095126	-1.919474
O	-0.383427	1.425717	-2.147112
C	2.786775	-0.471813	-0.316373
C	2.855512	-1.859216	-0.454830
C	3.987384	-2.560485	-0.074832
C	5.074734	-1.885686	0.463769
C	5.020747	-0.506516	0.606194
C	3.890445	0.195573	0.216469
O	0.752171	3.259124	-2.335823
H	-2.848442	0.281167	-1.210803
H	-3.998704	-2.133118	-1.638446
H	-2.437574	-1.735942	-2.351145
H	-1.931675	-3.783042	-1.117915
H	-2.917698	-3.265932	0.244502
H	-0.210902	-2.223471	-0.603018
H	-0.817294	-2.480048	1.033465
H	0.857454	-0.379579	-1.298029
H	1.539953	0.502117	2.832232
H	1.885569	1.593546	1.514936
H	3.877033	1.269188	0.326275
H	5.864312	0.028151	1.018389
H	5.958289	-2.429580	0.764815
H	4.021158	-3.633147	-0.199737
H	2.012281	-2.391299	-0.872602
H	-2.434419	1.376399	1.406432
H	0.759975	-0.962643	1.184990
H	2.475842	2.217260	-1.006881
H	-5.793894	-0.036825	0.468296
H	-1.950655	1.888659	-0.197127
H	-0.032107	3.067609	0.656838
H	-1.361146	3.452924	1.726727
H	0.626764	2.862288	3.075231
H	-0.584914	1.606884	3.269027

E_0 = -1148.5092866
E_{0+ZPE} = -1148.087084
E_{298} = -1148.065102
H_{298} = -1148.064158
G_{298} = -1148.138885
NImag = 1 (-369.1137)

C	-3.513866	0.638690	-0.939208
C	-2.407976	0.816172	-0.107117
C	-2.581525	0.664745	1.270646
C	-3.818138	0.331339	1.795001
C	-4.908967	0.144693	0.954271
C	-4.753620	0.304526	-0.414176
C	-1.115606	1.201849	-0.698202
C	-0.312072	2.101036	0.006041
N	0.710901	2.749785	-0.609794
O	1.355279	3.601574	0.023864
O	1.006603	2.464012	-1.785373
C	-0.060151	-0.588629	-1.156066
C	0.285649	-1.015284	0.124993
C	-0.543303	-2.024014	0.855883
C	-1.705384	-2.574346	0.043276
C	-1.299879	-2.773356	-1.403497
C	-0.946245	-1.435815	-2.034547
N	1.337199	-0.504870	0.770746
C	1.624737	-0.759384	2.186016
C	3.043161	-0.248409	2.389526
C	3.235363	0.761026	1.269436
C	2.459166	0.135303	0.111824
C	3.300689	-0.893023	-0.619202
O	3.207049	-2.086022	-0.509776
O	4.195149	-0.304364	-1.404179
H	2.158341	0.883360	-0.614885
H	4.276191	0.944485	1.019991
H	2.771582	1.714843	1.511574
H	3.176555	0.189309	3.374757
H	3.754728	-1.066114	2.289105
H	0.907555	-0.217759	2.801849
H	1.537413	-1.817995	2.415071
H	-1.129538	1.329253	-1.771299
H	-2.029147	-3.512947	0.491326
H	-2.553411	-1.892305	0.090732
H	-1.744277	0.803629	1.938906
H	-3.933225	0.216060	2.863155
H	-5.873189	-0.116123	1.365747
H	-5.597849	0.174893	-1.075688
H	-3.404950	0.782950	-2.004661
H	0.677020	-0.005166	-1.688523
H	0.128223	-2.840981	1.130977
H	-0.447929	2.365623	1.037848
H	4.728898	-0.986006	-1.827283
H	-0.897085	-1.599599	1.796756
H	-0.438185	-3.443112	-1.450477
H	-2.103336	-3.248128	-1.965734
H	-0.438134	-1.595228	-2.985935
H	-1.867799	-0.901663	-2.275666

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syn-addition

(1-2)'*syn* $(re\text{-}re)_{180}$

E_0 = -1148.5080791
E_{0+ZPE} = -1148.085733
E_{298} = -1148.063711
H_{298} = -1148.062767
G_{298} = -1148.137976
NImag = 1 (-424.6252)

C	3.238837	-0.908277	-0.393803
C	1.942708	-0.567411	-0.787732
C	1.160035	-1.540209	-1.411426
C	1.655205	-2.815460	-1.636374

(1-2)'*syn* $(re\text{-}re)_{300}$

E_0 = -1148.5024339
E_{0+ZPE} = -1148.080080
E_{298} = -1148.058145
H_{298} = -1148.057201
G_{298} = -1148.132417
NImag = 1 (-403.2155)

C	0.528736	2.063392	1.067585
C	-0.496225	2.101875	0.122060
C	-0.530120	3.164637	-0.783510
C	0.431154	4.161259	-0.748517

(1-2)'*syn* $(si\text{-}si)_{180}$

E_0 = -1148.5067758
E_{0+ZPE} = -1148.084147
E_{298} = -1148.062179
H_{298} = -1148.061235
G_{298} = -1148.136732
NImag = 1 (-422.0564)

C	-3.106198	-0.496204	-0.631168
C	-1.773429	-0.260688	-0.972472
C	-1.129330	-1.178808	-1.803935
C	-1.793094	-2.301147	-2.275599

C	2.942228	-3.143897	-1.235494
C	3.730475	-2.184559	-0.612992
C	1.389006	0.787661	-0.623613
C	2.262483	1.872599	-0.553245
N	1.806724	3.147149	-0.705869
O	2.612032	4.086184	-0.605440
O	0.603913	3.355746	-0.942256
C	0.376020	0.809365	1.257312
C	-0.744822	-0.016228	1.109213
C	-0.679004	-1.439608	1.569071
C	0.133588	-1.578714	2.849406
C	1.511757	-0.976553	2.673513
C	1.420143	0.493545	2.296550
N	-1.860010	0.432900	0.524880
C	-2.060553	1.845388	0.187875
C	-3.393250	1.870583	-0.531298
C	-4.154037	0.727906	0.115336
C	-3.071237	-0.338781	0.318231
C	-2.978834	-1.235147	-0.896616
O	-2.160959	-1.153350	-1.772501
O	-3.958665	-2.131686	-0.900233
H	-3.310155	-0.961569	1.175332
H	-4.989314	0.361646	-0.474329
H	-4.532303	1.022614	1.092237
H	-3.895958	2.827014	-0.418031
H	-3.253435	1.687004	-1.595306
H	-2.096978	2.423762	1.113488
H	-1.240081	2.226771	-0.412377
H	0.462768	0.959590	-1.150645
H	2.390161	0.859578	1.952108
H	1.191343	1.076924	3.192992
H	2.093384	-1.081413	3.589389
H	2.040317	-1.530572	1.898795
H	-0.392647	-1.083065	3.667837
H	0.203565	-2.634265	3.109613
H	0.155946	-1.288983	-1.723003
H	1.035309	-3.551127	-2.128725
H	3.331185	-4.136572	-1.410609
H	4.735515	-2.429852	-0.301148
H	3.873280	-0.179806	0.087943
H	0.188411	1.866129	1.130192
H	-1.671745	-1.852630	1.715411
H	3.306309	1.811628	-0.311422
H	-3.895957	-2.652865	-1.708596
H	-0.210992	-2.028648	0.775729

C	1.450445	4.110467	0.193551
C	1.492445	3.059490	1.099567
C	-1.571935	1.093393	0.064973
C	-1.957455	0.428675	1.227537
N	-3.242186	-0.005453	1.409875
O	-3.527347	-0.553574	2.486286
O	-4.101129	0.163166	0.532506
C	-0.846226	-0.126692	-1.557405
C	-0.003421	-1.028256	-0.901112
C	-0.637224	-2.213245	-0.258570
C	-1.672931	-2.865240	-1.166794
C	-2.722918	-1.857513	-1.587990
C	-2.090534	-0.643120	-2.245097
N	1.307822	-0.811456	-0.754195
C	2.018020	0.260391	-1.458325
C	3.437885	0.152808	-0.945693
C	3.604501	-1.337009	-0.712282
C	2.234568	-1.766486	-0.170810
C	2.214091	-1.761500	1.342387
O	1.675659	-0.952434	2.046498
O	2.899631	-2.795900	1.819547
H	2.013028	-2.781253	-0.492187
H	4.413658	-1.589624	-0.033598
H	3.781367	-1.853465	-1.653452
H	4.157892	0.550794	-1.655279
H	3.541975	0.702442	-0.011383
H	1.964106	0.077063	-2.533810
H	1.571827	1.224811	-1.247855
H	-2.390988	1.352862	-0.590588
H	-2.825073	0.157795	-2.332606
H	-1.808352	-0.898399	-3.271505
H	-3.430228	-2.314691	-2.280273
H	-3.295545	-1.540843	-0.718288
H	-1.173603	-3.283431	-2.043567
H	-2.132335	-3.698342	-0.636223
H	-1.323320	3.209409	-1.517507
H	0.383002	4.978740	-1.453572
H	2.201827	4.886360	0.224586
H	2.280410	3.013619	1.837871
H	0.593488	1.245437	1.767599
H	-0.363371	0.678496	-2.092653
H	0.088149	-2.947311	0.074400
H	-1.325002	0.260452	2.078903
H	2.885479	-2.755339	2.782380
H	-1.139485	-1.831231	0.640817

C	-3.115801	-2.527584	-1.922995
C	-3.768863	-1.619143	-1.100076
C	-1.025976	0.935402	-0.537586
C	-1.716975	2.126374	-0.300642
N	-1.034367	3.300768	-0.197068
O	-1.670353	4.351153	-0.008631
O	0.205531	3.307293	-0.288436
C	-0.282373	-1.924734	1.569384
C	0.512861	-0.744047	1.103471
C	-0.016340	0.542355	1.260965
C	-0.985286	0.814356	2.381018
C	-1.853641	-0.373474	2.754537
C	-1.020805	-1.633287	2.869990
N	1.687155	-0.970558	0.505818
C	2.219178	-2.308560	0.218769
C	3.579757	-2.040178	-0.394576
C	4.009336	-0.755211	0.290545
C	2.706082	0.051081	0.332049
C	2.563733	0.828603	-0.956395
O	1.936981	0.475711	-1.920634
O	3.280997	1.940523	-0.920029
H	2.689875	0.752207	1.162761
H	4.809245	-0.228224	-0.221717
H	4.329962	-0.950359	1.312143
H	4.268346	-2.861861	-0.219312
H	3.494510	-1.891933	-1.469412
H	2.330487	-2.870155	1.146141
H	1.549370	-2.853839	-0.440403
H	-0.075316	1.046281	-1.031778
H	-1.646012	-2.490562	3.117528
H	-0.295360	-1.526144	3.679104
H	-2.368437	-0.170667	3.693613
H	-2.624006	-0.524967	1.999454
H	-0.412215	1.133499	3.256377
H	-1.604946	1.670884	2.105502
H	-0.101527	-0.997783	-2.085444
H	-1.278200	-2.995192	-2.924483
H	-3.636446	-3.399891	-2.290748
H	-4.801119	-1.782866	-0.825728
H	-3.636192	0.198223	0.003480
H	0.354764	-2.794073	1.694220
H	0.656758	1.368452	1.069795
H	-2.774267	2.213132	-0.135987
H	3.161233	2.411557	-1.752269
H	-1.002297	-2.175270	0.786066

(1-2)'$_{syn}$ $(si\text{-}si)_{300}$

E_0 = -1148.5013791
E_{0+ZPE} = -1148.079165
E_{298} = -1148.057196
H_{298} = -1148.056252
G_{298} = -1148.131064
NImag = 1 (-381.0101)

C	-2.587146	-1.564899	-0.404948
C	-2.432943	-0.417545	0.373254
C	-3.567719	0.324632	0.698675
C	-4.824967	-0.074108	0.268954
C	-4.965942	-1.217079	-0.503490
C	-3.840865	-1.959951	-0.840058
C	-1.122318	0.018783	0.894174
C	-0.278895	-0.936812	1.452088
N	0.675142	-0.583613	2.366055
O	1.289959	-1.476148	2.963047
O	0.893415	0.616204	2.605286
C	0.954073	2.653827	0.235726
C	0.875498	1.297585	-0.403263
C	-0.338229	0.860621	-0.928498
C	-1.353713	1.859691	-1.417638
C	-1.352437	3.150320	-0.619378

(1-2)'$_{syn}$ $(si\text{-}re)_{60}$

E_0 = -1148.5039153
E_{0+ZPE} = -1148.081615
E_{298} = -1148.059688
H_{298} = -1148.058744
G_{298} = -1148.133243
NImag = 1 (-384.6762)

C	-2.306252	1.841436	-0.483050
C	-2.318482	0.449471	-0.383854
C	-3.502593	-0.175418	0.012733
C	-4.635397	0.570241	0.298277
C	-4.609887	1.953979	0.192020
C	-3.439604	2.587489	-0.202302
C	-1.096618	-0.301486	-0.737579
C	-1.225021	-1.592062	-1.255010
N	-0.251482	-2.130635	-2.045181
O	-0.459643	-3.237679	-2.572766
O	0.812745	-1.519593	-2.231764
C	1.217354	-2.205618	0.920909
C	1.094271	-0.718794	0.841950
C	-0.134382	-0.141940	1.176817
C	-1.016063	-0.804126	2.205056
C	-0.912814	-2.318851	2.215371

(1-2)'$_{syn}$ $(re\text{-}si)_{60}$

E_0 = -1148.5059406
E_{0+ZPE} = -1148.083189
E_{298} = -1148.061349
H_{298} = -1148.060405
G_{298} = -1148.134691
NImag = 1 (-407.6710)

C	3.501326	0.865691	-0.126182
C	2.188072	0.639284	-0.539694
C	1.954085	-0.316260	-1.530844
C	3.005117	-1.032908	-2.079010
C	4.308104	-0.805048	-1.653834
C	4.553126	0.150762	-0.678613
C	1.108161	1.460140	0.033770
C	0.102562	1.926112	-0.811896
N	-0.668331	2.985771	-0.448167
O	-1.501916	3.429566	-1.254300
O	-0.546875	3.482791	0.687415
C	0.336465	0.367757	1.693718
C	-0.451685	-0.637041	1.127238
C	0.128649	-2.003978	0.923301
C	1.065416	-2.390686	2.060178
C	2.141903	-1.342526	2.245534

C	0.062222	3.671201	-0.462841
N	1.951369	0.497900	-0.381295
C	3.179316	0.818196	0.351259
C	4.175988	-0.228963	-0.107141
C	3.714698	-0.536088	-1.522458
C	2.191488	-0.527914	-1.397670
C	1.712158	-1.918290	-1.019036
O	2.161407	-2.593254	-0.135096
O	0.767770	-2.358708	-1.849836
H	1.699532	-0.237173	-2.321103
H	4.095171	-1.476037	-1.913511
H	4.008225	0.260967	-2.204028
H	5.195475	0.145634	-0.071314
H	4.110523	-1.118630	0.512419
H	3.528437	1.812759	0.076811
H	2.977456	0.803082	1.420392
H	-1.129784	0.975564	1.395659
H	0.073229	4.597876	0.110184
H	0.474945	3.904721	-1.446598
H	-1.980080	3.890995	-1.114533
H	-1.787381	2.980768	0.367489
H	-1.132799	2.085825	-2.465372
H	-2.344737	1.408856	-1.417233
H	-3.464207	1.215027	1.302724
H	-5.693054	0.510748	0.536978
H	-5.943321	-1.527575	-0.843256
H	-3.941629	-2.849824	-1.444603
H	-1.719910	-2.145600	-0.681228
H	1.979838	3.010023	0.242777
H	-0.334523	-0.079471	-1.463033
H	-0.365057	-1.995467	1.294200
H	0.548097	-3.263978	-1.600715
H	0.657965	2.546905	1.280096

C	0.536626	-2.758053	2.168091
N	2.137542	0.000857	0.421239
C	3.324374	-0.582891	-0.204553
C	4.192038	0.618179	-0.528638
C	3.829020	1.605321	0.567648
C	2.312966	1.412102	0.702267
C	1.607941	2.338289	-0.262684
O	1.195765	2.053711	-1.353899
O	1.535787	3.567537	0.240399
H	1.961146	1.644237	1.705612
H	4.100455	2.632944	0.343392
H	4.298782	1.326579	1.509022
H	5.248669	0.365564	-0.533172
H	3.935405	1.020182	-1.506969
H	3.834308	-1.241681	0.498863
H	3.029306	-1.158696	-1.078610
H	-0.310548	0.289193	-1.186636
H	0.611438	-3.844782	2.155984
H	1.062862	-2.412748	3.060521
H	-1.405270	-2.713561	3.103951
H	-1.436098	-2.732480	1.352588
H	-0.729069	-0.418075	3.188248
H	-2.049924	-0.493019	2.060248
H	-3.547567	-1.250933	0.098317
H	-5.542117	0.067083	0.601874
H	-5.495643	2.532638	0.410668
H	-3.410369	3.663458	-0.297239
H	-1.401041	2.338637	-0.800772
H	2.255938	-2.516318	0.879327
H	-0.170678	0.939483	1.205261
H	-2.088522	-2.220030	-1.143440
H	1.140239	4.146291	-0.421062
H	0.723783	-2.630932	0.045059

C	1.528661	0.015102	2.547736
N	-1.701437	-0.389796	0.720520
C	-2.476475	0.774558	1.163720
C	-3.716233	0.725770	0.301374
C	-3.974147	-0.763747	0.174471
C	-2.563918	-1.365159	0.073319
C	-2.173651	-1.626772	-1.364359
O	-1.359688	-1.022195	-2.006656
O	-2.869551	-2.647190	-1.855590
H	-2.538390	-2.324790	0.585057
H	-4.595622	-1.032680	-0.674199
H	-4.451311	-1.146141	1.074276
H	-4.547600	1.259984	0.752618
H	-3.511545	1.169987	-0.671336
H	-2.723890	0.644279	2.220527
H	-1.922862	1.698072	1.062137
H	1.432385	2.164116	0.786857
H	2.286482	0.796234	2.463149
H	1.206984	0.035302	3.593175
H	2.815392	-1.625032	3.054625
H	2.742092	-1.289914	1.337908
H	0.490560	-2.506736	2.981267
H	1.506567	-3.361473	1.837482
H	0.944386	-0.501207	-1.868139
H	2.807554	-1.770299	-2.843945
H	5.126036	-1.363473	-2.085685
H	5.564067	0.343987	-0.349679
H	3.699721	1.617972	0.624104
H	-0.187280	1.252687	2.025759
H	-0.654963	-2.749689	0.828834
H	-0.134270	1.511010	-1.772726
H	-2.616735	-2.774990	-2.776707
H	0.681640	-2.009113	-0.018357

Oxazolidinone pathway anti addition

(3-4)*anti* (*re-re*)$_{60}$

E_0 = -1148.0270762
E_{0+ZPE} = -1147.618684
E_{298} = -1147.596702
H_{298} = -1147.595757
G_{298} = -1147.671036
NImag = 1 (-286.7505)

C	2.538843	-1.655278	0.197820
C	2.509889	-0.291738	0.501839
C	3.682561	0.448293	0.345712
C	4.853318	-0.155520	-0.090634
C	4.868993	-1.509797	-0.386421
C	3.705212	-2.256351	-0.241277
C	1.304001	0.379766	1.005621
C	0.457565	-0.271463	1.876609
N	-0.469626	0.416286	2.618312
O	-1.173668	-0.217853	3.417682
O	-0.581260	1.643070	2.499074
C	0.297384	0.672383	-1.056950
C	-0.969359	0.995725	-0.590801
C	-1.422234	2.430120	-0.527281
C	-0.653853	3.343372	-1.469843
C	0.839714	3.107120	-1.373935
C	1.156997	1.675800	-1.765947
N	-1.788101	0.060430	-0.106343
C	-3.059140	0.346321	0.547322
C	-3.733598	-1.010766	0.684963
C	-2.576300	-1.996184	0.646520
C	-1.619371	-1.365154	-0.358445
C	-1.971423	-1.783018	-1.811323
O	-2.658746	-1.002804	-2.492171
O	-1.537150	-2.909425	-2.126676
H	-0.596413	-1.666800	-0.164116

(3-4)*anti* (*re-re*)$_{180}$

E_0 = -1148.0228559
E_{0+ZPE} = -1147.614351
E_{298} = -1147.592442
H_{298} = -1147.591498
G_{298} = -1147.666740
NImag = 1 (-323.6208)

C	-2.251902	2.076009	-0.011387
C	-1.402243	1.264545	-0.769403
C	-0.381048	1.878250	-1.496968
C	-0.211163	3.254151	-1.471766
C	-1.061055	4.046883	-0.714555
C	-2.083493	3.450264	0.013296
C	-1.563271	-0.190633	-0.873937
C	-2.802696	-0.784402	-0.703389
N	-3.029098	-2.065297	-1.136180
O	-4.167980	-2.540421	-0.998629
O	-2.115891	-2.719344	-1.655005
C	-0.211753	-1.109432	0.694905
C	0.663966	-0.076999	1.038212
C	0.345001	0.815211	2.202037
C	-0.461491	0.122830	3.289735
C	-1.646443	-0.617935	2.706169
C	-1.177711	-1.652871	1.702246
N	1.746102	0.211064	0.321931
C	2.680881	1.289656	0.633801
C	3.819480	1.104068	-0.359109
C	3.177248	0.345814	-1.508938
C	2.209001	-0.593804	-0.798579
C	2.925546	-1.906616	-0.374738
O	3.308294	-2.001980	0.803459
O	3.068646	-2.719690	-1.308031
H	1.374574	-0.859050	-1.440866

(3-4)*anti* (*re-re*)$_{300}$

E_0 = -1148.018527
E_{0+ZPE} = -1147.610545
E_{298} = -1147.588472
H_{298} = -1147.587528
G_{298} = -1147.663527
NImag = 1 (-296.2941)

C	0.331296	2.399480	0.954036
C	-0.333281	2.083824	-0.232466
C	0.122724	2.658359	-1.422220
C	1.209084	3.514940	-1.429747
C	1.867185	3.814658	-0.243548
C	1.421109	3.255808	0.945670
C	-1.520160	1.221122	-0.276774
C	-2.293584	1.021563	0.851259
N	-3.621095	0.678840	0.766780
O	-4.251412	0.529531	1.824152
O	-4.172712	0.548606	-0.332201
C	-0.441167	-0.645241	-1.158954
C	-0.143519	-1.295137	0.034958
C	-1.206109	-2.152476	0.646454
C	-1.973855	-2.946235	-0.402847
C	-2.541891	-2.035222	-1.472626
C	-1.442118	-1.216711	-2.125026
N	0.999459	-1.109411	0.696589
C	1.316116	-1.733413	1.980299
C	2.799501	-1.459327	2.185482
C	3.068434	-0.240591	1.318977
C	2.173259	-0.473468	0.108248
C	2.889659	-1.351035	-0.954270
O	2.608798	-2.560958	-0.998053
O	3.718118	-0.722234	-1.642905
H	1.904935	0.467915	-0.358143

H	-2.869882	-2.998712	0.347427
H	-2.099348	-2.050734	1.624666
H	-4.320114	-1.078071	1.598260
H	-4.397171	-1.180978	-0.160190
H	-2.866196	0.807041	1.519280
H	-3.662539	1.034895	-0.039088
H	1.362487	1.452925	1.098762
H	2.208642	1.452416	-1.578129
H	1.025468	1.563364	-2.847366
H	1.381325	3.799539	-2.018951
H	1.173230	3.300162	-0.351640
H	-0.977106	3.160732	-2.496831
H	-0.902795	4.379520	-1.240287
H	3.679131	1.503025	0.582664
H	5.751712	0.434841	-0.200218
H	5.777353	-1.981502	-0.732293
H	3.705082	-3.310398	-0.478832
H	1.639321	-2.247338	0.287205
H	0.494517	-0.359369	-1.301927
H	-2.481268	2.476137	-0.772352
H	0.455150	-1.330796	2.054815
H	-1.325094	2.777395	0.500787

H	3.889016	-0.201070	-2.120355
H	2.628371	1.029998	-2.156668
H	4.251729	2.055453	-0.660137
H	4.605211	0.500128	0.089096
H	2.189190	2.255270	0.509076
H	3.032508	1.217611	1.660473
H	-0.911613	-0.670142	-1.585513
H	-2.037926	-2.078179	1.181248
H	-0.707991	-2.489959	2.229015
H	-2.224743	-1.098437	3.495674
H	-2.311712	0.094302	2.214175
H	0.181682	-0.581518	3.821152
H	-0.784402	0.866824	4.018161
H	0.272952	1.267332	-2.101812
H	0.581890	3.706512	-2.050057
H	-0.932964	5.119530	-0.694789
H	-2.753377	4.059096	0.603602
H	-3.051764	1.634406	0.564154
H	0.153381	-1.844024	-0.007590
H	1.259386	1.218639	2.626760
H	-3.651892	-0.331429	-0.226996
H	-0.216224	1.669891	1.811792

H	4.110296	-0.133559	1.031103
H	2.762384	0.669073	1.835660
H	3.039634	-1.301864	3.234509
H	3.382394	-2.305467	1.828534
H	0.708904	-1.289689	2.770352
H	1.114401	-2.801762	1.959377
H	-2.048051	1.199680	-1.217995
H	-1.876679	-0.418107	-2.730038
H	-0.894692	-1.851135	-2.831065
H	-3.061422	-2.621384	-2.231699
H	-3.277772	-1.365879	-1.028066
H	-1.302505	-3.679888	-0.854196
H	-2.770674	-3.504850	0.088295
H	-0.383990	2.425452	-2.348569
H	1.545867	3.946300	-2.361301
H	2.718750	4.479494	-0.246804
H	1.925534	3.486005	1.873159
H	0.003845	1.977100	1.891977
H	0.355398	-0.088402	-1.628220
H	-0.793762	-2.824750	1.391189
H	-1.956193	1.145778	1.863081
H	-1.893581	-1.481005	1.175917

(3-4)$_{anti}$ $(si\text{-}si)_{60}$

E_0 = -1148.0212339
E_{0+ZPE} = -1147.612792
E_{298} = -1147.590974
H_{298} = -1147.590029
G_{298} = -1147.665098
NImag = 1 (-313.7967)

C	-0.536114	2.279550	-1.073018
C	-1.309428	1.887026	0.020849
C	-1.435704	2.769203	1.097590
C	-0.804600	4.000767	1.087320
C	-0.025770	4.374205	-0.001301
C	0.101969	3.510249	-1.079975
C	-2.034703	0.611815	0.064172
C	-2.403062	-0.027516	-1.105065
N	-3.468352	-0.893064	-1.147516
O	-3.752274	-1.411323	-2.236875
O	-4.133984	-1.128443	-0.132306
C	0.137568	-2.143560	-0.299785
C	0.387049	-0.895975	0.485779
C	-0.563772	-0.517156	1.431414
C	-1.419783	-1.547657	2.120481
C	-1.687482	-2.793242	1.292308
C	-0.435540	-3.252867	0.572438
N	1.450771	-0.149559	0.197682
C	1.900982	0.946822	1.051351
C	3.272789	1.315174	0.505500
C	3.217155	0.840727	-0.938424
C	2.430528	-0.461376	-0.835763
C	3.379664	-1.641321	-0.485367
O	3.373706	-2.062344	0.683420
O	4.075193	-2.024478	-1.446635
H	1.931079	-0.696587	-1.772098
H	4.194385	0.680842	-1.384037
H	2.671897	1.557840	-1.552230
H	3.471243	2.380435	0.599030
H	4.049314	0.776633	1.044618
H	1.211731	1.785503	0.984848
H	1.935628	0.617486	2.089297
H	-2.706586	0.483777	0.899533
H	-0.650112	-4.119777	-0.052327
H	0.320673	-3.564315	1.295483
H	-2.063980	-3.585910	1.940060
H	-2.472566	-2.585551	0.567510
H	-0.908822	-1.839176	3.044887
H	-2.364062	-1.101293	2.436803

(3-4)$_{anti}$ $(si\text{-}si)_{180}$

E_0 = -1148.0268314
E_{0+ZPE} = -1147.618417
E_{298} = -1147.596555
H_{298} = -1147.595610
G_{298} = -1147.670734
NImag = 1 (-331.6299)

C	1.962539	2.318920	0.326187
C	1.414904	1.409179	-0.582894
C	0.376608	1.845895	-1.407874
C	-0.106788	3.142810	-1.324526
C	0.442798	4.033157	-0.414093
C	1.481868	3.614824	0.408268
C	1.906962	0.035313	-0.738503
C	3.210228	-0.300750	-0.413433
N	3.742330	-1.492505	-0.830687
O	4.922858	-1.745995	-0.545032
O	3.050229	-2.289052	-1.479356
C	-0.872457	0.327844	1.760651
C	-0.583421	-0.605626	0.623755
C	0.631057	-1.291716	0.577828
C	1.452254	-1.491002	1.813825
C	1.274092	-0.388640	2.841227
C	-0.196948	-0.095742	3.055713
N	-1.477578	-0.687300	-0.356017
C	-1.369016	-1.647112	-1.447934
C	-2.692417	-1.528728	-2.187059
C	-3.141794	-0.110840	-1.872278
C	-2.729992	0.057497	-0.413330
C	-3.840853	-0.472613	0.536397
O	-3.637741	-1.544233	1.130430
O	-4.846111	0.263525	0.580125
H	-2.554881	1.102314	-0.169936
H	-4.207325	0.050153	-2.004018
H	-2.606740	0.604405	-2.498329
H	-2.581113	-1.719945	-3.251680
H	-3.408713	-2.243837	-1.787384
H	-0.529872	-1.388880	-2.094328
H	-1.192843	-2.647555	-1.055788
H	1.473436	-0.511892	-1.558309
H	-0.333099	0.689493	3.799207
H	-0.693823	-0.987509	3.443013
H	1.748315	-0.675602	3.780161
H	1.774825	0.517839	2.498313
H	1.193524	-2.455467	2.262714
H	2.505550	-1.571722	1.531180

(3-4)$_{anti}$ $(si\text{-}si)_{300}$

E_0 = -1148.0267495
E_{0+ZPE} = -1147.618001
E_{298} = -1147.596191
H_{298} = -1147.595247
G_{298} = -1147.670139
NImag = 1 (-310.7915)

C	-3.019683	-1.313253	-0.875636
C	-2.828865	-0.367029	0.134721
C	-3.902072	0.452608	0.485845
C	-5.131625	0.327073	-0.145385
C	-5.307969	-0.617362	-1.144627
C	-4.244592	-1.436241	-1.507513
C	-1.558446	-0.230434	0.862872
C	-0.826807	-1.353748	1.191367
N	0.129287	-1.320314	2.175887
O	0.699577	-2.379143	2.474678
O	0.385858	-0.262570	2.762842
C	1.439978	1.941511	0.606871
C	0.789091	0.901405	-0.262204
C	-0.516241	1.063014	-0.713765
C	-1.210043	2.392136	-0.639303
C	-0.673244	3.278693	0.470434
C	0.840649	3.324413	0.409737
N	1.464237	-0.217359	-0.510149
C	1.061272	-1.170520	-1.539214
C	2.212947	-2.165397	-1.609992
C	2.907364	-2.010739	-0.264753
C	2.793065	-0.513775	0.003589
C	3.942271	0.260323	-0.698864
O	3.666449	0.899133	-1.729590
O	5.048495	0.131558	-0.139617
H	2.833513	-0.296663	1.068472
H	3.943782	-2.335162	-0.270762
H	2.372943	-2.560908	0.509043
H	1.862917	-3.178468	-1.795468
H	2.891611	-1.891037	-2.414815
H	0.127010	-1.651087	-1.259186
H	0.902789	-0.649156	-2.483368
H	-1.495404	0.600328	1.548649
H	1.242231	3.996829	1.167570
H	1.151021	3.719391	-0.560161
H	-1.094386	4.280410	0.381195
H	-0.983301	2.891471	1.443884
H	-1.096551	2.912351	-1.596502
H	-2.284155	2.239594	-0.518983

H	-2.037665	2.480847	1.948404
H	-0.919552	4.670251	1.927574
H	0.471545	5.333287	-0.011104
H	0.700232	3.795875	-1.933231
H	-0.425263	1.625445	-1.924423
H	1.042578	-2.487691	-0.787491
H	-0.339318	0.351842	2.033744
H	-1.937121	0.115927	-2.061854
H	-0.583797	-1.893834	-1.088020

H	-0.046771	1.161579	-2.128628
H	-0.910813	3.457521	-1.974287
H	0.068551	5.044349	-0.346379
H	1.919304	4.301758	1.118552
H	2.769223	2.016603	0.977205
H	-1.944126	0.397419	1.915851
H	0.723716	-2.082553	-0.152457
H	3.875122	0.286053	0.192095
H	-0.526326	1.324133	1.469269

H	-3.775038	1.183903	1.271649
H	-5.950592	0.968712	0.146436
H	-6.262905	-0.715147	-1.640340
H	-4.370419	-2.171575	-2.289208
H	-2.200846	-1.949170	-1.180673
H	2.502375	1.970033	0.381567
H	-0.855381	0.404580	-1.499250
H	-0.959611	-2.324866	0.752242
H	1.338384	1.631457	1.646249

(3-4)*anti* $(si\text{-}re)_{60}$

E_0 = -1148.0231327
E_{0+ZPE} = -1147.614814
E_{298} = -1147.592829
H_{298} = -1147.591884
G_{298} = -1147.667929
NImag = 1 (-347.0578)

C	2.750103	-1.905271	-0.487348
C	2.756996	-0.519714	-0.310665
C	3.878536	0.064483	0.283425
C	4.950211	-0.715099	0.690857
C	4.928883	-2.090320	0.507404
C	3.823759	-2.683076	-0.089100
C	1.609639	0.263999	-0.790694
C	1.759928	1.593025	-1.133815
N	0.820706	2.228070	-1.906841
O	1.007140	3.420461	-2.191719
O	-0.174651	1.614904	-2.310863
C	-1.569209	1.575881	0.796893
C	-0.947078	0.217094	0.640132
C	0.348224	-0.020007	1.103294
C	0.994143	0.899910	2.101023
C	0.465521	2.322796	2.040276
C	-1.048510	2.319992	2.015743
N	-1.656386	-0.717389	0.014489
C	-1.222164	-2.100807	-0.101347
C	-2.396300	-2.811294	-0.756049
C	-3.082584	-1.699071	-1.533417
C	-2.962872	-0.504502	-0.591967
C	-4.142213	-0.481561	0.419311
O	-3.916493	-0.856327	1.582666
O	-5.218867	-0.094689	-0.075819
H	-2.969982	0.432579	-1.142609
H	-4.118961	-1.911693	-1.778726
H	-2.544730	-1.496159	-2.460183
H	-2.072222	-3.638696	-1.383117
H	-3.066852	-3.203842	0.005696
H	-0.328448	-2.162104	-0.723089
H	-0.975992	-2.505648	0.879983
H	0.859771	-0.282275	-1.340248
H	-1.440315	3.336757	2.004105
H	-1.430242	1.843171	2.921026
H	0.837606	2.891968	2.892785
H	0.836186	2.818254	1.141471
H	0.833001	0.503886	3.109415
H	2.076954	0.894610	1.959132
H	3.925982	1.133311	0.428279
H	5.807058	-0.243727	1.150385
H	5.766938	-2.694670	0.823137
H	3.798131	-3.752065	-0.244313
H	1.892932	-2.374121	-0.949558
H	-2.647899	1.474592	0.866708
H	0.657722	-1.052859	1.164851
H	2.569155	2.229223	-0.829593
H	-1.363147	2.151201	-0.106921

(3-4)*anti* $(si\text{-}re)_{180}$

E_0 = -1148.0236979
E_{0+ZPE} = -1147.615220
E_{298} = -1147.593411
H_{298} = -1147.592467
G_{298} = -1147.667354
NImag = 1 (-309.8510)

C	-0.484217	2.206449	-1.229349
C	-1.350229	1.741755	-0.239829
C	-1.644065	2.581226	0.838777
C	-1.077743	3.839876	0.926557
C	-0.213096	4.292351	-0.065111
C	0.076431	3.473218	-1.145372
C	-1.954394	0.413372	-0.396218
C	-3.242720	0.168348	0.032093
N	-4.003731	-0.837783	-0.518039
O	-5.149287	-1.005580	-0.077717
O	-3.564124	-1.526427	-1.445561
C	0.589125	-2.178935	-0.629985
C	0.556563	-0.957844	0.244344
C	-0.560403	-0.730915	1.049555
C	-1.426431	-1.869536	1.497383
C	-1.441384	-3.052228	0.542981
C	-0.042619	-3.378538	0.062090
N	1.579216	-0.109593	0.182181
C	1.777516	0.969024	1.146573
C	3.175960	1.489714	0.850967
C	3.389106	1.114566	-0.607373
C	2.731262	-0.257958	-0.699754
C	3.735385	-1.362145	-0.265912
O	3.621519	-1.831638	0.878667
O	4.581650	-1.637179	-1.138967
H	2.404117	-0.475426	-1.713247
H	4.434316	1.075246	-0.899862
H	2.874809	1.820348	-1.259879
H	3.255504	2.558540	1.034867
H	3.906170	0.980111	1.475919
H	1.029502	1.745223	1.003808
H	1.676299	0.581782	2.159818
H	-1.631428	-0.146756	-1.259907
H	-0.059247	-4.219212	-0.631412
H	0.586382	-3.675134	0.904035
H	-1.886905	-3.915782	1.038089
H	-2.068626	-2.818137	-0.316968
H	-1.079348	-2.202783	2.481485
H	-2.445922	-1.504412	1.654906
H	-2.304680	2.242285	1.623446
H	-1.308664	4.472324	1.771838
H	0.226945	5.276572	0.005459
H	0.741350	3.817479	-1.924428
H	-0.256378	1.572666	-2.074803
H	1.608967	-2.417226	-0.910778
H	-0.501122	0.093227	1.746350
H	-3.759930	0.726493	0.790638
H	0.047133	-1.960001	-1.554257

(3-4)*anti* $(si\text{-}re)_{300}$

E_0 = -1148.0243126
E_{0+ZPE} = -1147.615553
E_{298} = -1147.593790
H_{298} = -1147.592846
G_{298} = -1147.667708
NImag = 1 (-312.9718)

C	-3.747937	0.353030	0.328439
C	-2.527780	0.512280	-0.331557
C	-2.373086	-0.073207	-1.591255
C	-3.398752	-0.809408	-2.158932
C	-4.603874	-0.970255	-1.486083
C	-4.776517	-0.380692	-0.242252
C	-1.487961	1.339089	0.290676
C	-0.673483	2.132582	-0.496658
N	0.016616	3.181851	0.046253
O	0.663367	3.922337	-0.708840
O	-0.003675	3.372048	1.271336
C	0.186684	-1.987621	-0.043475
C	0.561353	-0.682813	0.594939
C	-0.273879	-0.117685	1.553465
C	-1.279497	-0.944101	2.305253
C	-1.704116	-2.214416	1.583447
C	-0.513731	-2.904957	0.949332
N	1.667039	-0.066178	0.184641
C	2.344670	0.963853	0.970316
C	3.639809	1.231893	0.212097
C	3.350251	0.724367	-1.192872
C	2.491001	-0.507440	-0.933036
C	3.386660	-1.740672	-0.631606
O	3.517177	-2.085935	0.555148
O	3.902286	-2.244566	-1.648602
H	1.863338	-0.746351	-1.787678
H	4.244114	0.478172	-1.758637
H	2.779255	1.463658	-1.754606
H	3.909320	2.285059	0.235727
H	4.455659	0.661745	0.650697
H	1.736045	1.859013	1.058835
H	2.523489	0.588721	1.977679
H	-1.730488	1.730451	1.266491
H	-0.826647	-3.813630	0.435379
H	0.198602	-3.206408	1.719853
H	-2.204454	-2.882713	2.285043
H	-2.428319	-1.976466	0.804850
H	-0.844713	-1.212465	3.273821
H	-2.157398	-0.338297	2.542052
H	-1.444565	0.041707	-2.131166
H	-3.257861	-1.260009	-3.130967
H	-5.402552	-1.544974	-1.932248
H	-5.713536	-0.489390	0.284846
H	-3.893434	0.820301	1.292020
H	1.074366	-2.479133	-0.427548
H	0.116778	0.729906	2.098381
H	-0.543911	2.026520	-1.557483
H	-0.470797	-1.799157	-0.895363

(3-4)*anti* $(re\text{-}si)_{60}$

E_0 = -1148.0204726
E_{0+ZPE} = -1147.611826

(3-4)*anti* $(re\text{-}si)_{180}$

E_0 = -1148.0203706
E_{0+ZPE} = -1147.612009

(3-4)*anti* $(re\text{-}si)_{300}$

E_0 = -1148.0228163
E_{0+ZPE} = -1147.614551

E_{298} = -1147.589950
H_{298} = -1147.589005
G_{298} = -1147.663788
NImag = 1 (-298.3973)

C	-3.523246	0.686011	-0.951994
C	-2.451327	0.829207	-0.068563
C	-2.678682	0.606024	1.292231
C	-3.932106	0.234179	1.747786
C	-4.987398	0.083830	0.856254
C	-4.778987	0.316879	-0.495325
C	-1.155399	1.268974	-0.595161
C	-0.341193	2.098671	0.149709
N	0.656058	2.820789	-0.454635
O	1.303046	3.623224	0.232717
O	0.893304	2.663964	-1.658979
C	-0.066837	-0.674673	-1.128137
C	0.392966	-1.068019	0.122254
C	-0.381476	-2.087777	0.907628
C	-1.053046	-3.109271	0.001368
C	-1.901193	-2.424867	-1.050557
C	-1.053133	-1.497723	-1.906424
N	1.473123	-0.518681	0.682883
C	1.904635	-0.797744	2.050781
C	3.260716	-0.111021	2.186818
C	3.313521	0.858207	1.015439
C	2.539087	0.127462	-0.073415
C	3.437808	-0.891178	-0.827364
O	3.315977	-2.095671	-0.541029
O	4.221819	-0.365084	-1.641209
H	2.142833	0.824305	-0.803159
H	4.324581	1.094964	0.697287
H	2.806498	1.791124	1.258666
H	3.367940	0.382483	3.150190
H	4.056201	-0.847894	2.099601
H	1.171408	-0.403813	2.754802
H	1.996085	-1.867941	2.221565
H	-1.110323	1.397131	-1.665716
H	-1.696940	-0.842651	-2.498115
H	-0.497394	-2.093775	-2.637947
H	-2.393585	-3.162035	-1.685492
H	-2.689140	-1.858602	-0.553963
H	-0.286204	-3.720674	-0.478199
H	-1.660073	-3.780327	0.609254
H	-1.871151	0.718684	2.000591
H	-4.087221	0.061028	2.803115
H	-5.964389	-0.206680	1.214516
H	-5.594680	0.213737	-1.196423
H	-3.370252	0.877691	-2.004482
H	0.604507	-0.086074	-1.735249
H	0.276362	-2.599584	1.603497
H	-0.433001	2.279515	1.204555
H	-1.137741	-1.579845	1.511402

E_{298} = -1147.589942
H_{298} = -1147.588997
G_{298} = -1147.665264
NImag = 1 (-290.6555)

C	-0.216575	2.272344	-1.309594
C	0.572632	1.954896	-0.204471
C	0.376472	2.663804	0.983882
C	-0.584645	3.654869	1.061287
C	-1.363060	3.967200	-0.048463
C	-1.171992	3.275659	-1.234290
C	1.617956	0.935580	-0.352805
C	2.841968	1.097372	0.259007
N	3.969048	0.464473	-0.214484
O	5.034549	0.646048	0.389117
O	3.916731	-0.239252	-1.229575
C	0.525956	-0.784629	0.785783
C	-0.163221	-1.392138	-0.261134
C	0.528916	-2.466847	-1.052137
C	1.388943	-3.350073	-0.158845
C	2.377081	-2.515174	0.628667
C	1.656219	-1.481975	1.479198
N	-1.395998	-1.031309	-0.620970
C	-2.128823	-1.601614	-1.749953
C	-3.548552	-1.076075	-1.591936
C	-3.378763	0.185153	-0.762290
C	-2.253567	-0.181326	0.197335
C	-2.808635	-0.897715	1.459262
O	-2.762870	-2.139346	1.490534
O	-3.284634	-0.118175	2.308359
H	-1.717840	0.704596	0.518770
H	-4.278875	0.480092	-0.230535
H	-3.068407	1.017655	-1.393486
H	-4.022277	-0.896754	-2.554471
H	-4.149723	-1.801162	-1.048073
H	-1.678523	-1.274249	-2.688471
H	-2.109706	-2.688170	-1.726650
H	1.624874	0.399974	-1.289104
H	2.371587	-0.736772	1.840108
H	1.257262	-1.966656	2.376564
H	2.992464	-3.149991	1.266869
H	3.046952	-2.015497	-0.069911
H	0.741174	-3.906537	0.521802
H	1.907990	-4.083416	-0.776324
H	0.963834	2.424272	1.858581
H	-0.733222	4.184173	1.991429
H	-2.113310	4.741938	0.015667
H	-1.769605	3.512907	-2.102847
H	-0.070900	1.735587	-2.236633
H	-0.036153	-0.114911	1.418852
H	-0.192109	-3.077420	-1.584635
H	3.027924	1.720545	1.114327
H	1.155194	-1.992416	-1.812151

E_{298} = -1147.592485
H_{298} = -1147.591541
G_{298} = -1147.667729
NImag = 1 (-301.0305)

C	-2.205274	-1.843169	-0.929547
C	-2.377743	-0.504696	-0.567943
C	-3.603915	-0.119807	-0.020106
C	-4.621449	-1.044579	0.155997
C	-4.437133	-2.369705	-0.212472
C	-3.222852	-2.765573	-0.758340
C	-1.283912	0.442119	-0.814022
C	-1.520098	1.797313	-0.934366
N	-0.619543	2.623625	-1.559516
O	-0.915949	3.822591	-1.681102
O	0.445414	2.175567	-2.003105
C	-0.104739	-0.171711	1.108371
C	1.057576	0.536158	0.818629
C	1.214141	1.929801	1.352843
C	0.525952	2.129637	2.693878
C	-0.916742	1.671655	2.633545
C	-0.985636	0.200141	2.265245
N	2.012656	0.054743	0.025187
C	3.130797	0.841217	-0.474951
C	3.966327	-0.155608	-1.260688
C	2.948965	-1.189177	-1.713201
C	1.999934	-1.292287	-0.520973
C	2.465178	-2.384516	0.478581
O	3.148348	-2.027726	1.453070
O	2.118816	-3.538923	0.155664
H	0.999654	-1.556692	-0.851743
H	3.387713	-2.151301	-1.963345
H	2.407203	-0.825994	-2.586841
H	4.491499	0.319249	-2.086255
H	4.703144	-0.618067	-0.607061
H	2.746735	1.643377	-1.110289
H	3.698883	1.287794	0.337992
H	-0.447079	0.060872	-1.377677
H	-2.016213	-0.088307	2.049399
H	-0.693537	-0.400145	3.133880
H	-1.414752	1.839130	3.589018
H	-1.448334	2.267604	1.889807
H	1.058735	1.565346	3.462158
H	0.589130	3.181839	2.971302
H	-3.772940	0.906737	0.268800
H	-5.562387	-0.726688	0.581618
H	-5.232028	-3.088341	-0.074995
H	-3.066863	-3.794380	-1.048992
H	-1.260789	-2.161302	-1.348814
H	-0.125090	-1.218643	0.845454
H	2.266321	2.184842	1.438193
H	-2.399202	2.308661	-0.590256
H	0.789105	2.620483	0.619852

Oxazolidinone Pathway *syn*-addition

(3-4)$_{syn}$ (*re-re*)$_{180}$

E_0 = -1148.0257813
E_{0+ZPE} = -1147.616939
E_{298} = -1147.595257
H_{298} = -1147.594313
G_{298} = -1147.668525
NImag = 1 (-349.7389)

C	3.309025	-0.646983	-0.464580
C	1.973511	-0.410457	-0.803392
C	1.235738	-1.445842	-1.383365
C	1.821217	-2.680516	-1.619351
C	3.146477	-2.906945	-1.274335
C	3.886986	-1.884574	-0.694633
C	1.329856	0.896081	-0.623270

(3-4)$_{syn}$ (*re-re*)$_{300}$

E_0 = -1148.0181618
E_{0+ZPE} = -1147.609761
E_{298} = -1147.588045
H_{298} = -1147.587101
G_{298} = -1147.661816
NImag = 1 (-340.0828)

C	0.913444	1.911806	0.962323
C	-0.174606	2.134671	0.115859
C	-0.150796	3.242159	-0.735081
C	0.928058	4.111471	-0.740121
C	2.004527	3.886008	0.108106
C	1.990646	2.784358	0.954109
C	-1.371421	1.280836	0.126634

(3-4)$_{syn}$ (*si-si*)$_{60}$

E_0 = -1148.0031643
E_{0+ZPE} = -1147.594299
E_{298} = -1147.572891
H_{298} = -1147.571947
G_{298} = -1147.644789
NImag = 1 (-314.2345)

C	0.195898	2.061446	-1.257813
C	-0.375459	1.955614	0.011418
C	0.111314	2.772105	1.032996
C	1.109767	3.699908	0.785718
C	1.652132	3.812506	-0.485606
C	1.199234	2.981880	-1.501233
C	-1.549295	1.122002	0.290638

C	2.098432	2.039710	-0.479651
N	1.543322	3.285051	-0.584613
O	2.268113	4.273917	-0.391990
O	0.343525	3.413795	-0.869037
C	0.265591	0.720627	1.361935
C	-0.818575	-0.133046	1.140501
C	-0.705065	-1.583196	1.506426
C	0.161348	-1.796079	2.738585
C	1.512370	-1.133931	2.564293
C	1.354494	0.360876	2.334352
N	-1.950310	0.295755	0.585156
C	-2.195613	1.702809	0.290532
C	-3.489169	1.698369	-0.501862
C	-4.212939	0.474237	0.030580
C	-3.089658	-0.542011	0.225906
C	-2.880054	-1.404491	-1.044994
O	-1.908613	-1.138424	-1.775534
O	-3.750596	-2.280768	-1.204307
H	-3.334929	-1.220693	1.038033
H	-4.980868	0.092077	-0.635543
H	-4.677803	0.701272	0.990764
H	-4.048875	2.621481	-0.370277
H	-3.275487	1.579353	-1.562627
H	-2.305394	2.250111	1.231204
H	-1.365535	2.147363	-0.252369
H	0.367634	1.005332	-1.097631
H	2.300834	0.792960	1.996132
H	1.143199	0.846478	3.293047
H	2.141225	-1.306359	3.438388
H	2.018949	-1.591020	1.714653
H	-0.345309	-1.385462	3.615211
H	0.275402	-2.866003	2.912060
H	0.193375	-1.281427	-1.634766
H	1.236656	-3.468083	-2.073422
H	3.601129	-3.869979	-1.457856
H	4.920252	-2.050013	-0.424568
H	3.907744	0.132311	-0.018005
H	0.059979	1.778238	1.286879
H	-1.688710	-2.012827	1.667408
H	3.137418	2.058693	-0.210573
H	-0.275238	-2.115433	0.654919

C	-1.745295	0.612444	1.279791
N	-3.056160	0.294078	1.526414
O	-3.326336	-0.289159	2.586876
O	-3.948783	0.602080	0.722834
C	-0.805658	-0.043121	-1.640855
C	-0.140985	-1.062610	-0.957393
C	-0.973229	-2.142544	-0.348550
C	-2.109867	-2.571681	-1.267087
C	-2.963574	-1.385712	-1.670156
C	-2.120781	-0.307007	-2.328190
N	1.179045	-1.065090	-0.777863
C	2.064999	-0.138274	-1.479558
C	3.440735	-0.451595	-0.925479
C	3.345156	-1.929885	-0.594293
C	1.932765	-2.074417	-0.036998
C	1.878487	-1.937266	1.509483
O	1.132135	-1.070920	1.997241
O	2.597042	-2.761657	2.105652
H	1.548015	-3.067018	-0.261354
H	4.080702	-2.271939	0.126330
H	3.451805	-2.523716	-1.503027
H	4.228945	-0.215226	-1.636480
H	3.618100	0.127461	-0.019667
H	2.010934	-0.336082	-2.553786
H	1.777250	0.893782	-1.310724
H	-2.185359	1.619900	-0.497170
H	-2.694266	0.618790	-2.407068
H	-1.906562	-0.603802	-3.361412
H	-3.753086	-1.700670	-2.353955
H	-3.453999	-0.973570	-0.789153
H	-1.694650	-3.054196	-2.155544
H	-2.714044	-3.320815	-0.755716
H	-0.990550	3.424316	-1.392243
H	0.926201	4.966721	-1.400909
H	2.846458	4.563601	0.109743
H	2.828888	2.598559	1.610855
H	0.940079	1.025473	1.582516
H	-0.194102	0.697859	-2.134687
H	-0.373622	-2.999213	-0.061907
H	-1.065333	0.295356	2.048614
H	-1.380081	-1.729078	0.580783

C	-2.500746	0.931038	-0.693857
N	-3.819494	0.688227	-0.391439
O	-4.615762	0.568537	-1.333390
O	-4.199070	0.614679	0.782035
C	-1.063478	-2.075398	-0.954477
C	-0.066603	-1.400086	-0.065825
C	-0.562448	-0.805282	1.090474
C	-1.714959	-1.445241	1.830133
C	-2.663276	-2.258510	0.960369
C	-1.931419	-3.020425	-0.126883
N	1.236517	-1.402565	-0.385969
C	1.755188	-1.944996	-1.643476
C	3.245103	-2.114480	-1.402329
C	3.319265	-2.327992	0.100140
C	2.288827	-1.335441	0.638815
C	2.973641	0.033328	0.868063
O	3.384353	0.634118	-0.139923
O	3.122272	0.345068	2.067872
H	1.862422	-1.661499	1.582666
H	4.310636	-2.151620	0.510883
H	3.020200	-3.345997	0.355969
H	3.649647	-2.946050	-1.975682
H	3.774427	-1.203254	-1.662850
H	1.302697	-2.914308	-1.850583
H	1.530487	-1.280845	-2.476084
H	-1.923848	1.168292	1.301811
H	-2.643641	-3.521813	-0.782591
H	-1.301077	-3.798489	0.309613
H	-3.228775	-2.947060	1.589500
H	-3.393999	-1.598183	0.500297
H	-1.278245	-2.105005	2.588029
H	-2.279021	-0.695987	2.385502
H	-0.314611	2.691411	2.023540
H	1.466871	4.330005	1.587463
H	2.435970	4.529997	-0.680386
H	1.635657	3.047957	-2.487422
H	-0.147762	1.427914	-2.062611
H	-0.595038	-2.609603	-1.772653
H	0.156032	-0.303369	1.725931
H	-2.323557	1.043068	-1.747351
H	-1.705094	-1.306273	-1.397461

(3-4)$_{syn}$ $(si\text{-}si)_{180}$

E_0 = -1148.0214368
E_{0+ZPE} = -1147.612168
E_{298} = -1147.590723
H_{298} = -1147.589779
G_{298} = -1147.662828
NImag = 1 (-353.4562)

C	-2.643602	-1.532125	-0.700298
C	-1.478653	-0.823629	-1.006932
C	-0.454542	-1.490381	-1.684157
C	-0.593596	-2.822915	-2.043381
C	-1.755031	-3.516747	-1.733346
C	-2.779354	-2.863744	-1.059578
C	-1.291662	0.605340	-0.691764
C	-2.410487	1.411820	-0.515533
N	-2.308321	2.774247	-0.479227
O	-3.349876	3.441680	-0.345004
O	-1.202540	3.321571	-0.573836
C	0.165828	-1.617129	1.810578
C	0.667581	-0.342764	1.194460
C	-0.167145	0.778819	1.185184
C	-1.215437	0.945977	2.246595
C	-1.805657	-0.366240	2.728128
C	-0.708550	-1.365486	3.032022
N	1.881164	-0.347424	0.645518
C	2.721776	-1.542098	0.545742
C	4.021931	-1.033856	-0.050869

(3-4)$_{syn}$ $(si\text{-}si)_{300}$

E_0 = -1148.0167429
E_{0+ZPE} = -1147.607740
E_{298} = -1147.586264
H_{298} = -1147.585320
G_{298} = -1147.658285
NImag = 1 (-340.4886)

C	-2.493722	-1.545946	-0.314464
C	-2.380068	-0.364536	0.421123
C	-3.536094	0.360834	0.712040
C	-4.781290	-0.088617	0.295987
C	-4.886799	-1.267807	-0.426553
C	-3.738215	-1.988866	-0.732229
C	-1.088901	0.126869	0.935617
C	-0.209812	-0.757202	1.540508
N	0.719910	-0.309170	2.440631
O	1.382548	-1.136655	3.081219
O	0.871155	0.909478	2.632194
C	1.181486	2.632460	0.008639
C	0.948711	1.244809	-0.524490
C	-0.304268	0.884955	-1.001417
C	-1.286792	1.927921	-1.455404
C	-1.137344	3.249410	-0.722587
C	0.318438	3.671167	-0.693174
N	1.940302	0.346266	-0.457123
C	3.191969	0.600864	0.251340
C	4.052111	-0.601774	-0.080249

(3-4)$_{syn}$ $(si\text{-}re)_{60}$

E_0 = -1148.0205551
E_{0+ZPE} = -1147.611731
E_{298} = -1147.590099
H_{298} = -1147.589155
G_{298} = -1147.662709
NImag = 1 (-344.8445)

C	-2.233871	1.758860	-0.504187
C	-2.249112	0.365115	-0.405145
C	-3.434836	-0.262240	-0.014421
C	-4.569313	0.482574	0.269213
C	-4.542961	1.866624	0.164723
C	-3.370555	2.500564	-0.225147
C	-1.023653	-0.375575	-0.757463
C	-1.128386	-1.679121	-1.233682
N	-0.144495	-2.246666	-1.992339
O	-0.334069	-3.394200	-2.439709
O	0.903254	-1.630683	-2.236227
C	1.456528	-2.102527	0.961388
C	1.181959	-0.631253	0.881193
C	-0.081644	-0.167476	1.247594
C	-0.927639	-0.931406	2.228767
C	-0.680358	-2.430631	2.212088
C	0.805192	-2.729633	2.187032
N	2.138262	0.179381	0.435868
C	3.322901	-0.289031	-0.272380
C	4.011913	0.993098	-0.701175

C	4.075519	0.399077	0.450084
C	2.629127	0.856271	0.282793
C	2.412510	1.390733	-1.154617
O	1.737096	0.701266	-1.942195
O	2.987586	2.471072	-1.374252
H	2.377053	1.655457	0.975869
H	4.757553	1.036154	-0.103883
H	4.358619	0.420378	1.503540
H	4.870419	-1.637012	0.263425
H	3.975037	-1.050479	-1.138169
H	2.905175	-1.954602	1.538833
H	2.240508	-2.307646	-0.058347
H	-0.420289	1.045918	-1.152975
H	-1.128302	-2.314188	3.366819
H	-0.087106	-0.990367	3.848479
H	-2.421965	-0.195825	3.611339
H	-2.460798	-0.777242	1.959438
H	-0.779039	1.484118	3.094555
H	-2.007601	1.593151	1.863152
H	0.448479	-0.937082	-1.912393
H	0.207813	-3.319286	-2.572827
H	-1.864438	-4.554228	-2.015644
H	-3.690103	-3.392158	-0.815400
H	-3.456076	-1.049173	-0.178139
H	0.994260	-2.263026	2.083931
H	0.267720	1.708413	0.846484
H	-3.409969	1.055325	-0.352101
H	-0.408322	-2.154612	1.051613

C	3.594116	-0.948763	-1.486246
C	2.082591	-0.767792	-1.419404
C	1.349369	-2.090297	-1.052949
O	0.249914	-2.259104	-1.625025
O	1.929627	-2.873327	-0.285211
H	1.666392	-0.430311	-2.366464
H	3.862925	-1.957470	-1.785728
H	4.018699	-0.245431	-2.205072
H	5.112707	-0.368427	-0.013990
H	3.824613	-1.429853	0.585378
H	3.663406	1.510923	-0.124498
H	2.999159	0.731809	1.315048
H	-1.114310	1.118115	1.363553
H	0.435137	4.629205	-0.186003
H	0.673890	3.811187	-1.716791
H	-1.748474	4.013699	-1.203599
H	-1.504832	3.153049	0.301470
H	-1.149072	2.096697	-2.528703
H	-2.302676	1.547173	-1.350439
H	-3.458953	1.278626	1.278753
H	-5.666118	0.483819	0.535741
H	-5.854098	-1.619491	-0.756115
H	-3.811709	-2.901271	-1.307280
H	-1.597170	-2.084929	-0.596514
H	2.229776	2.900674	-0.097561
H	-0.384718	-0.093243	-1.460366
H	-0.204775	-1.820858	1.395254
H	0.969849	2.627359	1.077441

C	3.632324	1.963878	0.405613
C	2.166438	1.619850	0.677669
C	1.248333	2.497897	-0.202306
O	0.929078	2.071325	-1.327273
O	0.950131	3.591490	0.316161
H	1.894227	1.804245	1.715227
H	3.757794	3.008078	0.131967
H	4.231794	1.772499	1.296686
H	5.086234	0.861848	-0.808659
H	3.605794	1.333766	-1.651002
H	3.967807	-0.864251	0.395936
H	3.027316	-0.925515	-1.104237
H	-0.223059	0.230690	-1.164872
H	0.982136	-3.805080	2.171388
H	1.278386	-2.343658	3.092845
H	-1.150972	-2.891968	3.080798
H	-1.142743	-2.872957	1.328897
H	-0.720889	-0.546011	3.233039
H	-1.982492	-0.718544	2.050364
H	-3.481783	-1.338176	0.067551
H	-5.477180	-0.020963	0.569867
H	-5.429155	2.445276	0.383285
H	-3.339188	3.577262	-0.313622
H	-1.317422	2.248057	-0.808619
H	2.526413	-2.290543	0.963959
H	-0.214322	0.905283	1.274837
H	-1.979089	-2.319886	-1.096176
H	1.057314	-2.579317	0.065987

(3-4)$_{syn}$ (*si-re*)$_{300}$

E_0 = -1148.0156059
E_{0+ZPE} = -1147.606520
E_{298} = -1147.585046
H_{298} = -1147.584102
G_{298} = -1147.656939
NImag = 1 (-376.4372)

C	-3.100092	-0.419256	-0.836168
C	-1.785578	0.027291	-0.979975
C	-0.949084	-0.619184	-1.891853
C	-1.428456	-1.685166	-2.638282
C	-2.740851	-2.118971	-2.496007
C	-3.577449	-1.480120	-1.591733
C	-1.340284	1.191467	-0.196629
C	-0.619399	2.196356	-0.822752
N	-0.470649	3.411966	-0.213700
O	0.107844	4.320874	-0.826990
O	-0.918612	3.591646	0.930691
C	-0.646199	-1.958648	1.477467
C	0.284058	-0.817051	1.176292
C	-0.117455	0.479461	1.508380
C	-1.060694	0.702238	2.664680
C	-2.089754	-0.401855	2.818016
C	-1.417667	-1.758771	2.775219
N	1.435734	-1.094050	0.560741
C	1.830547	-2.443337	0.149869
C	3.273327	-2.296916	-0.303198
C	3.758722	-1.103877	0.502321
C	2.557151	-0.161625	0.446073
C	2.631945	0.661375	-0.863277
O	2.045260	0.209473	-1.866235
O	3.350996	1.672494	-0.783098
H	2.541589	0.525916	1.286535
H	4.655292	-0.640509	0.100488
H	3.955822	-1.395221	1.535242
H	3.843814	-3.204383	-0.118718
H	3.314719	-2.068705	-1.365028
H	1.776497	-3.122608	1.000985
H	1.173346	-2.821130	-0.630304
H	-2.027967	1.519675	0.568849

(3-4)$_{syn}$ (*re-si*)$_{60}$

E_0 = -1148.0219491
E_{0+ZPE} = -1147.613068
E_{298} = -1147.591426
H_{298} = -1147.590482
G_{298} = -1147.664415
NImag = 1 (-349.8379)

C	3.440813	0.962604	-0.129915
C	2.126256	0.719523	-0.531624
C	1.888568	-0.236939	-1.522532
C	2.946321	-0.932005	-2.086096
C	4.252353	-0.684956	-1.679164
C	4.496661	0.267273	-0.699870
C	1.046977	1.525142	0.051423
C	0.008728	1.964686	-0.750360
N	-0.782661	3.002425	-0.347285
O	-1.659213	3.418429	-1.119490
O	-0.631098	3.503599	0.780321
C	0.280116	0.278935	1.759307
C	-0.468068	-0.715005	1.129531
C	0.155228	-2.057170	0.877713
C	1.120971	-2.451038	1.985517
C	2.162485	-1.372866	2.199092
C	1.504298	-0.053029	2.570127
N	-1.718606	-0.506394	0.716226
C	-2.526462	0.629477	1.152176
C	-3.728982	0.584418	0.235181
C	-3.938016	-0.906858	0.042753
C	-2.517178	-1.469935	-0.041122
C	-2.067428	-1.700571	-1.508100
O	-1.190379	-0.960074	-1.984844
O	-2.667442	-2.641545	-2.062249
H	-2.484786	-2.444790	0.440844
H	-4.512560	-1.161477	-0.842479
H	-4.452972	-1.323449	0.908958
H	-4.590490	1.089231	0.665953
H	-3.488822	1.065215	-0.711543
H	-2.820943	0.474614	2.195505
H	-1.986275	1.565783	1.100771
H	1.344439	2.192782	0.846266

(3-4)$_{syn}$ (*re-si*)$_{180}$

E_0 = -1148.0209693
E_{0+ZPE} = -1147.612587
E_{298} = -1147.590664
H_{298} = -1147.589720
G_{298} = -1147.665899
NImag = 1 (-342.8930)

N	1.537915	-0.871009	-0.746956
C	2.071763	0.283338	-1.467423
C	3.485698	0.431436	-0.938724
C	3.865586	-0.991001	-0.567566
C	2.576002	-1.554936	0.017418
C	2.472005	-1.349747	1.554416
O	1.503721	-0.704525	1.992674
C	0.259078	-1.230907	-0.807302
C	-0.721360	-0.426029	-1.393454
C	-1.189343	-3.237311	-1.091052
O	3.393947	-1.892992	2.191351
C	-1.350841	0.727559	0.454566
H	2.528934	-2.627850	-0.151771
H	4.677332	-1.059658	0.149254
H	4.147081	-1.549055	-1.461335
H	4.149672	0.880698	-1.673421
H	3.485938	1.064270	-0.052039
H	2.062309	0.067629	-2.539008
H	1.474865	1.171526	-1.294882
H	-0.860955	0.039417	1.126556
C	-0.159558	-2.542029	-0.210127
C	-1.993586	-1.016327	-1.927733
H	-2.806652	-0.294756	-1.803604
H	-1.879017	-1.149067	-3.008897
C	-2.395081	-2.344702	-1.302979
H	-3.132654	-2.836944	-1.937731
H	-2.865481	-2.175442	-0.336349
H	-0.734019	-3.495085	-2.050739
H	-1.485640	-4.174577	-0.620098
C	-0.613639	1.976611	0.196306
C	0.552565	2.223304	0.921793
C	1.243460	3.415775	0.758353
C	0.790579	4.370636	-0.140329

H	-2.150455	-2.559483	2.876212	H	2.232079	0.758703	2.492785	C	-0.364812	4.127311	-0.874994
H	-0.731574	-1.851459	3.620238	H	1.219936	-0.083934	3.627489	C	-1.063644	2.944308	-0.705063
H	-2.634901	-0.274980	3.753766	H	2.864069	-1.664404	2.981496	H	0.921270	1.455524	1.589770
H	-2.824921	-0.340419	2.014411	H	2.740747	-1.258162	1.282777	H	2.142315	3.594647	1.331569
H	-0.475999	0.774229	3.588493	H	0.564191	-2.620753	2.910196	H	1.331568	5.297002	-0.270936
H	-1.547317	1.670487	2.549224	H	1.594580	-3.397210	1.724004	H	-0.722305	4.863697	-1.580795
H	0.085574	-0.306538	-1.985669	H	0.870519	-0.450486	-1.826821	H	-1.956717	2.767636	-1.287792
H	-0.770283	-2.181366	-3.338003	H	2.749235	-1.673365	-2.847672	H	-0.378843	0.441274	-1.937787
H	-3.107673	-2.947694	-3.084866	H	5.072809	-1.228878	-2.125148	H	0.696770	-3.189228	-0.055335
H	-4.601509	-1.804956	-1.474071	H	5.508902	0.472195	-0.381423	H	-0.585793	-2.344200	0.773584
H	-3.757806	0.078713	-0.137178	H	3.636305	1.712058	0.624272	C	-2.734025	0.764329	0.483357
H	-0.103854	-2.897222	1.522555	H	-0.257734	1.149494	2.106101	H	-3.335849	1.529466	0.028625
H	0.609257	1.265942	1.370956	H	-0.612713	-2.817443	0.774435	N	-3.468881	-0.186150	1.144946
H	-0.091875	2.088756	-1.751903	H	-0.277100	1.519328	-1.684620	O	-2.910585	-1.118899	1.734540
H	-1.346009	-2.048808	0.642901	H	0.678678	-2.020667	-0.078857	O	-4.704890	-0.071899	1.146493

Optimized Goemetries in solven phase with **enaime-DBU (lowest energy)** carboxylate Pathway

(3-4)$_{\textbf{DBU-}\textit{anti}}$ (*re-re*)$_{60}$

E_0 = -1610.5785535
E_{0+ZPE} = -1609.901588
E_{298} = -1609.868146
H_{298} = -1609.867201
G_{298} = -1609.971049
NImag = 1 (-315.4675)

N	-5.757593	-0.037396	0.781615
C	-6.152658	-1.245690	1.499694
C	-4.944349	-1.983455	2.028951
C	-3.943287	-2.181030	0.916710
N	-3.687942	-0.912466	0.270528
C	-4.557630	0.061683	0.227942
C	-4.158011	1.306074	-0.500327
C	-4.924341	1.532873	-1.804092
C	-6.320199	2.101280	-1.618100
C	-7.248429	1.248017	-0.770806
C	-6.758208	1.017160	0.649758
O	-1.314090	-0.502414	-0.844113
C	-0.430439	-1.290330	-0.402415
O	-0.582297	-2.150924	0.469739
C	0.935808	-1.129767	-1.093339
N	2.022680	-1.765456	-0.363737
C	2.379246	-3.057799	-0.938647
C	1.386536	-3.258256	-2.073364
C	0.968647	-1.843749	-2.441402
C	2.516852	-1.292060	0.781214
C	2.271346	0.015561	1.183700
C	2.646811	0.494350	2.555722
C	3.812268	-0.272964	3.152321
C	3.559144	-1.761772	3.031914
C	3.429220	-2.184909	1.577367
H	1.122725	-0.069066	-1.214527
H	0.011051	-1.791121	-2.951765
H	1.725517	-1.382704	-3.074140
H	1.830442	-3.798603	-2.905692
H	0.527145	-3.824745	-1.720258
H	3.409266	-3.014567	-1.300157
H	2.311988	-3.852407	-0.199926
H	2.641043	-2.012036	3.567867
H	4.361435	-2.334737	3.496196
H	1.436580	0.529005	0.732012
H	3.052588	-3.204485	1.532275
H	-2.739360	-0.761094	-0.163574
H	-6.736196	-1.883288	0.833844
H	-6.798584	-0.942277	2.319304
H	-7.591202	0.710761	1.273964
H	-6.370931	1.943633	1.075641
H	-8.215816	1.746551	-0.704831

(3-4)$_{\textbf{DBU-}\textit{anti}}$ (*re-re*)$_{180}$

E_0 = -1610.5755987
E_{0+ZPE} = -1609.898545
E_{298} = -1609.865139
H_{298} = -1609.864195
G_{298} = -1609.966997
NImag = 1 (-351.9992)

N	-5.184031	0.089958	0.764276
C	-5.700550	-0.911277	1.692038
C	-4.621662	-1.899086	2.073235
C	-3.980352	-2.457497	0.825675
N	-3.595035	-1.368583	-0.044520
C	-4.166378	-0.192473	-0.034728
C	-3.646331	0.832843	-0.989447
C	-4.628770	1.174711	-2.111020
C	-5.730486	2.139385	-1.706422
C	-6.613604	1.660008	-0.567166
C	-5.861872	1.382405	0.724822
O	-1.362789	-1.626362	-1.479773
C	-0.439185	-2.032062	-0.721867
O	-0.568743	-2.663710	0.330812
C	0.974331	-1.693649	-1.234302
N	1.996080	-1.805674	-0.205917
C	2.748993	-3.053705	-0.321823
C	2.075716	-3.795940	-1.466537
C	1.437375	-2.691184	-2.291861
C	2.133276	-0.924927	0.783282
C	1.396680	0.259124	0.837085
C	1.269174	1.020376	2.121448
C	2.468106	0.874473	3.039282
C	2.857171	-0.583213	3.172426
C	3.186342	-1.191119	1.817331
H	0.943850	-0.685501	-1.635509
H	0.614060	-3.032959	-2.912556
H	2.176637	-2.222137	-2.940878
H	2.785254	-4.394853	-2.031913
H	1.308093	-4.460695	-1.076116
H	3.795730	-2.838248	-0.538430
H	2.704110	-3.624097	0.602432
H	2.035218	-1.140758	3.626443
H	3.718243	-0.698798	3.830244
H	0.523676	0.322923	0.204293
H	3.350368	-2.258839	1.925220
H	-2.743550	-1.503517	-0.640997
H	-6.550845	-1.420100	1.235232
H	-6.061664	-0.386075	2.571640
H	-3.383144	1.734144	-0.435546
H	-2.727508	0.436328	-1.411364
H	-5.273800	3.089023	-1.417075

(3-4)$_{\textbf{DBU-}\textit{anti}}$ (*re-re*)$_{300}$

E_0 = -1610.5695515
E_{0+ZPE} = -1609.892685
E_{298} = -1609.860182
H_{298} = -1609.859238
G_{298} = -1609.959718
NImag = 1 (-321.3954)

N	5.785588	-0.810674	-0.771089
C	6.137275	-2.161536	-0.342417
C	4.899452	-2.979482	-0.054392
C	3.990659	-2.215137	0.877720
N	3.774040	-0.886140	0.350772
C	4.631319	-0.265439	-0.415491
C	4.269302	1.112536	-0.871290
C	5.132403	2.213167	-0.252646
C	6.500568	2.370083	-0.892547
C	7.373548	1.128105	-0.840912
C	6.780427	-0.079206	-1.549243
O	1.499881	0.370245	0.868381
C	0.563023	-0.398226	1.225111
O	0.627234	-1.623404	1.361549
C	-0.747982	0.342890	1.546210
N	-1.905690	-0.539469	1.596139
C	-2.283855	-0.858847	2.972978
C	-1.215029	-0.192920	3.824905
C	-0.710173	0.941037	2.949365
C	-2.415729	-1.133701	0.516306
C	-2.081798	-0.761496	-0.784212
C	-2.202496	-1.746819	-1.917884
C	-3.291837	-2.789291	-1.734786
C	-3.310856	-3.313973	-0.313388
C	-3.472920	-2.175464	0.685863
H	-0.886288	1.119937	0.802571
H	0.284825	1.286818	3.214776
H	-1.388655	1.791633	2.998448
H	-1.612229	0.147916	4.777906
H	-0.411567	-0.898424	4.026553
H	-3.277292	-0.463198	3.187470
H	-2.303906	-1.932965	3.135885
H	-2.384406	-3.850655	-0.097368
H	-4.126799	-4.023541	-0.178230
H	-1.269521	-0.059133	-0.900879
H	-3.496393	-2.565129	1.697313
H	2.860320	-0.407936	0.570645
H	6.779014	-2.102630	0.537980
H	6.712807	-2.619365	-1.142340
H	4.333436	1.153928	-1.959090
H	3.229004	1.269356	-0.602172
H	6.368518	2.659291	-1.938252

H	-7.426240	0.281886	-1.246835
H	-6.238097	3.088831	-1.157074
H	-6.772629	2.255855	-2.597856
C	3.719971	1.053812	-0.221131
H	4.534316	0.757782	0.422011
C	3.208756	2.418999	-0.021666
C	2.073509	2.898197	-0.679626
C	3.895447	3.281933	0.832720
C	1.647579	4.201895	-0.494553
H	1.510939	2.244027	-1.330455
C	3.470702	4.590310	1.015328
H	4.778357	2.927912	1.346108
C	2.345338	5.055199	0.352646
H	0.765465	4.553626	-1.010070
H	4.021077	5.244309	1.676326
H	2.010833	6.072536	0.495191
C	3.693091	0.488486	-1.481678
H	3.108071	0.853566	-2.305505
N	4.449003	-0.613181	-1.784088
O	5.159151	-1.140600	-0.917777
O	4.413880	-1.055737	-2.942195
H	4.406360	-2.193059	1.095840
H	3.950118	0.011252	4.195655
H	4.737261	-0.018008	2.630080
H	2.869940	1.561799	2.521160
H	1.780022	0.399784	3.218090
H	-2.988622	-2.552570	1.277201
H	-4.322169	-2.891888	0.180762
H	-4.488927	-1.413141	2.837964
H	-5.256629	-2.942903	2.433520
H	-4.289863	2.161958	0.162293
H	-3.096160	1.219871	-0.710644
H	-4.340161	2.229227	-2.404251
H	-4.963453	0.601122	-2.370229

(3-4)$_{\textbf{DBU-}\textit{anti}}$ $(si\text{-}si)_{60}$

E_0 = -1610.5719208
E_{0+ZPE} = -1609.894553
E_{298} = -1609.861364
H_{298} = -1609.860420
G_{298} = -1609.963376
NImag = 1 (-337.2864)

N	6.174931	0.425978	-0.462095
C	6.549935	-0.001052	-1.807061
C	5.325920	-0.283515	-2.647252
C	4.402953	-1.218941	-1.904069
N	4.170495	-0.704722	-0.572686
C	5.014267	0.063911	0.064011
C	4.629033	0.513689	1.437440
C	5.479652	-0.102251	2.549373
C	6.841157	0.546152	2.728571
C	7.733266	0.502896	1.500097
C	7.152891	1.209850	0.285914
O	1.838338	-1.205450	0.599924
C	0.876541	-1.202983	-0.217887
O	0.952264	-1.127123	-1.447617
C	-0.502526	-1.347603	0.452891
N	-1.621036	-0.998534	-0.411605
C	-2.247546	-2.184016	-0.994070
C	-1.381311	-3.338747	-0.516836
C	-0.779726	-2.813648	0.777180
C	-1.934980	0.241996	-0.777911
C	-1.087067	1.381822	-0.316930
C	-0.932604	2.437511	-1.404544
C	-2.284769	2.924751	-1.885556
C	-3.142487	1.771034	-2.376371
C	-3.086522	0.541711	-1.505750
H	-0.508245	-0.734867	1.350295
H	0.121236	-3.336725	1.084606
H	-6.353048	2.350081	-2.576444
H	-4.052129	1.623217	-2.918636
H	-5.057011	0.254814	-2.513056
C	2.503135	1.638639	-0.526555
H	1.901059	1.220609	-1.316076
C	3.910772	1.217895	-0.538588
C	4.880855	1.777660	0.297305
C	4.311731	0.240665	-1.451400
C	6.201761	1.368313	0.223786
H	4.607425	2.539844	1.011526
C	5.633718	-0.171318	-1.524205
H	3.578295	-0.188848	-2.118244
C	6.585024	0.389621	-0.684674
H	6.935835	1.816016	0.878248
H	5.921399	-0.925182	-2.242999
H	7.616417	0.072945	-0.740484
C	2.146082	2.910247	-0.105174
H	2.766790	3.575840	0.464788
N	0.890768	3.396432	-0.355580
O	0.056264	2.690509	-0.938629
O	0.616132	4.548634	0.015135
H	4.124296	-0.771721	1.440095
H	2.241538	1.300620	4.016738
H	3.311999	1.437012	2.637672
H	1.100398	2.075891	1.893354
H	0.367017	0.683216	2.642083
H	-3.867021	-1.400308	2.680766
H	-3.077296	-3.018390	1.049019
H	-4.670204	-3.117354	0.297816
H	-5.055462	-2.698888	2.668109
H	-7.356210	2.429490	-0.354139
H	-7.166057	0.763948	-0.856758
H	-5.141918	2.176606	0.924890
H	-6.558514	1.373694	1.556743

(3-4)$_{\textbf{DBU-}\textit{anti}}$ $(si\text{-}si)_{180}$

E_0 = -1610.5767092
E_{0+ZPE} = -1609.899693
E_{298} = -1609.866228
H_{298} = -1609.865283
G_{298} = -1609.970212
NImag = 1 (-361.8048)

N	6.279350	-0.673384	-0.780928
C	6.474953	-2.119220	-0.732121
C	5.148566	-2.843896	-0.718629
C	4.270994	-2.275392	0.369942
N	4.219928	-0.835607	0.239613
C	5.171426	-0.124519	-0.305462
C	4.980466	1.357787	-0.349686
C	5.924885	2.120647	0.580961
C	7.329179	2.302328	0.031388
C	8.066142	1.011188	-0.280803
C	7.372701	0.135115	-1.311831
O	2.019424	0.444303	1.037234
C	1.010223	-0.311806	0.993766
O	0.996369	-1.509125	0.693084
C	-0.304160	0.391006	1.385977
N	-1.494356	-0.400515	1.109219
C	-1.990334	-1.068904	2.308285
C	-0.970727	-0.724620	3.382271
C	-0.380374	0.589792	2.897318
C	-2.017287	-0.590688	-0.098170
C	-1.349701	0.069427	-1.266932
C	-1.554329	-0.690547	-2.569023
C	-3.015874	-1.022346	-2.791068
C	-3.553472	-1.852320	-1.639960
C	-3.200347	-1.308224	-0.288586
H	-0.346744	1.341481	0.860950
H	0.592902	0.816141	3.322391
H	7.024359	3.194889	-0.408917
H	4.586721	3.149871	-0.358742
H	5.232187	2.036600	0.819402
C	-3.733492	0.758609	-1.171075
H	-3.532737	0.539178	-2.209075
C	-3.040159	1.935431	-0.628727
C	-3.341870	2.484335	0.618701
C	-2.073020	2.565888	-1.416020
C	-2.687824	3.621866	1.065453
H	-4.091467	2.028781	1.247885
C	-1.422045	3.703032	-0.970655
H	-1.834756	2.156209	-2.388003
C	-1.723937	4.234164	0.276961
H	-2.934849	4.033335	2.033598
H	-0.680103	4.176822	-1.597153
H	-1.216620	5.120878	0.628427
C	-5.002993	0.426778	-0.728355
H	-5.422988	0.714839	0.217194
N	-5.880407	-0.275488	-1.516121
O	-5.559678	-0.636633	-2.654895
O	-7.007475	-0.516622	-1.059052
H	-4.436098	-1.677106	0.516057
H	-3.134224	-3.607276	-2.438767
H	-4.258832	-2.349450	-1.974369
H	-2.347053	-1.216380	-2.860726
H	-1.236129	-2.254226	-2.012850
H	3.015076	-2.681388	0.979668
H	4.431479	-2.143157	1.873177
H	4.375062	-3.193016	-0.985326
H	5.188868	-3.928441	0.389865
H	8.326281	1.351578	-1.321495
H	7.599607	0.857945	0.192411
H	6.353017	0.212949	-2.509369
H	7.568155	-0.793925	-1.763066

(3-4)$_{\textbf{DBU-}\textit{anti}}$ $(si\text{-}si)_{300}$

E_0 = -1610.5784044
E_{0+ZPE} = -1609.900719
E_{298} = -1609.867586
H_{298} = -1609.866642
G_{298} = -1609.968582
NImag = 1 (-340.0630)

N	6.479740	-0.988668	-0.028452
C	6.616337	-2.092449	0.916909
C	5.268123	-2.690183	1.247724
C	4.318237	-1.596303	1.671157
N	4.336490	-0.536307	0.686911
C	5.355585	-0.290126	-0.092954
C	5.219068	0.841212	-1.061755
C	6.111658	2.041084	-0.740867
C	7.562455	1.872920	-1.158195
C	8.275042	0.688219	-0.528327
C	7.641232	-0.656880	-0.847234
O	2.131895	0.902467	0.354641
C	1.090796	0.264113	0.672315
O	1.040244	-0.881497	1.132386
C	-0.210630	1.061033	0.464690
N	-1.420236	0.277936	0.651180
C	-1.939724	0.404057	2.011512
C	-0.989121	1.379974	2.692816
C	-0.359665	2.139498	1.534570
C	-1.897798	-0.601131	-0.226083
C	-1.120013	-0.846590	-1.489051
C	-1.444792	-2.190693	-2.122071
C	-2.942710	-2.394006	-2.236114
C	-3.578426	-2.371015	-0.857458
C	-3.136600	-1.201789	-0.025427
H	-0.195564	1.491715	-0.533842
H	0.593942	2.596901	1.780583

H	-1.505357	-2.877735	1.587217
H	-1.961146	-4.247941	-0.377909
H	-0.594414	-3.543084	-1.239843
H	-3.269935	-2.285956	-0.637208
H	-2.271911	-2.093029	-2.078972
H	-2.809071	1.480011	-3.378543
H	-4.176152	2.098734	-2.495640
H	-0.112092	1.046257	0.018558
H	-3.654706	-0.295654	-1.885051
H	-1.592752	1.828196	0.548760
H	3.245987	-0.918367	-0.119082
H	7.187951	-0.883456	-1.738326
H	7.135574	0.798068	-2.253083
H	7.949311	1.432380	-0.416355
H	6.713172	2.165436	0.574495
H	8.679155	0.989685	1.738738
H	7.970509	-0.528260	1.231205
H	6.697781	1.590282	3.017872
H	7.355194	0.064114	3.560400
C	-4.507440	0.968586	0.190173
H	-5.095426	1.453286	-0.574969
C	-4.887161	-0.419687	0.490977
C	-5.822529	-1.052352	-0.332160
C	-4.386501	-1.121474	1.588723
C	-6.237853	-2.347439	-0.075721
H	-6.226724	-0.516674	-1.180193
C	-4.797237	-2.421293	1.841720
H	-3.673711	-0.658315	2.254127
C	-5.719748	-3.041470	1.010700
H	-6.966428	-2.815590	-0.721848
H	-4.396890	-2.950375	2.694619
H	-6.039014	-4.053652	1.212698
C	-4.043822	1.800887	1.197338
H	-3.592537	1.468987	2.113272
N	-4.181398	3.163258	1.125587
O	-4.723040	3.695439	0.148567
O	-3.763809	3.841359	2.076441
H	-0.345283	3.267197	-1.011719
H	-0.366790	2.012818	-2.236159
H	-2.798648	3.437608	-1.074415
H	-2.161350	3.653048	-2.687751
H	4.806140	0.649190	-2.864030
H	5.630616	-0.722704	-3.593760
H	3.433190	-1.305308	-2.385700
H	4.836923	-2.217585	-1.836856
H	4.919290	-0.002147	3.477965
H	5.589420	-1.173133	2.371424
H	4.685429	1.601776	1.482270
H	3.588009	0.237872	1.578016

H	-1.052693	1.416684	3.125361
H	-1.427653	-0.651101	4.365759
H	-0.198203	-1.489738	3.424692
H	-2.979502	-0.691184	2.565648
H	-2.074076	-2.140340	2.135203
H	-3.173309	-2.875672	-1.718379
H	-4.640879	-1.935656	-1.713641
H	-0.287240	0.184828	-1.077860
H	-3.535226	-1.922934	0.534586
H	-1.765632	1.077455	-1.355615
H	3.350065	-0.343093	0.563000
H	7.065182	-2.371913	0.150030
H	7.050623	-2.400932	-1.609499
H	5.108202	1.703635	-1.375741
H	3.949825	1.552098	-0.067811
H	7.271619	2.898743	-0.882591
H	7.915057	2.884857	0.742671
H	5.486726	3.102825	0.752928
H	5.954964	1.624318	1.552362
C	-4.784058	0.158821	0.183321
H	-4.658246	-0.134615	1.211858
C	-4.271691	1.499418	-0.135203
C	-3.566433	2.196084	0.847768
C	-4.489485	2.129534	-1.363325
C	-3.086025	3.475455	0.613267
H	-3.406921	1.731441	1.809977
C	-4.011459	3.407985	-1.597768
H	-5.036368	1.622292	-2.143952
C	-3.305056	4.086719	-0.612496
H	-2.547270	3.996612	1.391708
H	-4.192581	3.878084	-2.553718
H	-2.935111	5.084649	-0.798123
C	-5.920635	-0.334529	-0.443021
H	-6.349207	0.046949	-1.350691
N	-6.561515	-1.434256	0.058346
O	-6.114703	-2.010028	1.061307
O	-7.589042	-1.834446	-0.511153
H	-3.586368	-0.096880	-2.878675
H	-3.145951	-1.562233	-3.729204
H	-1.161303	-0.093515	-3.391718
H	-0.970905	-1.612905	-2.539856
H	4.657214	-2.728976	-1.684447
H	5.317805	-3.905027	-0.554814
H	3.248254	-2.635666	0.309223
H	4.661016	-2.535855	1.354991
H	9.052478	1.259714	-0.673497
H	8.228801	0.429736	0.628504
H	7.006928	0.740315	-2.142213
H	8.084982	-0.569691	-1.728402

H	-1.032963	2.912759	1.168320
H	-1.509389	2.029523	3.392667
H	-0.225873	0.834925	3.244931
H	-2.958851	0.781450	1.990207
H	-1.951231	-0.573617	2.493160
H	-3.326795	-3.298224	-0.332114
H	-4.666419	-2.371160	-0.939044
H	-0.057552	-0.796042	-1.267770
H	-3.546712	-1.165521	0.972648
H	-1.343275	-0.040552	-2.186832
H	3.457029	0.029873	0.561319
H	7.114623	-1.733722	1.818812
H	7.258598	-2.838733	0.457635
H	8.361283	-1.449061	-0.670754
H	7.369365	-0.707651	-1.902311
H	5.434767	0.475461	-2.066213
H	4.176786	1.145967	-1.046095
H	5.694912	2.900900	-1.263601
H	6.044890	2.270081	0.323789
C	-4.430043	0.515612	-0.690986
H	-4.235530	0.253933	-1.720005
C	-5.688746	0.001678	-0.126301
C	-6.601414	-0.635549	-0.966909
C	-6.022104	0.157431	1.221263
C	-7.817167	-1.094803	-0.479971
H	-6.362306	-0.757611	-2.013995
C	-7.232646	-0.303779	1.707872
H	-5.323756	0.631349	1.896587
C	-8.137144	-0.931432	0.858816
H	-8.512722	-1.579867	-1.149582
H	-7.471562	-0.176904	2.754031
H	-9.081429	-1.291151	1.241026
C	-3.949562	1.742734	-0.268509
H	-4.271371	2.252102	0.620587
N	-3.030182	2.442906	-1.003242
O	-2.568897	1.965724	-2.048517
O	-2.694806	3.569523	-0.606908
H	-0.968359	-2.244801	-3.100782
H	-1.016600	-2.993031	-1.517112
H	-3.367599	-1.603455	-2.858723
H	-3.166346	-3.339052	-2.731378
H	3.291405	-1.943308	1.743044
H	4.605218	-1.192558	2.643185
H	4.870562	-3.205647	0.374049
H	5.382195	-3.422765	2.042755
H	8.335028	0.805558	0.555315
H	9.300774	0.661773	-0.897155
H	7.603954	1.765941	-2.245067
H	8.107359	2.786400	-0.918478

(3-4)$_{\textbf{DBU-}\textit{anti}}$ $(\textit{si-re})_{60}$

E_0 = -1610.5747416
E_{0+ZPE} = -1609.897845
E_{298} = -1609.864429
H_{298} = -1609.863484
G_{298} = -1609.967326
NImag = 1 (-345.2359)

N	-6.484303	-0.496091	0.834827
C	-6.663371	-1.908035	1.158554
C	-5.329636	-2.594345	1.343645
C	-4.444037	-2.310182	0.154685
N	-4.406979	-0.884230	-0.083805
C	-5.373248	-0.071104	0.250971
C	-5.194596	1.377330	-0.072485
C	-6.126891	1.872076	-1.179489
C	-7.542581	2.168705	-0.716104
C	-8.274976	0.987549	-0.102226
C	-7.596157	0.403539	1.126498
O	-2.196803	0.155503	-1.115613

(3-4)$_{\textbf{DBU-}\textit{anti}}$ $(\textit{si-re})_{180}$

E_0 = -1610.57384
E_{0+ZPE} = -1609.896772
E_{298} = -1609.863402
H_{298} = -1609.862458
G_{298} = -1609.967056
NImag = 1 (-339.5862)

N	6.379422	0.700361	-0.397325
C	6.638728	0.672428	-1.833627
C	5.345491	0.693022	-2.615619
C	4.427396	-0.391215	-2.106013
N	4.313882	-0.284152	-0.667988
C	5.239722	0.236255	0.093366
C	4.981634	0.266818	1.565596
C	5.875066	-0.687602	2.359824
C	7.276700	-0.161351	2.614717
C	8.078195	0.153552	1.363441
C	7.441928	1.204486	0.467557
O	2.033112	-1.049406	0.477092

(3-4)$_{\textbf{DBU-}\textit{anti}}$ $(\textit{si-re})_{300}$

E_0 = -1610.5749458
E_{0+ZPE} = -1609.896934
E_{298} = -1609.863962
H_{298} = -1609.863018
G_{298} = -1609.964731
NImag = 1 (-334.7702)

N	6.299806	-0.740119	0.527474
C	6.616906	-0.297007	1.882455
C	5.358110	-0.036634	2.677257
C	4.440780	0.871340	1.894531
N	4.264129	0.338172	0.561772
C	5.148876	-0.411423	-0.040671
C	4.821495	-0.879153	-1.423213
C	5.694631	-0.251073	-2.510272
C	7.075462	-0.869471	-2.638443
C	7.925051	-0.795613	-1.381340
C	7.322354	-1.505272	-0.179626
O	1.963487	0.814608	-0.690151

C	-1.170093	-0.519723	-0.826058
O	-1.140522	-1.584662	-0.201170
C	0.139306	0.093866	-1.354830
N	1.338269	-0.566878	-0.868940
C	1.915821	-1.457149	-1.865419
C	0.904548	-1.452575	-2.999303
C	0.248193	-0.087538	-2.867667
C	1.885094	-0.363596	0.326644
C	1.150247	0.488527	1.317832
C	1.421360	0.069192	2.754546
C	2.911127	0.002822	3.021970
C	3.574883	-0.997284	2.090598
C	3.144413	-0.862792	0.656546
H	0.157889	1.147144	-1.084493
H	-0.721024	-0.018337	-3.352265
H	0.894509	0.685642	-3.281888
H	1.376985	-1.609538	-3.965792
H	0.168895	-2.240865	-2.849457
H	2.881855	-1.074729	-2.199153
H	2.076216	-2.447733	-1.441291
H	3.339988	-2.011346	2.431044
H	4.661111	-0.915122	2.158683
H	0.083736	0.462143	1.119166
H	3.567297	-1.597117	-0.013137
H	1.472514	1.521951	1.176732
H	-3.527620	-0.479596	-0.500623
H	-7.240967	-2.387707	0.366920
H	-7.246165	-1.961635	2.073917
H	-8.311930	-0.187455	1.688421
H	-7.256500	1.199911	1.789848
H	-5.344584	1.964185	0.834200
H	-4.160106	1.508942	-0.375740
H	-9.270169	1.314600	0.200337
H	-8.417615	0.195747	-0.840107
C	4.414849	0.795200	-0.227359
H	3.865315	0.689362	-1.149633
C	5.675577	0.042884	-0.150318
C	6.606456	0.220393	0.875610
C	5.976203	-0.866835	-1.166590
C	7.796746	-0.490614	0.880526
H	6.411569	0.918868	1.675609
C	7.167673	-1.571407	-1.166101
H	5.265667	-1.016777	-1.967924
C	8.083423	-1.388094	-0.138200
H	8.504100	-0.339321	1.683064
H	7.382300	-2.263022	-1.967944
H	9.013310	-1.937909	-0.132873
C	4.272547	2.018247	0.404885
H	4.877561	2.378223	1.215132
N	3.305502	2.904599	0.007092
O	2.522260	2.611760	-0.906994
O	3.249011	4.004915	0.577758
H	0.938422	0.777887	3.426951
H	0.966808	-0.906058	2.940728
H	3.342479	0.993849	2.873345
H	3.104430	-0.274227	4.058602
H	-5.485789	-3.664293	1.455253
H	-4.851867	-2.229477	2.252348
H	-4.819594	-2.816535	-0.735770
H	-3.418653	-2.630311	0.316045
H	-5.693013	2.784626	-1.585971
H	-6.136269	1.147342	-1.995217
H	-8.119721	2.546065	-1.560557
H	-7.507647	2.976361	0.019271

C	1.058537	-0.929855	-0.315499
O	1.103975	-0.561103	-1.493194
C	-0.294046	-1.337355	0.298395
N	-1.448411	-0.852404	-0.446034
C	-1.993604	-1.882165	-1.329131
C	-1.048513	-3.061615	-1.162296
C	-0.466488	-2.852513	0.226879
C	-1.873593	0.407872	-0.445733
C	-1.078835	1.433153	0.309960
C	-1.060456	2.766801	-0.424383
C	-2.469855	3.243992	-0.707951
C	-3.239497	2.221393	-1.528111
C	-3.055878	0.802737	-1.076485
H	-0.324931	-0.980702	1.324134
H	0.472455	-3.374177	0.389963
H	-1.174604	-3.175938	0.988983
H	-1.567366	-4.011229	-1.266859
H	-0.259033	-3.020060	-1.909536
H	-3.004935	-2.141600	-1.026185
H	-2.028424	-1.509950	-2.351906
H	-2.931504	2.290157	-2.576524
H	-4.306444	2.462144	-1.517259
H	-0.063123	1.090500	0.474074
H	-3.538744	0.066809	-1.703605
H	-1.530735	1.563729	1.297041
H	3.413101	-0.593235	-0.223123
H	7.226012	-0.214680	-2.075581
H	7.239539	1.545170	-2.074543
H	5.110746	1.286956	1.928219
H	3.938639	0.000618	1.709808
H	7.204355	0.746649	3.218647
H	7.823692	-0.888081	3.215687
H	5.388348	-0.865474	3.317736
H	5.915560	-1.652942	1.852575
C	-4.538955	0.595282	0.608027
H	-3.841139	0.889453	1.377235
C	-4.789065	-0.849840	0.502019
C	-5.638913	-1.396264	-0.463676
C	-4.195477	-1.705650	1.428744
C	-5.875887	-2.758456	-0.503417
H	-6.106035	-0.755767	-1.198059
C	-4.439659	-3.071508	1.393234
H	-3.547405	-1.295606	2.190511
C	-5.275804	-3.603872	0.424214
H	-6.531046	-3.165300	-1.260342
H	-3.975972	-3.717869	2.124615
H	-5.465061	-4.667054	0.392082
C	-5.559752	1.494843	0.356616
H	-6.414607	1.298806	-0.263920
N	-5.569435	2.746974	0.921376
O	-4.680268	3.091978	1.709837
O	-6.510361	3.503657	0.642922
H	-2.984437	3.412840	0.237348
H	-2.451375	4.196688	-1.237859
H	-0.520484	3.496523	0.178829
H	-0.505091	2.651758	-1.357589
H	4.864191	1.664159	-2.503165
H	5.558457	0.546138	-3.671323
H	3.422544	-0.306938	-2.509703
H	4.813728	-1.377757	-2.366459
H	8.192663	1.617115	-0.198423
H	7.060973	2.033879	1.064637
H	9.057116	0.529291	1.662415
H	8.255777	-0.751733	0.780087

C	1.018812	0.993895	0.127178
O	1.092878	0.965021	1.359620
C	-0.331349	1.300249	-0.547899
N	-1.469181	1.259637	0.358790
C	-1.766856	2.586884	0.899492
C	-0.769882	3.511625	0.211874
C	-0.367363	2.744221	-1.038645
C	-2.035943	0.145452	0.808898
C	-1.406795	-1.174496	0.479072
C	-1.588389	-2.168438	1.618208
C	-3.051868	-2.313296	1.984651
C	-3.651520	-0.975248	2.389447
C	-3.237554	0.176609	1.514655
H	-0.471044	0.595475	-1.362982
H	0.587165	3.054848	-1.453063
H	-1.129615	2.847655	-1.809864
H	-1.209143	4.480439	-0.011459
H	0.098264	3.671480	0.848002
H	-2.793657	2.874798	0.690711
H	-1.641459	2.569400	1.981494
H	-3.347614	-0.743592	3.415512
H	-4.740250	-1.047527	2.420915
H	-0.349641	-1.047824	0.271063
H	-3.562817	1.145698	1.865234
H	-1.865950	-1.572044	-0.428968
H	3.352789	0.530299	0.073547
H	7.237065	0.599084	1.830336
H	7.204347	-1.080357	2.353517
H	8.100096	-1.699082	0.551477
H	6.917485	-2.475155	-0.471590
H	8.889209	-1.262161	-1.584421
H	8.129577	0.242970	-1.114456
H	6.965685	-1.918945	-2.923394
H	7.606074	-0.382318	-3.456754
C	-4.703889	0.298241	-0.164835
H	-5.353656	0.693294	0.601148
C	-4.961900	-1.100649	-0.531968
C	-4.274116	-1.755708	-1.557450
C	-5.981936	-1.790912	0.125689
C	-4.581049	-3.063407	-1.892400
H	-3.492769	-1.244084	-2.099730
C	-6.291645	-3.099424	-0.211575
H	-6.545542	-1.290860	0.900318
C	-5.587414	-3.743950	-1.217730
H	-4.035179	-3.553608	-2.685789
H	-7.086743	-3.612969	0.309595
H	-5.825488	-4.764076	-1.482105
C	-4.310406	1.204820	-1.139889
H	-3.889232	0.942339	-2.092275
N	-4.489604	2.545804	-0.964537
O	-4.931052	2.981006	0.111813
O	-4.197463	3.313851	-1.894835
H	-1.171368	-3.130444	1.320903
H	-1.016017	-1.827650	2.483296
H	-3.590737	-2.720214	1.129331
H	-3.171218	-3.026797	2.800354
H	5.619756	0.417198	3.629719
H	4.852502	-0.979295	2.884471
H	4.856904	1.877763	1.829915
H	3.452482	0.944956	2.339331
H	5.773158	0.823271	-2.337460
H	5.168290	-0.370653	-3.456398
H	4.903890	-1.965960	-1.458980
H	3.779926	-0.628671	-1.601268

(3-4)$_{\text{DBU-}anti}$ $(re\text{-}si)_{60}$
E_0 = -1610.5732478
E_{0+ZPE} = -1609.895740
E_{298} = -1609.862535

(3-4)$_{\text{DBU-}anti}$ $(re\text{-}si)_{300}$
E_0 = -1610.5739661
E_{0+ZPE} = -1609.896626
E_{298} = -1609.863231

H_{298} = -1609.861591
G_{298} = -1609.963957
NImag = 1 (-321.6881)

N	6.001766	-0.943875	-0.699308
C	6.295851	-2.193803	-0.005427
C	5.023937	-2.864288	0.460270
C	4.190007	-1.879709	1.243259
N	4.040625	-0.661560	0.477879
C	4.898370	-0.262601	-0.422927
C	4.600608	1.020204	-1.131853
C	5.563860	2.156123	-0.783725
C	6.901215	2.085704	-1.500569
C	7.699826	0.820320	-1.239206
C	6.989878	-0.457847	-1.656837
O	1.825402	0.743570	0.813526
C	0.853381	0.024481	1.176920
O	0.884835	-1.186335	1.420411
C	-0.464448	0.807354	1.333381
N	-1.602912	-0.065729	1.577725
C	-1.858704	-0.204692	3.011632
C	-0.857946	0.730197	3.680545
C	-0.447894	1.690188	2.575168
C	-2.166668	-0.833127	0.642171
C	-2.037555	-0.554787	-0.714673
C	-2.357316	-1.582389	-1.764148
C	-3.322352	-2.663322	-1.304696
C	-2.972111	-3.137542	0.089815
C	-3.021333	-1.985677	1.083095
H	-0.596163	1.400621	0.435407
H	0.525263	2.145137	2.732706
H	-1.181486	2.486062	2.457271
H	-1.290037	1.233232	4.542115
H	0.005385	0.163338	4.023914
H	-2.889151	0.077313	3.227712
H	-1.714301	-1.230698	3.341067
H	-1.970976	-3.573349	0.096478
H	-3.659906	-3.917371	0.416156
H	-1.267728	0.147180	-0.999703
H	-2.699944	-2.335439	2.059408
H	3.157658	-0.100744	0.620062
H	6.959210	-1.990387	0.836707
H	6.828752	-2.837023	-0.700219
H	7.715714	-1.257546	-1.762500
H	6.519480	-0.329995	-2.632539
H	4.609199	0.841882	-2.207633
H	3.587696	1.302956	-0.860455
H	5.071189	3.089492	-1.052237
H	5.712027	2.189234	0.296771
C	-3.552340	1.087703	-0.983338
H	-3.033485	1.208079	-1.922177
C	-4.846032	0.399323	-1.067727
C	-5.330080	0.024870	-2.322510
C	-5.643845	0.153270	0.052569
C	-6.566311	-0.588536	-2.455037
H	-4.734671	0.227579	-3.201349
C	-6.876381	-0.463477	-0.079184
H	-5.298673	0.441059	1.034911
C	-7.341816	-0.841039	-1.332904
H	-6.923165	-0.867949	-3.435882
H	-7.477023	-0.650362	0.799432
H	-8.304171	-1.321692	-1.433129
C	-3.367714	2.100142	-0.057450
H	-3.995982	2.285611	0.793805
N	-2.351617	3.004155	-0.207933
O	-1.527469	2.865858	-1.123788
O	-2.275116	3.949189	0.590516
H	-4.052897	-1.644510	1.198979
H	-3.303171	-3.494801	-2.009589
H	-4.341112	-2.276661	-1.299401
H	-2.747351	-1.088381	-2.656824

H_{298} = -1609.862287
G_{298} = -1609.966252
NImag = 1 (-333.6441)

N	-5.729169	0.017747	0.883108
C	-6.060171	-1.067021	1.802353
C	-4.809247	-1.746964	2.308962
C	-3.931910	-2.127783	1.141555
N	-3.731215	-0.970238	0.297804
C	-4.591009	0.009368	0.204909
C	-4.255629	1.130081	-0.727346
C	-5.146751	1.182878	-1.969568
C	-6.514106	1.800750	-1.732907
C	-7.358602	1.100327	-0.681994
C	-6.726452	1.067499	0.700499
O	-1.436743	-0.727368	-1.023419
C	-0.540126	-1.478764	-0.546351
O	-0.673963	-2.292022	0.372351
C	0.820778	-1.335051	-1.251154
N	1.922996	-1.915551	-0.506110
C	2.392447	-3.161181	-1.099908
C	1.368569	-3.467040	-2.179443
C	0.853599	-2.094385	-2.576867
C	2.496330	-1.321690	0.539416
C	2.154381	-0.035551	0.952649
C	2.506668	0.460425	2.326816
C	3.744919	-0.193559	2.914117
C	3.686660	-1.694853	2.723447
C	3.604866	-2.044017	1.246096
H	0.986404	-0.274782	-1.418890
H	-0.121031	-2.114774	-3.056204
H	1.555614	-1.610258	-3.255135
H	1.807659	-4.014780	-3.009511
H	0.560011	-4.067140	-1.766105
H	3.391042	-3.005853	-1.514441
H	2.445431	-3.956630	-0.360802
H	2.815490	-2.100227	3.242495
H	4.565029	-2.176061	3.152875
H	1.248922	0.387868	0.544060
H	3.496036	-3.117281	1.123932
H	-2.822515	-0.894436	-0.229127
H	-6.713041	-1.779924	1.296502
H	-6.617986	-0.635400	2.629003
H	-7.491976	0.879132	1.446064
H	-6.284489	2.035177	0.941064
H	-4.317903	2.075096	-0.187142
H	-3.219911	0.993658	-1.023980
H	-4.621345	1.773689	-2.718790
H	-5.248679	0.180671	-2.388186
C	3.482773	1.130067	-0.496444
H	3.036216	0.570022	-1.302986
C	2.865157	2.432430	-0.210634
C	1.678180	2.769860	-0.864805
C	3.430692	3.367427	0.659190
C	1.078163	4.001236	-0.665790
H	1.225879	2.056535	-1.539740
C	2.826210	4.598176	0.864406
H	4.350661	3.142380	1.177649
C	1.649635	4.921361	0.203503
H	0.165095	4.243202	-1.190423
H	3.279347	5.307996	1.541320
H	1.182701	5.882605	0.362307
C	4.838960	0.925094	-0.315480
H	5.484063	1.524349	0.298664
N	5.486546	-0.099412	-0.956117
O	4.860241	-0.879906	-1.686868
O	6.711782	-0.210128	-0.794407
H	4.543822	-1.773401	0.757593
H	3.830005	0.058685	3.971382
H	4.639491	0.191843	2.422705
H	2.625166	1.545118	2.306285

H	-1.419017	-2.050450	-2.079179
H	4.460264	-3.219257	-0.402062
H	5.272219	-3.726237	1.074449
H	3.188713	-2.250330	1.443690
H	4.661891	-1.650193	2.199756
H	7.973411	0.747132	-0.184880
H	8.632723	0.873977	-1.801164
H	6.726576	2.170451	-2.576161
H	7.500278	2.951587	-1.217263
H	1.656042	0.274524	2.991351
H	-4.267035	-1.073049	2.971720
H	-5.083776	-2.628820	2.882256
H	-2.948374	-2.468883	1.450637
H	-4.393808	-2.925104	0.557362
H	-7.590589	0.079195	-0.990416
H	-8.310699	1.624311	-0.594323
H	-6.380602	2.843211	-1.432554
H	-7.060925	1.820380	-2.675893

(3-4)$_{\text{DBU1-}anti}$ (*re-re*)$_{60}$

E_0 = -1610.5778275
E_{0+ZPE} = -1609.900592
E_{298} = -1609.867193
H_{298} = -1609.866249
G_{298} = -1609.970511
NImag = 1 (-325.8187)

N	-5.675683	0.177406	0.754439
C	-6.269339	-1.016800	1.347152
C	-5.201934	-1.946260	1.875769
C	-4.178629	-2.203615	0.796981
N	-3.728623	-0.943593	0.245981
C	-4.452535	0.146900	0.246196
C	-3.859295	1.366168	-0.379015
C	-4.572964	1.798819	-1.661737
C	-5.862120	2.570431	-1.443335
C	-6.930196	1.812786	-0.674947
C	-6.498294	1.383670	0.717665
O	-1.175460	-1.184877	-0.421713
C	-0.534986	-0.434767	-1.199945
O	-0.972607	0.554131	-1.806187
C	0.939905	-0.781510	-1.476637
N	1.528614	-1.650622	-0.467161
C	1.581409	-3.039350	-0.910225
C	0.915857	-3.030688	-2.278108
C	1.091933	-1.598329	-2.756152
C	1.831622	-1.244153	0.765347
C	1.937488	0.109722	1.068064
C	2.070925	0.583712	2.485995
C	2.712382	-0.446124	3.397555
C	2.020738	-1.782977	3.223996
C	2.150284	-2.291878	1.796839
H	1.485340	0.152394	-1.545250
H	0.373520	-1.301086	-3.515215
H	2.095711	-1.458227	-3.154405
H	1.366041	-3.758319	-2.948704
H	-0.141599	-3.267524	-2.179796
H	2.625776	-3.354719	-0.966692
H	1.066400	-3.697243	-0.214994
H	0.963895	-1.672732	3.477317
H	2.431929	-2.528777	3.903876
H	1.464606	0.808901	0.395795
H	1.483542	-3.139854	1.655299
H	-2.741132	-0.912529	-0.107396
H	-6.887941	-1.518725	0.601778
H	-6.919445	-0.692730	2.154603
H	-7.374615	1.159856	1.317101
H	-5.971214	2.196191	1.218884
H	-3.868113	2.178083	0.349539
H	-2.822479	1.139090	-0.620022
H	-7.804458	2.454625	-0.562505
H	-7.256592	0.933483	-1.233305
C	3.946874	0.494155	0.120020
H	4.423772	0.034311	0.971697
C	3.879284	1.964070	0.140122
C	3.196721	2.696195	-0.834474
C	4.542118	2.660271	1.151211
C	3.185247	4.079598	-0.799146

(3-4)$_{\text{DBU1-}anti}$ (*si-si*)$_{300}$

E_0 = -1610.5772056
E_{0+ZPE} = -1609.899565
E_{298} = -1609.866328
H_{298} = -1609.865384
G_{298} = -1609.967816
NImag = 1 (-342.8028)

N	-6.054226	-1.319258	-0.032365
C	-6.192158	-2.448665	-0.946146
C	-4.847657	-3.069714	-1.244041
C	-3.883874	-1.998565	-1.692803
N	-3.908862	-0.895038	-0.756816
C	-4.934122	-0.612387	0.005934
C	-4.816302	0.575031	0.904326
C	-5.748379	1.723795	0.512013
C	-7.188689	1.561225	0.964361
C	-7.889144	0.329519	0.418241
C	-7.209898	-0.977765	0.792193
O	-1.479281	0.154835	-0.639644
C	-1.197613	1.327286	-0.281653
O	-1.986604	2.185916	0.135169
C	0.272276	1.769953	-0.405613
N	1.224072	0.675389	-0.511843
C	1.553628	0.374507	-1.903457
C	0.758538	1.392038	-2.710903
C	0.496155	2.515843	-1.719175
C	1.601444	-0.094286	0.505411
C	0.972672	0.141406	1.850827
C	1.048427	-1.079932	2.752603
C	2.454478	-1.644084	2.789857
C	2.878294	-2.076676	1.397588
C	2.622211	-1.028488	0.352234
H	0.516795	2.392267	0.451199
H	-0.354882	3.137829	-1.982649
H	1.373044	3.153359	-1.618546
H	1.303258	1.724665	-3.591137
H	-0.180879	0.953516	-3.039821
H	2.623498	0.475323	-2.066460
H	1.272819	-0.653060	-2.134140
H	2.337161	-2.989579	1.127931
H	3.933621	-2.352519	1.389007
H	-0.065984	0.432001	1.717865
H	2.885874	-1.308977	-0.656549
H	1.479816	0.984350	2.318614
H	-3.017036	-0.352360	-0.650169
H	-6.676230	-2.111128	-1.863757
H	-6.846623	-3.175712	-0.474225
H	-7.909197	-1.798869	0.673949
H	-6.913944	-0.964936	1.841565
H	-5.010272	0.265236	1.931994
H	-3.789083	0.928777	0.844359
H	-5.341100	2.630461	0.956833
H	-5.704236	1.869867	-0.568607
C	4.363070	0.379503	0.483894
H	4.249027	0.418037	1.556675
C	5.376331	-0.562872	-0.019943
C	6.224440	-1.198549	0.886604
C	5.542801	-0.822143	-1.382190

(3-4)$_{\text{DBU1-}anti}$ (*si-si*)$_{180}$

E_0 = -1610.5764967
E_{0+ZPE} = -1609.899203
E_{298} = -1609.865898
H_{298} = -1609.864953
G_{298} = -1609.967714
NImag = 1 (-360.8896)

N	-5.963027	1.106258	-0.504376
C	-6.094582	2.496065	-0.077627
C	-4.742842	3.163444	0.023018
C	-3.818702	2.311473	0.858503
N	-3.836389	0.951064	0.365934
C	-4.854144	0.422505	-0.264809
C	-4.737209	-1.006751	-0.682222
C	-5.668722	-1.941530	0.092700
C	-7.110448	-1.938946	-0.384854
C	-7.800938	-0.587950	-0.317979
C	-7.123363	0.492965	-1.144533
O	-1.443164	-0.121199	0.771885
C	-1.081396	-1.311261	0.600394
O	-1.783238	-2.260207	0.223883
C	0.387428	-1.654478	0.919448
N	1.257605	-0.489840	1.008239
C	1.500713	-0.097775	2.392303
C	0.639857	-1.045458	3.212434
C	0.502709	-2.264618	2.314154
C	1.691952	0.211648	-0.033442
C	1.293414	-0.246945	-1.403954
C	1.249453	0.884487	-2.420093
C	2.514483	1.716288	-2.373709
C	2.713292	2.300968	-0.988351
C	2.564581	1.293385	0.111922
H	0.746041	-2.341494	0.158292
H	-0.353869	-2.888559	2.552914
H	1.398754	-2.882242	2.370037
H	1.092332	-1.273299	4.174226
H	-0.336510	-0.601204	3.393480
H	2.557507	-0.213286	2.631656
H	1.234340	0.947058	2.541298
H	1.996200	3.112172	-0.826417
H	3.701139	2.761866	-0.916856
H	0.328600	-0.743132	-1.371820
H	2.665432	1.707721	1.104598
H	2.021954	-1.000124	-1.718960
H	-2.960299	0.392320	0.493600
H	-6.616532	2.528920	0.879783
H	-6.712782	3.006656	-0.810620
H	-4.936752	-1.082369	-1.751846
H	-3.707023	-1.316445	-0.512555
H	-7.137250	-2.292113	-1.418933
H	-7.679480	-2.660888	0.201524
H	-5.267651	-2.948922	-0.009223
H	-5.619403	-1.701171	1.156124
C	4.555851	0.353370	0.301398
H	4.375143	0.342895	1.363045
C	4.496639	-0.967744	-0.340532
C	4.090699	-2.065080	0.420783
C	4.868030	-1.185978	-1.669812

H	2.660549	2.182603	-1.619833
C	4.533988	4.047516	1.184421
H	5.080744	2.108890	1.909161
C	3.854862	4.762312	0.209980
H	2.648708	4.628253	-1.559818
H	5.059050	4.567159	1.972967
H	3.843682	5.842371	0.234909
C	4.073308	-0.168442	-1.087719
H	3.879869	0.267977	-2.050056
N	4.480502	-1.473789	-1.143229
O	4.722322	-2.097811	-0.100608
O	4.611984	-2.008357	-2.255171
H	2.635306	1.517117	2.506395
H	1.078533	0.836014	2.874290
H	3.773385	-0.551684	3.160138
H	2.653021	-0.113646	4.434020
H	3.160507	-2.656222	1.614904
H	-3.878150	2.425975	-2.218268
H	-4.756806	0.921436	-2.284307
H	-5.632491	3.492664	-0.903515
H	-6.263329	2.872205	-2.411247
H	-3.308354	-2.722802	1.188178
H	-4.601365	-2.817323	0.000632
H	-4.718302	-1.495525	2.741774
H	-5.658987	-2.879006	2.196060
C	7.217978	-2.061636	0.446190
H	6.113621	-1.002529	1.943864
C	6.530965	-1.685753	-1.821420
H	4.885997	-0.354494	-2.102078
C	7.374412	-2.309099	-0.908743
H	7.868729	-2.539313	1.164445
H	6.642871	-1.877164	-2.878993
H	8.144726	-2.983350	-1.253875
C	4.143948	1.564570	-0.197038
H	4.458836	1.757094	-1.205753
N	3.529948	2.631088	0.403738
O	3.109271	2.539116	1.564572
O	3.430932	3.689601	-0.235266
H	0.712694	-0.802598	3.751509
H	0.361066	-1.846989	2.388868
H	3.138571	-0.882924	3.171605
H	2.512238	-2.490536	3.474255
H	-2.865072	-2.372984	-1.735708
H	-4.145484	-1.635115	-2.687179
H	-4.464311	-3.561519	-0.350844
H	-4.960288	-3.825292	-2.017395
H	-7.978163	0.386662	-0.668260
H	-8.904583	0.296700	0.814311
H	-7.211507	1.520359	2.056340
H	-7.751836	2.450076	0.678396
C	4.053011	-3.339375	-0.125140
H	3.818008	-1.915573	1.455654
C	4.833187	-2.458481	-2.214839
H	5.186647	-0.357968	-2.285248
C	4.423485	-3.541225	-1.446378
H	3.740881	-4.175066	0.484744
H	5.126984	-2.606432	-3.244116
H	4.397969	-4.533014	-1.873948
C	5.455691	1.314956	-0.138611
H	5.959191	1.311280	-1.087141
N	5.732520	2.407063	0.637045
O	5.156140	2.559294	1.724349
O	6.565717	3.231042	0.227525
H	3.368313	1.089169	-2.634016
H	2.473685	2.516288	-3.113151
H	1.096655	0.460825	-3.412403
H	0.386525	1.520077	-2.210753
H	-4.321780	3.296083	-0.972864
H	-4.857539	4.147732	0.469593
H	-2.793939	2.668064	0.809028
H	-4.123987	2.321610	1.905418
H	-8.818996	-0.696110	-0.693178
H	-7.883742	-0.246452	0.715537
H	-6.834328	0.101022	-2.120143
H	-7.821802	1.303093	-1.326417

(3-4)$_{\text{DBU2-}anti}$ (*re-re*)$_{60}$

E_0 = -1610.5785737
E_{0+ZPE} = -1609.901283
E_{298} = -1609.867939
H_{298} = -1609.866995
G_{298} = -1609.970096
NImag = 1 (-318.6306)

N	-5.957905	-0.238140	0.608574
C	-6.103377	-0.614353	2.011360
C	-4.915803	-1.425289	2.476824
C	-3.638918	-0.692685	2.142349
N	-3.658572	-0.303696	0.749429
C	-4.755422	-0.115866	0.065368
C	-4.608642	0.263622	-1.374228
C	-5.044518	1.694466	-1.692568
C	-6.547599	1.880565	-1.804287
C	-7.332074	1.504156	-0.559099
C	-7.175915	0.050034	-0.141918
O	-1.341992	-0.087394	-0.507430
C	-0.517638	-0.984283	-0.169541
O	-0.683158	-1.847487	0.696640
C	0.784382	-0.955685	-0.989971
N	1.854941	-1.743335	-0.396437
C	1.997362	-3.041229	-1.047904
C	0.870718	-3.081077	-2.067872
C	0.592980	-1.614281	-2.353177
C	2.518007	-1.378862	0.701924
C	2.475341	-0.068244	1.165652
C	3.052021	0.306586	2.499804
C	4.177759	-0.612740	2.935477
C	3.735019	-2.055762	2.809472
C	3.389901	-2.406814	1.370890
H	1.083291	0.080424	-1.097343
H	-0.399127	-1.428987	-2.755302
H	1.330643	-1.222185	-3.051711
H	1.151664	-3.640631	-2.956533
H	-0.008461	-3.552813	-1.632916
H	2.979541	-3.094447	-1.523380
H	1.922775	-3.855772	-0.332294
H	2.860245	-2.216234	3.443257
H	4.509202	-2.736376	3.162969
H	1.662037	0.553858	0.825495
H	2.878656	-3.366878	1.351400

(3-4)$_{\text{DBU2-}anti}$ (*si-si*)$_{300}$

E_0 = -1610.5782112
E_{0+ZPE} = -1609.900668
E_{298} = -1609.867495
H_{298} = -1609.866551
G_{298} = -1609.968957
NImag = 1 (-336.1154)

N	-6.603872	0.771808	0.479264
C	-6.629545	2.222135	0.644025
C	-5.311705	2.729167	1.182829
C	-4.179907	2.192780	0.340120
N	-4.314537	0.758344	0.216734
C	-5.458380	0.131914	0.293733
C	-5.435741	-1.356076	0.142689
C	-6.077382	-1.855914	-1.152500
C	-7.595230	-1.891211	-1.124432
C	-8.259591	-0.551034	-0.860706
C	-7.887580	0.076821	0.473584
O	-2.122819	-0.695507	-0.116096
C	-1.099825	-0.153862	0.386719
O	-1.056971	0.927778	0.982647
C	0.183122	-0.989985	0.231406
N	1.403896	-0.270222	0.553715
C	1.828976	-0.511834	1.931138
C	0.781670	-1.466268	2.487869
C	0.204113	-2.130081	1.246747
C	1.966521	0.650193	-0.226175
C	1.277330	1.021095	-1.510320
C	1.678435	2.401129	-2.005798
C	3.185679	2.556857	-2.023039
C	3.742206	2.397032	-0.619453
C	3.211442	1.184024	0.089895
H	0.231352	-1.364053	-0.788647
H	-0.784854	-2.552578	1.399540
H	0.865557	-2.916179	0.886214
H	1.213093	-2.178046	3.187431
H	0.007902	-0.906817	3.009560
H	2.823364	-0.951548	1.946622
H	1.866746	0.431653	2.475455
H	3.495139	3.288493	-0.033725
H	4.832221	2.359321	-0.644067
H	0.201525	0.985972	-1.363759
H	3.563278	1.048843	1.101555

(3-4)$_{\text{DBU2-}anti}$ (*re-si*)$_{300}$

E_0 = -1610.5737969
E_{0+ZPE} = -1609.896610
E_{298} = -1609.863174
H_{298} = -1609.862230
G_{298} = -1609.966475
NImag = 1 (-331.8091)

N	-6.097687	-0.182716	0.701517
C	-6.164146	-0.308404	2.154052
C	-4.887937	-0.905055	2.700679
C	-3.702358	-0.127178	2.182230
N	-3.800800	-0.000307	0.744826
C	-4.929704	-0.050281	0.089865
C	-4.864316	0.071569	-1.399596
C	-5.455044	1.374293	-1.941368
C	-6.971685	1.388137	-2.019967
C	-7.681113	1.170436	-0.694473
C	-7.360856	-0.158787	-0.029117
O	-1.519124	0.046226	-0.601536
C	-0.731650	-0.845287	-0.173621
O	-0.914821	-1.585558	0.796113
C	0.549934	-0.986252	-1.015137
N	1.571233	-1.797897	-0.379273
C	1.683319	-3.116512	-0.990779
C	0.514433	-3.178989	-1.959076
C	0.282802	-1.723257	-2.326545
C	2.382771	-1.348690	0.576822
C	2.403885	-0.015400	0.980714
C	3.024904	0.394548	2.286121
C	4.146098	-0.522701	2.740359
C	3.720813	-1.970825	2.616584
C	3.367275	-2.308099	1.176665
H	0.919894	0.015980	-1.212963
H	-0.714039	-1.520568	-2.707370
H	1.005152	-1.403907	-3.077050
H	0.735453	-3.806308	-2.818971
H	-0.363238	-3.585594	-1.459483
H	2.644459	-3.187864	-1.504856
H	1.631273	-3.906065	-0.244910
H	2.856105	-2.157085	3.257083
H	4.513475	-2.639395	2.951663
H	1.582825	0.608652	0.661387
H	2.987804	-3.323620	1.116876

H	-2.731687	-0.226822	0.250590	H	1.523803	0.267809	-2.257624	H	-2.898600	0.028302	0.200105
H	-2.760490	-1.315634	2.285828	H	-3.435462	0.189238	0.096785	H	-2.763085	-0.631793	2.390227
H	-3.528340	0.195254	2.766234	H	-3.207321	2.383652	0.784681	H	-3.664446	0.865417	2.632856
H	-4.921088	-2.397851	1.985409	H	-4.190892	2.645216	-0.652580	H	-4.807739	-1.946366	2.389890
H	-4.988323	-1.592688	3.548419	H	-5.187116	2.403737	2.215261	H	-4.912436	-0.881538	3.787227
H	-7.016751	-1.195621	2.101836	H	-5.311359	3.816247	1.173508	H	-7.012277	-0.945639	2.387753
H	-6.220515	0.286504	2.615730	H	-7.435859	2.457480	1.333174	H	-6.353860	0.672589	2.592311
H	-7.229523	-0.604207	-1.013017	H	-6.862947	2.688515	-0.314193	H	-7.371832	-0.964986	-0.763896
H	-7.996936	-0.229391	0.510119	H	-7.899102	-0.674228	1.264751	H	-8.126887	-0.391957	0.703142
H	-3.559780	0.136257	-1.626106	H	-8.627053	0.824772	0.740621	H	-3.815659	0.002157	-1.674187
H	-5.176761	-0.440435	-1.983434	H	-4.393548	-1.659662	0.175200	H	-5.374022	-0.781976	-1.847706
H	-7.057671	2.146284	0.280025	H	-5.932900	-1.807026	1.002129	H	-7.455605	1.980182	0.001880
H	-8.391517	1.676673	-0.750427	H	-8.033734	0.155741	-1.661313	H	-8.757341	1.197353	-0.867220
H	-6.757062	2.920097	-2.057643	H	-9.340766	-0.692047	-0.864002	H	-7.294948	2.338191	-2.445826
H	-6.914057	1.280038	-2.640668	H	-7.957187	-2.287983	-2.073229	H	-7.293783	0.611725	-2.718522
H	-4.630427	2.376973	-0.949248	H	-7.915654	-2.596432	-0.353327	H	-5.097308	2.213606	-1.343339
H	-4.587105	1.965851	-2.643199	H	-5.725480	-1.251712	-1.989861	H	-5.051797	1.519578	-2.942605
C	3.867420	0.867764	-0.353679	H	-5.706454	-2.864757	-1.327811	C	3.784788	0.778654	-0.657327
H	4.707719	0.463675	0.189222	C	4.472551	-0.530848	-0.644709	H	3.107492	0.352691	-1.380724
C	3.531238	2.271218	-0.066516	H	4.326338	-0.196293	-1.660369	C	3.558462	2.193169	-0.330163
C	2.400858	2.893773	-0.601515	C	5.723291	-0.097902	-0.000336	C	2.403588	2.817135	-0.807181
C	4.382614	3.022662	0.743830	C	6.694654	0.546821	-0.765801	C	4.465614	2.955238	0.409205
C	2.137134	4.226428	-0.338107	C	5.989603	-0.337225	1.349681	C	2.163867	4.158337	-0.563263
H	1.715412	2.329732	-1.217773	C	7.903845	0.931139	-0.203499	H	1.688476	2.240422	-1.377683
C	4.120386	4.360155	1.004863	H	6.505987	0.734032	-1.813563	C	4.223272	4.297198	0.658843
H	5.265350	2.557895	1.160082	C	7.193676	0.049415	1.911582	H	5.370499	2.506112	0.790104
C	2.996517	4.966737	0.465646	H	5.242728	-0.815839	1.967327	C	3.073822	4.904883	0.174022
H	1.255755	4.689482	-0.757986	C	8.157701	0.684436	1.136716	H	1.267195	4.621265	-0.949261
H	4.795960	4.926007	1.630132	H	8.645851	1.423822	-0.815217	H	4.937810	4.869943	1.232308
H	2.787784	6.006800	0.670333	H	7.381115	-0.141193	2.958512	H	2.888858	5.951493	0.367786
C	3.649173	0.357586	-1.619631	H	9.096647	0.986077	1.577726	C	5.059378	0.239417	-0.651112
H	3.025166	0.814037	-2.365478	C	3.935181	-1.763589	-0.320209	H	5.909606	0.657480	-0.146182
N	4.240946	-0.807403	-2.028116	H	4.203952	-2.337156	0.547221	N	5.343016	-0.908905	-1.343367
O	4.973729	-1.439662	-1.255436	N	3.023044	-2.383879	-1.132530	O	4.450871	-1.509230	-1.959367
O	4.036023	-1.202735	-3.186196	O	2.621125	-1.827634	-2.162843	O	6.515228	-1.316271	-1.347716
H	4.297703	-2.524799	0.780323	O	2.633918	-3.519549	-0.820480	H	4.272380	-2.282203	0.565081
H	4.466131	-0.386867	3.962177	H	1.259017	2.555934	-2.999522	H	4.422344	-0.288624	3.768678
H	5.061257	-0.447529	2.314749	H	1.243299	3.163726	-1.356085	H	5.033747	-0.358612	2.127671
H	3.394136	1.342073	2.470161	H	3.617914	1.805101	-2.687291	H	3.381784	1.423434	2.214701
H	2.258936	0.283017	3.254555	H	3.468447	3.530335	-2.423741	H	2.243399	0.411187	3.053536

(3-4)$_{\text{DBU6-}anti}$ (*re-re*)$_{60}$

E_0 = -1610.5785206
E_{0+ZPE} = -1609.900558
E_{298} = -1609.867500
H_{298} = -1609.866556
G_{298} = -1609.967905
NImag = 1 (-323.4316)

N	-5.402185	0.986607	-0.284597
C	-5.953069	1.281008	-1.603987
C	-4.853331	1.385206	-2.635931
C	-3.977950	0.157361	-2.570668
N	-3.571672	-0.070250	-1.201270
C	-4.250161	0.343226	-0.164065
C	-3.688587	0.037310	1.187274
C	-4.504047	-0.994861	1.967381
C	-5.752269	-0.435153	2.627385
C	-6.752601	0.195314	1.673447
C	-6.199859	1.366839	0.877291
O	-1.195428	-1.193499	-0.784019
C	-0.361958	-0.764299	-1.623438
O	-0.605360	-0.044304	-2.602447
C	1.108066	-1.192916	-1.463785
N	1.416270	-1.736119	-0.148173
C	1.455124	-3.194689	-0.160428
C	1.078961	-3.575833	-1.584014
C	1.455853	-2.348204	-2.397360
C	1.495790	-0.993316	0.956076

(3-4)$_{\text{DBU6-}anti}$ (*re-re*)$_{180}$

E_0 = -1610.5743363
E_{0+ZPE} = -1609.896787
E_{298} = -1609.863509
H_{298} = -1609.862565
G_{298} = -1609.966385
NImag = 1 (-351.0302)

N	-5.722474	-0.331137	0.406641
C	-6.467195	0.618524	1.227378
C	-5.535385	1.404259	2.121056
C	-4.429056	2.012112	1.292877
N	-3.837327	0.991790	0.455377
C	-4.460897	-0.092846	0.079522
C	-3.698487	-1.067562	-0.759799
C	-4.196241	-1.164700	-2.202378
C	-5.447530	-2.007177	-2.378325
C	-6.653638	-1.531867	-1.586562
C	-6.437297	-1.506170	-0.081618
O	-1.276791	1.350863	-0.195902
C	-0.635081	1.719255	0.820855
O	-1.099965	1.969665	1.940539
C	0.888152	1.915135	0.678146
N	1.421489	1.456005	-0.593763
C	1.577622	2.561563	-1.539123
C	1.097958	3.788196	-0.774760
C	1.256242	3.394298	0.684492
C	1.648697	0.178518	-0.886440

(3-4)$_{\text{DBU6-}anti}$ (*re-re*)$_{300}$

E_0 = -1610.5695014
E_{0+ZPE} = -1609.892402
E_{298} = -1609.858984
H_{298} = -1609.858040
G_{298} = -1609.961771
NImag = 1 (-329.7996)

N	-5.507873	-0.050602	-0.949502
C	-6.049861	-1.280954	-1.518771
C	-4.944128	-2.253109	-1.858992
C	-4.039701	-2.431475	-0.663465
N	-3.623465	-1.132327	-0.182218
C	-4.333058	-0.045809	-0.337084
C	-3.778393	1.221925	0.228251
C	-4.555548	1.738004	1.440576
C	-5.838881	2.471735	1.092593
C	-6.849693	1.651801	0.309098
C	-6.337581	1.147438	-1.030842
O	-1.217287	-0.878335	0.935217
C	-0.419450	-1.747557	0.497359
O	-0.700982	-2.701424	-0.241297
C	1.050323	-1.662536	0.949479
N	1.423071	-0.350567	1.463080
C	1.448092	-0.328987	2.925590
C	0.976650	-1.715581	3.336126
C	1.316140	-2.583266	2.136492
C	1.519153	0.732805	0.691149

C	1.633258	0.388776	0.883836
C	1.506314	1.250711	2.106011
C	1.882217	0.524474	3.383947
C	1.154039	-0.802429	3.451413
C	1.527718	-1.701396	2.283005
H	1.724119	-0.326485	-1.675545
H	0.929627	-2.274677	-3.344932
H	2.527185	-2.343573	-2.592110
H	1.596705	-4.474537	-1.909515
H	0.008192	-3.758553	-1.651039
H	2.463653	-3.525683	0.098171
H	0.763900	-3.615983	0.565042
H	0.077253	-0.618731	3.440159
H	1.374100	-1.324308	4.382440
H	1.364403	0.868857	-0.044524
H	0.843574	-2.546534	2.248006
H	-2.636503	-0.524131	-1.041508
H	-3.067532	0.269467	-3.152899
H	-4.513011	-0.718350	-2.940473
H	-4.254724	2.275428	-2.444511
H	-5.293254	1.486000	-3.624826
H	-6.493003	2.220745	-1.530361
H	-6.669423	0.504304	-1.876012
H	-5.614442	2.023656	1.521827
H	-7.020748	1.960876	0.488934
H	-2.678865	-0.331854	1.032463
H	-3.610914	0.962810	1.758836
H	-7.149471	-0.549527	0.980977
H	-7.599260	0.565155	2.252456
H	-6.244804	-1.231781	3.185445
H	-5.451802	0.316262	3.362066
H	-4.759980	-1.826750	1.309276
H	-3.854217	-1.404789	2.739343
C	3.824244	0.458934	0.333110
H	4.082788	0.232215	1.356093
C	3.865723	1.882432	-0.037416
C	3.428022	2.347004	-1.280060
C	4.383782	2.804577	0.872156
C	3.516844	3.689972	-1.602761
H	3.000409	1.657547	-1.994368
C	4.476278	4.150446	0.547297
H	4.730601	2.460371	1.836443
C	4.043045	4.598160	-0.691150
H	3.169435	4.031195	-2.567359
H	4.886665	4.847186	1.264008
H	4.110178	5.646044	-0.945514
C	4.138728	-0.504823	-0.606931
H	4.174363	-0.338178	-1.667668
N	4.447004	-1.786044	-0.235387
O	4.424751	-2.113099	0.959157
O	4.759340	-2.600251	-1.117743
H	2.525242	-2.114884	2.426832
H	1.638101	1.141513	4.248895
H	2.959966	0.350359	3.414301
H	2.113899	2.148311	1.983623
H	0.474195	1.607886	2.188129

(3-4)$_{\text{DBU6-}anti}$ (*si-si*)$_{60}$

E_0 = -1610.571551
E_{0+ZPE} = -1609.894067
E_{298} = -1609.860805
H_{298} = -1609.859861
G_{298} = -1609.963322
NImag = 1 (-343.5992)

N	-5.986424	0.379660	-0.272474
C	-6.704975	-0.310401	-1.339809
C	-5.758340	-0.758633	-2.429282
C	-4.607357	-1.521148	-1.819608
N	-4.028957	-0.737422	-0.749987
C	1.529861	-0.844036	0.058437
C	1.398389	-2.270891	-0.380704
C	2.118634	-2.573784	-1.680124
C	1.771056	-1.538765	-2.729481
C	2.142294	-0.138174	-2.267142
H	1.360196	1.393050	1.504496
H	0.625036	3.961579	1.361481
H	2.291580	3.513334	1.002742
H	1.664877	4.676386	-1.041882
H	0.050172	3.979721	-0.998043
H	2.623220	2.651235	-1.833256
H	0.985149	2.394269	-2.435906
H	0.699508	-1.576053	-2.937431
H	2.282064	-1.747582	-3.669090
H	0.981191	-0.613774	0.959746
H	1.768441	0.592677	-2.977725
H	-2.826547	1.111689	0.196863
H	-3.629794	2.412984	1.910114
H	-4.813526	2.817572	0.665558
H	-5.109849	0.744752	2.876664
H	-6.095328	2.181914	2.634379
H	-7.175220	0.051231	1.824964
H	-7.036881	1.285209	0.578092
H	-5.919014	-2.408831	0.244325
H	-7.397846	-1.496993	0.422776
H	-2.660468	-0.748296	-0.749980
H	-3.738689	-2.047757	-0.283525
H	-6.967170	-0.539867	-1.917727
H	-7.487637	-2.205507	-1.785141
H	-5.705363	-2.040063	-3.437174
H	-5.221926	-3.035135	-2.083699
H	-4.354004	-0.161548	-2.601318
H	-3.393276	-1.604921	-2.792149
C	3.456108	-0.781111	1.164738
H	2.966858	-0.094091	1.835447
C	4.456936	-0.163197	0.283220
C	5.319733	-0.900204	-0.532812
C	4.582432	1.227149	0.288360
C	6.269249	-0.265224	-1.316016
H	5.255299	-1.977597	-0.559880
C	5.531454	1.863817	-0.496899
H	3.935301	1.811116	0.926624
C	6.378633	1.119711	-1.304931
H	6.928098	-0.854774	-1.937372
H	5.614046	2.941010	-0.470173
H	7.121719	1.611789	-1.915616
C	3.636889	-2.066605	1.654522
H	4.313459	-2.798476	1.254960
N	2.883598	-2.519502	2.704143
O	2.019162	-1.790166	3.209290
O	3.089845	-3.667418	3.129490
H	3.231029	-0.026638	-2.254841
H	1.857079	-3.573604	-2.026828
H	3.196463	-2.569272	-1.511744
H	1.773770	-2.921971	0.412134
H	0.335772	-2.513765	-0.483927

(3-4)$_{\text{DBU6-}anti}$ (*si-si*)$_{180}$

E_0 = -1610.5769283
E_{0+ZPE} = -1609.899615
E_{298} = -1609.866333
H_{298} = -1609.865389
G_{298} = -1609.968210
NImag = 1 (-366.4766)

N	-6.031022	0.165232	-0.524916
C	-6.846430	-1.022557	-0.286635
C	-6.006944	-2.277819	-0.352235
C	-4.801698	-2.131689	0.545281
N	-4.132042	-0.884532	0.249018
C	1.550513	0.672347	-0.700600
C	1.100798	1.847105	-1.529950
C	1.306832	3.200177	-0.871416
C	0.928255	3.158284	0.595526
C	1.704804	2.071432	1.328343
H	1.673010	-1.938757	0.105842
H	0.731194	-3.496919	2.079360
H	2.370253	-2.856655	2.150127
H	1.456469	-2.049506	4.252879
H	-0.098498	-1.706369	3.501771
H	2.459942	-0.125302	3.277912
H	0.791013	0.442621	3.317888
H	-0.141733	2.966821	0.703452
H	1.127548	4.118609	1.070548
H	1.345393	-0.285478	-1.155984
H	1.433878	2.058589	2.378227
H	-2.676159	-1.053197	0.267210
H	-3.136154	-2.983897	-0.903978
H	-4.558237	-2.964233	0.135066
H	-4.367005	-1.874497	-2.702097
H	-5.377956	-3.205396	-2.153205
H	-6.604282	-1.010584	-2.413693
H	-6.753547	-1.723562	-0.812157
H	-5.790560	1.934424	-1.551143
H	-7.178856	0.880858	-1.661929
H	-2.749621	1.017885	0.509657
H	-3.758641	1.980850	-0.554730
H	-7.197257	0.801883	0.899529
H	-7.723824	2.272790	0.111324
H	-6.303892	2.826992	2.012524
H	-5.586877	3.362106	0.511009
H	-4.763483	0.907376	2.117162
H	-3.899071	2.417668	1.982324
C	3.798079	0.582672	-1.021355
H	3.553506	0.943043	-2.009410
C	3.953661	-0.873914	-0.902233
C	4.472051	-1.491312	0.237272
C	3.615673	-1.674304	-1.996680
C	4.638605	-2.866892	0.279409
H	4.751128	-0.903279	1.098707
C	3.783483	-3.047177	-1.954786
H	3.217006	-1.208854	-2.887597
C	4.293206	-3.650883	-0.812200
H	5.042662	-3.327968	1.169298
H	3.517610	-3.647019	-2.813190
H	4.424610	-4.722587	-0.775540
C	4.571091	1.436747	-0.252271
H	5.036861	1.177667	0.679661
N	4.865891	2.711766	-0.664512
O	4.445883	3.141619	-1.745826
O	5.581439	3.409286	0.069655
H	2.777707	2.298555	1.281618
H	0.716315	3.953463	-1.394181
H	2.350131	3.495365	-0.970581
H	1.592784	1.827367	-2.503851
H	0.034153	1.709757	-1.739461

(3-4)$_{\text{DBU6-}anti}$ (*si-si*)$_{300}$

E_0 = -1610.577716
E_{0+ZPE} = -1609.900256
E_{298} = -1609.867029
H_{298} = -1609.866084
G_{298} = -1609.968635
NImag = 1 (-345.6221)

N	6.019548	0.547867	0.244740
C	6.939921	-0.582347	0.169006
C	6.233550	-1.876640	0.499793
C	4.989669	-2.007973	-0.345639
N	4.211096	-0.792396	-0.248713

C	-4.702700	0.139031	-0.052695
C	-3.974632	0.853638	1.040383
C	-4.423234	0.442193	2.443607
C	-5.720580	1.087936	2.899260
C	-6.921371	0.807594	2.011379
C	-6.757275	1.282936	0.576244
O	-1.417046	-1.007680	-0.257768
C	-0.800863	-1.401489	-1.281284
O	-1.293801	-1.671167	-2.385157
C	0.718584	-1.619915	-1.155535
N	1.330530	-0.942857	-0.020083
C	1.506329	-1.844349	1.117552
C	0.895638	-3.158642	0.655286
C	1.013057	-3.088055	-0.859399
C	1.541212	0.369145	0.053266
C	1.105825	1.244813	-1.075614
C	0.555977	2.574242	-0.574159
C	1.562851	3.281123	0.310988
C	1.988775	2.401158	1.473940
C	2.241435	0.961431	1.104729
H	1.181115	-1.301836	-2.085509
H	0.329467	-3.750889	-1.382469
H	2.028287	-3.327091	-1.174189
H	1.411358	-4.015253	1.082204
H	-0.151296	-3.209855	0.946181
H	2.562607	-1.960496	1.348299
H	1.008715	-1.432121	1.994388
H	1.202699	2.413485	2.237076
H	2.871392	2.824031	1.955830
H	0.373447	0.751519	-1.705381
H	2.491223	0.326289	1.942693
H	1.991108	1.432517	-1.696298
H	-3.002353	-0.848987	-0.560651
H	-3.812753	-1.716776	-2.533728
H	-4.947446	-2.478801	-1.422738
H	-5.379623	0.109256	-2.968195
H	-6.294651	-1.383296	-3.139122
H	-7.439646	0.383278	-1.739499
H	-7.243511	-1.160219	-0.917716
H	-6.309900	2.277271	0.552020
H	-7.732093	1.367213	0.107153
H	-2.919217	0.632192	0.913749
H	-4.100408	1.928616	0.909319
H	-7.158209	-0.258086	2.007357
H	-7.789210	1.319088	2.428462
H	-5.942177	0.758220	3.914492
H	-5.572968	2.169579	2.951475
H	-4.498688	-0.645042	2.496728
H	-3.629729	0.727185	3.133234
C	4.317261	0.945569	0.246547
H	4.518010	1.681705	1.010873
C	4.676180	-0.437038	0.596009
C	5.077746	-0.715553	1.904899
C	4.675868	-1.477282	-0.334624
C	5.459569	-1.993011	2.276887
H	5.093948	0.083349	2.633680
C	5.052009	-2.758192	0.039342
H	4.384318	-1.293724	-1.357713
C	5.441404	-3.023322	1.344972
H	5.772957	-2.185425	3.292940
H	5.044803	-3.551701	-0.694271
H	5.736997	-4.022124	1.631920
C	4.458696	1.390414	-1.059204
H	4.472926	0.758083	-1.926967
N	4.665003	2.713832	-1.351347
O	4.714178	3.562042	-0.451443
O	4.818754	3.030193	-2.540514
H	0.296616	3.195713	-1.430953
H	-0.368768	2.393168	-0.022299
H	2.438223	3.554037	-0.275476
C	-4.734245	0.159937	-0.254536
C	-3.903491	1.378373	-0.500796
C	-4.239217	2.547641	0.426476
C	-5.475610	3.331038	0.021340
C	-6.756551	2.516755	-0.040348
C	-6.709999	1.357642	-1.023149
O	-1.496721	-0.781797	0.670162
C	-0.978852	-1.906241	0.450795
O	-1.564792	-2.933519	0.082769
C	0.538412	-2.054588	0.679821
N	1.228647	-0.799433	0.943564
C	1.447557	-0.595632	2.372624
C	0.771967	-1.787495	3.032518
C	0.810527	-2.854348	1.950243
C	1.542622	0.107382	0.023718
C	1.168635	-0.174224	-1.400509
C	0.942301	1.093310	-2.211007
C	2.094953	2.063202	-2.051308
C	2.281557	2.433721	-0.591496
C	2.275454	1.255405	0.335061
H	0.959283	-2.544867	-0.193681
H	0.081025	-3.646640	2.087813
H	1.800737	-3.306183	1.895005
H	1.279358	-2.085062	3.946516
H	-0.259026	-1.543942	3.282219
H	2.515147	-0.578058	2.588798
H	1.025242	0.356963	2.687949
H	1.491918	3.127468	-0.285972
H	3.219414	2.980177	-0.461628
H	0.279190	-0.794641	-1.440029
H	2.351979	1.517931	1.380520
H	1.980912	-0.757769	-1.844246
H	-3.095131	-0.841416	0.404832
H	-4.074121	-2.923456	0.391135
H	-5.098807	-2.142665	1.594918
H	-5.682596	-2.450037	-1.378136
H	-6.607410	-3.130667	-0.045756
H	-7.620700	-1.046552	-1.048749
H	-7.336278	-0.932211	0.684021
H	-6.251611	1.671981	-1.961539
H	-7.721435	1.043613	-1.258888
H	-2.866557	1.086628	-0.361969
H	-4.018768	1.681850	-1.542017
H	-7.020320	2.134837	0.947656
H	-7.571306	3.172394	-0.348736
H	-5.612561	4.159320	0.716918
H	-5.300416	3.778324	-0.960338
H	-4.337639	2.182761	1.449953
H	-3.382407	3.220050	0.422647
C	4.366102	0.539622	0.388031
H	4.179473	0.266913	1.413226
C	4.479409	-0.598039	-0.536119
C	4.229664	-1.882378	-0.049917
C	4.862502	-0.460897	-1.872983
C	4.351430	-2.994401	-0.869504
H	3.950751	-2.007907	0.986176
C	4.986108	-1.570886	-2.691683
H	5.064011	0.517812	-2.281882
C	4.729218	-2.842948	-2.195444
H	4.157330	-3.979227	-0.469322
H	5.284649	-1.442872	-3.722287
H	4.827329	-3.707017	-2.836426
C	5.136809	1.679438	0.204276
H	5.649847	1.947134	-0.700140
N	5.251640	2.604419	1.205803
O	4.639810	2.444464	2.272254
O	5.974008	3.595993	1.018463
H	3.006373	1.604337	-2.436290
H	1.921848	2.962582	-2.642544
H	0.802966	0.823061	-3.257495
C	4.722176	0.375444	0.037511
C	3.784446	1.539347	0.099192
C	3.969023	2.539726	-1.043054
C	5.141558	3.488250	-0.860785
C	6.494732	2.812745	-0.717557
C	6.593637	1.870217	0.471800
O	1.571694	-0.945249	-0.543762
C	1.122097	-2.036927	-0.104842
O	1.786091	-2.986993	0.329318
C	-0.404425	-2.240694	-0.134218
N	-1.167475	-1.030775	-0.396331
C	-1.486328	-0.891049	-1.815937
C	-0.903768	-2.141652	-2.461661
C	-0.803811	-3.129320	-1.308910
C	-1.385907	-0.066848	0.493572
C	-0.773689	-0.204612	1.859826
C	-0.625936	1.131318	2.570209
C	-1.918163	1.921927	2.520243
C	-2.297740	2.209959	1.078333
C	-2.238498	0.993638	0.198775
H	-0.709739	-2.675705	0.814129
H	-0.082874	-3.924207	-1.476307
H	-1.773925	-3.577759	-1.100511
H	-1.526484	-2.503532	-3.276125
H	0.085000	-1.928943	-2.862817
H	-2.562620	-0.830191	-1.953536
H	-1.043292	0.025856	-2.204468
H	-1.622776	2.973440	0.677768
H	-3.294513	2.650470	1.027852
H	0.199632	-0.679347	1.771145
H	-2.464873	1.167563	-0.842360
H	-1.402213	-0.872825	2.446777
H	3.168364	-0.868032	-0.365199
H	4.349377	-2.820431	-0.013752
H	5.249701	-2.188252	-1.389632
H	5.964907	-1.889105	1.555625
H	6.904965	-2.711770	0.317609
H	7.743340	-0.398874	0.876814
H	7.377568	-0.622628	-0.829634
H	6.134204	2.320093	1.352782
H	7.637306	1.700660	0.715894
H	2.777126	1.134272	0.072887
H	3.907834	2.043674	1.058137
H	6.752337	2.266803	-1.627060
H	7.256303	3.582559	-0.589424
H	5.173098	4.177565	-1.704861
H	4.962170	4.097796	0.028442
H	4.056044	2.001624	-1.988167
H	3.053291	3.125878	-1.109730
C	-4.192634	-0.055166	0.517382
H	-4.076694	0.072310	1.582945
C	-5.034527	0.945589	-0.159889
C	-5.742354	1.870912	0.606993
C	-5.178988	0.983358	-1.548831
C	-6.578185	2.802171	0.006702
H	-5.648794	1.849716	1.683677
C	-6.009723	1.914034	-2.147841
H	-4.627583	0.287866	-2.165898
C	-6.714586	2.827785	-1.372483
H	-7.122252	3.506319	0.619619
H	-6.106725	1.929872	-3.223928
H	-7.362436	3.553408	-1.842521
C	-4.188647	-1.359030	0.051689
H	-4.546881	-1.663846	-0.914035
N	-3.754339	-2.395994	0.833555
O	-3.304219	-2.179614	1.966615
O	-3.846227	-3.549267	0.386473
H	-0.318528	0.951826	3.600068
H	0.170734	1.711145	2.098487
H	-2.708893	1.350032	3.010783

H	1.142148	4.211183	0.694946

(3-4)$_{\mathbf{DBU6}\text{-}anti}$ (*si-re*)$_{60}$

E_0 = -1610.5741068
E_{0+ZPE} = -1609.896936
E_{298} = -1609.863617
H_{298} = -1609.862673
G_{298} = -1609.966528
NImag = 1 (-357.0693)

N	6.074250	0.476756	0.379933
C	6.983676	-0.657578	0.248039
C	6.239190	-1.964008	0.400541
C	5.056675	-1.985877	-0.536601
N	4.288175	-0.771297	-0.369997
C	4.792346	0.351420	0.068602
C	3.865773	1.519276	0.186988
C	4.160596	2.641724	-0.809996
C	5.316663	3.543542	-0.413832
C	6.649991	2.836943	-0.240010
C	6.640349	1.748098	0.820552
O	1.660800	-0.898655	-0.804006
C	1.218825	-2.022867	-0.450493
O	1.888546	-2.991598	-0.067079
C	-0.303683	-2.249833	-0.513972
N	-1.082880	-1.049293	-0.771304
C	-1.515360	-0.965695	-2.159329
C	-0.828951	-2.141004	-2.835190
C	-0.665298	-3.139781	-1.701071
C	-1.409062	-0.145495	0.148110
C	-0.806146	-0.269730	1.516020
C	-0.628860	1.079743	2.194491
C	-1.926449	1.861191	2.183631
C	-2.395394	2.096111	0.757559
C	-2.333161	0.868188	-0.107599
H	-0.615944	-2.702295	0.424015
H	0.094302	-3.893681	-1.884311
H	-1.609354	-3.646421	-1.502370
H	-1.412172	-2.528104	-3.666892
H	0.145227	-1.839337	-3.215674
H	-2.600248	-1.057238	-2.221700
H	-1.235131	-0.003431	-2.586464
H	-1.776640	2.877111	0.302766
H	-3.411041	2.495798	0.755225
H	0.149126	-0.781549	1.457692
H	-2.601233	1.028824	-1.141466
H	-1.463404	-0.898190	2.119123
H	3.254179	-0.822057	-0.551328
H	4.382914	-2.813211	-0.332679
H	5.387481	-2.064087	-1.573225
H	5.896984	-2.072937	1.429237
H	6.910097	-2.791065	0.183033
H	7.742543	-0.561237	1.019364
H	7.484052	-0.605751	-0.720156
H	6.114098	2.090148	1.712552
H	7.658538	1.527858	1.123803
H	2.860225	1.140914	0.027739
H	3.909174	1.905062	1.206071
H	6.987920	2.409603	-1.185930
H	7.398248	3.572990	0.054903
H	5.424137	4.329297	-1.162010
H	5.063782	4.044338	0.524134
H	4.331084	2.214142	-1.799345
H	3.258170	3.246407	-0.890812
C	-4.246485	-0.258918	0.294692
H	-3.880331	-1.066589	-0.319394
C	-5.122837	0.706771	-0.386025
C	-5.823212	1.707164	0.291562
C	-5.296993	0.596024	-1.767268
C	-6.666533	2.567614	-0.394485
H	0.016166	1.568184	-1.880794

(3-4)$_{\mathbf{DBU6}\text{-}anti}$ (*si-re*)$_{180}$

E_0 = -1610.5737477
E_{0+ZPE} = -1609.896245
E_{298} = -1609.863053
H_{298} = -1609.862109
G_{298} = -1609.964843
NImag = 1 (-343.5265)

N	-6.040492	0.419479	-0.244736
C	-6.842311	-0.565933	-0.964211
C	-5.978626	-1.400434	-1.881486
C	-4.811475	-1.961978	-1.106192
N	-4.150527	-0.889385	-0.394648
C	-4.753608	0.206488	-0.015532
C	-3.937493	1.218778	0.722966
C	-4.323391	1.359845	2.196460
C	-5.562999	2.202578	2.441034
C	-6.824921	1.695430	1.764232
C	-6.724954	1.610264	0.249766
O	-1.508478	-1.091371	-0.027850
C	-0.987748	-1.776289	-0.945018
O	-1.576050	-2.324244	-1.887446
C	0.535009	-2.004167	-0.886535
N	1.242908	-1.085899	-0.003749
C	1.506784	-1.689957	1.301020
C	0.841333	-3.055388	1.228710
C	0.835372	-3.363373	-0.259917
C	1.483192	0.193726	-0.274968
C	0.959630	0.765144	-1.561063
C	0.498730	2.205278	-1.383518
C	1.600745	3.055633	-0.786052
C	2.054840	2.497299	0.552203
C	2.246407	1.009228	0.564808
H	0.923348	-1.939398	-1.899107
H	0.102745	-4.111049	-0.549977
H	1.818507	-3.704685	-0.581589
H	1.378817	-3.797019	1.814368
H	-0.178682	-2.998427	1.602559
H	2.578008	-1.782408	1.461862
H	1.096356	-1.060186	2.088999
H	1.320656	2.756775	1.322255
H	2.986908	2.978410	0.861717
H	0.143757	0.164417	-1.947981
H	2.507477	0.599098	1.530310
H	1.758757	0.725841	-2.306462
H	-3.115877	-0.972162	-0.242548
H	-4.065341	-2.417956	-1.750691
H	-5.149517	-2.714906	-0.392672
H	-5.612105	-0.785025	-2.702495
H	-6.574299	-2.203889	-2.307013
H	-7.589586	-0.024261	-1.537432
H	-7.366551	-1.196382	-0.244535
H	-6.240325	2.501035	-0.151951
H	-7.721422	1.576417	-0.178226
H	-2.900554	0.906224	0.644413
H	-4.025115	2.182603	0.220540
H	-7.107605	0.716967	2.157078
H	-7.643879	2.375284	2.000269
H	-5.737024	2.271368	3.515046
H	-5.367780	3.220426	2.094418
H	-4.442705	0.368994	2.637338
H	-3.480281	1.822237	2.708100
C	4.321693	0.757091	-0.280457
H	3.990842	0.737217	-1.307738
C	4.642918	-0.553268	0.302557
C	5.103232	-0.702334	1.613985
C	4.534393	-1.689408	-0.498137
C	5.433407	-1.951787	2.106960
H	-1.819109	2.857772	3.070357

(3-4)$_{\mathbf{DBU6}\text{-}anti}$ (*si-re*)$_{300}$

E_0 = -1610.5746715
E_{0+ZPE} = -1609.896740
E_{298} = -1609.863654
H_{298} = -1609.862710
G_{298} = -1609.965228
NImag = 1 (-342.8168)

N	5.901033	-0.692350	-0.449480
C	6.691365	0.073457	-1.408634
C	5.798512	0.791055	-2.394302
C	4.749708	1.579394	-1.648154
N	4.093537	0.715752	-0.691020
C	4.659009	-0.335693	-0.158615
C	3.854609	-1.121656	0.827051
C	4.372691	-1.017821	2.262826
C	5.574946	-1.896579	2.561282
C	6.794978	-1.626178	1.697617
C	6.554902	-1.818910	0.208935
O	1.529640	1.169993	-0.086694
C	0.930751	1.720934	-1.046025
O	1.433109	2.100404	-2.112562
C	-0.579058	1.985857	-0.889423
N	-1.200251	1.295932	0.232544
C	-1.230926	2.142125	1.426539
C	-0.637666	3.469174	0.969808
C	-0.827048	3.449674	-0.539389
C	-1.511211	0.004443	0.246534
C	-1.095913	-0.854757	-0.909594
C	-0.756176	-2.267485	-0.453359
C	-1.901122	-2.877002	0.330704
C	-2.250117	-2.028528	1.543894
C	-2.271648	-0.547978	1.276888
H	-1.064841	1.709401	-1.820984
H	-0.151880	4.112092	-1.073237
H	-1.850502	3.718153	-0.798370
H	-1.129183	4.313606	1.446029
H	0.422139	3.512141	1.212471
H	-2.244843	2.260003	1.798330
H	-0.643831	1.672094	2.214792
H	-1.516879	-2.217466	2.334767
H	-3.208916	-2.346325	1.957514
H	-0.241577	-0.418381	-1.416550
H	-2.400725	0.064985	2.157563
H	-1.910878	-0.892428	-1.635797
H	3.089834	0.914427	-0.457150
H	3.976966	1.966752	-2.305956
H	5.201452	2.422890	-1.124137
H	5.316479	0.066246	-3.049621
H	6.400561	1.451104	-3.013593
H	7.343445	-0.624907	-1.925951
H	7.322137	0.781582	-0.869293
H	5.979510	-2.728045	0.030871
H	7.505060	-1.944990	-0.299759
H	2.838390	-0.742407	0.776864
H	3.828309	-2.165990	0.513694
H	7.174220	-0.617145	1.869112
H	7.589226	-2.312669	1.992039
H	5.846850	-1.777851	3.610371
H	5.284464	-2.942653	2.434959
H	4.595918	0.024814	2.493882
H	3.555657	-1.307610	2.922319
C	-4.341163	-0.035606	0.632170
H	-4.566753	-0.197293	1.675162
C	-4.732522	-1.133982	-0.261312
C	-4.571796	-1.075806	-1.648374
C	-5.346041	-2.261494	0.287837
C	-4.990492	-2.121593	-2.453064

H	-5.720027	1.817274	1.360594
C	-6.145561	1.449351	-2.451484
H	-4.764853	-0.176220	-2.305573
C	-6.832430	2.443176	-1.766540
H	-7.199458	3.335581	0.147417
H	-6.272643	1.338056	-3.518659
H	-7.493931	3.112428	-2.297256
C	-4.440312	-0.572345	1.629179
H	-4.974542	0.027939	2.340895
N	-3.944204	-1.736778	2.154307
O	-3.293768	-2.518403	1.446280
O	-4.177261	-1.987613	3.346732
H	-0.281629	0.919859	3.214925
H	0.149155	1.647247	1.679330
H	-2.681588	1.300738	2.736134
H	-1.805327	2.817004	2.693890

(3-4)$_{\textbf{DBU6-}\textit{anti}}$ $(\textit{re-si})_{60}$

E_0 = -1610.5721705
E_{0+ZPE} = -1609.894852
E_{298} = -1609.861513
H_{298} = -1609.860569
G_{298} = -1609.963849
NImag = 1 (-324.4205)

N	5.649420	-0.426437	-0.750123
C	6.504512	0.742734	-0.929643
C	5.674825	1.986369	-1.152936
C	4.644219	2.113999	-0.057607
N	3.931346	0.863288	0.082639
C	4.422929	-0.295427	-0.265907
C	3.552093	-1.495812	-0.073652
C	4.042628	-2.440436	1.025020
C	5.181096	-3.353708	0.604357
C	6.434611	-2.636898	0.132533
C	6.215145	-1.732874	-1.070136
O	1.387283	1.035009	0.843326
C	0.836000	1.963033	0.194688
O	1.396895	2.759226	-0.570101
C	-0.683372	2.163602	0.361988
N	-1.307427	1.129633	1.175878
C	-1.398452	1.551004	2.574901
C	-0.873144	2.981627	2.587571
C	-0.993401	3.434628	1.141669
C	-1.525102	-0.118178	0.757850
C	-1.582457	-0.444217	-0.594007
C	-1.450952	-1.866553	-1.064116
C	-1.832257	-2.907721	-0.023554
C	-1.275462	-2.540042	1.336066
C	-1.789009	-1.179973	1.785034
H	-1.111006	2.203328	-0.634227
H	-0.313793	4.239645	0.879699
H	-2.008531	3.757697	0.916881
H	-1.430070	3.609226	3.278879
H	0.170615	2.989662	2.896466
H	-2.434347	1.492897	2.908041
H	-0.800812	0.909833	3.218175
H	-0.184304	-2.516795	1.299489
H	-1.551478	-3.287358	2.079798
H	-1.201379	0.289449	-1.289116
H	-1.325891	-0.911344	2.729322
H	2.927223	0.916043	0.392608
H	3.900337	2.872930	-0.283725
H	5.118127	2.368561	0.891363
H	5.177308	1.925813	-2.120294
H	6.324562	2.857764	-1.166161
H	7.141470	0.553576	-1.788999
H	7.147707	0.855694	-0.055439
H	5.585686	-2.229581	-1.809483
H	7.166220	-1.532925	-1.552758

(3-4)$_{\textbf{DBU6-}\textit{anti}}$ $(\textit{re-si})_{180}$

E_0 = -1610.5713338
E_{0+ZPE} = -1609.894422
E_{298} = -1609.860886
H_{298} = -1609.859941
G_{298} = -1609.964706
NImag = 1 (-328.9950)

N	-5.482813	0.096976	-1.131567
C	-5.915205	-0.991762	-2.003340
C	-4.732011	-1.789043	-2.502084
C	-3.866609	-2.195410	-1.334502
N	-3.561095	-1.026988	-0.538427
C	-4.336958	0.022347	-0.470817
C	-3.896767	1.146595	0.410445
C	-4.767019	1.319347	1.656639
C	-6.074344	2.051346	1.408098
C	-6.992990	1.391102	0.394134
C	-6.383244	1.237282	-0.989992
O	-1.231642	-0.960800	0.754658
C	-0.388473	-1.714790	0.203338
O	-0.587589	-2.462113	-0.764474
C	1.026871	-1.768517	0.807897
N	1.348956	-0.610304	1.632968
C	1.246996	-0.919578	3.059904
C	0.708831	-2.340371	3.103701
C	1.159837	-2.935605	1.781845
C	1.542557	0.609870	1.132110
C	1.694013	0.853170	-0.233714
C	1.366882	2.199374	-0.809703
C	1.519453	3.360136	0.160331
C	0.962093	3.006309	1.523415
C	1.651875	1.768807	2.080744
H	1.733451	-1.869052	-0.007882
H	0.572654	-3.793377	1.466148
H	2.203301	-3.241592	1.837886
H	1.080603	-2.886058	3.967391
H	-0.377548	-2.321033	3.156017
H	2.230114	-0.845470	3.527131
H	0.578321	-0.229837	3.566836
H	-0.111587	2.816235	1.455452
H	1.095195	3.832580	2.221608
H	1.488681	0.029423	-0.901721
H	1.236489	1.519986	3.050655
H	-2.642145	-1.009026	-0.027637
H	-2.917207	-2.621048	-1.646018
H	-4.378560	-2.932161	-0.713528
H	-4.149448	-1.186185	-3.198150
H	-5.086922	-2.666403	-3.036765
H	-6.450734	-0.547699	-2.837945
H	-6.613885	-1.630118	-1.460653
H	-5.863399	2.150649	-1.281826
H	-7.172284	1.080037	-1.718072

(3-4)$_{\textbf{DBU6-}\textit{anti}}$ $(\textit{re-si})_{300}$

E_0 = -1610.5736467
E_{0+ZPE} = -1609.896848
E_{298} = -1609.863305
H_{298} = -1609.862361
G_{298} = -1609.967047
NImag = 1 (-334.8414)

N	-5.513375	0.888618	0.086365
C	-6.237458	1.192638	-1.143675
C	-5.277975	1.394128	-2.294048
C	-4.344173	0.211530	-2.389534
N	-3.770566	-0.056052	-1.088856
C	-4.332364	0.289465	0.038749
C	-3.600733	-0.042551	1.299154
C	-4.282933	-1.132468	2.127265
C	-5.454765	-0.643619	2.960599
C	-6.584581	-0.012048	2.165154
C	-6.165849	1.203650	1.353144
O	-1.359106	-1.166723	-1.009017
C	-0.593287	-0.635368	-1.853812
O	-0.909239	0.193675	-2.718502
C	0.885260	-1.067361	-1.854561
N	1.292550	-1.771047	-0.650974
C	1.459545	-3.200698	-0.880483
C	0.938833	-3.416099	-2.291410
C	1.176982	-2.075345	-2.965177
C	1.581713	-1.161898	0.496936
C	1.638192	0.225381	0.619044
C	1.563112	0.891842	1.963552
C	2.110860	0.041797	3.095969
C	1.564608	-1.367665	3.005580
C	1.943402	-2.009590	1.679825
H	1.478922	-0.168405	-1.994380
H	0.552812	-1.906406	-3.838149
H	2.219033	-1.986896	-3.270721
H	1.447560	-4.238509	-2.788097
H	-0.125754	-3.641871	-2.266702
H	2.518870	-3.451902	-0.791647
H	0.903967	-3.787305	-0.152708
H	0.476938	-1.348387	3.103255
H	1.944831	-1.985622	3.818582
H	1.225023	0.808084	-0.190742
H	1.484543	-2.990189	1.597831
H	-2.813964	-0.494037	-1.061312
H	-3.515635	0.399160	-3.066901
H	-4.875848	-0.673912	-2.740331
H	-4.702571	2.305728	-2.134953
H	-5.838249	1.510371	-3.218315
H	-6.815409	2.095955	-0.970405
H	-6.937950	0.384347	-1.358961
H	-5.517515	1.850842	1.945092
H	-7.042448	1.789099	1.096732

H	2.559938	-1.128257	0.172151
H	3.472808	-2.032749	-1.019546
H	6.872547	-2.050939	0.942765
H	7.176984	-3.383502	-0.150420
H	5.436213	-4.007255	1.438931
H	4.829299	-4.004354	-0.200296
H	4.325538	-1.859519	1.904288
H	3.194963	-3.055330	1.325076
C	-3.670702	0.199410	-1.126484
H	-3.280872	0.128027	-2.130447
C	-4.520016	-0.921363	-0.706017
C	-4.796686	-1.936385	-1.623709
C	-5.115596	-0.987151	0.556289
C	-5.629889	-2.992524	-1.288620
H	-4.363858	-1.888109	-2.612625
C	-5.945196	-2.043513	0.892183
H	-4.927684	-0.210504	1.283012
C	-6.203178	-3.053320	-0.026940
H	-5.833300	-3.765829	-2.015262
H	-6.394441	-2.078846	1.874298
H	-6.851695	-3.875941	0.237428
C	-3.942037	1.480938	-0.677963
H	-4.564604	1.726013	0.162322
N	-3.457525	2.570039	-1.349262
O	-2.687213	2.416796	-2.308649
O	-3.802743	3.700116	-0.974034
H	-2.864093	-1.237852	1.971813
H	-1.467667	-3.886948	-0.335432
H	-2.916796	-2.983914	0.048884
H	-2.041012	-2.012023	-1.971490
H	-0.411271	-2.028609	-1.367382
H	-2.872153	0.936321	0.702690
H	-3.886628	2.070471	-0.168742
H	-7.318900	0.411611	0.749233
H	-7.891262	2.000154	0.289263
H	-6.605454	2.157904	2.354252
H	-5.848505	3.064366	1.065900
H	-4.956876	0.342813	2.105404
H	-4.183943	1.882364	2.384200
C	3.952743	0.722308	-0.466379
H	4.153749	1.109898	0.520345
C	4.074872	-0.734652	-0.612024
C	4.512602	-1.483746	0.479539
C	3.823920	-1.394065	-1.818337
C	4.702038	-2.854042	0.370731
H	4.721204	-0.984373	1.415335
C	4.001802	-2.761699	-1.922463
H	3.472063	-0.838258	-2.675441
C	4.442803	-3.498873	-0.828462
H	5.050828	-3.416446	1.225047
H	3.794047	-3.258193	-2.859391
H	4.582979	-4.566656	-0.914381
C	4.292977	1.555978	-1.514572
H	4.296973	1.274167	-2.551368
N	4.687350	2.854480	-1.297274
O	4.785764	3.299929	-0.147179
O	4.969155	3.550549	-2.282453
H	2.711603	1.982236	2.243327
H	1.017563	4.240390	-0.242504
H	2.573975	3.612398	0.265204
H	1.988345	2.370978	-1.693429
H	0.335752	2.167416	-1.177083
H	-2.605053	-0.366697	1.010586
H	-3.488225	0.865305	1.892708
H	-7.043500	-0.744439	1.498287
H	-7.362014	0.309615	2.858749
H	-5.849330	-1.478531	3.539997
H	-5.087651	0.088058	3.684796
H	-4.596605	-1.944110	1.468639
H	-3.531212	-1.552896	2.794005
C	3.777176	0.499743	-0.121916
H	3.496553	-0.029052	-1.019487
C	3.691445	1.964774	-0.196421
C	3.107202	2.547541	-1.323322
C	4.201114	2.805313	0.795535
C	3.039220	3.923347	-1.460835
H	2.707061	1.910593	-2.100468
C	4.128009	4.183061	0.660884
H	4.663381	2.388088	1.677579
C	3.548274	4.748256	-0.466145
H	2.589604	4.351961	-2.344830
H	4.528608	4.816709	1.439043
H	3.495566	5.822307	-0.569993
C	4.745065	-0.120217	0.649866
H	5.285044	0.337506	1.457063
N	5.124287	-1.413315	0.400998
O	4.574911	-2.069118	-0.495731
O	6.039722	-1.897853	1.084876
H	3.023703	-2.172957	1.653698
H	1.856367	0.493329	4.055019
H	3.199781	0.005839	3.041160
H	2.079359	1.852506	1.927426
H	0.515479	1.134211	2.173604

Other conformations in enamine-DBU carboxylate pathway

(3-4)$_{\textbf{DBU3-}\textit{anti}}$ (*re-re*)$_{60}$

E_0 = -1610.5781509
E_{0+ZPE} = -1609.901061
E_{298} = -1609.867669
H_{298} = -1609.866725
G_{298} = -1609.969740
NImag = 1 (-321.3942)

N	-5.929504	0.637611	-0.252637
C	-6.272966	1.987364	-0.688884
C	-5.302970	2.478021	-1.737795
C	-3.889313	2.306251	-1.237704
N	-3.704254	0.952747	-0.760682
C	-4.678588	0.204121	-0.311105
C	-4.327511	-1.170089	0.159491
C	-4.509404	-1.372044	1.665133
C	-5.942619	-1.606270	2.108706
C	-6.903532	-0.479773	1.771175
C	-7.008563	-0.187230	0.283402
O	-1.192400	0.244864	-1.176378
C	-0.576335	-0.760631	-0.728964
O	-1.023954	-1.629592	0.026716
C	0.863896	-0.885184	-1.258309
N	1.702227	-1.747058	-0.437600
C	1.834629	-3.081695	-1.011437
C	0.953751	-3.053472	-2.250736
C	0.893273	-1.579198	-2.616874
C	2.162307	-1.398061	0.764113
C	2.155803	-0.070258	1.177967
C	2.477267	0.307313	2.594662
C	3.389396	-0.692145	3.281844
C	2.846929	-2.093945	3.092454
C	2.782316	-2.468573	1.620214
H	1.284605	0.111134	-1.320763

(3-4)$_{\textbf{DBU4-}\textit{anti}}$ (*re-re*)$_{60}$

E_0 = -1610.5786376
E_{0+ZPE} = -1609.901211
E_{298} = -1609.867932
H_{298} = -1609.866988
G_{298} = -1609.969382
NImag = 1 (-311.8496)

N	-5.726149	1.062790	0.327067
C	-5.996768	2.395335	-0.202026
C	-4.716712	3.180826	-0.362032
C	-3.721023	2.366401	-1.151036
N	-3.601471	1.048795	-0.564842
C	-4.556357	0.474805	0.120959
C	-4.295594	-0.896902	0.650939
C	-5.126561	-1.982024	-0.036207
C	-6.556202	-2.086361	0.465815
C	-7.382321	-0.820964	0.307365
C	-6.813622	0.389378	1.031138
O	-1.230934	0.050263	-1.170049
C	-0.601691	-0.830844	-0.523140
O	-1.020121	-1.483398	0.438905
C	0.814951	-1.094729	-1.066435
N	1.658909	-1.821581	-0.129234
C	1.751454	-3.237267	-0.468580
C	0.826594	-3.404154	-1.664299
C	0.784610	-2.016042	-2.282279
C	2.148912	-1.283504	0.988602
C	2.185575	0.094849	1.165413
C	2.538995	0.704525	2.490419
C	3.430516	-0.188839	3.333223
C	2.842264	-1.583607	3.396680
C	2.749348	-2.207099	2.013021
H	1.255216	-0.136790	-1.318304

(3-4)$_{\textbf{DBU5-}\textit{anti}}$ (*re-re*)$_{60}$

E_0 = -1610.5784448
E_{0+ZPE} = -1609.901010
E_{298} = -1609.867709
H_{298} = -1609.866765
G_{298} = -1609.969370
NImag = 1 (-319.9735)

N	-5.756195	0.130866	0.017797
C	-6.447800	-0.898359	0.786563
C	-5.826373	-2.254499	0.549101
C	-4.336720	-2.175021	0.779033
N	-3.790310	-1.071836	0.018684
C	-4.483393	-0.014660	-0.320430
C	-3.780680	1.049241	-1.097042
C	-3.555033	2.335771	-0.301147
C	-4.775751	3.234361	-0.208270
C	-5.991706	2.591645	0.436464
C	-6.498078	1.351739	-0.284551
O	-1.193116	-1.448704	-0.393115
C	-0.504076	-0.912069	-1.295738
O	-0.910331	-0.153083	-2.188749
C	0.999532	-1.242398	-1.345874
N	1.515161	-1.799726	-0.102946
C	1.652975	-3.250538	-0.175319
C	1.115391	-3.617788	-1.549816
C	1.295887	-2.343874	-2.359062
C	1.691532	-1.083926	1.008141
C	1.725772	0.305833	0.969910
C	1.710121	1.123805	2.228229
C	2.298549	0.390151	3.419238
C	1.676129	-0.986514	3.530673
C	1.956298	-1.822843	2.291837
H	1.523471	-0.329340	-1.603984

H	0.032103	-1.317371	-3.225851	H	-0.090729	-1.840117	-2.901320	H	0.645632	-2.282405	-3.227234
H	1.797333	-1.288724	-3.149869	H	1.676467	-1.847793	-2.883944	H	2.328696	-2.256785	-2.692756
H	1.360429	-3.671015	-3.047655	H	1.190868	-4.163342	-2.351912	H	1.643976	-4.467546	-1.974599
H	-0.040663	-3.421681	-2.006995	H	-0.166496	-3.697229	-1.328913	H	0.059946	-3.873992	-1.480794
H	2.883530	-3.260431	-1.259131	H	2.788093	-3.476070	-0.717871	H	2.707632	-3.513333	-0.065433
H	1.516017	-3.847870	-0.309488	H	1.450459	-3.866060	0.365217	H	1.097134	-3.742348	0.618771
H	1.846604	-2.151227	3.527226	H	1.845683	-1.531640	3.840368	H	0.597174	-0.880643	3.663525
H	3.460713	-2.826189	3.616532	H	3.439527	-2.232265	4.037089	H	2.050883	-1.516206	4.406188
H	1.496678	0.610459	0.661477	H	1.541154	0.695285	0.542216	H	1.302817	0.791573	0.104188
H	2.210576	-3.387223	1.508436	H	2.148964	-3.112657	2.066466	H	1.343393	-2.721059	2.317932
H	-2.734159	0.556214	-0.832751	H	-2.692274	0.543770	-0.717981	H	-2.775928	-1.129515	-0.242800
H	-6.281883	2.653582	0.174963	H	-2.735794	2.824009	-1.141224	H	-3.835600	-3.082750	0.454614
H	-7.280520	1.955078	-1.093117	H	-4.034344	2.274744	-2.191712	H	-4.115194	-2.033613	1.837618
H	-7.923643	0.360979	0.084414	H	-4.305236	3.416164	0.619015	H	-6.024379	-2.574070	-0.473496
H	-7.068863	-1.117406	-0.282576	H	-4.926911	4.118450	-0.870246	H	-6.275080	-2.982489	1.220039
H	-4.929507	-1.896073	-0.389172	H	-6.661846	2.896105	0.495962	H	-7.487836	-0.900294	0.472489
H	-3.282281	-1.344560	-0.090157	H	-6.519263	2.304908	-1.155466	H	-6.419618	-0.636990	1.845524
H	-7.899670	-0.751229	2.121892	H	-6.482466	0.114018	2.032869	H	-6.508237	1.514462	-1.362839
H	-6.625118	0.436096	2.295933	H	-7.591500	1.136050	1.152961	H	-7.523138	1.153763	0.011626
C	3.924189	0.647588	-0.037461	H	-3.233042	-1.100496	0.524594	H	-2.826614	0.640370	-1.427634
H	4.587852	0.182201	0.674860	H	-4.494527	-0.903754	1.723638	H	-4.361191	1.265458	-1.995046
C	3.692226	2.088957	0.148278	H	-7.512991	-0.574654	-0.748075	H	-5.786498	2.336924	1.478025
C	2.759941	2.801738	-0.609532	H	-8.378895	-1.002258	0.710811	H	-6.805571	3.317279	0.446819
C	4.446788	2.781642	1.095395	H	-7.056319	-2.905417	-0.051838	H	-4.513179	4.135715	0.346222
C	2.596116	4.163998	-0.428907	H	-6.535558	-2.357862	1.524421	H	-5.047587	3.560158	-1.215499
H	2.147556	2.287304	-1.336597	H	-5.112818	-1.824069	-1.115860	H	-3.189079	2.087189	0.696535
C	4.285413	4.148358	1.273658	H	-4.623740	-2.932482	0.138645	H	-2.751942	2.883281	-0.792655
H	5.176576	2.246523	1.686777	C	3.956272	0.535848	-0.180036	C	3.816603	0.540955	0.139907
C	3.359158	4.844743	0.512832	H	4.617015	0.172884	0.591962	H	4.221030	0.309384	1.113091
H	1.866918	4.696959	-1.022050	C	3.774037	1.994845	-0.235713	C	3.715816	1.971787	-0.188067
H	4.884572	4.666405	2.008611	C	2.848256	2.602035	-1.087695	C	3.086327	2.430826	-1.347161
H	3.228550	5.908077	0.652291	C	4.571813	2.809788	0.567880	C	4.293162	2.907257	0.670759
C	3.915531	0.111358	-1.311650	C	2.732352	3.980231	-1.137300	C	3.044505	3.782890	-1.639572
H	3.509617	0.598651	-2.178612	H	2.204734	1.992784	-1.706616	H	2.613428	1.726851	-2.017086
N	4.455892	-1.119788	-1.570818	C	4.458474	4.191838	0.515132	C	4.255077	4.262668	0.375568
O	4.947845	-1.792446	-0.654701	H	5.297107	2.356408	1.228822	H	4.788931	2.567027	1.569171
O	4.451877	-1.533585	-2.740385	C	3.538020	4.782170	-0.336836	C	3.630133	4.705399	-0.780002
H	3.780935	-2.675493	1.237045	H	2.008275	4.431679	-1.800293	H	2.549281	4.119810	-2.538886
H	3.472518	-0.451724	4.341851	H	5.090445	4.805019	1.141373	H	4.713881	4.970729	1.050617
H	4.396928	-0.631844	2.864046	H	3.444988	5.857780	-0.377306	H	3.595571	5.760343	-1.010557
H	2.919806	1.304183	2.614105	C	3.900044	-0.206579	-1.344122	C	4.067966	-0.374905	-0.864556
H	1.545510	0.391489	3.163811	H	3.491977	0.142991	-2.274402	H	3.951835	-0.179642	-1.914641
H	-3.163973	2.480853	-2.027307	N	4.389804	-1.484515	-1.398952	N	4.515231	-1.637660	-0.580939
H	-3.676306	3.007561	-0.430132	O	4.879860	-2.009917	-0.390485	O	4.680044	-1.993904	0.593904
H	-5.502935	3.523866	-1.956424	O	4.341846	-2.091304	-2.479738	O	4.762393	-2.404528	-1.524070
H	-5.440354	1.911616	-2.658431	H	3.737089	-2.508849	1.666487	H	2.993763	-2.155391	2.286893
H	-3.910439	-2.237808	1.944139	H	3.538224	0.230182	4.333764	H	2.129079	0.963824	4.330644
H	-4.081024	-0.522537	2.199231	H	4.432594	-0.237876	2.900816	H	3.380346	0.291676	3.304477
H	-5.956567	-1.778851	3.185273	H	3.010678	1.675122	2.330631	H	2.238712	2.062616	2.057877
H	-6.308259	-2.525786	1.644500	H	1.618529	0.916002	3.044699	H	0.677953	1.408601	2.458220

(3-4)$_{\textbf{DBU7-}\textit{anti}}$ $(\textit{re-re})_{60}$

E_0 = -1610.578597
E_{0+ZPE} = -1609.901082
E_{298} = -1609.867897
H_{298} = -1609.866952
G_{298} = -1609.968707
NImag = 1 (-318.7860)

N	5.722129	-1.128986	0.270773
C	5.952026	-1.656195	1.611559
C	4.654910	-2.099977	2.245959
C	3.639913	-0.986581	2.155776
N	3.563083	-0.513176	0.790845
C	4.554898	-0.595017	-0.058664
C	4.337191	-0.043455	-1.429146
C	5.130955	1.235237	-1.701047
C	6.592983	1.001503	-2.041436
C	7.388566	0.265761	-0.976083
C	6.857462	-1.120833	-0.647056

O	1.249280	0.699120	0.345963
C	0.622780	0.639176	-0.741591
O	1.019391	0.126362	-1.798712
C	-0.765852	1.302157	-0.806819
N	-1.349714	1.553979	0.503610
C	-1.193788	2.947366	0.907424
C	-0.392174	3.584234	-0.217044
C	-0.687952	2.698618	-1.416551
C	-1.822590	0.590785	1.295748
C	-2.122520	-0.670131	0.792383
C	-2.447825	-1.818641	1.702106
C	-3.045077	-1.374923	3.024720
C	-2.185634	-0.286470	3.634338
C	-2.116155	0.934556	2.730751
H	-1.408116	0.658775	-1.397113
H	0.064260	2.758145	-2.198244
H	-1.655147	2.959081	-1.843303
H	-0.676986	4.621228	-0.376222
H	0.669731	3.555777	0.019449
H	-2.182796	3.399721	1.009933
H	-0.682718	3.029503	1.863200
H	-1.178503	-0.676446	3.798066
H	-2.568519	0.016492	4.608701
H	-1.686093	-0.946666	-0.154859
H	-1.345942	1.609329	3.098020
H	2.667115	-0.051704	0.493550
H	6.441520	-0.893040	2.218630
H	6.634413	-2.496792	1.521576
H	7.634570	-1.700979	-0.159875
H	6.592272	-1.654481	-1.560096
H	8.414150	0.147779	-1.327142
H	7.438925	0.853330	-0.057267
H	6.647965	0.430788	-2.971991
H	7.069144	1.961658	-2.241712
C	-4.076326	-0.135856	-0.215865
H	-4.562962	-0.116622	0.747139
C	-4.226548	-1.382481	-0.982832
C	-3.544641	-1.614920	-2.179559
C	-5.105348	-2.360926	-0.517355
C	-3.745757	-2.785333	-2.890436
H	-2.841439	-0.882667	-2.550871
C	-5.310080	-3.532414	-1.232074
H	-5.644898	-2.194247	0.404483
C	-4.630828	-3.749150	-2.421037
H	-3.206239	-2.949406	-3.812186
H	-6.000669	-4.274259	-0.857458
H	-4.785277	-4.662012	-2.977869
C	-3.980313	1.072967	-0.879144
H	-3.747782	1.183839	-1.922196
N	-4.196672	2.258820	-0.229186
O	-4.465212	2.269429	0.979990
O	-4.129891	3.312784	-0.880099
H	-3.055254	1.485657	2.766240
H	-3.126288	-2.226078	3.700889
H	-4.057482	-0.994447	2.871702
H	-3.120535	-2.508637	1.191030
H	-1.535242	-2.392374	1.895747
H	2.649869	-1.327458	2.445803
H	3.911776	-0.159589	2.812933
H	4.277779	-2.983590	1.732072
H	4.832062	-2.367944	3.284425
H	4.605429	-0.808808	-2.158845
H	3.269273	0.136903	-1.541719
H	4.653199	1.741018	-2.539088
H	5.041453	1.908841	-0.847134

***syn*-addition**

(3-4) **DBU-*syn*** $(re\text{-}re)_{180}$
E_0 = -1610.5758495
E_{0+ZPE} = -1609.897980

(3-4)$_{DBU2\text{-}syn}$ $(re\text{-}re)_{180}$
E_0 = -1610.5758048
E_{0+ZPE} = -1609.898143

(3-4)$_{DBUx\text{-}syn}$ $(re\text{-}re)_{180}$
E_0 = -1610.5761759
E_{0+ZPE} = -1609.898270

E_{298} = -1609.864859
H_{298} = -1609.863914
G_{298} = -1609.966232
NImag = 1 (-370.9171)

N	5.451061	1.125960	-0.583586
C	5.163415	1.871791	-1.805864
C	3.676218	1.933109	-2.067480
C	3.091657	0.543308	-2.003333
N	3.504437	-0.092543	-0.770856
C	4.606912	0.208017	-0.136240
C	4.905524	-0.551940	1.116369
C	6.097361	-1.502424	0.985177
C	7.452401	-0.825227	1.093918
C	7.713187	0.249196	0.052129
C	6.720658	1.400342	0.083373
O	1.813969	-1.820649	0.366802
C	0.621687	-1.540843	0.068551
O	0.241057	-0.606385	-0.645499
C	-0.410310	-2.509085	0.670833
N	-1.793267	-2.085536	0.493315
C	-2.479011	-2.888945	-0.515363
C	-1.374128	-3.708226	-1.153939
C	-0.371598	-3.868623	-0.025204
C	-2.406257	-1.126920	1.185732
C	-3.716911	-0.733367	0.894789
C	-4.546390	0.002551	1.911918
C	-3.734594	0.780490	2.935318
C	-2.567975	-0.045073	3.437018
C	-1.655111	-0.436365	2.284693
H	-0.170774	-2.620301	1.724807
H	0.632191	-4.117983	-0.355626
H	-0.704204	-4.642111	0.667034
H	-1.742645	-4.655849	-1.538589
H	-0.929702	-3.157291	-1.981555
H	-3.214193	-3.528358	-0.019739
H	-3.012077	-2.263007	-1.226352
H	-2.933259	-0.946273	3.934646
H	-1.990058	0.511470	4.174552
H	-4.279156	-1.403551	0.261357
H	-0.845884	-1.061841	2.647814
H	2.844352	-0.779800	-0.330647
H	5.685689	1.404390	-2.641879
H	5.566835	2.872813	-1.680478
H	7.143870	2.255984	-0.432457
H	6.533123	1.715071	1.110796
H	8.704466	0.669269	0.224721
H	7.726530	-0.181032	-0.950886
H	7.542013	-0.377079	2.086700
H	8.232889	-1.583640	1.027310
C	-3.573087	0.660374	-0.830125
H	-2.862789	-0.003374	-1.297397
C	-3.000679	1.889368	-0.263828
C	-3.786157	2.971608	0.142435
C	-1.611135	2.001898	-0.174130
C	-3.198434	4.126418	0.632265
H	-4.862531	2.922026	0.079898
C	-1.026223	3.161839	0.310347
H	-0.991726	1.166556	-0.477196
C	-1.816015	4.227617	0.718922
H	-3.822485	4.952084	0.943103
H	0.050834	3.231873	0.368919
H	-1.360255	5.131231	1.097670
C	-4.857674	0.670661	-1.355746
H	-5.610424	1.404392	-1.139243
N	-5.304969	-0.350213	-2.145491
O	-4.545393	-1.281969	-2.453876
O	-6.478846	-0.319180	-2.546780
H	-1.188496	0.458657	1.866975
H	-4.378759	1.078219	3.763098
H	-3.349004	1.696983	2.489530

E_{298} = -1609.865014
H_{298} = -1609.864070
G_{298} = -1609.966252
NImag = 1 (-375.7360)

N	5.710876	0.886245	-0.922818
C	5.330658	2.208777	-1.410922
C	3.884527	2.228677	-1.850350
C	3.011400	1.673982	-0.751135
N	3.542534	0.402581	-0.311342
C	4.802226	0.068942	-0.412055
C	5.196473	-1.277355	0.105958
C	6.054193	-1.216580	1.371189
C	7.518238	-0.899006	1.120582
C	7.774710	0.426991	0.424836
C	7.129772	0.543581	-0.947458
O	1.859184	-1.407632	0.688495
C	0.683710	-1.255925	0.258887
O	0.285059	-0.361964	-0.495626
C	-0.293000	-2.341007	0.743077
N	-1.694759	-2.042190	0.479936
C	-2.237872	-2.881556	-0.583867
C	-1.019168	-3.556387	-1.182052
C	-0.071985	-3.659047	-0.000115
C	-2.438364	-1.166416	1.154036
C	-3.762428	-0.894785	0.791739
C	-4.715090	-0.257284	1.765750
C	-4.039851	0.580671	2.840067
C	-2.832600	-0.139347	3.404385
C	-1.820156	-0.435422	2.307896
H	-0.120548	-2.476602	1.807071
H	0.969427	-3.791580	-0.277921
H	-0.359968	-4.491538	0.641785
H	-1.263099	-4.520467	-1.621101
H	-0.589536	-2.928332	-1.960853
H	-2.923562	-3.612180	-0.146387
H	-2.798462	-2.294403	-1.306306
H	-3.142447	-1.074837	3.875446
H	-2.352593	0.459838	4.177892
H	-4.220067	-1.607865	0.121945
H	-0.987873	-1.000636	2.715914
H	2.868186	-0.303250	0.076512
H	1.992886	1.495611	-1.083344
H	2.973299	2.361748	0.094911
H	3.765637	1.629610	-2.752629
H	3.593278	3.248656	-2.088049
H	5.981877	2.449651	-2.246639
H	5.508469	2.945293	-0.625949
H	7.272889	-0.377220	-1.513735
H	7.614520	1.334831	-1.509634
H	4.276898	-1.816934	0.312666
H	5.722531	-1.823012	-0.677909
H	7.442691	1.260425	1.046692
H	8.850057	0.547359	0.290701
H	8.050145	-0.911131	2.072252
H	7.951521	-1.698933	0.514984
H	5.622119	-0.496172	2.067620
H	5.984894	-2.189399	1.856028
C	-3.666952	0.524558	-0.911112
H	-2.871706	-0.058371	-1.348461
C	-3.245817	1.794863	-0.304594
C	-4.150454	2.795802	0.059323
C	-1.880258	2.032772	-0.130691
C	-3.701682	3.994838	0.588514
H	-5.211830	2.647962	-0.068619
C	-1.434483	3.236692	0.392580
H	-1.169831	1.260520	-0.399503
C	-2.342118	4.221374	0.757905
H	-4.416124	4.756766	0.865424
H	-0.374029	3.405366	0.516115
H	-1.994305	5.159603	1.165882

E_{298} = -1609.865114
H_{298} = -1609.864170
G_{298} = -1609.966761
NImag = 1 (-367.9092)

N	-5.076617	-0.172436	0.051283
C	-5.793661	0.464001	1.151887
C	-5.179522	1.802172	1.493788
C	-3.695163	1.637848	1.712984
N	-3.121850	0.916348	0.597985
C	-3.795876	0.090109	-0.159238
C	-3.055706	-0.580892	-1.271724
C	-2.866649	-2.084793	-1.064893
C	-4.090637	-2.921897	-1.392959
C	-5.330046	-2.583626	-0.582279
C	-5.805913	-1.149490	-0.751666
O	-0.571763	1.390822	-0.059280
C	-0.285611	2.609964	0.076131
O	-0.968102	3.469286	0.647793
C	1.019191	3.107059	-0.568745
N	1.968993	2.048357	-0.884512
C	2.005547	1.758965	-2.314885
C	0.861459	2.570120	-2.893354
C	0.743093	3.740559	-1.932540
C	2.744186	1.417173	-0.004219
C	3.530810	0.320730	-0.372832
C	4.694498	-0.117833	0.473167
C	4.582393	0.272329	1.938651
C	4.104370	1.702553	2.078083
C	2.744302	1.884449	1.420855
H	1.457887	3.836420	0.105005
H	-0.223864	4.235020	-1.957833
H	1.509274	4.485238	-2.147630
H	1.059762	2.876788	-3.917329
H	-0.053461	1.980615	-2.887266
H	2.969519	2.082326	-2.716011
H	1.907531	0.693317	-2.507684
H	4.823406	2.383500	1.617140
H	4.030643	1.984310	3.128238
H	3.671854	0.178472	-1.433810
H	2.444743	2.926169	1.479218
H	-2.120986	1.108562	0.357018
H	-5.785023	-0.200418	2.017305
H	-6.826701	0.589948	0.840568
H	-6.842789	-1.069506	-0.442291
H	-5.768330	-0.857630	-1.801688
H	-6.143362	-3.238079	-0.897059
H	-5.162427	-2.779517	0.478483
H	-4.324540	-2.800898	-2.453614
H	-3.846220	-3.974617	-1.249982
C	2.148258	-1.421978	-0.398504
H	1.399993	-0.814504	-0.883067
C	1.898003	-1.704148	1.021185
C	2.610593	-2.667636	1.740061
C	0.868026	-1.015936	1.666624
C	2.307166	-2.924886	3.067008
H	3.407717	-3.224428	1.271121
C	0.561986	-1.280829	2.992427
H	0.313499	-0.265275	1.116868
C	1.282536	-2.233337	3.699937
H	2.870537	-3.671753	3.607888
H	-0.240177	-0.740083	3.474596
H	1.046101	-2.439139	4.734022
C	2.799772	-2.357930	-1.189035
H	3.425695	-3.149482	-0.823605
N	2.764569	-2.277881	-2.552255
O	2.092861	-1.396182	-3.111086
O	3.409717	-3.108051	-3.211369
H	1.990958	1.316689	1.971890
H	5.548530	0.141416	2.426875
H	3.878705	-0.384432	2.449397

H	-5.244053	0.668216	1.396635
H	-5.174925	-0.723952	2.436846
H	2.005564	0.550128	-2.007203
H	3.429142	-0.056475	-2.849813
H	3.196755	2.568108	-1.323100
H	3.499526	2.374980	-3.044738
H	5.078722	0.153026	1.929700
H	4.011274	-1.116525	1.363798
H	6.010589	-2.241416	1.780638
H	6.021903	-2.053148	0.046290
C	-4.916766	0.416586	-1.505803
H	-5.751824	1.064171	-1.317357
N	-5.216542	-0.629680	-2.331445
O	-4.349091	-1.470218	-2.616912
O	-6.366834	-0.713693	-2.789009
H	-1.400967	0.500277	1.930935
H	-4.755616	0.807277	3.630646
H	-3.717133	1.534177	2.422856
H	-5.442789	0.346630	1.216977
H	-5.299496	-1.047492	2.247811
H	4.824903	-1.199158	0.377894
H	5.607986	0.320717	0.059033
H	-5.356395	2.505879	0.681031
H	-5.652662	2.200352	2.387813
H	-3.179928	2.592349	1.772427
H	-3.500773	1.090310	2.636247
H	-2.541115	-2.273634	-0.040979
H	-2.045614	-2.397589	-1.708400
H	-3.580483	-0.396198	-2.209690
H	-2.086209	-0.096676	-1.343617

3_{DBU}

E_0 = -1096.5680552
E_{0+ZPE} = -1096.034119
E_{298} = -1096.010082
H_{298} = -1096.009138
G_{298} = -1096.091391
NImag = 0

C	-5.037874	-0.741660	0.463817
C	-4.012129	-0.268937	-0.276231
C	-3.337497	-1.127040	-1.313266
C	-4.111153	-2.396216	-1.631664
C	-4.609507	-3.066115	-0.366069
C	-5.571803	-2.140401	0.357214
N	-3.541504	1.016505	-0.162698
C	-2.277556	1.474671	-0.693354
C	-2.381457	2.985310	-0.491241
C	-3.105465	3.103664	0.843327
C	-4.043911	1.899376	0.866123
C	-1.028221	0.920093	0.009716
O	-1.137930	0.368417	1.110436
O	0.052149	1.112242	-0.622922
N	2.128937	0.182107	0.710218
C	2.035568	0.140896	2.152668
C	2.848829	-1.018739	2.674655
C	4.243381	-0.964084	2.094484
N	4.202609	-0.822278	0.642080
C	3.152729	-0.276853	0.042881
C	5.388018	-1.233471	-0.103434
C	6.145229	-0.090832	-0.762227
C	5.545329	0.375802	-2.077761
C	4.117639	0.885166	-1.984039
C	3.117996	-0.139905	-1.445817
H	-2.185191	1.237503	-1.750773
H	-1.409551	3.471404	-0.501697
H	-2.984876	3.412082	-1.292360
H	-3.639870	4.045144	0.950399
H	-2.391528	3.033467	1.661631
H	-5.079373	2.177610	0.649262
H	-4.039801	1.408414	1.842890
H	-5.777305	-2.528354	1.357399
H	-6.537056	-2.149972	-0.162812
H	-2.333892	-1.377934	-0.962141
H	-5.516153	-0.094849	1.185750
H	-3.202737	-0.549750	-2.227832
H	-3.477494	-3.069864	-2.209102
H	-4.967929	-2.150978	-2.264070
H	-3.759150	-3.289184	0.283087
H	-5.094752	-4.015247	-0.596473
H	1.294546	0.555422	0.174623
H	4.808944	-0.133788	2.520137
H	4.781486	-1.881413	2.318586
H	6.033040	-1.727156	0.616388
H	5.110989	-1.984422	-0.844367

3_{DBU1}

E_0 = -1096.5682627
E_{0+ZPE} = -1096.034206
E_{298} = -1096.010225
H_{298} = -1096.009281
G_{298} = -1096.090772
NImag = 0

N	3.991761	1.175408	-0.003564
C	3.999407	2.393687	-0.805984
C	2.633490	3.039161	-0.814352
C	1.595187	2.018168	-1.210789
N	1.745692	0.833362	-0.393918
C	2.877475	0.474335	0.154422
C	2.882634	-0.782455	0.961340
C	3.663261	-1.923835	0.307820
C	5.170101	-1.828035	0.475279
C	5.796164	-0.562210	-0.085089
C	5.268773	0.720834	0.537838
O	-0.525762	-0.492857	-0.311025
C	-0.905794	-1.279354	0.595675
O	-0.239917	-1.645907	1.577722
C	-2.315778	-1.878528	0.464729
N	-3.246366	-1.121548	-0.343832
C	-3.265353	-1.569669	-1.717936
C	-2.367806	-2.803178	-1.739663
C	-2.268991	-3.213852	-0.276736
C	-3.753670	0.105731	0.004059
C	-4.389241	0.913574	-0.872270
C	-4.959749	2.254457	-0.511573
C	-4.416827	2.772200	0.808571
C	-4.470511	1.671628	1.849898
C	-3.595147	0.494969	1.450150
H	-2.695417	-2.017744	1.473941
H	-1.373234	-3.785692	-0.047033
H	-3.134500	-3.810886	0.010975
H	-2.766180	-3.593154	-2.372725
H	-1.383427	-2.535505	-2.117020
H	-4.290707	-1.797866	-2.024305
H	-2.893603	-0.793400	-2.391903
H	-5.504440	1.334712	1.957310
H	-4.156577	2.039440	2.826957
H	-4.511960	0.595484	-1.898034
H	-3.833189	-0.360573	2.081599
H	0.888493	0.232695	-0.261290
H	4.322802	2.155659	-1.820587
H	4.732986	3.068672	-0.373667
H	5.970385	1.527874	0.354113
H	5.189182	0.614763	1.620365
H	3.301786	-0.564954	1.944738
H	1.845160	-1.077870	1.116561
H	6.870904	-0.595179	0.096431
H	5.663506	-0.512126	-1.167555
H	-4.741192	2.969472	-1.307982

3_{DBU2}

E_0 = -1096.5679216
E_{0+ZPE} = -1096.034121
E_{298} = -1096.009994
H_{298} = -1096.009050
G_{298} = -1096.091968
NImag = 0

N	-4.348036	-0.709561	-0.654754
C	-4.209508	-1.987600	-1.346485
C	-2.820531	-2.144300	-1.921905
C	-1.793658	-1.870564	-0.849989
N	-2.087038	-0.603470	-0.217747
C	-3.287079	-0.093724	-0.150738
C	-3.437901	1.215498	0.556216
C	-4.189788	1.106462	1.884268
C	-5.700237	1.035036	1.742336
C	-6.209601	-0.140156	0.925323
C	-5.696384	-0.171295	-0.505342
O	-0.045104	0.808435	0.680716
C	0.988407	0.605660	-0.022792
O	1.101369	-0.233523	-0.923420
C	2.165411	1.541312	0.297201
N	3.443436	1.135619	-0.242929
C	3.685456	1.711515	-1.546800
C	2.535045	2.691735	-1.761430
C	1.962899	2.902764	-0.366259
C	4.157507	0.044013	0.186735
C	3.742202	-0.531099	1.514889
C	4.769302	-1.488459	2.096636
C	5.285384	-2.444719	1.039246
C	5.990583	-1.664203	-0.056048
C	5.193058	-0.475062	-0.507104
H	2.210236	1.647267	1.378624
H	0.920873	3.211692	-0.367299
H	2.540127	3.653114	0.173998
H	2.863420	3.618325	-2.227294
H	1.782737	2.243233	-2.407169
H	4.660517	2.207446	-1.563619
H	3.702465	0.940146	-2.321233
H	6.184073	-2.317563	-0.909823
H	6.979071	-1.354995	0.303948
H	2.783054	-1.039679	1.392474
H	5.481531	-0.027065	-1.447470
H	3.566644	0.280086	2.221166
H	4.325365	-2.029668	2.932408
H	5.609550	-0.918728	2.500829
H	4.444785	-2.996600	0.611665
H	5.961079	-3.179446	1.478599
H	-1.271033	-0.038565	0.151346
H	-0.785740	-1.795527	-1.248184
H	-1.802810	-2.660777	-0.097534
H	-2.683650	-1.446321	-2.747499
H	-2.703129	-3.151445	-2.313976

H	7.162799	-0.436394	-0.946838
H	6.219912	0.738784	-0.056623
H	5.575109	-0.454653	-2.787718
H	6.174172	1.161396	-2.497421
H	0.980491	0.051448	2.396066
H	2.399731	1.082984	2.565663
H	2.908014	-0.984741	3.759700
H	2.370012	-1.957042	2.396513
H	4.074357	1.788496	-1.373246
H	3.783042	1.173545	-2.979683
H	3.299285	-1.114298	-1.900299
H	2.107816	0.158386	-1.710640
H	-6.053741	2.207776	-0.454803
H	-3.380671	3.094110	0.678050
H	-4.983751	3.643816	1.137476
H	-2.544883	0.727624	1.642043
H	3.319021	-2.851676	0.763103
H	3.399736	-1.987961	-0.749351
H	5.407350	-1.889408	1.540519
H	5.636690	-2.694687	0.005954
H	0.587642	2.397034	-1.064184
H	1.697781	1.750518	-2.263226
H	2.406227	3.428929	0.177393
H	2.629890	3.873889	-1.510567
H	-4.951774	-2.013194	-2.139820
H	-4.436109	-2.798133	-0.652042
H	-5.742052	0.824662	-0.947968
H	-6.336278	-0.809617	-1.105787
H	-2.435982	1.596873	0.730163
H	-3.944910	1.922173	-0.101353
H	-5.962186	-1.085011	1.412879
H	-7.297827	-0.087627	0.880630
H	-6.147692	0.999272	2.735984
H	-6.052752	1.959989	1.278896
H	-3.818715	0.245312	2.442346
H	-3.934939	1.986074	2.473999

3_{DBU3}

E_0 = -1096.5681456
E_{0+ZPE} = -1096.033940
E_{298} = -1096.009994
H_{298} = -1096.009050
G_{298} = -1096.090453
NImag = 0

N	4.343898	0.066607	-0.247980
C	5.290067	-0.810408	0.432851
C	4.741372	-2.213982	0.540156
C	3.354110	-2.171117	1.134171
N	2.544814	-1.217576	0.406949
C	3.042729	-0.185597	-0.223644
C	2.083540	0.730247	-0.910720
C	1.956770	2.096895	-0.236041
C	3.086535	3.060586	-0.556161
C	4.475149	2.567397	-0.185059
C	4.880167	1.272059	-0.871776
O	-0.015821	-1.702917	0.759371
C	-0.967061	-1.339241	0.010176
O	-0.862191	-0.756198	-1.076013
C	-2.362131	-1.710436	0.538242
N	-3.460323	-0.968983	-0.040639
C	-4.020384	-1.643048	-1.191102
C	-3.319842	-2.998612	-1.231867
C	-2.716097	-3.147199	0.158294
C	-3.678900	0.371786	0.164634
C	-2.956988	0.981527	1.336685
C	-3.490205	2.352958	1.718638
C	-3.716279	3.214053	0.491365
C	-4.765804	2.571107	-0.398236
C	-4.512381	1.105901	-0.603083
H	-2.337293	-1.597077	1.619556
H	-1.853035	-3.807663	0.187041
H	-3.459131	-3.529012	0.858469
H	-4.001793	-3.808293	-1.482497
H	-2.530896	-2.984645	-1.980773
H	-5.104218	-1.740224	-1.078730
H	-3.841052	-1.074567	-2.107450
H	-4.788561	3.074865	-1.367290
H	-5.757117	2.736902	0.039820
H	-1.891810	1.045419	1.101659
H	-5.036953	0.633946	-1.421919
H	-3.036951	0.313917	2.194316
H	-2.796158	2.830182	2.410936
H	-4.437499	2.238631	2.251230
H	-2.777731	3.308658	-0.060634
H	-4.023561	4.220908	0.776669
H	1.497663	-1.352452	0.437444
H	5.512285	-0.403038	1.420412
H	6.211867	-0.808307	-0.142222
H	5.959441	1.164727	-0.838867
H	4.597986	1.293827	-1.924799
H	2.401597	0.858548	-1.946310
H	1.114374	0.233288	-0.935307
H	5.202364	3.329064	-0.468136
H	4.563034	2.437875	0.895382

3_{DBU4}

E_0 = -1096.5680525
E_{0+ZPE} = -1096.034012
E_{298} = -1096.009948
H_{298} = -1096.009004
G_{298} = -1096.091462
NImag = 0

N	-4.377337	-0.755740	-0.357104
C	-5.055279	-1.706024	0.517916
C	-4.065518	-2.656632	1.149126
C	-2.949538	-1.870043	1.793071
N	-2.414822	-0.920909	0.841239
C	-3.110439	-0.424311	-0.148544
C	-2.432528	0.566223	-1.037647
C	-2.971636	1.989820	-0.885977
C	-4.273520	2.247542	-1.624206
C	-5.429631	1.354527	-1.207497
C	-5.173520	-0.130849	-1.409227
O	0.047123	-0.284004	1.519405
C	0.928219	0.241620	0.780867
O	0.804551	0.530044	-0.415650
C	2.247672	0.556672	1.505427
N	3.373072	0.849411	0.647179
C	3.496068	2.264872	0.381057
C	2.458861	2.924588	1.286055
C	2.123849	1.848985	2.310864
C	4.013325	-0.074313	-0.141576
C	3.743076	-1.518775	0.186538
C	4.729944	-2.472411	-0.467474
C	4.966433	-2.104425	-1.919327
C	5.582196	-0.718691	-2.001645
C	4.864949	0.271321	-1.130820
H	2.461483	-0.283132	2.162653
H	1.139498	1.965876	2.756573
H	2.862807	1.841915	3.112124
H	2.831116	3.839660	1.741493
H	1.571615	3.177804	0.709269
H	4.513024	2.601469	0.603981
H	3.306816	2.487440	-0.672395
H	5.570000	-0.369224	-3.036473
H	6.642155	-0.781052	-1.727678
H	2.723709	-1.765540	-0.119813
H	5.055115	1.316948	-1.327786
H	3.775064	-1.654519	1.267302
H	4.359876	-3.493901	-0.376460
H	5.681923	-2.433127	0.067584
H	4.013081	-2.113459	-2.453234
H	5.612323	-2.837654	-2.403731
H	-1.416528	-0.610519	0.988019
H	-2.136921	-2.518920	2.107702
H	-3.308877	-1.338300	2.675084
H	-3.655828	-3.318867	0.387051
H	-4.572498	-3.271334	1.888520
H	-5.773056	-2.254809	-0.085652
H	-5.610881	-1.159517	1.281607
H	-4.703708	-0.309348	-2.376955
H	-6.118950	-0.663159	-1.417679

3_{DBU5}

E_0 = -1096.5681425
E_{0+ZPE} = -1096.033983
E_{298} = -1096.010005
H_{298} = -1096.009061
G_{298} = -1096.090736
NImag = 0

N	-4.108682	-0.307864	0.549066
C	-4.378096	-0.727770	1.920043
C	-3.384852	-1.773941	2.368695
C	-1.981057	-1.286845	2.102968
N	-1.874155	-0.842214	0.730416
C	-2.887747	-0.389809	0.038969
C	-2.623659	0.055437	-1.361759
C	-2.739961	1.568216	-1.555248
C	-4.166581	2.076204	-1.678246
C	-5.059982	1.765608	-0.488945
C	-5.215524	0.280781	-0.198407
O	0.639002	-0.951735	-0.043092
C	1.067445	-0.994031	-1.225688
O	0.378975	-0.987550	-2.259214
C	2.589072	-1.092667	-1.424863
N	3.398090	-0.727689	-0.282932
C	3.721678	-1.872692	0.538586
C	3.199614	-3.075786	-0.242262
C	3.007855	-2.543463	-1.655847
C	3.500799	0.546292	0.218561
C	3.028323	1.650132	-0.690007
C	3.479992	3.029864	-0.239085
C	3.293782	3.208027	1.255245
C	4.150365	2.200364	2.001758
C	4.020840	0.816502	1.435210
H	2.834451	-0.483874	-2.292067
H	2.272338	-3.098211	-2.232582
H	3.951543	-2.560886	-2.201052
H	3.880272	-3.923238	-0.199261
H	2.243163	-3.395260	0.166522
H	4.801874	-1.923681	0.704227
H	3.248572	-1.797768	1.521413
H	3.872370	2.188968	3.058175
H	5.195052	2.532538	1.979471
H	1.938082	1.612985	-0.750240
H	4.375176	0.004771	2.054894
H	3.391946	1.466053	-1.700547
H	2.931040	3.789403	-0.796236
H	4.536748	3.163799	-0.482684
H	2.241998	3.054138	1.509260
H	3.550708	4.223974	1.557604
H	-0.914379	-0.869965	0.293741
H	-1.251259	-2.077430	2.253466
H	-1.722338	-0.465608	2.772471
H	-3.560544	-2.703630	1.828394
H	-3.522305	-1.973747	3.428320
H	-5.387353	-1.128891	1.947961
H	-4.347983	0.143482	2.576110
H	-5.366745	-0.275346	-1.124250
H	-6.099341	0.120839	0.410732

H	4.704602	-2.670506	-0.448433
H	5.400583	-2.815512	1.160847
H	2.865569	-3.139502	1.070486
H	3.392997	-1.887859	2.186846
H	2.898671	4.008842	-0.051773
H	3.069643	3.273896	-1.627984
H	1.017900	2.535505	-0.571174
H	1.862359	1.962983	0.842876

3_{DBU6}

E_0 = -1096.568233
E_{0+ZPE} = -1096.034190
E_{298} = -1096.010170
H_{298} = -1096.009226
G_{298} = -1096.091084
NImag = 0

N	-4.021193	-0.004117	-0.411209
C	-4.729030	-1.245507	-0.707699
C	-3.797723	-2.262782	-1.326256
C	-2.570791	-2.419901	-0.460982
N	-2.016645	-1.116488	-0.169386
C	-2.717361	-0.014897	-0.168141
C	-1.994395	1.255878	0.144953
C	-2.389659	1.873488	1.487315
C	-3.696795	2.646184	1.458806
C	-4.910810	1.828642	1.051872
C	-4.812006	1.220204	-0.338198
O	0.566917	-0.964794	0.325808
C	1.233673	-1.772375	-0.376950
O	0.770287	-2.589976	-1.186911
C	2.761067	-1.775643	-0.199430
N	3.322203	-0.614907	0.456087
C	3.447213	-0.806144	1.883558
C	3.071574	-2.266699	2.116928
C	3.190589	-2.902639	0.738644
C	3.364933	0.643681	-0.089885
C	3.115513	0.726638	-1.572174
C	3.510082	2.067986	-2.169493
C	3.035001	3.216951	-1.301340
C	3.696575	3.134911	0.063093
C	3.640550	1.748992	0.636121
H	3.193405	-1.917371	-1.187357
H	2.582381	-3.795270	0.618336
H	4.227237	-3.166121	0.528796
H	3.708853	-2.743920	2.858218
H	2.044149	-2.332646	2.468910
H	4.469924	-0.586170	2.204241
H	2.785317	-0.129456	2.430878
H	3.214331	3.833046	0.751119
H	4.734090	3.479449	-0.020985
H	2.058346	0.526485	-1.762330
H	3.839877	1.655068	1.694354
H	3.666871	-0.066666	-2.076221
H	3.106865	2.146209	-3.179359
H	4.597790	2.118822	-2.260089
H	1.949780	3.156916	-1.186081
H	3.254036	4.174819	-1.774477
H	-0.975352	-1.058106	0.013843
H	-1.789159	-2.991339	-0.954021
H	-2.819848	-2.925209	0.473368
H	-3.505660	-1.933983	-2.323281
H	-4.315394	-3.213288	-1.427844
H	-5.537038	-1.007463	-1.393925
H	-5.174772	-1.634332	0.209263
H	-4.419016	1.951405	-1.045751
H	-5.803747	0.950576	-0.686112
H	-0.933611	1.022994	0.146739
H	-2.169367	1.970659	-0.659978
H	-5.100452	1.033624	1.775460
H	-5.787629	2.476781	1.062399

H	-1.368208	0.543363	-0.805060
H	-2.540006	0.239189	-2.072834
H	-5.694771	1.530025	-0.163106
H	-6.305973	1.617932	-1.800470
H	-4.560777	3.290419	-1.486365
H	-4.099817	2.114710	-2.695006
H	-3.080465	2.228144	0.173518
H	-2.210024	2.665646	-1.272926

3_{DBU7}

E_0 = -1096.568193
E_{0+ZPE} = -1096.033982
E_{298} = -1096.009960
H_{298} = -1096.009016
G_{298} = -1096.090932
NImag = 0

N	4.018421	1.149056	0.099211
C	4.016126	2.514897	-0.413426
C	2.695586	3.194289	-0.135658
C	1.563628	2.316909	-0.612833
N	1.725108	0.984751	-0.072820
C	2.886214	0.474724	0.244830
C	2.902697	-0.924542	0.767328
C	3.498127	-1.930768	-0.217992
C	5.017063	-1.937802	-0.255103
C	5.656492	-0.606443	-0.613258
C	5.317639	0.529175	0.340296
O	-0.533083	-0.367408	-0.078364
C	-0.893889	-1.112146	0.870595
O	-0.226229	-1.390312	1.879742
C	-2.279043	-1.772487	0.767327
N	-3.172738	-1.210409	-0.221106
C	-3.040244	-1.871819	-1.499905
C	-2.137724	-3.074113	-1.229305
C	-2.153219	-3.216594	0.287229
C	-3.738975	0.037806	-0.133605
C	-3.725541	0.669927	1.232771
C	-4.662896	1.861327	1.347885
C	-4.543476	2.771071	0.140878
C	-4.949907	2.015623	-1.111987
C	-4.311190	0.659442	-1.186969
H	-2.719947	-1.738341	1.761004
H	-1.270656	-3.709471	0.686307
H	-3.031208	-3.776989	0.608331
H	-2.481147	-3.971262	-1.739725
H	-1.126986	-2.863537	-1.573169
H	-4.024914	-2.168510	-1.872314
H	-2.601090	-1.202536	-2.244748
H	-4.680295	2.595082	-1.997957
H	-6.042774	1.931969	-1.140500
H	-2.702776	0.972058	1.470524
H	-4.325657	0.169836	-2.150527
H	-4.000711	-0.076348	1.977600
H	-4.448360	2.402279	2.269956
H	-5.693527	1.506240	1.423476
H	-3.508401	3.108442	0.045311
H	-5.160539	3.661717	0.265684
H	0.858189	0.386954	0.015414
H	4.226847	2.497412	-1.483928
H	4.825454	3.050223	0.076022
H	6.048128	1.324163	0.229539
H	5.375764	0.190672	1.375411
H	3.466366	-0.943147	1.700828
H	1.876221	-1.188288	1.016252
H	6.740002	-0.728457	-0.603063
H	5.385703	-0.308961	-1.628320
H	2.593266	3.377328	0.933525
H	2.669719	4.155695	-0.642425
H	0.600520	2.695780	-0.282387
H	1.544035	2.268758	-1.702436

H	-1.622190	-0.279953	-1.630623
H	-3.320375	-0.454405	-2.028478
H	-4.694193	2.266272	0.409601
H	-6.054775	2.166036	-0.686193
H	-4.147873	3.154581	-1.838776
H	-4.616764	1.639519	-2.573377
H	-2.221799	2.082038	-0.744064
H	-2.199540	1.818600	-2.467388

$3_{DBU-conf}$

E_0 = -1096.5686704
E_{0+ZPE} = -1096.034544
E_{298} = -1096.010591
H_{298} = -1096.009646
G_{298} = -1096.091407
NImag = 0

N	-4.384357	-0.359631	0.545272
C	-4.448852	-0.880109	1.906963
C	-3.075381	-0.935842	2.534419
C	-2.117651	-1.626292	1.592231
N	-2.182955	-0.987352	0.296869
C	-3.260881	-0.406943	-0.155606
C	-3.184673	0.240189	-1.502425
C	-3.440330	1.748412	-1.489588
C	-4.905930	2.145505	-1.425287
C	-5.648496	1.665336	-0.189997
C	-5.626305	0.156190	-0.017754
O	0.010627	-0.896917	-1.157502
C	1.060383	-0.964414	-0.451786
O	1.104440	-1.023239	0.782124
C	2.363342	-1.013455	-1.265107
N	3.570142	-0.734094	-0.520223
C	4.169593	-1.938746	0.009133
C	3.357543	-3.079768	-0.598007
C	2.624159	-2.433291	-1.765715
C	3.904725	0.498538	-0.015575
C	3.137449	1.667192	-0.574197
C	3.768641	3.009753	-0.241639
C	4.202337	3.066327	1.210164
C	5.263793	2.011424	1.467542
C	4.880111	0.675598	0.901398
H	2.249206	-0.328618	-2.102207
H	1.707611	-2.948964	-2.040325
H	3.267195	-2.390208	-2.644650
H	3.983921	-3.914839	-0.904374
H	2.640226	-3.451880	0.130546
H	5.225841	-1.987648	-0.271920
H	4.125848	-1.953754	1.101430
H	5.436965	1.914837	2.541707
H	6.217769	2.352936	1.048376
H	2.113991	1.629570	-0.193376
H	5.427732	-0.181005	1.268344
H	3.061644	1.564055	-1.656463
H	3.062239	3.807631	-0.471823
H	4.641885	3.168808	-0.878999
H	3.338058	2.878963	1.852136
H	4.580547	4.057668	1.462491
H	-1.293945	-0.941234	-0.278671
H	-4.908380	-1.869591	1.886434
H	-5.101767	-0.222872	2.476654
H	-5.826950	-0.338823	-0.967948
H	-6.411461	-0.152938	0.665804
H	-2.191004	0.038768	-1.891589
H	-3.895214	-0.252457	-2.168126
H	-5.242897	2.131061	0.710038
H	-6.690728	1.977269	-0.262956
H	-4.978912	3.231606	-1.485946
H	-5.412802	1.752891	-2.310562
H	-2.885468	2.205083	-0.668755
H	-3.013281	2.152729	-2.406518

H	-3.872505	3.081221	2.442976
H	-3.593029	3.484195	0.764890
H	-2.425733	1.093596	2.249769
H	-1.588338	2.550408	1.780182
H	5.352573	-2.695279	-0.964076
H	5.387983	-2.247817	0.725260
H	3.150700	-2.920121	0.076897
H	3.091671	-1.748437	-1.214372
H	-1.085849	-1.557279	1.924497
H	-2.371703	-2.682781	1.491583
H	-3.131590	-1.467778	3.480782
H	-2.720527	0.073965	2.738976

3_{DBU8}

E_0 = -1096.5677059
E_{0+ZPE} = -1096.033596
E_{298} = -1096.009572
H_{298} = -1096.008628
G_{298} = -1096.090416
NImag = 0

N	3.521201	-0.801561	-0.355498
C	4.153368	-1.937179	0.276947
C	3.391504	-3.150266	-0.247750
C	2.687357	-2.631172	-1.493689
C	2.360516	-1.183695	-1.127510
C	1.017543	-1.108195	-0.382304
O	0.003393	-1.129052	-1.142867
C	3.802512	0.478231	0.052713
C	3.006721	1.570832	-0.610753
C	5.073312	2.152561	1.438266
O	1.001666	-1.063790	0.851350
H	2.267017	-0.577079	-2.025472
H	1.800283	-3.200260	-1.759635
H	3.365728	-2.640678	-2.346819
H	4.047685	-3.993118	-0.453766
H	2.656618	-3.471744	0.487384
H	5.215443	-1.971523	0.015165
H	4.092897	-1.865407	1.365990
C	4.750639	0.762888	0.971768
C	3.581348	2.958028	-0.371885
C	3.980484	3.143708	1.078999
H	5.226897	2.146713	2.519724
H	6.022834	2.496518	1.011011
H	1.976980	1.523761	-0.248537
H	5.320509	-0.041538	1.415118
H	2.958910	1.382676	-1.683064
H	2.851790	3.708299	-0.677859
H	4.462189	3.100163	-1.002778
H	3.109656	2.974605	1.717067
H	4.317383	4.165168	1.259741
H	-1.362314	-1.107868	-0.374514
N	-2.317192	-1.126770	0.088665
C	-2.547668	-2.108756	1.124422
H	-1.960656	-2.990464	0.883096
H	-2.184058	-1.722543	2.076691
C	-4.021640	-2.427372	1.199603
H	-4.325217	-2.980604	0.311279
H	-4.231693	-3.048570	2.066642
C	-4.813728	-1.144160	1.296926
H	-5.875384	-1.345811	1.185031
H	-4.665198	-0.669124	2.267961
C	-3.215569	-0.258846	-0.291136
N	-4.428962	-0.212210	0.242068
C	-5.395837	0.815991	-0.128346
H	-5.590969	0.764528	-1.200147
H	-6.320217	0.544989	0.371342
C	-4.995356	2.227435	0.271148
C	-2.817529	0.719057	-1.350614
H	-1.861656	0.384985	-1.743246
H	-3.540605	0.674824	-2.165805
C	-2.690071	2.155316	-0.839903
C	-4.012629	2.885201	-0.682569
H	-4.593796	2.208365	1.286072
H	-5.903963	2.829176	0.305600
H	-3.816037	3.903498	-0.346364
H	-4.485242	2.970734	-1.664374
H	-2.139346	2.157226	0.101814
H	-2.073931	2.698992	-1.554851

3_{DBU9}

E_0 = -1096.5676643
E_{0+ZPE} = -1096.033580
E_{298} = -1096.009553
H_{298} = -1096.008609
G_{298} = -1096.090305
NImag = 0

N	-4.388220	-1.083295	-0.073630
C	-4.363905	-2.172488	-1.044194
C	-3.033543	-2.888579	-1.016179
C	-1.913688	-1.884955	-1.149048
N	-2.099398	-0.820384	-0.187468
C	-3.265493	-0.480086	0.293410
C	-3.302559	0.658271	1.262429
C	-3.973911	1.911393	0.696904
C	-5.491946	1.874636	0.724284
C	-6.115844	0.732829	-0.059675
C	-5.693113	-0.648511	0.414205
O	-0.033081	0.538237	0.732041
C	0.981862	0.550665	-0.026315
O	1.109817	-0.078236	-1.081425
C	2.111217	1.480640	0.443940
N	3.410765	1.207473	-0.128195
C	3.647847	1.980022	-1.327313
C	2.457920	2.930524	-1.422890
C	1.855455	2.912543	-0.024607
C	4.153601	0.084162	0.142750
C	3.740329	-0.698710	1.360318
C	4.786176	-1.709473	1.803743
C	5.349560	-2.472332	0.620384
C	6.044083	-1.509744	-0.326738
C	5.213206	-0.291645	-0.604849
H	2.141143	1.434212	1.529991
H	0.799997	3.172685	-0.005355
H	2.387329	3.603028	0.629938
H	2.750670	3.928385	-1.742440
H	1.737023	2.547624	-2.141871
H	4.599319	2.514341	-1.247917
H	3.713360	1.333109	-2.205996
H	6.272680	-2.016479	-1.266948
H	7.015901	-1.228777	0.096382
H	2.795226	-1.204923	1.149387
H	5.499454	0.303532	-1.460599
H	3.537253	-0.010133	2.180211
H	4.345463	-2.388298	2.534205
H	5.601986	-1.188389	2.310686
H	4.534433	-2.977024	0.095811
H	6.043103	-3.245053	0.954420
H	-1.245345	-0.288902	0.145939
H	-4.569076	-1.773443	-2.038717
H	-5.167901	-2.857269	-0.789005
H	-6.402692	-1.387347	0.056571
H	-5.710044	-0.698836	1.503374
H	-7.200112	0.794033	0.037871
H	-5.891659	0.827546	-1.123695
H	-5.821240	1.804305	1.764104
H	-5.876201	2.821153	0.343320
H	-0.944153	-2.335576	-0.961226
H	-1.887711	-1.463596	-2.154147
H	-2.992769	-3.609938	-1.828495
H	-2.930831	-3.435798	-0.079523
H	-3.615185	2.085398	-0.318880
H	-3.633485	2.758256	1.291156
H	-3.812051	0.338694	2.172113
H	-2.273317	0.881935	1.526124

3_{DBU10}

E_0 = -1096.5679001
E_{0+ZPE} = -1096.033825
E_{298} = -1096.009845
H_{298} = -1096.008901
G_{298} = -1096.090302
NImag = 0

N	-4.271481	-0.925009	-0.429361
C	-4.722545	-2.190237	0.139421
C	-3.548745	-3.091813	0.443456
C	-2.530570	-2.339227	1.266063
N	-2.226975	-1.078009	0.626259
C	-3.064335	-0.450088	-0.156510
C	-2.623229	0.858597	-0.727338
C	-3.353927	2.059282	-0.124524
C	-4.742054	2.291857	-0.697199
C	-5.704065	1.125846	-0.541589
C	-5.239250	-0.159944	-1.208554
O	0.057336	-0.030155	1.402325
C	0.894609	0.435576	0.575898
O	0.755272	0.487538	-0.652073
C	2.161315	1.021990	1.219678
N	3.318982	1.094350	0.356330
C	3.410309	2.365965	-0.325269
C	2.305000	3.220346	0.288762
C	1.944830	2.492582	1.577173
C	4.021734	0.002986	-0.093094
C	3.775761	-1.286901	0.643379
C	4.816805	-2.353235	0.342006
C	5.112555	-2.427200	-1.143384
C	5.690454	-1.105349	-1.617238
C	4.904966	0.069589	-1.112478
H	2.372000	0.439549	2.113124
H	0.932102	2.693419	1.918388
H	2.632357	2.768142	2.377101
H	2.623808	4.246357	0.461916
H	1.445580	3.244932	-0.377195
H	4.402546	2.801711	-0.175129
H	3.270409	2.246332	-1.402611
H	5.716382	-1.082976	-2.709182
H	6.737604	-1.037261	-1.299758
H	2.778877	-1.655368	0.388922
H	5.076479	1.014690	-1.608013
H	3.761549	-1.092568	1.715362
H	4.468700	-3.314345	0.720789
H	5.740329	-2.119607	0.876805
H	4.187544	-2.637914	-1.685141
H	5.803080	-3.243561	-1.359150
H	-1.294768	-0.627044	0.845867
H	-1.603242	-2.898404	1.357170
H	-2.906704	-2.155686	2.273251
H	-3.093253	-3.428462	-0.487511
H	-3.895487	-3.970433	0.981211
H	-5.381551	-2.660245	-0.585930
H	-5.305451	-1.992555	1.040384
H	-4.829894	0.049319	-2.197260
H	-6.087666	-0.820328	-1.354624
H	-1.550844	0.933848	-0.563698
H	-2.773845	0.839205	-1.807294
H	-5.901696	0.926192	0.513471
H	-6.658796	1.400717	-0.991157
H	-5.175992	3.176203	-0.229541
H	-4.645968	2.521976	-1.761261
H	-3.402018	1.950784	0.960488
H	-2.744431	2.941275	-0.316359

3_{DBU11}

E_0 = -1096.5683306
E_{0+ZPE} = -1096.034086
E_{298} = -1096.010136
H_{298} = -1096.009192
G_{298} = -1096.090577
NImag = 0

N	-3.969851	0.067836	-0.530325
C	-4.631948	-1.098043	-1.107223
C	-3.631821	-2.018101	-1.768838
C	-2.507428	-2.320125	-0.807766
N	-1.989751	-1.082020	-0.268171
C	-2.698346	0.009407	-0.157930
C	-2.027579	1.205510	0.438295
C	-2.561921	1.574820	1.822977
C	-3.873829	2.339975	1.804167
C	-5.028139	1.611276	1.137339
C	-4.782984	1.261458	-0.321731
O	0.560618	-0.968147	0.397835
C	1.261304	-1.785484	-0.259277
O	0.836498	-2.629555	-1.063368
C	2.779981	-1.765440	-0.023013
N	3.311749	-0.545152	0.543326
C	3.388556	-0.603644	1.985861
C	3.007967	-2.038251	2.340411
C	3.174386	-2.798239	1.031673
C	3.365549	0.658034	-0.115170
C	3.174773	0.598262	-1.607781
C	3.583277	1.880675	-2.314156
C	3.065157	3.100352	-1.577639
C	3.674079	3.155493	-0.187606
C	3.606500	1.829435	0.512893
H	3.251783	-1.995682	-0.975301
H	2.570687	-3.700498	0.974296
H	4.217449	-3.077600	0.882834
H	3.621709	-2.442079	3.142749
H	1.969653	-2.076470	2.662520
H	4.399414	-0.349616	2.318886
H	2.706977	0.116863	2.445960
H	3.160506	3.910610	0.411822
H	4.711533	3.501718	-0.264709
H	2.127660	0.370405	-1.820841
H	3.766389	1.837752	1.581906
H	3.751445	-0.233291	-2.011780
H	3.220072	1.858114	-3.341875
H	4.673315	1.934810	-2.366858
H	1.976844	3.038369	-1.498471
H	3.294470	4.012190	-2.130498
H	-0.966555	-1.052440	0.001206
H	-1.674571	-2.827623	-1.286308
H	-2.860046	-2.950651	0.009939
H	-3.232894	-1.544866	-2.665700
H	-4.130295	-2.935694	-2.071058
H	-5.353135	-0.736908	-1.835410
H	-5.182821	-1.621969	-0.324408
H	-4.334927	2.106320	-0.846047
H	-5.730950	1.059315	-0.809708
H	-0.968653	0.973632	0.503884
H	-2.132688	2.051007	-0.242167
H	-5.275802	0.699550	1.684298
H	-5.912045	2.248564	1.176125
H	-4.152836	2.588486	2.828422
H	-3.717276	3.290731	1.288385
H	-2.656595	0.670658	2.426686
H	-1.804980	2.189030	2.308784

Different conformation of Enamine intermediate

$\mathbf{1_i}$ ($Cyhex_{Conf}$)

E_0 = -634.5121219
E_{0+ZPE} = -634.232212
E_{298} = -634.219850
H_{298} = -634.218906
G_{298} = -634.271259
NImag = 0

N	0.429174	0.556919	0.168744
C	0.850716	1.944364	0.339694
C	2.340376	1.912056	0.066273
C	2.438676	0.885663	-1.049497
C	1.406925	-0.170159	-0.640985
C	2.064270	-1.276208	0.174932
O	1.759830	-1.264690	1.460519
C	-0.941911	0.279354	0.042229
C	-1.295427	-1.129760	-0.351401
C	-3.357286	0.916966	0.242995
O	2.815424	-2.087093	-0.299844
H	0.966018	-0.642131	-1.514941
H	3.430182	0.462110	-1.181910
H	2.130320	1.328643	-1.994670
H	2.725562	2.887318	-0.219367
H	2.887764	1.579793	0.948610
H	0.340572	2.586772	-0.384865
H	0.602602	2.300074	1.337789
C	-1.885197	1.193108	0.310012
C	-2.734633	-1.478652	-0.010149
C	-3.674595	-0.382990	-0.475580
H	-3.770649	0.886469	1.256444
H	-3.858733	1.750867	-0.251586
H	-0.623357	-1.833225	0.141166
H	-1.597707	2.187035	0.622183
H	-1.135582	-1.259352	-1.424364
H	1.119188	-0.532801	1.559394
H	-2.992209	-2.434045	-0.466145
H	-3.556375	-0.244538	-1.552792
H	-4.713142	-0.664930	-0.303010
H	-2.832175	-1.604678	1.070323

$\mathbf{1_i}$

E_0 = -634.5116771
E_{0+ZPE} = -634.231616
E_{298} = -634.219261
H_{298} = -634.218317
G_{298} = -634.270692
NImag = 0

N	0.440206	0.577722	0.148412
C	0.859575	1.965803	0.310052
C	2.365056	1.904825	0.167629
C	2.533658	0.875858	-0.937510
C	1.436462	-0.154048	-0.636837
C	2.003889	-1.317824	0.163034
O	1.685904	-1.308393	1.445160
C	-0.929776	0.299677	-0.014842
C	-1.288375	-1.152474	-0.177574
C	-3.343562	0.973899	0.046506
O	2.710340	-2.165496	-0.316464
H	1.033512	-0.565141	-1.559301
H	3.520621	0.423814	-0.980823
H	2.330149	1.331284	-1.904849
H	2.794273	2.870624	-0.085759
H	2.826925	1.563103	1.093987
H	0.432414	2.594987	-0.477135
H	0.524241	2.351745	1.270621
C	-1.870011	1.250104	0.072649
C	-2.737158	-1.351225	-0.592758
C	-3.662135	-0.496845	0.251989
H	-3.836170	1.575806	0.812445
H	-3.763352	1.311978	-0.906153
H	-1.101260	-1.670263	0.767119
H	-1.579331	2.283734	0.193303
H	-0.637868	-1.625605	-0.912234
H	-2.993377	-2.406838	-0.508527
H	-2.855381	-1.079500	-1.643963
H	-3.528793	-0.756831	1.304817
H	-4.705088	-0.694971	0.005563
H	1.081349	-0.547362	1.548408

$\mathbf{1_i}$ (*down*)

E_0 = -634.5076091
E_{0+ZPE} = -634.227694
E_{298} = -634.215177
H_{298} = -634.214233
G_{298} = -634.266710
NImag = 0

N	0.517020	0.652260	0.139246
C	0.956517	2.043420	0.255810
C	2.278145	2.096756	-0.492210
C	2.807899	0.681340	-0.376816
C	1.535887	-0.165348	-0.496148
C	1.757966	-1.474378	0.233230
O	1.415170	-1.454929	1.513722
C	-0.851007	0.371270	0.005719
C	-1.208561	-0.993033	-0.521707
C	-3.270635	0.954802	0.341057
O	2.265261	-2.440005	-0.270963
H	1.330059	-0.388983	-1.542998
H	3.270534	0.530173	0.598941
H	3.533052	0.415320	-1.139736
C	-1.799160	1.242553	0.385621
C	-2.673561	-1.102987	-0.912909
C	-3.567728	-0.523564	0.165112
H	-3.735805	1.324115	1.256966
H	-3.736735	1.520552	-0.472205
H	-0.979829	-1.746627	0.236130
H	-1.514505	2.208428	0.777747
H	-0.592032	-1.233445	-1.386606
H	-2.914243	-2.148501	-1.102864
H	-2.841520	-0.564091	-1.847938
H	-3.385587	-1.049936	1.105170
H	-4.618489	-0.671559	-0.083762
H	0.979535	-0.601455	1.670954
H	1.066997	2.325644	1.304068
H	0.220046	2.709328	-0.190614
H	2.960338	2.837096	-0.082001
H	2.101021	2.342606	-1.538603

$\mathbf{1_{iii}}$

E_0 = -634.5066239
E_{0+ZPE} = -634.227352
E_{298} = -634.214552
H_{298} = -634.213608
G_{298} = -634.267540
NImag = 0

N	0.419858	0.660896	-0.077249
C	0.878163	2.001900	0.211003
C	2.389600	1.883203	0.180099
C	2.618873	0.814897	-0.875981
C	1.447681	-0.158942	-0.667137
C	1.896418	-1.326273	0.188226
O	1.813714	-1.106570	1.494824
C	-0.926862	0.356177	-0.110573
C	-1.275028	-1.088897	-0.345833
C	-3.344255	0.966197	0.209778
O	2.337827	-2.350735	-0.268955
H	1.149088	-0.593271	-1.619415
H	3.588438	0.327468	-0.807119
H	2.530738	1.243142	-1.872856
H	2.875363	2.824401	-0.065005
H	2.760835	1.551063	1.148194
H	0.521052	2.711837	-0.544433
H	0.499924	2.334295	1.178151
C	-1.880318	1.280093	0.115049
C	-2.756215	-1.302691	-0.613742
C	-3.604114	-0.521577	0.371016
H	-3.780294	1.512340	1.049002
H	-3.868806	1.331104	-0.680002

$\mathbf{1_{iv}}$

E_0 = -634.5070037
E_{0+ZPE} = -634.227800
E_{298} = -634.215013
H_{298} = -634.214069
G_{298} = -634.267788
NImag = 0

N	0.389938	0.683279	-0.035153
C	0.807578	2.044683	0.217032
C	2.321378	1.965222	0.207994
C	2.590995	0.883740	-0.824573
C	1.444839	-0.116778	-0.598764
C	1.909632	-1.221967	0.328170
O	2.540787	-2.180792	-0.350177
C	-0.948786	0.346087	-0.092249
C	-1.260164	-1.113584	-0.286102
C	-3.386605	0.911083	0.148331
O	1.782476	-1.253352	1.522610
H	1.165904	-0.580819	-1.543850
H	3.573396	0.426448	-0.735087
H	2.500972	1.288697	-1.830874
H	2.786192	2.913953	-0.048415
H	2.688529	1.660638	1.186866
H	0.443643	2.721728	-0.565210
H	0.407122	2.396149	1.168166
C	-1.927852	1.254478	0.079779
C	-2.727557	-1.367724	-0.590928
C	-3.619330	-0.576787	0.346232
H	-3.855039	1.471186	0.960474
H	-3.896233	1.239225	-0.764151

$\mathbf{1_{ii}}$

E_0 = -634.5016601
E_{0+ZPE} = -634.222666
E_{298} = -634.209810
H_{298} = -634.208866
G_{298} = -634.262846
NImag = 0

N	0.392938	0.674816	-0.074338
C	0.826532	2.026448	0.202818
C	2.340425	1.934496	0.186266
C	2.599185	0.842049	-0.837635
C	1.449533	-0.148374	-0.588330
C	1.900582	-1.225339	0.390562
O	2.606329	-2.221129	-0.155340
C	-0.947324	0.343565	-0.110323
C	-1.272768	-1.108568	-0.334036
C	-3.377010	0.921262	0.178344
O	1.703461	-1.215535	1.571720
H	1.171973	-0.639140	-1.523808
H	3.582849	0.386176	-0.748022
H	2.502147	1.236543	-1.847511
H	2.811276	2.877181	-0.080503
H	2.711119	1.635374	1.165298
H	0.462225	2.720499	-0.563457
H	0.436226	2.363510	1.163534
C	-1.916881	1.255310	0.095578
C	-2.746835	-1.344669	-0.621008
C	-3.617855	-0.568757	0.347486
H	-3.828235	1.466663	1.009933
H	-3.898371	1.273156	-0.718594

H	-0.969117	-1.669061	0.528918
H	-1.596551	2.312353	0.264921
H	-0.702048	-1.481372	-1.185174
H	-2.979833	-2.368303	-0.566190
H	-2.992998	-0.975304	-1.628643
H	-3.349095	-0.829861	1.387935
H	-4.662680	-0.739499	0.227627
H	2.160981	-1.883686	1.946457

H	-0.969026	-1.653816	0.617815
H	-1.670893	2.296936	0.204759
H	-0.652979	-1.523209	-1.093026
H	-2.930204	-2.436076	-0.516768
H	-2.942285	-1.076118	-1.621600
H	-3.386171	-0.849807	1.378319
H	-4.668697	-0.821901	0.180399
H	2.865335	-2.833729	0.279268

H	-0.970459	-1.673765	0.550539
H	-1.650240	2.292697	0.240632
H	-0.682898	-1.502413	-1.161377
H	-2.956227	-2.412938	-0.567846
H	-2.975570	-1.027892	-1.641233
H	-3.370448	-0.866157	1.369361
H	-4.671401	-0.802843	0.192836
H	2.671644	-2.121580	-1.108775

$\mathbf{1_{iv}}$ ($\text{Cyhex}_{\text{Conf}}$)

E_0 = -634.5074761
E_{0+ZPE} = -634.228349
E_{298} = -634.215512
H_{298} = -634.214568
G_{298} = -634.268602
NImag = 0

N	0.369386	0.657322	-0.080297
C	0.820717	1.990419	0.252369
C	2.325535	1.941725	0.038541
C	2.496114	0.851494	-1.007408
C	1.413225	-0.163624	-0.621077
C	1.966143	-1.157792	0.383574
O	2.697511	-2.095472	-0.219192
C	-0.962181	0.310457	-0.030151
C	-1.308244	-1.074866	-0.507962
C	-3.377172	0.832733	0.434995
O	1.807995	-1.127423	1.574441
H	1.092028	-0.730437	-1.492931
H	3.493135	0.419569	-1.033924
H	2.265471	1.233280	-2.000412
H	2.726793	2.898879	-0.284532
H	2.829407	1.662759	0.962687
H	0.341611	2.726434	-0.402384
H	0.561078	2.249878	1.279870
C	-1.913815	1.161929	0.400408
C	-2.714043	-1.497340	-0.115024
C	-3.712394	-0.391812	-0.398230
H	-0.594634	-1.795065	-0.107635
H	-1.630093	2.142413	0.756157
H	-1.200409	-1.113234	-1.595218
H	-2.735625	-1.736064	0.950604
H	-2.977857	-2.410068	-0.649060
H	3.054992	-2.682252	0.455890
H	-3.952648	1.691012	0.081870
H	-3.704487	0.666923	1.467460
H	-4.728503	-0.726776	-0.188706
H	-3.673315	-0.135280	-1.459845

$\mathbf{1_{iv}}$ (*down*)

E_0 = -634.505846
E_{0+ZPE} = -634.226735
E_{298} = -634.213871
H_{298} = -634.212926
G_{298} = -634.267008
NImag = 0

N	-0.502111	-0.756039	-0.265757
C	-1.057302	-1.972772	0.275926
C	-2.424990	-2.024949	-0.376189
C	-2.854162	-0.564700	-0.395520
C	-1.528765	0.220436	-0.530987
C	-1.558980	1.365324	0.454817
O	-2.147976	2.440097	-0.068499
C	0.835934	-0.429354	-0.132691
C	1.281103	0.795136	-0.887935
C	3.171222	-0.887257	0.665590
O	-1.153950	1.333771	1.586233
H	-1.430193	0.645845	-1.529247
H	-3.344057	-0.312349	0.544050
H	-3.541072	-0.324256	-1.201318
C	1.704315	-1.181623	0.565026
C	2.789163	0.848089	-1.075025
C	3.507911	0.525632	0.221163
H	3.500684	-1.041237	1.694921
H	3.743851	-1.602950	0.065375
H	0.951906	1.693592	-0.359407
H	1.347151	-2.057133	1.089499
H	0.790290	0.813534	-1.861529
H	3.073697	1.833120	-1.444712
H	3.085496	0.125627	-1.838993
H	3.195504	1.235160	0.991025
H	4.585735	0.638382	0.102378
H	-2.198681	3.119891	0.612365
H	-1.133277	-1.944372	1.369358
H	-0.430802	-2.821385	0.006338
H	-3.127590	-2.654618	0.164128
H	-2.331140	-2.409303	-1.390858

$\mathbf{1_{iii}}$ (*down*)

E_0 = -634.5057508
E_{0+ZPE} = -634.226642
E_{298} = -634.213813
H_{298} = -634.212869
G_{298} = -634.266630
NImag = 0

N	-0.537761	-0.727635	-0.280364
C	-1.124074	-1.929267	0.262878
C	-2.492871	-1.948837	-0.387779
C	-2.881803	-0.478256	-0.407917
C	-1.540208	0.267470	-0.582514
C	-1.555782	1.480875	0.318109
O	-1.205625	1.214408	1.571456
C	0.807496	-0.436503	-0.143943
C	1.288487	0.775268	-0.897737
C	3.124361	-0.947211	0.676058
O	-1.901040	2.578057	-0.041763
H	-1.435529	0.650534	-1.596552
H	-3.339158	-0.206378	0.542355
H	-3.581273	-0.221665	-1.197740
C	1.651426	-1.206578	0.565025
C	2.798364	0.788582	-1.075406
C	3.498912	0.454813	0.227912
H	3.442313	-1.104700	1.708519
H	3.683771	-1.679282	0.083354
H	0.982147	1.684027	-0.373212
H	1.269659	-2.072925	1.087307
H	0.802640	0.807313	-1.873235
H	3.110151	1.764053	-1.448269
H	3.080974	0.054473	-1.833339
H	3.198219	1.175965	0.991802
H	4.580044	0.540669	0.117406
H	-1.284119	2.026382	2.083861
H	-1.198482	-1.897049	1.356584
H	-0.518554	-2.793760	-0.004564
H	-3.210695	-2.559131	0.154672
H	-2.410304	-2.336944	-1.402062

$\mathbf{1_{i}}$-*syn*

E_0 = -634.5071916
E_{0+ZPE} = -634.228103
E_{298} = -634.215271
H_{298} = -634.214327
G_{298} = -634.268093
NImag = 0

N	0.409833	0.672368	-0.083688
C	0.826414	2.049045	0.120708
C	2.338135	1.945438	0.177773
C	2.637089	0.827077	-0.806558
C	1.465844	-0.146303	-0.599867
C	1.867347	-1.248508	0.360648
O	2.451237	-2.259100	-0.284655
C	-0.905276	0.258271	-0.133110
C	-1.916273	1.263240	0.348107
C	-2.691415	-1.471229	-0.507361
O	1.743081	-1.232517	1.555557
H	1.192010	-0.620153	-1.544647
H	3.607408	0.359953	-0.656573
H	2.600805	1.199599	-1.828693

$\mathbf{1_{i}}$-*syn* ($\text{Cyhex}_{\text{Conf}}$)

E_0 = -634.5071025
E_{0+ZPE} = -634.228011
E_{298} = -634.215161
H_{298} = -634.214217
G_{298} = -634.268141
NImag = 0

N	0.407945	0.656782	-0.035759
C	0.786960	2.060187	-0.005172
C	2.300622	2.002546	0.019344
C	2.604753	0.812038	-0.874770
C	1.454088	-0.164050	-0.573999
C	1.908989	-1.226295	0.405432
O	2.491084	-2.245379	-0.228398
C	-0.905776	0.226810	-0.061829
C	-1.920350	1.233172	0.410873
C	-2.691731	-1.491277	-0.475437
O	1.821961	-1.176660	1.602515
H	1.143010	-0.674788	-1.488099
H	3.585470	0.375618	-0.701379
H	2.550441	1.100218	-1.922885

H	2.827442	2.879775	-0.086024	H	2.757128	2.922569	-0.337234
H	2.655561	1.665540	1.181018	H	2.649382	1.818311	1.034341
H	0.515221	2.693104	-0.709173	H	0.434590	2.593557	-0.895147
H	0.408612	2.457439	1.038098	H	0.380397	2.561688	0.869116
C	-1.276613	-0.971468	-0.538602	C	-1.271118	-1.011068	-0.445912
C	-3.346040	0.865503	0.022116	C	-3.279215	0.615458	0.698133
C	-3.591447	-0.595358	0.346349	C	-3.687161	-0.347453	-0.399846
H	-3.098649	-1.527753	-1.522755	H	-2.858843	-2.070751	-1.385708
H	-2.704953	-2.496127	-0.130680	H	-2.874752	-2.186157	0.351528
H	-0.531664	-1.674497	-0.885081	H	-2.018065	2.022244	-0.339384
H	-4.637760	-0.856691	0.185967	H	-0.521037	-1.731817	-0.740966
H	-3.375941	-0.770219	1.403140	H	-1.546536	1.718513	1.312006
H	2.742883	-2.905465	0.367225	H	-4.017426	1.408063	0.819426
H	-1.702301	2.236418	-0.092883	H	-3.236745	0.075651	1.646688
H	-1.798670	1.388551	1.427647	H	-3.710749	0.182591	-1.355282
H	-3.537090	1.033180	-1.040438	H	-4.692329	-0.730889	-0.223186
H	-4.032872	1.509459	0.571236	H	2.815722	-2.866183	0.432645