Supporting Information

Full Conformational Analyses of the Ultrafast Isomerization in Penta-coordinated $Ru(S_2C_2(CF_3)_2)(CO)(PPh_3)_2$: One Compound, Two Crystal Structures, Three CO Frequencies, 24 Stereoisomers, and 48 Transition States

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Table S1. DFT optimized geometries (bond lengths (Å) and angles (°)) of isomer **1** at singlet and triplet states at DFT/BS1 level.

	Exp.	BP86		TPSS	
		$S = 0$	$S = 1$	$S = 0$	$S = 1$
Ru-S1	2.298	2.315	2.309	2.315	2.312
Ru-S2	2.287	2.322	2.387	2.319	2.384
Ru-P1	2.353	2.397	2.397	2.396	2.396
Ru-P2	2.274	2.301	2.415	2.298	2.416
Ru-C1	1.849	1.871	1.875	1.879	1.883
C1-O	1.133	1.171	1.170	1.167	1.166
S1-Ru-S2	86.5	84.9	85.3	84.9	85.2
S1-Ru-C1	87.5	90.1	90.0	90.4	90.4
S1-Ru-P1	162.3	155.9	114.4	156.7	113.8
S2-Ru-P1	88.3	84.9	86.9	84.7	86.8
S2-Ru-C1	153.2	155.9	174.6	156.4	174.9
S1-Ru-P2	92.5	96.0	106.3	95.5	105.3
S2-Ru-P2	111.8	111.6	94.9	111.1	94.5
P1-Ru-P2	105.2	107.6	139.3	107.8	140.9
C1-Ru-P2	94.3	92.3	88.9	92.3	89.2
Ru-C1-O	171.8	174.0	176.2	174.2	176.4
τ_5	0.2	0.0	0.6	0.0	0.6

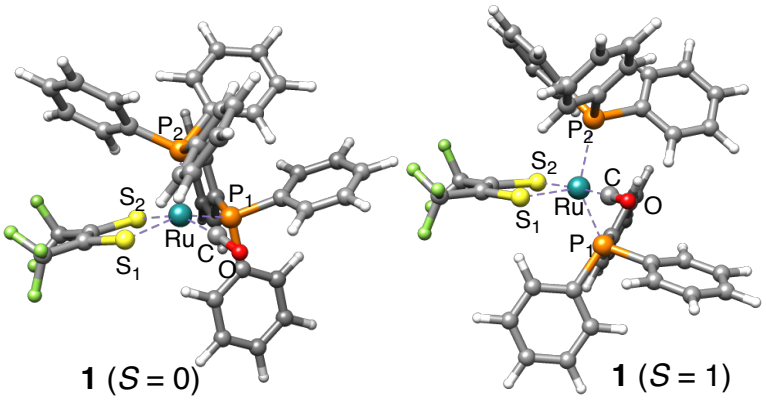


Table S2. DFT optimized geometries (bond lengths (Å) and angles (°)) of isomer **5′** at singlet and triplet states at DFT/BS1 level.

	Exp.	BP86		TPSS	
		S = 0	S = 1	S = 0	S = 1
Ru-S1	2.286	2.291	2.309	2.289	2.313
Ru-S2	2.336	2.326	2.384	2.328	2.382
Ru-P2	2.397	2.401	2.363	2.399	2.359
Ru-P1	2.381	2.385	2.458	2.379	2.461
Ru-C1	1.827	1.820	1.897	1.827	1.907
C1-O	1.152	1.176	1.169	1.172	1.165
S1-Ru-S2	85.1	84.9	84.7	84.8	84.7
S1-Ru-P2	85.8	85.7	88.6	85.6	88.4
S2-Ru-P1	84.0	84.5	85.4	84.4	85.2
P1-Ru-P2	100.8	101.0	101.1	101.2	100.3
S1-Ru-P1	150.6	148.0	116.8	146.8	117.0
S2-Ru-P2	168.7	169.2	172.3	169.4	172.6
S1-Ru-C1	116.7	114.7	106.4	115.7	105.0
S2-Ru-C1	100.8	97.0	87.9	96.9	88.9
P2-Ru-C1	89.3	91.5	90.3	91.4	90.4
P1-Ru-C1	92.2	96.9	135.3	96.8	136.7
Ru-C1-O	173.8	172.9	174.0	173.0	174.6
τ_5	0.3	0.4	0.6	0.4	0.6

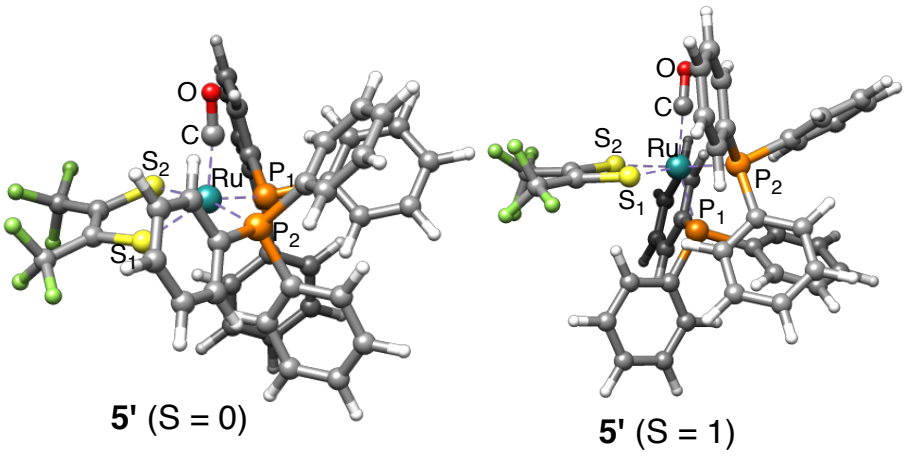


Table S3. Relative free energies (kcal/mol) of the singlet (S = 0) and triplet (S = 1) states for isomers **0-b**, **1-a**, and **2-c** at different levels.

	1-a		**2-c**		**0-b**	
	S = 0	S = 1	S = 0	S = 1	S = 0	S = 1
$BP86_g$[a]	0.0	17.2	0.0	33.8	—[c]	—[c]
$TPSS_g$[a]	0.0	21.9	0.0	33.7	0.0	5.4
$B3P86_g$[a]	0.0	17.5	0.0	34.8	0.0	2.3
$B3LYP_g$[a]	0.0	21.4	0.0	34.3	0.0	7.2
$BP86_g$[b]	0.0	17.4	0.0	33.8	—[c]	—[c]
$BP86_s$[a]	0.0	17.0	0.0	33.0	0.0	1.9
$B3P86_s$[a]	0.0	16.4	0.0	35.1	0.0	4.7

[a]Optimization using def2−TZVP (Ru, S, P, and O) and def2−SVP (H and C).

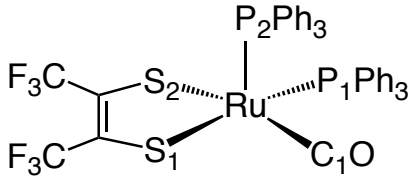
[b]Optimization using def2−TZVP for all atoms. "g" indicates of optimization in the gas phase. "s" indicates of optimization in the solvent phase. [c]BP86 functional always converge **0-b** smoothly to isomer **2-c**.

Table S4. DFT optimized geometries (bond lengths (Å) and angles (°)) of isomer **1** in the gas phase at different levels.[a]

	Exp.	B3LYP$_g$[a]	B3P86$_g$[a]	BP86$_g$[a]	TPSS$_g$[a]	M06$_g$[a]	ωb97xd$_g$[b]	BP86-GD3$_g$[a]	BP86$_g$[b]	M06$_g$[b]	ωb97xd$_g$[b]	BP86$_g$[a] ORCA
Ru-S1	2.298	2.327	2.299	2.315	2.315	2.328	2.312	2.305	2.315	2.316	2.302	2.335
Ru-S2	2.287	2.334	2.305	2.322	2.319	2.324	2.310	2.307	2.323	2.327	2.312	2.341
Ru-P1	2.353	2.434	2.380	2.397	2.396	2.394	2.385	2.323	2.400	2.380	2.365	2.427
Ru-P2	2.274	2.319	2.279	2.301	2.298	2.265	2.262	2.262	2.302	2.294	2.291	2.324
Ru-C1	1.849	1.876	1.862	1.871	1.879	1.877	1.870	1.875	1.867	1.878	1.872	1.892
C1-O	1.133	1.155	1.154	1.171	1.167	1.154	1.151	1.170	1.167	1.148	1.145	1.165
S1-Ru-S2	86.5	84.6	85.1	84.9	84.9	84.8	84.8	86.1	84.8	85.2	85.3	84.3
S1-Ru-C1	87.5	89.9	90.1	90.1	90.4	93.6	92.9	88.0	89.9	88.4	87.3	90.4
S1-Ru-P1	162.3	156.4	157.2	155.9	156.7	163.0	163.1	157.0	155.9	156.9	156.1	156.1
S2-Ru-P1	88.3	85.5	85.0	84.9	84.7	85.3	85.1	89.5	85.1	89.4	90.2	85.2
S2-Ru-C1	153.2	156.8	156.9	155.9	156.4	159.4	159.7	157.9	155.9	158.3	158.2	156.9
S1-Ru-P2	92.5	95.5	95.1	96.0	95.5	90.7	90.5	103.3	96.3	100.5	103.2	95.8
S2-Ru-P2	111.8	110.5	110.8	111.6	111.1	108.6	107.7	103.3	111.7	105.6	104.7	111.0
P1-Ru-P2	105.2	108.1	107.5	107.6	107.8	105.6	105.4	99.7	107.7	102.6	100.7	108.0
C1-Ru-P2	94.3	92.4	92.0	92.3	92.3	91.9	92.5	98.8	92.3	95.9	97.0	91.9
Ru-C1-O	171.8	174.2	174.4	174.0	174.2	176.3	176.2	172.3	174.0	173.1	173.1	174.0

[a]Optimization using def2−TZVP (Ru, S, P, and O) and def2−SVP (H and C).

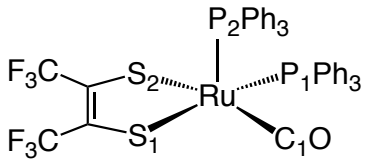
[b]Optimization using def2−TZVP for all atoms.



(**1**)

Table S5. DFT optimized geometries (bond lengths (Å) and angles (°)) of isomer **1** in the solvent phase at DFT/B1 level.

	Exp.	B3P86	BP86	M06	ωb97xd	BP86-GD3BJ
Ru-S1	2.298	2.310	2.324	2.337	2.321	2.318
Ru-S2	2.287	2.320	2.334	2.345	2.326	2.321
Ru-P1	2.353	2.373	2.394	2.382	2.370	2.332
Ru-P2	2.274	2.289	2.313	2.301	2.297	2.266
Ru-C1	1.849	1.858	1.866	1.871	1.867	1.866
C1-O	1.133	1.155	1.173	1.154	1.150	1.172
S1-Ru-S2	86.5	85.3	85.2	85.3	85.3	86.1
S1-Ru-C1	87.5	88.0	88.0	89.0	87.8	88.2
S1-Ru-P1	162.3	154.8	154.0	158.5	156.9	156.5
S2-Ru-P1	88.3	88.8	88.4	89.7	90.9	89.4
S2-Ru-C1	153.2	158.4	157.6	158.4	159.0	159.0
S1-Ru-P2	92.5	101.7	101.2	99.4	102.8	103.9
S2-Ru-P2	111.8	106.2	106.8	106.0	104.3	104.2
P1-Ru-P2	105.2	103.5	104.8	102.1	100.2	99.6
C1-Ru-P2	94.3	95.2	95.4	95.5	96.6	96.8
Ru-C1-O	171.8	171.5	171.1	171.1	171.3	171.4



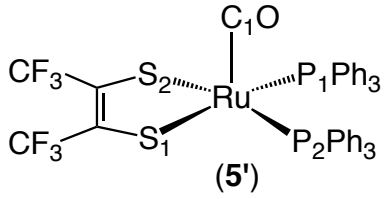
(**1**)

Table S6. DFT optimized geometries (bond lengths (Å) and angles (°)) of isomer **5′** in the gas phase at different levels.[a]

	Exp.	B3LYP$_g$[a]	B3P86$_g$[a]	BP86$_g$[a]	TPSS$_g$[a]	M06$_g$[a]	ωb97xd$_g$[a]	BP86-GD3BJ$_g$[a]	BP86$_g$[b]	M06$_g$[b]	ωb97xd$_g$[b]	BP86$_g$[a] ORCA
Ru-S1	2.286	2.300	2.275	2.291	2.289	2.300	2.293	2.296	2.291	2.300	2.295	2.312
Ru-S2	2.336	2.337	2.312	2.326	2.328	2.341	2.324	2.327	2.327	2.341	2.324	2.341
Ru-P2	2.397	2.435	2.383	2.401	2.399	2.400	2.390	2.345	2.404	2.405	2.393	2.431
Ru-P1	2.381	2.424	2.364	2.385	2.379	2.336	2.306	2.274	2.387	2.335	2.303	2.423
Ru-C1	1.827	1.817	1.807	1.820	1.827	1.834	1.841	1.848	1.816	1.832	1.842	1.834
C1-O	1.152	1.160	1.159	1.176	1.172	1.156	1.152	1.174	1.172	1.152	1.148	1.170
S1-Ru-S2	85.1	84.6	85.0	84.9	84.8	84.7	84.6	85.2	84.7	84.5	84.4	84.3
S1-Ru-P2	85.8	86.1	85.8	85.7	85.6	85.5	84.7	84.2	85.7	85.4	84.8	85.1
S2-Ru-P1	84.0	84.6	84.6	84.5	84.4	85.7	87.3	87.1	84.6	85.9	88.0	84.5
P1-Ru-P2	100.8	101.0	100.9	101.0	101.2	101.0	101.2	100.2	101.2	101.0	101.4	101.1
S1-Ru-P1	150.6	150.0	148.1	148.0	146.8	137.6	128.4	126.1	147.8	137.0	126.6	150.8
S2-Ru-P2	168.7	169.3	169.7	169.2	169.4	170.1	169.0	169.4	169.3	169.9	168.6	168.2
S1-Ru-C1	116.7	112.1	114.8	114.7	115.7	129.3	138.9	140.6	114.8	130.4	141.2	111.4
S2-Ru-C1	100.8	96.7	96.7	97.0	96.9	95.7	94.6	95.3	96.8	95.7	94.2	97.8
P2-Ru-C1	89.3	91.6	91.4	91.5	91.4	91.2	91.9	92.0	91.6	91.4	91.9	91.9
P1-Ru-C1	92.2	96.9	96.3	96.9	96.8	92.7	92.5	93.3	96.6	92.2	92.0	96.7
Ru-C1-O	173.8	173.7	173.5	172.9	173.0	173.4	173.8	173.3	172.9	173.5	174.0	173.1

[a]Optimization using def2−TZVP (Ru, S, P, and O) and def2−SVP (H and C).

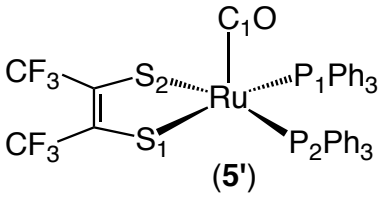
[b]Optimization using def2−TZVP for all atoms.



(**5'**)

Table S7. DFT optimized geometries (bond lengths (Å) and angles (°)) of isomer **5′** in the solvent phase at DFT/B1 level.

	Exp.	B3P86	BP86	M06	ωb97xd	BP86-GD3BJ
Ru-S1	2.286	2.306	2.319	2.328	2.317	2.315
Ru-S2	2.336	2.322	2.335	2.346	2.333	2.331
Ru-P2	2.397	2.393	2.411	2.405	2.395	2.347
Ru-P1	2.381	2.410	2.432	2.421	2.405	2.351
Ru-C1	1.827	1.784	1.797	1.791	1.788	1.796
C1-O	1.152	1.161	1.179	1.159	1.156	1.178
S1-Ru-S2	85.1	85.2	85.1	85.1	85.2	85.8
S1-Ru-P2	85.8	87.1	86.9	88.4	88.0	87.8
S2-Ru-P1	84.0	84.8	84.6	85.7	86.4	86.8
P1-Ru-P2	100.8	100.2	100.4	98.6	97.6	95.9
S1-Ru-P1	150.6	158.6	157.9	158.8	158.7	157.2
S2-Ru-P2	168.7	169.7	169.3	171.3	170.2	169.6
S1-Ru-C1	116.7	102.5	103.0	103.4	102.7	104.6
S2-Ru-C1	100.8	96.2	96.6	96.4	96.1	97.3
P2-Ru-C1	89.3	92.1	92.2	90.7	92.3	92.4
P1-Ru-C1	92.2	97.4	97.5	96.5	97.6	97.8
Ru-C1-O	173.8	173.0	172.3	172.9	173.4	172.1



(**5'**)

Table S8. Comparisons of the energies of isomer **5′** at different levels.

Level	ΔG(kcal/mol)
BP86/BS3[a]//BP86$_{g}$/BS1[b]	1.8
BP86/BS3[a]//BP86$_{g+GD3BJ}$/BS1[c]	1.7
BP86/BS3[a]//BP86$_{sol+GD3BJ}$/BS1[d]	0.0

[a]Gibbs free energies include the BS3 electronic energy in solution, DFT−D3 with BJ damping, gas-phase thermal correction at 298.15 K, and solvation free energy. [b]Geometry optimization in the gas phase without DFT−D3 with BJ damping. [c]Geometry optimization in the gas phase with DFT−D3 with BJ damping. [d]Geometry optimization in the solvent phase with DFT−D3 with BJ damping.

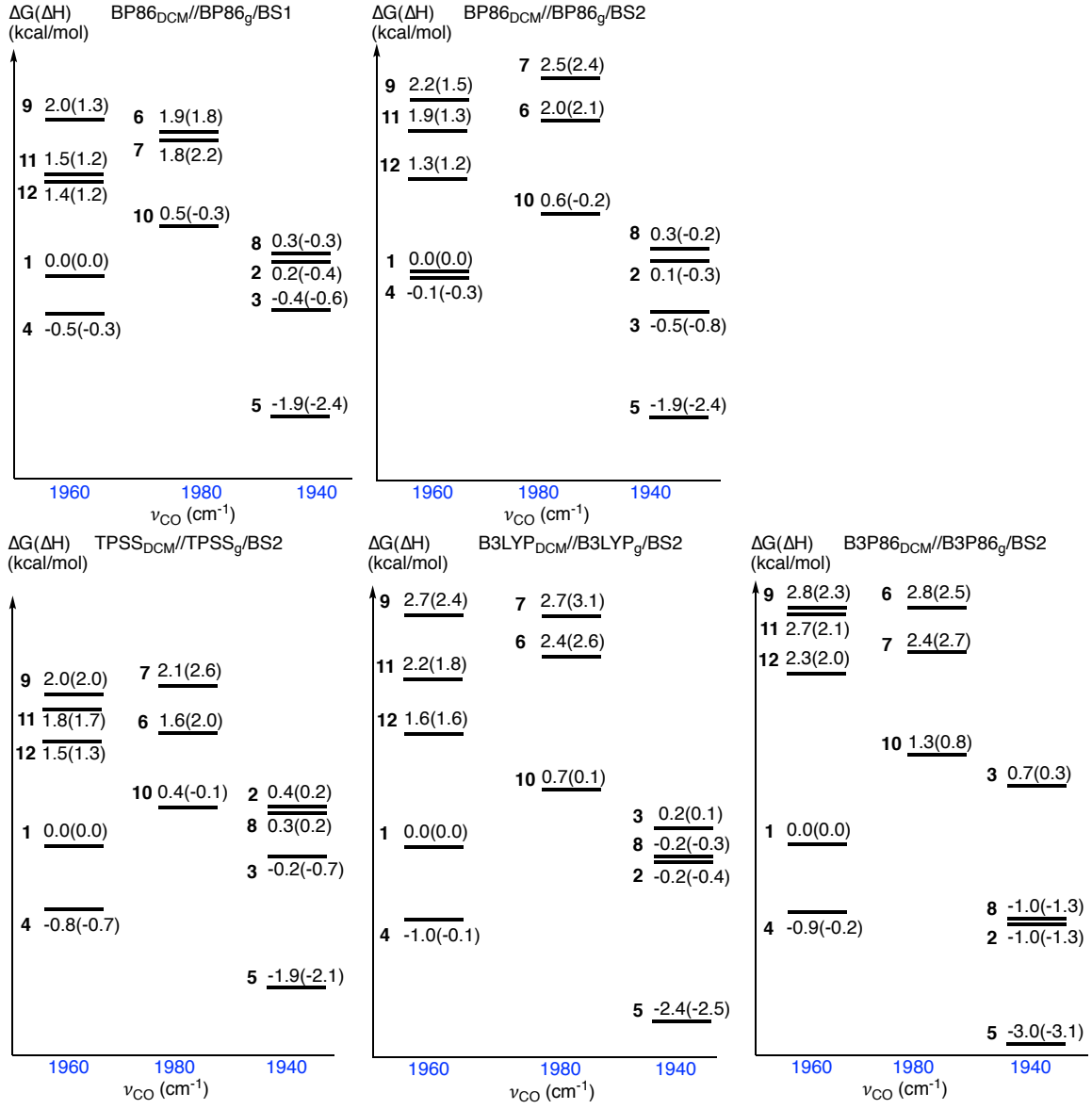
The energetic difference between the gas-phase optimized structures with (BP86/BS3//BP86$_{g+GD3BJ}$ /BS1) and without dispersion correction (BP86/BS3//BP86$_{g}$/BS1) is just 0.1 kcal/mol. The energy at the solvent-phase optimized structures with dispersion correction (BP86/BS3//BP86$_{sol+GD3BJ}$/BS1) is lower by 1.7 and 1.8 kcal/mol as compared to those at the gas-phase optimized structures with (BP86/BS3//BP86$_{g+GD3BJ}$/BS1) and without dispersion correction (BP86/BS3//BP86$_{g}$/BS1), respectively.

Table S9. The scaled CO frequencies (ν_{CO} cm^{-1}) of isomers **1**–**12** with the CF_3 group conformation $\mathbf{L_U}$ at different DFT levels.[a]

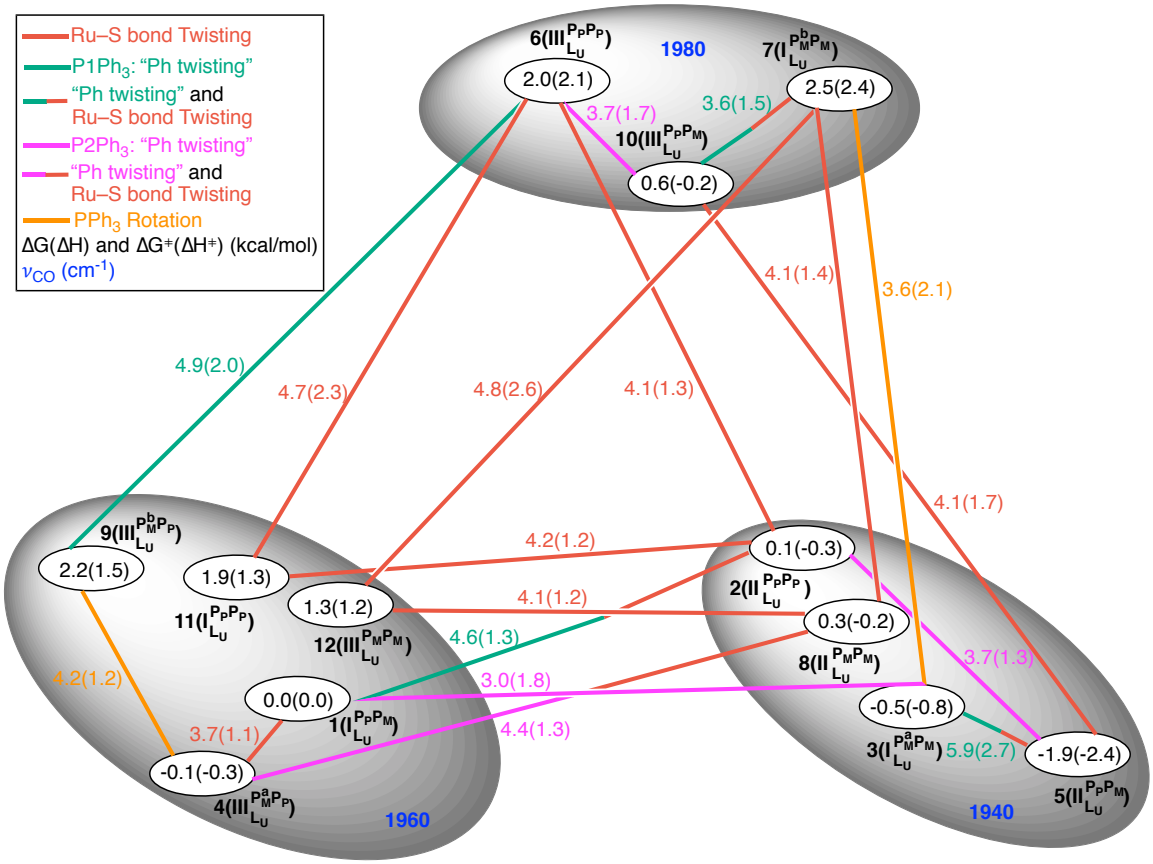
Species	stereocenter	BP86/BS1	BP86/BS2	TPSS/BS2	B3P86/BS2	B3LYP/BS2
1	$\mathbf{I}^{\mathbf{P_P P_M}}_{\mathbf{L_U}}$	1957	1957	1958	1959	1959
2	$\mathbf{II}^{\mathbf{P_P P_P}}_{\mathbf{L_U}}$	1940	1940	1940	1937	1938
3	$\mathbf{I}^{\mathbf{P^a_M P_M}}_{\mathbf{L_U}}$	1941	1942	1946	1945	1945
4	$\mathbf{III}^{\mathbf{P^a_M P_P}}_{\mathbf{L_U}}$	1955	1956	1956	1956	1957
5	$\mathbf{II}^{\mathbf{P_P P_M}}_{\mathbf{L_U}}$	1943	1943	1942	1941	1941
6	$\mathbf{III}^{\mathbf{P_P P_P}}_{\mathbf{L_U}}$	1972	1971	1972	1974	1974
7	$\mathbf{I}^{\mathbf{P^b_M P_M}}_{\mathbf{L_U}}$	1972	1971	1971	1974	1973
8	$\mathbf{II}^{\mathbf{P_M P_M}}_{\mathbf{L_U}}$	1941	1939	1939	1937	1938
9	$\mathbf{III}^{\mathbf{P^b_M P_P}}_{\mathbf{L_U}}$	1956	1955	1957	1957	1958
10	$\mathbf{III}^{\mathbf{P_P P_M}}_{\mathbf{L_U}}$	1975	1974	1975	1977	1976
11	$\mathbf{I}^{\mathbf{P_P P_P}}_{\mathbf{L_U}}$	1953	1954	1954	1956	1958
12	$\mathbf{III}^{\mathbf{P_M P_M}}_{\mathbf{L_U}}$	1953	1954	1957	1956	1958

[a]The scaling factor for ν_{CO} is obtained by averaging the two individual scaling factors of experimentally observed two crystals **1** and **5′**.

Scheme S1. Relative free energies of isomers **1**–**12** at DFT-GD3BJ(SMD)/B3//DFT/B1 and DFT-GD3BJ(SMD)/B3//DFT/B2 levels.



Scheme S2. The relative free energies (ΔG) and entropy (ΔH) of the isomers **1**–**12** and the kinetic barriers ($\Delta G^{\ddagger}/\Delta H^{\ddagger}$) for all the possible interchange pathways among the isomers with the CO frequencies near 1980, 1960, and 1940 cm^{-1} at the BP86-GD3BJ(SMD)/B3//BP86/B2 level.[a]



[a]The vermilion line indicates interchange of the Ru stereochemistry (**I**, **II**, **III**) by twisting either of the Ru–S bonds. The bluish green and magenta lines indicate permutations of the conformation of two respective $P1Ph_3$ and $P2Ph_3$ (see Figure 2 for the definitions of $P1Ph_3$ and $P2Ph_3$) between $\mathbf{P_M}$ and $\mathbf{P_P}$ via Ph twisting. The lines in two colors indicate coupling of Ph twisting with the proximal Ru–S bond twisting. The orange line indicates a change in the PPh_3 position by rotation about the Ru–P bond without stereomutation. All the energies and barriers are relative to that of isomer **1**.

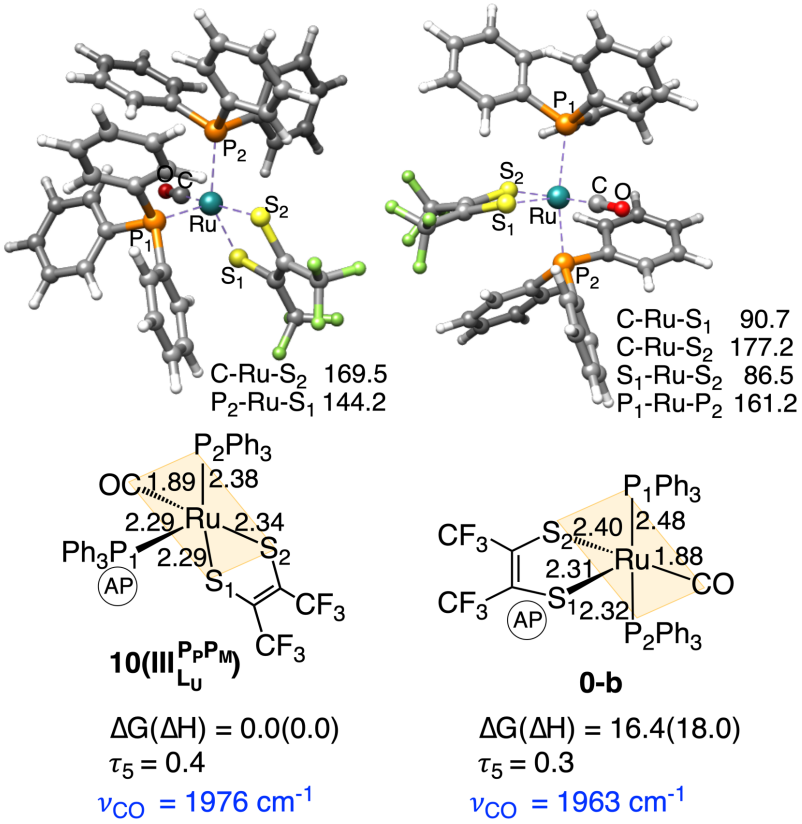


Figure S1. Assignment the isomer that corresponds to ν_{CO} near 1980 cm^{-1} by comparisons of the relative energies (kcal/mol), geometric parameters (bond distances are in Å, and angles are in °), and scaled CO frequencies between calculated isomers **10** and **0-b** at the TPSS-GD3BJ(SMD)/BS3//TPSS/BS1 level.

From comparisons of the thermodynamic predictions with experiment, DFT calculations predict that isomer **10** with a distorted SP-like geometry (τ_5 = 0.4) is consistent with the experimentally observed CO frequency near 1980 cm^{-1}.[44a] To get the information of isomer **0-b**, we performed the geometry optimization on the basis of the reported geometric data for **0-b** as the initial geometries. BP86 functional always converge **0-b** smoothly to isomer **5**, while other tested functionals like TPSS functional could converge the isomer **0-b**. Close inspection of our DFT optimized structure reveals that this proposed TBP-like **0-b** has slightly more distorted SP-like character (τ_5 = 0.3) with one S in the apical position. Moreover, the scaled CO frequency of isomer **0-b** is near 1960 cm^{-1}, which is not in accord with the experimentally observed CO frequency near 1980 cm^{-1}.[44a] In addition, the isomer **0-**

b is quite high in the relative free energy as compared to isomer **10** by about 18 kcal/mol, indicating that such less stable isomer **0-b** can be ruled out as the intermediate in this ultrafast isomerization.

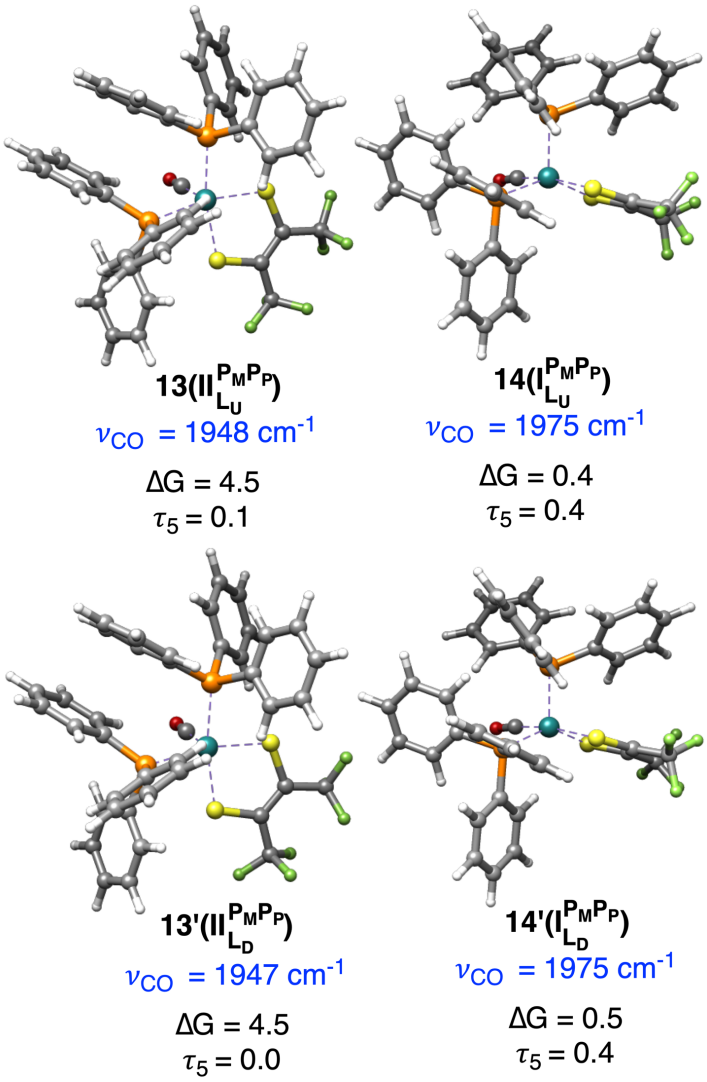


Figure S2. Relative free energies (kcal/mol) relative to **1**, the parameter τ_5, and scaled CO frequencies for optimized isomers **13**(**13**′) and **14**(**14**′) at the BP86-GD3BJ(SMD)/BS3//BP86/BS1 level.[a] [a]The scaling factor for ν_{CO} is obtained by averaging the two individual scaling factors of two crystals **1** and **5**′.

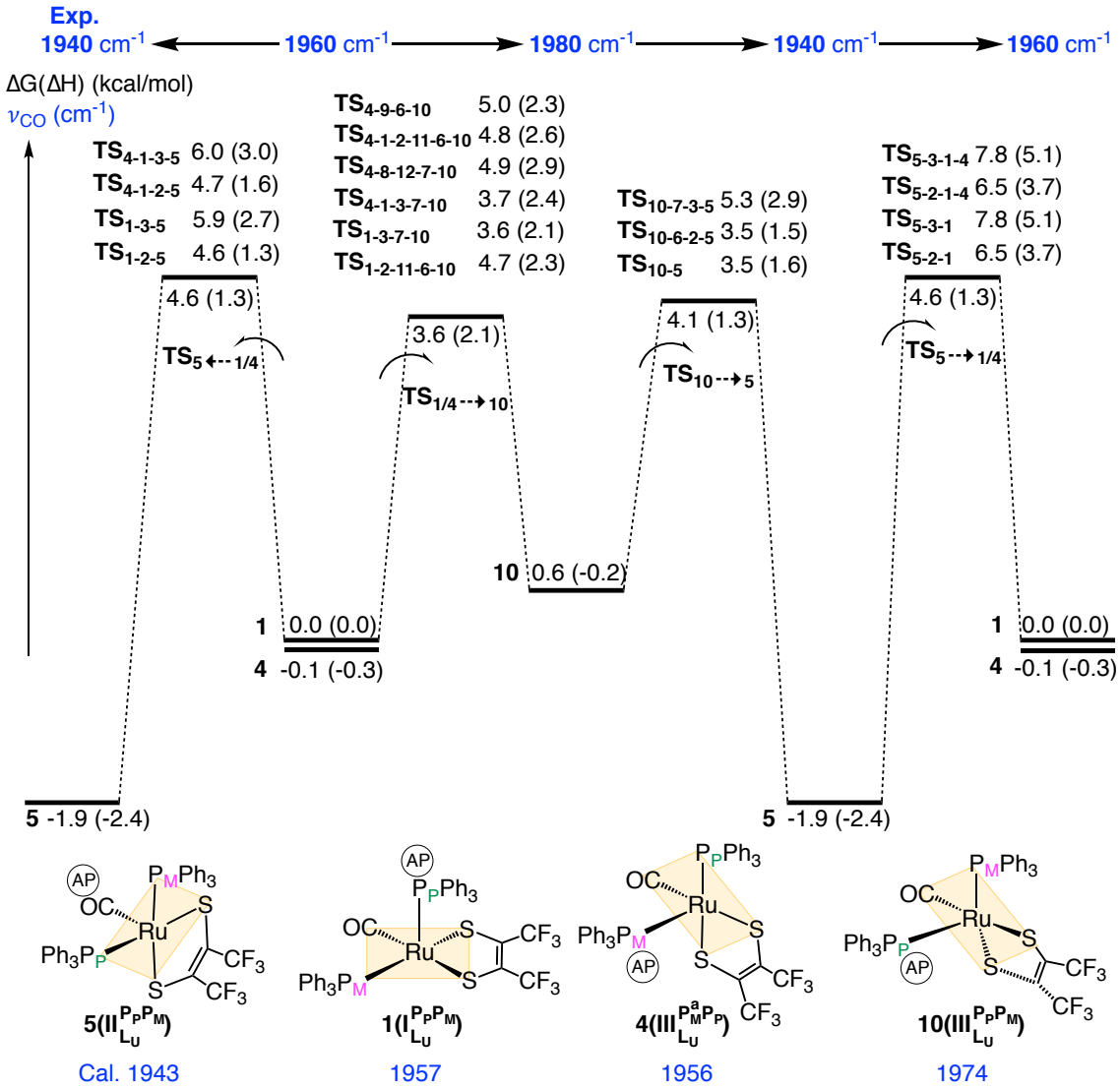


Figure S3. Overall energy profile of the Ru($S_2C_2(CF_3)_2$)(CO)(PPh_3)$_2$ isomerization based on the most stable $\mathbf{L_U}$ isomers in each CO frequency pattern (ν_{CO} ≈ 1960 cm^{-1} (**1** and **4**), 1940 cm^{-1} (**5**), and 1980 cm^{-1} (**10**)) at the BP86-GD3BJ(SMD)/BS3//BP86/BS2 level. The vertical energy scale refers to **1** as zero point.

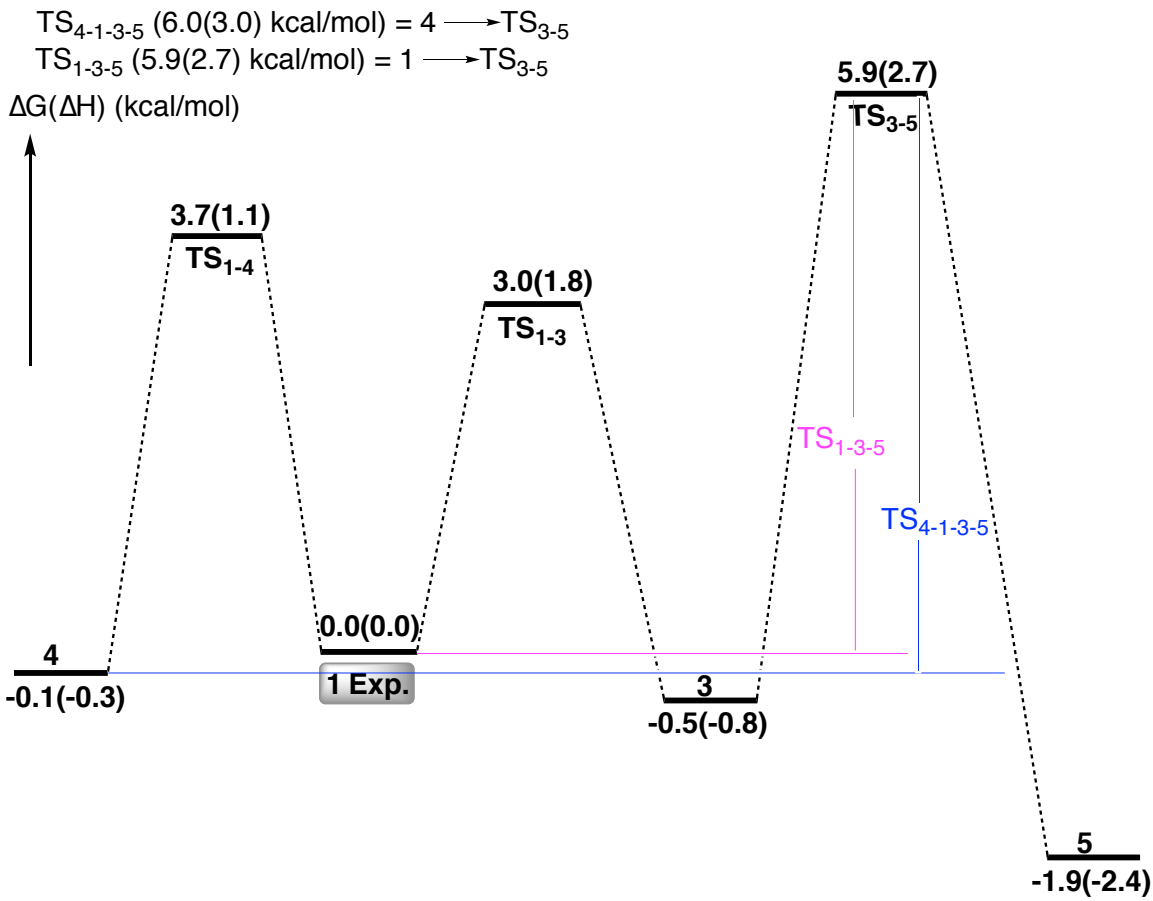


Figure S3a. Energy profiles of interchange pathways from the isomers **1** or **4** (ν_{CO} ≈ 1960 cm^{-1}) to **10** (ν_{CO} ≈ 1940 cm^{-1}) at the BP86-GD3BJ(SMD)/BS3//BP86/BS2 level. The overall barrier **TS$_{4\text{-}1\text{-}3\text{-}5}$** indicates of the difference between **TS$_{3\text{-}5}$** and the starting isomer **4**. The overall barrier **TS$_{1\text{-}3\text{-}5}$** indicates of the difference between **TS$_{3\text{-}5}$** and the starting isomer **1**.

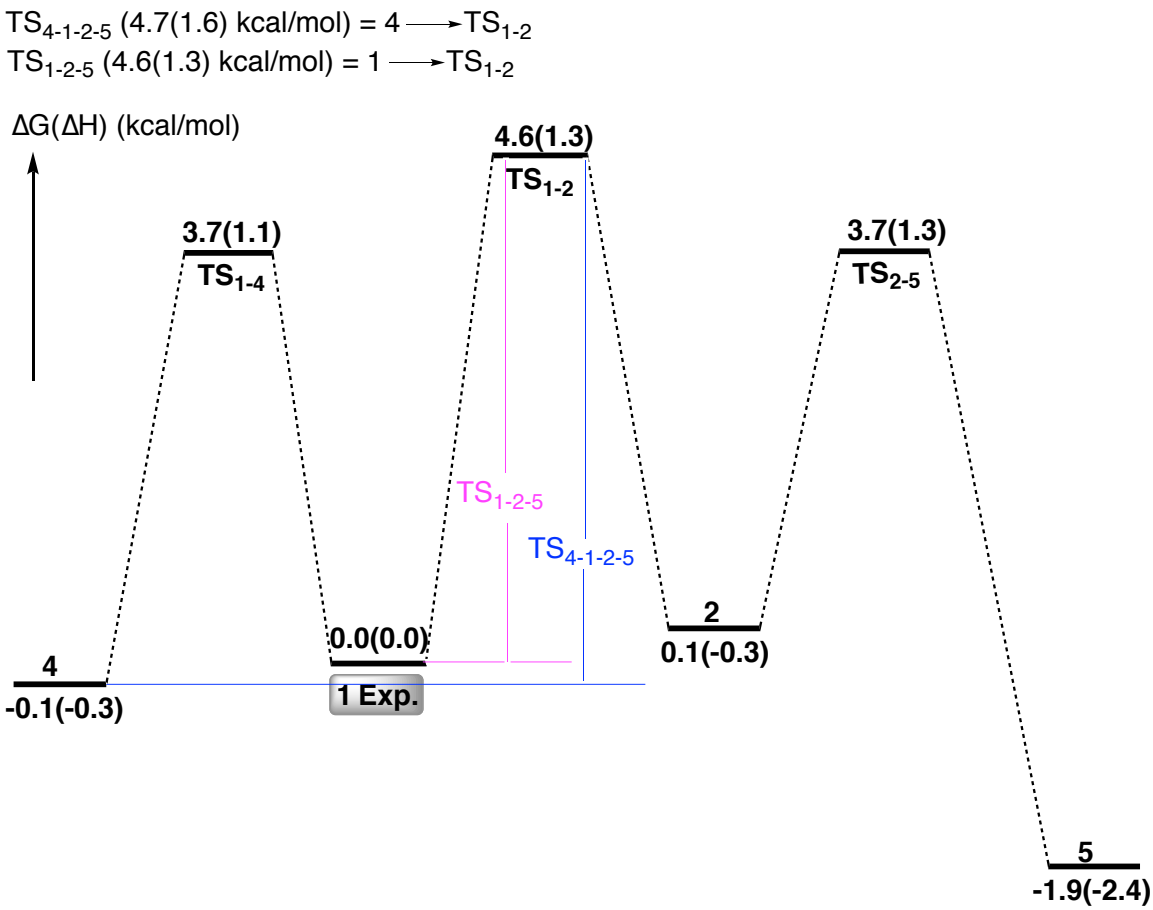


Figure S3b. Energy profiles of interchange pathways from the isomers **1** and **4** (ν_{CO} ≈ 1960 cm^{-1}) to **10** (ν_{CO} ≈ 1940 cm^{-1}) at the BP86-GD3BJ(SMD)/BS3//BP86/BS2 level. The overall barrier **TS$_{4\text{-}1\text{-}2\text{-}5}$** indicates of the difference between **TS$_{1\text{-}2}$** and the starting isomer **4**. The overall barrier **TS$_{1\text{-}2\text{-}5}$** indicates of the difference between **TS$_{1\text{-}2}$** and the starting isomer **1**.

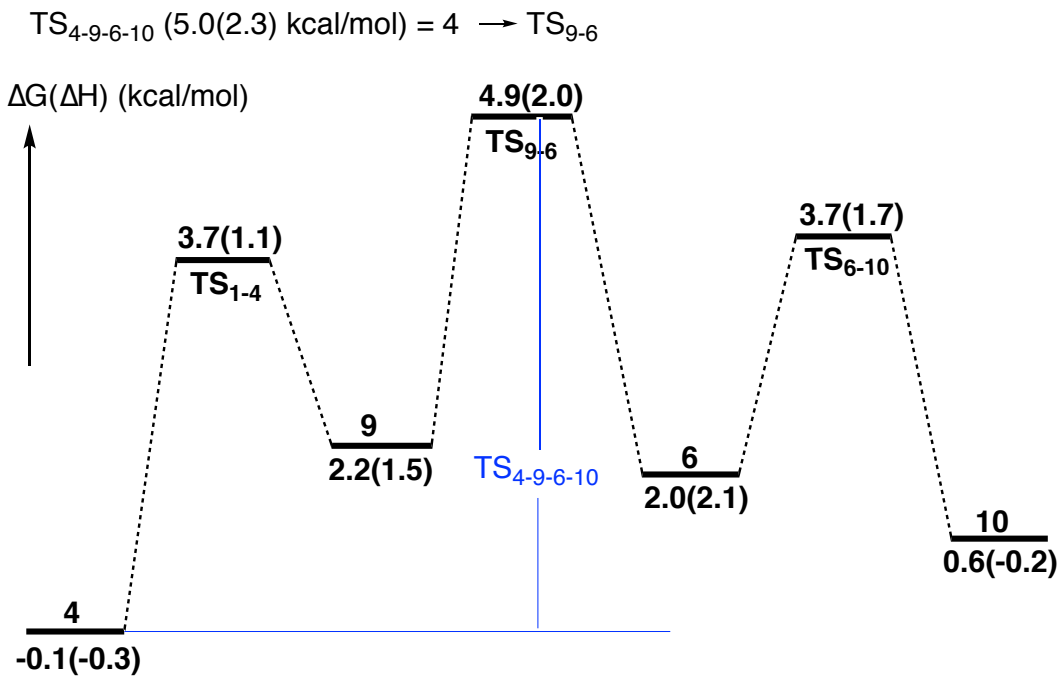


Figure S3c. Energy profiles of interchange pathways from the isomer **4** (ν_{CO} ≈ 1960 cm^{-1}) to **10** (ν_{CO} ≈ 1980 cm^{-1}) at the BP86-GD3BJ(SMD)/BS3//BP86/BS2 level. The overall barrier **$TS_{4\text{-}9\text{-}6\text{-}10}$** indicates of the difference between **$TS_{9\text{-}6}$** and the starting isomer **4**.

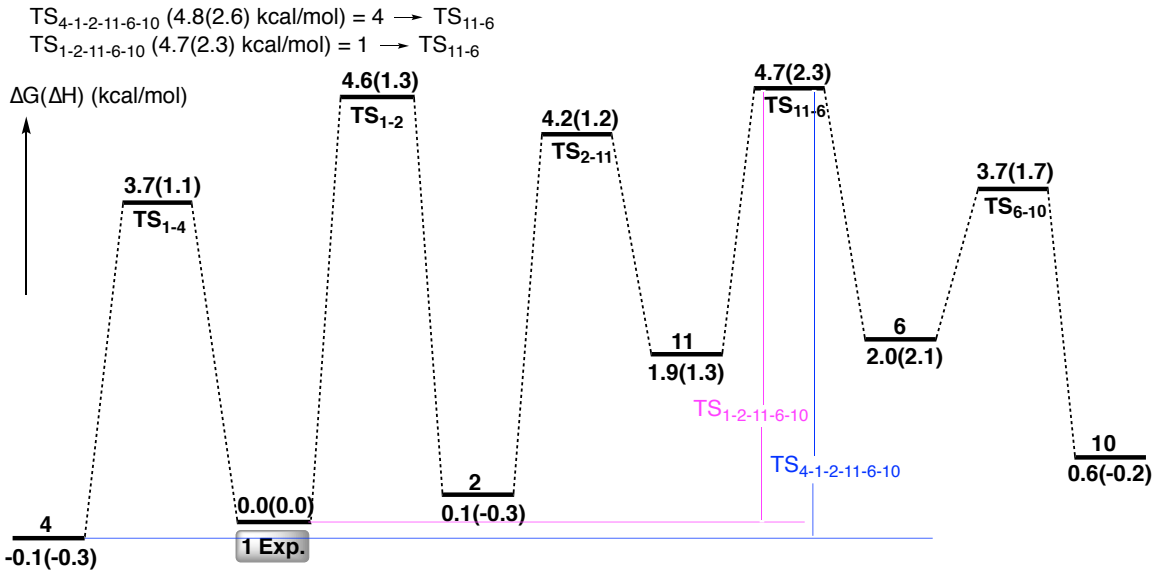


Figure S3d. Energy profiles of interchange pathways from the isomers **1** or **4** (ν_{CO} ≈ 1960 cm^{-1}) to **10** (ν_{CO} ≈ 1980 cm^{-1}) at the BP86-GD3BJ(SMD)/BS3//BP86/BS2 level. The overall barrier **$TS_{4\text{-}1\text{-}2\text{-}11\text{-}6\text{-}10}$** indicates of the difference between **$TS_{11\text{-}6}$** and the starting isomer **4**. The overall barrier **$TS_{1\text{-}2\text{-}11\text{-}6\text{-}10}$** indicates of the difference between **$TS_{11\text{-}6}$** and the starting isomer **1**.

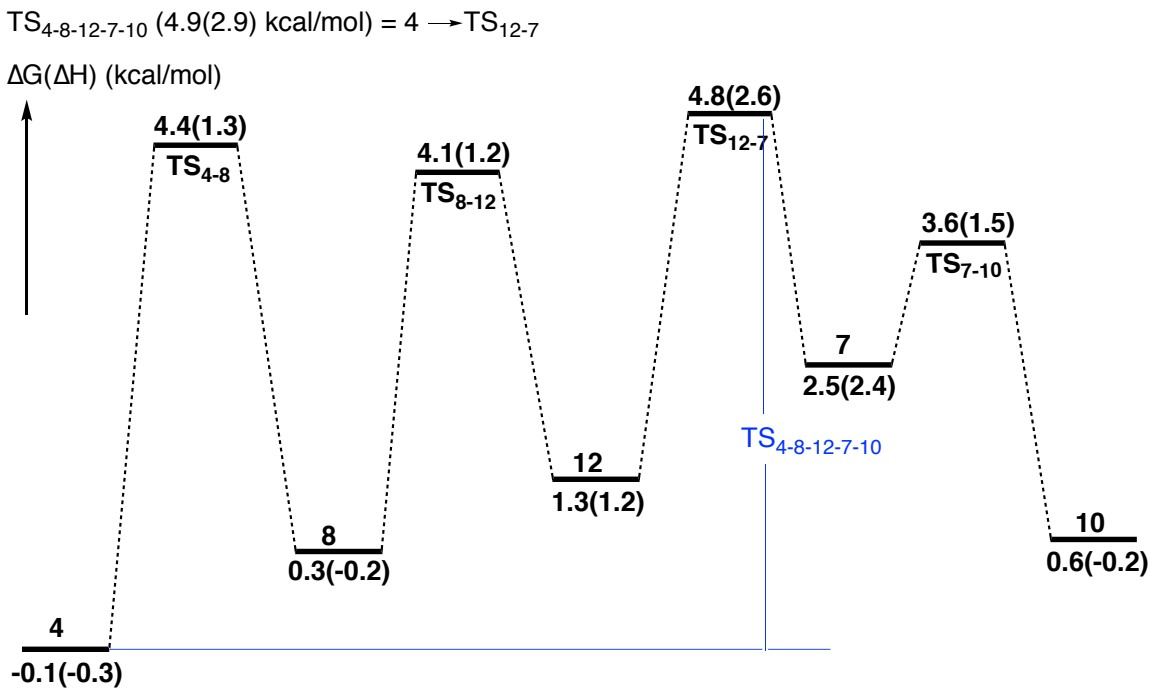


Figure S3e. Energy profiles of interchange pathways from the isomer **4** (ν_{CO} ≈ 1960 cm^{-1}) to **10** (ν_{CO} ≈ 1980 cm^{-1}) at the BP86-GD3BJ(SMD)/BS3//BP86/BS2 level. The overall barrier **TS$_{4\text{-}8\text{-}12\text{-}7\text{-}10}$** indicates of the difference between **TS$_{12\text{-}7}$** and the starting isomer **4**.

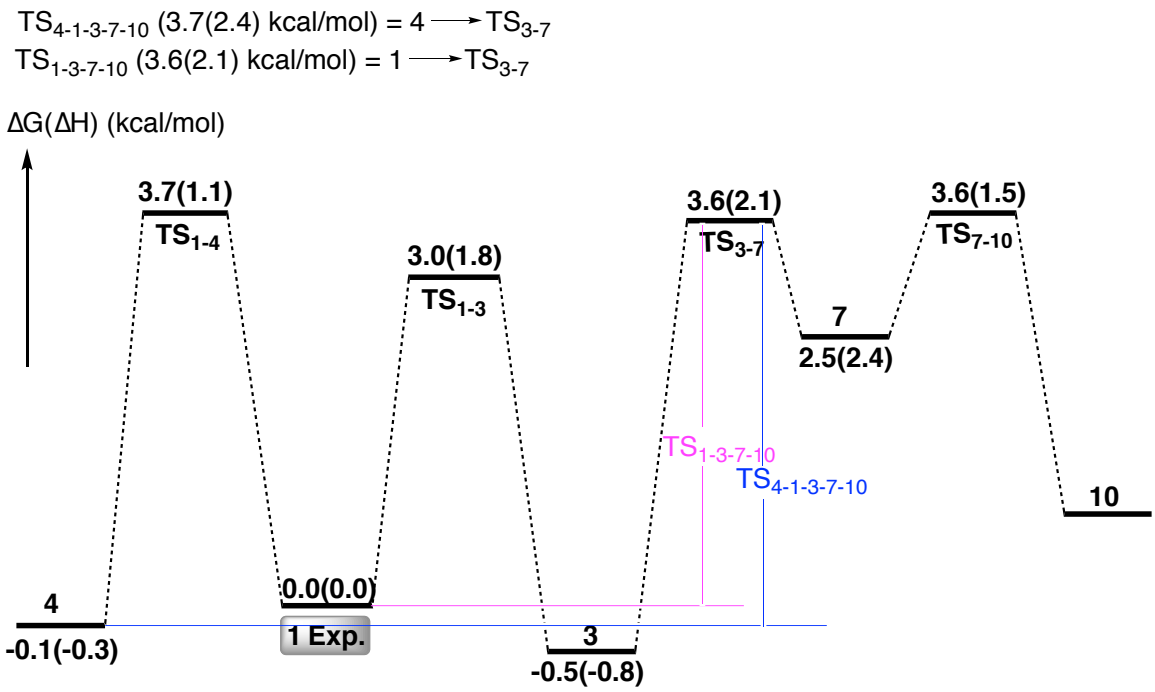


Figure S3f. Energy profiles of interchange pathways from the isomers **1** or **4** (ν_{CO} ≈ 1960 cm^{-1}) to **10** (ν_{CO} ≈ 1980 cm^{-1}) at the BP86-GD3BJ(SMD)/BS3//BP86/BS2 level. The overall barrier **TS$_{4\text{-}1\text{-}3\text{-}7\text{-}10}$** indicates of the difference between **TS$_{3\text{-}7}$** and the starting isomer **4**. The overall barrier **TS$_{1\text{-}3\text{-}7\text{-}10}$** indicates of the difference between **TS$_{3\text{-}7}$** and the starting isomer **1**.

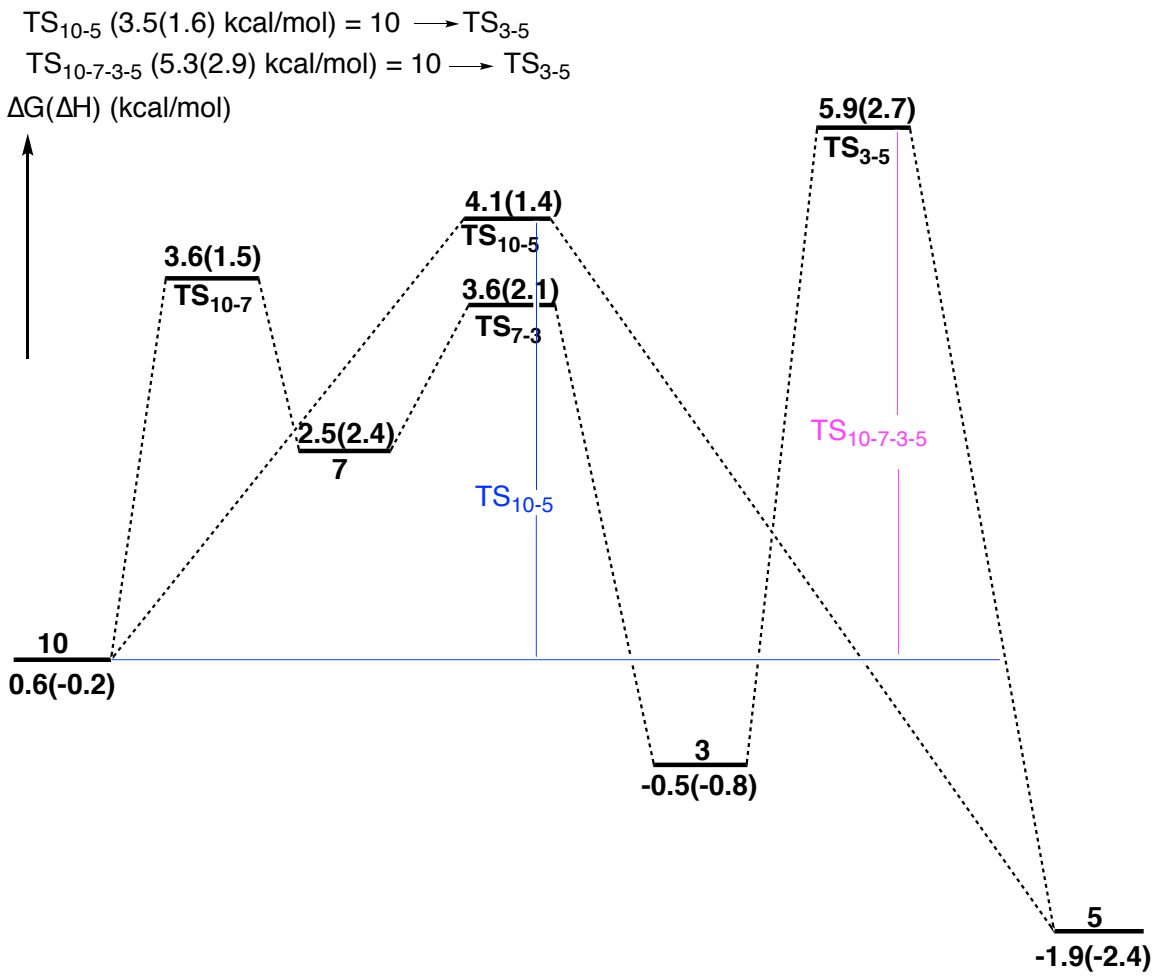


Figure S3g. Energy profiles of interchange pathways from the isomer **10** (ν_{CO} ≈ 1980 cm^{-1}) to **5** (ν_{CO} ≈ 1940 cm^{-1}) at the BP86-GD3BJ(SMD)/BS3//BP86/BS2 level. The overall barrier **$TS_{10\text{-}5}$** indicates of the difference between **$TS_{10\text{-}5}$** and the starting isomer **10**. The overall barrier **$TS_{10\text{-}7\text{-}3\text{-}5}$** indicates of the difference between **$TS_{3\text{-}5}$** and the starting isomer **10**.

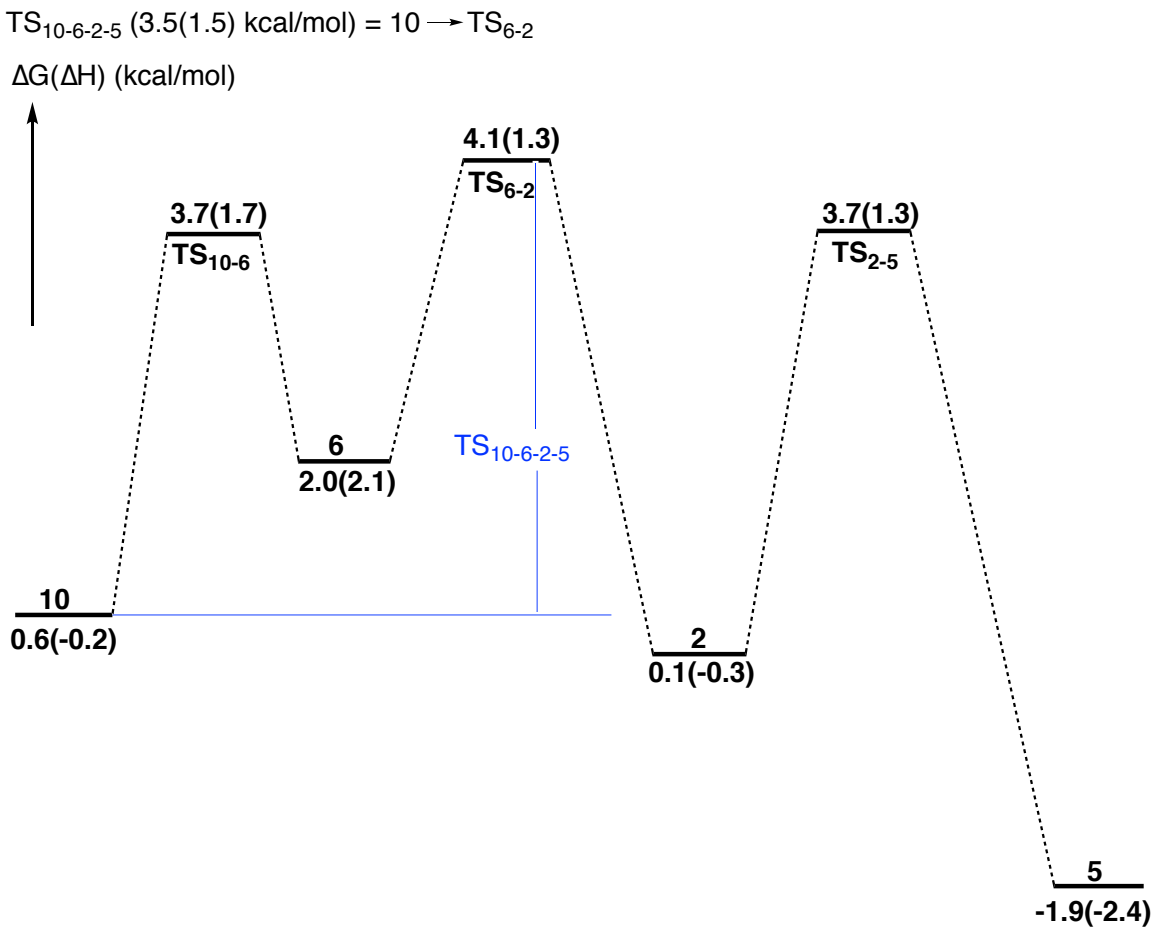


Figure S3h. Energy profiles of interchange pathways from the isomer **10** (ν_{CO} ≈ 1980 cm^{-1}) to **5** (ν_{CO} ≈ 1940 cm^{-1}) at the BP86-GD3BJ(SMD)/BS3//BP86/BS2 level. The overall barrier **TS$_{10\text{-}6\text{-}2\text{-}5}$** indicates of the difference between **TS$_{6\text{-}2}$** and the starting isomer **10**.

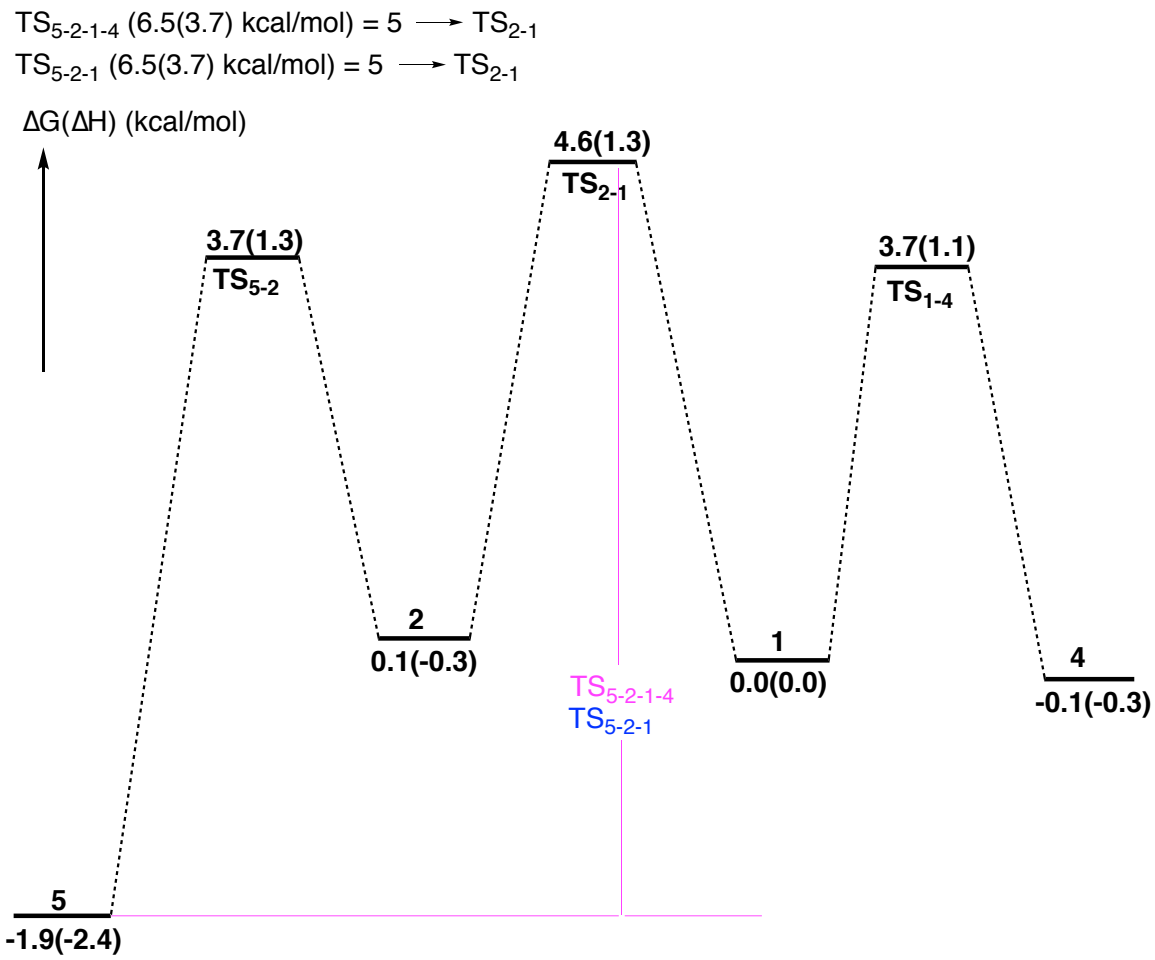


Figure S3i. Energy profiles of interchange pathways from the isomer **5** (ν_{CO} ≈ 1940 cm^{-1}) to **1** or **4** (ν_{CO} ≈ 1960 cm^{-1}) at the BP86-GD3BJ(SMD)/BS3//BP86/BS2 level. The overall barrier **TS$_{5\text{-}2\text{-}1\text{-}4}$** indicates of the difference between **TS$_{2\text{-}1}$** and the starting isomer **5**. The overall barrier **TS$_{5\text{-}2\text{-}1}$** indicates of the difference between **TS$_{2\text{-}1}$** and the starting isomer **5**.

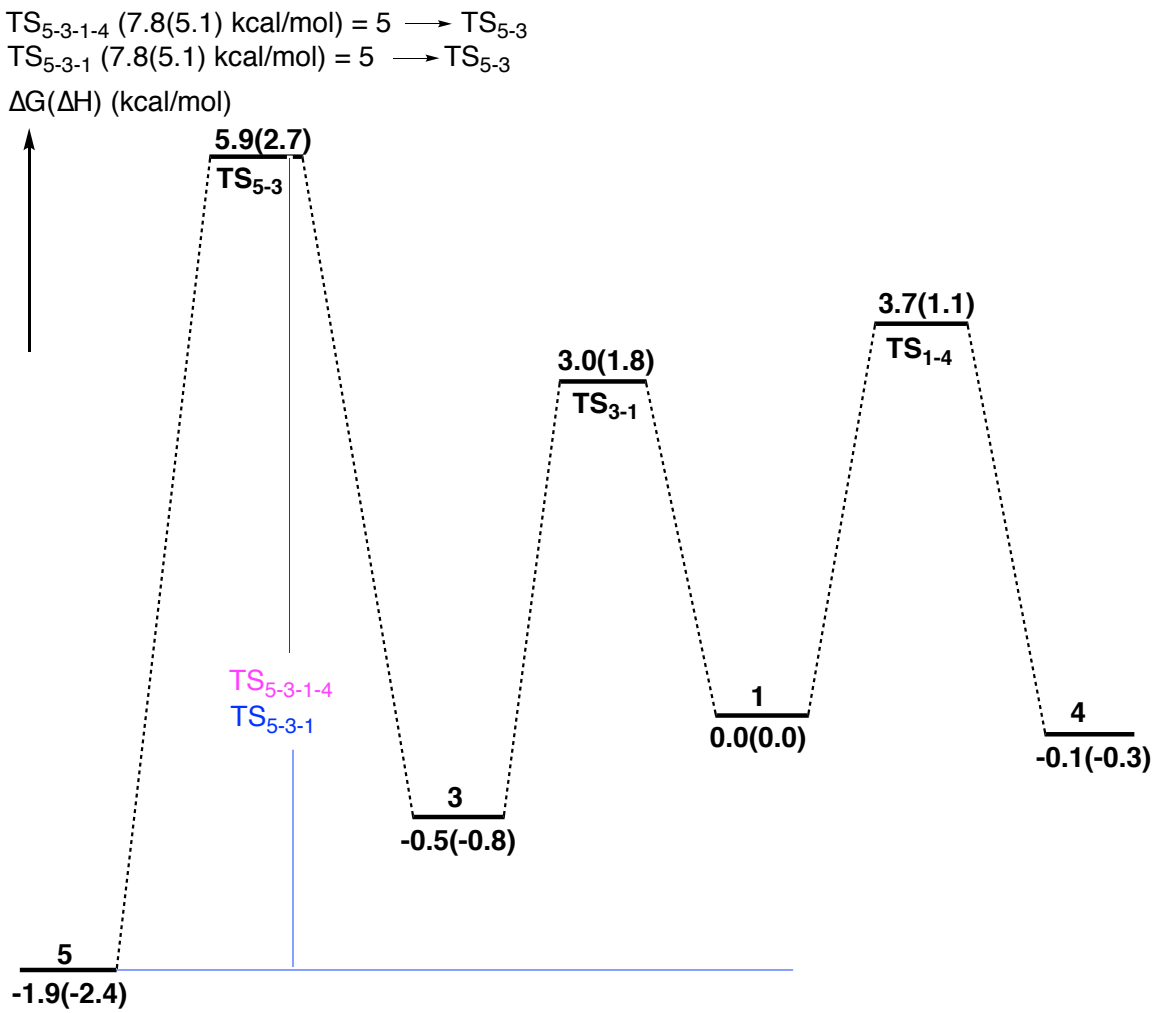


Figure S3j. Energy profiles of interchange pathways from the isomer **5** (ν_{CO} ≈ 1940 cm^{-1}) to **1** or **4** (ν_{CO} ≈ 1960 cm^{-1}) at the BP86-GD3BJ(SMD)/BS3//BP86/BS2 level. The overall barrier **TS$_{5\text{-}3\text{-}1\text{-}4}$** indicates of the difference between **TS$_{5\text{-}3}$** and the starting isomer **5**. The overall barrier **TS$_{5\text{-}3\text{-}1}$** indicates of the difference between **TS$_{5\text{-}3}$** and the starting isomer **5**.

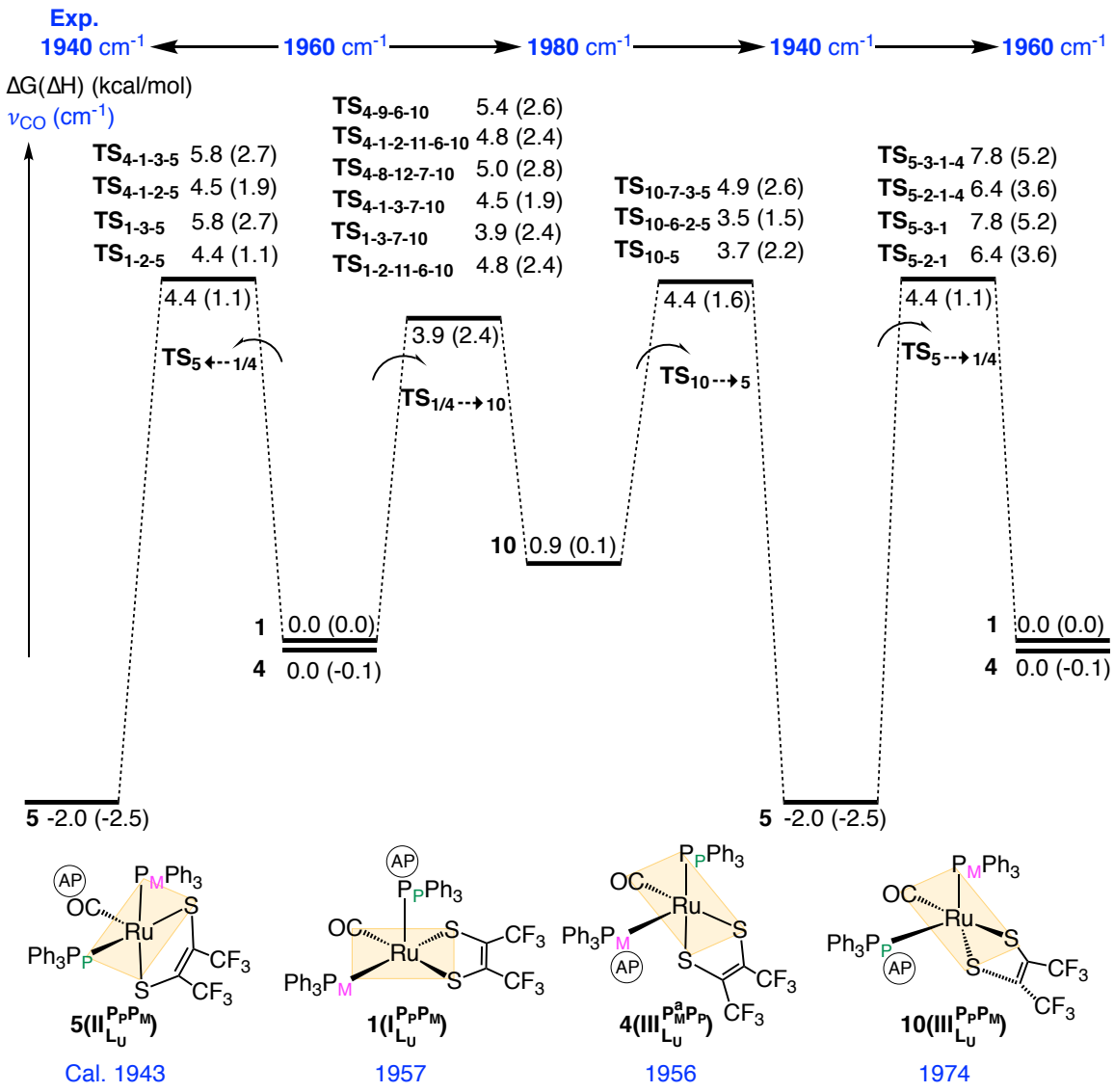


Figure S4. Overall energy profile of the $Ru(S_2C_2(CF_3)_2)(CO)(PPh_3)_2$ isomerization at the B3LYP-GD3BJ(SMD)/BS3//BP86/BS2 level based on the most stable isomers in each CO frequency pattern (ν_{CO} ≈ 1960 cm^{-1} (**1** and **4**), 1940 cm^{-1} (**5**), and 1980 cm^{-1} (**10**)). The vertical energy scale refers to **1** as 0.0. The overall barriers in each path refer to their starting isomer.

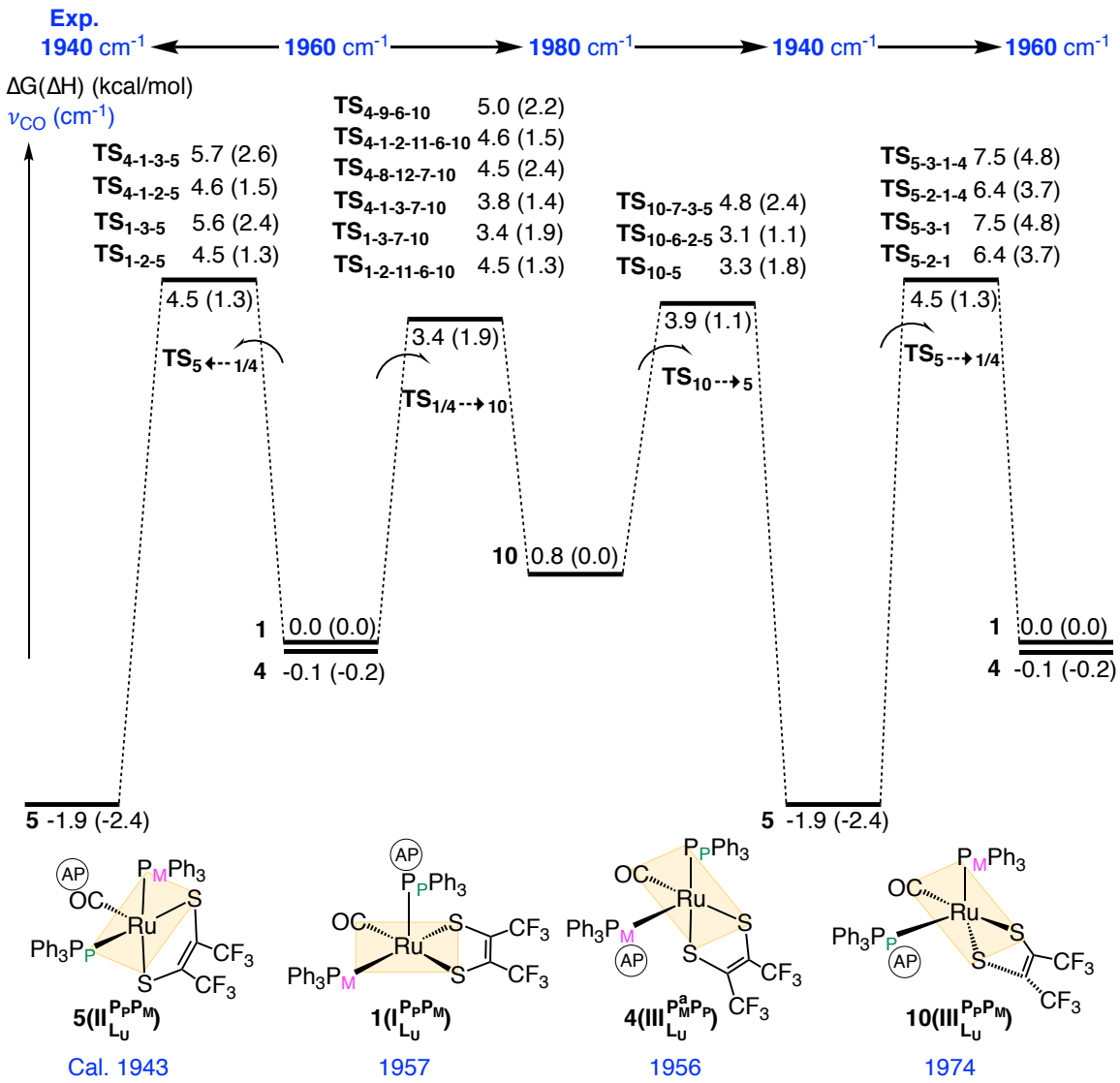
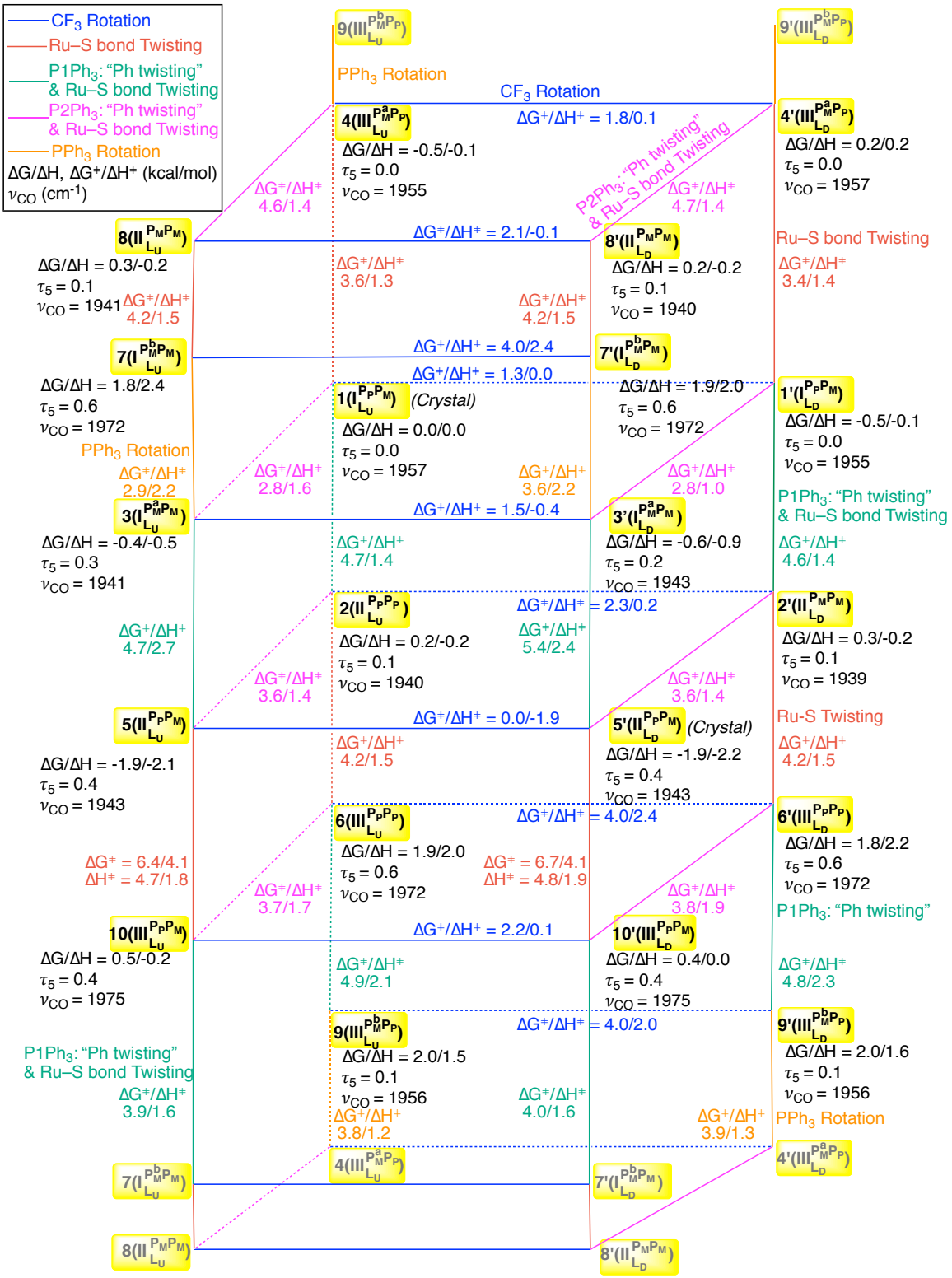
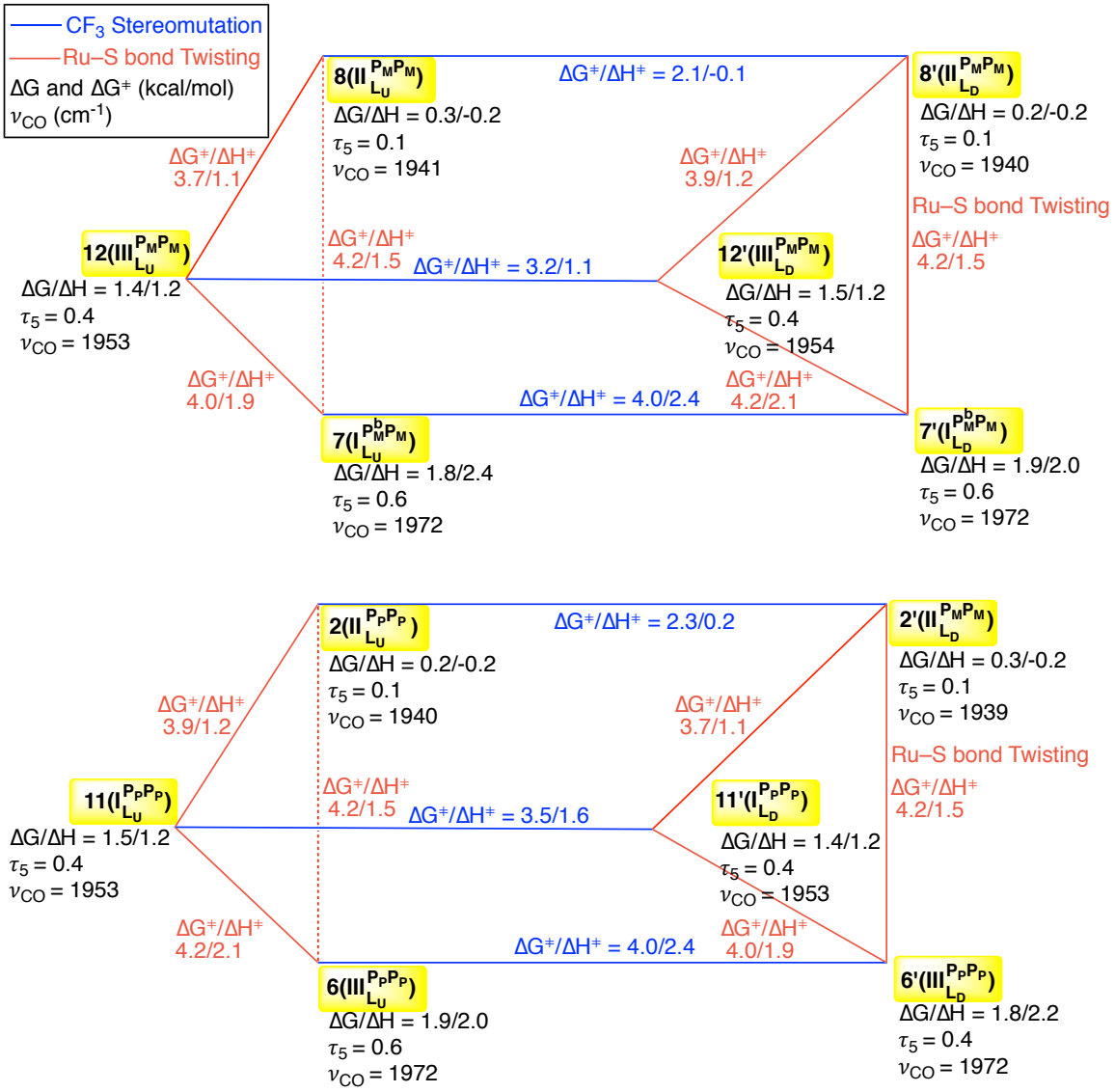


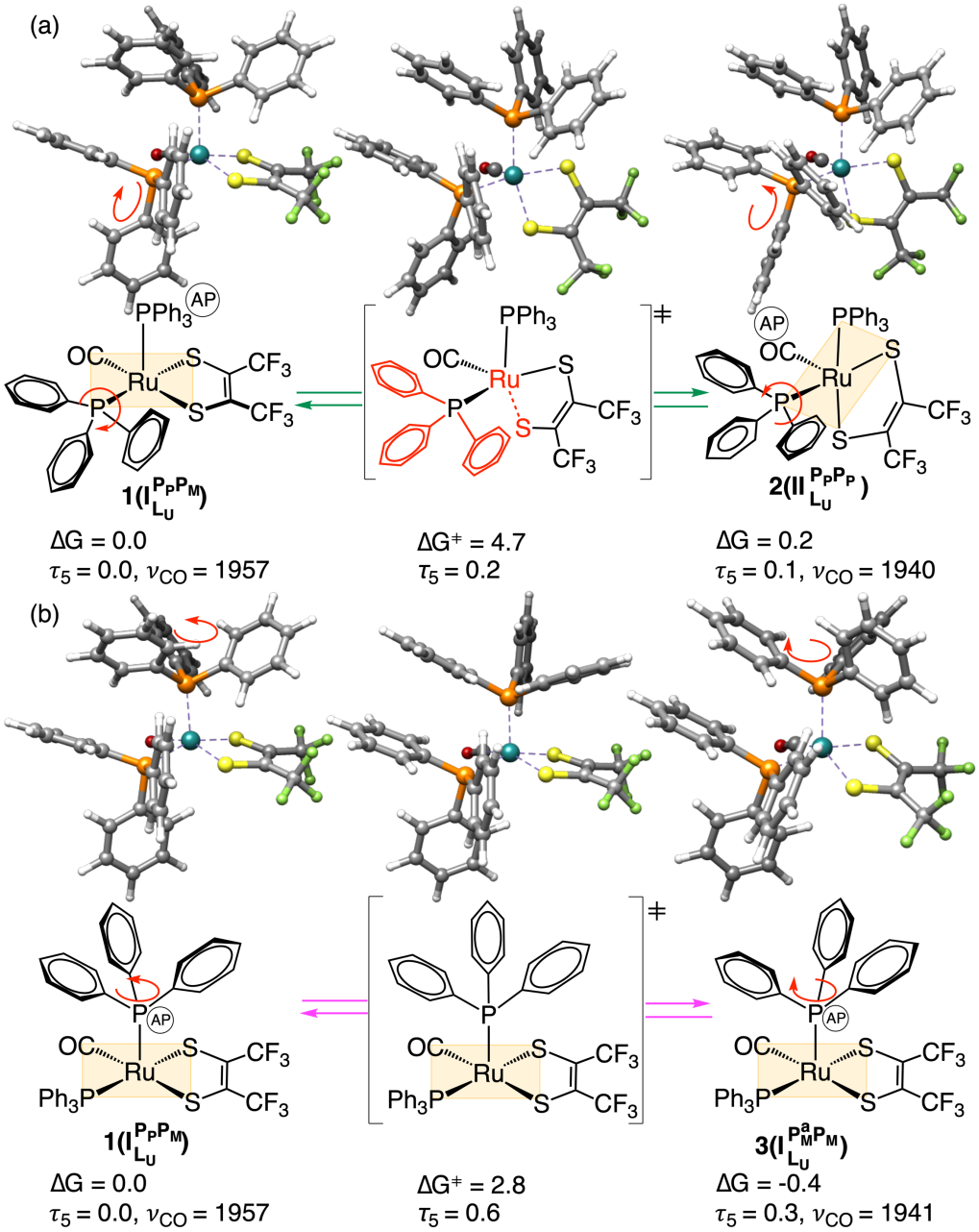
Figure S5. Overall energy profile of the $Ru(S_2C_2(CF_3)_2)(CO)(PPh_3)_2$ isomerization at the TPSS-GD3BJ(SMD)/BS3//BP86/BS2 level based on the most stable isomers in each CO frequency pattern (ν_{CO} ≈ 1960 cm^{-1} (**1** and **4**), 1940 cm^{-1} (**5**), and 1980 cm^{-1} (**10**)). The vertical energy scale refers to **1** as 0.0. The overall barriers in each path refer to their starting isomer.

Scheme S3. Calculated stereomutation mechanisms based on experimentally observed two crystals at the BP86-GD3BJ(SMD)/BS3//BP86/BS1 level.[a]





[a]All the energies of the isomers and barriers are relative to crystal structure **1**. The scaling factor for ν_{CO} is obtained by averaging the two individual scaling factors of experimentally observed two crystals (**1** and **5′**). The vermilion line indicates of the Ru stereochemistry (**I**, **II**, **III**) interchange by twisting one of Ru–S bond. The bluish green and magenta lines indicate of the conformation of two different PPh_3 permutations between $\mathbf{P_M}$ and $\mathbf{P_P}$ via Ph group twisting, or simultaneous twisting the proximal Ru-S bond. The orange line indicates of only changing the PPh_3 position without stereomutation.


(a)
PPh3
AP
OC
Ru
S
CF3
P
1(I PPPM LU)
ΔG = 0.0
τ5 = 0.0, νCO = 1957
ΔG‡ = 4.7
τ5 = 0.2
2(II PPPP LU)
ΔG = 0.2
τ5 = 0.1, νCO = 1940
(b)
Ph3P
1(I PPPM LU)
ΔG = 0.0
τ5 = 0.0, νCO = 1957
ΔG‡ = 2.8
τ5 = 0.6
3(I PaMPM LU)
ΔG = -0.4
τ5 = 0.3, νCO = 1941

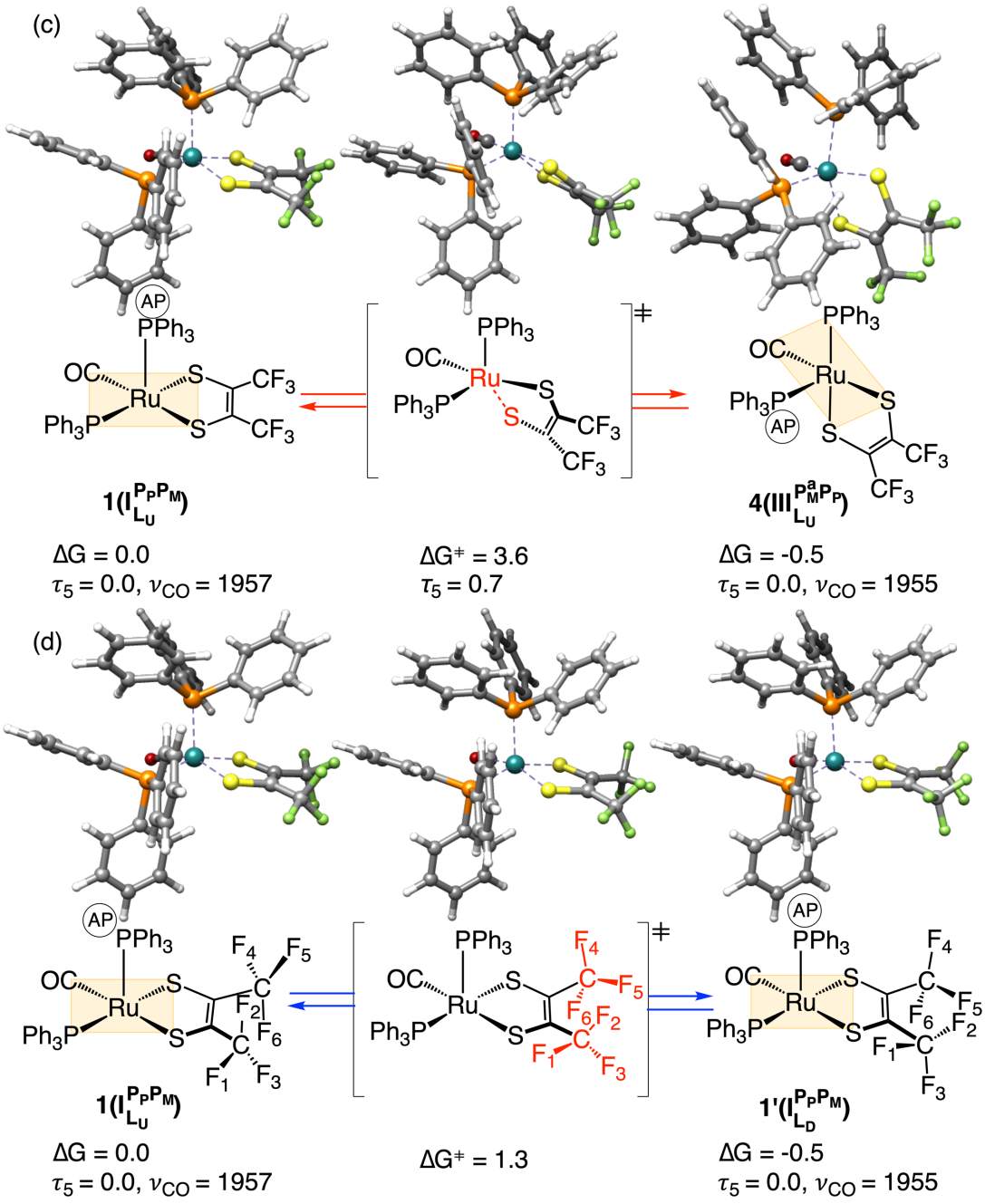


Figure S6. Permutation of isomer **1** at the BP86-GD3BJ(SMD)/BS3//BP86/BS1 level.

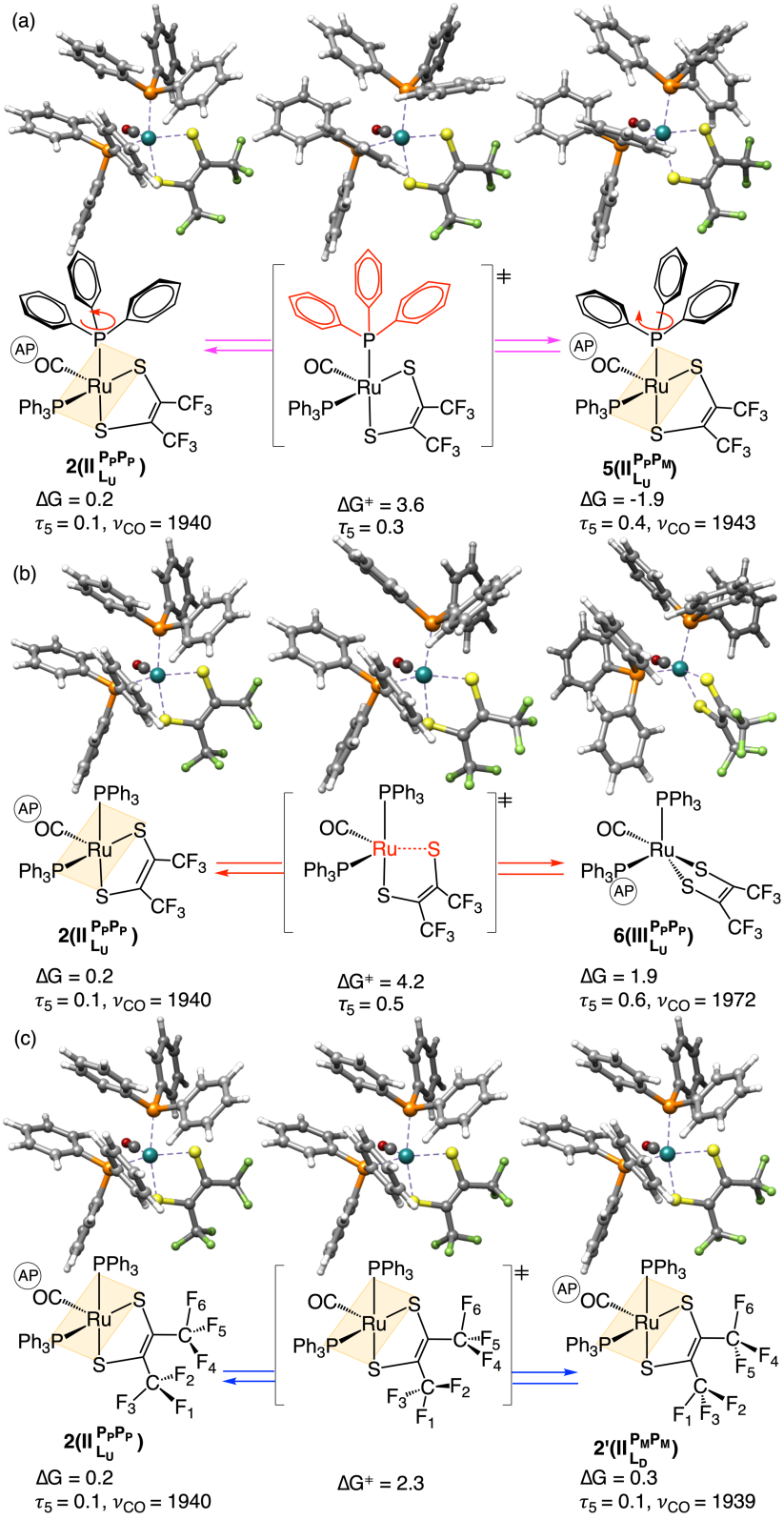


Figure S7. Permutation of isomer **2** at the BP86-GD3BJ(SMD)/BS3//BP86/BS1 level.

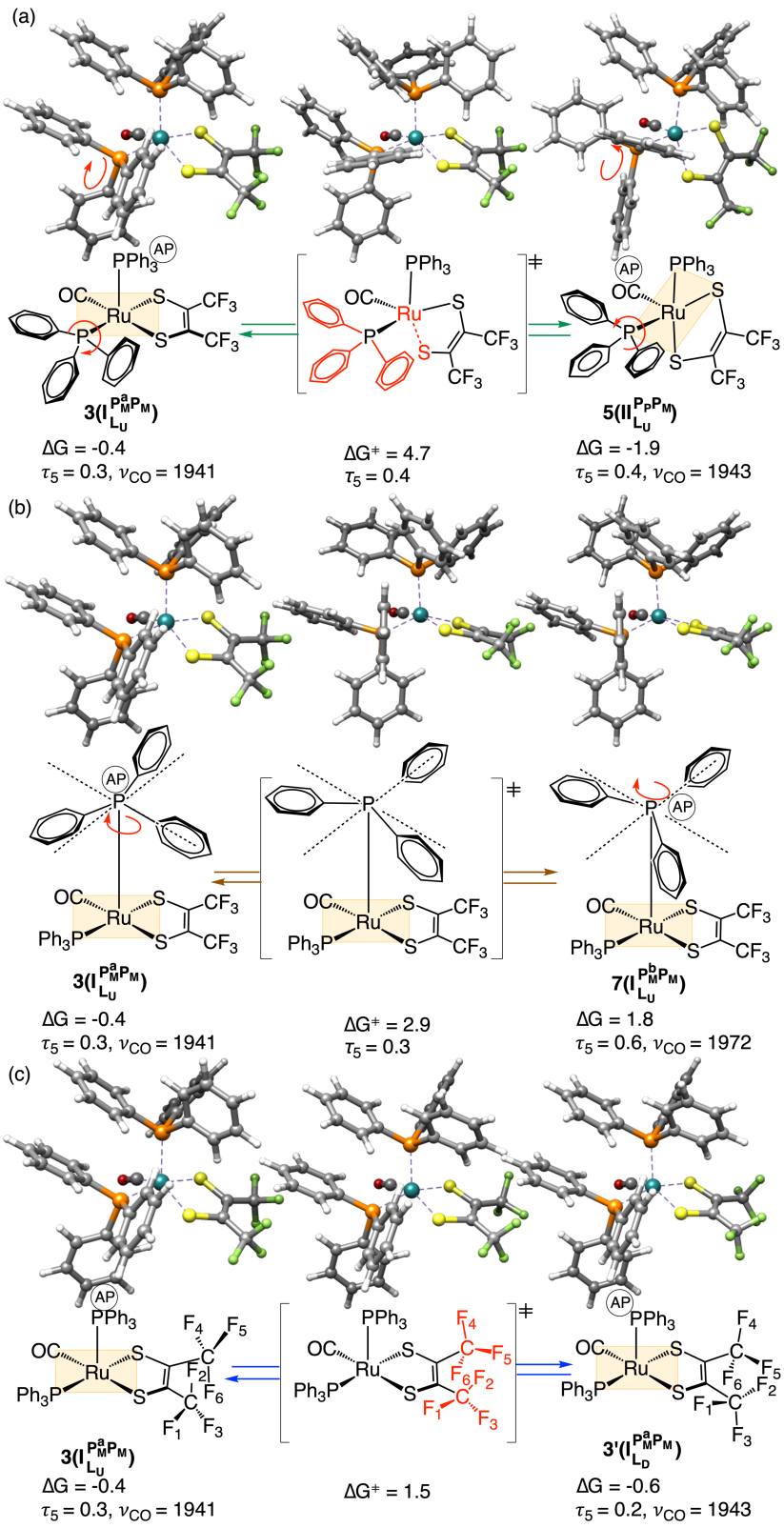


Figure S8. Permutation of isomer **3** at the BP86-GD3BJ(SMD)/BS3//BP86/BS1 level.

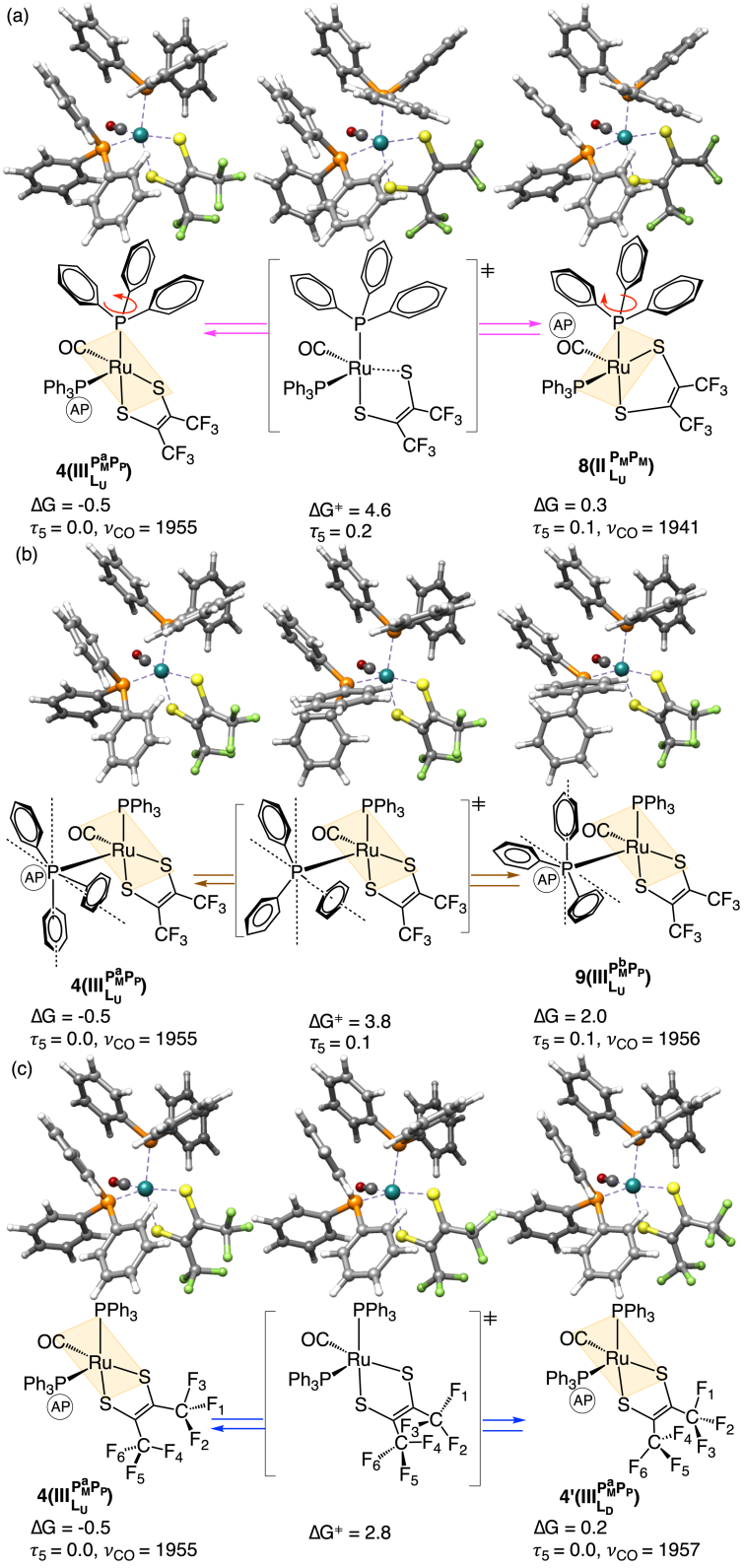


Figure S9. Permutation of isomer **4** at the BP86-GD3BJ(SMD)/BS3//BP86/BS1 level.

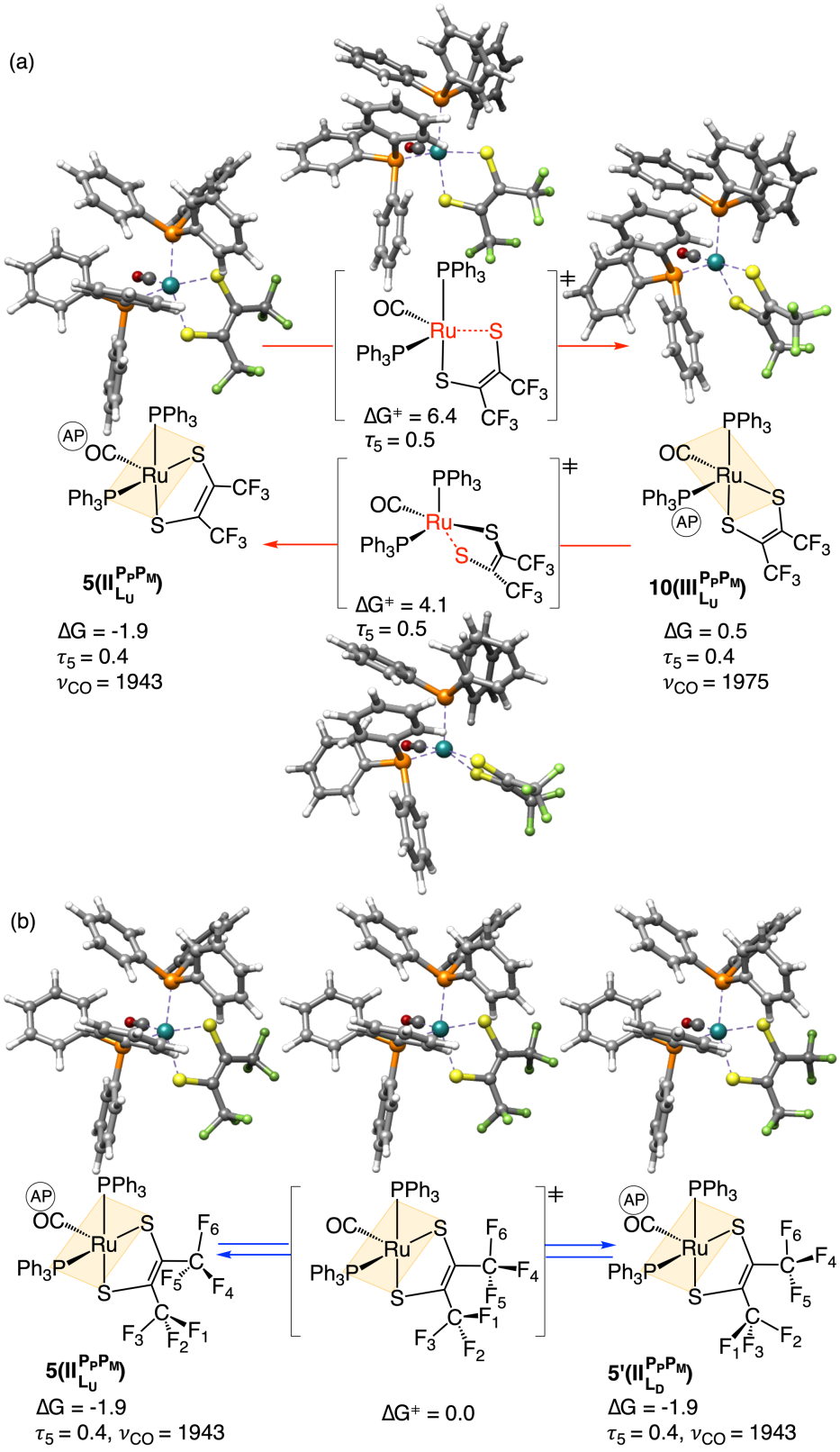


Figure S10. Permutation of isomer **5** at the BP86-GD3BJ(SMD)/BS3//BP86/BS1 level.

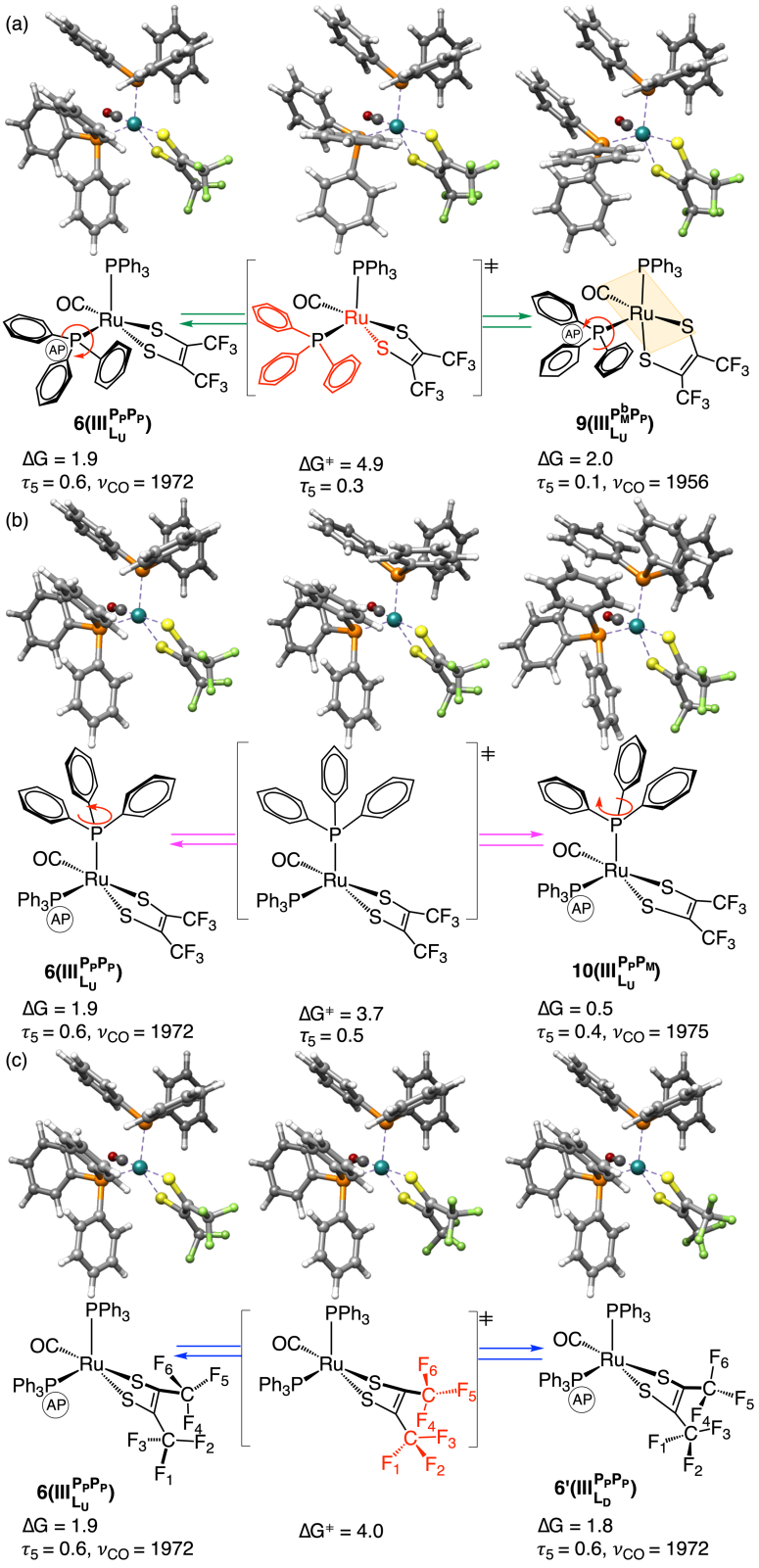


Figure S11. Permutation of isomer **6** at the BP86-GD3BJ(SMD)/BS3//BP86/BS1 level.

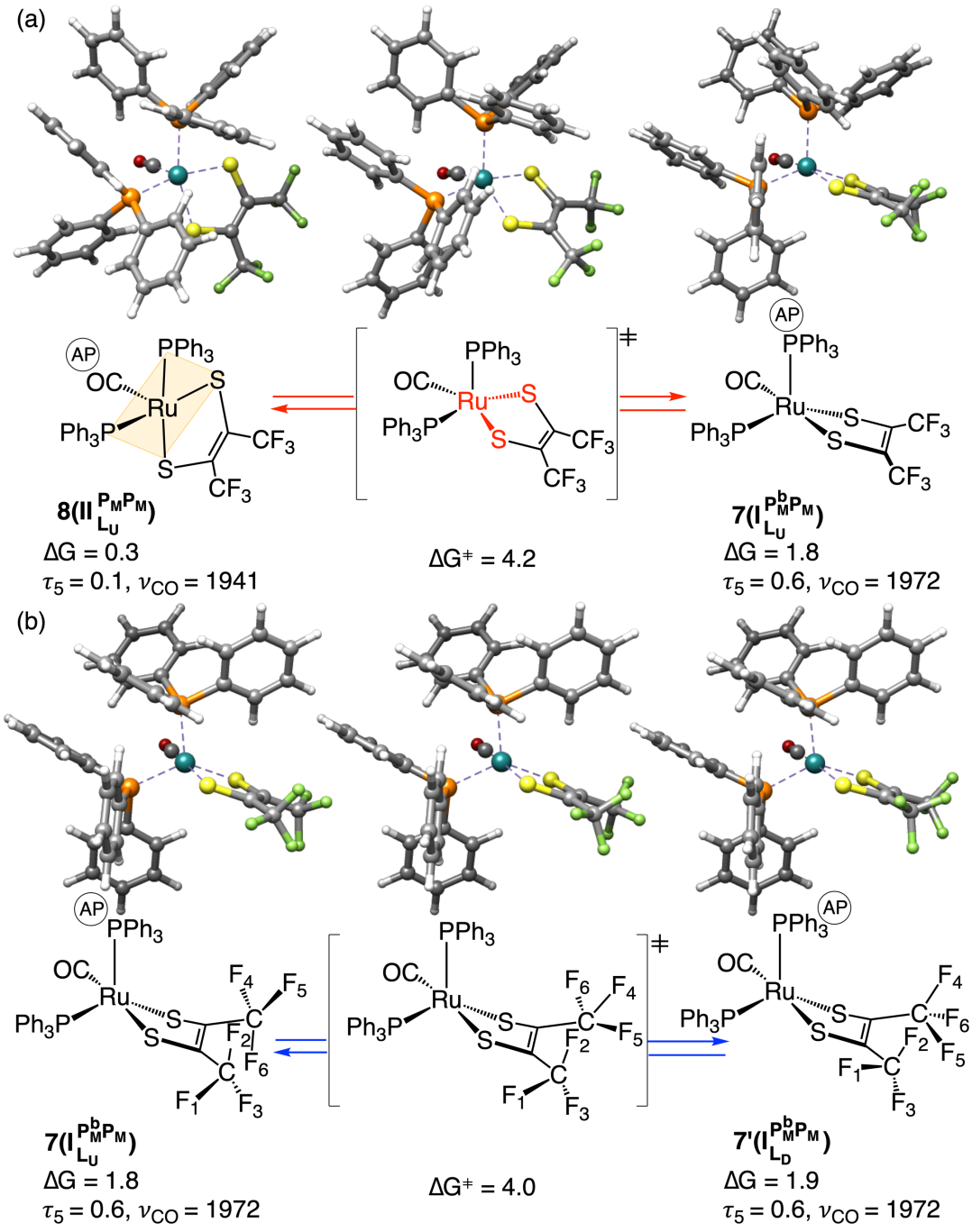


Figure S12. Permutation of isomer **7** at the BP86-GD3BJ(SMD)/BS3//BP86/BS1 level.

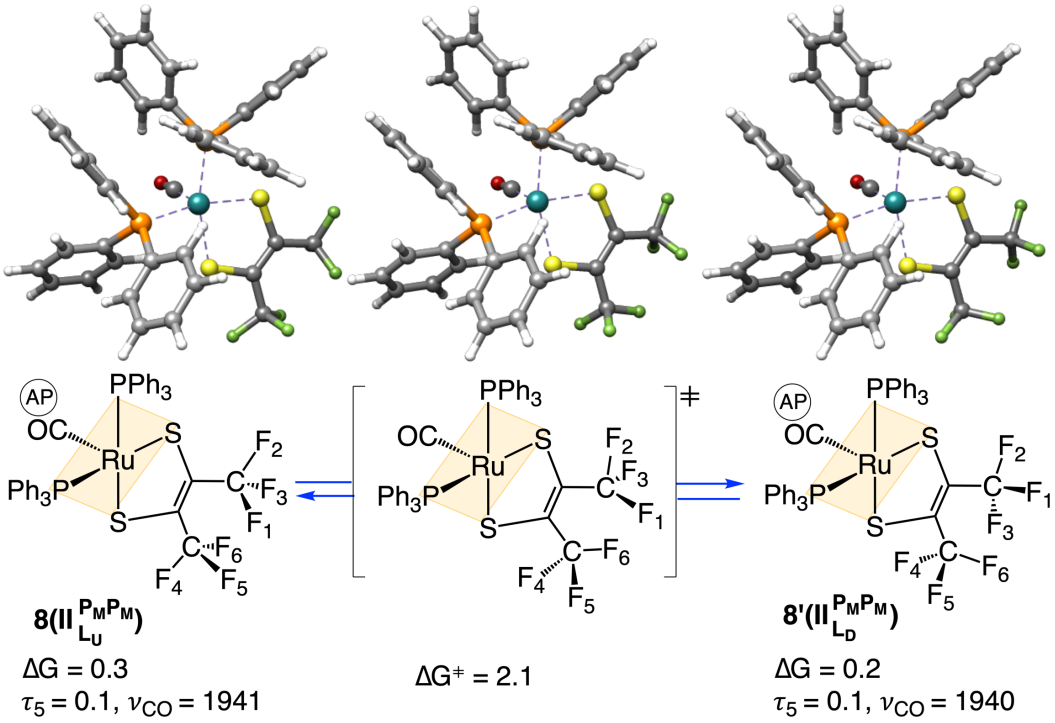


Figure S13. Permutation of isomer **8** at the BP86-GD3BJ(SMD)/BS3//BP86/BS1 level.

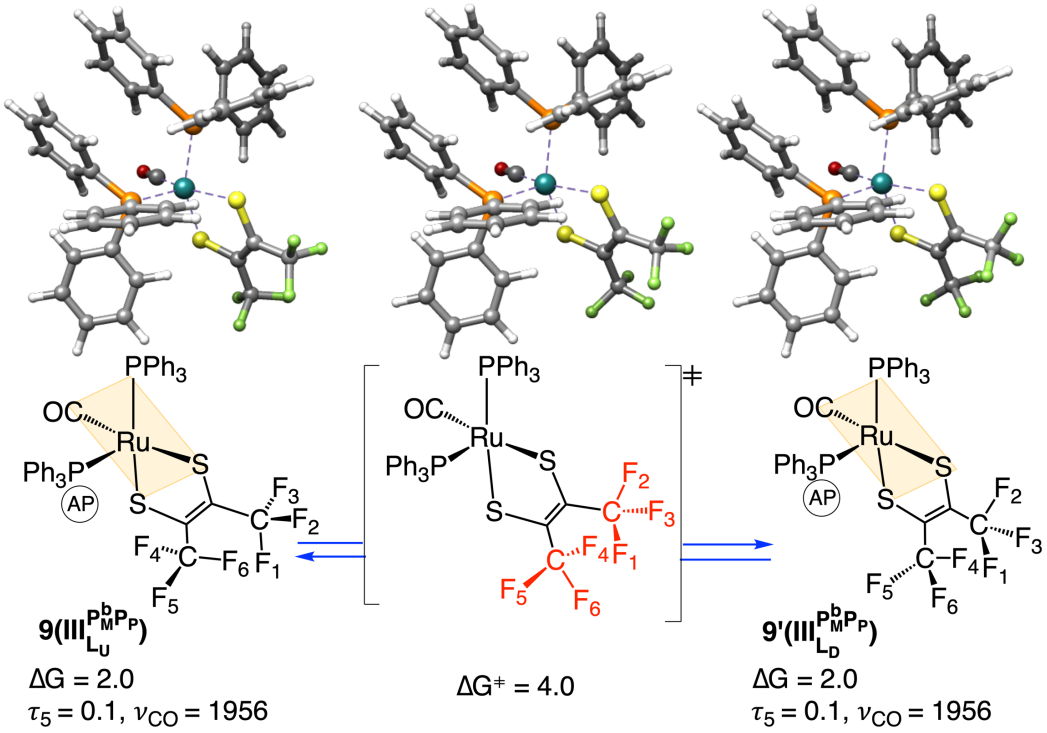


Figure S14. Permutation of isomer **9** at the BP86-GD3BJ(SMD)/BS3//BP86/BS1 level.

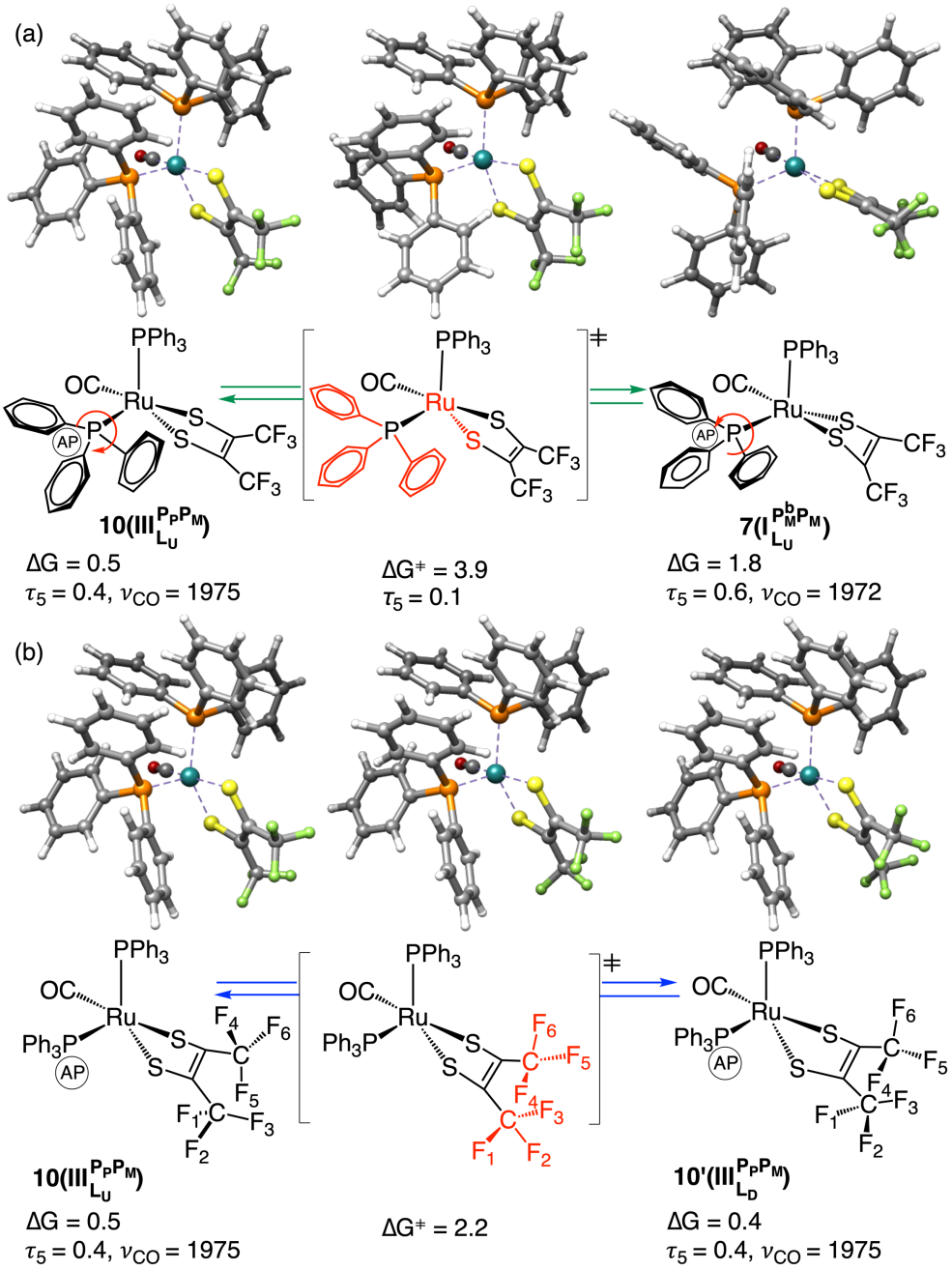


Figure S15. Permutation of isomer **10** at the BP86-GD3BJ(SMD)/BS3//BP86/BS1 level.

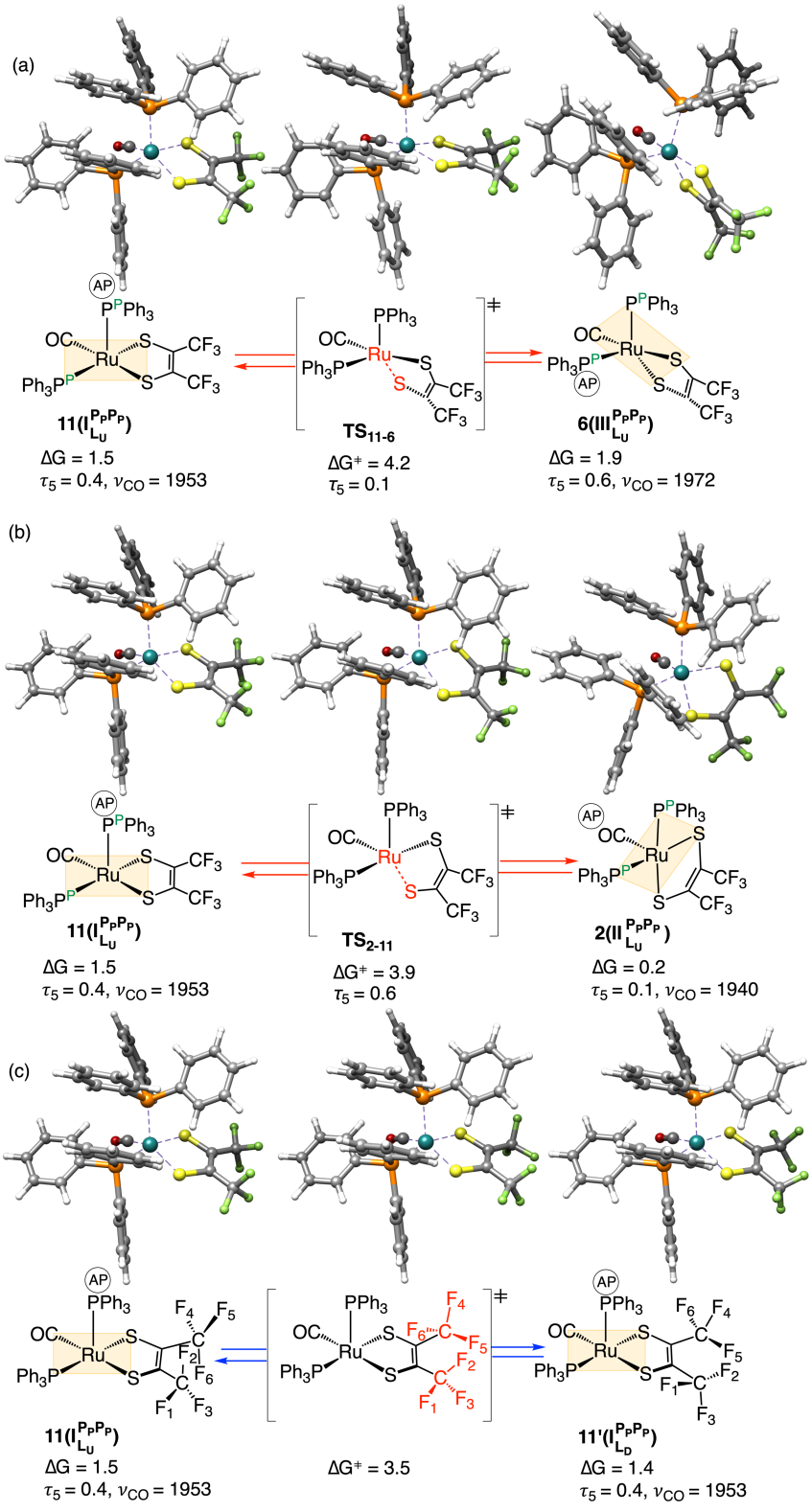


Figure S16. Permutation of isomer **11** at the BP86-GD3BJ(SMD)/BS3//BP86/BS1 level.

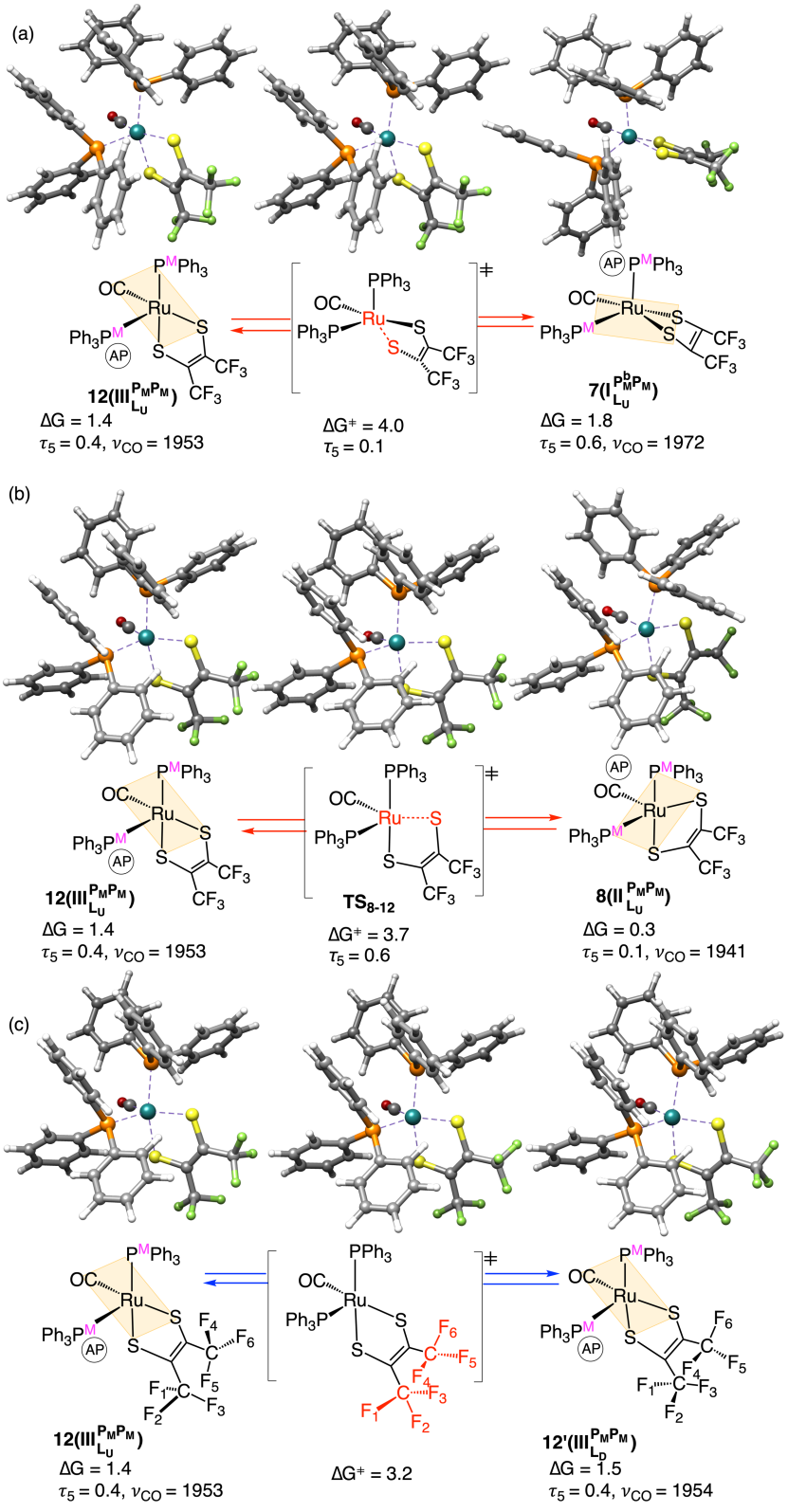


Figure S17. Permutation of isomer **12** at the BP86-GD3BJ(SMD)/BS3//BP86/BS1 level.

Cartesian Coordinate

1

C	-0.63504486	0.45130012	-2.39029838
C	0.98314577	4.30214810	-3.19617051
C	0.26010301	5.48560906	-2.96486255
C	-0.51471536	5.60730474	-1.79943109
C	-0.57253973	4.55237075	-0.87122961
C	1.72358812	2.29193198	1.04459990
C	2.25395661	1.31865490	1.92015255
C	3.40735125	1.58844344	2.67575817
C	4.05477054	2.83040917	2.55882680
C	3.53621928	3.80385163	1.68817385
C	2.37707327	3.54179796	0.93817780
C	-1.13396169	2.45425326	1.32657788
C	-2.00661190	-1.91224002	1.51737974
C	-1.76368000	-1.06681666	2.62535032
C	-1.77109728	-1.58511846	3.93015761
C	-2.00073160	-2.95607706	4.14533055
C	-2.22802572	-3.80396104	3.04865125
C	-2.23466217	-3.28697496	1.74087405
C	-2.29613444	-2.61128917	-1.28981094
C	-1.22747472	-3.23632750	-1.96994722
C	-1.46041431	-4.34194292	-2.80666079
C	-2.76389493	-4.83761224	-2.97632158
C	-2.46813942	2.62293679	0.88687604
C	-3.83543849	-4.22316858	-2.30340766
C	-3.60564699	-3.11754687	-1.46821403
C	-3.59927998	-0.30006277	-0.27792633
C	-4.52867182	-0.29176631	0.78449420
C	-5.77889327	0.33669412	0.63517022
C	-6.11837947	0.96382217	-0.57490954
C	-5.19979637	0.95575134	-1.64162341
C	-3.95223917	0.32836672	-1.49616111
C	2.75139270	-1.81409345	0.26353532
C	3.27039523	-1.04649696	-0.77289559
C	-3.46949887	3.02896325	1.78357484
C	4.73709557	-1.03822117	-1.20313694
C	3.56037402	-2.74186340	1.16153122
C	-3.16090471	3.25108985	3.13791637
C	-1.84132800	3.07419074	3.58691910
C	-0.83135690	2.68657850	2.68830407
C	0.13499031	3.35067165	-1.10496306
C	0.91876926	3.24287187	-2.27713274
F	2.76892236	-3.66337331	1.78193461
F	4.20667147	-2.05739390	2.16180594
F	4.51107366	-3.44535358	0.48451420
F	5.03420727	0.04157083	-1.98023796
F	5.59213022	-0.99664824	-0.14119466
F	5.05940752	-2.14382990	-1.94166178
H	1.60075626	4.19602072	-4.10176207
H	0.30272962	6.31249873	-3.69147129
H	-1.07891684	6.53300482	-1.60306151
H	-1.16970703	4.67573370	0.04334861
H	1.76652584	0.33478120	2.00360004
H	3.80882018	0.81180330	3.34489740
H	4.96819716	3.03578794	3.13923167
H	4.03808534	4.77914231	1.58507207
H	1.98532964	4.31742846	0.26484511
H	-1.56732129	0.00488587	2.46696119
H	-1.58497916	-0.91340248	4.78302532
H	-1.99386738	-3.36435876	5.16844041
H	-2.39735069	-4.88079608	3.20736743
H	-2.40926861	-3.96255435	0.89074041
H	-0.20215665	-2.85535394	-1.84344737
H	-0.61404601	-4.81327098	-3.33063693
H	-2.94695176	-5.70086974	-3.63584581
H	-2.72797020	2.44855044	-0.16778683
H	-4.86122056	-4.60405170	-2.43212134
H	-4.45511959	-2.64367173	-0.95354398
H	-4.28087121	-0.78235533	1.73694759
H	-6.49227723	0.33002868	1.47483595
H	-7.09877209	1.45263172	-0.69161305
H	-5.45729913	1.43616766	-2.59890693
H	-3.25626933	0.32156682	-2.34754264
H	-4.49895448	3.16525455	1.41813716
H	-3.94863861	3.56461620	3.84125100
H	-1.58711081	3.25152442	4.64414623
H	0.20088383	2.57398131	3.05021320
H	1.49914908	2.32735646	-2.46887838
O	-1.05263650	0.73823334	-3.44645787
P	-1.96895725	-1.17033857	-0.16856183
P	0.16176714	1.95455247	0.10992030
Ru	0.11512727	-0.16242019	-0.79026384
S	1.05943190	-1.72308696	0.64684936
S	2.22470848	-0.06691365	-1.73930959

Sum of electronic and zero-point Energies= -3827.802267

Sum of electronic and thermal Energies= -3827.751634

Sum of electronic and thermal Enthalpies= -3827.750690

Sum of electronic and thermal Free Energies= -3827.893356

$TS_{1\text{-}1'}$

C	-0.64891429	0.50697970	-2.39968354
C	1.43859224	4.28349402	-3.06964106
C	0.91353299	5.55176738	-2.77029812
C	0.14583127	5.72650240	-1.60582830
C	-0.10112450	4.64017564	-0.74973908
C	1.55087985	2.13566360	1.30997127
C	1.70875422	1.21349949	2.37024370
C	2.73980985	1.37365696	3.30962645
C	3.64194715	2.44636427	3.19455315
C	3.50069621	3.36024806	2.13787596
C	2.46047726	3.21197173	1.20341241
C	-1.30983055	2.53049880	1.06427202
C	-1.96983271	-1.86363757	1.53821716
C	-1.82186187	-0.96219944	2.61867334
C	-1.81255676	-1.43119979	3.94216256
C	-1.92823234	-2.80831761	4.20484135
C	-2.05904614	-3.71073920	3.13659226
C	-2.08346861	-3.24363678	1.81025355
C	-2.24070540	-2.67289902	-1.24053772
C	-1.17940150	-3.24927975	-1.97181329
C	-1.39533229	-4.38732957	-2.76933554
C	-2.67372053	-4.96428983	-2.84517667
C	-2.51758099	2.74589661	0.35940704
C	-3.73826444	-4.39824046	-2.11979417
C	-3.52603431	-3.25961627	-1.32602523
C	-3.59209829	-0.35535002	-0.32567341
C	-4.51003423	-0.26880122	0.74300077
C	-5.77406532	0.31914808	0.55296269
C	-6.14020179	0.82566288	-0.70476838
C	-5.23305180	0.73944978	-1.77756703
C	-3.97111978	0.15342688	-1.59100046
C	2.77733689	-1.75828903	0.28543791
C	3.28026664	-1.05039989	-0.79909492
C	-3.64880957	3.24933621	1.01933842
C	4.72382538	-0.98300086	-1.28850463
C	3.58810687	-2.66803316	1.20629578

C	-3.59867757	3.52861711	2.39767767
C	-2.40636220	3.31100803	3.10784357
C	-1.26429687	2.82302665	2.44606285
C	0.41209324	3.35498135	-1.04928721
C	1.18868109	3.19400324	-2.21800590
F	2.80226591	-3.27553039	2.14143135
F	4.54788297	-1.98659121	1.90283288
F	4.21293525	-3.67529329	0.52547640
F	5.16860698	0.31187696	-1.33582095
F	5.61279046	-1.66774688	-0.52797668
F	4.83220924	-1.47594434	-2.56294065
H	2.04635188	4.13263986	-3.97554207
H	1.10248080	6.40356077	-3.44287634
H	-0.26669525	6.71734912	-1.35719031
H	-0.69613267	4.80028495	0.16085259
H	1.03327281	0.34838766	2.45207268
H	2.84864304	0.64187351	4.12535259
H	4.46115252	2.56140468	3.92183937
H	4.20778742	4.19812519	2.03116212
H	2.36535018	3.93930673	0.38491499
H	-1.71904489	0.11669077	2.42367874
H	-1.70512845	-0.71557017	4.77274276
H	-1.90862619	-3.17748349	5.24249976
H	-2.13837771	-4.79184767	3.33221481
H	-2.18186832	-3.96237852	0.98376846
H	-0.17315213	-2.80477756	-1.91682404
H	-0.55556752	-4.82024528	-3.33537205
H	-2.84356799	-5.85392515	-3.47241189
H	-2.56972408	2.53586928	-0.71974985
H	-4.74447004	-4.84355719	-2.17558914
H	-4.36964696	-2.82229866	-0.77042172
H	-4.24515225	-0.66803225	1.73265175
H	-6.47805337	0.37424249	1.39866086
H	-7.13267060	1.28034233	-0.85328815
H	-5.51114165	1.12415257	-2.77168139
H	-3.28515138	0.07910219	-2.44759095
H	-4.57676120	3.41822546	0.45163422
H	-4.48842806	3.92022648	2.91582604
H	-2.35406248	3.53665096	4.18500535
H	-0.32887416	2.68634767	3.00828971
H	1.61995417	2.21180549	-2.46103503
O	-1.08298146	0.84713703	-3.43336623
P	-1.94384270	-1.18497377	-0.17488683
P	0.15541926	1.93354175	0.11295098
Ru	0.11938588	-0.15750747	-0.82491256
S	1.08175386	-1.67421087	0.65187084
S	2.21056321	-0.12950246	-1.80438200

Sum of electronic and zero-point Energies= -3827.800848

Sum of electronic and thermal Energies= -3827.751070

Sum of electronic and thermal Enthalpies= -3827.750126

Sum of electronic and thermal Free Energies= -3827.890621

1'

C	-0.66448927	0.48649615	-2.40122491
C	1.30671036	4.30147940	-3.11550873
C	0.78221938	5.56523267	-2.79677590
C	0.05262292	5.73261116	-1.60694096
C	-0.15714285	4.64329615	-0.74480434
C	1.57465372	2.15741778	1.26272936
C	1.78345043	1.22816663	2.30795314
C	2.83703599	1.40221392	3.21972034
C	3.71131704	2.49600316	3.09093966
C	3.51947949	3.41731084	2.04865177
C	2.45675801	3.25519593	1.14244635
C	-1.29551202	2.51429638	1.09890188
C	-1.95916378	-1.89127897	1.53442248
C	-1.78053431	-1.00528994	2.62292401
C	-1.76204512	-1.49001829	3.94054211
C	-1.89914951	-2.86786959	4.18873603
C	-2.06066161	-3.75526862	3.11210825
C	-2.09438591	-3.27211801	1.79169576
C	-2.25738969	-2.66615768	-1.25084378
C	-1.19698270	-3.24982289	-1.97795222
C	-1.41978013	-4.37920398	-2.78566626
C	-2.70441902	-4.93999143	-2.87686376
C	-2.52159956	2.73474471	0.42802398
C	-3.76796757	-4.36674669	-2.15589276
C	-3.54867976	-3.23706292	-1.35115174
C	-3.59593837	-0.35637341	-0.29258562
C	-4.50386143	-0.28957909	0.78602402
C	-5.76875746	0.30356486	0.61927534
C	-6.14570815	0.83496724	-0.62493080
C	-5.24844880	0.76891309	-1.70746278
C	-3.98555555	0.17797437	-1.54407592
C	2.78254706	-1.73055971	0.26795737
C	3.27623490	-1.02560580	-0.82319645
C	-3.63868254	3.22045728	1.12437073
C	4.74022638	-0.98962863	-1.25620790
C	3.61050542	-2.64075544	1.16813668
C	-3.55581640	3.47668153	2.50557098
C	-2.34503814	3.25391680	3.18208208
C	-1.21732489	2.78363132	2.48400249
C	0.35550891	3.36242835	-1.06327915
C	1.09394863	3.20914404	-2.25740836
F	2.98113279	-2.89456649	2.35322013
F	4.82474793	-2.10656193	1.48630643
F	3.84514265	-3.86070665	0.59160759
F	5.48695417	-0.15400429	-0.47196205
F	5.33047895	-2.21845138	-1.21342097
F	4.87886319	-0.54171591	-2.53737338
H	1.88467921	4.15647000	-4.04162505
H	0.94204306	6.41930480	-3.47398902
H	-0.35875043	6.71999638	-1.34310685
H	-0.72227478	4.79729979	0.18569245
H	1.12972578	0.34730639	2.39983658
H	2.98491803	0.66468532	4.02409133
H	4.54827530	2.62205753	3.79582478
H	4.20421050	4.27219874	1.93138839
H	2.32188305	3.98917335	0.33548654
H	-1.65996191	0.07366472	2.43852806
H	-1.62996967	-0.78648226	4.77784484
H	-1.87205895	-3.24954782	5.22169099
H	-2.15713790	-4.83698235	3.29640964
H	-2.21739771	-3.97893082	0.95819717
H	-0.18609134	-2.81780788	-1.91100879
H	-0.58050238	-4.81810972	-3.34779847
H	-2.87969479	-5.82256214	-3.51252597
H	-2.59968253	2.54283849	-0.65290283
H	-4.77898007	-4.79937077	-2.22342308
H	-4.39149421	-2.79453176	-0.79861522
H	-4.22992482	-0.70820094	1.76516941
H	-6.46480795	0.34316069	1.47238384
H	-7.13888139	1.29362877	-0.75544094
H	-5.53510195	1.17358940	-2.69116800
H	-3.30727983	0.12050900	-2.40806063
H	-4.58125277	3.39377484	0.58269299
H	-4.43440875	3.85453590	3.05218657
H	-2.26701021	3.46174771	4.26126164
H	-0.26757737	2.64301651	3.02062642
H	1.52383877	2.23089067	-2.51720763
O	-1.10652958	0.80858097	-3.43758968
P	-1.94826874	-1.19158078	-0.17020077
P	0.14900918	1.93774182	0.10453893
Ru	0.11346570	-0.15811891	-0.82475421

S	1.08726692	-1.68182923	0.63407777
S	2.20737846	-0.08466892	-1.80343175

Sum of electronic and zero-point Energies= -3827.802406
Sum of electronic and thermal Energies= -3827.751727
Sum of electronic and thermal Enthalpies= -3827.750783
Sum of electronic and thermal Free Energies= -3827.894462

2

Ru	0.43143578	-0.03275648	-0.50458473
S	2.09164089	1.51694316	-0.10895996
S	2.14044191	-1.58228313	-0.32225670
P	-1.03388051	-1.82507385	0.05930471
P	-1.05494436	1.82908671	-0.10955265
O	0.04714394	-0.12207905	-3.46448748
C	0.11960060	-0.09275169	-2.28978926
C	3.63274464	-0.70085877	-0.19871919
C	3.61454587	0.67842661	-0.09976902
C	4.88605431	-1.56836115	-0.14741092
C	4.84196679	1.57696203	-0.01024208
F	5.90386912	-1.06630538	-0.90290847
F	4.65122440	-2.83182567	-0.60438447
F	5.36048097	-1.70579303	1.13060280
F	4.52594042	2.81964307	0.45711403
F	5.43149809	1.76243717	-1.23209521
F	5.79937672	1.08360594	0.82639946
C	-1.06076436	3.14513627	-1.41299880
C	0.00673934	3.25329730	-2.33042467
C	0.01967442	4.27568742	-3.29557450
C	-1.03241785	5.20391547	-3.35875116
C	-2.09979696	5.10801562	-2.44776981
C	-2.11573387	4.08793067	-1.48261194
C	-0.55779156	2.73348598	1.42412164
C	-0.28420797	1.97673204	2.58763547
C	0.08106061	2.61516117	3.78324682
C	0.20050194	4.01611739	3.82861642
C	-0.05439530	4.77299928	2.67342600
C	-0.43670709	4.13821842	1.47783614
C	-2.87315972	1.60039956	0.14704318
C	-3.49212586	1.78492335	1.40293115
C	-4.88341025	1.62737065	1.54253402
C	-5.67437367	1.28724098	0.43253143
C	-5.06678422	1.10779666	-0.82353690
C	-3.67909012	1.26221178	-0.96456425
C	-1.32483468	-1.73579571	1.87406782
C	-0.21925895	-1.96290878	2.73198164
C	-0.35731484	-1.83349389	4.12295182
C	-1.59307189	-1.45374430	4.68003902
C	-2.68658566	-1.20135061	3.83507063
C	-2.55708995	-1.33995725	2.44096397
C	-0.36274377	-3.52690923	-0.22005566
C	-0.41824853	-4.55065182	0.75016992
C	0.02777248	-5.84721429	0.43946474
C	0.52513073	-6.13821843	-0.84204685
C	0.57326478	-5.12595204	-1.81635746
C	0.13388238	-3.82873484	-1.50887127
C	-2.67971755	-2.11954325	-0.73221027
C	-2.90164294	-1.67206167	-2.05087490
C	-4.06784366	-2.03852245	-2.74607616
C	-5.03417940	-2.84764069	-2.12690041
C	-4.81883625	-3.30609079	-0.81430787
C	-3.64513608	-2.95865687	-0.12698087
H	0.84039500	2.53800994	-2.28769685
H	0.86079976	4.33991339	-4.00350655
H	-1.02324581	6.00171118	-4.11842830
H	-2.92989589	5.83130145	-2.48855739
H	-2.96032934	4.02468348	-0.78011069
H	-0.34592323	0.87733722	2.55853439
H	0.28896881	2.01059484	4.67993507
H	0.50341362	4.51573575	4.76248152
H	0.05055300	5.86936448	2.69550987
H	-0.62625149	4.74500544	0.58053120
H	-2.88917762	2.06601348	2.27847582
H	-5.35038448	1.78382965	2.52816731
H	-6.76409304	1.16929936	0.54234376
H	-5.67691632	0.84591086	-1.70199673
H	-3.22084707	1.14287085	-1.95767068
H	0.75959818	-2.23337146	2.30438554
H	0.51019203	-2.02454438	4.77424225
H	-1.69998756	-1.34913324	5.77138425
H	-3.65463133	-0.89201811	4.26019536
H	-3.42193432	-1.12793855	1.79638334
H	-0.81002867	-4.34236872	1.75681812
H	-0.01570513	-6.63489928	1.20850822
H	0.87730231	-7.15402211	-1.08162467
H	0.96412419	-5.34275755	-2.82286006
H	0.18209910	-3.04478018	-2.28025079
H	-2.15075985	-1.04461510	-2.55076380
H	-4.21652297	-1.68820953	-3.77984649
H	-5.94970608	-3.13272519	-2.66923401
H	-5.56325608	-3.95479870	-0.32567027
H	-3.47469057	-3.36375479	0.88185593

Sum of electronic and zero-point Energies= -3827.799682
Sum of electronic and thermal Energies= -3827.749041
Sum of electronic and thermal Enthalpies= -3827.748097
Sum of electronic and thermal Free Energies= -3827.889976

$TS_{1\text{-}2}$

Ru	0.40146293	-0.03379902	-0.54286977
S	2.24154133	1.38780496	-0.59776773
S	1.94642616	-1.63641377	0.02214328
P	-1.18831113	-1.75635055	-0.02247412
P	-0.84911864	1.92424711	0.00136603
O	-0.24653649	-0.00341669	-3.46360706
C	-0.06321517	0.00582259	-2.30058354
C	3.53422440	-0.92600219	-0.05543126
C	3.65688345	0.42377457	-0.32954868
C	4.68551688	-1.87586784	0.24631060
C	4.97719908	1.17763159	-0.46420685
F	5.74777289	-1.70167857	-0.59121690
F	4.31105259	-3.18319128	0.12918412
F	5.15349074	-1.72590445	1.52567849
F	4.80313451	2.52718528	-0.37057135
F	5.57373257	0.94718360	-1.67354859
F	5.87715979	0.83702450	0.50155090
C	-0.86399690	3.31662538	-1.22047354
C	0.05247817	3.35936426	-2.29261622
C	0.04332693	4.43354977	-3.20009382
C	-0.88114582	5.47982086	-3.05046039
C	-1.80088093	5.44778685	-1.98667715
C	-1.79554570	4.37523816	-1.08055919
C	-0.11961933	2.66361710	1.53039076
C	0.23536666	1.79208773	2.58633525
C	0.78703150	2.29726854	3.77434118
C	1.01188073	3.67858343	3.91646687
C	0.67597746	4.54903946	2.86640301
C	0.10886655	4.04803256	1.68079271
C	-2.64909277	1.85120859	0.41185407
C	-3.14107340	2.07251079	1.71731574
C	-4.52590006	2.05595761	1.96857658
C	-5.43304720	1.82934670	0.92046699

C	-4.95054373	1.61513870	-0.38372890
C	-3.57034730	1.62102648	-0.63591154
C	-1.22050721	-2.07735876	1.79073732
C	-0.39994152	-3.07561240	2.36593496
C	-0.34385259	-3.23576571	3.76066921
C	-1.10420126	-2.40638825	4.60341160
C	-1.91378548	-1.40356909	4.04180457
C	-1.96561275	-1.23311360	2.64774140
C	-0.82461602	-3.41639876	-0.76571012
C	-1.49513918	-4.56523215	-0.28248763
C	-1.30862406	-5.81161500	-0.89907372
C	-0.46196083	-5.92732352	-2.01740479
C	0.19412349	-4.78977049	-2.51351406
C	0.01643550	-3.54077399	-1.89107523
C	-2.96271668	-1.67662613	-0.54970161
C	-3.21380187	-1.41445965	-1.91665750
C	-4.51675686	-1.49229632	-2.43276446
C	-5.59301892	-1.82438256	-1.59020324
C	-5.35275498	-2.08566134	-0.23129394
C	-4.04642008	-2.02144957	0.28623538
H	0.78522890	2.55127359	-2.42589592
H	0.76594699	4.44470160	-4.03100456
H	-0.88942192	6.31895120	-3.76419145
H	-2.53346404	6.26124183	-1.86253526
H	-2.53026014	4.35969249	-0.26139889
H	0.09395820	0.70481795	2.47479897
H	1.05850165	1.60338504	4.58536664
H	1.46078043	4.07393816	4.84145925
H	0.86229181	5.63048964	2.96298294
H	-0.13830305	4.74278798	0.86502178
H	-2.44182792	2.27746416	2.54171383
H	-4.89454617	2.23709669	2.99095818
H	-6.51691064	1.82541494	1.11693117
H	-5.65344577	1.44002224	-1.21268518
H	-3.20632933	1.46779228	-1.66325975
H	0.20916122	-3.72775090	1.72292940
H	0.30368933	-4.01675629	4.18957536
H	-1.06142450	-2.53770048	5.69624653
H	-2.50873695	-0.74248013	4.69193032
H	-2.59023307	-0.43065547	2.22678120
H	-2.17470429	-4.48712729	0.58030624
H	-1.83290030	-6.69768171	-0.50699663
H	-0.31712866	-6.90598509	-2.50198729
H	0.85745274	-4.86877345	-3.38905344
H	0.54447227	-2.65959339	-2.28107887
H	-2.38372880	-1.16646562	-2.59491461
H	-4.68940110	-1.29606690	-3.50295162
H	-6.61573290	-1.88718736	-1.99489544
H	-6.18670488	-2.35410130	0.43675634
H	-3.87863033	-2.25511977	1.34747498

Sum of electronic and zero-point Energies= -3827.802406

Sum of electronic and thermal Energies= -3827.751727

Sum of electronic and thermal Enthalpies= -3827.750783

Sum of electronic and thermal Free Energies= -3827.894462

3

C	-0.51429377	0.27371693	-2.35961817
C	1.45322055	4.33704098	-2.97536120
C	2.28432759	5.25890704	-2.31568285
C	2.42060173	5.19107534	-0.91947073
C	1.72967106	4.21265640	-0.18370364
C	0.65439145	2.16101879	1.81641744
C	0.16163677	3.12978592	2.72405411
C	0.75473873	3.28803914	3.98839169
C	1.85121519	2.49136644	4.36233447
C	2.35566050	1.53685968	3.46231614
C	1.76106794	1.37131941	2.19990624
C	-1.70564405	2.76762293	0.28268562
C	-1.82483092	-2.16208247	1.46637435
C	-1.37607352	-1.45381348	2.60477713
C	-1.39047101	-2.05744641	3.87256986
C	-1.83626271	-3.38339640	4.01711015
C	-2.26843567	-4.10038803	2.88843102
C	-2.26589035	-3.49453805	1.61951601
C	-2.13531168	-2.66826959	-1.38018608
C	-1.03929214	-3.33579085	-1.97317901
C	-1.24788603	-4.39038102	-2.87797170
C	-2.55317397	-4.79051858	-3.21116350
C	-2.12040038	3.84591232	-0.52974235
C	-3.65039614	-4.13148519	-2.63028588
C	-3.44543088	-3.07861729	-1.72207842
C	-3.48015326	-0.46798482	-0.17547598
C	-4.44438325	-0.70518765	0.82927085
C	-5.72573048	-0.13213051	0.73733201
C	-6.06083483	0.68085883	-0.35814345
C	-5.10436698	0.92608925	-1.36011255
C	-3.82317598	0.36038987	-1.26871172
C	2.94644982	-1.75108451	0.17345633
C	3.43499977	-0.75701120	-0.66297292
C	-3.38026872	4.44084448	-0.33779402
C	4.91152898	-0.56079575	-1.01128326
C	3.79237643	-2.76611123	0.92968645
C	-4.23578446	3.97844924	0.67519010
C	-3.83295635	2.90301618	1.48756048
C	-2.58527899	2.29480912	1.28461364
C	0.89491337	3.27922656	-0.83763638
C	0.76894292	3.35183176	-2.24455501
F	3.05730369	-3.84537764	1.32364173
F	4.33360139	-2.23259559	2.07436872
F	4.82913489	-3.25453493	0.19206204
F	5.14718954	0.66083410	-1.56637534
F	5.72041760	-0.64861226	0.08488496
F	5.34819713	-1.48760770	-1.91539351
H	1.34291167	4.37335987	-4.07064526
H	2.83070339	6.02331077	-2.89048407
H	3.07552470	5.90242769	-0.39163206
H	1.85454300	4.17421848	0.90770220
H	-0.68648666	3.77092966	2.44342084
H	0.35565124	4.04372253	4.68377517
H	2.31327159	2.61597362	5.35464621
H	3.21652683	0.90880614	3.73953567
H	2.16054729	0.61590739	1.50813771
H	-0.98717114	-0.42932787	2.49387534
H	-1.03418189	-1.49308172	4.74862389
H	-1.83521197	-3.86192047	5.00933947
H	-2.60629089	-5.14380411	2.99176871
H	-2.60324114	-4.06656408	0.74237057
H	-0.01317566	-3.02589830	-1.72457204
H	-0.37976094	-4.89618477	-3.32927498
H	-2.71581727	-5.61202183	-3.92696161
H	-1.45124363	4.24077875	-1.30768244
H	-4.67804473	-4.43442121	-2.88730267
H	-4.31635515	-2.57208877	-1.28086872
H	-4.19950913	-1.35034470	1.68597967
H	-6.46790216	-0.33156685	1.52703880
H	-7.06657663	1.12423502	-0.43242834
H	-5.35569477	1.56421609	-2.22172408
H	-3.09131028	0.55827067	-2.06510676
H	-3.68456629	5.28336585	-0.97909641
H	-5.21636275	4.45461562	0.83361172
H	-4.49704160	2.52926207	2.28208005
H	-2.28395733	1.45550393	1.92920588
H	0.13695000	2.63312712	-2.78510838
O	-0.90190097	0.41440873	-3.45982422

P	-1.82890795	-1.29852088	-0.16356418
P	-0.04185021	1.98949076	0.10902967
Ru	0.20442103	-0.15803488	-0.70740743
S	1.23383335	-1.84679374	0.48190110
S	2.35795614	0.35473966	-1.43349952

Sum of electronic and zero-point Energies= -3827.801679
Sum of electronic and thermal Energies= -3827.751038
Sum of electronic and thermal Enthalpies= -3827.750094
Sum of electronic and thermal Free Energies= -3827.892670

$TS_{1\text{-}3}$

C	-0.74464793	0.58642816	-2.32805361
C	1.78409608	4.37338635	-2.73156241
C	1.99761280	5.57200592	-2.03416272
C	1.66704193	5.65180236	-0.66755063
C	1.12554352	4.53895516	-0.00851612
C	1.36497782	1.79367607	1.66088847
C	1.02552215	1.31718096	2.94726141
C	1.99933943	1.19553395	3.95103460
C	3.33973906	1.52143032	3.68403214
C	3.69815593	1.95979444	2.39914702
C	2.72270799	2.09461013	1.39747511
C	-1.38531714	2.73533486	0.80766475
C	-1.98361917	-2.19364393	1.32807297
C	-1.73448344	-1.58545151	2.57926340
C	-1.69949317	-2.35056438	3.75510518
C	-1.89752676	-3.74177976	3.69564868
C	-2.13720110	-4.35708271	2.45594417
C	-2.18378077	-3.58964825	1.27831561
C	-2.44410227	-2.33309853	-1.52286260
C	-1.40164827	-3.02034525	-2.18721150
C	-1.69122462	-3.95312809	-3.19716940
C	-3.02459267	-4.20570654	-3.56449357
C	-1.99305180	3.65775051	-0.07968294
C	-4.06710762	-3.52593645	-2.91109093
C	-3.78153233	-2.59728677	-1.89513211
C	-3.59810393	-0.20636581	0.01420379
C	-4.55116639	-0.54858705	1.00101336
C	-5.79242613	0.10961830	1.05327169
C	-6.10319193	1.11092590	0.11801462
C	-5.16050696	1.45834519	-0.86551824
C	-3.91527924	0.81122924	-0.91363857
C	2.75682325	-1.72663942	0.19718583
C	3.23314799	-0.98208874	-0.87549700
C	-3.18646775	4.31236834	0.26296617
C	4.67816747	-0.98106498	-1.36822417
C	3.61221741	-2.62104144	1.08871059
C	-3.80658771	4.05752590	1.49756205
C	-3.22943893	3.12694274	2.37679988
C	-2.03741081	2.46774971	2.03232680
C	0.91063069	3.32280514	-0.70325250
C	1.24491995	3.25372911	-2.06870824
F	2.85346802	-3.50432983	1.79907380
F	4.32854411	-1.90248822	2.00876067
F	4.50882721	-3.36844245	0.38094908
F	4.94226912	0.09014913	-2.17150959
F	5.58196668	-0.92666476	-0.34731433
F	4.96942135	-2.09528854	-2.10705235
H	2.04142021	4.29753618	-3.79955656
H	2.42357877	6.44613128	-2.55189482
H	1.83279251	6.58788326	-0.11087865
H	0.86926795	4.61415634	1.06001808
H	0.00035686	1.00453178	3.17986566
H	1.70647162	0.82756817	4.94698749
H	4.10455643	1.41487441	4.46909074
H	4.74829350	2.19397961	2.16486238
H	3.02821056	2.43093163	0.39602405
H	-1.57176476	-0.49846881	2.62985263
H	-1.50606884	-1.86001822	4.72218191
H	-1.85888514	-4.34576681	4.61592787
H	-2.28834798	-5.44671924	2.39941272
H	-2.37311903	-4.08465959	0.31464192
H	-0.35343630	-2.82228558	-1.91123395
H	-0.86625954	-4.47869961	-3.70348161
H	-3.25112478	-4.92982265	-4.36324433
H	-1.52153742	3.88087849	-1.04800286
H	-5.11469749	-3.71602754	-3.19438479
H	-4.60833747	-2.07339068	-1.39319633
H	-4.33038836	-1.34326940	1.72843703
H	-6.52381270	-0.17161478	1.82789397
H	-7.07915580	1.62062100	0.15493586
H	-5.39264590	2.24269288	-1.60287287
H	-3.19220556	1.09501600	-1.69120308
H	-3.63001362	5.03277049	-0.44268612
H	-4.73853574	4.57665555	1.77112192
H	-3.70738236	2.90813103	3.34460171
H	-1.61970596	1.74692222	2.74577508
H	1.09308967	2.32143190	-2.62802865
O	-1.22174137	0.94167867	-3.33883499
P	-2.01055990	-1.13245384	-0.17951568
P	0.17470775	1.90440154	0.24305427
Ru	0.07239642	-0.11649728	-0.79480405
S	1.07506383	-1.66722079	0.61483316
S	2.14248499	-0.02985213	-1.82268560

Sum of electronic and zero-point Energies= -3827.794330
Sum of electronic and thermal Energies= -3827.744361
Sum of electronic and thermal Enthalpies= -3827.743416
Sum of electronic and thermal Free Energies= -3827.884159

4

Ru	-0.11178343	-0.15960177	-0.81249259
S	-2.21207250	-0.08500964	-1.77963010
S	-1.06845014	-1.70323317	0.63560517
P	-0.16479231	1.94361116	0.10569557
P	1.96231961	-1.17733464	-0.17016086
O	1.08954210	0.79177509	-3.43805373
C	0.65531335	0.47943676	-2.39554344
C	-2.76491482	-1.76326095	0.27263931
C	-3.26820336	-1.04704822	-0.80683310
C	-3.58107273	-2.69498821	1.16118356
C	-4.73489926	-1.01722241	-1.23239271
F	-4.80070342	-2.17905293	1.48968991
F	-2.94646874	-2.95826113	2.34153005
F	-3.80361920	-3.90914362	0.56807484
F	-4.88436307	-0.54664164	-2.50401753
F	-5.48565409	-0.20434549	-0.42872811
F	-5.31217360	-2.25279514	-1.21008070
C	2.28493524	-2.63652657	-1.26818993
C	1.22341953	-3.23853811	-1.97894765
C	1.45488807	-4.35677338	-2.79943135
C	2.74959220	-4.88806650	-2.92080284
C	3.81419791	-4.29655798	-2.21660986
C	3.58607453	-3.17812011	-1.39850992
C	1.98295290	-1.89521486	1.52662709
C	1.77248551	-1.02629479	2.62311557
C	1.76427711	-1.52535358	3.93541589
C	1.94431455	-2.90063508	4.16993323
C	2.13812943	-3.77146439	3.08504717
C	2.16124612	-3.27373778	1.76987435
C	3.60119112	-0.32374892	-0.28284981

C	4.51452292	-0.27919098	0.79239447
C	5.77328436	0.32970508	0.63575791
C	6.13812392	0.90005573	-0.59478630
C	5.23536360	0.85642706	-1.67396832
C	3.97891785	0.24907609	-1.52088210
C	1.23216806	2.50239935	1.17515008
C	1.08002038	2.75761404	2.55707161
C	2.17163285	3.20732871	3.32232756
C	3.42087983	3.42368992	2.71723324
C	3.57811221	3.18099100	1.34020134
C	2.49661920	2.71487480	0.57689075
C	-1.64089710	2.19258316	1.19340469
C	-2.45555829	3.34147398	1.07065571
C	-3.55267550	3.53103189	1.92883314
C	-3.84707855	2.58616067	2.92547511
C	-3.03969602	1.44283065	3.05741261
C	-1.95081603	1.24248343	2.19324423
C	-0.30318640	3.35890515	-1.08227462
C	-1.05663814	3.21147147	-2.26850885
C	-1.22756242	4.29233478	-3.14942644
C	-0.64474093	5.53856472	-2.86312657
C	0.09971427	5.70009910	-1.68212256
C	0.26629718	4.62250779	-0.79542008
H	0.20482467	-2.82965380	-1.88909985
H	0.61438576	-4.81006054	-3.34816870
H	2.93163649	-5.76159574	-3.56695995
H	4.83308232	-4.70577850	-2.30762684
H	4.42993199	-2.72156935	-0.85929760
H	1.61676363	0.04991591	2.44945726
H	1.60581356	-0.83525073	4.77924372
H	1.92518665	-3.29370791	5.19880125
H	2.26841429	-4.85139706	3.25876124
H	2.30980716	-3.96735028	0.92942541
H	4.24875825	-0.72711404	1.76082211
H	6.47375671	0.35165480	1.48590382
H	7.12611748	1.37185733	-0.71748702
H	5.51266240	1.29197568	-2.64709915
H	3.29616890	0.21087914	-2.38233216
H	0.10106739	2.61961896	3.03892939
H	2.03550563	3.40358606	4.39788571
H	4.27153067	3.78561271	3.31631900
H	4.55120687	3.34927345	0.85371461
H	2.63456357	2.53151384	-0.49936620
H	-2.24009446	4.09447781	0.29952305
H	-4.18322448	4.42652324	1.81041156
H	-4.71140834	2.73393832	3.59208457
H	-3.26707580	0.68791049	3.82631489
H	-1.34680648	0.32664424	2.28637789
H	-1.53067694	2.24705584	-2.50354634
H	-1.81848931	4.15257776	-4.06814920
H	-0.77133298	6.38327867	-3.55883071
H	0.55605528	6.67399939	-1.44325787
H	0.84188687	4.77354338	0.12893874

Sum of electronic and zero-point Energies= -3827.802412

Sum of electronic and thermal Energies= -3827.751730

Sum of electronic and thermal Enthalpies= -3827.750785

Sum of electronic and thermal Free Energies= -3827.894630

$TS_{1\text{-}4}$

Ru	-0.23621423	-0.08030234	-0.79196558
S	-2.19603789	-0.33500936	-1.95290621
S	-1.61514128	-0.03499608	1.10457745
P	0.78337318	1.87824270	-0.04261619
P	1.18931659	-1.74723754	-0.01189485
O	1.12496777	-0.23113504	-3.51678466
C	0.64570578	-0.14637454	-2.45275056
C	-3.24027568	-0.19242118	0.54219911
C	-3.50898152	-0.35694645	-0.81158737
C	-4.30271966	-0.18107457	1.64392103
C	-4.89628761	-0.50284972	-1.42538241
F	-5.39703230	0.55841040	1.30339479
F	-3.82699328	0.35066046	2.80546344
F	-4.73761746	-1.44102708	1.94433444
F	-4.84297593	-1.04851193	-2.67412394
F	-5.52730071	0.70753146	-1.56140221
F	-5.72100747	-1.30288709	-0.69103487
C	1.17083246	-3.15978273	-1.21291724
C	-0.04661958	-3.52455009	-1.83196779
C	-0.10092604	-4.61731754	-2.71210201
C	1.06188322	-5.35567006	-2.99646069
C	2.27670721	-4.99957845	-2.38737451
C	2.33254612	-3.91237733	-1.49710582
C	0.70201022	-2.56506605	1.57101226
C	0.64961989	-1.79817091	2.75830685
C	0.29061048	-2.39420101	3.97678134
C	-0.03715085	-3.76152206	4.02758797
C	0.00603839	-4.52893610	2.85270418
C	0.37791114	-3.93808567	1.63108338
C	3.00684900	-1.48027610	0.20539630
C	3.72732699	-2.02995747	1.29092867
C	5.11634678	-1.83530368	1.39502965
C	5.80527964	-1.10225698	0.41310267
C	5.09757514	-0.56093301	-0.67527949
C	3.70823469	-0.74248746	-0.77568832
C	1.19265231	2.03064039	1.75170028
C	0.35172922	2.75410454	2.62814433
C	0.64005526	2.82151342	4.00219226
C	1.77559072	2.17815257	4.52300724
C	2.61263668	1.44605195	3.66234352
C	2.31686558	1.35995020	2.29096874
C	-0.32373577	3.34647450	-0.31252037
C	0.21649717	4.64749278	-0.16601561
C	-0.59435397	5.77888872	-0.34138020
C	-1.95431255	5.63019748	-0.67330060
C	-2.49616692	4.34421204	-0.82590107
C	-1.68575305	3.20766881	-0.64583380
C	2.28992342	2.49455862	-0.92735591
C	2.17918468	2.66282544	-2.32859997
C	3.24951845	3.17411668	-3.07796589
C	4.45098634	3.53479747	-2.44055089
C	4.56436284	3.39143279	-1.04821897
C	3.49209679	2.87902710	-0.29442926
H	-0.95708590	-2.93786123	-1.63208819
H	-1.05872268	-4.88537437	-3.18531602
H	1.02121299	-6.20547094	-3.69631654
H	3.19400573	-5.56933014	-2.60581424
H	3.29116635	-3.65122638	-1.02576628
H	0.89285145	-0.72576467	2.73565557
H	0.25417731	-1.78015523	4.89024680
H	-0.33151594	-4.22538727	4.98237431
H	-0.25236937	-5.59945599	2.87980970
H	0.40987992	-4.55452576	0.72135801
H	3.20187619	-2.61616876	2.05907354
H	5.66304415	-2.26758992	2.24844324
H	6.89380332	-0.95368795	0.49494516
H	5.62597629	0.01480460	-1.45090312
H	3.16832780	-0.30467445	-1.62788208
H	-0.53877650	3.26699145	2.23723896
H	-0.03171191	3.38530664	4.66863619
H	2.00472788	2.24122869	5.59862904
H	3.50001116	0.92751094	4.05860921
H	2.96654074	0.75672902	1.63998814
H	1.28021972	4.77897308	0.08576038
H	-0.15955059	6.78427575	-0.22309539

H	-2.58878504	6.51944439	-0.81620307
H	-3.55759461	4.21440806	-1.08894370
H	-2.11664008	2.20468884	-0.77729382
H	1.23833722	2.41024061	-2.83979622
H	3.13993487	3.29604066	-4.16705596
H	5.29163700	3.93667345	-3.02820597
H	5.49328975	3.68664973	-0.53456864
H	3.59852114	2.79671594	0.79615864

Sum of electronic and zero-point Energies= -3827.798095
Sum of electronic and thermal Energies= -3827.748421
Sum of electronic and thermal Enthalpies= -3827.747477
Sum of electronic and thermal Free Energies= -3827.884964

2'

C	-0.12940700	0.10147600	-2.28956200
C	0.00237700	-4.26568900	-3.31366200
C	1.05454300	-5.19420500	-3.37108000
C	2.11406800	-5.10208800	-2.45058400
C	2.12221900	-4.08536400	-1.48181200
C	0.54091400	-2.73831500	1.41638900
C	0.26444500	-1.98434000	2.58108500
C	-0.11386200	-2.62505900	3.77134500
C	-0.24359100	-4.02536300	3.80996000
C	0.01449600	-4.77931000	2.65357000
C	0.40998400	-4.14235600	1.46337200
C	2.86841200	-1.60565600	0.16137200
C	1.34180100	1.73096400	1.87117600
C	0.24287100	1.95893300	2.73736600
C	0.39095800	1.82823900	4.12717300
C	1.63020800	1.44630900	4.67492200
C	2.71717000	1.19332200	3.82178500
C	2.57764800	1.33328000	2.42877400
C	0.36757200	3.52618800	-0.21366700
C	-0.13930000	3.83035500	-1.49793800
C	-0.57798600	5.12895500	-1.80059000
C	-0.51914300	6.14022700	-0.82580700
C	3.68185400	-1.25680700	-0.94143000
C	-0.01190300	5.84679300	0.45125100
C	0.43354200	4.54885800	0.75701500
C	2.67971200	2.11588300	-0.74293200
C	2.89576300	1.66566200	-2.06162600
C	4.05975900	2.02909500	-2.76214600
C	5.02955500	2.83826200	-2.14842000
C	4.81983900	3.29984400	-0.83600100
C	3.64847800	2.95516600	-0.14333600
C	-3.63071900	0.70367400	-0.16378100
C	-3.61873500	-0.67870300	-0.12861800
C	5.06873500	-1.10497800	-0.78994800
C	-4.85027900	-1.56933600	-0.00779400
C	-4.88049300	1.57619900	-0.14716600
C	5.66813200	-1.29869100	0.46799400
C	4.86979000	-1.65035400	1.56909400
C	3.47920100	-1.80453200	1.41906000
C	1.06717900	-3.14224000	-1.41806200
C	0.00747700	-3.24665200	-2.34488800
F	-4.59373100	2.86242400	0.21046300
F	-5.82147100	1.13380300	0.73556100
F	-5.47878000	1.64094000	-1.37585900
F	-5.32890100	-1.61325500	1.27453400
F	-5.87623200	-1.15728900	-0.80639300
F	-4.58083200	-2.85976700	-0.35931900
H	-0.83278800	-4.32716200	-4.02885000
H	1.05147000	-5.98936400	-4.13356700
H	2.94409500	-5.82570300	-2.48667900
H	2.96069100	-4.02506700	-0.77176200
H	0.33421500	-0.88521700	2.55698600
H	-0.32398400	-2.02283800	4.66909600
H	-0.55689200	-4.52660700	4.73950700
H	-0.09812900	-5.87500800	2.67043300
H	0.60210200	-4.74666700	0.56491900
H	-0.73862400	2.23143500	2.31718300
H	-0.47141400	2.02016400	4.78500500
H	1.74492800	1.34056400	5.76536700
H	3.68795100	0.88242100	4.23943300
H	3.43773200	1.12129200	1.77786400
H	-0.19596400	3.04715000	-2.26949700
H	-0.97660000	5.34769500	-2.80364100
H	-0.87077600	7.15712300	-1.06151500
H	3.23025500	-1.12681300	-1.93615100
H	0.03974300	6.63359200	1.22069000
H	0.83300400	4.33862200	1.76024100
H	2.14221300	1.03806500	-2.55728900
H	4.20389600	1.67646700	-3.79577100
H	5.94332800	3.12102000	-2.69491600
H	5.56694900	3.94867100	-0.35165200
H	3.48264300	3.36219400	0.86549900
H	5.68457000	-0.83413800	-1.66169200
H	6.75723600	-1.18297800	0.58604900
H	5.33028900	-1.81814900	2.55590600
H	2.87043000	-2.09394700	2.28782100
H	-0.82658500	-2.53163900	-2.30660000
O	-0.06345500	0.13594400	-3.46453700
P	1.03821200	1.82293100	0.05843100
P	1.05185300	-1.83048600	-0.11043900
Ru	-0.43303400	0.03469300	-0.50345900
S	-2.13612100	1.58278300	-0.28192400
S	-2.09800300	-1.52050000	-0.14156400

Sum of electronic and zero-point Energies= -3827.799705
Sum of electronic and thermal Energies= -3827.749054
Sum of electronic and thermal Enthalpies= -3827.748110
Sum of electronic and thermal Free Energies= -3827.890079

$TS_{2\text{-}2'}$

C	-0.12472957	0.08454171	-2.29416565
C	0.04227342	-4.28508442	-3.30409314
C	1.09862144	-5.20959636	-3.34748882
C	2.15008130	-5.10800140	-2.41876035
C	2.14595457	-4.08589402	-1.45569131
C	0.54732049	-2.72934000	1.42497242
C	0.26383963	-1.96958645	2.58417808
C	-0.11472626	-2.60481295	3.77729692
C	-0.23756612	-4.00548652	3.82420113
C	0.02748735	-4.76522870	2.67318630
C	0.42311125	-4.13368951	1.48016703
C	2.87122240	-1.58898919	0.16888182
C	1.32465493	1.74225525	1.86641481
C	0.22388919	1.96786687	2.73089071
C	0.37164999	1.84274047	4.12127425
C	1.61233571	1.46893000	4.67133899
C	2.70121965	1.21831697	3.81994576
C	2.56202272	1.35263813	2.42635582
C	0.33820936	3.52310429	-0.22428192
C	-0.17694423	3.81793989	-1.50736140
C	-0.62600540	5.11214943	-1.81360408
C	-0.56963818	6.12802103	-0.84349733
C	3.68373159	-1.23714676	-0.93363190
C	-0.05431703	5.84383565	0.43244548
C	0.40171032	4.55044393	0.74167613
C	2.66368196	2.13034892	-0.74633149
C	2.88458967	1.67991636	-2.06418018

C	4.04724257	2.04994541	-2.76344420
C	5.01084850	2.86622889	-2.14935649
C	4.79616381	3.32813950	-0.83787166
C	3.62610222	2.97663582	-0.14640905
C	-3.64453302	0.66754628	-0.17890621
C	-3.62543708	-0.71400366	-0.13361142
C	5.06941692	-1.07629999	-0.78068850
C	-4.84459183	-1.62723903	-0.02732742
C	-4.85315054	1.59293653	-0.13337712
C	5.66838709	-1.26398489	0.47839077
C	4.87093022	-1.61862066	1.57917864
C	3.48149653	-1.78172383	1.42774771
C	1.08635273	-3.14706143	-1.40574656
C	0.03498849	-3.26079764	-2.34086034
F	-4.80811659	2.40069152	0.97572916
F	-6.05071009	0.95851561	-0.10437675
F	-4.88023777	2.42947057	-1.21728752
F	-5.58270112	-1.38041135	1.09640322
F	-5.67977144	-1.50893132	-1.10223597
F	-4.48833605	-2.94251839	0.03553927
H	-0.78644135	-4.35381483	-4.02609714
H	1.10519979	-6.00890948	-4.10559429
H	2.98345847	-5.82820746	-2.44409447
H	2.97846843	-4.01768494	-0.73935534
H	0.32837811	-0.87031479	2.55355692
H	-0.33021332	-1.99806094	4.67071762
H	-0.55085469	-4.50259621	4.75597343
H	-0.07972089	-5.86135083	2.69650863
H	0.62054340	-4.74259545	0.58598829
H	-0.75882325	2.23393523	2.30943149
H	-0.49224047	2.03283480	4.77763925
H	1.72677394	1.36773790	5.76225139
H	3.67324763	0.91381344	4.23941122
H	3.42368844	1.14273247	1.77685636
H	-0.23267603	3.03071244	-2.27479985
H	-1.03139714	5.32349714	-2.81549405
H	-0.92977310	7.14131614	-1.08187517
H	3.23248612	-1.11178129	-1.92912224
H	-0.00483304	6.63428247	1.19827231
H	0.80713711	4.34726663	1.74396718
H	2.13588191	1.04689306	-2.56025010
H	4.19517585	1.69692747	-3.79639829
H	5.92357287	3.15420613	-2.69488054
H	5.53829966	3.98245509	-0.35325662
H	3.45635041	3.38359437	0.86179270
H	5.68465670	-0.80312191	-1.65211806
H	6.75658973	-1.14119423	0.59759880
H	5.33126139	-1.78163295	2.56686768
H	2.87335660	-2.07316180	2.29627265
H	-0.80214291	-2.54886261	-2.31389065
O	-0.05412166	0.11649914	-3.46899567
P	1.02310086	1.82652474	0.05287467
P	1.05707625	-1.82792812	-0.10594510
Ru	-0.43605896	0.02485887	-0.50957936
S	-2.14899868	1.55497411	-0.27578551
S	-2.09456523	-1.54224666	-0.16530484

Sum of electronic and zero-point Energies= -3827.798481

Sum of electronic and thermal Energies= -3827.748725

Sum of electronic and thermal Enthalpies= -3827.747780

Sum of electronic and thermal Free Energies= -3827.886991

5

C	0.00071600	-0.06672600	-2.29853900
C	0.72596800	4.49284500	-2.91591700
C	1.06307200	5.66550200	-2.21841600
C	0.88165400	5.72163400	-0.82620700
C	0.35959400	4.61637200	-0.13264600
C	-0.47758700	2.36956300	1.82922900
C	-1.37900400	3.22489400	2.50766800
C	-1.16361500	3.56654300	3.85322700
C	-0.04574300	3.06349200	4.54257600
C	0.85792100	2.21856600	3.87666600
C	0.64281400	1.87195600	2.53134100
C	-2.51078500	2.21638400	-0.19706000
C	-2.07281300	-1.61934600	1.61544200
C	-1.18792600	-1.35516200	2.68629100
C	-1.65531500	-1.33177500	4.01113500
C	-3.01607400	-1.55752900	4.28383100
C	-3.90493400	-1.81249000	3.22463200
C	-3.43844100	-1.84701600	1.89856700
C	-0.78022400	-3.41715100	-0.22986500
C	-0.31502400	-3.85346100	-1.49279500
C	0.14212200	-5.16793500	-1.66609200
C	0.15211300	-6.06209000	-0.57921300
C	-3.02939600	3.03851800	-1.22224600
C	-0.30125100	-5.63391100	0.67859000
C	-0.76774200	-4.31775200	0.85485400
C	-2.83824000	-1.74343900	-1.20628600
C	-3.20193000	-0.64198700	-2.00706500
C	-4.31697000	-0.71248200	-2.86063600
C	-5.08511000	-1.88632400	-2.92408000
C	-4.72966000	-2.99431600	-2.13342600
C	-3.61246700	-2.92728900	-1.28561800
C	3.44538300	-1.14000000	0.05506700
C	3.65710700	0.17985600	-0.30583500
C	-4.41923700	3.17915100	-1.38942400
C	5.02404500	0.85487600	-0.40005000
C	4.53401500	-2.16042000	0.36005700
C	-5.30919600	2.51197100	-0.53120400
C	-4.80101500	1.69828600	0.49740800
C	-3.41531200	1.54686400	0.66050900
C	0.01642800	3.43414300	-0.82495600
C	0.21429400	3.38198200	-2.22472400
F	5.55255000	-1.64032200	1.10481800
F	5.09196900	-2.67859300	-0.77738800
F	4.04600900	-3.22188900	1.06724400
F	5.95366900	0.07240400	-1.01705700
F	4.96920800	2.02043200	-1.10474300
F	5.51837100	1.17589800	0.83621400
H	0.87494000	4.43225100	-4.00547000
H	1.47681100	6.53161700	-2.75877800
H	1.15386000	6.63197200	-0.26878500
H	0.23083100	4.67580000	0.95772500
H	-2.25519600	3.63288200	1.98234100
H	-1.87512800	4.23438200	4.36468200
H	0.12104100	3.33287000	5.59772800
H	1.74120800	1.82387400	4.40321400
H	1.36278900	1.21801100	2.01533900
H	-0.12258400	-1.16824900	2.47624400
H	-0.95113300	-1.12696200	4.83263200
H	-3.38462000	-1.53116000	5.32162800
H	-4.97311700	-1.98849800	3.42980100
H	-4.14616200	-2.04480800	1.07994700
H	-0.30657300	-3.15842000	-2.34727300
H	0.50250700	-5.49334300	-2.65468000
H	0.51986400	-7.09161700	-0.71405500
H	-2.34790600	3.58344000	-1.89185500
H	-0.29191800	-6.32589400	1.53567000
H	-1.12002700	-3.99611100	1.84603200
H	-2.60570200	0.27928200	-1.97041400
H	-4.57833800	0.15747100	-3.48282100
H	-5.95546000	-1.94379800	-3.59709600
H	-5.31883500	-3.92382300	-2.18515800
H	-3.33035800	-3.81036700	-0.69206800

H	-4.80505800	3.82714600	-2.19260000
H	-6.39692800	2.62869100	-0.65992300
H	-5.48772100	1.17318500	1.17997000
H	-3.03541000	0.90940000	1.47242100
H	-0.02126400	2.46480700	-2.78404800
O	-0.12063800	-0.11394800	-3.46757900
P	-1.36412800	-1.66902000	-0.09146200
P	-0.69472000	1.96031400	0.03537100
Ru	0.39155800	-0.08847300	-0.52112700
S	1.82021400	-1.76271100	0.11576700
S	2.31137700	1.22026000	-0.63634800

Sum of electronic and zero-point Energies= -3827.803735
Sum of electronic and thermal Energies= -3827.753065
Sum of electronic and thermal Enthalpies= -3827.752121
Sum of electronic and thermal Free Energies= -3827.894355

$TS_{2\text{-}5}$

C	0.01581200	-0.06256100	-2.25736100
C	0.54671100	4.55068500	-2.88635400
C	0.13809200	5.80695900	-2.41274800
C	-0.54826400	5.90115900	-1.18681800
C	-0.81981300	4.74470000	-0.44104000
C	-0.42077000	2.44858200	1.79460200
C	-1.00347500	1.82508100	2.92152400
C	-0.60130500	2.16722600	4.22411000
C	0.40566500	3.12375300	4.42952000
C	1.01593500	3.72790000	3.31712100
C	0.61123200	3.39324500	2.01515500
C	-2.70287300	2.04702800	-0.06850700
C	-1.73991800	-1.80648300	1.74594400
C	-0.70065900	-1.76153900	2.70644300
C	-0.99150800	-1.84253500	4.07840300
C	-2.32499800	-1.94281000	4.51465300
C	-3.36498200	-1.96982100	3.56910000
C	-3.07660000	-1.90954600	2.19333200
C	-0.64521600	-3.43771500	-0.37313400
C	-0.29683400	-3.74941400	-1.70833200
C	0.15631800	-5.03391500	-2.04324000
C	0.27439200	-6.02346200	-1.05002600
C	-3.30612900	2.79446900	-1.10926100
C	-0.06753000	-5.72059700	0.27763900
C	-0.52691000	-4.43461600	0.61720900
C	-2.84129400	-1.80412900	-0.98323200
C	-3.21769300	-0.77301500	-1.86591400
C	-4.39586800	-0.87603500	-2.62708100
C	-5.21406100	-2.01098900	-2.51094500
C	-4.84441300	-3.05123300	-1.63785400
C	-3.66280200	-2.95453600	-0.88698400
C	3.50495200	-1.01461200	-0.12454800
C	3.64258200	0.35661700	-0.23934500
C	-4.70426000	2.84954900	-1.24296100
C	4.96732700	1.11301600	-0.23020800
C	4.65079000	-2.01391100	-0.03318900
C	-5.53336200	2.16622300	-0.33835000
C	-4.94777000	1.40474000	0.68632200
C	-3.55066200	1.33365000	0.80964100
C	-0.40295600	3.47255200	-0.90617000
C	0.27866600	3.38927400	-2.13731900
F	5.66114100	-1.58641200	0.77772100
F	5.20280500	-2.28008900	-1.25707000
F	4.23540700	-3.21317700	0.47089400
F	5.92070000	0.51189000	-0.99728600
F	4.83144300	2.38418100	-0.70776200
F	5.47984800	1.23194500	1.03385800
H	1.08463400	4.46506200	-3.84335200
H	0.35304600	6.71599000	-2.99676600
H	-0.87603500	6.88283400	-0.80933700
H	-1.36613600	4.83059400	0.51097500
H	-1.76715100	1.04641000	2.80565700
H	-1.07897600	1.66913500	5.08243400
H	0.72274200	3.38851700	5.45058900
H	1.82116900	4.46612100	3.45794600
H	1.11777500	3.86849800	1.16366400
H	0.34571700	-1.66253000	2.37384600
H	-0.16823600	-1.81709000	4.80954100
H	-2.55374600	-1.99836700	5.59084000
H	-4.41261100	-2.04637500	3.90170300
H	-3.90091700	-1.94081300	1.46555500
H	-0.37735200	-2.98206000	-2.49417100
H	0.42707900	-5.26039900	-3.08650500
H	0.63791600	-7.02960300	-1.31238200
H	-2.68288300	3.34544100	-1.82724600
H	0.02470900	-6.48833400	1.06225800
H	-0.78972700	-4.21366900	1.66212100
H	-2.58079000	0.11552200	-1.96798100
H	-4.66789400	-0.06252700	-3.31720400
H	-6.13536300	-2.09354100	-3.10939800
H	-5.47230100	-3.95248200	-1.55270800
H	-3.36527900	-3.79103800	-0.23573000
H	-5.14481000	3.44264500	-2.06029400
H	-6.62910400	2.21948600	-0.43640600
H	-5.58121300	0.84879500	1.39552900
H	-3.13179100	0.69484000	1.59649400
H	0.61114400	2.41366400	-2.51627300
O	-0.10061600	-0.10941200	-3.42749700
P	-1.25621300	-1.72406200	-0.03642200
P	-0.84787300	1.95475600	0.05372600
Ru	0.38717000	-0.03866600	-0.48217300
S	1.91816500	-1.72693800	-0.14178200
S	2.22881800	1.35624100	-0.35005200

Sum of electronic and zero-point Energies= -3827.795849
Sum of electronic and thermal Energies= -3827.746051
Sum of electronic and thermal Enthalpies= -3827.745107
Sum of electronic and thermal Free Energies= -3827.884283

6

C	0.68282000	0.09693900	-2.43821400
C	0.25329200	-4.77690900	-2.26868100
C	1.37936400	-5.61579500	-2.30124500
C	2.56188400	-5.22009300	-1.64935800
C	2.61887900	-3.99051200	-0.97372200
C	1.45833600	-2.12734000	1.75102200
C	1.58950700	-1.19923400	2.80959500
C	1.50436800	-1.62100600	4.14679400
C	1.26510300	-2.97205600	4.44976100
C	1.11054700	-3.89795900	3.40457800
C	1.20804700	-3.48256000	2.06566900
C	3.32379400	-1.07321100	-0.23423200
C	1.07881600	2.20076000	1.65307300
C	0.23282600	1.97131900	2.76614200
C	0.70480100	2.16248100	4.07377100
C	2.03456000	2.56825800	4.29560000
C	2.88350700	2.78857500	3.19822700
C	2.40918400	2.61427400	1.88431600
C	-1.09654200	3.10410300	0.08068300
C	-2.28511800	2.86658000	-0.63750800
C	-3.35534800	3.77740600	-0.57550300
C	-3.25012200	4.93993900	0.20461700
C	3.82064500	-1.01498300	-1.56004800
C	-2.06454100	5.19217700	0.91906700

C	-0.99586500	4.28397900	0.85971200
C	1.50189800	2.90077600	-1.14354500
C	2.79494700	2.39096800	-1.40553800
C	3.67901200	3.08057800	-2.25050400
C	3.28018100	4.28030400	-2.86559800
C	1.99022100	4.78302100	-2.62953600
C	1.10684600	4.10298800	-1.77264800
C	-3.41201500	-0.76701300	-0.86235000
C	-3.12774200	-0.85777500	0.49508600
C	5.15307500	-0.65103300	-1.81084900
C	-4.16404000	-1.15621500	1.58047700
C	-4.79402400	-0.91301200	-1.48797200
C	6.01321500	-0.33001500	-0.74422000
C	5.53018600	-0.38542600	0.57364700
C	4.19772300	-0.75854900	0.82965000
C	1.49136500	-3.13491200	-0.94298100
C	0.30872400	-3.54395800	-1.59405700
F	-5.52922100	0.24067800	-1.38593500
F	-5.53306400	-1.90878600	-0.92162100
F	-4.71738700	-1.20108000	-2.81917900
F	-5.32469200	-0.46463900	1.39707600
F	-4.48270200	-2.48463200	1.62970900
F	-3.71095900	-0.82283000	2.82284100
H	-0.67814900	-5.07668600	-2.77422900
H	1.33793200	-6.57869100	-2.83492100
H	3.44919100	-5.87294800	-1.66736900
H	3.54941600	-3.69615200	-0.46486800
H	1.74593000	-0.13328300	2.59413900
H	1.61350000	-0.87982000	4.95393800
H	1.18831600	-3.30078900	5.49827600
H	0.90848700	-4.95746500	3.62848900
H	1.07908900	-4.22228100	1.26329700
H	-0.80517900	1.63976300	2.60755100
H	0.02727500	1.98970000	4.92488600
H	2.40525900	2.71728600	5.32224300
H	3.92332800	3.11505600	3.35941200
H	3.08086200	2.82198200	1.03909500
H	-2.37649300	1.95619900	-1.24869000
H	-4.27831200	3.56457000	-1.13695400
H	-4.09127900	5.64917300	0.26010200
H	3.16597700	-1.26870700	-2.40725100
H	-1.96969600	6.10268500	1.53212500
H	-0.07567600	4.49935400	1.42301900
H	3.11343000	1.43715500	-0.96072200
H	4.68217700	2.66596300	-2.43636700
H	3.97052300	4.81628500	-3.53610600
H	1.66093900	5.71465900	-3.11656200
H	0.10148600	4.51273100	-1.60125000
H	5.52070200	-0.62233700	-2.84886100
H	7.05917100	-0.04575200	-0.94077500
H	6.19708300	-0.14858100	1.41799000
H	3.84859200	-0.81942600	1.87011000
H	-0.57703900	-2.88923500	-1.57998100
O	1.15810100	0.22270300	-3.49844300
P	0.36070300	1.96012300	-0.03799000
P	1.54744800	-1.53901300	0.00257200
Ru	-0.19351000	-0.15530900	-0.79094200
S	-2.13380600	-0.41217800	-1.98659700
S	-1.50376600	-0.70523500	1.06880900

Sum of electronic and zero-point Energies= -3827.799842

Sum of electronic and thermal Energies= -3827.749223

Sum of electronic and thermal Enthalpies= -3827.748279

Sum of electronic and thermal Free Energies= -3827.891120

$TS_{2\text{-}6}$

C	0.45450200	0.22806900	-2.33650900
C	0.65356800	-4.32039700	-3.13739700
C	1.79766500	-5.13220900	-3.19588800
C	2.88569500	-4.86304000	-2.34547000
C	2.82871200	-3.78781900	-1.44419700
C	1.42154700	-2.42864000	1.47520400
C	1.08174000	-1.65286600	2.60720500
C	0.98399600	-2.24458600	3.87721700
C	1.20029600	-3.62475700	4.03198300
C	1.51430500	-4.40773300	2.90855200
C	1.62672700	-3.81611100	1.63835600
C	3.33244400	-0.99218500	-0.14687000
C	0.08654900	1.98205400	1.96147200
C	-1.25075700	1.82115600	2.40016600
C	-1.54518300	1.74047900	3.76969700
C	-0.51017600	1.79884500	4.72210800
C	0.82165600	1.93487200	4.29492100
C	1.12155000	2.02535500	2.92320500
C	-0.56010400	3.44024600	-0.48937900
C	-0.60210700	3.63183000	-1.88924400
C	-1.25448400	4.74746800	-2.43607400
C	-1.87426800	5.68795600	-1.59402500
C	4.02827200	-0.85858900	-1.37205800
C	-1.83014500	5.50809600	-0.20170400
C	-1.17326200	4.39409200	0.35089400
C	2.08257000	2.75577300	-0.05208700
C	2.95296500	2.30171500	-1.06053900
C	4.15567400	2.98125100	-1.32615100
C	4.50286100	4.11982200	-0.58281100
C	3.63537700	4.58680400	0.42261200
C	2.42904200	3.91882500	0.67921400
C	-3.53207000	-0.23104600	-0.63343200
C	-3.18537700	-1.37641200	0.06402000
C	5.36453500	-0.42757000	-1.39123200
C	-4.16013800	-2.40666500	0.61687700
C	-4.96461800	0.23334100	-0.89488600
C	6.02335900	-0.10717600	-0.19048400
C	5.33505200	-0.22141900	1.02874100
C	4.00069800	-0.66475500	1.05267000
C	1.67766200	-2.96391100	-1.37464500
C	0.59302900	-3.24469700	-2.23332200
F	-5.51964800	0.81387700	0.21486400
F	-5.78511700	-0.78658900	-1.27180500
F	-5.02543400	1.16576700	-1.88681000
F	-5.24882200	-1.83811400	1.21368400
F	-4.63084500	-3.24830300	-0.35645200
F	-3.57666500	-3.20135800	1.56033400
H	-0.20301600	-4.51897100	-3.80048500
H	1.84548200	-5.97325200	-3.90582800
H	3.78890500	-5.49272800	-2.38525200
H	3.69341500	-3.58525000	-0.79408900
H	0.87327600	-0.57867800	2.49386900
H	0.71821000	-1.62156400	4.74551700
H	1.10920800	-4.09239100	5.02523700
H	1.66575200	-5.49365600	3.01535400
H	1.85916300	-4.44890700	0.77014500
H	-2.06473900	1.74690300	1.66133100
H	-2.59095700	1.62104900	4.09358000
H	-0.74321200	1.73145400	5.79662600
H	1.63895400	1.97204100	5.03277800
H	2.16950700	2.12532500	2.60337500
H	-0.12473800	2.90342400	-2.56298400
H	-1.28385100	4.87760400	-3.52933700
H	-2.39302400	6.55924500	-2.02404300
H	3.52903300	-1.11163900	-2.32040700
H	-2.31212600	6.23949600	0.46654400
H	-1.14733500	4.27180200	1.44378900
H	2.68615600	1.41655300	-1.65260000
H	4.82158000	2.61286800	-2.12158900

H	5.44497000	4.65174900	-0.79038400
H	3.89272200	5.48803400	1.00168300
H	1.74361500	4.31977700	1.44140800
H	5.89559100	-0.34695900	-2.35329800
H	7.07271400	0.22729100	-0.20568300
H	5.84286100	0.02268600	1.97542800
H	3.48496300	-0.77557700	2.01841400
H	-0.30915300	-2.61671700	-2.19160800
O	0.81056200	0.32468300	-3.45248000
P	0.41112000	1.99818700	0.15073500
P	1.57437100	-1.56994700	-0.15689400
Ru	-0.24266200	-0.07731300	-0.65963700
S	-2.31315700	0.84695000	-1.22060000
S	-1.50003300	-1.74011100	0.31711000

Sum of electronic and zero-point Energies= -3827.798047
Sum of electronic and thermal Energies= -3827.748353
Sum of electronic and thermal Enthalpies= -3827.747409
Sum of electronic and thermal Free Energies= -3827.885729

3'

C	-0.58091400	0.32391900	-2.37719400
C	1.61196200	4.32142900	-2.91747600
C	2.23209900	5.36851100	-2.21495700
C	2.19528500	5.37783600	-0.81013500
C	1.54284600	4.34851100	-0.11088400
C	0.80340900	2.07129000	1.78925100
C	0.23810700	2.77333000	2.87887700
C	0.92619600	2.86056400	4.10316000
C	2.18979500	2.26520100	4.25143700
C	2.76871700	1.58428200	3.16510700
C	2.08080100	1.48437400	1.94602700
C	-1.63698300	2.76391200	0.36597500
C	-1.89138900	-2.11779400	1.46471900
C	-1.41088200	-1.43187700	2.60354100
C	-1.44925100	-2.03716900	3.87034200
C	-1.95410700	-3.34148800	4.01368600
C	-2.42032100	-4.03680600	2.88456600
C	-2.39121200	-3.43011400	1.61671600
C	-2.16189400	-2.63745800	-1.37636700
C	-1.06396600	-3.42441100	-1.79651700
C	-1.24874600	-4.48650900	-2.69661000
C	-2.52923500	-4.77278000	-3.20186700
C	-2.03214600	3.88785000	-0.39379900
C	-3.62556000	-3.99441600	-2.79422500
C	-3.44634500	-2.93575000	-1.88616600
C	-3.51738100	-0.41412900	-0.19407100
C	-4.51094500	-0.69130800	0.77172800
C	-5.78266100	-0.09819800	0.67777200
C	-6.08071400	0.77446400	-0.38219400
C	-5.09605300	1.05912600	-1.34526800
C	-3.82319800	0.47481800	-1.24982100
C	2.90265300	-1.70756600	0.23524400
C	3.38094700	-0.85698800	-0.75243300
C	-3.28000100	4.49671300	-0.17211300
C	4.85099500	-0.70547500	-1.14073400
C	3.75085100	-2.68759300	1.03632400
C	-4.14340000	4.00352700	0.81976900
C	-3.76277400	2.88095900	1.57676000
C	-2.52816000	2.25708800	1.34082000
C	0.92057000	3.28797900	-0.80875500
C	0.96436300	3.28731300	-2.22018600
F	3.10528600	-3.12314100	2.15619000
F	4.92873900	-2.14038900	1.46100600
F	4.06615500	-3.80833200	0.31521900
F	5.53752400	0.06575200	-0.23967200
F	5.49842100	-1.90125900	-1.22375700
F	4.99711500	-0.10172000	-2.35348800
H	1.63924000	4.29799800	-4.01820600
H	2.74939700	6.17286900	-2.76158200
H	2.68270400	6.19055100	-0.24842200
H	1.52649500	4.37084400	0.98854500
H	-0.73851400	3.26729500	2.77639700
H	0.46835900	3.40669900	4.94346000
H	2.72627400	2.33480000	5.21107500
H	3.76226500	1.12015000	3.26402600
H	2.54572800	0.95004200	1.10450800
H	-0.97655800	-0.42572300	2.49491100
H	-1.06495300	-1.49124800	4.74617200
H	-1.97294900	-3.82114800	5.00518200
H	-2.80628500	-5.06347400	2.98736300
H	-2.75555700	-3.98430600	0.73873100
H	-0.05548400	-3.20136000	-1.41579500
H	-0.38084000	-5.08796100	-3.00998400
H	-2.67144100	-5.59936700	-3.91613200
H	-1.35779400	4.30144300	-1.15754100
H	-4.63299100	-4.20852400	-3.18550900
H	-4.31683400	-2.33923600	-1.57717000
H	-4.29583000	-1.38166100	1.60061400
H	-6.54660200	-0.32818500	1.43783200
H	-7.07903900	1.23407600	-0.45807600
H	-5.31697200	1.74478300	-2.17818800
H	-3.06721700	0.71056100	-2.01173200
H	-3.56993600	5.37266000	-0.77404700
H	-5.11458300	4.49027000	1.00204700
H	-4.43557900	2.47944600	2.35014700
H	-2.25097400	1.37307000	1.93396500
H	0.49349500	2.47446800	-2.78968800
O	-0.99227000	0.49742300	-3.46332100
P	-1.87267700	-1.25879500	-0.16715600
P	0.00761200	1.96740800	0.12129700
Ru	0.17215200	-0.15478800	-0.74466900
S	1.19918200	-1.74630200	0.58724000
S	2.30113900	0.18711800	-1.61116400

Sum of electronic and zero-point Energies= -3827.801686
Sum of electronic and thermal Energies= -3827.751100
Sum of electronic and thermal Enthalpies= -3827.750156
Sum of electronic and thermal Free Energies= -3827.892437

$TS_{3\text{-}3'}$

C	-0.57293801	0.34370812	-2.37783504
C	1.69833387	4.30783689	-2.87678283
C	2.28922447	5.36317020	-2.16168787
C	2.21101821	5.37917458	-0.75853949
C	1.54623261	4.34820132	-0.07374765
C	0.80384896	2.05177422	1.80465503
C	0.23263941	2.74675473	2.89556342
C	0.91216785	2.82219944	4.12552049
C	2.17269186	2.22162108	4.27813987
C	2.75763165	1.54788643	3.19044419
C	2.07867854	1.46047119	1.96549693
C	-1.61990386	2.76771768	0.35942003
C	-1.90402483	-2.10357779	1.45887282
C	-1.42776824	-1.41753060	2.59939906
C	-1.47467834	-2.02114957	3.86673367
C	-1.98388727	-3.32387795	4.00898485
C	-2.44581751	-4.01935669	2.87819335
C	-2.40819949	-3.41434845	1.60979057
C	-2.16331904	-2.62550221	-1.38316010
C	-1.06572758	-3.41628439	-1.79703907
C	-1.24913614	-4.47779667	-2.69809956

C	-2.52780975	-4.75974882	-3.21034894
C	-2.00123631	3.88985349	-0.41016187
C	-3.62376772	-3.97772498	-2.80872932
C	-3.44598572	-2.91951692	-1.89985883
C	-3.51712805	-0.39686604	-0.20821672
C	-4.51439078	-0.66867002	0.75534942
C	-5.78406439	-0.07205788	0.65624666
C	-6.07649864	0.79890410	-0.40667449
C	-5.08819726	1.07822285	-1.36755699
C	-3.81737412	0.49032844	-1.26705768
C	2.89645644	-1.73550020	0.25199477
C	3.38567779	-0.88252521	-0.72799182
C	-3.24708580	4.50778379	-0.20309670
C	4.83409079	-0.71295578	-1.18277295
C	3.72591448	-2.71219315	1.08105276
C	-4.12241662	4.02556878	0.78374959
C	-3.75602365	2.90443880	1.54977816
C	-2.52340930	2.27130213	1.32822971
C	0.95261344	3.27961844	-0.78435672
C	1.03826852	3.27213409	-2.19352845
F	2.94950759	-3.45346307	1.92102041
F	4.64306391	-2.07566675	1.87571371
F	4.40903162	-3.60739176	0.30662886
F	5.23132968	0.59424698	-1.08057387
F	5.73632414	-1.44412973	-0.48321078
F	4.97747292	-1.06187511	-2.49872752
H	1.75866213	4.27894421	-3.97604989
H	2.81636722	6.16877932	-2.69695327
H	2.67566577	6.19828339	-0.18690759
H	1.49755497	4.37541858	1.02466760
H	-0.74172715	3.24453399	2.78999221
H	0.44989811	3.36300527	4.96684166
H	2.70225834	2.28147204	5.24226083
H	3.74848129	1.07897304	3.29348117
H	2.54808739	0.93248254	1.12229232
H	-0.99036117	-0.41256938	2.49214112
H	-1.09378542	-1.47507452	4.74395219
H	-2.00956074	-3.80218918	5.00097838
H	-2.83523085	-5.04480038	2.98018177
H	-2.76939421	-3.96859856	0.73055033
H	-0.05867452	-3.19673376	-1.41045570
H	-0.38159746	-5.08217593	-3.00681560
H	-2.66887470	-5.58585084	-3.92539695
H	-1.31739592	4.29475650	-1.17013496
H	-4.62974823	-4.18856143	-3.20547901
H	-4.31609830	-2.31997569	-1.59568355
H	-4.30385852	-1.35760967	1.58656047
H	-6.55085852	-0.29800418	1.41464324
H	-7.07323749	1.26127020	-0.48657628
H	-5.30457900	1.76245586	-2.20283490
H	-3.05886274	0.72201567	-2.02758256
H	-3.52609066	5.38212263	-0.81248166
H	-5.09197107	4.51957367	0.95480898
H	-4.43850616	2.51113397	2.31889268
H	-2.25804880	1.38791489	1.92762313
H	0.59093172	2.45261578	-2.77225385
O	-0.98149371	0.53254569	-3.46217305
P	-1.87515099	-1.24679161	-0.17395155
P	0.02144441	1.96020538	0.12974493
Ru	0.17603859	-0.15570912	-0.74748965
S	1.19024859	-1.74178706	0.60369921
S	2.30810353	0.14876275	-1.61208203

Sum of electronic and zero-point Energies= -3827.799952

Sum of electronic and thermal Energies= -3827.750253

Sum of electronic and thermal Enthalpies= -3827.749309

Sum of electronic and thermal Free Energies= -3827.888897

$TS_{3\text{-}5}$

C	-0.43500151	0.11734357	-2.30561220
C	-0.77903074	4.13994055	-3.27105827
C	0.37501027	4.93339161	-3.39860593
C	1.40475083	4.81863378	-2.45020071
C	1.27907164	3.92982025	-1.36815765
C	1.21106178	2.43537960	1.37934832
C	1.11732974	3.74711958	1.90688377
C	2.03744446	4.19409092	2.86642013
C	3.05365079	3.33480014	3.32660214
C	3.14302596	2.02887938	2.82031352
C	2.22730506	1.58173721	1.84913866
C	-1.55577277	2.40250536	1.05879471
C	-2.31623680	-1.76582145	1.62045382
C	-1.34275031	-1.71251189	2.64032926
C	-1.65126778	-2.11023047	3.95375196
C	-2.94437638	-2.55688401	4.27021070
C	-3.92707882	-2.60529673	3.26460305
C	-3.61624529	-2.21709665	1.95182992
C	-2.02017659	-2.95556539	-0.99086842
C	-0.87972264	-3.62983301	-1.47638607
C	-0.99778634	-4.88385825	-2.10326045
C	-2.25827814	-5.48075619	-2.25979172
C	-2.43613888	3.43197414	0.66381737
C	-3.40457690	-4.81334337	-1.79028387
C	-3.28764381	-3.56273135	-1.16474314
C	-3.34503710	-0.42978088	-0.75210163
C	-4.15191142	0.37239302	0.08498303
C	-5.25168264	1.07353344	-0.44095015
C	-5.55815545	0.99282423	-1.80951153
C	-4.75664709	0.20292446	-2.65311418
C	-3.66207549	-0.50460849	-2.13023658
C	3.09442363	-1.69322986	0.24927737
C	3.50840013	-0.73570335	-0.66695737
C	-3.50409357	3.81404137	1.49729104
C	4.96159983	-0.50312455	-1.08431087
C	4.01073269	-2.61874238	1.03770452
C	-3.70410809	3.18004176	2.73442488
C	-2.82490127	2.15823557	3.14047996
C	-1.76118295	1.77489208	2.31013772
C	0.11802717	3.13802015	-1.22469441
C	-0.90294732	3.24028877	-2.20019344
F	3.34100765	-3.70298347	1.52339547
F	4.56018264	-1.98805191	2.12835381
F	5.04638750	-3.10474843	0.29805835
F	5.12301516	0.68557400	-1.73075468
F	5.81088092	-0.47870324	-0.01585096
F	5.40731384	-1.47154213	-1.93812709
H	-1.58548161	4.20929744	-4.01795832
H	0.47587374	5.63132622	-4.24474569
H	2.32070091	5.42204831	-2.55096329
H	2.09730240	3.84712898	-0.63837527
H	0.31900674	4.42457951	1.56589883
H	1.95702982	5.21914535	3.26208954
H	3.77298921	3.68599889	4.08348890
H	3.93009184	1.34532463	3.17459329
H	2.30005247	0.55501545	1.46430640
H	-0.32591893	-1.36426488	2.40429090
H	-0.87109349	-2.06990598	4.73023616
H	-3.18860942	-2.86784685	5.29846309
H	-4.94602740	-2.95015312	3.50251737
H	-4.40327898	-2.25819904	1.18523891
H	0.11340157	-3.17193892	-1.36092121
H	-0.09254411	-5.39086395	-2.47279009
H	-2.35154170	-6.46155055	-2.75269750
H	-2.28585814	3.95817014	-0.28930963

H	-4.40053752	-5.26715992	-1.91668643
H	-4.20074309	-3.04974670	-0.82890189
H	-3.92730226	0.45257585	1.15827306
H	-5.87102822	1.68750178	0.23160260
H	-6.42178029	1.54094936	-2.21865654
H	-4.98692040	0.12766590	-3.72768926
H	-3.05884636	-1.13142575	-2.80319087
H	-4.17850470	4.62319509	1.17441042
H	-4.53703885	3.48649045	3.38706858
H	-2.96303648	1.65878506	4.11229811
H	-1.07094191	0.98733337	2.64717828
H	-1.79871419	2.60348880	-2.13617916
O	-0.75472962	0.24292144	-3.42469133
P	-1.85282440	-1.31759149	-0.11990325
P	-0.03963873	1.89276250	0.12432428
Ru	0.25697284	-0.27221423	-0.62506188
S	1.39770491	-1.84746801	0.62152628
S	2.35830397	0.27780958	-1.46459933

Sum of electronic and zero-point Energies= -3827.796318
Sum of electronic and thermal Energies= -3827.746729
Sum of electronic and thermal Enthalpies= -3827.745785
Sum of electronic and thermal Free Energies= -3827.885334

7

C	-0.65498200	0.33722500	-2.42485300
C	3.12272500	3.82415500	-1.75007200
C	3.82412300	4.42934700	-0.68974000
C	3.34748800	4.29325200	0.62277200
C	2.17613900	3.55539400	0.88140800
C	-0.43604000	2.18309900	1.86920200
C	-1.54197100	2.93427600	2.32915900
C	-1.77430900	3.09145900	3.70795200
C	-0.89920400	2.51742200	4.64525800
C	0.20417600	1.76779700	4.19643600
C	0.42732400	1.59076300	2.82192200
C	-1.31728700	3.12651900	-0.69880400
C	-1.85689300	-1.94285500	1.65310000
C	-1.94361800	-0.97915300	2.68458100
C	-2.00136000	-1.37646900	4.03108100
C	-1.94667700	-2.73915900	4.37014800
C	-1.83277900	-3.70211100	3.35353500
C	-1.79062100	-3.31002400	2.00478400
C	-1.80458900	-2.97527700	-1.04679600
C	-0.63800700	-3.45659300	-1.67773700
C	-0.65241700	-4.68069700	-2.37079200
C	-1.83245700	-5.43894100	-2.44038500
C	-1.03907700	4.50997300	-0.80377600
C	-3.00075900	-4.96999200	-1.81121000
C	-2.98898400	-3.74767100	-1.12076800
C	-3.49366000	-0.77273300	-0.45019500
C	-4.41458700	-0.41236500	0.55764400
C	-5.69398600	0.06500800	0.21886000
C	-6.07598900	0.18275900	-1.12778700
C	-5.16852700	-0.18223700	-2.13970400
C	-3.88916600	-0.65386400	-1.80550100
C	2.93382900	-1.35478700	0.44870500
C	3.32414100	-0.92614900	-0.81488400
C	-1.99416700	5.38884400	-1.34085400
C	4.74099400	-1.02801700	-1.37368100
C	3.87184200	-1.92567300	1.50914300
C	-3.23927800	4.90250500	-1.77759100
C	-3.52476200	3.53098300	-1.67175100
C	-2.56962900	2.64897700	-1.13716100
C	1.47856000	2.92923000	-0.17339400
C	1.96487200	3.07687700	-1.49364600
F	3.19296400	-2.61370600	2.47156400
F	4.56431000	-0.93706000	2.15932800
F	4.79165000	-2.78976100	0.99606000
F	4.91369100	-0.24064400	-2.47308700
F	5.68937800	-0.64397900	-0.47103100
F	5.04778500	-2.30435700	-1.76452200
H	3.48659300	3.92476700	-2.78460000
H	4.74248500	5.00361100	-0.88999100
H	3.88649100	4.76359000	1.46047300
H	1.81030600	3.47711300	1.91486400
H	-2.22695900	3.40572700	1.60977800
H	-2.64306600	3.67786300	4.04743700
H	-1.07674200	2.65111200	5.72432700
H	0.89352900	1.30558100	4.92043800
H	1.27368000	0.97219000	2.48605000
H	-1.95598700	0.09333000	2.44078100
H	-2.07499300	-0.60929100	4.81743800
H	-1.98107900	-3.04950900	5.42653000
H	-1.77246600	-4.77213200	3.60828700
H	-1.69727900	-4.07746400	1.22348500
H	0.29167600	-2.86742700	-1.63189800
H	0.26748600	-5.03741200	-2.86020000
H	-1.84484600	-6.39576000	-2.98633700
H	-0.06961000	4.90520800	-0.46680500
H	-3.93049100	-5.55912500	-1.86029700
H	-3.91042300	-3.39182400	-0.63469700
H	-4.14355100	-0.51661500	1.61813000
H	-6.39970400	0.33680700	1.02004100
H	-7.08081600	0.55040600	-1.38982100
H	-5.45803500	-0.10474900	-3.19972600
H	-3.19734300	-0.94417100	-2.61067000
H	-1.75939800	6.46221300	-1.42141100
H	-3.98434400	5.59291600	-2.20414300
H	-4.49401800	3.13452100	-2.01200800
H	-2.80460300	1.57861200	-1.06409900
H	1.43508100	2.59875300	-2.33150700
O	-1.07775400	0.60079000	-3.48359500
P	-1.77842900	-1.37851600	-0.10217400
P	-0.09237000	1.97074900	0.06457000
Ru	0.13933800	-0.15305700	-0.79296300
S	1.27950600	-1.22020200	0.94286100
S	2.14368000	-0.29012200	-1.91155500

Sum of electronic and zero-point Energies= -3827.799543
Sum of electronic and thermal Energies= -3827.748880
Sum of electronic and thermal Enthalpies= -3827.747936
Sum of electronic and thermal Free Energies= -3827.891233

$TS_{3\text{-}7}$

C	-0.63139700	0.44728900	-2.38374600
C	2.79789300	3.97661000	-2.17235000
C	3.52284000	4.71747500	-1.22023300
C	3.16917200	4.63701200	0.13543500
C	2.09563900	3.82297700	0.54315000
C	-0.11308400	2.23147100	1.91580600
C	-0.99392300	3.15175200	2.53041900
C	-0.96058200	3.35025900	3.92293100
C	-0.03955900	2.64830700	4.71834700
C	0.84867100	1.74001800	4.11349300
C	0.80797400	1.52839900	2.72628600
C	-1.50046500	3.02737100	-0.48218100
C	-1.85937400	-1.89711200	1.63474700
C	-1.87836100	-0.90496900	2.64225600
C	-1.93540400	-1.26525100	3.99863500
C	-1.95087600	-2.62166000	4.36862600
C	-1.91153300	-3.61376500	3.37459300

C	-1.86929700	-3.25684300	2.01555000
C	-1.79678700	-2.95446100	-1.07209200
C	-0.61918100	-3.44190900	-1.67902200
C	-0.62681900	-4.66142000	-2.37965500
C	-1.81027800	-5.41072900	-2.48146300
C	-1.33758900	4.27053600	-1.13377800
C	-2.98960200	-4.93520200	-1.87913700
C	-2.98546700	-3.71582500	-1.18304100
C	-3.51426800	-0.78855900	-0.46494700
C	-4.49672700	-0.66348400	0.54230500
C	-5.80299100	-0.25121200	0.21771300
C	-6.14760700	0.03245100	-1.11447700
C	-5.17629100	-0.09615700	-2.12457800
C	-3.87144700	-0.50088900	-1.80387900
C	2.90838200	-1.48003400	0.40667400
C	3.33486600	-0.92560900	-0.79446000
C	-2.45989700	5.02283700	-1.52434400
C	4.76626400	-0.98275600	-1.32331400
C	3.80993100	-2.16854200	1.42631100
C	-3.75699200	4.55380700	-1.25949100
C	-3.92864900	3.32321300	-0.60050900
C	-2.80978400	2.56470600	-0.22185400
C	1.37232400	3.06520600	-0.40293600
C	1.73800000	3.15223500	-1.76681700
F	3.09847800	-2.95230200	2.28666900
F	4.48553300	-1.26105400	2.20238500
F	4.74354900	-2.97760500	0.85217900
F	4.97307600	-0.09282700	-2.33459200
F	5.69069500	-0.69630600	-0.36126900
F	5.07686600	-2.21684800	-1.82874800
H	3.06796000	4.02869300	-3.23871900
H	4.36570000	5.35173100	-1.53740400
H	3.73116300	5.20963300	0.89025800
H	1.82897100	3.78067100	1.60861000
H	-1.70776800	3.72582200	1.92274000
H	-1.65799100	4.06779200	4.38408200
H	-0.01214100	2.80886100	5.80797000
H	1.57678000	1.18329700	4.72406400
H	1.49279200	0.79832800	2.26900400
H	-1.83653100	0.16045500	2.36882600
H	-1.95235900	-0.47804700	4.76841700
H	-1.98295200	-2.90493000	5.43268300
H	-1.90898200	-4.67890500	3.65556500
H	-1.83454300	-4.04474500	1.24939200
H	0.31433400	-2.86251200	-1.60712200
H	0.30172000	-5.02191000	-2.84961200
H	-1.81671400	-6.36449400	-3.03282600
H	-0.33071000	4.66139100	-1.33712300
H	-3.92298500	-5.51565200	-1.95503900
H	-3.91754900	-3.35327900	-0.72339800
H	-4.24907900	-0.89821100	1.58803200
H	-6.55764400	-0.16445300	1.01586800
H	-7.17234400	0.34783600	-1.36761600
H	-5.43498200	0.11913100	-3.17332000
H	-3.13029900	-0.60617600	-2.60982700
H	-2.31307900	5.98685300	-2.03695300
H	-4.63407300	5.14582800	-1.56586600
H	-4.93840900	2.94110900	-0.38457600
H	-2.96158000	1.60216000	0.28616600
H	1.19166500	2.56955300	-2.52349400
O	-1.05434800	0.77157600	-3.42631500
P	-1.78461400	-1.35675800	-0.12636700
P	-0.06934500	2.00159800	0.07831400
Ru	0.15253900	-0.12502000	-0.77730500
S	1.24208500	-1.36805200	0.87062200
S	2.19128600	-0.16525600	-1.84784200

Sum of electronic and zero-point Energies= -3827.799055

Sum of electronic and thermal Energies= -3827.749164

Sum of electronic and thermal Enthalpies= -3827.748220

Sum of electronic and thermal Free Energies= -3827.889712

4'

C	0.63499700	0.45088300	-2.39045900
C	1.46012900	-4.34249400	-2.80614100
C	2.76364900	-4.83794200	-2.97615000
C	3.83529000	-4.22321500	-2.30365300
C	3.60555700	-3.11753400	-1.46852000
C	2.00655900	-1.91232900	1.51738800
C	1.76368200	-1.06688600	2.62535600
C	1.77114400	-1.58516300	3.93017200
C	2.00078700	-2.95611700	4.14536500
C	2.22805000	-3.80401900	3.04869300
C	2.23463600	-3.28705700	1.74090600
C	3.59916200	-0.30020100	-0.27799400
C	1.13398300	2.45409100	1.32692000
C	2.46830500	2.62255900	0.88755600
C	3.46947800	3.02853700	1.78448200
C	3.16055900	3.25084100	3.13872000
C	1.84084000	3.07417500	3.58738600
C	0.83105500	2.68660600	2.68853900
C	-1.72351400	2.29205600	1.04419500
C	-2.25398100	1.31903600	1.91998300
C	-3.40753800	1.58899100	2.67527500
C	-4.05504600	2.83085900	2.55779000
C	3.95208200	0.32830400	-1.49619800
C	-3.53640400	3.80404100	1.68690300
C	-2.37708300	3.54182800	0.93723000
C	-0.13422800	3.35053100	-1.10497600
C	0.57348800	4.55210500	-0.87120900
C	0.51597300	5.60700600	-1.79947200
C	-0.25871800	5.48539800	-2.96499400
C	-0.98194700	4.30205200	-3.19634000
C	-0.91787400	3.24281000	-2.27724800
C	-2.75161400	-1.81374600	0.26371900
C	-3.27051100	-1.04629100	-0.77289700
C	5.19962200	0.95573000	-1.64164900
C	-4.73718000	-1.03799300	-1.20327800
C	-3.56073600	-2.74120100	1.16190200
C	6.11822200	0.96377100	-0.57495200
C	5.77877400	0.33656200	0.63510100
C	4.52857600	-0.29194100	0.78441100
C	2.29600900	-2.61149700	-1.28976800
C	1.22725200	-3.23681100	-1.96950100
F	-2.76937700	-3.66259900	1.78262600
F	-4.51144500	-3.44480400	0.48504600
F	-4.20702700	-2.05639300	2.16194800
F	-5.05948400	-2.14370700	-1.94165400
F	-5.59231800	-0.99618500	-0.14144900
F	-5.03414400	0.04168000	-1.98059700
H	0.61368500	-4.81404700	-3.32979300
H	2.94666000	-5.70124700	-3.63562500
H	4.86110300	-4.60392200	-2.43264600
H	4.45510000	-2.64344300	-0.95416600
H	1.56733400	0.00481600	2.46696000
H	1.58505600	-0.91343000	4.78303300
H	1.99396200	-3.36437500	5.16848400
H	2.39739400	-4.88084900	3.20742400
H	2.40922200	-3.96265700	0.89078600
H	2.72839100	2.44803300	-0.16701900
H	4.49905100	3.16465600	1.41930800
H	3.94815300	3.56432900	3.84222800
H	1.58635500	3.25164500	4.64452500
H	-0.20129000	2.57418100	3.05019900
H	-1.76649800	0.33522800	2.00387500

H	-3.80906200	0.81254500	3.34460600
H	-4.96860500	3.03636300	3.13794100
H	3.25610000	0.32155000	-2.34756700
H	-4.03832800	4.77925600	1.58336900
H	-1.98526200	4.31727300	0.26373000
H	1.17056400	4.67540700	0.04343800
H	1.08032000	6.53261000	-1.60306600
H	-0.30110500	6.31225700	-3.69165000
H	-1.59946200	4.19600000	-4.10200500
H	-1.49838800	2.32738600	-2.46901900
H	5.45708900	1.43621100	-2.59890900
H	7.09859600	1.45262100	-0.69163400
H	6.49217600	0.32987600	1.47475100
H	4.28079400	-0.78258100	1.73684400
H	0.20190700	-2.85599900	-1.84273600
O	1.05250400	0.73755100	-3.44672300
P	-0.16147300	1.95444600	0.10993300
P	1.96884900	-1.17049200	-0.16858700
Ru	-0.11515100	-0.16253800	-0.79029200
S	-1.05967300	-1.72286800	0.64703100
S	-2.22469000	-0.06698600	-1.73941000

Sum of electronic and zero-point Energies= -3827.802267
Sum of electronic and thermal Energies= -3827.751634
Sum of electronic and thermal Enthalpies= -3827.750690
Sum of electronic and thermal Free Energies= -3827.893361

$TS_{4\text{-}4'}$

C	0.63419281	0.47984692	-2.39509781
C	1.53303290	-4.31362950	-2.82575588
C	2.84330863	-4.79470663	-2.98444597
C	3.90201745	-4.16972555	-2.30092548
C	3.65265352	-3.06802691	-1.46624224
C	2.02076988	-1.88577585	1.50693954
C	1.77291749	-1.04305559	2.61589929
C	1.77661942	-1.56385652	3.91965121
C	2.00674370	-2.93512288	4.13272146
C	2.23853765	-3.78041182	3.03508101
C	2.24944014	-3.26066217	1.72834832
C	3.60313879	-0.24982256	-0.27719741
C	1.12145706	2.47975419	1.28431366
C	2.42936842	2.69417433	0.78930814
C	3.45297358	3.13361705	1.64366698
C	3.19346888	3.34549664	3.01004437
C	1.90036951	3.12509906	3.51335992
C	0.86731258	2.70304681	2.65714174
C	-1.74185892	2.21253684	1.10409013
C	-2.17249682	1.23243659	2.02652350
C	-3.30971170	1.44987517	2.82223266
C	-4.04216196	2.64317375	2.69878913
C	3.95663881	0.37759818	-1.49576049
C	-3.62481793	3.62100935	1.78034490
C	-2.48115661	3.41276397	0.99045799
C	-0.25665591	3.35702980	-1.08308808
C	0.37147284	4.59583378	-0.81512203
C	0.25910510	5.66491347	-1.72130139
C	-0.49100725	5.51984672	-2.90042830
C	-1.13447246	4.29872956	-3.16657789
C	-1.01628543	3.22595963	-2.26818221
C	-2.74302738	-1.82668678	0.25260471
C	-3.26687382	-1.08299414	-0.79745207
C	5.19791179	1.01848851	-1.63592410
C	-4.73158661	-1.07869883	-1.24043152
C	-3.47698795	-2.78043565	1.18407849
C	6.10931308	1.04161716	-0.56329860
C	5.76887277	0.41638127	0.64748281
C	4.52519783	-0.22600445	0.79130070
C	2.33608668	-2.57638529	-1.29899894
C	1.28040271	-3.21196848	-1.98947580
F	-2.97219701	-4.05078946	1.08652980
F	-4.81215113	-2.87345445	0.97056559
F	-3.32110720	-2.40794474	2.49854442
F	-5.16281863	-2.32160299	-1.60927910
F	-5.56862813	-0.62384745	-0.26184056
F	-4.93398000	-0.27194728	-2.32060327
H	0.69652187	-4.79365244	-3.35759157
H	3.04169078	-5.65500621	-3.64340874
H	4.93297135	-4.53938525	-2.42073797
H	4.49214910	-2.58585253	-0.94296242
H	1.57603498	0.02883938	2.45894045
H	1.58700679	-0.89423509	4.77341661
H	1.99659106	-3.34555495	5.15493050
H	2.40807730	-4.85745588	3.19206070
H	2.42769296	-3.93429988	0.87745133
H	2.64933589	2.53125984	-0.27627256
H	4.46119386	3.30464573	1.23605049
H	3.99869922	3.68574996	3.68037107
H	1.68439268	3.29554964	4.58018499
H	-0.14532538	2.55824611	3.06072634
H	-1.62246967	0.28263504	2.11506922
H	-3.63151585	0.66937905	3.52909810
H	-4.94316903	2.80619044	3.31114839
H	3.26645410	0.35838543	-2.35178760
H	-4.19443647	4.55757195	1.67065660
H	-2.16955314	4.19159690	0.28009947
H	0.94964119	4.73563420	0.10926968
H	0.76154222	6.61958833	-1.49781953
H	-0.57583310	6.35780932	-3.61047649
H	-1.73159219	4.17311247	-4.08334013
H	-1.53610489	2.28112115	-2.48745211
H	5.45639286	1.49729217	-2.59376992
H	7.08504523	1.54062710	-0.67593497
H	6.47658786	0.42181455	1.49191314
H	4.27723549	-0.71574541	1.74413083
H	0.24966101	-2.84342225	-1.87050377
O	1.05467730	0.78537992	-3.44508406
P	-0.20169404	1.94494533	0.11311358
P	1.98411289	-1.14139369	-0.17776360
Ru	-0.11338920	-0.16074182	-0.80476191
S	-1.04239607	-1.74146412	0.61440764
S	-2.22365990	-0.08712276	-1.75445839

Sum of electronic and zero-point Energies= -3827.801280
Sum of electronic and thermal Energies= -3827.751538
Sum of electronic and thermal Enthalpies= -3827.750593
Sum of electronic and thermal Free Energies= -3827.890539

8

Ru	0.43295900	0.03471500	-0.50348900
S	2.09804900	-1.52035700	-0.14167900
S	2.13594800	1.58293200	-0.28200300
P	-1.05172200	-1.83064300	-0.11044700
P	-1.03834500	1.82286900	0.05850200
O	0.06311100	0.13604600	-3.46452800
C	0.12915700	0.10151700	-2.28955600
C	3.63062200	0.70391800	-0.16384600
C	3.61872700	-0.67845800	-0.12870100
C	4.88029900	1.57659200	-0.14722700
C	4.85031900	-1.56901500	-0.00791000
F	5.82135000	1.13427900	0.73547600
F	4.59339000	2.86276500	0.21046200
F	5.47855800	1.64146300	-1.37592000

F	4.58091000	-2.85945900	-0.35947600
F	5.32894100	-1.61297700	1.27442100
F	5.87625000	-1.15692600	-0.80649300
C	-0.36789600	3.52615800	-0.21390900
C	0.13914200	3.83016900	-1.49814600
C	0.57757800	5.12881300	-1.80098600
C	0.51831700	6.14027800	-0.82642800
C	0.01091100	5.84699100	0.45060200
C	-0.43428900	4.54901800	0.75654800
C	-1.34148600	1.73100500	1.87133100
C	-2.57705800	1.33267300	2.42910600
C	-2.71633400	1.19268400	3.82213400
C	-1.62938800	1.44626900	4.67512400
C	-0.39041500	1.82882700	4.12720000
C	-0.24257400	1.95957400	2.73737000
C	-2.68006200	2.11568300	-0.74247300
C	-3.64906600	2.95443300	-0.14254200
C	-4.82053200	3.29905400	-0.83506900
C	-5.03012500	2.83793900	-2.14766500
C	-4.06010000	2.02928700	-2.76172100
C	-2.89600000	1.66591500	-2.06135700
C	-0.54062200	-2.73837900	1.41636900
C	-0.40923200	-4.14237700	1.46329600
C	-0.01353400	-4.77924100	2.65347400
C	0.24430100	-4.02524800	3.80989400
C	0.11411100	-2.62498700	3.77133400
C	-0.26440700	-1.98434600	2.58109200
C	-1.06696400	-3.14237600	-1.41806000
C	-2.12189200	-4.08563400	-1.48170400
C	-2.11371100	-5.10235100	-2.45048500
C	-1.05426300	-5.19432200	-3.37109200
C	-0.00221900	-4.26566200	-3.31378600
C	-0.00734900	-3.24663100	-2.34500600
C	-2.86828300	-1.60593500	0.16136200
C	-3.68166800	-1.25682600	-0.94139700
C	-5.06856700	-1.10511600	-0.78995800
C	-5.66802900	-1.29920800	0.46789600
C	-4.86974300	-1.65113800	1.56895000
C	-3.47913700	-1.80521200	1.41895400
H	0.19614900	3.04682500	-2.26953100
H	0.97632700	5.34743900	-2.80400600
H	0.86975500	7.15720600	-1.06228500
H	-0.04105500	6.63393800	1.21986600
H	-0.83388900	4.33889500	1.75974000
H	-3.43711100	1.12020900	1.77831400
H	-3.68689800	0.88128700	4.23992000
H	-1.74391000	1.34049700	5.76558800
H	0.47194800	2.02121500	4.78490700
H	0.73873100	2.23257200	2.31706300
H	-3.48336700	3.36109100	0.86646600
H	-5.56782000	3.94746400	-0.35043500
H	-5.94398000	3.12064600	-2.69405600
H	-4.20416600	1.67702100	-3.79548000
H	-2.14228800	1.03870700	-2.55726400
H	-0.60114800	-4.74671400	0.56481800
H	0.09945800	-5.87490200	2.67030700
H	0.55776500	-4.52643400	4.73941700
H	0.32403200	-2.02271600	4.66910200
H	-0.33452700	-0.88524300	2.55703600
H	-2.96030900	-4.02544200	-0.77157600
H	-2.94364700	-5.82607500	-2.48649600
H	-1.05115400	-5.98947500	-4.13358200
H	0.83287400	-4.32701200	-4.02907100
H	0.82661300	-2.53149000	-2.30679800
H	-3.23001100	-1.12651400	-1.93605300
H	-5.68436600	-0.83406800	-1.66166300
H	-6.75714500	-1.18357500	0.58591900
H	-5.33030300	-1.81923000	2.55568500
H	-2.87039600	-2.09485500	2.28766500

Sum of electronic and zero-point Energies= -3827.799706
Sum of electronic and thermal Energies= -3827.749055
Sum of electronic and thermal Enthalpies= -3827.748110
Sum of electronic and thermal Free Energies= -3827.890078

$TS_{4\text{-}8}$

Ru	-0.43250600	-0.04820500	-0.51173000
S	-2.23363800	1.37727900	-0.30114600
S	-1.99575700	-1.70073800	-0.13927600
P	0.91231800	1.92509200	-0.10426500
P	1.16783700	-1.74604300	0.05407800
O	-0.03023700	0.02327600	-3.47142600
C	-0.11189600	-0.00508500	-2.29842200
C	-3.56676000	-0.95763300	-0.08968300
C	-3.67318100	0.41736300	-0.18524700
C	-4.73270500	-1.93180200	0.01226000
C	-4.97626600	1.20818900	-0.13538600
F	-5.71599400	-1.49244600	0.84959600
F	-4.33470800	-3.14712500	0.49140800
F	-5.31544600	-2.16791900	-1.20337300
F	-4.81688400	2.48267700	-0.59692600
F	-5.45800500	1.32096300	1.14126900
F	-5.96085500	0.64338800	-0.88993200
C	0.58155300	-3.49676600	-0.10448900
C	-0.00213600	-3.88317400	-1.33277400
C	-0.36474300	-5.22014300	-1.55981200
C	-0.15209400	-6.18918500	-0.56391400
C	0.43439700	-5.81454500	0.65673800
C	0.80479200	-4.47778600	0.88553300
C	1.56117100	-1.54356700	1.83971000
C	2.76013900	-0.95009200	2.29536500
C	2.96124600	-0.71616000	3.66771200
C	1.97275400	-1.06733100	4.60191900
C	0.76820600	-1.64238000	4.15569800
C	0.55757800	-1.86892000	2.78633300
C	2.77786200	-2.02993800	-0.81868000
C	3.86140500	-2.68332700	-0.18815300
C	5.00935000	-3.02895700	-0.92017000
C	5.08350800	-2.75296200	-2.29715100
C	3.99784400	-2.13289000	-2.93900600
C	2.85442500	-1.77279600	-2.20471000
C	0.43666700	2.76636000	1.46759100
C	0.58339600	4.16194000	1.63990700
C	0.25165200	4.76447800	2.86540800
C	-0.21853300	3.98151800	3.93459200
C	-0.35389000	2.59146100	3.77486100
C	-0.03304900	1.98779100	2.54746900
C	0.72724300	3.26866200	-1.37060000
C	1.75201400	3.59541300	-2.28679300
C	1.54965400	4.57959100	-3.27041700
C	0.32457700	5.26060500	-3.35288800
C	-0.69719900	4.95444600	-2.43761400
C	-0.50060800	3.96967200	-1.45625200
C	2.74838200	1.80128400	0.07008000
C	3.49672100	1.18596600	-0.95864700
C	4.89670300	1.09874700	-0.87888300
C	5.57223000	1.61766700	0.23945400
C	4.83767300	2.22592700	1.27224100
C	3.43726100	2.31938200	1.19033900
H	-0.18015600	-3.13328800	-2.11872800
H	-0.82547700	-5.50252200	-2.51941200
H	-0.44430500	-7.23661400	-0.73940500
H	0.60907200	-6.56781200	1.44149400
H	1.27234800	-4.20556400	1.84330000
H	3.54227800	-0.65781900	1.57991500

H	3.90191600	-0.25247000	4.00435000
H	2.13611200	-0.88690200	5.67620100
H	-0.01853400	-1.91307800	4.87766800
H	-0.39995800	-2.29486400	2.44666800
H	3.80943400	-2.94118200	0.88003600
H	5.84730100	-3.53106100	-0.41070400
H	5.98114600	-3.03328700	-2.87091800
H	4.03497800	-1.92832600	-4.02076600
H	2.01158300	-1.29469700	-2.72473300
H	0.95307800	4.78369500	0.81064900
H	0.35888300	5.85462500	2.98266500
H	-0.48443700	4.45675500	4.89223000
H	-0.72330000	1.97044200	4.60573400
H	-0.15686600	0.89980500	2.42749600
H	2.72732500	3.09204400	-2.23530700
H	2.36423600	4.81579000	-3.97350000
H	0.16745900	6.03116500	-4.12418800
H	-1.66172300	5.48431700	-2.48331000
H	-1.31455500	3.75395400	-0.74984400
H	2.98238800	0.76688800	-1.83463800
H	5.45656200	0.61147300	-1.69233600
H	6.66950400	1.54673300	0.30618500
H	5.35717300	2.63632600	2.15296900
H	2.87964500	2.79793900	2.00782000

Sum of electronic and zero-point Energies= -3827.795879
Sum of electronic and thermal Energies= -3827.746101
Sum of electronic and thermal Enthalpies= -3827.745156
Sum of electronic and thermal Free Energies= -3827.884151

5'

C	-0.00083600	0.06668500	-2.29855900
C	-0.72541200	-4.49306400	-2.91578900
C	-1.06238600	-5.66574500	-2.21826000
C	-0.88102000	-5.72180400	-0.82604300
C	-0.35915300	-4.61644000	-0.13249500
C	0.47772400	-2.36948300	1.82933100
C	1.37924700	-3.22461700	2.50787600
C	1.16383600	-3.56623500	3.85344200
C	0.04582700	-3.06335700	4.54269400
C	-0.85793500	-2.21861400	3.87668100
C	-0.64279200	-1.87201800	2.53136400
C	2.51095300	-2.21620900	-0.19694500
C	2.07262900	1.61964900	1.61545300
C	1.18769300	1.35564100	2.68629500
C	1.65501100	1.33254300	4.01117500
C	3.01573400	1.55842700	4.28390400
C	3.90464600	1.81323200	3.22470500
C	3.43823200	1.84747400	1.89861200
C	0.78005900	3.41716100	-0.23008000
C	0.31487700	3.85331700	-1.49306900
C	-0.14233200	5.16774800	-1.66652400
C	-0.15241400	6.06201700	-0.57974000
C	3.02959300	-3.03852000	-1.22197300
C	0.30092400	5.63398800	0.67812500
C	0.76747900	4.31787400	0.85454300
C	2.83817100	1.74338700	-1.20628200
C	3.20185200	0.64191500	-2.00704400
C	4.31689000	0.71238000	-2.86061100
C	5.08506300	1.88620200	-2.92406000
C	4.72964600	2.99420400	-2.13340800
C	3.61244600	2.92720900	-1.28560200
C	-3.44549100	1.13977200	0.05506000
C	-3.65710700	-0.18009000	-0.30588900
C	4.41944000	-3.17909500	-1.38916100
C	-5.02401200	-0.85519700	-0.40010900
C	-4.53420800	2.16008200	0.36003900
C	5.30938100	-2.51171300	-0.53108200
C	4.80117100	-1.69788100	0.49740000
C	3.41546300	-1.54649400	0.66048800
C	-0.01612400	-3.43418800	-0.82482600
C	-0.21392200	-3.38211100	-2.22461300
F	-4.04631800	3.22157400	1.06729700
F	-5.55275200	1.63989700	1.10468500
F	-5.09211400	2.67828200	-0.77744400
F	-5.51839700	-1.17607800	0.83612700
F	-5.95364200	-0.07278200	-1.01728000
F	-4.96910600	-2.02079500	-1.10469500
H	-0.87434200	-4.43253600	-4.00535100
H	-1.47597700	-6.53194000	-2.75861000
H	-1.15311300	-6.63216200	-0.26860300
H	-0.23043500	-4.67581900	0.95788300
H	2.25553100	-3.63250600	1.98262600
H	1.87543700	-4.23392700	4.36496700
H	-0.12099500	-3.33273100	5.59784100
H	-1.74131700	-1.82403300	4.40315800
H	-1.36282100	-1.21817700	2.01529600
H	0.12237300	1.16864200	2.47622700
H	0.95078400	1.12785300	4.83266400
H	3.38422500	1.53230000	5.32172600
H	4.97280600	1.98934200	3.42991000
H	4.14598200	2.04514300	1.07998500
H	0.30649100	3.15818700	-2.34747500
H	-0.50269200	5.49302900	-2.65516200
H	-0.52022200	7.09150700	-0.71470000
H	2.34812800	-3.58361700	-1.89146300
H	0.29151200	6.32605700	1.53513800
H	1.11973900	3.99635500	1.84577000
H	2.60560600	-0.27934500	-1.97038100
H	4.57824400	-0.15758500	-3.48278600
H	5.95542300	1.94363800	-3.59706700
H	5.31884100	3.92369800	-2.18514100
H	3.33036300	3.81029900	-0.69206200
H	4.80527800	-3.82720500	-2.19223800
H	6.39711700	-2.62839100	-0.65980400
H	5.48786400	-1.17264200	1.17986900
H	3.03554600	-0.90891200	1.47230400
H	0.02156900	-2.46493400	-2.78395500
O	0.12046800	0.11394100	-3.46760100
P	1.36403600	1.66905200	-0.09148600
P	0.69486600	-1.96022300	0.03547200
Ru	-0.39158500	0.08848300	-0.52111100
S	-1.82033100	1.76255000	0.11583700
S	-2.31133000	-1.22041800	-0.63640100

Sum of electronic and zero-point Energies= -3827.803735
Sum of electronic and thermal Energies= -3827.753065
Sum of electronic and thermal Enthalpies= -3827.752121
Sum of electronic and thermal Free Energies= -3827.894354

$TS_{5\text{-}5'}$

C	0.02440192	0.03997184	-2.31058526
C	-0.75979334	-4.50799531	-2.90306494
C	-1.11892971	-5.67046618	-2.19957924
C	-0.95352513	-5.71681665	-0.80502749
C	-0.42566570	-4.61210313	-0.11503174
C	0.41961837	-2.35978034	1.83752260
C	1.30044963	-3.22512561	2.53017753
C	1.06745837	-3.55297246	3.87621716
C	-0.04768587	-3.02573574	4.55180061
C	-0.93087078	-2.17048175	3.87173775
C	-0.69823448	-1.83782045	2.52580682

C	2.47513077	-2.24812839	-0.16936305
C	2.07926906	1.60249390	1.60976994
C	1.18527309	1.35532665	2.67713348
C	1.64516978	1.33421060	4.00463895
C	3.00701631	1.54539717	4.28360822
C	3.90465950	1.78372349	3.22794384
C	3.44589961	1.81586854	1.89911743
C	0.81517539	3.40367529	-0.25145424
C	0.35508147	3.83653247	-1.51740548
C	-0.08784477	5.15458286	-1.69959089
C	-0.08879285	6.05593360	-0.61861178
C	2.99354657	-3.08026542	-1.18660093
C	0.35943116	5.63130542	0.64219225
C	0.81196133	4.31145880	0.82732737
C	2.86433419	1.70525744	-1.20648997
C	3.22773312	0.59290563	-1.99222389
C	4.35015159	0.64727388	-2.83722566
C	5.12603131	1.81567466	-2.90706966
C	4.77110666	2.93425876	-2.13126062
C	3.64670686	2.88325990	-1.29186753
C	-3.43992959	1.17125966	0.02355411
C	-3.66689196	-0.14932575	-0.32315286
C	4.38306673	-3.23918461	-1.33920241
C	-5.03726147	-0.82025527	-0.43186159
C	-4.46021363	2.24157834	0.38060500
C	5.27276482	-2.58046223	-0.47419101
C	4.76466095	-1.75701641	0.54664751
C	3.37941413	-1.58749286	0.69533297
C	-0.06026039	-3.44009619	-0.81334022
C	-0.24199932	-3.39761606	-2.21563253
F	-4.29881346	2.65580014	1.68100039
F	-5.75447317	1.85719751	0.25418315
F	-4.30589585	3.35695027	-0.39832599
F	-5.72883554	-0.77095315	0.74662769
F	-5.81962897	-0.25228635	-1.39496508
F	-4.93235403	-2.14080553	-0.75417179
H	-0.89586191	-4.45491094	-3.99470149
H	-1.53722786	-6.53610263	-2.73719036
H	-1.24302350	-6.61892183	-0.24295785
H	-0.30998464	-4.66382713	0.97718248
H	2.17420277	-3.65163797	2.01559365
H	1.76299917	-4.22884156	4.39896103
H	-0.22822385	-3.28414302	5.60743233
H	-1.81146467	-1.75631241	4.38772715
H	-1.40188302	-1.17482423	1.99897849
H	0.11884563	1.18026442	2.46261320
H	0.93397797	1.14283351	4.82333195
H	3.36947385	1.52089462	5.32359652
H	4.97366918	1.94855760	3.43805145
H	4.16023690	2.00081843	1.08322805
H	0.33863252	3.13562562	-2.36695569
H	-0.44487580	5.47713947	-2.69030246
H	-0.44593134	7.08825940	-0.76034859
H	2.31201394	-3.61879842	-1.86129159
H	0.35682815	6.32888444	1.49477519
H	1.16050492	3.99267869	1.82072914
H	2.62560774	-0.32429246	-1.95041928
H	4.61120402	-0.23099065	-3.44775636
H	6.00217929	1.86050813	-3.57349405
H	5.36657339	3.85945347	-2.18798228
H	3.36567172	3.77407413	-0.70951630
H	4.76865090	-3.89476773	-2.13630936
H	6.36016384	-2.71141881	-0.59153120
H	5.45104188	-1.23847356	1.23451720
H	2.99958535	-0.94277438	1.50148493
H	0.01128746	-2.48852946	-2.78033489
O	0.16079207	0.07601857	-3.47835149
P	1.38191353	1.65089855	-0.10171585
P	0.66016242	-1.96821722	0.04309505
Ru	-0.38971754	0.08735393	-0.53784773
S	-1.80259322	1.76947792	0.10383909
S	-2.32618499	-1.19649924	-0.66650320

Sum of electronic and zero-point Energies= -3827.802574

Sum of electronic and thermal Energies= -3827.752795

Sum of electronic and thermal Enthalpies= -3827.751851

Sum of electronic and thermal Free Energies= -3827.891416

10

C	0.65288900	0.14961000	-2.42250500
C	0.90739100	-4.73716800	-2.22127100
C	1.88239900	-5.65119900	-1.79017700
C	2.84340700	-5.25125500	-0.84264600
C	2.82676200	-3.94560600	-0.32805700
C	2.30691500	-1.64611000	1.67329100
C	3.54461700	-1.29502000	2.25624300
C	3.83370300	-1.64590100	3.58752600
C	2.89566600	-2.35432400	4.35633800
C	1.66563200	-2.72150000	3.78074500
C	1.37494900	-2.37490500	2.45182000
C	3.39531600	-0.57748100	-0.80856900
C	1.11820600	2.24774400	1.49815700
C	1.05107100	1.38938200	2.61982500
C	1.82548500	1.64804300	3.76237000
C	2.69079500	2.75676000	3.79416000
C	2.76706800	3.61310900	2.68201200
C	1.98027400	3.36742000	1.54214000
C	-1.61514800	2.53222200	0.69502400
C	-2.78091500	2.35687600	-0.08432500
C	-4.01290700	2.87793100	0.34315300
C	-4.10245900	3.57351100	1.56162400
C	4.04729000	-1.18725300	-1.90354200
C	-2.94890000	3.75483600	2.34246800
C	-1.71152300	3.24439000	1.91275400
C	0.49204100	3.19413500	-1.16058300
C	1.71318700	3.06389000	-1.86188800
C	2.11721600	4.04290100	-2.78298800
C	1.30349800	5.16375800	-3.02770300
C	0.08867600	5.30203000	-2.33666400
C	-0.31424200	4.32865400	-1.40491200
C	-3.33156000	-1.07946300	-0.84123500
C	-3.01472600	-1.25407000	0.50074300
C	5.18894300	-0.59739800	-2.47486800
C	-4.00333500	-1.70217600	1.57720500
C	-4.71250800	-1.27920300	-1.45467400
C	5.70422800	0.60203500	-1.95656300
C	5.05923400	1.22101300	-0.87061100
C	3.90749300	0.64446400	-0.30879000
C	1.84970500	-3.01674200	-0.75950200
C	0.89121600	-3.42691100	-1.70911600
F	-5.52720200	-0.19261500	-1.25706600
F	-5.36656600	-2.36403600	-0.95224200
F	-4.64299700	-1.46322600	-2.80453900
F	-5.21267100	-1.08227700	1.46799500
F	-4.23096600	-3.05064600	1.53061400
F	-3.54551600	-1.43499600	2.83361600
H	0.14691800	-5.04121900	-2.95765800
H	1.89260900	-6.67863300	-2.18764300
H	3.60902000	-5.96381700	-0.49634900
H	3.57849300	-3.64777400	0.41918800
H	4.30242600	-0.75550400	1.67111400
H	4.80701400	-1.36548600	4.02107200
H	3.12481200	-2.62889900	5.39836400
H	0.92461100	-3.28783200	4.36676600
H	0.41424200	-2.68400500	2.01319900

H	0.37796000	0.51813800	2.60282800
H	1.75666800	0.97118200	4.62792000
H	3.30467900	2.95409700	4.68738200
H	3.43663200	4.48795600	2.70183600
H	2.03360300	4.05610300	0.68615100
H	-2.72585200	1.80251900	-1.03407300
H	-4.90942500	2.72286700	-0.27671200
H	-5.07197100	3.96868800	1.90401900
H	3.66166900	-2.12986700	-2.31838400
H	-3.00663800	4.29876600	3.29877800
H	-0.82011600	3.40552200	2.53502000
H	2.36133600	2.19221500	-1.68820500
H	3.07107900	3.92089000	-3.31983900
H	1.61552800	5.92611200	-3.75912200
H	-0.55720800	6.17534600	-2.52027700
H	-1.26503200	4.45650800	-0.86830800
H	5.67888600	-1.08580600	-3.33208900
H	6.60398100	1.05719100	-2.40004300
H	5.44919700	2.16524900	-0.45835000
H	3.40456500	1.15450500	0.52688700
H	0.11597300	-2.71916200	-2.04505800
O	1.10180600	0.31868700	-3.48748900
P	0.00660600	1.89937400	0.06481900
P	1.85148100	-1.28652100	-0.08757900
Ru	-0.17077100	-0.23392600	-0.77218100
S	-2.11179100	-0.54690800	-1.95661700
S	-1.38924100	-1.04005600	1.05255500

Sum of electronic and zero-point Energies= -3827.801163
Sum of electronic and thermal Energies= -3827.750655
Sum of electronic and thermal Enthalpies= -3827.749710
Sum of electronic and thermal Free Energies= -3827.891382

$TS_{5\text{-}10}$

C	0.24868200	0.15532400	-2.35301100
C	0.39951900	-4.59017800	-2.67841100
C	1.26443900	-5.63745400	-2.32153300
C	2.21587200	-5.43861300	-1.30437100
C	2.30218600	-4.20000900	-0.64937000
C	2.09378200	-2.00362700	1.53391100
C	3.44525000	-2.08649900	1.94330500
C	3.78087300	-2.57000900	3.22078200
C	2.77675500	-2.99271700	4.10696200
C	1.43124000	-2.92854000	3.70508800
C	1.09279400	-2.43566400	2.43448500
C	3.16095800	-0.84373900	-0.89985200
C	1.18599800	1.82926600	1.83185200
C	0.61678200	0.95730500	2.78868300
C	1.15064400	0.87192700	4.08490600
C	2.27827100	1.63414800	4.43699700
C	2.86499600	2.48637000	3.48615800
C	2.32058700	2.59078500	2.19377000
C	-1.02459100	3.11479600	0.49823800
C	-1.59984100	3.79294100	-0.60284900
C	-2.68586700	4.65997400	-0.41688700
C	-3.22108800	4.85922800	0.86957700
C	3.62937200	-1.30819700	-2.14926900
C	-2.65640400	4.19005100	1.96647900
C	-1.56125500	3.32451800	1.78491200
C	1.49966000	3.06915100	-0.78736900
C	2.29620000	2.59123600	-1.84680900
C	3.13087300	3.46479800	-2.56760500
C	3.18661700	4.82698100	-2.23331400
C	2.40273300	5.31532000	-1.17160000
C	1.56278400	4.44680400	-0.45734400
C	-3.64906700	-0.31238500	-0.59996800
C	-3.29389900	-1.37046300	0.22204700
C	4.80712400	-0.78242200	-2.71052000
C	-4.25228800	-2.34359600	0.88984500
C	-5.08710500	0.08916600	-0.93012500
C	5.54130100	0.20156300	-2.02707500
C	5.07902200	0.67472700	-0.78586900
C	3.89236400	0.16733500	-0.23226300
C	1.43570900	-3.13866100	-1.00173000
C	0.48168500	-3.34971300	-2.02059500
F	-5.67817500	0.76161800	0.10283300
F	-5.87255300	-0.98750700	-1.21713700
F	-5.15010200	0.91323900	-2.01406200
F	-5.36396300	-1.73247800	1.39117100
F	-4.68483300	-3.32050800	0.03201400
F	-3.66377400	-2.99203800	1.93986300
H	-0.35411600	-4.73621900	-3.46813100
H	1.19407800	-6.61192800	-2.83056800
H	2.89391700	-6.25662800	-1.01304600
H	3.04671000	-4.06339500	0.14936000
H	4.25260200	-1.78189900	1.26249800
H	4.84062700	-2.62233400	3.51780800
H	3.04189800	-3.37694700	5.10484200
H	0.63194400	-3.26737100	4.38331000
H	0.03274900	-2.40149300	2.14137700
H	-0.24873700	0.33487700	2.50877000
H	0.69022400	0.19180400	4.81808200
H	2.70392800	1.55762700	5.45003200
H	3.75358700	3.08189700	3.75022500
H	2.78611100	3.27076500	1.46543400
H	-1.19516000	3.64460000	-1.61629000
H	-3.12282700	5.17782500	-1.28516900
H	-4.07900500	5.53475900	1.01350000
H	3.07568200	-2.09084700	-2.68870500
H	-3.06572500	4.34020800	2.97808000
H	-1.12677900	2.81742900	2.65860200
H	2.26858300	1.52900900	-2.11967700
H	3.73602900	3.07004300	-3.39830500
H	3.83549800	5.51181400	-2.80227200
H	2.43615300	6.38318300	-0.90281500
H	0.94076100	4.84672600	0.35760000
H	5.15562700	-1.15625200	-3.68638000
H	6.47134300	0.60151900	-2.46130900
H	5.64144600	1.45234700	-0.24531700
H	3.53709100	0.56012600	0.73264000
H	-0.21409700	-2.54237000	-2.29275200
O	0.50353400	0.20748500	-3.49667800
P	0.38015100	1.94967400	0.17232100
P	1.58632500	-1.48215300	-0.17778300
Ru	-0.36228500	-0.11745200	-0.62809400
S	-2.43985000	0.69507500	-1.30451300
S	-1.60305200	-1.70582600	0.46678600

Sum of electronic and zero-point Energies= -3827.793219
Sum of electronic and thermal Energies= -3827.743447
Sum of electronic and thermal Enthalpies= -3827.742503
Sum of electronic and thermal Free Energies= -3827.882394

$TS_{10\text{-}5}$

C	-0.63668700	0.20450700	-2.40562100
C	1.21059000	4.52897400	-2.61463100
C	0.81937400	5.78405300	-2.12333100
C	-0.01064100	5.85956400	-0.98868200
C	-0.44423500	4.68684700	-0.35311500
C	-0.30045400	2.42303800	1.77686800
C	-1.26519300	2.84807500	2.71638200
C	-0.87163700	3.30009100	3.99041900

C	0.48722100	3.34764500	4.33888700
C	1.45731000	2.95023800	3.40029600
C	1.06784600	2.49347600	2.13252000
C	-2.50893000	2.10762400	-0.14585200
C	-2.18175800	-1.61659400	1.55909500
C	-1.50905700	-1.09249100	2.68734900
C	-2.14938700	-1.03595500	3.93664400
C	-3.47340700	-1.49129100	4.07448800
C	-4.15016900	-2.01190000	2.95754700
C	-3.50932700	-2.07838500	1.70737100
C	-0.37030700	-3.29592000	0.07632600
C	0.54379200	-3.63663000	-0.94769200
C	1.24328900	-4.85224400	-0.90186600
C	1.05044300	-5.73906700	0.17369200
C	-3.03351600	2.80046600	-1.26260100
C	0.14643100	-5.40645600	1.19573700
C	-0.56653600	-4.19444500	1.14678700
C	-2.63543300	-2.12359900	-1.24851600
C	-3.48599600	-1.10661400	-1.73881800
C	-4.53164000	-1.41535400	-2.62362600
C	-4.74051400	-2.74203300	-3.03962000
C	-3.89883500	-3.75959000	-2.56030400
C	-2.85484700	-3.45557900	-1.66888700
C	3.52718300	-0.29281200	-0.83611700
C	3.24645500	-0.59205200	0.49163600
C	-4.42228900	2.89655600	-1.45862100
C	4.29893900	-0.86908500	1.56544400
C	4.92012700	-0.25535500	-1.45417700
C	-5.31132400	2.31297000	-0.53960900
C	-4.80098500	1.61172700	0.56722500
C	-3.41351300	1.49727700	0.75676300
C	-0.06017500	3.41589100	-0.84698500
C	0.77315200	3.35097400	-1.98008100
F	5.40124100	-1.51066000	-1.71731400
F	5.83496100	0.36508100	-0.65355600
F	4.93125700	0.41521600	-2.64176700
F	5.30860700	-1.66670200	1.12006500
F	4.86787300	0.28998500	2.02493500
F	3.76586200	-1.49224700	2.65370800
H	1.86685800	4.45646700	-3.49610300
H	1.16474400	6.70576400	-2.61815000
H	-0.31775700	6.84001500	-0.59096300
H	-1.08464800	4.76226800	0.53940000
H	-2.33361700	2.84757100	2.46053600
H	-1.64075900	3.62379600	4.70988000
H	0.79296400	3.70109800	5.33643200
H	2.52791100	2.99343900	3.65437400
H	1.83904800	2.19376300	1.40788500
H	-0.47561300	-0.72437100	2.59403900
H	-1.60881500	-0.62732100	4.80464700
H	-3.97701000	-1.44099500	5.05304300
H	-5.18633400	-2.37317800	3.05729000
H	-4.04851200	-2.48995800	0.84127800
H	0.71991400	-2.93551600	-1.77924600
H	1.95400200	-5.10128100	-1.70558000
H	1.61092500	-6.68639200	0.21670700
H	-2.35315900	3.27173900	-1.98696800
H	-0.00754700	-6.09258900	2.04380600
H	-1.27328100	-3.94932100	1.95304100
H	-3.33360100	-0.06278000	-1.43035800
H	-5.18067200	-0.60755000	-2.99610500
H	-5.55548400	-2.98123100	-3.74120700
H	-4.05066800	-4.80230900	-2.88181500
H	-2.20586400	-4.26363700	-1.30163800
H	-4.80868600	3.43946300	-2.33581900
H	-6.39939500	2.39927000	-0.68810700
H	-5.48549000	1.13778800	1.28807500
H	-3.03739800	0.91388400	1.60856700
H	1.10261700	2.37312900	-2.35994600
O	-1.11447400	0.36855100	-3.45933900
P	-1.28834100	-1.69521200	-0.05733000
P	-0.68315400	1.90198500	0.03758100
Ru	0.25055700	-0.05740700	-0.76545900
S	2.21863000	0.00207400	-1.94021800
S	1.61441100	-0.61397800	1.05541800

Sum of electronic and zero-point Energies= -3827.798456

Sum of electronic and thermal Energies= -3827.748716

Sum of electronic and thermal Enthalpies= -3827.747772

Sum of electronic and thermal Free Energies= -3827.886816

6'

C	0.67864700	0.09695600	-2.43767500
C	0.11697900	-4.78785200	-2.23555500
C	1.22432900	-5.65087900	-2.27849500
C	2.42409200	-5.27653500	-1.64585000
C	2.51682200	-4.04432900	-0.97893900
C	1.42546700	-2.14248100	1.75080500
C	1.58170400	-1.21056400	2.80254300
C	1.50345600	-1.62341000	4.14296000
C	1.24623900	-2.96883900	4.45608500
C	1.06676200	-3.89807500	3.41789100
C	1.15723300	-3.49178900	2.07569700
C	3.29643900	-1.14435000	-0.25519400
C	1.10242600	2.19171000	1.66465600
C	0.24139800	1.97151500	2.76793100
C	0.70163500	2.15349800	4.08103700
C	2.03418000	2.54102100	4.31815000
C	2.89781700	2.75270400	3.23053100
C	2.43548700	2.58760300	1.91121300
C	-1.02997300	3.13900400	0.05238400
C	-2.19332600	2.94332600	-0.71866700
C	-3.24108300	3.88114900	-0.68719600
C	-3.13991300	5.02858200	0.11571300
C	3.78386800	-1.10186800	-1.58503600
C	-1.97955600	5.23893200	0.88268500
C	-0.93208900	4.30465000	0.85248500
C	1.58204400	2.87321000	-1.12563700
C	2.86407100	2.32976400	-1.37348800
C	3.77663400	2.99813100	-2.20525500
C	3.41788400	4.21030900	-2.82058600
C	2.13950400	4.74736500	-2.59756300
C	1.22775300	4.08842300	-1.75406700
C	-3.43010800	-0.68828600	-0.85329200
C	-3.13857400	-0.82552000	0.49893700
C	5.12282200	-0.77173000	-1.84733100
C	-4.17946700	-1.08598800	1.58969100
C	-4.81153200	-0.85649200	-1.47674500
C	5.99922300	-0.46970500	-0.78839400
C	5.52560500	-0.50980900	0.53348900
C	4.18639000	-0.84908700	0.80100900
C	1.40839600	-3.16453500	-0.93800600
C	0.20826300	-3.55218800	-1.56989900
F	-4.87447300	-0.31093800	-2.72581500
F	-5.79770100	-0.25868400	-0.74727100
F	-5.15592600	-2.17495900	-1.61596700
F	-4.87335300	0.04946300	1.90787800
F	-5.09148100	-2.03238600	1.22918700
F	-3.60738700	-1.52421300	2.74647000
H	-0.82780700	-5.07067500	-2.72588000
H	1.15481400	-6.61595400	-2.80527600
H	3.29696600	-5.94830000	-1.67203100
H	3.46039400	-3.76705400	-0.48478400
H	1.75279200	-0.14853200	2.57885700
H	1.63228500	-0.87947700	4.94462600

H	1.17488700	-3.29040500	5.50720500
H	0.85042900	-4.95300500	3.64994100
H	1.00864500	-4.23388500	1.27895700
H	-0.79928300	1.65480800	2.59719900
H	0.01278600	1.98774500	4.92440900
H	2.39570800	2.68267300	5.34909900
H	3.94004600	3.06504100	3.40379500
H	3.11879700	2.78782400	1.07348800
H	-2.28367900	2.04365900	-1.34597900
H	-4.14454200	3.70255200	-1.29100400
H	-3.96456900	5.75832300	0.14763800
H	3.11631700	-1.34122500	-2.42628800
H	-1.88746000	6.13724100	1.51388400
H	-0.03048200	4.48911100	1.45516700
H	3.15188600	1.36728200	-0.92662200
H	4.77044600	2.55717400	-2.38027300
H	4.13053900	4.72965200	-3.48078300
H	1.84172200	5.68968500	-3.08432100
H	0.23218400	4.52510100	-1.59250800
H	5.48263400	-0.75433400	-2.88831700
H	7.05031900	-0.21204600	-0.99403000
H	6.20498800	-0.28754400	1.37182300
H	3.84388300	-0.89863300	1.84431600
H	-0.66271300	-2.87825100	-1.54822500
O	1.15306000	0.21943100	-3.49863600
P	0.40305200	1.96131000	-0.03522700
P	1.51136500	-1.56522200	-0.00168400
Ru	-0.19846600	-0.14269700	-0.78846900
S	-2.14423800	-0.37414400	-1.98072700
S	-1.51425900	-0.67788400	1.07153000

Sum of electronic and zero-point Energies= -3827.799587
Sum of electronic and thermal Energies= -3827.748934
Sum of electronic and thermal Enthalpies= -3827.747990
Sum of electronic and thermal Free Energies= -3827.891470

$TS_{6\text{-}6'}$

C	0.66582688	0.09157599	-2.43533162
C	0.06792438	-4.79171483	-2.22582353
C	1.17049246	-5.66059803	-2.27377565
C	2.37544331	-5.29210487	-1.64762805
C	2.47813078	-4.05983022	-0.98226811
C	1.40397369	-2.15091270	1.75183614
C	1.56318037	-1.21818798	2.80236275
C	1.48456304	-1.62913748	4.14327727
C	1.22427231	-2.97361384	4.45809189
C	1.04222215	-3.90367343	3.42109360
C	1.13294072	-3.49923707	2.07831226
C	3.27782276	-1.16584719	-0.25743651
C	1.13233257	2.19267877	1.66002320
C	0.27492334	1.98798782	2.76921873
C	0.74441087	2.17154640	4.07885667
C	2.08222598	2.54611816	4.30674106
C	2.94195771	2.74309561	3.21332198
C	2.47082132	2.57562059	1.89744478
C	-1.00499300	3.14738516	0.06226457
C	-2.18975944	2.94336914	-0.67289348
C	-3.23190242	3.88723898	-0.62988546
C	-3.10274621	5.04888907	0.14807830
C	3.76415036	-1.12719220	-1.58777754
C	-1.92077742	5.26723412	0.87932666
C	-0.87951810	4.32665119	0.83834799
C	1.59559835	2.85764427	-1.13902519
C	2.87725478	2.31176865	-1.38403396
C	3.78543902	2.96842890	-2.22978796
C	3.42257845	4.17048749	-2.86232571
C	2.14421700	4.70901047	-2.64283630
C	1.23686025	4.06205030	-1.78546160
C	-3.44342831	-0.68222699	-0.82362679
C	-3.15209466	-0.79235486	0.53009085
C	5.10495325	-0.80584084	-1.85149703
C	-4.17869790	-1.07033211	1.63294245
C	-4.79431138	-0.82170389	-1.51162277
C	5.98422246	-0.50872113	-0.79354751
C	5.51162018	-0.54488022	0.52883122
C	4.17053362	-0.87553906	0.79782020
C	1.37457112	-3.17415221	-0.93651683
C	0.16908283	-3.55598809	-1.56173973
F	-5.07001220	0.27806644	-2.28468580
F	-5.84928131	-0.97471310	-0.67400053
F	-4.80404927	-1.89951361	-2.35971928
F	-5.11310870	-0.07862449	1.72835179
F	-4.84011383	-2.24839456	1.43590340
F	-3.59628883	-1.16251768	2.86157927
H	-0.88086790	-5.06971236	-2.71112627
H	1.09321250	-6.62568181	-2.79946263
H	3.24462965	-5.96847240	-1.67771077
H	3.42564308	-3.78722267	-0.49312593
H	1.73628905	-0.15681719	2.57719418
H	1.61537086	-0.88452488	4.94400020
H	1.15254964	-3.29376314	5.50962048
H	0.82364927	-4.95784079	3.65453067
H	0.98218130	-4.24189671	1.28250644
H	-0.77004308	1.68162656	2.60592236
H	0.05839651	2.01767218	4.92679178
H	2.45088697	2.68934187	5.33494187
H	3.98826974	3.04563470	3.37919249
H	3.15181195	2.76462339	1.05532199
H	-2.30171969	2.03362426	-1.28180813
H	-4.15205526	3.70152047	-1.20554132
H	-3.92232900	5.78393966	0.18847456
H	3.09426621	-1.36272503	-2.42824714
H	-1.80709575	6.17662062	1.49084509
H	0.03883355	4.51609905	1.41381211
H	3.16815063	1.35615889	-0.92453971
H	4.77909454	2.52608155	-2.40219176
H	4.13189235	4.68048329	-3.53330281
H	1.84295420	5.64298182	-3.14333497
H	0.24102095	4.49935658	-1.62717415
H	5.46391327	-0.79137841	-2.89281843
H	7.03676172	-0.25795617	-1.00033288
H	6.19319312	-0.32636307	1.36636815
H	3.82856641	-0.92222440	1.84145488
H	-0.69827325	-2.87760804	-1.53632450
O	1.13728374	0.20858417	-3.49808061
P	0.41936080	1.96011390	-0.03420606
P	1.49073799	-1.57538881	-0.00113592
Ru	-0.20736676	-0.13930019	-0.78217790
S	-2.15704980	-0.37967366	-1.95977152
S	-1.52026178	-0.64286369	1.08909398

Sum of electronic and zero-point Energies= -3827.798655
Sum of electronic and thermal Energies= -3827.748923
Sum of electronic and thermal Enthalpies= -3827.747979
Sum of electronic and thermal Free Energies= -3827.888057

$TS_{6\text{-}10}$

C	0.74156947	0.05982620	-2.41569351
C	0.54649506	-4.73025248	-2.41623179
C	1.54480665	-5.67244461	-2.12343575
C	2.55070713	-5.35772523	-1.18885033
C	2.55580287	-4.10725622	-0.55392738

C	1.50568836	-2.10518931	1.78666654
C	2.09133196	-1.44340211	2.88845273
C	1.94220982	-1.94488365	4.19378394
C	1.18170442	-3.10041648	4.43063739
C	0.56162316	-3.74819759	3.34851672
C	0.72195164	-3.25826668	2.04348009
C	3.32551447	-0.98614679	-0.34293398
C	1.23888036	2.08667940	1.63640360
C	0.61204028	1.56040892	2.79120854
C	1.18441738	1.74521353	4.05965463
C	2.40613005	2.43078628	4.19352324
C	3.04497329	2.94059904	3.04989048
C	2.46146668	2.78086829	1.77912180
C	-1.13019073	2.96954420	0.32771658
C	-2.28135939	2.83863158	-0.47752012
C	-3.38685072	3.68624081	-0.29153929
C	-3.35936601	4.67631722	0.70487553
C	3.84249942	-1.31043588	-1.62263024
C	-2.21464630	4.82051169	1.50810871
C	-1.10638020	3.97742004	1.32199298
C	1.35741548	2.95869989	-1.12922867
C	2.61033451	2.49077868	-1.58982443
C	3.38848907	3.27178247	-2.45902465
C	2.92193533	4.52450995	-2.89572273
C	1.67414641	4.99243769	-2.45230475
C	0.89734512	4.21953984	-1.57110133
C	-3.40901926	-0.68985833	-0.93848222
C	-3.15161466	-0.84266384	0.41882753
C	5.11864016	-0.87855301	-2.01912836
C	-4.21394723	-1.14871107	1.47559398
C	-4.78356272	-0.77343554	-1.59138154
C	5.91386411	-0.11640228	-1.14593324
C	5.40834823	0.22620945	0.11898103
C	4.12504453	-0.19241761	0.51238758
C	1.55512877	-3.14954943	-0.84764749
C	0.55150000	-3.47329956	-1.78103408
F	-5.48992873	0.39489373	-1.45646813
F	-5.55856265	-1.76972852	-1.07643098
F	-4.69183667	-1.01180154	-2.93152683
F	-5.35168906	-0.41874878	1.29947793
F	-4.57132201	-2.46919583	1.47182228
F	-3.77252635	-0.87466927	2.73642815
H	-0.24649222	-4.96766377	-3.14275793
H	1.54155637	-6.65549115	-2.62075871
H	3.33588796	-6.09345046	-0.95218145
H	3.34426504	-3.87215545	0.17858739
H	2.66172575	-0.51732951	2.75644336
H	2.42316885	-1.41485030	5.03104835
H	1.06313097	-3.48922205	5.45436061
H	-0.05446060	-4.64549214	3.51677610
H	0.22939543	-3.78442819	1.21331645
H	-0.33842870	1.01045127	2.69773398
H	0.67334991	1.34223602	4.94805389
H	2.85678206	2.57184880	5.18890282
H	3.99760916	3.48610211	3.14484564
H	2.95576750	3.21522020	0.89796399
H	-2.31590354	2.05875374	-1.25353658
H	-4.27814272	3.55821904	-0.92520174
H	-4.23064328	5.33257417	0.85899638
H	3.24414266	-1.91307644	-2.32116950
H	-2.18078049	5.59477107	2.29118071
H	-0.21845815	4.11112303	1.95645031
H	2.98367371	1.50637583	-1.27152867
H	4.36159180	2.88940776	-2.80451308
H	3.52826711	5.13154766	-3.58664652
H	1.29521120	5.96899348	-2.79334918
H	-0.07546731	4.60267791	-1.23159525
H	5.49299865	-1.14830476	-3.01931696
H	6.91966760	0.21248279	-1.45166639
H	6.01265129	0.83239870	0.81234583
H	3.75646381	0.12843136	1.49325132
H	-0.23766553	-2.73914159	-2.01130705
O	1.24686969	0.15674299	-3.46456514
P	0.36036129	1.91075475	0.01805445
P	1.58517573	-1.51201883	0.03000489
Ru	-0.17799880	-0.17920250	-0.78944288
S	-2.10394978	-0.33153819	-2.02893890
S	-1.53195912	-0.77376275	1.02076271

Sum of electronic and zero-point Energies= -3827.797172

Sum of electronic and thermal Energies= -3827.747460

Sum of electronic and thermal Enthalpies= -3827.746516

Sum of electronic and thermal Free Energies= -3827.885900

$TS_{6\text{-}9}$

Ru	0.22198359	0.14889253	-0.75418717
S	2.18243727	0.10246948	-1.96263644
S	1.55261060	0.98847643	0.97109802
P	-0.43101661	-1.93501598	-0.00664464
P	-1.53367526	1.53715316	0.02543139
O	-1.06780934	-0.25593938	-3.48134390
C	-0.63360351	-0.13338454	-2.40213458
C	3.18902164	0.96225422	0.40259898
C	3.46765519	0.60169156	-0.91083436
C	4.22869419	1.42841303	1.42029157
C	4.85859238	0.56862028	-1.53655426
F	5.36718305	0.67787928	1.38613719
F	3.75847705	1.35435805	2.69888497
F	4.59401301	2.73118446	1.21983608
F	4.80173294	0.57808134	-2.89812416
F	5.55041591	-0.56262983	-1.18646864
F	5.62738713	1.63523220	-1.17572015
C	-1.44012494	3.14519027	-0.89496890
C	-0.23757910	3.54314467	-1.51756517
C	-0.15340698	4.77715690	-2.18704703
C	-1.26986026	5.62778009	-2.24255669
C	-2.47231133	5.24145000	-1.62228579
C	-2.55901887	4.00970675	-0.95379128
C	-1.45801605	2.07711513	1.78696474
C	-1.67283753	1.12683465	2.81172955
C	-1.60237867	1.50270387	4.16331034
C	-1.29543340	2.82940350	4.51256452
C	-1.06100865	3.77618066	3.50138183
C	-1.14410145	3.40640987	2.14788079
C	-3.31907582	1.11785437	-0.23111208
C	-4.26951463	1.07504707	0.81299026
C	-5.62247641	0.80243471	0.53735258
C	-6.04773071	0.58081248	-0.78282036
C	-5.10935287	0.62899468	-1.82968819
C	-3.75819980	0.89094378	-1.55720466
C	-0.66406282	-2.33669039	1.79426898
C	-1.48231361	-3.41680616	2.20643099
C	-1.52367300	-3.80818456	3.55483959
C	-0.73575438	-3.14466050	4.51195301
C	0.09414603	-2.08512439	4.10927279
C	0.12689308	-1.68171571	2.76288051
C	0.83115076	-3.25548117	-0.35102601
C	0.45387512	-4.60502643	-0.54342617
C	1.43156850	-5.60421128	-0.68263172
C	2.79671737	-5.27547750	-0.61227325
C	3.17901944	-3.94080588	-0.39649706
C	2.20291883	-2.93814458	-0.26706005
C	-1.96161683	-2.55266606	-0.81657194
C	-1.88980595	-3.11979095	-2.11108043
C	-3.05625314	-3.52956803	-2.77690418

C	-4.31237059	-3.37628108	-2.16422014
C	-4.39636128	-2.79223648	-0.88875505
C	-3.23181479	-2.37504069	-0.22255970
H	0.64168559	2.88043984	-1.48313386
H	0.79247732	5.06878794	-2.67001265
H	-1.20563179	6.59212308	-2.77134819
H	-3.35258329	5.90283457	-1.66149268
H	-3.50660051	3.71893844	-0.47527754
H	-1.89089006	0.07919754	2.55753573
H	-1.77734249	0.74743324	4.94564432
H	-1.23082684	3.12269853	5.57235703
H	-0.80788460	4.81553019	3.76416902
H	-0.95653112	4.15945575	1.36915031
H	-3.96343006	1.27483137	1.84995875
H	-6.34927268	0.77938368	1.36523692
H	-7.10901870	0.37773553	-0.99762125
H	-5.42937440	0.46230338	-2.87019874
H	-3.04550826	0.93676036	-2.39310266
H	-2.08661754	-3.96964749	1.47273853
H	-2.17130841	-4.64730866	3.85549910
H	-0.76482365	-3.45833223	5.56762963
H	0.72520641	-1.56150259	4.84458427
H	0.78175941	-0.84882205	2.46232191
H	-0.60878826	-4.88590649	-0.58770524
H	1.12058481	-6.64851099	-0.84595899
H	3.56169488	-6.06035053	-0.72312415
H	4.24418306	-3.66919742	-0.33333621
H	2.51426834	-1.89713539	-0.10046593
H	-0.91419667	-3.24523778	-2.60481972
H	-2.97957165	-3.97245912	-3.78242165
H	-5.22593418	-3.70472899	-2.68476428
H	-5.37565380	-2.65156404	-0.40572277
H	-3.31931454	-1.90872464	0.76972185

Sum of electronic and zero-point Energies= -3827.797369
Sum of electronic and thermal Energies= -3827.747787
Sum of electronic and thermal Enthalpies= -3827.746843
Sum of electronic and thermal Free Energies= -3827.885160

9

Ru	-0.23144200	-0.15954000	-0.76506400
S	-2.24579100	0.01000800	-1.88267200
S	-1.45955200	-1.32653100	0.82878900
P	0.28115500	1.93658500	0.03976600
P	1.65076900	-1.43685300	-0.05093700
O	0.97133400	0.37902100	-3.50429000
C	0.56902400	0.22384600	-2.41510900
C	-3.12507300	-1.24734500	0.35098300
C	-3.46783500	-0.68160100	-0.87143500
C	-4.10426800	-1.90536700	1.31830700
C	-4.88751700	-0.58030300	-1.42281300
F	-5.26081600	-1.19515300	1.45727800
F	-3.57649000	-2.02845600	2.57111500
F	-4.45016800	-3.16916800	0.92261800
F	-4.89500800	-0.35540000	-2.76675500
F	-5.58266500	0.45565000	-0.85344600
F	-5.61676700	-1.71329200	-1.21731600
C	1.73222600	-2.97660300	-1.08241500
C	0.58493600	-3.43621800	-1.76507300
C	0.63139200	-4.61698600	-2.52754300
C	1.82485100	-5.35231700	-2.61788800
C	2.97319400	-4.90338700	-1.94014700
C	2.92966700	-3.72418200	-1.17898800
C	1.57341800	-2.09511600	1.66856600
C	1.69694600	-1.19618300	2.75319700
C	1.61994900	-1.65751300	4.07726900
C	1.39807800	-3.02167200	4.33752900
C	1.25723200	-3.91920300	3.26612100
C	1.34711200	-3.46222700	1.93956000
C	3.39938100	-0.84900000	-0.20288300
C	4.34516700	-0.95656100	0.84123100
C	5.68571000	-0.58375500	0.63256200
C	6.10270600	-0.10815400	-0.62107800
C	5.16818300	0.00023900	-1.66668600
C	3.82852300	-0.36224200	-1.45979600
C	0.15752300	2.30676700	1.85621200
C	0.55484000	3.58649300	2.31936300
C	0.38443400	3.94279200	3.66522000
C	-0.20351000	3.03764900	4.56911100
C	-0.61828400	1.77635000	4.11471100
C	-0.43674300	1.41197800	2.76687100
C	-0.88747900	3.26320200	-0.53840100
C	-0.47051400	4.52240500	-1.02337700
C	-1.41835500	5.51077900	-1.34817700
C	-2.78944900	5.26336000	-1.17658200
C	-3.21184500	4.02095700	-0.66947900
C	-2.26965800	3.03082300	-0.35347700
C	1.94735200	2.57117100	-0.41977700
C	2.20337700	2.95925600	-1.75717500
C	3.47014200	3.43340100	-2.13474800
C	4.50810900	3.51006000	-1.18949100
C	4.27465700	3.09431000	0.13199800
C	3.00583300	2.62744100	0.51475200
H	-0.35475700	-2.86493600	-1.70139500
H	-0.27307800	-4.95778500	-3.05557600
H	1.86287100	-6.27462100	-3.21923700
H	3.91356900	-5.47349700	-2.00734500
H	3.83711600	-3.38194600	-0.65872700
H	1.85447500	-0.12333400	2.56495700
H	1.72417600	-0.94273600	4.90882700
H	1.32823900	-3.38296500	5.37576800
H	1.07268600	-4.98768700	3.45994100
H	1.23453900	-4.17635900	1.11096800
H	4.04450400	-1.35089400	1.82249300
H	6.40935600	-0.68022100	1.45790700
H	7.15467700	0.17445800	-0.78579600
H	5.48263400	0.36888000	-2.65555200
H	3.11860500	-0.28157200	-2.29516200
H	0.99107000	4.31771500	1.62193700
H	0.70295400	4.94026800	4.00780600
H	-0.34529300	3.32281900	5.62377400
H	-1.09333600	1.06318800	4.80662800
H	-0.77867000	0.42546100	2.41814300
H	0.59811700	4.74768700	-1.14896800
H	-1.07450300	6.48277300	-1.73670900
H	-3.52958000	6.03757300	-1.43386500
H	-4.28347600	3.81492800	-0.52247400
H	-2.61567500	2.06496900	0.04355400
H	1.40628800	2.90297000	-2.51319500
H	3.64389000	3.74477300	-3.17698200
H	5.50043400	3.88565500	-1.48525800
H	5.08515200	3.13326600	0.87643600
H	2.83905600	2.31547500	1.55631600

Sum of electronic and zero-point Energies= -3827.797865
Sum of electronic and thermal Energies= -3827.747351
Sum of electronic and thermal Enthalpies= -3827.746407
Sum of electronic and thermal Free Energies= -3827.888182

7'

C	-0.68261600	0.09690400	-2.43810900
C	3.35252100	3.77998900	-0.57681400

C	3.24630200	4.94293000	0.20256100
C	2.06050200	5.19462200	0.91684500
C	0.99259300	4.28548800	0.85804300
C	-1.07952400	2.20078400	1.65331400
C	-2.40966500	2.61466300	1.88523100
C	-2.88322500	2.78923700	3.19938100
C	-2.03373300	2.56885700	4.29632200
C	-0.70418400	2.16278700	4.07381600
C	-0.23297100	1.97136600	2.76594800
C	-1.50457200	2.89933000	-1.14342800
C	-1.45728200	-2.12799000	1.75116600
C	-1.58848200	-1.19959100	2.80947600
C	-1.50354500	-1.62100100	4.14679700
C	-1.26448700	-2.97201000	4.45013000
C	-1.10995000	-3.89821100	3.40521300
C	-1.20722800	-3.48316400	2.06617500
C	-1.48897900	-3.13590800	-0.94273100
C	-0.30572400	-3.54449000	-1.59299900
C	-0.24929100	-4.77748500	-2.26745300
C	-1.37495500	-5.61689100	-2.30066900
C	-1.11021200	4.10087000	-1.77423200
C	-2.55807000	-5.22167400	-1.64957300
C	-2.61606100	-3.99205000	-0.97409600
C	-3.32292800	-1.07527400	-0.23446900
C	-4.19711200	-0.76107800	0.82934100
C	-5.52978800	-0.38877600	0.57322900
C	-6.01275700	-0.33378100	-0.74467900
C	-5.15235000	-0.65434400	-1.81122800
C	-3.81970600	-1.01743500	-1.56032200
C	3.12827400	-0.85633100	0.49524400
C	3.41247300	-0.76552200	-0.86219500
C	-1.99440400	4.77986300	-2.63110800
C	4.79455500	-0.91089600	-1.48787600
C	4.16467700	-1.15428300	1.58066700
C	-3.28450900	4.27673800	-2.86548300
C	-3.68265900	3.07764400	-2.24869400
C	-2.79779400	2.38907100	-1.40372400
C	1.09426500	3.10523700	0.07971900
C	2.28306300	2.86821600	-0.63827500
F	3.71144800	-0.82105500	2.82300700
F	5.32504900	-0.46223200	1.39725100
F	4.48391900	-2.48258500	1.62995800
F	5.52913000	0.24320100	-1.38616600
F	5.53417600	-1.90614500	-0.92132800
F	4.71802500	-1.19934500	-2.81901700
H	4.27567800	3.56757900	-1.13810800
H	4.08686600	5.65290100	0.25761000
H	1.96489100	6.10542100	1.52934800
H	0.07221900	4.50041400	1.42121900
H	-3.08174000	2.82248500	1.04035700
H	-3.92287800	3.11599000	3.36109300
H	-2.40385700	2.71808100	5.32314600
H	-0.02621300	1.98999000	4.92457900
H	0.80487800	1.63955000	2.60684900
H	-1.74476700	-0.13368600	2.59367400
H	-1.61266400	-0.87958900	4.95373600
H	-1.18784200	-3.30048200	5.49873900
H	-0.90807300	-4.95768700	3.62943000
H	-1.07827100	-4.22310100	1.26400200
H	0.57972400	-2.88936500	-1.57846400
H	0.68261700	-5.07688600	-2.77236600
H	-1.33274200	-6.57982000	-2.83422500
H	-0.10473900	4.51092100	-1.60419000
H	-3.44505900	-5.87494600	-1.66808600
H	-3.54705300	-3.69809100	-0.46584600
H	-3.84799500	-0.82164200	1.86982800
H	-6.19688200	-0.15226700	1.41750900
H	-7.05887800	-0.05019100	-0.94133500
H	-5.51992200	-0.62592400	-2.84926700
H	-3.16481200	-1.27078600	-2.40745800
H	-1.66562500	5.71099800	-3.11943200
H	-3.97551900	4.81188200	-3.53596400
H	-4.68594400	2.66272300	-2.43321200
H	-3.11579900	1.43575700	-0.95749900
H	2.37522000	1.95750300	-1.24884600
O	-1.15779700	0.22263300	-3.49838500
P	-1.54633000	-1.53993300	0.00263600
P	-0.36211100	1.96001300	-0.03806500
Ru	0.19369000	-0.15507800	-0.79078600
S	1.50422700	-0.70439600	1.06895700
S	2.13410200	-0.41132800	-1.98644600

Sum of electronic and zero-point Energies= -3827.799842

Sum of electronic and thermal Energies= -3827.749223

Sum of electronic and thermal Enthalpies= -3827.748279

Sum of electronic and thermal Free Energies= -3827.891116

$TS_{7\text{-}7'}$

C	-0.66581870	0.09148582	-2.43539629
C	3.23193866	3.88715442	-0.62998636
C	3.10293826	5.04867118	0.14820378
C	1.92106602	5.26695022	0.87962645
C	0.87975240	4.32642713	0.83860429
C	-1.13244119	2.19257911	1.65992015
C	-2.47103001	2.57526465	1.89719947
C	-2.94233708	2.74265426	3.21302606
C	-2.08268132	2.54584052	4.30653535
C	-0.74477552	2.17150618	4.07879302
C	-0.27511350	1.98803209	2.76920536
C	-1.59550495	2.85777679	-1.13905379
C	-1.40398280	-2.15087738	1.75183384
C	-1.56331196	-1.21815535	2.80234607
C	-1.48469218	-1.62908344	4.14326722
C	-1.22427290	-2.97352969	4.45810432
C	-1.04210187	-3.90358289	3.42112201
C	-1.13282570	-3.49917106	2.07833370
C	-1.37452374	-3.17417596	-0.93648807
C	-0.16897852	-3.55606146	-1.56157138
C	-0.06777482	-4.79181731	-2.22559341
C	-1.17035432	-5.66068211	-2.27362280
C	-1.23692803	4.06252521	-1.78494087
C	-2.37536024	-5.29214217	-1.64760933
C	-2.47809248	-4.05983902	-0.98230864
C	-3.27782171	-1.16587629	-0.25749269
C	-4.17055253	-0.87550929	0.79773022
C	-5.51163368	-0.54486391	0.52869892
C	-5.98421193	-0.50877114	-0.79368971
C	-5.10492406	-0.80594933	-1.85160715
C	-3.76412640	-1.12729031	-1.58784522
C	3.15207471	-0.79224625	0.53011479
C	3.44342132	-0.68220045	-0.82360801
C	-2.14429104	4.70962478	-2.64220379
C	4.79430521	-0.82174671	-1.51158625
C	4.17867516	-1.07014341	1.63299009
C	-3.42249718	4.17090425	-2.86211822
C	-3.78519968	2.96851930	-2.23011116
C	-2.87700644	2.31172640	-1.38446979
C	1.00507917	3.14728470	0.06230756
C	2.18974221	2.94334773	-0.67304020
F	3.59625344	-1.16232195	2.86162123
F	5.11303734	-0.07838847	1.72838635
F	4.84014816	-2.24818046	1.43599001
F	5.06998234	0.27792068	-2.28480401
F	5.84928030	-0.97461720	-0.67394443
F	4.80406432	-1.89967536	-2.35953224

H	4.15201076	3.70149348	-1.20578961
H	3.92256556	5.78367005	0.18863541
H	1.80750111	6.17623675	1.49131537
H	-0.03852458	4.51582468	1.41420452
H	-3.15196588	2.76412293	1.05499729
H	-3.98872293	3.04499804	3.37878713
H	-2.45147438	2.68900264	5.33469739
H	-0.05882550	2.01775246	4.92680222
H	0.76992312	1.68185199	2.60602207
H	-1.73652474	-0.15680283	2.57716357
H	-1.61560077	-0.88447613	4.94397852
H	-1.15254624	-3.29365941	5.50963852
H	-0.82343139	-4.95772599	3.65457669
H	-0.98197646	-4.24182562	1.28254068
H	0.69838674	-2.87769531	-1.53610167
H	0.88106176	-5.06985204	-2.71078839
H	-1.09303951	-6.62578801	-2.79926427
H	-0.24121473	4.49999449	-1.62631057
H	-3.24455508	-5.96849626	-1.67774938
H	-3.42564626	-3.78720191	-0.49326380
H	-3.82860736	-0.92214099	1.84137417
H	-6.19322128	-0.32630248	1.36621251
H	-7.03674632	-0.25801282	-1.00050758
H	-5.46386591	-0.79154473	-2.89293565
H	-3.09422776	-1.36287327	-2.42828947
H	-1.84315572	5.64386348	-3.14228010
H	-4.13181181	4.68100846	-3.53301198
H	-4.77873258	2.52602558	-2.40284640
H	-3.16776838	1.35588381	-0.92537503
H	2.30157716	2.03371445	-1.28214435
O	-1.13726894	0.20844085	-3.49815440
P	-1.49073505	-1.57538990	-0.00115095
P	-0.41934111	1.96010735	-0.03426500
Ru	0.20736346	-0.13931169	-0.78222666
S	1.52023797	-0.64272745	1.08910267
S	2.15705005	-0.37974843	-1.95979079

Sum of electronic and zero-point Energies= -3827.798655
Sum of electronic and thermal Energies= -3827.748923
Sum of electronic and thermal Enthalpies= -3827.747979
Sum of electronic and thermal Free Energies= -3827.888060

8'

Ru	0.43132100	0.03280400	-0.50464900
S	2.09146500	-1.51707000	-0.10916500
S	2.14043100	1.58214300	-0.32207700
P	-1.05513900	-1.82906300	-0.10962000
P	-1.03373600	1.82529400	0.05929400
O	0.04722700	0.12155900	-3.46457200
C	0.11952200	0.09241800	-2.28986500
C	3.63272000	0.70063800	-0.19868800
C	3.61443500	-0.67865100	-0.09998900
C	4.88600900	1.56813300	-0.14706600
C	4.84182900	-1.57720100	-0.01065200
F	5.36014000	1.70543300	1.13105800
F	4.65126800	2.83163000	-0.60400400
F	5.90401600	1.06614800	-0.90237500
F	5.43163000	-1.76208400	-1.23247300
F	4.52573900	-2.82012000	0.45604700
F	5.79903800	-1.08420800	0.82643600
C	-0.36255600	3.52710600	-0.22008400
C	0.13432100	3.82889300	-1.50880900
C	0.57372200	5.12611000	-1.81626100
C	0.52537000	6.13841600	-0.84200000
C	0.02775600	5.84745200	0.43942100
C	-0.41828900	4.55088700	0.75008600
C	-1.32437200	1.73585900	1.87409500
C	-2.55636600	1.33931800	2.44108900
C	-2.68563700	1.20044000	3.83518500
C	-1.59215100	1.45325900	4.68006700
C	-0.35665500	1.83371200	4.12288800
C	-0.21881900	1.96340700	2.73192300
C	-2.67965900	2.11993700	-0.73198800
C	-3.64536400	2.95839600	-0.12634800
C	-4.81907200	3.30596900	-0.81361100
C	-5.03412200	2.84833700	-2.12652800
C	-4.06746700	2.03990900	-2.74612700
C	-2.90126600	1.67330100	-2.05101200
C	-2.87325900	-1.60029500	0.14736000
C	-3.49219400	-1.78590800	1.40310500
C	-4.88344300	-1.62824300	1.54292500
C	-5.67440500	-1.28692000	0.43328600
C	-5.06685200	-1.10642400	-0.82265600
C	-3.67919400	-1.26096000	-0.96389500
C	-0.55779200	-2.73365400	1.42385900
C	-0.43693900	-4.13841200	1.47736400
C	-0.05453300	-4.77340800	2.67280800
C	0.20065700	-4.01670500	3.82805300
C	0.08139300	-2.61572500	3.78289300
C	-0.28396500	-1.97707800	2.58742700
C	-1.06124300	-3.14498300	-1.41320000
C	0.00646100	-3.25347200	-2.33036800
C	0.01928000	-4.27581000	-3.29556800
C	-1.03313300	-5.20365600	-3.35909000
C	-2.10070400	-5.10742200	-2.44837600
C	-2.11651600	-4.08740100	-1.48314100
H	0.18271800	3.04489900	-2.28014200
H	0.96477500	5.34288700	-2.82269400
H	0.87757200	7.15421600	-1.08154800
H	-0.01591200	6.63515500	1.20843400
H	-0.81027800	4.34264600	1.75666400
H	-3.42118000	1.12696300	1.79658500
H	-3.65347600	0.89055100	4.26037000
H	-1.69888600	1.34841600	5.77140700
H	0.51083200	2.02510600	4.77410400
H	0.75986000	2.23442400	2.30427800
H	-3.47518100	3.36285800	0.88278700
H	-5.56373200	3.95414600	-0.32463100
H	-5.94965600	3.13352800	-2.66879500
H	-4.21590900	1.69026000	-3.78015700
H	-2.15016200	1.04638100	-2.55123400
H	-2.88924200	-2.06789600	2.27835600
H	-5.35039500	-1.78554500	2.52843400
H	-6.76409400	-1.16886000	0.54326900
H	-5.67697700	-0.84360600	-1.70084100
H	-3.22098000	-1.14078900	-1.95690800
H	-0.62677000	-4.74502600	0.57999700
H	0.05024300	-5.86979300	2.69474400
H	0.50364100	-4.51648800	4.76180500
H	0.28951000	-2.01131100	4.67963900
H	-0.34557400	-0.87766900	2.55848000
H	0.84035700	-2.53847800	-2.28742700
H	0.86057200	-4.34029800	-4.00328000
H	-1.02404100	-6.00139800	-4.11882200
H	-2.93106600	-5.83039200	-2.48940600
H	-2.96123900	-4.02396400	-0.78081600

Sum of electronic and zero-point Energies= -3827.799682
Sum of electronic and thermal Energies= -3827.749041
Sum of electronic and thermal Enthalpies= -3827.748097
Sum of electronic and thermal Free Energies= -3827.889974

$TS_{8\text{-}8'}$

Ru	0.43409906	0.04221202	-0.50213349
S	2.10402295	-1.48607660	-0.08287195
S	2.13545388	1.60371961	-0.33307509
P	-1.04034019	-1.83284195	-0.11451912
P	-1.04019308	1.82191553	0.06468013
O	0.04340560	0.13291226	-3.46114338
C	0.11853838	0.10462301	-2.28661352
C	3.63867446	0.73775364	-0.19511066
C	3.62797037	-0.64162120	-0.10556615
C	4.88033625	1.62668267	-0.16350390
C	4.81337466	-1.59014494	0.00311549
F	5.61490505	1.44996657	0.97599872
F	4.55679073	2.95154688	-0.20194222
F	5.70884259	1.40448166	-1.22612782
F	4.80319873	-2.51083981	-1.01267381
F	4.76531153	-2.30605163	1.17169160
F	6.02679344	-0.98652231	-0.03595234
C	-0.38342339	3.52931695	-0.21432535
C	0.10821154	3.83663684	-1.50373881
C	0.53586245	5.13790186	-1.81071196
C	0.48070007	6.14877219	-0.83532659
C	-0.01180377	5.85222073	0.44679629
C	-0.44602583	4.55156811	0.75703568
C	-1.32253049	1.72516556	1.88013596
C	-2.54797672	1.31390864	2.45091313
C	-2.66994715	1.16956834	3.84507993
C	-1.57554499	1.43121955	4.68612755
C	-0.34639154	1.82612076	4.12501951
C	-0.21575196	1.96166530	2.73392018
C	-2.69099470	2.10557979	-0.72015883
C	-3.66283633	2.93121228	-0.10680601
C	-4.84125676	3.27260633	-0.78911328
C	-5.05516232	2.82175562	-2.10453428
C	-4.08262290	2.02626777	-2.73164320
C	-2.91157386	1.66560554	-2.04163275
C	-2.86051565	-1.61885507	0.13980159
C	-3.47961068	-1.81333623	1.39416975
C	-4.87187658	-1.66450157	1.53332910
C	-5.66385426	-1.32364258	0.42425312
C	-5.05619518	-1.13448610	-0.83033695
C	-3.66743730	-1.27975818	-0.97082150
C	-0.53960766	-2.74227598	1.41477880
C	-0.41476327	-4.14697578	1.46101345
C	-0.03195479	-4.78712873	2.65352393
C	0.21981658	-4.03563180	3.81293268
C	0.09658810	-2.63483177	3.77500190
C	-0.26937457	-1.99093518	2.58253747
C	-1.03012609	-3.14109273	-1.42552497
C	0.05051161	-3.24339540	-2.32835767
C	0.07813875	-4.26084580	-3.29832512
C	-0.97207469	-5.18969862	-3.38129833
C	-2.05214197	-5.09974223	-2.48485310
C	-2.08268875	-4.08488032	-1.51446058
H	0.16160582	3.05392233	-2.27607040
H	0.92292050	5.35911601	-2.81773366
H	0.82358202	7.16783062	-1.07454697
H	-0.06073752	6.63876127	1.21668097
H	-0.83422549	4.33892563	1.76417111
H	-3.41310057	1.09418051	1.80929382
H	-3.63266293	0.84826855	4.27340219
H	-1.67656513	1.32190160	5.77757022
H	0.52178655	2.02425868	4.77328147
H	0.75813045	2.24427469	2.30281833
H	-3.49397769	3.33062689	0.90454307
H	-5.59065032	3.91068326	-0.29412623
H	-5.97450925	3.10215325	-2.64282924
H	-4.23030024	1.68207608	-3.76760999
H	-2.15611367	1.04879639	-2.54783828
H	-2.87572544	-2.09532826	2.26879490
H	-5.33881439	-1.82852979	2.51775124
H	-6.75434453	-1.21263203	0.53362659
H	-5.66708346	-0.87189526	-1.70805996
H	-3.20900148	-1.15244323	-1.96285686
H	-0.60199424	-4.74926491	0.56017378
H	0.07605916	-5.88329142	2.66987671
H	0.52350381	-4.53935105	4.74433363
H	0.30240288	-2.03457948	4.67504590
H	-0.33414113	-0.89160580	2.55924170
H	0.88328469	-2.52814821	-2.26957291
H	0.92956639	-4.32079603	-3.99419067
H	-0.95133180	-5.98353045	-4.14489503
H	-2.88067798	-5.82381169	-2.54084525
H	-2.93665120	-4.02704695	-0.82295108

Sum of electronic and zero-point Energies= -3827.798535

Sum of electronic and thermal Energies= -3827.748781

Sum of electronic and thermal Enthalpies= -3827.747837

Sum of electronic and thermal Free Energies= -3827.887046

$TS_{8\text{-}7}$

Ru	0.24054900	-0.07449200	-0.66770400
S	1.49630900	-1.73082500	0.32245600
S	2.31210200	0.84336700	-1.23410300
P	-1.57617600	-1.56703700	-0.16241900
P	-0.40802100	1.99523100	0.15504800
O	-0.82349100	0.34665000	-3.45547400
C	-0.46361300	0.24331900	-2.34149600
C	3.53059600	-0.22601000	-0.63072500
C	3.18132700	-1.38180300	0.04880000
C	4.96498500	0.20469600	-0.93915300
C	4.15503700	-2.37911200	0.66075800
F	5.79623500	0.05515900	0.13293400
F	5.03708800	1.51701200	-1.30075900
F	5.49994700	-0.51174600	-1.97238000
F	3.56184600	-3.58315400	0.90358600
F	4.64749700	-1.94411200	1.86580100
F	5.23016200	-2.63309900	-0.13898200
C	0.56884800	3.43849000	-0.47411700
C	0.60582400	3.64398900	-1.87217100
C	1.26235400	4.76117900	-2.41058600
C	1.89135000	5.68952800	-1.56180600
C	1.85233100	5.49578200	-0.17127600
C	1.19136000	4.38000400	0.37300400
C	-0.09007800	1.97021300	1.96691400
C	-1.12694500	2.02412700	2.92598900
C	-0.83165300	1.92692900	4.29829500
C	0.49727600	1.77356500	4.72854600
C	1.53402100	1.70463700	3.77867300
C	1.24399700	1.79226900	2.40868800
C	-2.07694300	2.75825300	-0.04924300
C	-2.41619000	3.92570000	0.67857400
C	-3.62115600	4.59694800	0.42427300
C	-4.49458500	4.12884300	-0.57551000
C	-4.15456400	2.98598700	-1.31552000
C	-2.95311200	2.30328600	-1.05212500
C	-3.33515200	-0.99178000	-0.14962900
C	-4.00295300	-0.66721900	1.05094900
C	-5.33769800	-0.22496700	1.02873300
C	-6.02688600	-0.10877500	-0.18981200
C	-5.36858200	-0.42634000	-1.39160200
C	-4.03199800	-0.85647100	-1.37409300
C	-1.42071400	-2.43001700	1.46716300
C	-1.61787900	-3.81922500	1.62540700
C	-1.50268800	-4.41462500	2.89357700

C	-1.19365300	-3.63381500	4.01989800
C	-0.98514400	-2.25191600	3.87002700
C	-1.08577000	-1.65627900	2.60204400
C	-1.67878800	-2.95801700	-1.38363100
C	-0.59507600	-3.23396100	-2.24501800
C	-0.65495400	-4.30702900	-3.15226500
C	-1.79739900	-5.12114500	-3.21103800
C	-2.88442700	-4.85691900	-2.35777400
C	-2.82814500	-3.78421600	-1.45347000
H	0.12086400	2.92533200	-2.55101200
H	1.28758100	4.90234200	-3.50259200
H	2.41326200	6.56211500	-1.98531700
H	2.34150500	6.21755800	0.50219400
H	1.16943700	4.24680900	1.46470700
H	-2.17278500	2.13731100	2.60373000
H	-1.65035000	1.97227000	5.03414300
H	0.72670100	1.70066700	5.80348100
H	2.57728000	1.57070300	4.10489800
H	2.05862400	1.70955300	1.67153100
H	-1.72601500	4.32741900	1.43609000
H	-3.87276800	5.50155800	1.00058000
H	-5.43564000	4.66329600	-0.78137100
H	-4.82502600	2.61661200	-2.10666000
H	-2.69199500	1.41486800	-1.64165700
H	-3.48657300	-0.77933500	2.01618200
H	-5.84508500	0.01682100	1.97624300
H	-7.07650300	0.22493300	-0.20368000
H	-5.90029500	-0.34429200	-2.35318500
H	-3.53324300	-1.10731000	-2.32328200
H	-1.84604000	-4.45034700	0.75486400
H	-1.64791400	-5.50177200	2.99647500
H	-1.10036700	-4.10437500	5.01156400
H	-0.72328400	-1.63038800	4.74057700
H	-0.88323500	-0.58058200	2.49270800
H	0.30585700	-2.60414500	-2.20308300
H	0.20076000	-4.50177100	-3.81761600
H	-1.84470300	-5.96017600	-3.92338900
H	-3.78627900	-5.48853800	-2.39771100
H	-3.69198500	-3.58546000	-0.80103300

Sum of electronic and zero-point Energies= -3827.797836

Sum of electronic and thermal Energies= -3827.748135

Sum of electronic and thermal Enthalpies= -3827.747191

Sum of electronic and thermal Free Energies= -3827.885592

9'

Ru	-0.23025400	-0.16380300	-0.76644500
S	-2.24236600	0.00500600	-1.88813400
S	-1.46374500	-1.31849400	0.83175000
P	0.28599700	1.93323100	0.03288700
P	1.64950200	-1.43734100	-0.04358600
O	0.97440600	0.35782100	-3.50903400
C	0.57233000	0.20838600	-2.41905800
C	-3.12591500	-1.25669400	0.34064400
C	-3.46984300	-0.66784100	-0.87097500
C	-4.11203500	-1.85661600	1.33773300
C	-4.88545400	-0.61257100	-1.44206700
F	-4.73350300	-0.88769000	2.08284900
F	-3.49492300	-2.68663800	2.22701300
F	-5.09175700	-2.59253300	0.74135800
F	-5.28232000	-1.81996700	-1.94750600
F	-4.98905600	0.28369200	-2.46352200
F	-5.81024900	-0.24079900	-0.50837200
C	1.73088700	-2.98302600	-1.06623300
C	0.58640400	-3.44177900	-1.75400800
C	0.63332500	-4.62676100	-2.50996200
C	1.82445500	-5.36718600	-2.58832600
C	2.97005800	-4.91909000	-1.90532500
C	2.92606200	-3.73567000	-1.15084100
C	1.57214800	-2.08648700	1.67944900
C	1.70594400	-1.18402700	2.75994100
C	1.62879200	-1.63909100	4.08620800
C	1.39647800	-3.00024600	4.35293700
C	1.24505800	-3.90105000	3.28573500
C	1.33505800	-3.45047000	1.95703400
C	3.39849900	-0.85092500	-0.19994600
C	4.34529700	-0.95191200	0.84392800
C	5.68549500	-0.57963600	0.63200100
C	6.10132000	-0.11120900	-0.62471600
C	5.16596600	-0.00985200	-1.67027300
C	3.82669300	-0.37184100	-1.46014900
C	0.17624300	2.30919400	1.84895800
C	0.57973300	3.58910700	2.30623700
C	0.41650700	3.95011200	3.65173400
C	-0.17058200	3.04981500	4.56101600
C	-0.59185700	1.78861600	4.11238800
C	-0.41728000	1.41946300	2.76496300
C	-0.89355500	3.25364600	-0.53655800
C	-0.48870600	4.51009900	-1.03814400
C	-1.44511600	5.49289900	-1.35484100
C	-2.81226900	5.24260400	-1.15823900
C	-3.22208000	4.00287900	-0.63438700
C	-2.27175100	3.01802200	-0.32685800
C	1.94620000	2.57096000	-0.44331600
C	2.18953900	2.95450800	-1.78439700
C	3.45208600	3.42925400	-2.17520100
C	4.49836800	3.51129500	-1.23962300
C	4.27749900	3.10019000	0.08548400
C	3.01304900	2.63245700	0.48139000
H	-0.35133300	-2.86624800	-1.69991200
H	-0.26889600	-4.96677700	-3.04234600
H	1.86290400	-6.29284300	-3.18447600
H	3.90862200	-5.49319500	-1.96327300
H	3.83136800	-3.39397000	-0.62645400
H	1.87181500	-0.11334500	2.56684600
H	1.74136300	-0.92164700	4.91437900
H	1.32674100	-3.35656600	5.39290200
H	1.05200700	-4.96709900	3.48455100
H	1.21404700	-4.16721000	1.13191300
H	4.04588800	-1.34078700	1.82772600
H	6.40980500	-0.67090500	1.45735900
H	7.15298800	0.17110100	-0.79186700
H	5.47940800	0.35288600	-2.66163500
H	3.11631300	-0.29664700	-2.29556500
H	1.01477900	4.31686900	1.60446900
H	0.73973700	4.94761500	3.98981400
H	-0.30685500	3.33878600	5.61536600
H	-1.06666700	1.07950800	4.80861700
H	-0.76435500	0.43333700	2.42048400
H	0.57700400	4.73782600	-1.18268700
H	-1.11105300	6.46295600	-1.75652300
H	-3.55912900	6.01251100	-1.40883400
H	-4.29069300	3.79597000	-0.46741500
H	-2.60706300	2.05399300	0.08385500
H	1.38595900	2.89350300	-2.53313100
H	3.61596200	3.73676400	-3.22017400
H	5.48735500	3.88737800	-1.54578500
H	5.09459800	3.14319400	0.82243700
H	2.85657600	2.32352000	1.52543400

Sum of electronic and zero-point Energies= -3827.797561

Sum of electronic and thermal Energies= -3827.747029

Sum of electronic and thermal Enthalpies= -3827.746085

Sum of electronic and thermal Free Energies= -3827.888151

$TS_{9\text{-}9'}$

Ru	-0.25344776	-0.14203034	-0.75494346
S	-2.26734579	0.02970487	-1.86665537
S	-1.50385265	-1.24169380	0.87373017
P	0.35194817	1.93521665	0.03841812
P	1.58244661	-1.48180781	-0.05030499
O	0.94236473	0.36201306	-3.50476167
C	0.54568079	0.21647869	-2.41250539
C	-3.17064446	-1.16589251	0.39386945
C	-3.50726485	-0.60136386	-0.83026891
C	-4.15123226	-1.78796401	1.38769162
C	-4.89378099	-0.48027778	-1.45475075
F	-5.04562607	-0.87486889	1.87416622
F	-3.51307570	-2.30890843	2.47446385
F	-4.86690498	-2.81476224	0.84010165
F	-4.97935536	-1.22011229	-2.60427935
F	-5.16425942	0.81674486	-1.80781502
F	-5.91328424	-0.87898617	-0.65480294
C	1.58291232	-3.03995411	-1.05695053
C	0.40905936	-3.46014638	-1.71935106
C	0.39549986	-4.65420879	-2.46221388
C	1.55458989	-5.44255874	-2.55246686
C	2.72904605	-5.03319472	-1.89464533
C	2.74565200	-3.84063484	-1.15356963
C	1.51057032	-2.10737212	1.68174363
C	1.67825128	-1.19317518	2.74738444
C	1.61005687	-1.62800640	4.08089846
C	1.35329751	-2.98017212	4.36982721
C	1.16845695	-3.89229744	3.31753397
C	1.24910377	-3.46212226	1.98150361
C	3.35089253	-0.96949535	-0.24312524
C	4.30737335	-1.08943269	0.78981196
C	5.65836574	-0.77601182	0.55285047
C	6.07468959	-0.34719487	-0.71777896
C	5.12942183	-0.22673350	-1.75237367
C	3.77993052	-0.53122689	-1.51786865
C	0.26779799	2.32640087	1.85312316
C	0.75006919	3.57977790	2.30725551
C	0.60793184	3.95496756	3.65136163
C	-0.03501767	3.09634041	4.56293233
C	-0.53296231	1.86202005	4.11785230
C	-0.38042423	1.47823204	2.77195637
C	-0.76847930	3.30350999	-0.53872849
C	-0.29870432	4.56324423	-0.97320796
C	-1.20510712	5.59041039	-1.29395290
C	-2.58792009	5.38173188	-1.16861718
C	-3.06296444	4.13886783	-0.71289131
C	-2.16145378	3.10985441	-0.40083733
C	2.03485248	2.50089792	-0.44926842
C	2.28044181	2.89410437	-1.78701026
C	3.56063816	3.31030296	-2.18692514
C	4.62089478	3.32522019	-1.26369803
C	4.39558160	2.90584427	0.05812830
C	3.11431304	2.49476552	0.46263167
H	-0.50387455	-2.84702621	-1.65625467
H	-0.52883387	-4.96346584	-2.97503686
H	1.54557839	-6.37550982	-3.13833037
H	3.64283559	-5.64499862	-1.96197633
H	3.67305888	-3.52985758	-0.64896116
H	1.86274209	-0.12896704	2.53648186
H	1.74838609	-0.90154809	4.89719589
H	1.29035101	-3.32055976	5.41554906
H	0.95603832	-4.95121009	3.53403278
H	1.10119652	-4.18727386	1.16824593
H	4.00606485	-1.44721937	1.78480262
H	6.39014686	-0.88182170	1.36984105
H	7.13436275	-0.11069015	-0.90433016
H	5.44319132	0.10532199	-2.75436308
H	3.06170987	-0.44381599	-2.34542378
H	1.23187871	4.27646479	1.60471912
H	0.99284003	4.93136591	3.98644964
H	-0.15376020	3.39662280	5.61624265
H	-1.05024975	1.18536617	4.81614206
H	-0.78525866	0.51283876	2.43155291
H	0.77969799	4.75705292	-1.06394448
H	-0.82020284	6.56183027	-1.64348884
H	-3.29586322	6.18634420	-1.42323404
H	-4.14432203	3.96210647	-0.60446968
H	-2.54816228	2.14262880	-0.04793940
H	1.46458082	2.88887481	-2.52490994
H	3.72707563	3.62593268	-3.22905896
H	5.62373443	3.65619824	-1.57679110
H	5.22237010	2.89755115	0.78537243
H	2.95478249	2.17821266	1.50398591

Sum of electronic and zero-point Energies= -3827.796226

Sum of electronic and thermal Energies= -3827.746576

Sum of electronic and thermal Enthalpies= -3827.745632

Sum of electronic and thermal Free Energies= -3827.885176

$TS_{4\text{-}9}$

Ru	-0.22722870	-0.15146218	-0.77233836
S	-2.27314112	0.03182801	-1.83214469
S	-1.38449278	-1.45223915	0.76667994
P	0.19608579	1.95452908	0.05447488
P	1.70685440	-1.37850383	-0.08742339
O	0.93076777	0.48865877	-3.50749064
C	0.54237264	0.29613137	-2.41845675
C	-3.06354822	-1.39381543	0.33284756
C	-3.44999811	-0.75760361	-0.84044950
C	-4.00005406	-2.14207081	1.27538493
C	-4.88562525	-0.65438121	-1.34926636
F	-5.16926843	-1.47327893	1.49313084
F	-3.43587874	-2.33876827	2.50285918
F	-4.32694322	-3.38411511	0.80131366
F	-4.93321759	-0.34222858	-2.67500553
F	-5.58727533	0.32587616	-0.69581326
F	-5.58417785	-1.81496434	-1.20110707
C	1.81526867	-2.93057426	-1.09876657
C	0.69345687	-3.39590087	-1.81814587
C	0.76739723	-4.58217133	-2.57026504
C	1.96279484	-5.31826273	-2.61169803
C	3.08660549	-4.86349624	-1.89725852
C	3.01619880	-3.67783348	-1.14877927
C	1.66903932	-2.00698854	1.64433092
C	1.78184492	-1.08145384	2.70772092
C	1.73371583	-1.51539692	4.04223220
C	1.55043975	-2.87906773	4.33434630
C	1.41928553	-3.80305066	3.28455120
C	1.48114401	-3.37299645	1.94723472
C	3.44302438	-0.76256233	-0.27413624
C	4.40643988	-0.84144246	0.75645981
C	5.74094549	-0.46649693	0.51758720
C	6.13474365	-0.01606095	-0.75284853
C	5.18271451	0.06476136	-1.78463234
C	3.84844633	-0.30064721	-1.54789589
C	-0.12442820	2.30704720	1.84854085
C	0.05644568	3.63498764	2.31144895
C	-0.22147039	3.96868295	3.64487817
C	-0.70164097	2.98866718	4.53478762
C	-0.89912208	1.67589615	4.08010351
C	-0.60986670	1.33611691	2.74440884

C	-0.90154908	3.27762961	-0.65635745
C	-0.43294531	4.46596760	-1.25722626
C	-1.34003153	5.44428307	-1.70745612
C	-2.72176837	5.25801083	-1.54894226
C	-3.19668840	4.08814757	-0.92748878
C	-2.29577012	3.10856094	-0.48587736
C	1.90179232	2.60077906	-0.20488343
C	2.34343204	2.91576940	-1.51303611
C	3.63819323	3.41272864	-1.73101695
C	4.52596345	3.57590413	-0.65310290
C	4.11094833	3.23122937	0.64365893
C	2.80884706	2.75188670	0.86786400
H	-0.24838711	-2.82567357	-1.79051240
H	-0.11765534	-4.92704794	-3.12772147
H	2.02198678	-6.24566153	-3.20343411
H	4.02872502	-5.43395289	-1.92633012
H	3.90551213	-3.32969204	-0.60158022
H	1.90981727	-0.00952546	2.49228498
H	1.82978040	-0.78067938	4.85723124
H	1.50283565	-3.21927709	5.38093944
H	1.26370348	-4.87121818	3.50378356
H	1.37622050	-4.10735452	1.13544502
H	4.12402208	-1.21551261	1.75093945
H	6.47843268	-0.54033511	1.33290243
H	7.18231573	0.26804498	-0.94117082
H	5.47954675	0.41269573	-2.78657544
H	3.12425066	-0.24543654	-2.37350571
H	0.40795033	4.41785568	1.62176618
H	-0.07348955	5.00488987	3.98854669
H	-0.93033903	3.25504895	5.57906933
H	-1.28840083	0.90279364	4.76106078
H	-0.78436136	0.30813835	2.39180904
H	0.64479477	4.64781585	-1.37182536
H	-0.95453614	6.36070725	-2.18227549
H	-3.42972282	6.02366378	-1.90384784
H	-4.27774663	3.93178317	-0.78805228
H	-2.68391209	2.20166779	0.00118117
H	1.67230098	2.78077628	-2.37370985
H	3.95547470	3.66828838	-2.75445175
H	5.54246116	3.96324982	-0.82546192
H	4.80240956	3.34088957	1.49394404
H	2.49486056	2.50615277	1.89322743

Sum of electronic and zero-point Energies= -3827.797863

Sum of electronic and thermal Energies= -3827.748219

Sum of electronic and thermal Enthalpies= -3827.747275

Sum of electronic and thermal Free Energies= -3827.885695

10'

C	0.65331700	0.14931100	-2.42914100
C	0.90567800	-4.73213600	-2.23733300
C	1.88447800	-5.64554300	-1.81362400
C	2.84819800	-5.24714900	-0.86813300
C	2.83048800	-3.94361700	-0.34831700
C	2.29816400	-1.65797500	1.66855900
C	3.53061600	-1.30297900	2.26026500
C	3.81562900	-1.66152800	3.59037400
C	2.87868000	-2.38169200	4.34951100
C	1.65403400	-2.75291500	3.76516500
C	1.36746600	-2.39878200	2.43731000
C	3.39601700	-0.57549200	-0.80298100
C	1.10033800	2.23525900	1.51911100
C	1.02171500	1.36734400	2.63263500
C	1.78234100	1.61753200	3.78637000
C	2.64563800	2.72701000	3.83751400
C	2.73392300	3.59248900	2.73332700
C	1.96086900	3.35529500	1.58242700
C	-1.62083500	2.53313000	0.66807000
C	-2.76098800	2.40509400	-0.15759400
C	-3.99939300	2.92908700	0.24644000
C	-4.12237700	3.57879200	1.48722400
C	4.05323500	-1.17973100	-1.89792700
C	-2.99491000	3.71179900	2.31421400
C	-1.75014400	3.19962700	1.90806100
C	0.52297800	3.20108900	-1.14094000
C	1.73641600	3.05191600	-1.85127700
C	2.16379000	4.03873500	-2.75346900
C	1.38159400	5.18751800	-2.96918400
C	0.17512400	5.34579600	-2.26774600
C	-0.25103200	4.36402900	-1.35539200
C	-3.34081400	-1.04035800	-0.83924200
C	-3.01034000	-1.27039800	0.49148100
C	5.19811700	-0.58749100	-2.46026400
C	-4.00000100	-1.70431300	1.57287000
C	-4.72083700	-1.26330300	-1.44944600
C	5.71153300	0.60876200	-1.93277800
C	5.06104600	1.22257800	-0.84717600
C	3.90592800	0.64388400	-0.29458400
C	1.84980000	-3.01524000	-0.77261300
C	0.88857700	-3.42387700	-1.72003100
F	-4.85583400	-0.62629600	-2.64858800
F	-5.73096300	-0.80211700	-0.65529400
F	-4.96902400	-2.58813300	-1.68857400
F	-4.77438500	-0.66456100	2.00618100
F	-4.84308000	-2.68747100	1.14659300
F	-3.36453800	-2.19664000	2.67570700
H	0.14292200	-5.03509700	-2.97180600
H	1.89553100	-6.67138300	-2.21517000
H	3.61669400	-5.95936600	-0.52755000
H	3.58421000	-3.64699400	0.39744100
H	4.28797000	-0.75460100	1.68290000
H	4.78500900	-1.37784600	4.03055300
H	3.10461400	-2.66228200	5.39064100
H	0.91389500	-3.32846000	4.34325900
H	0.41090500	-2.71128100	1.99226000
H	0.35086900	0.49478800	2.60039700
H	1.70462400	0.93309200	4.64518900
H	3.24893300	2.91761800	4.73937200
H	3.40247700	4.46764500	2.76799900
H	2.02394700	4.05064700	0.73251100
H	-2.68055600	1.88554000	-1.12507600
H	-4.87620300	2.81416300	-0.40971400
H	-5.09771200	3.97545500	1.81068500
H	3.66924600	-2.11990400	-2.31974900
H	-3.07893400	4.21920200	3.28846600
H	-0.87884100	3.32376800	2.56627200
H	2.36074300	2.15940900	-1.69890700
H	3.11108300	3.90104100	-3.29808700
H	1.71159800	5.95630900	-3.68584100
H	-0.44596100	6.24140300	-2.42810200
H	-1.19459800	4.50794500	-0.81023000
H	5.69212200	-1.07160000	-3.31759200
H	6.61393500	1.06564900	-2.36903900
H	5.44903500	2.16469600	-0.42830300
H	3.39820300	1.15059000	0.54029400
H	0.11021300	-2.71658100	-2.04973200
O	1.10063300	0.31673700	-3.49513000
P	0.01079500	1.89852300	0.06587200
P	1.84913200	-1.28827600	-0.09230100
Ru	-0.16993100	-0.23151100	-0.77757600
S	-2.11622100	-0.52805000	-1.95857300
S	-1.38545900	-1.05176700	1.04125100

Sum of electronic and zero-point Energies= -3827.800825

Sum of electronic and thermal Energies= -

3827.750298
Sum of electronic and thermal Enthalpies= -3827.749354
Sum of electronic and thermal Free Energies= -3827.891346

$TS_{10\text{-}10'}$

C	0.64042381	0.15812622	-2.42591489
C	0.92515161	-4.72480488	-2.24468506
C	1.91296797	-5.63143607	-1.82744139
C	2.87793955	-5.22754354	-0.88554897
C	2.85252170	-3.92527797	-0.36292485
C	2.31073388	-1.64813493	1.66137984
C	3.54420523	-1.28894422	2.24840360
C	3.83647265	-1.64882658	3.57658827
C	2.90590507	-2.37453117	4.33829657
C	1.68035008	-2.74990717	3.75850925
C	1.38652652	-2.39436730	2.43262993
C	3.39188326	-0.55308720	-0.81224096
C	1.09163851	2.24299310	1.52047536
C	1.02814057	1.37303466	2.63339750
C	1.79349512	1.62916099	3.78270160
C	2.64622617	2.74696830	3.82998951
C	2.71926081	3.61464570	2.72641921
C	1.94159557	3.37126466	1.57991961
C	-1.63754320	2.51605298	0.68521401
C	-2.78245171	2.37329320	-0.13150508
C	-4.02379169	2.88344923	0.28141846
C	-4.14472260	3.53377007	1.52213007
C	4.04709696	-1.14919404	-1.91282897
C	-3.01247115	3.68143214	2.34015278
C	-1.76498133	3.18317895	1.92510186
C	0.49048209	3.20346084	-1.13647935
C	1.70442069	3.06776908	-1.84873892
C	2.11751968	4.05765532	-2.75417626
C	1.32031954	5.19583871	-2.97129199
C	0.11313943	5.34048056	-2.26814969
C	-0.29881911	4.35573391	-1.35249433
C	-3.34234560	-1.06805721	-0.81129421
C	-3.00971196	-1.28127678	0.52070734
C	5.18529874	-0.54774703	-2.47893575
C	-3.97719966	-1.75047471	1.61042435
C	-4.69688227	-1.25770987	-1.48117689
C	5.69399117	0.64976024	-1.94972264
C	5.04541262	1.25549123	-0.85844799
C	3.89686224	0.66754167	-0.30194765
C	1.86273314	-3.00366793	-0.78085077
C	0.90029566	-3.41773060	-1.72466153
F	-5.07116070	-0.13036616	-2.16905813
F	-5.71711844	-1.54312573	-0.63506621
F	-4.65102545	-2.27168645	-2.40259686
F	-4.98059902	-0.85314410	1.83739656
F	-4.55462316	-2.94996002	1.30340698
F	-3.34896349	-1.92916639	2.80781779
H	0.16132136	-5.03204244	-2.97625514
H	1.93017443	-6.65630842	-2.23123830
H	3.65352436	-5.93445466	-0.55001627
H	3.60737196	-3.62438753	0.37997982
H	4.29670026	-0.73623488	1.66881545
H	4.80648301	-1.36178522	4.01318541
H	3.13750609	-2.65612045	5.37790831
H	0.94519391	-3.32966898	4.33874234
H	0.42928902	-2.70960380	1.99093461
H	0.36539607	0.49421047	2.60435691
H	1.72765899	0.94300675	4.64114423
H	3.25310305	2.94236107	4.72841679
H	3.37940856	4.49626963	2.75811705
H	1.99282641	4.06815697	0.73047315
H	-2.70490838	1.85296296	-1.09875412
H	-4.90341912	2.75665657	-0.36867785
H	-5.12201329	3.91989790	1.85247196
H	3.66675678	-2.09019498	-2.33611936
H	-3.09477678	4.18959602	3.31416490
H	-0.89016561	3.31840791	2.57644935
H	2.34020689	2.18346536	-1.69550871
H	3.06544790	3.93068202	-3.30028614
H	1.63917913	5.96695980	-3.69048019
H	-0.51967529	6.22759944	-2.42979705
H	-1.24329763	4.48877339	-0.80613871
H	5.67780417	-1.02559348	-3.34062592
H	6.59122004	1.11388832	-2.38899624
H	5.42971688	2.19845685	-0.43808736
H	3.39040503	1.16795026	0.53745055
H	0.11485620	-2.71607472	-2.04949728
O	1.08241073	0.33103052	-3.49311695
P	-0.00327641	1.89718670	0.07355705
P	1.85278502	-1.27816249	-0.09705051
Ru	-0.17415895	-0.23289197	-0.77196186
S	-2.12029505	-0.55674012	-1.93973986
S	-1.37866381	-1.05116291	1.05599112

Sum of electronic and zero-point Energies= -3827.799875
Sum of electronic and thermal Energies= -3827.750239
Sum of electronic and thermal Enthalpies= -3827.749295
Sum of electronic and thermal Free Energies= -3827.888554

$TS_{10\text{-}7}$

C	0.70131998	0.36684706	-2.27263642
C	1.37105098	-4.29824466	-2.83739067
C	2.43245329	-5.17273067	-2.55376570
C	3.34648830	-4.85376358	-1.53162705
C	3.19761349	-3.66732086	-0.79717717
C	2.34417346	-1.85680491	1.58528900
C	3.43146441	-1.41356453	2.37090829
C	3.66999644	-1.96894003	3.64124122
C	2.82929351	-2.97375350	4.14813314
C	1.75208604	-3.43187136	3.36883040
C	1.51395168	-2.88402221	2.09829007
C	3.45508057	-0.25270293	-0.58609236
C	0.79773025	2.27666965	1.74268254
C	0.96767184	1.23254412	2.67595790
C	1.51926874	1.48951707	3.94383536
C	1.91304901	2.79258410	4.29064290
C	1.73554072	3.84247313	3.37061440
C	1.17132549	3.59169765	2.10931947
C	-1.75366999	2.58869117	0.68263170
C	-2.65488854	1.74905285	1.37000822
C	-3.86213033	2.25849074	1.87632706
C	-4.18585009	3.61462214	1.70245881
C	4.24308934	-0.61845065	-1.70016967
C	-3.28902829	4.46105237	1.02819735
C	-2.07787684	3.95655684	0.52537570
C	0.48866928	3.15350934	-1.06410236
C	1.79995919	3.67508963	-1.06228883
C	2.22986093	4.52712877	-2.09541104
C	1.35879750	4.86674094	-3.14313389
C	0.05515080	4.33764326	-3.16235952
C	-0.37518376	3.48250823	-2.13697825
C	-3.31825433	-1.01012192	-0.85983293
C	-2.92578115	-1.63109423	0.32035894
C	5.36378732	0.14788566	-2.06662181
C	-3.83647053	-2.46081662	1.21880593
C	-4.74266036	-1.00127733	-1.41067126
C	5.72450412	1.28132564	-1.32026433
C	4.94186866	1.65954102	-0.21477829

C	3.80761849	0.91034714	0.13999597
C	2.13367137	-2.77705589	-1.07921484
C	1.22240981	-3.10692064	-2.10368793
F	-4.77358278	-0.65860752	-2.73020207
F	-5.54024809	-0.10075542	-0.75868069
F	-5.34900857	-2.21926931	-1.31565256
F	-3.30234521	-2.63643923	2.46314019
F	-5.06047885	-1.88525623	1.40627602
F	-4.05374767	-3.71478393	0.71563088
H	0.64645609	-4.54186858	-3.63018938
H	2.54689550	-6.10778291	-3.12495038
H	4.17865731	-5.53774889	-1.30042918
H	3.91317086	-3.43233351	0.00617398
H	4.11527243	-0.64190575	1.99066682
H	4.52876824	-1.61392782	4.23324821
H	3.01793631	-3.40655573	5.14343862
H	1.09093978	-4.22739780	3.74707944
H	0.67949693	-3.27085569	1.49522056
H	0.65436613	0.21150913	2.41022937
H	1.64089566	0.66130218	4.65897524
H	2.35038952	2.99448726	5.28139256
H	2.02826033	4.86983525	3.64044710
H	1.01028122	4.43010509	1.41532690
H	-2.40980337	0.68617703	1.51335834
H	-4.55624103	1.58357873	2.40063820
H	-5.13728339	4.01168177	2.09036787
H	3.98145909	-1.50722610	-2.29222412
H	-3.53090027	5.52690923	0.88892494
H	-1.38798328	4.63799877	0.00666231
H	2.50079644	3.40882218	-0.25906377
H	3.25785572	4.92234672	-2.07948592
H	1.69743331	5.53394765	-3.95145671
H	-0.63146370	4.58481501	-3.98728261
H	-1.39118656	3.05805049	-2.17526225
H	5.96009473	-0.15086190	-2.94330736
H	6.60981273	1.87316131	-1.60188639
H	5.21179303	2.54944428	0.37634098
H	3.19162002	1.23596931	0.99215727
H	0.37896869	-2.43253439	-2.32449408
O	1.19156509	0.63838733	-3.29682621
P	-0.10181439	1.91993189	0.16551580
P	1.94963206	-1.20863098	-0.10752489
Ru	-0.15230409	-0.20507666	-0.69679331
S	-2.16813407	-0.13913146	-1.81573818
S	-1.26707644	-1.54991534	0.83125248

Sum of electronic and zero-point Energies= -3827.797182

Sum of electronic and thermal Energies= -3827.747485

Sum of electronic and thermal Enthalpies= -3827.746541

Sum of electronic and thermal Free Energies= -3827.885626

11

C	-0.43857093	0.31341316	-2.48866220
C	0.77906206	4.45390843	-3.09808162
C	0.15723394	5.66152604	-2.73982331
C	-0.54119785	5.74693165	-1.52290857
C	-0.62248406	4.63118608	-0.67259990
C	1.36718110	2.31564817	1.26952585
C	1.92625680	1.28282507	2.05447460
C	2.95277710	1.55729847	2.97382827
C	3.44581590	2.86583622	3.11291230
C	2.90203205	3.89814782	2.32982502
C	1.86824485	3.62926050	1.41676977
C	-1.50522164	2.28460120	1.16501049
C	-2.43439735	-1.14482137	1.53667890
C	-1.51477216	-1.43856326	2.57161893
C	-1.92815054	-1.44967822	3.91336308
C	-3.26137329	-1.14858987	4.24601075
C	-4.17426865	-0.83101226	3.22722088
C	-3.76685868	-0.83087602	1.88079631
C	-1.71037094	-3.06363286	-0.49607929
C	-1.24832954	-3.49136375	-1.76280484
C	-1.15120804	-4.85820294	-2.06133367
C	-1.50062286	-5.81941592	-1.09407652
C	-2.73902425	2.65316451	0.57916505
C	-1.95547319	-5.40327315	0.16715872
C	-2.06642494	-4.03195315	0.46575796
C	-3.37905667	-0.88010826	-1.19583693
C	-3.54613215	0.34321249	-1.87543994
C	-4.71527603	0.60682845	-2.61086455
C	-5.73791421	-0.35345960	-2.67602316
C	-5.58236055	-1.58058888	-2.00607093
C	-4.41258421	-1.84467722	-1.27584903
C	3.45504285	-0.72688601	-0.69814770
C	2.96036709	-1.72689384	0.12783470
C	-3.85858469	2.93420473	1.37819102
C	3.80099118	-2.72131316	0.91591919
C	4.93641604	-0.50790879	-1.00911819
C	-3.76787553	2.84316323	2.77830215
C	-2.55179773	2.46366493	3.37007014
C	-1.42826351	2.18704499	2.57237911
C	-0.01158002	3.40402564	-1.03047798
C	0.69446755	3.33535065	-2.25180279
F	5.41251153	-1.43307858	-1.89513284
F	5.71603326	-0.57473188	0.10817071
F	5.16554332	0.71378373	-1.56768913
F	4.87024484	-3.19444724	0.21684640
F	4.29432839	-2.16912072	2.07393316
F	3.07448853	-3.81167971	1.29548427
H	1.33471020	4.37384858	-4.04540156
H	0.21781781	6.53610554	-3.40686385
H	-1.02738957	6.69048935	-1.22772223
H	-1.16564044	4.72223097	0.27921141
H	1.56751209	0.24911920	1.93088703
H	3.38010037	0.73517623	3.56873170
H	4.26154678	3.07845863	3.82194747
H	3.28820482	4.92580859	2.42207950
H	1.46274835	4.45100311	0.80950743
H	-0.46799802	-1.67733844	2.32514853
H	-1.20104438	-1.69671333	4.70327675
H	-3.58600959	-1.15870297	5.29876530
H	-5.21846631	-0.58386841	3.47682292
H	-4.49740105	-0.58737809	1.09601934
H	-0.95207283	-2.74618987	-2.51818221
H	-0.78884324	-5.17513145	-3.05200214
H	-1.41168576	-6.89298278	-1.32421236
H	-2.82277321	2.75690702	-0.51200026
H	-2.22635365	-6.14872218	0.93177397
H	-2.42778933	-3.72133794	1.45712328
H	-2.74441827	1.09264436	-1.84651751
H	-4.81816489	1.56478693	-3.14460993
H	-6.65174162	-0.15171452	-3.25724122
H	-6.37426197	-2.34460980	-2.05915111
H	-4.29850530	-2.81562020	-0.77043932
H	-4.80550023	3.23279004	0.90103885
H	-4.64423699	3.06876366	3.40633061
H	-2.46906241	2.38694004	4.46547618
H	-0.47962929	1.90873291	3.05382584
H	1.19647146	2.40403576	-2.54873855
O	-0.74718335	0.48482083	-3.60639172
P	-1.84877647	-1.23845579	-0.21531637
P	-0.02900501	1.94203170	0.10641395
Ru	0.21916396	-0.16922028	-0.81630010
S	2.37831443	0.34232475	-1.52088221
S	1.24032412	-1.87911962	0.34348252

Sum of electronic and zero-point Energies= -3827.797330
Sum of electronic and thermal Energies= -3827.746735
Sum of electronic and thermal Enthalpies= -3827.745791
Sum of electronic and thermal Free Energies= -3827.887899

11'

C	-0.41413224	0.28874482	-2.48581280
C	0.73101517	4.46263636	-3.10699391
C	0.09195357	5.66391972	-2.75804887
C	-0.61905943	5.74463666	-1.54805719
C	-0.69505807	4.63055122	-0.69519585
C	1.28260510	2.35181472	1.29240059
C	1.83941600	1.32835707	2.09128687
C	2.83745966	1.62054352	3.03606661
C	3.30525671	2.93708596	3.18635568
C	2.76471390	3.95973817	2.38858324
C	1.75828023	3.67338027	1.45056558
C	-1.58537782	2.27484580	1.12223263
C	-2.40551943	-1.17940661	1.53680758
C	-1.48419163	-1.44813175	2.57713538
C	-1.90132265	-1.45176574	3.91779304
C	-3.24017547	-1.16848231	4.24363816
C	-4.15511001	-0.87632240	3.21909683
C	-3.74381994	-0.88347169	1.87388648
C	-1.63426393	-3.10095910	-0.47670601
C	-1.16162359	-3.52949577	-1.73925280
C	-1.03575803	-4.89645355	-2.02618867
C	-1.36661808	-5.85662555	-1.05140279
C	-2.81184319	2.61547601	0.50490630
C	-1.83183392	-5.43956847	0.20574469
C	-1.97155911	-4.06839504	0.49274539
C	-3.34558581	-0.96108789	-1.20227646
C	-3.53044862	0.24622498	-1.90521755
C	-4.70083554	0.47610283	-2.65001461
C	-5.70687997	-0.50235499	-2.70077047
C	-5.53345970	-1.71390742	-2.00715871
C	-4.36228247	-1.94450590	-1.26799955
C	3.47987729	-0.66698730	-0.68438904
C	3.00141522	-1.66403094	0.15386277
C	-3.95439841	2.88295468	1.27561821
C	3.85543905	-2.69107345	0.88398591
C	4.95845487	-0.39975373	-0.96907902
C	-3.89389947	2.80723215	2.67830517
C	-2.68479727	2.45628730	3.30120705
C	-1.53858816	2.19248745	2.53189479
C	-0.06519826	3.41002229	-1.04301713
C	0.65214950	3.34573844	-2.25784505
F	5.13033085	0.37536971	-2.07717685
F	5.66141127	-1.54700276	-1.18798709
F	5.56537634	0.25982856	0.06301824
F	4.24157992	-3.72122385	0.06973988
F	4.99157286	-2.15197146	1.41450873
F	3.18001055	-3.26075187	1.92691226
H	1.29568321	4.38609517	-4.04925648
H	0.14834202	6.53715119	-3.42722105
H	-1.11975087	6.68302652	-1.26073714
H	-1.25000627	4.71713634	0.25026899
H	1.50138697	0.28882410	1.95834723
H	3.26320824	0.80687659	3.64388816
H	4.09921683	3.16347898	3.91551606
H	3.13200696	4.99350964	2.48915097
H	1.35440658	4.48787493	0.83250238
H	-0.43320367	-1.67366430	2.33576934
H	-1.17279740	-1.67924781	4.71225742
H	-3.56759301	-1.17276329	5.29557214
H	-5.20383132	-0.64332588	3.46322424
H	-4.47564725	-0.65899398	1.08467876
H	-0.87963523	-2.78467499	-2.50035634
H	-0.66525920	-5.21403805	-3.01361921
H	-1.25507298	-6.92998153	-1.27248556
H	-2.87202845	2.70849170	-0.58887390
H	-2.08831611	-6.18408905	0.97620493
H	-2.34068145	-3.75712641	1.48104311
H	-2.74146654	1.00930749	-1.88694181
H	-4.81766872	1.42195484	-3.20216975
H	-6.62160233	-0.32708682	-3.28912878
H	-6.31218101	-2.49205116	-2.04881130
H	-4.23368002	-2.90397164	-0.74443315
H	-4.89550327	3.15944492	0.77426591
H	-4.78833023	3.02280086	3.28401474
H	-2.62542860	2.39212273	4.39893053
H	-0.59637202	1.93631455	3.03755246
H	1.16646667	2.41917977	-2.54839281
O	-0.71255593	0.44244025	-3.60920144
P	-1.81218149	-1.27683247	-0.21220595
P	-0.07995696	1.95189878	0.09884087
Ru	0.23427315	-0.16208949	-0.80415626
S	2.38856504	0.40380481	-1.48542089
S	1.28211821	-1.86570448	0.33810287

Sum of electronic and zero-point Energies= -3827.797387
Sum of electronic and thermal Energies= -3827.746771
Sum of electronic and thermal Enthalpies= -3827.745826
Sum of electronic and thermal Free Energies= -3827.888259

$TS_{11\text{-}11'}$

C	-0.43941958	0.34244267	-2.48347868
C	0.92448740	4.43803687	-3.07151988
C	0.33715578	5.66171522	-2.70967786
C	-0.36483392	5.76135443	-1.49584408
C	-0.48425724	4.64379780	-0.65255209
C	1.41778987	2.26393997	1.29199581
C	1.91995857	1.21930367	2.09952421
C	2.94336398	1.46239103	3.03098284
C	3.49126358	2.74997048	3.15956812
C	3.00531168	3.79305825	2.35330213
C	1.97440093	3.55624818	1.42820536
C	-1.45521270	2.31732713	1.16012600
C	-2.47236260	-1.09605194	1.52441230
C	-1.56806521	-1.40774069	2.56761739
C	-1.99240231	-1.40465239	3.90597651
C	-3.32086284	-1.07136765	4.22685823
C	-4.21806723	-0.73646218	3.19971667
C	-3.80003021	-0.75047199	1.85663665
C	-1.76115911	-3.03228329	-0.49783325
C	-1.29144715	-3.46976580	-1.75838634
C	-1.21139188	-4.83859669	-2.05292297
C	-1.58580288	-5.79223653	-1.08751832
C	-2.67135739	2.71890681	0.55927619
C	-2.04864157	-5.36643723	0.16761206
C	-2.14264827	-3.99292773	0.46194847
C	-3.39520880	-0.82659780	-1.21267853
C	-3.54900395	0.40532589	-1.87979132
C	-4.71135032	0.68565784	-2.61968117
C	-5.74049596	-0.26633881	-2.70213261
C	-5.59843589	-1.50158293	-2.04429608
C	-4.43556682	-1.78219384	-1.30916172
C	3.43918688	-0.81613082	-0.69096304
C	2.92558071	-1.77724167	0.16840424
C	-3.79341835	3.02807279	1.34417283
C	3.73542690	-2.80573058	0.95143494

C	4.90519937	-0.56277253	-1.04085243
C	-3.72288593	2.93333738	2.74525580
C	-2.52442866	2.52265683	3.35189447
C	-1.39834224	2.21749037	2.56822100
C	0.09112480	3.40072442	-1.01447063
C	0.80182439	3.31776168	-2.23213375
F	5.12216579	-0.73251479	-2.38199489
F	5.78578872	-1.36780881	-0.39761525
F	5.26584664	0.72425015	-0.74724407
F	4.47501677	-3.62204112	0.14397016
F	4.59698606	-2.22120616	1.84187744
F	2.93378829	-3.62769315	1.68892246
H	1.48288573	4.34666717	-4.01619178
H	0.42759482	6.53779457	-3.37135279
H	-0.82374537	6.71752597	-1.19759725
H	-1.02877002	4.74578860	0.29736825
H	1.51829254	0.20055765	1.98423987
H	3.32533427	0.63174188	3.64484146
H	4.30470676	2.93726309	3.87828700
H	3.43505248	4.80402252	2.43666748
H	1.61434212	4.38609486	0.80366998
H	-0.52531285	-1.67219682	2.33027698
H	-1.27772686	-1.66609876	4.70257467
H	-3.65407580	-1.07039400	5.27697984
H	-5.25829548	-0.46465251	3.44007611
H	-4.51845513	-0.49340450	1.06501935
H	-0.97544179	-2.73075878	-2.51189459
H	-0.84269287	-5.16315030	-3.03876967
H	-1.51022296	-6.86754412	-1.31428560
H	-2.73743533	2.82725992	-0.53277466
H	-2.33922232	-6.10601789	0.93069417
H	-2.51067737	-3.67459796	1.44841608
H	-2.74262631	1.14879539	-1.83676233
H	-4.80383604	1.65022054	-3.14333787
H	-6.64895904	-0.05154012	-3.28706617
H	-6.39570127	-2.25897639	-2.11042937
H	-4.33260200	-2.75878031	-0.81244516
H	-4.72606512	3.35181342	0.85546574
H	-4.60105571	3.18085049	3.36240469
H	-2.45743385	2.44351007	4.44820726
H	-0.46334693	1.91504018	3.06161162
H	1.27836595	2.37376128	-2.53094124
O	-0.74796842	0.53441697	-3.59760254
P	-1.87562496	-1.20462660	-0.22279069
P	0.02165367	1.93515985	0.11591736
Ru	0.21363275	-0.17336178	-0.81731253
S	2.38096650	0.25785390	-1.53900456
S	1.19868453	-1.88626051	0.37325406

Sum of electronic and zero-point Energies= -3827.795574

Sum of electronic and thermal Energies= -3827.745848

Sum of electronic and thermal Enthalpies= -3827.744904

Sum of electronic and thermal Free Energies= -3827.884627

$TS_{11\text{-}2}$

C	-0.20917715	0.08798380	-2.45035478
C	0.21315715	4.44339525	-3.20620076
C	-0.58882460	5.56481631	-2.93728223
C	-1.36811384	5.59642073	-1.76739588
C	-1.34708529	4.51292049	-0.87329143
C	0.70697851	2.59056684	1.36832086
C	1.34132603	1.66558965	2.22798076
C	2.18866700	2.10868918	3.25679220
C	2.42787120	3.48297945	3.43162168
C	1.80930400	4.40923814	2.57521391
C	0.95027152	3.96918816	1.55308366
C	-2.07815186	2.08514656	0.92394265
C	-2.17221203	-1.44267458	1.56330471
C	-1.22444030	-1.54781632	2.60937400
C	-1.63835512	-1.55823234	3.95101777
C	-3.00395328	-1.44680328	4.27056345
C	-3.94879795	-1.32103737	3.23907228
C	-3.53872531	-1.32042409	1.89349158
C	-1.14934509	-3.30249451	-0.39542330
C	-0.66655723	-3.70640775	-1.66235173
C	-0.37438850	-5.05429453	-1.91594310
C	-0.54785906	-6.01778907	-0.90453158
C	-3.27580922	2.20933853	0.18146453
C	-1.02172175	-5.62419852	0.35681206
C	-1.32619017	-4.27360138	0.61178809
C	-3.08744905	-1.41876533	-1.20573138
C	-3.34757949	-0.32223858	-2.05095606
C	-4.50890792	-0.28195712	-2.84350186
C	-5.43021775	-1.34051655	-2.79729588
C	-5.18019234	-2.44423296	-1.96106424
C	-4.01648303	-2.48752536	-1.17738221
C	3.61679138	-0.15796275	-0.52477017
C	3.27667900	-1.35891990	0.07873534
C	-4.51484883	2.32766610	0.83146089
C	4.25572858	-2.35052860	0.69056558
C	5.04878904	0.32658854	-0.75779394
C	-4.57979585	2.32135307	2.23606624
C	-3.39751863	2.18865125	2.98296483
C	-2.15607462	2.07100059	2.33462280
C	-0.54609538	3.37449735	-1.13770776
C	0.23318776	3.35676219	-2.31501823
F	5.64431350	-0.33069327	-1.79702637
F	5.83981321	0.15574622	0.33992771
F	5.09423626	1.65403765	-1.06340198
F	5.37462429	-2.53569710	-0.06577264
F	4.67678853	-1.94971863	1.93498985
F	3.69434789	-3.58224864	0.85829808
H	0.82887637	4.40568847	-4.11838310
H	-0.60851073	6.41375256	-3.63902997
H	-2.00028158	6.47116882	-1.54599102
H	-1.96437148	4.55580590	0.03618712
H	1.18737704	0.58540612	2.07637838
H	2.67884347	1.37161582	3.91206607
H	3.10576400	3.83043784	4.22729208
H	2.00011662	5.48759241	2.69529355
H	0.48338758	4.71013259	0.88823500
H	-0.15303741	-1.63833491	2.36859259
H	-0.88730325	-1.65524941	4.75109083
H	-3.32907491	-1.45489661	5.32316503
H	-5.01962821	-1.22306713	3.47846767
H	-4.29293445	-1.22073232	1.09976065
H	-0.51003954	-2.95754597	-2.45473670
H	0.00182737	-5.35289924	-2.90712710
H	-0.30723040	-7.07467902	-1.10067293
H	-3.24297881	2.24969452	-0.91654795
H	-1.15575081	-6.37076485	1.15577606
H	-1.69934657	-3.98152508	1.60441243
H	-2.62323354	0.50116634	-2.10717191
H	-4.68479551	0.57871198	-3.50797497
H	-6.33767920	-1.31337574	-3.42132445
H	-5.89090750	-3.28529131	-1.92704138
H	-3.82199670	-3.36830274	-0.54641656
H	-5.43370545	2.43458806	0.23337349
H	-5.55086111	2.42249387	2.74629318
H	-3.43488253	2.18236265	4.08352515
H	-1.24020348	1.98217981	2.93635012
H	0.86814464	2.48973959	-2.54548150
O	-0.41353319	0.10964122	-3.60663024
P	-1.55075157	-1.50814387	-0.17594053
P	-0.44762934	1.96434434	0.05726080

Ru	0.33348774	-0.11871251	-0.70486921
S	2.39136160	0.89520125	-1.13364999
S	1.59517208	-1.79905897	0.20867570

Sum of electronic and zero-point Energies= -3827.797188
Sum of electronic and thermal Energies= -3827.747478
Sum of electronic and thermal Enthalpies= -3827.746534
Sum of electronic and thermal Free Energies= -3827.884899

$TS_{11\text{-}6}$

C	0.69975274	-0.49085287	-2.40391331
C	-1.67237711	-4.33137337	-2.87207823
C	-1.60468470	-5.60643753	-2.29045074
C	-1.09136468	-5.75036056	-0.98739740
C	-0.64554189	-4.62585840	-0.27767760
C	-1.27431363	-1.90458856	1.59765545
C	-1.01052100	-1.08458421	2.72010891
C	-1.87970042	-1.07672329	3.82121301
C	-3.04696388	-1.86170401	3.80845783
C	-3.33737824	-2.64969388	2.68418812
C	-2.45778957	-2.67566874	1.58664183
C	1.45598581	-2.63161726	0.78059519
C	2.59764150	1.07327241	1.52605943
C	1.76715303	1.48056370	2.59920029
C	2.21756515	1.38658231	3.92606045
C	3.49971267	0.87800009	4.20587466
C	4.32899078	0.47218009	3.14759090
C	3.88472128	0.57148628	1.81624823
C	1.78075774	3.05801458	-0.39997812
C	1.01945222	3.54935861	-1.48489043
C	0.91985242	4.93001686	-1.71921728
C	1.56953939	5.83945750	-0.86502552
C	2.28200432	-3.30460758	-0.15416038
C	2.32928634	5.35985596	0.21538248
C	2.44190884	3.97670707	0.44434065
C	3.43038231	0.88034785	-1.24333955
C	3.84457238	-0.45752430	-1.42691431
C	4.97337182	-0.75910694	-2.20537630
C	5.69996405	0.27199527	-2.82618363
C	5.29203782	1.60541953	-2.65590649
C	4.16865798	1.91095541	-1.86743415
C	-3.31434805	0.92989292	-0.87033414
C	-2.85948356	1.64124202	0.23338304
C	3.48570385	-3.90314209	0.25043149
C	-3.73874135	2.45298744	1.17862269
C	-4.76039340	0.89813224	-1.35633342
C	3.89134102	-3.83731766	1.59592008
C	3.08137810	-3.17043529	2.52927235
C	1.87299645	-2.57249737	2.12777508
C	-0.71337690	-3.33203920	-0.85436788
C	-1.23116857	-3.20137696	-2.15757614
F	-5.10004228	2.03968374	-2.03096087
F	-5.65330570	0.75302284	-0.33525475
F	-4.98728106	-0.13595919	-2.21677457
F	-4.67409492	3.19680700	0.52136806
F	-4.41042527	1.65770317	2.06820382
F	-3.00650404	3.32972177	1.92566831
H	-2.07215266	-4.20440239	-3.89021421
H	-1.95054296	-6.49036732	-2.84961889
H	-1.03492736	-6.74661029	-0.52052936
H	-0.24220719	-4.75506742	0.73860390
H	-0.13228881	-0.42251302	2.72531201
H	-1.65355521	-0.43501177	4.68723978
H	-3.73729828	-1.84209511	4.66636790
H	-4.26106069	-3.24870725	2.65017179
H	-2.70838114	-3.29524420	0.71425907
H	0.76660831	1.89545932	2.39674344
H	1.56263081	1.72082400	4.74652595
H	3.85238144	0.80634768	5.24709377
H	5.33740651	0.07921087	3.35357015
H	4.55238466	0.25876650	1.00040317
H	0.48939332	2.84339958	-2.14459221
H	0.31989772	5.29652948	-2.56698015
H	1.47923014	6.92333903	-1.03986442
H	1.96850825	-3.38350652	-1.20699942
H	2.84012981	6.06582937	0.88946503
H	3.04693290	3.61446582	1.28876637
H	3.28250313	-1.27409962	-0.95189570
H	5.28040158	-1.80923828	-2.33332472
H	6.57956142	0.03575812	-3.44585903
H	5.85085709	2.42154144	-3.14099378
H	3.86643261	2.96068479	-1.74413696
H	4.10500850	-4.43415988	-0.49005031
H	4.83244116	-4.31224379	1.91549845
H	3.38264271	-3.11852464	3.58733853
H	1.24737194	-2.07838699	2.88334568
H	-1.30362478	-2.21059937	-2.62459597
O	1.17061695	-0.83881311	-3.41686828
P	1.94610368	1.22715445	-0.19812347
P	-0.12202345	-1.88803599	0.15021979
Ru	-0.12157309	0.17021391	-0.84771848
S	-2.19045861	0.06560749	-1.86285409
S	-1.17318060	1.62629097	0.62304234

Sum of electronic and zero-point Energies= -3827.796471
Sum of electronic and thermal Energies= -3827.746696
Sum of electronic and thermal Enthalpies= -3827.745752
Sum of electronic and thermal Free Energies= -3827.885111

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Ru	-0.23201426	-0.16271730	-0.80538502
S	-1.27581583	-1.86576451	0.34215247
S	-2.38700502	0.39278283	-1.49221376
P	0.07207573	1.95101787	0.10013212
P	1.81767273	-1.27142361	-0.21285108
O	0.71857519	0.44986187	-3.60783269
C	0.41809402	0.29318816	-2.48546094
C	-3.47601722	-0.67755679	-0.68741789
C	-2.99539115	-1.66979469	0.15536394
C	-4.95505251	-0.41569370	-0.97435933
C	-3.84722214	-2.69629195	0.88886994
F	-5.65457498	-1.56586533	-1.18912529
F	-5.12822585	0.35434782	-2.08579059
F	-5.56478567	0.24634946	0.05448263
F	-3.17113025	-3.26006149	1.93456986
F	-4.22997079	-3.73062955	0.07841456
F	-4.98522935	-2.15815085	1.41643157
C	1.64406151	-3.09580877	-0.47837785
C	1.17076224	-3.52479958	-1.74052268
C	1.04784400	-4.89190064	-2.02807574
C	1.38233120	-5.85180866	-1.05426724
C	1.84825481	-5.43432453	0.20247693
C	1.98507536	-4.06297676	0.49005179
C	2.41180166	-1.17377298	1.53587938
C	3.74979837	-0.87556637	1.87218131
C	4.16211668	-0.86888420	3.21708283
C	3.24853504	-1.16382140	4.24204125
C	1.90997656	-1.44936175	3.91697303
C	1.49179069	-1.44521528	2.57664816
C	3.34989833	-0.95071694	-1.20310898
C	4.36754517	-1.93279513	-1.27355920
C	5.53805555	-1.69788521	-2.01245027

C	5.70992634	-0.48318564	-2.70089072
C	4.70298834	0.49410667	-2.64528137
C	3.53322733	0.25984501	-1.90090375
C	1.57418505	2.27781737	1.12714298
C	1.52480413	2.19237271	2.53653648
C	2.66855168	2.45832857	3.30875208
C	3.87777370	2.81452511	2.68907720
C	3.94088394	2.89343163	1.28668912
C	2.80079655	2.62379208	0.51309197
C	-1.29464065	2.34638615	1.29050682
C	-1.77630990	3.66614701	1.44588903
C	-2.78571487	3.94953675	2.38159742
C	-3.32341107	2.92574145	3.17982601
C	-2.84971463	1.61101835	3.03228846
C	-1.84864049	1.32173291	2.08980571
C	0.05507391	3.40964090	-1.04106412
C	-0.66068196	3.34400025	-2.25676935
C	-0.74163411	4.46109080	-3.10546078
C	-0.10631285	5.66396857	-2.75517332
C	0.60290497	5.74609206	-1.54422512
C	0.68093374	4.63180972	-0.69179757
H	0.88587468	-2.78023397	-2.50080344
H	0.67678374	-5.20982625	-3.01518478
H	1.27305790	-6.92530752	-1.27579490
H	2.10759333	-6.17865065	0.97216911
H	2.35483091	-3.75136678	1.47800157
H	4.48059219	-0.64911140	1.08257030
H	5.21058460	-0.63413813	3.46063181
H	3.57679949	-1.16852912	5.29371071
H	1.18251154	-1.67901110	4.71178547
H	0.44104650	-1.67248966	2.33588376
H	4.24026555	-2.89454832	-0.75389499
H	6.31750602	-2.47508701	-2.05788755
H	6.62415185	-0.30448509	-3.28898906
H	4.81864058	1.44247974	-3.19334448
H	2.74355566	1.02210841	-1.87884882
H	0.58239475	1.93209205	3.03973302
H	2.60715923	2.39165006	4.40621206
H	4.77025264	3.03171135	3.29707956
H	4.88209192	3.17408989	0.78785555
H	2.86293271	2.71929787	-0.58036506
H	-1.37474963	4.48151381	0.82749143
H	-3.15756053	4.98188824	2.47999887
H	-4.11970282	3.14979662	3.90716290
H	-3.27312238	0.79638657	3.64044824
H	-1.50593923	0.28345478	1.95913920
H	-1.17226416	2.41621362	-2.54824830
H	-1.30499132	4.38345244	-4.04841811
H	-0.16428798	6.53735927	-3.42400237
H	1.10052114	6.68576284	-1.25575552
H	1.23417188	4.71960831	0.25455295

Sum of electronic and zero-point Energies= -3827.796818

Sum of electronic and thermal Energies= -3827.746132

Sum of electronic and thermal Enthalpies= -3827.745187

Sum of electronic and thermal Free Energies= -3827.888716

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Ru	-0.21920011	-0.16923385	-0.81611338
S	-1.24035477	-1.87937889	0.34320375
S	-2.37839353	0.34267198	-1.52039276
P	0.02890140	1.94217617	0.10639987
P	1.84878778	-1.23845415	-0.21530055
O	0.74748639	0.48422594	-3.60620200
C	0.43863614	0.31310168	-2.48849151
C	-3.45511452	-0.72682196	-0.69797493
C	-2.96040055	-1.72710513	0.12765418
C	-4.93648937	-0.50768829	-1.00884473
C	-3.80101832	-2.72172640	0.91546735
F	-5.41268087	-1.43262034	-1.89505030
F	-5.16561732	0.71414147	-1.56713681
F	-5.71607231	-0.57472221	0.10843356
F	-4.29416858	-2.16986397	2.07371036
F	-3.07457578	-3.81229436	1.29456784
F	-4.87041607	-3.19453064	0.21638476
C	1.71046270	-3.06361561	-0.49617870
C	1.24823676	-3.49135323	-1.76282915
C	1.15123832	-4.85819370	-2.06140722
C	1.50097113	-5.81940205	-1.09426369
C	1.95600531	-5.40326061	0.16690592
C	2.06683230	-4.03194159	0.46554694
C	2.43454666	-1.14494180	1.53664856
C	3.76708045	-0.83118709	1.88065661
C	4.17461270	-0.83146364	3.22704515
C	3.26176653	-1.14900307	4.24589338
C	1.92847404	-1.44990360	3.91334843
C	1.51497633	-1.43864409	2.57164170
C	3.37895878	-0.87986907	-1.19588738
C	4.41241076	-1.84446107	-1.27649151
C	5.58210882	-1.58008704	-2.00674520
C	5.73765788	-0.35263682	-2.67610454
C	4.71509133	0.60768890	-2.61033590
C	3.54602253	0.34377910	-1.87490284
C	1.50517857	2.28472123	1.16493121
C	1.42835186	2.18630213	2.57225685
C	2.55185441	2.46274751	3.37004386
C	3.76780285	2.84289902	2.77842288
C	3.85838942	2.93480434	1.37836383
C	2.73884141	2.65397194	0.57923863
C	-1.36721782	2.31576080	1.26964716
C	-1.86807560	3.62941001	1.41721493
C	-2.90177268	3.89824054	2.33039304
C	-3.44567840	2.86582637	3.11325957
C	-2.95286791	1.55724110	2.97381998
C	-1.92643213	1.28283009	2.05435079
C	0.01142017	3.40409275	-1.03053745
C	-0.69419375	3.33520032	-2.25210319
C	-0.77879767	4.45371280	-3.09843753
C	-0.15740125	5.66150175	-2.74000452
C	0.54063811	5.74711395	-1.52287883
C	0.62193441	4.63140876	-0.67251940
H	0.95172810	-2.74618476	-2.51811074
H	0.78872780	-5.17512267	-3.05202115
H	1.41212718	-6.89296987	-1.32443661
H	2.22713745	-6.14870980	0.93143259
H	2.42833512	-3.72132736	1.45686167
H	4.49757912	-0.58773064	1.09582314
H	5.21886161	-0.58446199	3.47657320
H	3.58649873	-1.15923917	5.29861761
H	1.20141214	-1.69690666	4.70331302
H	0.46814876	-1.67726267	2.32524164
H	4.29835077	-2.81563817	-0.77153140
H	6.37394589	-2.34414100	-2.06030283
H	6.65142183	-0.15065543	-3.25733961
H	4.81798311	1.56590855	-3.14361229
H	2.74434079	1.09322587	-1.84549975
H	0.47982825	1.90746505	3.05361744
H	2.46920068	2.38534584	4.46540728
H	4.64415088	3.06834937	3.40652307
H	4.80519087	3.23392746	0.90132262
H	2.82249800	2.75843421	-0.51186978
H	-1.46253093	4.45123679	0.81010276
H	-3.28778431	4.92593705	2.42291037
H	-4.26133421	3.07840857	3.82239373
H	-3.38029668	0.73503658	3.56853396

H	-1.56785730	0.24909642	1.93049033
H	-1.19581275	2.40373242	-2.54920411
H	-1.33411148	4.37348668	-4.04593875
H	-0.21799982	6.53605019	-3.40708446
H	1.02651755	6.69079299	-1.22756933
H	1.16482567	4.72259329	0.27943433

Sum of electronic and zero-point Energies= -3827.797329
Sum of electronic and thermal Energies= -3827.746734
Sum of electronic and thermal Enthalpies= -3827.745790
Sum of electronic and thermal Free Energies= -3827.887898

$TS_{12\text{-}12'}$

Ru	-0.22463703	-0.16621772	-0.82075493
S	-1.23596934	-1.89604652	0.30958208
S	-2.38925208	0.34519531	-1.51191964
P	0.01096459	1.94415770	0.10844888
P	1.85030841	-1.22549059	-0.22242998
O	0.73295744	0.49553813	-3.61041396
C	0.42633111	0.32215383	-2.49225059
C	-3.46526092	-0.74293817	-0.70729818
C	-2.96249827	-1.73592573	0.12035313
C	-4.94693109	-0.51198136	-1.01690029
C	-3.72766435	-2.77650667	0.92084794
F	-5.53129293	-1.60882605	-1.58137455
F	-5.12966401	0.51205593	-1.89739035
F	-5.66264769	-0.18850335	0.10027650
F	-3.44672060	-2.66607816	2.26423479
F	-3.36606126	-4.04727316	0.56096610
F	-5.07637603	-2.70555443	0.80686722
C	1.72448958	-3.05111416	-0.50463289
C	1.27062614	-3.48095860	-1.77359007
C	1.18378376	-4.84818419	-2.07338305
C	1.53554613	-5.80768401	-1.10533697
C	1.98232327	-5.38948009	0.15809654
C	2.08281330	-4.01769014	0.45813736
C	2.42879318	-1.12774246	1.53131775
C	3.75630664	-0.79866778	1.88021392
C	4.15839472	-0.79341853	3.22822185
C	3.24507968	-1.12055357	4.24362899
C	1.91668371	-1.43726575	3.90602224
C	1.50839329	-1.43182141	2.56266047
C	3.38085372	-0.85685149	-1.19837209
C	4.42254927	-1.81309067	-1.27233282
C	5.59220673	-1.54144814	-1.99991333
C	5.73940966	-0.31511061	-2.67326050
C	4.70865879	0.63683089	-2.61402087
C	3.53963488	0.36576030	-1.88108674
C	1.49467936	2.30188778	1.15168636
C	1.43687599	2.20118671	2.55970961
C	2.56686965	2.49155431	3.34335273
C	3.77027717	2.88745056	2.73662057
C	3.84172985	2.98223160	1.33559948
C	2.71550453	2.68854202	0.55061809
C	-1.37765645	2.28702204	1.28963389
C	-1.91214203	3.58688407	1.44015355
C	-2.93962560	3.83066843	2.36740989
C	-3.44329374	2.78690505	3.16192401
C	-2.91705135	1.49168804	3.01928603
C	-1.89757676	1.24168945	2.08535161
C	-0.03589214	3.41344970	-1.01780071
C	-0.73080209	3.34000085	-2.24501159
C	-0.83331146	4.46403974	-3.08218491
C	-0.24110315	5.68171389	-2.70834090
C	0.44658348	5.77150056	-1.48551674
C	0.54621929	4.65015519	-0.64477371
H	0.97261821	-2.73730955	-2.52974528
H	0.82731816	-5.16684386	-3.06561792
H	1.45448205	-6.88164347	-1.33651250
H	2.25478996	-6.13367354	0.92336272
H	2.43785782	-3.70536291	1.45125213
H	4.48693544	-0.54708560	1.09806698
H	5.19873862	-0.53434532	3.48176192
H	3.56564799	-1.12623425	5.29766747
H	1.18938864	-1.69240014	4.69316631
H	0.46552903	-1.68339677	2.31208862
H	4.31495338	-2.78345292	-0.76437355
H	6.39063297	-2.29895868	-2.04835791
H	6.65320188	-0.10755208	-3.25248813
H	4.80518974	1.59397686	-3.15041357
H	2.73164360	1.10848383	-1.85629759
H	0.49838564	1.90970618	3.05301292
H	2.49910055	2.41236082	4.43960222
H	4.65169443	3.12341167	3.35369189
H	4.77836161	3.29429096	0.84692041
H	2.78265111	2.79729378	-0.54129825
H	-1.53818443	4.41727076	0.82447987
H	-3.35245302	4.84770022	2.46193747
H	-4.25370724	2.97989027	3.88256614
H	-3.31240602	0.66044158	3.62371912
H	-1.51476473	0.21702885	1.95890100
H	-1.20901774	2.40038414	-2.55465149
H	-1.37956624	4.38027877	-4.03463065
H	-0.31598706	6.56075165	-3.36803356
H	0.91016607	6.72267312	-1.17864597
H	1.08163499	4.74352708	0.31126331

Sum of electronic and zero-point Energies= -3827.796542
Sum of electronic and thermal Energies= -3827.746841
Sum of electronic and thermal Enthalpies= -3827.745897
Sum of electronic and thermal Free Energies= -3827.885267

$TS_{12\text{-}7}$

Ru	-0.11426633	-0.17297089	-0.85151963
S	-1.15438584	-1.63431659	0.62371031
S	-2.17685641	-0.10479037	-1.87989286
P	-0.14790240	1.88002828	0.15523955
P	1.96531172	-1.20667114	-0.19930947
O	1.17294541	0.87125407	-3.40886127
C	0.70296302	0.50922487	-2.40041318
C	-3.29393115	-0.98227220	-0.89090856
C	-2.84195318	-1.65170455	0.23949502
C	-4.74468078	-0.92110994	-1.35671064
C	-3.71243986	-2.49469365	1.16552822
F	-5.38450556	-2.12055510	-1.25155353
F	-4.84161116	-0.54733830	-2.66545696
F	-5.47528386	-0.01074079	-0.64038557
F	-3.10242158	-2.73130696	2.36384913
F	-3.99325379	-3.72324611	0.63109313
F	-4.90498783	-1.89791731	1.45228238
C	1.82176669	-3.03966001	-0.39830286
C	1.05809027	-3.54332647	-1.47579964
C	0.97505239	-4.92574810	-1.70662837
C	1.64418250	-5.82460794	-0.85634885
C	2.40666197	-5.33268800	0.21665190
C	2.50242573	-3.94777120	0.44210413
C	2.61421630	-1.04406017	1.52518504
C	3.89628698	-0.53029050	1.81657865
C	4.33802434	-0.42607994	3.14841124
C	3.51136657	-0.83913668	4.20593606
C	2.23437916	-1.35985387	3.92487885
C	1.78632253	-1.45854259	2.59755692

C	3.44493995	-0.84260838	-1.24503615
C	4.18660642	-1.86329626	-1.88119353
C	5.30526545	-1.54428618	-2.67109718
C	5.70514612	-0.20714459	-2.83068192
C	4.97498405	0.81421409	-2.19800611
C	3.85074155	0.49932864	-1.41825544
C	1.42028941	2.64634085	0.78262321
C	1.83934577	2.60087087	2.12967539
C	3.03986385	3.21769530	2.52634768
C	3.83938029	3.89057753	1.58835385
C	3.43130860	3.94329024	0.24298036
C	2.23579745	3.32553472	-0.15686212
C	-1.29888313	1.87378176	1.60347376
C	-2.50305051	2.61196790	1.58621721
C	-3.38429558	2.56678600	2.68183029
C	-3.07489930	1.79229430	3.81047764
C	-1.88670482	1.03937646	3.82930209
C	-1.01551684	1.06602275	2.73003941
C	-0.76427275	3.31819753	-0.84270149
C	-1.28134838	3.18519939	-2.14588642
C	-1.74154903	4.31132046	-2.85455030
C	-1.69371265	5.58453022	-2.26689202
C	-1.18140978	5.73053361	-0.96365847
C	-0.71672664	4.61004326	-0.25976379
H	0.51310718	-2.84593786	-2.13243083
H	0.37275856	-5.30199556	-2.54843207
H	1.56693702	-6.90994963	-1.02836307
H	2.93272240	-6.03041281	0.88761301
H	3.10952067	-3.57560129	1.28073181
H	4.56219631	-0.21214472	1.00140412
H	5.34250487	-0.02364752	3.35535547
H	3.86214397	-0.76365463	5.24752349
H	1.58157823	-1.69980080	4.74469819
H	0.78950791	-1.88200389	2.39435919
H	3.89080179	-2.91579650	-1.76622896
H	5.86683787	-2.35282922	-3.16560374
H	6.58119451	0.03964343	-3.45126640
H	5.27563290	1.86717824	-2.31759062
H	3.28557549	1.30871412	-0.93452972
H	1.22136467	2.10289183	2.88891693
H	3.34300196	3.17593083	3.58433886
H	4.77412854	4.38033147	1.90417156
H	4.04223844	4.47885900	-0.50116841
H	1.92021090	3.39375652	-1.20984603
H	-2.76880815	3.21993269	0.71016759
H	-4.32405623	3.13983270	2.64266793
H	-3.76625495	1.75811011	4.66716282
H	-1.64499325	0.40777396	4.69851208
H	-0.12006803	0.42761011	2.74013790
H	-1.33856741	2.19535002	-2.61709684
H	-2.14035727	4.18282631	-3.87288417
H	-2.05436928	6.46542624	-2.82147707
H	-1.14064144	6.72533297	-0.49209273
H	-0.31458088	4.74075847	0.75681669

Sum of electronic and zero-point Energies= -3827.796798

Sum of electronic and thermal Energies= -3827.747024

Sum of electronic and thermal Enthalpies= -3827.746080

Sum of electronic and thermal Free Energies= -3827.885410

$TS_{12\text{-}8}$

Ru	-0.32088068	-0.12413268	-0.71671525
S	-1.55376957	-1.80596969	0.23548689
S	-2.39753682	0.83191467	-1.18882403
P	0.40145218	1.96887987	0.06081514
P	1.58433378	-1.48211543	-0.18134197
O	0.45894239	0.14581979	-3.60800171
C	0.23957728	0.11033300	-2.45508588
C	-3.60374796	-0.22688098	-0.55223766
C	-3.24150665	-1.38660448	0.11537773
C	-5.04300783	0.24472286	-0.76639545
C	-4.20318302	-2.41036944	0.70071264
F	-5.87103467	-0.76896048	-1.14621285
F	-5.12705608	1.19706705	-1.73779234
F	-5.56961187	0.79997862	0.36655585
F	-3.59360260	-3.19677015	1.63762312
F	-4.70063327	-3.26143229	-0.24937229
F	-5.27337874	-1.83540615	1.32256223
C	1.20558563	-3.28169763	-0.39862476
C	0.71823434	-3.69230123	-1.66166651
C	0.44108847	-5.04389952	-1.91247880
C	0.63423475	-6.00462642	-0.90195239
C	1.11293146	-5.60452207	0.35552533
C	1.40262119	-4.25009735	0.60750296
C	2.20763222	-1.40806018	1.55715367
C	3.57387046	-1.27128572	1.88295334
C	3.98843474	-1.26863250	3.22715528
C	3.04842444	-1.40596490	4.26156233
C	1.68310660	-1.53194791	3.94634102
C	1.26443683	-1.52447302	2.60614241
C	3.12013229	-1.37034731	-1.21033334
C	4.05457890	-2.43458202	-1.19860202
C	5.21995047	-2.37143990	-1.97855875
C	5.46682633	-1.25142223	-2.79367312
C	4.54066329	-0.19643719	-2.82259916
C	3.37733667	-0.25702272	-2.03441042
C	2.01859162	2.11724737	0.94716127
C	2.07966552	2.09235947	2.35852927
C	3.31061324	2.22878059	3.02293971
C	4.49892490	2.39127023	2.29161621
C	4.45092931	2.40827780	0.88645746
C	3.22242648	2.27093859	0.22041660
C	-0.78178535	2.56863284	1.35861946
C	-1.04411290	3.94316060	1.54941656
C	-1.92230975	4.36595216	2.56231408
C	-2.54187023	3.42647749	3.40355427
C	-2.28418200	2.05652237	3.22238549
C	-1.41727907	1.63027365	2.20264707
C	0.48554026	3.38505268	-1.12838898
C	-0.28642240	3.35971121	-2.31042162
C	-0.27907967	4.45018962	-3.19703077
C	0.50278089	5.58350590	-2.91886140
C	1.27432132	5.62302131	-1.74414598
C	1.26577184	4.53561643	-0.85453129
H	0.54556501	-2.94569480	-2.45284043
H	0.06087276	-5.34768324	-2.90054958
H	0.40503913	-7.06449336	-1.09572124
H	1.26222915	-6.34889956	1.15382343
H	1.77958128	-3.95274749	1.59710840
H	4.32431827	-1.16380791	1.08666631
H	5.05895886	-1.15948543	3.46310807
H	3.37714759	-1.41195516	5.31306701
H	0.93581818	-1.63828709	4.74875629
H	0.19319687	-1.62670048	2.36935643
H	3.86339866	-3.32689305	-0.58310414
H	5.93470507	-3.20950309	-1.95789628
H	6.37574382	-1.20843814	-3.41468024
H	4.71429424	0.67729615	-3.47039782
H	2.64939402	0.56391054	-2.07768303
H	1.15833689	1.98024881	2.94796765
H	3.33495851	2.21348519	4.12376449
H	5.46155488	2.50703098	2.81453709
H	5.37469943	2.53839551	0.30065860
H	3.20191491	2.31978060	-0.87759839
H	-0.57651999	4.69426048	0.89659984

H	-2.12726183	5.44115907	2.68724472
H	-3.23488675	3.76032220	4.19197031
H	-2.77485077	1.30939218	3.86578838
H	-1.24792457	0.55310005	2.04606217
H	-0.90631345	2.48388847	-2.54830100
H	-0.88884583	4.40610715	-4.11291390
H	0.51267411	6.43553466	-3.61705457
H	1.89052502	6.50717097	-1.51521179
H	1.87638579	4.58532142	0.05906582

Sum of electronic and zero-point Energies= -3827.797356
Sum of electronic and thermal Energies= -3827.747640
Sum of electronic and thermal Enthalpies= -3827.746696
Sum of electronic and thermal Free Energies= -3827.885122

$TS_{1'\text{-}3'}$

C	-0.72664958	0.51850539	-2.34344966
C	1.64730901	4.37447380	-2.75400644
C	1.70188894	5.61081202	-2.09279247
C	1.27129798	5.70591401	-0.75539274
C	0.78695941	4.57090765	-0.08999272
C	1.30956282	1.88700096	1.61548827
C	1.03817640	1.74469820	2.99438158
C	2.08398798	1.71132812	3.93372068
C	3.42059992	1.80575020	3.51580908
C	3.70576514	1.93326898	2.14541806
C	2.66354704	1.97334714	1.20746363
C	-1.54032184	2.60261013	0.73819937
C	-2.03546912	-1.94211865	1.53348352
C	-1.48758270	-1.23235134	2.62422373
C	-1.56697903	-1.74810066	3.92865851
C	-2.18681417	-2.98797551	4.15887019
C	-2.72480310	-3.70832434	3.07792383
C	-2.65088355	-3.19118432	1.77366479
C	-2.21639130	-2.66219596	-1.26142102
C	-1.09426959	-3.37342676	-1.74398590
C	-1.26132423	-4.50796544	-2.55612163
C	-2.55077464	-4.94699412	-2.90187987
C	-2.27648768	3.22617902	-0.30043928
C	-3.67402411	-4.24850730	-2.42541005
C	-3.51068680	-3.11500937	-1.61049364
C	-3.56809182	-0.32261282	-0.29675974
C	-4.40666863	-0.11160175	0.81914576
C	-5.65516163	0.51728454	0.66469104
C	-6.08515688	0.94015142	-0.60343115
C	-5.25380376	0.73959490	-1.72035024
C	-4.00422133	0.11845017	-1.56961347
C	2.85072512	-1.59858323	0.25856432
C	3.27135073	-0.97521321	-0.91022376
C	-3.52061194	3.82213670	-0.04899351
C	4.70693073	-0.94337773	-1.42460108
C	3.75145376	-2.41391533	1.18262545
C	-4.06102435	3.81403641	1.24887779
C	-3.35534766	3.17949742	2.28247914
C	-2.11463773	2.56834764	2.02853698
C	0.72705210	3.31949877	-0.75036901
C	1.16359339	3.23313743	-2.08549623
F	3.18500079	-2.61044949	2.40672434
F	4.95589920	-1.81185251	1.40773691
F	4.01150200	-3.65950040	0.67638335
F	5.46563352	-0.00631596	-0.76913428
F	5.34663531	-2.13893408	-1.29122188
F	4.76431948	-0.62191168	-2.74879817
H	1.98626373	4.28650780	-3.79808982
H	2.08256233	6.50257729	-2.61569416
H	1.31445617	6.67134255	-0.22648990
H	0.45370606	4.65686811	0.95645061
H	0.01197159	1.65379136	3.36813745
H	1.84394978	1.60561528	5.00359740
H	4.23775450	1.77078412	4.25319740
H	4.74804190	1.99464415	1.79658862
H	2.90968229	2.06661052	0.13862952
H	-0.97622132	-0.27616474	2.44321796
H	-1.12554950	-1.18544635	4.76628750
H	-2.24021090	-3.39907461	5.17944953
H	-3.20233679	-4.68635622	3.24811520
H	-3.06943172	-3.76967163	0.93692675
H	-0.07946429	-3.03649814	-1.48050457
H	-0.37377906	-5.04684118	-2.92344926
H	-2.68116120	-5.83202351	-3.54481430
H	-1.86300127	3.26240773	-1.31986934
H	-4.68899180	-4.58555456	-2.69032812
H	-4.40021259	-2.57940010	-1.24708684
H	-4.09209594	-0.45262098	1.81627088
H	-6.29844547	0.66802744	1.54621386
H	-7.06795392	1.42320283	-0.72360936
H	-5.58076725	1.06407215	-2.72104454
H	-3.37894272	-0.04591542	-2.45904472
H	-4.06724865	4.30330474	-0.87504210
H	-5.03139641	4.29419913	1.45056727
H	-3.76927508	3.15412715	3.30304505
H	-1.60854987	2.06973025	2.86257021
H	1.14248911	2.27008582	-2.61267685
O	-1.19432944	0.87825509	-3.35647215
P	-1.94868800	-1.19905176	-0.15397274
P	0.08268118	1.87298744	0.22427202
Ru	0.10025889	-0.15577295	-0.80148563
S	1.18008395	-1.55655162	0.71751674
S	2.13269809	-0.11767085	-1.89414743

Sum of electronic and zero-point Energies= -3827.794805
Sum of electronic and thermal Energies= -3827.744893
Sum of electronic and thermal Enthalpies= -3827.743949
Sum of electronic and thermal Free Energies= -3827.883770

$TS_{3'\text{-}5'}$

C	-0.63179400	0.31058400	-2.33666900
C	1.56723400	4.13495800	-3.09061500
C	1.50945900	5.44434800	-2.59014800
C	0.99657100	5.67283100	-1.29927900
C	0.54358200	4.59818100	-0.52073800
C	1.14620900	2.23040400	1.53163200
C	0.78420700	2.99901600	2.66142200
C	1.73335000	3.28965300	3.65823900
C	3.05606700	2.83421700	3.53507300

C	3.43067300	2.09155400	2.40126400
C	2.48455100	1.79144800	1.40930100
C	-1.63396400	2.51578200	0.62185400
C	-2.41133600	-1.43169000	1.66515100
C	-1.50260200	-1.11500000	2.69697100
C	-1.85295100	-1.29568200	4.04729000
C	-3.12516700	-1.78359200	4.38674000
C	-4.04479000	-2.09181900	3.36761200
C	-3.69092900	-1.92169700	2.01976300
C	-1.89506600	-3.04983600	-0.66858000
C	-0.69333600	-3.72977000	-0.95984400
C	-0.70658500	-5.08192000	-1.34879500
C	-1.92150800	-5.77580600	-1.45641900
C	-2.40656600	3.31642500	-0.25112600
C	-3.12784400	-5.10687900	-1.17901300
C	-3.11568200	-3.75783600	-0.79341400
C	-3.39525700	-0.63574300	-0.95806500
C	-4.30242700	0.23886900	-0.32175600
C	-5.41845100	0.73800200	-1.01609300
C	-5.64058400	0.37970200	-2.35603300
C	-4.73506800	-0.48009400	-3.00266100
C	-3.62278800	-0.98474900	-2.31100500
C	2.96511700	-1.57836900	0.41113900
C	3.36978300	-1.04247300	-0.80520600
C	-3.66376600	3.80151400	0.14698900
C	4.79826800	-1.05016800	-1.34006100
C	3.87509900	-2.32442800	1.38332000
C	-4.17097000	3.49739000	1.42212200
C	-3.42638700	2.67383900	2.28568300
C	-2.17475200	2.17612700	1.88470000
C	0.58726400	3.27322900	-1.02089000
C	1.11001800	3.05628900	-2.31033600
F	3.32347900	-2.42431800	2.62557200
F	5.08325800	-1.70888900	1.54717300
F	4.12671000	-3.60432700	0.96970600
F	5.56589500	-0.07282600	-0.76013100
F	5.43473600	-2.23662000	-1.13074700
F	4.83815600	-0.82256200	-2.68360700
H	1.97458000	3.94034800	-4.09502500
H	1.86907100	6.28809400	-3.20031500
H	0.95466400	6.69564600	-0.89217900
H	0.15745800	4.79447800	0.49124600
H	-0.23793700	3.38760400	2.77167600
H	1.43086100	3.88376800	4.53547600
H	3.79644300	3.06200100	4.31821500
H	4.46624200	1.73639600	2.28456600
H	2.79456300	1.21907500	0.52247300
H	-0.50331400	-0.72833400	2.44656200
H	-1.12146600	-1.05296900	4.83416800
H	-3.40197200	-1.92521500	5.44362100
H	-5.04724800	-2.47105000	3.62263700
H	-4.42840600	-2.16568800	1.24173400
H	0.26706200	-3.20138000	-0.87628000
H	0.24568600	-5.58930100	-1.56958500
H	-1.93240500	-6.83418800	-1.76186900
H	-2.01883900	3.57611400	-1.24740800
H	-4.08918200	-5.63760800	-1.26855000
H	-4.07379300	-3.25090000	-0.60798300
H	-4.14312600	0.53446300	0.72519600
H	-6.11778100	1.41382500	-0.49905300
H	-6.51690200	0.77015800	-2.89749200
H	-4.89438500	-0.76465400	-4.05468300
H	-2.93039400	-1.66464500	-2.82984600
H	-4.24614900	4.42889000	-0.54611900
H	-5.14804100	3.89448900	1.74033800
H	-3.81919200	2.41327600	3.28124100
H	-1.61618400	1.52203000	2.56862000
H	1.18183400	2.03800300	-2.71341300
O	-1.08699400	0.59092900	-3.37671200
P	-1.88644100	-1.27082400	-0.10745900
P	0.02219500	1.89691100	0.09535000
Ru	0.18682300	-0.22935400	-0.73586500
S	1.30291800	-1.47840400	0.89148600
S	2.21934900	-0.23877500	-1.82294900

Sum of electronic and zero-point Energies= -3827.795687

Sum of electronic and thermal Energies= -3827.746160

Sum of electronic and thermal Enthalpies= -3827.745216

Sum of electronic and thermal Free Energies= -3827.883033

$TS_{1'\text{-}2'}$

C	0.05213900	0.00665000	-2.29741600
C	-0.01698600	-4.41878000	-3.21903000
C	0.91920700	-5.45618500	-3.08093400
C	1.84423000	-5.42112400	-2.02185200
C	1.83260800	-4.35429400	-1.10904700
C	0.14543200	-2.67532600	1.51852400
C	-0.21514100	-1.81353300	2.58054600
C	-0.76032900	-2.33091600	3.76626700
C	-0.97309700	-3.71498500	3.89999200
C	-0.63148300	-4.57592500	2.84394000
C	-0.07071300	-4.06259500	1.66056800
C	2.66606600	-1.83517300	0.40127800
C	1.21067100	2.07079000	1.80074000
C	0.37912500	3.05327500	2.38727500
C	0.32721700	3.20198400	3.78339100
C	1.10231300	2.37630800	4.61634400
C	1.92254200	1.38868100	4.04343900
C	1.97066400	1.22986500	2.64783600
C	0.79345700	3.42685900	-0.74377900
C	-0.04659000	3.55119200	-1.86997300
C	-0.23689000	4.80321800	-2.48248000
C	0.40557900	5.94382300	-1.97562200
C	3.58373700	-1.58951700	-0.64610900
C	1.25125700	5.82822500	-0.85655600
C	1.45028600	4.57895300	-0.24975000
C	2.94630500	1.70230300	-0.55050800
C	3.19395900	1.44463300	-1.91887700
C	4.49380000	1.53637800	-2.44060600
C	5.57033500	1.87807300	-1.60226900
C	5.33343100	2.13509900	-0.24192600
C	4.03010900	2.05709300	0.28117900
C	-3.54082800	0.89685400	-0.03221500
C	-3.65632000	-0.44680600	-0.33659400
C	4.96421100	-1.57274000	-0.39584200
C	-4.97156600	-1.21747100	-0.42226600
C	-4.69597500	1.85768000	0.20960100
C	5.45056600	-1.79156400	0.90614500
C	4.54701000	-2.03384500	1.95386700
C	3.16202800	-2.06120000	1.70442600
C	0.88951400	-3.30449500	-1.23754100
C	-0.03240900	-3.35030200	-2.30492500
F	-4.29031000	2.97381000	0.88554500
F	-5.69951000	1.30534900	0.94898300
F	-5.25496100	2.29882000	-0.96037400
F	-5.47430600	-1.51024300	0.81577200
F	-5.93515900	-0.52922800	-1.09865200
F	-4.82264900	-2.40963000	-1.06757400
H	-0.74412200	-4.43246200	-4.04595100
H	0.93237500	-6.29077100	-3.79990600
H	2.58582300	-6.22769400	-1.90657500
H	2.57133300	-4.33632900	-0.29357200
H	-0.08295600	-0.72442500	2.47558000
H	-1.03633900	-1.64460500	4.58218000
H	-1.41708100	-4.11998000	4.82317700

H	-0.80823700	-5.65953500	2.93409900
H	0.18141500	-4.74999800	0.84006900
H	-0.24208100	3.70171700	1.75217000
H	-0.32887500	3.97085400	4.22109900
H	1.06267000	2.49857400	5.71035100
H	2.52895600	0.73040500	4.68577800
H	2.60391400	0.43892900	2.21813600
H	-0.56401900	2.66753200	-2.26853200
H	-0.89934000	4.88206700	-3.35870200
H	0.25084000	6.92480300	-2.45238400
H	3.21696000	-1.43254700	-1.67188900
H	1.76490300	6.71676900	-0.45610700
H	2.12877100	4.50135500	0.61392000
H	2.36342900	1.18891500	-2.59368000
H	4.66372400	1.34335100	-3.51180800
H	6.59059200	1.95165900	-2.01131900
H	6.16759100	2.41095000	0.42283400
H	3.86457200	2.28757300	1.34348100
H	5.66423000	-1.38542000	-1.22457700
H	6.53463000	-1.77904500	1.10114600
H	4.91876200	-2.21877000	2.97444600
H	2.46587600	-2.27788200	2.52843600
H	-0.77480900	-2.54953600	-2.42882700
O	0.22970300	0.02154600	-3.46128300
P	1.17380500	1.76427400	-0.01491800
P	0.86591400	-1.91998000	-0.00682800
Ru	-0.40358300	0.03267800	-0.53787800
S	-1.95958200	1.62352600	0.02834400
S	-2.23317100	-1.40277100	-0.59389000

Sum of electronic and zero-point Energies= -3827.798096
Sum of electronic and thermal Energies= -3827.748422
Sum of electronic and thermal Enthalpies= -3827.747478
Sum of electronic and thermal Free Energies= -3827.884969

$TS_{2'\text{-}5'}$

C	-0.01616076	0.06235681	-2.25751406
C	-0.54949745	-4.55135333	-2.88480426
C	-0.14247261	-5.80778042	-2.41022512
C	0.54327316	-5.90196191	-1.18395638
C	0.81580590	-4.74532824	-0.43880154
C	0.42037079	-2.44760681	1.79536752
C	1.00508260	-1.82495190	2.92171233
C	0.60310542	-2.16597626	4.22466257
C	-0.40550229	-3.12056874	4.43100579
C	-1.01758467	-3.72396308	3.31918206
C	-0.61313299	-3.39040779	2.01686435
C	2.70174333	-2.04853504	-0.06907147
C	1.74101980	1.80581280	1.74558066
C	0.70180197	1.76151286	2.70614990
C	0.99276266	1.84264889	4.07807630
C	2.32631887	1.94239086	4.51423899
C	3.36626492	1.96872121	3.56862536
C	3.07777430	1.90833432	2.19288476
C	0.64699860	3.43729229	-0.37364574
C	0.29810846	3.74886102	-1.70873965
C	-0.15425710	5.03360546	-2.04377182
C	-0.27103262	6.02353551	-1.05078328
C	3.30422841	-2.79724507	-1.10934169
C	0.07139706	5.72080459	0.27678004
C	0.53000748	4.43457818	0.61646870
C	2.84214104	1.80241875	-0.98376848
C	3.21745530	0.77132707	-1.86694725
C	4.39541184	0.87374928	-2.62853223
C	5.21449085	2.00805561	-2.51230533
C	4.84593382	3.04827311	-1.63872179
C	3.66451544	2.95220262	-0.88746770
C	-3.50449463	1.01600819	-0.12429284
C	-3.64277509	-0.35506103	-0.24021611
C	4.70229106	-2.85310980	-1.24347103
C	-4.96783561	-1.11090940	-0.23149766
C	-4.64988507	2.01571562	-0.03176857
C	5.53204542	-2.16946351	-0.33969389
C	4.94720407	-1.40682225	0.68455261
C	3.55017642	-1.33484265	0.80821106
C	0.40056440	-3.47302234	-0.90491984
C	-0.28046976	-3.38976367	-2.13640469
F	-4.23369325	3.21465218	0.47242099
F	-5.65972308	1.58823633	0.77983803
F	-5.20280411	2.28255273	-1.25508045
F	-5.47931751	-1.23200712	1.03280143
F	-5.92163508	-0.50799463	-0.99659500
F	-4.83284854	-2.38122554	-0.71157512
H	-1.08693761	-4.46574505	-3.84207485
H	-0.35819682	-6.71694324	-2.99375375
H	0.86978399	-6.88376054	-0.80570806
H	1.36163558	-4.83122253	0.51349565
H	1.77033876	-1.04790919	2.80518622
H	1.08232966	-1.66860091	5.08253354
H	-0.72237478	-3.38447512	5.45236053
H	-1.82405855	-4.46068697	3.46074912
H	-1.12112316	-3.86494054	1.16582672
H	-0.34463932	1.66295127	2.37362675
H	0.16951657	1.81771919	4.80925954
H	2.55515051	1.99804855	5.59040346
H	4.41394966	2.04483276	3.90115428
H	3.90208152	1.93903204	1.46507242
H	0.37759389	2.98121256	-2.49439403
H	-0.42543222	5.25998589	-3.08695146
H	-0.63394600	7.02987215	-1.31323458
H	2.68045145	-3.34853670	-1.82662090
H	-0.01983341	6.48884006	1.06122576
H	0.79321265	4.21372779	1.66130440
H	2.57988950	-0.11673628	-1.96903865
H	4.66657132	0.06028679	-3.31905088
H	6.13562732	2.09013593	-3.11107792
H	5.47450904	3.94903766	-1.55351406
H	3.36778994	3.78876504	-0.23592680
H	5.14227112	-3.44712745	-2.06044120
H	6.62772776	-2.22340192	-0.43805931
H	5.58117566	-0.85062538	1.39308950
H	3.13182755	-0.69513965	1.59465407
H	-0.61171709	-2.41402924	-2.51611902
O	0.09991135	0.10908519	-3.42769161
P	1.25712743	1.72336385	-0.03675051
P	0.84692219	-1.95506058	0.05402353
Ru	-0.38713987	0.03882232	-0.48225674
S	-1.91733194	1.72754198	-0.14078995
S	-2.22954416	-1.35536049	-0.35150597

Sum of electronic and zero-point Energies= -3827.795846
Sum of electronic and thermal Energies= -3827.746050
Sum of electronic and thermal Enthalpies= -3827.745106
Sum of electronic and thermal Free Energies= -3827.884271

$TS_{1'\text{-}4'}$

C	0.64030300	-0.14017500	-2.45341900
C	-0.12490900	-4.63507400	-2.65011900
C	1.04043200	-5.34752100	-2.98642000
C	2.27305600	-4.96422900	-2.43231600
C	2.34452500	-3.87560100	-1.54463100
C	0.77151200	-2.54720300	1.58248000

C	0.71537800	-1.77003900	2.76272200
C	0.39386600	-2.36369800	3.99282500
C	0.10863900	-3.73956600	4.06264800
C	0.15621100	-4.51772300	2.89490300
C	0.48995000	-3.92874700	1.66146800
C	3.03545200	-1.44910700	0.16578000
C	1.20819700	2.02609700	1.74517600
C	2.36352000	1.38210000	2.25039100
C	2.68894000	1.46159500	3.61539300
C	1.85164300	2.15916300	4.50401800
C	0.68582700	2.77475400	4.01748200
C	0.36756500	2.71481700	2.64969500
C	-0.38201600	3.33547300	-0.26236200
C	-1.75390700	3.17686800	-0.54203500
C	-2.58862900	4.30141000	-0.68179300
C	-2.06139500	5.59501300	-0.54329000
C	3.71057100	-0.69103500	-0.81819400
C	-0.69179300	5.76340700	-0.26496400
C	0.14296100	4.64407900	-0.12861900
C	2.22854500	2.53514800	-0.95810600
C	3.43893400	2.93968700	-0.35389500
C	4.48115800	3.47747200	-1.13182200
C	4.32878400	3.62724600	-2.51975600
C	3.11834800	3.24718000	-3.12820100
C	2.07823200	2.70989400	-2.35486600
C	-3.23738900	-0.25737600	0.54695800
C	-3.51134500	-0.34842900	-0.81286700
C	5.09974000	-0.49622600	-0.74143500
C	-4.89578900	-0.53339800	-1.42316000
C	-4.30020100	-0.24398200	1.64813400
C	5.83343500	-1.04465300	0.32591200
C	5.17065700	-1.79778300	1.31071200
C	3.78199300	-2.00511800	1.23032500
C	1.18030100	-3.14914700	-1.20887900
C	-0.05553600	-3.54082200	-1.77318500
F	-3.76676100	-0.49300300	2.87664400
F	-5.26917300	-1.18144100	1.45104600
F	-4.92067500	0.97281100	1.73594300
F	-5.32709700	-1.83078400	-1.33477400
F	-5.84571100	0.24577200	-0.82811400
F	-4.91276600	-0.21306600	-2.74863400
H	-1.09665900	-4.92497400	-3.08001900
H	0.98733100	-6.19852800	-3.68396500
H	3.19204400	-5.51360400	-2.69194400
H	3.31693800	-3.59283500	-1.11594800
H	0.92695400	-0.69155300	2.72506600
H	0.35342100	-1.74139400	4.90047100
H	-0.15605200	-4.20210000	5.02673400
H	-0.06875200	-5.59530100	2.93708400
H	0.52595400	-4.55344900	0.75753100
H	3.01402600	0.80382500	1.57813200
H	3.59977100	0.96433400	3.98473200
H	2.10430100	2.21695900	5.57465700
H	0.01413900	3.31154000	4.70596900
H	-0.54580400	3.20681600	2.28546000
H	-2.17428300	2.16830400	-0.66207500
H	-3.65783500	4.15652600	-0.90187400
H	-2.71500200	6.47477800	-0.65521200
H	3.15032200	-0.24641700	-1.65339400
H	-0.26835700	6.77487300	-0.15781500
H	1.21343400	4.79114300	0.08240400
H	3.57499100	2.85369300	0.73308400
H	5.41721500	3.78772100	-0.64044900
H	5.14597300	4.04895700	-3.12629400
H	2.97811800	3.37360100	-4.21324500
H	1.12961500	2.44113800	-2.84309400
H	5.60735000	0.09551200	-1.51891400
H	6.92172400	-0.88570400	0.38936000
H	5.73767800	-2.23514400	2.14812200
H	3.27682300	-2.60553600	2.00110700
H	-0.96886000	-2.97395200	-1.53310900
O	1.11618100	-0.22080200	-3.51920400
P	0.75698700	1.88366100	-0.04022800
P	1.21612400	-1.73220200	-0.01453300
Ru	-0.23796100	-0.08449500	-0.78996100
S	-1.61215000	-0.10136700	1.10991300
S	-2.19830600	-0.31788500	-1.95393500

Sum of electronic and zero-point Energies= -3827.799460

Sum of electronic and thermal Energies= -3827.749751

Sum of electronic and thermal Enthalpies= -3827.748807

Sum of electronic and thermal Free Energies= -3827.887848

$TS_{4'\text{-}8'}$

Ru	0.40151500	0.03377400	-0.54280600
S	2.24144700	-1.38800100	-0.59734000
S	1.94663000	1.63636700	0.02188700
P	-0.84932300	-1.92417900	0.00132100
P	-1.18812100	1.75644800	-0.02242800
O	-0.24632000	0.00346500	-3.46357400
C	-0.06305700	-0.00577900	-2.30054000
C	3.53435700	0.92579000	-0.05551600
C	3.65690000	-0.42405000	-0.32937000
C	4.68571700	1.87557500	0.24621700
C	4.97711200	-1.17807000	-0.46407400
F	5.74798400	1.70124900	-0.59126800
F	5.15362900	1.72563800	1.52560900
F	4.31136600	3.18292300	0.12901800
F	4.80294300	-2.52757500	-0.36990000
F	5.87736500	-0.83719700	0.50130800
F	5.57334500	-0.94812300	-1.67366300
C	-0.82431600	3.41649400	-0.76561500
C	0.01664800	3.54082800	-1.89105100
C	0.19440500	4.78983000	-2.51345800
C	-0.46152300	5.92743000	-2.01725000
C	-1.30810300	5.81176200	-0.89885200
C	-1.49468700	4.56537500	-0.28229600
C	-1.22030500	2.07739100	1.79079500
C	-1.96549800	1.23319000	2.64776600
C	-1.91365600	1.40358900	4.04183500
C	-1.10397400	2.40630700	4.60348100
C	-0.34353700	3.23563700	3.76077100
C	-0.39963500	3.07553700	2.36603200
C	-2.96252100	1.67686100	-0.54969000
C	-4.04621800	2.02176800	0.28622000
C	-5.35253000	2.08610600	-0.23135000
C	-5.59277300	1.82487600	-1.59027300
C	-4.51651600	1.49270500	-2.43280600
C	-3.21358500	1.41473600	-1.91665700
C	-2.64931600	-1.85098700	0.41170900
C	-3.14137200	-2.07223500	1.71715100
C	-4.52620700	-2.05555500	1.96835700
C	-5.43329100	-1.82887200	0.92020900
C	-4.95071500	-1.61471700	-0.38396800
C	-3.57050800	-1.62072900	-0.63609500
C	-0.12001600	-2.66368800	1.53037200
C	0.10813700	-4.04815300	1.68081300
C	0.67507700	-4.54926800	2.86646000
C	1.01113600	-3.67886700	3.91652100
C	0.78661700	-2.29750300	3.77435600
C	0.23512500	-1.79222000	2.58631400
C	-0.86424100	-3.31650900	-1.22057500
C	0.05239600	-3.35934100	-2.29257700
C	0.04323100	-4.43349000	-3.20009700
C	-0.88141700	-5.47963300	-3.05065000

C	-1.80131200	-5.44750700	-1.98700900
C	-1.79596300	-4.37499400	-1.08084700
H	0.54456100	2.65961300	-2.28114300
H	0.85766700	4.86880000	-3.38905200
H	-0.31663500	6.90609500	-2.50180800
H	-1.83226200	6.69786400	-0.50669900
H	-2.17418800	4.48730500	0.58055200
H	-2.59019500	0.43080600	2.22677700
H	-2.50867200	0.74253400	4.69193600
H	-1.06118800	2.53757600	5.69632100
H	0.30408400	4.01654500	4.18970800
H	0.20954600	3.72762800	1.72305200
H	-3.87843700	2.25540700	1.34746800
H	-6.18647800	2.35460900	0.43667800
H	-6.61546800	1.88778500	-1.99499700
H	-4.68914400	1.29650900	-3.50300200
H	-2.38350900	1.16667100	-2.59488600
H	-2.44217900	-2.27724800	2.54157900
H	-4.89491000	-2.23665300	2.99072500
H	-6.51716200	-1.82484100	1.11662900
H	-5.65356700	-1.43954400	-1.21295400
H	-3.20643800	-1.46753900	-1.66343100
H	-0.13916100	-4.74286900	0.86504700
H	0.86113500	-5.63075900	2.96307200
H	1.45990000	-4.07430800	4.84154100
H	1.05821200	-1.60366600	4.58537900
H	0.09397800	-0.70492000	2.47474000
H	0.78529000	-2.55135400	-2.42570200
H	0.76598000	-4.44471400	-4.03089500
H	-0.88970400	-6.31873300	-3.76441500
H	-2.53403300	-6.26086000	-1.86301200
H	-2.53080500	-4.35937600	-0.26180300

Sum of electronic and zero-point Energies= -3827.797917
Sum of electronic and thermal Energies= -3827.748245
Sum of electronic and thermal Enthalpies= -3827.747301
Sum of electronic and thermal Free Energies= -3827.884759

$TS_{8'\text{-}12'}$

Ru	-0.33347300	-0.11871200	-0.70491100
S	-1.59506400	-1.79908600	0.20872400
S	-2.39140900	0.89505100	-1.13376400
P	0.44751600	1.96434200	0.05729300
P	1.55083500	-1.50805200	-0.17598200
O	0.41347700	0.10980600	-3.60667900
C	0.20915900	0.08809400	-2.45039800
C	-3.61678000	-0.15816400	-0.52483800
C	-3.27659200	-1.35903900	0.07878800
C	-5.04880200	0.32616600	-0.75813900
C	-4.25556100	-2.35052400	0.69093700
F	-5.64405400	-0.33128300	-1.79742200
F	-5.09439200	1.65358300	-1.06386400
F	-5.83998100	0.15528700	0.33946700
F	-4.67654500	-1.94936800	1.93527900
F	-3.69411300	-3.58217400	0.85898700
F	-5.37450400	-2.53595400	-0.06526200
C	1.14950900	-3.30241800	-0.39550400
C	0.66669400	-3.70631700	-1.66242600
C	0.37461300	-5.05421600	-1.91605600
C	0.54819800	-6.01773700	-0.90469000
C	1.02208900	-5.62416000	0.35664800
C	1.32647200	-4.27355100	0.61166200
C	2.17227500	-1.44258000	1.56327400
C	3.53877200	-1.32018400	1.89347400
C	3.94883700	-1.32077400	3.23905700
C	3.00400100	-1.44665700	4.27054000
C	1.63841700	-1.55822900	3.95098300
C	1.22450900	-1.54784000	2.60933700
C	3.08755500	-1.41861900	-1.20574200
C	4.01669300	-2.48728400	-1.17722700
C	5.18041900	-2.44398400	-1.96088300
C	5.43035800	-1.34035600	-2.79725700
C	4.50894800	-0.28189100	-2.84362700
C	3.34760400	-0.32217800	-2.05110200
C	2.07802900	2.08520600	0.92397900
C	2.15596000	2.07118600	2.33465900
C	3.39740600	2.18892200	2.98298400
C	4.57967400	2.32159200	2.23606700
C	4.51471900	2.32777900	0.83146100
C	3.27567900	2.20936200	0.18148200
C	-0.70715200	2.59044200	1.36835600
C	-0.95056100	3.96904200	1.55312800
C	-1.80966800	4.40901000	2.57523100
C	-2.42819900	3.48269000	3.43159800
C	-2.18888400	2.10842100	3.25675500
C	-1.34146500	1.66540100	2.22797300
C	0.54591800	3.37455700	-1.13760700
C	-0.23337900	3.35685400	-2.31490900
C	-0.21339700	4.44353500	-3.20603500
C	0.58854800	5.56497000	-2.93706600
C	1.36785200	5.59654000	-1.76718800
C	1.34687400	4.51299200	-0.87314100
H	0.51008900	-2.95743800	-2.45477600
H	-0.00162300	-5.35281000	-2.90723500
H	0.30763800	-7.07463700	-1.10086100
H	1.15620800	-6.37074800	1.15557700
H	1.69965000	-3.98148600	1.60428200
H	4.29297700	-1.22040300	1.09975100
H	5.01965500	-1.22269100	3.47845900
H	3.32911600	-1.45473000	5.32314400
H	0.88737000	-1.65533900	4.75104900
H	0.15311600	-1.63846600	2.36855200
H	3.82227500	-3.36799500	-0.54614800
H	5.89121500	-3.28496800	-1.92672900
H	6.33783200	-1.31321100	-3.42126700
H	4.68476900	0.57870700	-3.50820800
H	2.62318400	0.50115300	-2.10744800
H	1.24009600	1.98239600	2.93639900
H	3.43477600	2.18272800	4.08354400
H	5.55074000	2.42280200	2.74627900
H	5.43356900	2.43467200	0.23335900
H	3.24284000	2.24961200	-0.91653400
H	-0.48370500	4.71003200	0.88830900
H	-2.00056800	5.48734800	2.69532000
H	-3.10615100	3.83008300	4.22724600
H	-2.67903400	1.37129900	3.91199400
H	-1.18743800	0.58523100	2.07635700
H	-0.86831100	2.48982300	-2.54540800
H	-0.82912500	4.40585400	-4.11821200
H	0.60819500	6.41394400	-3.63876900
H	1.99999200	6.47129900	-1.54574600
H	1.96417200	4.55584600	0.03633100

Sum of electronic and zero-point Energies= -3827.797188
Sum of electronic and thermal Energies= -3827.747478
Sum of electronic and thermal Enthalpies= -3827.746534
Sum of electronic and thermal Free Energies= -3827.884900

$TS_{2'\text{-}11'}$

C	-0.23984900	0.11060100	-2.45519100
C	0.27973800	4.45031300	-3.19686900
C	-0.50202500	5.58368600	-2.91865700

C	-1.27358300	5.62320900	-1.74395500
C	-1.26514800	4.53575700	-0.85439500
C	0.78238800	2.56841100	1.35856600
C	1.41810300	1.62992900	2.20228500
C	2.28510300	2.05604100	3.22200100
C	2.54265900	3.42598100	3.40345500
C	1.92287400	4.36558300	2.56252100
C	1.04458600	3.94292600	1.54964900
C	-2.01807300	2.11744100	0.94734500
C	-2.20782000	-1.40774800	1.55714900
C	-1.26457600	-1.52416700	2.60609200
C	-1.68318300	-1.53168400	3.94631000
C	-3.04848700	-1.40573300	4.26159800
C	-3.98854800	-1.26838400	3.22723900
C	-3.57404600	-1.27099700	1.88301800
C	-1.20613000	-3.28147500	-0.39872000
C	-0.71906400	-3.69214300	-1.66185200
C	-0.44207500	-5.04376800	-1.91269100
C	-0.63509400	-6.00445900	-0.90210500
C	-3.22196400	2.27138000	0.22074800
C	-1.11351000	-5.60429100	0.35545800
C	-1.40304300	-4.24983800	0.60746600
C	-3.12046100	-1.36984900	-1.21029000
C	-3.37762100	-0.25643200	-2.03425700
C	-4.54098900	-0.19568100	-2.82237100
C	-5.46724000	-1.25059000	-2.79348200
C	-5.22041200	-2.37069700	-1.97847700
C	-4.05500000	-2.43400400	-1.19859400
C	3.60363800	-0.22742500	-0.55242600
C	3.24122100	-1.38699800	0.11535800
C	-4.45037500	2.40882700	0.88693600
C	4.20275100	-2.41080500	0.70086100
C	5.04296600	0.24396100	-0.76660800
C	-4.49821700	2.39167700	2.29209800
C	-3.30985000	2.22893800	3.02327600
C	-2.07899500	2.09240700	2.35871700
C	-0.48501700	3.38513500	-1.12829700
C	0.28696400	3.35978800	-2.31031800
F	5.12716700	1.19613800	-1.73815600
F	5.87087800	-0.76988800	-1.14623000
F	5.56959900	0.79933400	0.36627200
F	4.70015000	-3.26203900	-0.24909600
F	5.27298400	-1.83588400	1.32269100
F	3.59304000	-3.19702100	1.63784000
H	0.88951800	4.40622300	-4.11274300
H	-0.51182800	6.43575200	-3.61680500
H	-1.88971300	6.50740100	-1.51498500
H	-1.87577500	4.58547400	0.05919200
H	1.24884100	0.55277300	2.04547900
H	2.77594600	1.30881500	3.86515900
H	3.23574500	3.75972100	4.19185500
H	2.12771800	5.44078400	2.68767600
H	0.57681600	4.69412600	0.89707400
H	-0.19334600	-1.62636600	2.36925500
H	-0.93585500	-1.63802900	4.74868600
H	-3.37716200	-1.41175800	5.31311800
H	-5.05906200	-1.15925600	3.46324400
H	-4.32453400	-1.16350400	1.08677100
H	-0.54650100	-2.94556900	-2.45308000
H	-0.06208400	-5.34760300	-2.90083300
H	-0.40602000	-7.06434800	-1.09589800
H	-3.20156200	2.32033600	-0.87726400
H	-1.26270700	-6.34863900	1.15380100
H	-1.77978500	-3.95243900	1.59713900
H	-2.64961700	0.56444700	-2.07750800
H	-4.71458300	0.67812100	-3.47008600
H	-6.37619000	-1.20747500	-3.41443200
H	-5.93523700	-3.20870100	-1.95784300
H	-3.86385800	-3.32638000	-0.58317900
H	-5.37419000	2.53913700	0.30125300
H	-5.46077300	2.50751900	2.81513700
H	-3.33407900	2.21352500	4.12410100
H	-1.15761600	1.98008700	2.94803700
H	0.90678200	2.48392500	-2.54823500
O	-0.45935000	0.14625700	-3.60807400
P	-1.58461900	-1.48184100	-0.18138500
P	-0.40104800	1.96888800	0.06083200
Ru	0.32078100	-0.12418000	-0.71689600
S	2.39758900	0.83144300	-1.18919700
S	1.55342500	-1.80610800	0.23549600

Sum of electronic and zero-point Energies= -3827.797355

Sum of electronic and thermal Energies= -3827.747640

Sum of electronic and thermal Enthalpies= -3827.746696

Sum of electronic and thermal Free Energies= -3827.885121

$TS_{4'\text{-}9'}$

Ru	-0.22990026	-0.14990025	-0.77239248
S	-2.27628537	0.05493410	-1.82859695
S	-1.39595883	-1.44606341	0.76306380
P	0.21306644	1.95360415	0.05042131
P	1.69513889	-1.38763474	-0.08357126
O	0.93224989	0.47096468	-3.51077220
C	0.54289840	0.28546950	-2.42090816
C	-3.07223526	-1.39322724	0.31866278
C	-3.45988830	-0.72105038	-0.83443485
C	-4.01651969	-2.09512703	1.28808072
C	-4.89182907	-0.65292409	-1.36289491
F	-4.99406460	-2.80668897	0.65876928
F	-4.64168249	-1.20632646	2.12452546
F	-3.35586275	-2.97739422	2.09213828
F	-5.04288779	0.32271829	-2.30300290
F	-5.79857152	-0.38252172	-0.37865899
F	-5.27488609	-1.82328767	-1.95752492
C	1.79530655	-2.94171407	-1.09279110
C	0.67407610	-3.39748107	-1.81907884
C	0.74228044	-4.58485256	-2.57005225
C	1.93124308	-5.33168336	-2.60316191
C	3.05444017	-4.88651676	-1.88169650
C	2.98980973	-3.69971796	-1.13455461
C	1.65163425	-2.01363335	1.64896926
C	1.77469577	-1.08828425	2.71139068
C	1.72249349	-1.52034967	4.04638683
C	1.52485066	-2.88170408	4.33993431
C	1.38320786	-3.80523897	3.29110429
C	1.44904744	-3.37720554	1.95335671
C	3.43576933	-0.78375503	-0.26973504
C	4.39812212	-0.86746162	0.76148137
C	5.73531992	-0.50216908	0.52265719
C	6.13288692	-0.05662941	-0.74831561
C	5.18196996	0.02888070	-1.78075057
C	3.84512765	-0.32701780	-1.54411311
C	-0.09743554	2.30974395	1.84537232
C	0.09962193	3.63522349	2.30869806
C	-0.17304096	3.97138982	3.64258428
C	-0.66426948	2.99667130	4.53231379
C	-0.87819354	1.68669030	4.07706034
C	-0.59401000	1.34432211	2.74096672
C	-0.87950130	3.28418226	-0.65464101
C	-0.40727171	4.46506971	-1.26704195
C	-1.31066682	5.44931771	-1.71179859
C	-2.69204364	5.27644933	-1.53633828
C	-3.17018329	4.11409061	-0.90337072
C	-2.27317019	3.12858646	-0.46726250
C	1.92164120	2.58832185	-0.21842916

C	2.35883377	2.89789317	-1.52939137
C	3.65529061	3.38713000	-1.75473516
C	4.54912901	3.54772080	-0.68147435
C	4.13856036	3.20779990	0.61795791
C	2.83495869	2.73609619	0.84947006
H	-0.26269744	-2.81868266	-1.79805939
H	-0.14213030	-4.92207870	-3.13319003
H	1.98597278	-6.25999085	-3.19390410
H	3.99157254	-5.46541872	-1.90428411
H	3.87868980	-3.35903713	-0.58195204
H	1.91385942	-0.01798028	2.49488732
H	1.82681678	-0.78586503	4.86058324
H	1.47418338	-3.22037371	5.38688665
H	1.21600194	-4.87141314	3.51142492
H	1.33543755	-4.11118186	1.14241640
H	4.11277751	-1.23794604	1.75645332
H	6.47185014	-0.57974003	1.33849430
H	7.18247682	0.21997879	-0.93656149
H	5.48169907	0.37298209	-2.78314975
H	3.12182204	-0.26840356	-2.37026155
H	0.45940840	4.41425919	1.61893089
H	-0.01243714	5.00554637	3.98676421
H	-0.88894858	3.26518741	5.57691611
H	-1.27666945	0.91818617	4.75788345
H	-0.78101892	0.31893493	2.38735837
H	0.67063237	4.63680576	-1.39469042
H	-0.92244427	6.35986353	-2.19560949
H	-3.39718647	6.04668987	-1.88685322
H	-4.25107763	3.96906792	-0.75081010
H	-2.66288377	2.22762377	0.02946668
H	1.68297727	2.76459103	-2.38660524
H	3.96902614	3.63864137	-2.78026686
H	5.56688671	3.92913930	-0.85953733
H	4.83481058	3.31506044	1.46462607
H	2.52488994	2.49364713	1.87679118

Sum of electronic and zero-point Energies= -3827.797541
Sum of electronic and thermal Energies= -3827.747887
Sum of electronic and thermal Enthalpies= -3827.746943
Sum of electronic and thermal Free Energies= -3827.885482

TS$_{9'\text{-}6'}$

Ru	-0.21637200	-0.15586600	-0.75312200
S	-2.17296200	-0.11906900	-1.96779100
S	-1.55059800	-0.98723200	0.97300200
P	0.42427000	1.93432200	-0.01482500
P	1.54349800	-1.53138500	0.03672200
O	1.08005400	0.23253500	-3.48016400
C	0.64356100	0.11569500	-2.40135700
C	-3.18308200	-0.98552900	0.39305200
C	-3.46272800	-0.60090600	-0.91378200
C	-4.22947600	-1.39731500	1.42674200
C	-4.84904400	-0.62116300	-1.55267400
F	-4.86992000	-0.30922200	1.95967800
F	-3.67327800	-2.06701200	2.47595000
F	-5.18853500	-2.21679700	0.91216800
F	-5.24474700	-1.88978500	-1.88005000
F	-4.88936500	0.10269200	-2.70640200
F	-5.80994300	-0.09733200	-0.73538300
C	1.46331600	-3.14147300	-0.88126300
C	0.26706000	-3.54558700	-1.51182400
C	0.19287100	-4.78130100	-2.17940800
C	1.31322400	-5.62738000	-2.22488500
C	2.50948100	-5.23488000	-1.59648200
C	2.58616000	-4.00148500	-0.92985400
C	1.46591100	-2.07051300	1.79857400
C	1.68069800	-1.12112800	2.82417900
C	1.60800000	-1.49759800	4.17550500
C	1.29883100	-2.82399700	4.52379600
C	1.06423400	-3.76984200	3.51179600
C	1.14947800	-3.39948700	2.15863500
C	3.32692200	-1.10007400	-0.21587900
C	4.27297200	-1.03819800	0.83129400
C	5.62415200	-0.75415000	0.55843200
C	6.05251600	-0.54036100	-0.76203000
C	5.11885100	-0.60812300	-1.81199800
C	3.76932600	-0.88120700	-1.54230400
C	0.67860800	2.34415900	1.78104700
C	1.49255700	3.43225700	2.18014300
C	1.54583700	3.82846700	3.52676300
C	0.77381200	3.16211000	4.49479100
C	-0.05229200	2.09475400	4.10503400
C	-0.09643300	1.68629900	2.76053200
C	-0.86308800	3.23501300	-0.33903500
C	-0.51218200	4.58742500	-0.55803400
C	-1.50886100	5.57021700	-0.67946200
C	-2.86599700	5.22223200	-0.56355900
C	-3.22120400	3.88476900	-0.32001900
C	-2.22687000	2.89809100	-0.20944000
C	1.93370500	2.56843200	-0.85053600
C	1.83450900	3.12962600	-2.14586800
C	2.98520100	3.55030500	-2.83192600
C	4.25278100	3.41337500	-2.23926800
C	4.36409200	2.83432500	-0.96362900
C	3.21536500	2.40644900	-0.27694300
H	-0.61499100	-2.88612000	-1.48544200
H	-0.74819500	-5.07775600	-2.66882100
H	1.25691700	-6.59303500	-2.75218700
H	3.39271300	-5.89272900	-1.62785800
H	3.52894700	-3.70584700	-0.44483000
H	1.90068800	-0.07372100	2.57100400
H	1.78331200	-0.74294700	4.95838900
H	1.23267200	-3.11778300	5.58335400
H	0.80921200	-4.80894800	3.77367700
H	0.96164300	-4.15193800	1.37942600
H	3.96541800	-1.23219700	1.86886300
H	6.34729800	-0.71616600	1.38895300
H	7.11254000	-0.32846000	-0.97453500
H	5.44126100	-0.44817300	-2.85283200
H	3.06072300	-0.94225400	-2.38068600
H	2.08327400	3.98797000	1.43757200
H	2.18986100	4.67387000	3.81741800
H	0.81189900	3.47982600	5.54896200
H	-0.67142700	1.56930300	4.84913700
H	-0.74859900	0.84795900	2.46952400
H	0.54431400	4.88367500	-0.63621600
H	-1.21889000	6.61701200	-0.86405000
H	-3.64585100	5.99426200	-0.65986100
H	-4.27997100	3.59948700	-0.21916800
H	-2.51728600	1.85490800	-0.01952500
H	0.84980200	3.24055200	-2.62486200
H	2.88723300	3.98825900	-3.83775000
H	5.15399100	3.75014500	-2.77578300
H	5.35268000	2.70572400	-0.49639400
H	3.32466600	1.94296700	0.71457900

Sum of electronic and zero-point Energies= -3827.797120
Sum of electronic and thermal Energies= -3827.747524
Sum of electronic and thermal Enthalpies= -3827.746580
Sum of electronic and thermal Free Energies= -3827.885198

TS$_{6'\text{-}10'}$

C	0.73532536	0.06734389	-2.41953401
C	0.54889807	-4.72660602	-2.41977165
C	1.55363022	-5.66499977	-2.13688051
C	2.56659782	-5.34710744	-1.21102448
C	2.57232532	-4.09724908	-0.57488623
C	1.53179607	-2.10097847	1.77697310
C	2.11960939	-1.43377690	2.87438880
C	1.98612268	-1.93726340	4.18060809
C	1.23870547	-3.10016183	4.42310569
C	0.61597608	-3.75331074	3.34580110
C	0.76126019	-3.26154030	2.03968875
C	3.33059311	-0.97245327	-0.36242480
C	1.20817649	2.08341653	1.65331902
C	0.58145563	1.53911104	2.79976106
C	1.14438553	1.71929976	4.07319071
C	2.35764622	2.41696618	4.22008842
C	2.99763543	2.94328422	3.08455653
C	2.42277854	2.78898363	1.80930642
C	-1.15344514	2.95883127	0.30773720
C	-2.24695558	2.88090522	-0.58174627
C	-3.36117813	3.72187207	-0.42362364
C	-3.40315281	4.65086551	0.62997473
C	3.84636567	-1.29944601	-1.64186142
C	-2.31700372	4.74195813	1.51706123
C	-1.19762335	3.90735903	1.35735135
C	1.35916035	2.97431370	-1.09964430
C	2.59694163	2.49553736	-1.58807450
C	3.38813362	3.29160443	-2.43166981
C	2.95011009	4.57218241	-2.81329611
C	1.71843003	5.05317198	-2.33951598
C	0.92878790	4.26424676	-1.48444939
C	-3.41258095	-0.66636042	-0.92892884
C	-3.14332083	-0.88177310	0.41791453
C	5.11882708	-0.86127585	-2.04357741
C	-4.20321068	-1.17671318	1.48011837
C	-4.78845787	-0.77711487	-1.57730306
C	5.91133004	-0.09002594	-1.17599136
C	5.40648822	0.25596920	0.08831944
C	4.12682495	-0.16870736	0.48670849
C	1.56523257	-3.14327473	-0.85873662
C	0.55458337	-3.47025344	-1.78340639
F	-4.82415365	-0.17175664	-2.79987873
F	-5.77242090	-0.19459604	-0.83249845
F	-5.15685689	-2.07987261	-1.78387782
F	-4.87821146	-0.04687926	1.85200651
F	-5.13034951	-2.08333945	1.05913727
F	-3.65472100	-1.68981709	2.61837520
H	-0.24971607	-4.96658463	-3.13925389
H	1.54989293	-6.64759117	-2.63510589
H	3.35680660	-6.07990257	-0.98211125
H	3.36626916	-3.85974621	0.15089189
H	2.67986259	-0.50208151	2.73815261
H	2.46875362	-1.40291119	5.01414891
H	1.13221363	-3.49049743	5.44757973
H	0.00959771	-4.65630526	3.51866704
H	0.26716182	-3.79213428	1.21333157
H	-0.36133118	0.97802611	2.69592242
H	0.63314980	1.30225011	4.95495938
H	2.80125686	2.55384824	5.21920563
H	3.94431166	3.49723387	3.18962684
H	2.91790402	3.23502756	0.93444182
H	-2.23065121	2.14634914	-1.40152747
H	-4.20622166	3.63781596	-1.12472879
H	-4.28304563	5.30028536	0.76229690
H	3.25004517	-1.90901327	-2.33609661
H	-2.33705804	5.46817103	2.34530582
H	-0.35473790	4.00235019	2.05650103
H	2.94905925	1.49154629	-1.31028039
H	4.34883130	2.89949194	-2.80013125
H	3.56618606	5.19150305	-3.48444023
H	1.36235950	6.05254400	-2.63625111
H	-0.03066066	4.65803034	-1.12014738
H	5.49242534	-1.13332584	-3.04343520
H	6.91429111	0.24372599	-1.48576178
H	6.00835056	0.86999165	0.77689521
H	3.75756638	0.15612595	1.46610741
H	-0.23962906	-2.73901007	-2.00565010
O	1.23424219	0.16832339	-3.47115907
P	0.35014413	1.91088507	0.02408154
P	1.59469888	-1.50631582	0.01990078
Ru	-0.17709802	-0.17893013	-0.79012813
S	-2.10844441	-0.31928636	-2.02317827
S	-1.52220039	-0.80771647	1.01436135

Sum of electronic and zero-point Energies= -3827.796842

Sum of electronic and thermal Energies= -3827.747119

Sum of electronic and thermal Enthalpies= -3827.746174

Sum of electronic and thermal Free Energies= -3827.885806

$TS_{10'\text{-}7'}$

C	0.70057900	0.38003400	-2.27148700
C	1.42215600	-4.29290400	-2.82587700
C	2.48874200	-5.15885700	-2.53530000
C	3.39727700	-4.82936400	-1.51167700
C	3.23794700	-3.64095600	-0.78246700
C	2.38920600	-1.81243000	1.58505600
C	3.49060900	-1.36076300	2.34589200
C	3.75058500	-1.90005100	3.61897000
C	2.91773700	-2.89716300	4.15325900
C	1.82645000	-3.36354900	3.39874600
C	1.56666400	-2.83164300	2.12563800
C	3.45860600	-0.21372900	-0.60853900
C	0.78482100	2.28333800	1.73474400
C	0.97214900	1.24438200	2.67058900
C	1.53551500	1.51061700	3.93123800
C	1.92393700	2.81795500	4.26818100
C	1.72931800	3.86249900	3.34564200
C	1.15334000	3.60240500	2.09147500
C	-1.78917600	2.54059300	0.71469100
C	-2.66968200	1.67552400	1.39720300
C	-3.88186900	2.15593300	1.92012100
C	-4.23094300	3.50836700	1.76772900
C	4.24462800	-0.57898600	-1.72402900
C	-3.35441100	4.38034800	1.09912800
C	-2.13854500	3.90474700	0.57997500
C	0.41432300	3.15856200	-1.06508400
C	1.72058600	3.69227200	-1.09184200
C	2.11790900	4.55312600	-2.13057900
C	1.21925500	4.88885500	-3.15610100
C	-0.07914800	4.34686900	-3.14750000
C	-0.47742700	3.48331000	-2.11611400
C	-3.31151400	-1.02075300	-0.85353300
C	-2.90006500	-1.69407600	0.29100400
C	5.35089000	0.20072900	-2.10597100
C	-3.80551200	-2.50354000	1.21094100
C	-4.73628300	-1.03239600	-1.40515100
C	5.69881500	1.34735000	-1.37384200
C	4.91835700	1.72446300	-0.26636100
C	3.79855600	0.96130500	0.10411500
C	2.16848900	-2.75959500	-1.07111500
C	1.26279100	-3.09995100	-2.09724700
F	-5.02568600	-2.20495400	-2.04786900
F	-4.94029500	-0.03709000	-2.31336000
F	-5.67592000	-0.86310500	-0.42972100
F	-3.09407400	-3.37240000	1.98692000

F	-4.50606500	-1.70236400	2.07936800
F	-4.72024700	-3.25281000	0.53555300
H	0.70188400	-4.54471100	-3.62006200
H	2.61149100	-6.09539600	-3.10230900
H	4.23349100	-5.50656200	-1.27515400
H	3.94958200	-3.39765500	0.02185100
H	4.16809600	-0.59444300	1.94406400
H	4.61971500	-1.53834900	4.19149400
H	3.12326200	-3.31752400	5.15056200
H	1.17105500	-4.15333200	3.79846800
H	0.72056600	-3.22478900	1.54315600
H	0.66378800	0.21996500	2.41218400
H	1.67095100	0.68639800	4.64849600
H	2.37068900	3.02713500	5.25320100
H	2.01800100	4.89298800	3.60780200
H	0.97959700	4.43650000	1.39541200
H	-2.40466100	0.61552100	1.52532700
H	-4.55812800	1.46034900	2.44057200
H	-5.18608900	3.88305100	2.16863100
H	3.99261400	-1.47778500	-2.30506800
H	-3.61606500	5.44366700	0.97729100
H	-1.46483200	4.60576600	0.06599400
H	2.44313200	3.42793300	-0.30733000
H	3.14219400	4.95812200	-2.13698800
H	1.53246500	5.56284800	-3.96903400
H	-0.78708100	4.59056700	-3.95526700
H	-1.48974000	3.04884400	-2.13293900
H	5.94591700	-0.09777700	-2.98360600
H	6.57268400	1.95007200	-1.66783800
H	5.17886500	2.62411600	0.31412800
H	3.18459000	1.28450600	0.95869500
H	0.41536800	-2.43232800	-2.32336500
O	1.18606000	0.66484400	-3.29424800
P	-0.13084200	1.91073200	0.17089400
P	1.97034300	-1.18636400	-0.11034900
Ru	-0.14621700	-0.21163500	-0.69884400
S	-2.16902000	-0.13814000	-1.80799900
S	-1.24374600	-1.59390700	0.80621000

Sum of electronic and zero-point Energies= -3827.797349
Sum of electronic and thermal Energies= -3827.747666
Sum of electronic and thermal Enthalpies= -3827.746722
Sum of electronic and thermal Free Energies= -3827.885635

TS$_{7'\text{-}12'}$

Ru	-0.12171100	-0.17021600	-0.84769800
S	-1.17348800	-1.62591400	0.62333500
S	-2.19058400	-0.06569600	-1.86284700
P	-0.12159800	1.88816700	0.15006900
P	1.94578600	-1.22744000	-0.19811200
O	1.17027300	0.83838000	-3.41711500
C	0.69951500	0.49058400	-2.40405700
C	-3.31458400	-0.92966700	-0.87017500
C	-2.85978000	-1.64083700	0.23367000
C	-4.76058900	-0.89793400	-1.35629200
C	-3.73910300	-2.45233800	1.17906500
F	-5.10013600	-2.03948600	-2.03097600
F	-4.98742100	0.13617000	-2.21673700
F	-5.65360600	-0.75286900	-0.33530800
F	-4.41089700	-1.65682700	2.06835600
F	-3.00690900	-3.32883400	1.92642900
F	-4.67436300	-3.19637800	0.52192200
C	1.78006500	-3.05830900	-0.39960600
C	1.01858700	-3.54972100	-1.48436700
C	0.91873700	-4.93040400	-1.71843600
C	1.56834600	-5.83979900	-0.86413500
C	2.32826900	-5.36013000	0.21611900
C	2.44114200	-3.97695900	0.44481700
C	2.59753000	-1.07337600	1.52597400
C	3.88474700	-0.57182100	1.81595100
C	4.32916800	-0.47239100	3.14723300
C	3.49990500	-0.87785300	4.20566600
C	2.21761700	-1.38619600	3.92606400
C	1.76705600	-1.48030100	2.59926300
C	3.43003300	-0.88114600	-1.24355200
C	4.16801300	-1.91202200	-1.86755200
C	5.29138300	-1.60686900	-2.65618700
C	5.69960000	-0.27356700	-2.82671900
C	4.97331400	0.75780000	-2.20599400
C	3.84452400	0.45659900	-1.42737200
C	1.45657900	2.63133900	0.78049700
C	1.87333500	2.57238600	2.12776300
C	3.08184200	3.17002000	2.52933500
C	3.89217700	3.83644100	1.59597600
C	3.48678600	3.90211200	0.25040600
C	2.28296500	3.30387200	-0.15426000
C	-1.27389700	1.90526400	1.59750100
C	-2.45690400	2.67706100	1.58659400
C	-3.33645600	2.65154500	2.68418100
C	-3.04646000	1.86331300	3.80838900
C	-1.87965400	1.07764900	3.82105000
C	-1.01052400	1.08505800	2.71990500
C	-0.71254500	3.33220700	-0.85470300
C	-1.23109200	3.20137800	-2.15759600
C	-1.67214100	4.33135500	-2.87222500
C	-1.60353400	5.60657400	-2.29104200
C	-1.08948600	5.75066200	-0.98829600
C	-0.64383400	4.62617400	-0.27844400
H	0.48859600	-2.84378900	-2.14415200
H	0.31865000	-5.29697000	-2.56608200
H	1.47784100	-6.92369700	-1.03877100
H	2.83905600	-6.06606700	0.89028200
H	3.04630600	-3.61466200	1.28911800
H	4.55239600	-0.25937600	0.99998800
H	5.33768900	-0.07960700	3.35304800
H	3.85269300	-0.80610700	5.24683800
H	1.56269000	-1.72015600	4.74665000
H	0.76641100	-1.89503500	2.39696800
H	3.86556300	-2.96166300	-1.74405800
H	5.84996500	-2.42319800	-3.14120000
H	6.57918900	-0.03763200	-3.44652200
H	5.28058200	1.80783900	-2.33413000
H	3.28271600	1.27337500	-0.95239000
H	1.24741600	2.07864300	2.88333200
H	3.38291100	3.11824300	3.58746300
H	4.83337500	4.31113400	1.91561100
H	4.10638000	4.43278300	-0.49008300
H	1.96964200	3.38268800	-1.20715600
H	-2.70716100	3.29684600	0.71426300
H	-4.25978000	3.25111700	2.65024900
H	-3.73676700	1.84406100	4.66633000
H	-1.65384200	0.43576400	4.68703500
H	-0.13265700	0.42250300	2.72504200
H	-1.30429800	2.21047400	-2.62423800
H	-2.07251000	4.20424800	-3.89011100
H	-1.94925000	6.49049200	-2.85031600
H	-1.03234800	6.74703100	-0.52176600
H	-0.23996100	4.75551300	0.73760500

Sum of electronic and zero-point Energies= -3827.796471
Sum of electronic and thermal Energies= -3827.746696
Sum of electronic and thermal Enthalpies= -3827.745752

Sum of electronic and thermal Free Energies= -3827.885110

$TS_{6'-11'}$

C	-0.70299600	0.50923600	-2.40040200
C	1.74206000	4.31107900	-2.85443400
C	1.69372500	5.58439700	-2.26705300
C	1.18085400	5.73055900	-0.96406100
C	0.71609600	4.61011900	-0.26013500
C	1.29842500	1.87411600	1.60361200
C	1.01492700	1.06654900	2.73028200
C	1.88595500	1.04014400	3.82967700
C	3.07411400	1.79312100	3.81089200
C	3.38363100	2.56744000	2.68215900
C	2.50254400	2.61238000	1.58640800
C	-1.42066900	2.64633200	0.78220700
C	-2.61427100	-1.04393800	1.52514800
C	-1.78643500	-1.45811500	2.59768400
C	-2.23462400	-1.35919500	3.92494400
C	-3.51169000	-0.83854900	4.20577400
C	-4.33829300	-0.42580300	3.14808700
C	-3.89642300	-0.53024700	1.81631600
C	-1.82125300	-3.03989000	-0.39768500
C	-1.05710800	-3.54378600	-1.47473900
C	-0.97384000	-4.92626700	-1.70514200
C	-1.64321600	-5.82495200	-0.85487500
C	-2.23623300	3.32497300	-0.15762700
C	-2.40617400	-5.33280300	0.21768300
C	-2.50216000	-3.94783400	0.44270600
C	-3.44467700	-0.84335700	-1.24527700
C	-3.85098100	0.49842100	-1.41857900
C	-4.97513500	0.81286600	-2.19863500
C	-5.70470100	-0.20877100	-2.83154800
C	-5.30430800	-1.54575000	-2.67189800
C	-4.18574200	-1.86432500	-1.88168800
C	3.29392900	-0.98235700	-0.89104900
C	2.84212900	-1.65122200	0.23976500
C	-3.43185200	3.94273600	0.24187800
C	3.71277400	-2.49377600	1.16605600
C	4.74460100	-0.92140100	-1.35710300
C	-3.83998000	3.89057000	1.58725800
C	-3.04040400	3.21824100	2.52559700
C	-1.83976800	2.60142500	2.12926300
C	0.76412400	3.31816900	-0.84280100
C	1.28177700	3.18501100	-2.14574000
F	4.84132600	-0.54822100	-2.66603300
F	5.38445800	-2.12079100	-1.25150300
F	5.47530900	-0.01070100	-0.64130100
F	3.99349100	-3.72257500	0.63214200
F	4.90536700	-1.89686200	1.45232300
F	3.10296000	-2.72982800	2.36458800
H	2.14132400	4.18245800	-3.87257300
H	2.05443600	6.46525500	-2.82166400
H	1.13969900	6.72544300	-0.49270800
H	0.31351800	4.74096000	0.75625800
H	0.11949000	0.42812100	2.74037200
H	1.64414800	0.40869000	4.69896800
H	3.76534500	1.75912500	4.66768500
H	4.32336000	3.14054200	2.64304200
H	2.76838100	3.22021900	0.71029500
H	-0.78956300	-1.88153000	2.39466500
H	-1.58186600	-1.69890800	4.74489400
H	-3.86257100	-0.76288500	5.24731300
H	-5.34283700	-0.02343800	3.35485300
H	-4.56230000	-0.21235800	1.00101600
H	-0.51194400	-2.84653100	-2.13136100
H	-0.37117600	-5.30269100	-2.54660200
H	-1.56579400	-6.91033500	-1.02655100
H	-1.92059600	3.39276700	-1.21062500
H	-2.93243500	-6.03039000	0.88863000
H	-3.10962600	-3.57548700	1.28098700
H	-3.28627600	1.30803500	-0.93469700
H	-5.27618100	1.86571100	-2.31827400
H	-6.58067800	0.03767600	-3.45236800
H	-5.86540300	-2.35451000	-3.16659200
H	-3.88953700	-2.91670700	-1.76668100
H	-4.04282600	4.47787800	-0.50254100
H	-4.77481800	4.38032500	1.90280800
H	-3.34358700	3.17691500	3.58359300
H	-1.22173300	2.10390300	2.88876100
H	1.33941200	2.19506400	-2.61670100
O	-1.17298900	0.87139700	-3.40879400
P	-1.96513600	-1.20686200	-0.19922900
P	0.14768600	1.88006000	0.15519500
Ru	0.11428900	-0.17297600	-0.85152400
S	2.17666400	-0.10538800	-1.88028000
S	1.15464900	-1.63361400	0.62429300

Sum of electronic and zero-point Energies= -3827.796798

Sum of electronic and thermal Energies= -3827.747024

Sum of electronic and thermal Enthalpies= -3827.746080

Sum of electronic and thermal Free Energies= -3827.885406

$TS_{5'-10'}$

C	0.24828100	0.16174600	-2.35604900
C	0.41612900	-4.57943100	-2.69741100
C	1.27779100	-5.62863900	-2.33827300
C	2.22224700	-5.43397000	-1.31390300
C	2.30508100	-4.19762700	-0.65412800
C	2.09340000	-2.00366600	1.53180500
C	3.44519700	-2.10005900	1.93761800
C	3.77944000	-2.58692700	3.21411500
C	2.77347700	-2.99976400	4.10292600
C	1.42765500	-2.92180800	3.70482500
C	1.09075700	-2.42507500	2.43527400
C	3.16380700	-0.83778400	-0.89639400
C	1.16711400	1.82003000	1.84207600
C	0.57792700	0.95723200	2.79517500
C	1.09785200	0.86848500	4.09676900
C	2.23148300	1.61734900	4.45821000
C	2.83827100	2.45959500	3.51115600
C	2.30772700	2.56791500	2.21329800
C	-1.02296600	3.11943500	0.48704400
C	-1.58358300	3.79914200	-0.62056600
C	-2.66628100	4.67272900	-0.44646300
C	-3.21249300	4.87740100	0.83448900
C	3.63133900	-1.29321800	-2.14944300
C	-2.66225300	4.20676800	1.93785600
C	-1.57064000	3.33435500	1.76818700
C	1.51101700	3.06249100	-0.77330100
C	2.30518100	2.58728000	-1.83559900
C	3.14624800	3.46075600	-2.54913600
C	3.21113500	4.81983000	-2.20420000
C	2.42974600	5.30535900	-1.13929800
C	1.58305000	4.43719500	-0.43275600
C	-3.64963000	-0.30991600	-0.59610200
C	-3.29286900	-1.39345900	0.19188100
C	4.81010400	-0.76523800	-2.70649100
C	-4.25257400	-2.32891900	0.90985500
C	-5.08753500	0.06793200	-0.95478500
C	5.54608500	0.21192800	-2.01521900
C	5.08468200	0.67606100	-0.77028600
C	3.89710500	0.16648400	-0.22071400
C	1.44195000	-3.13436100	-1.00866200
C	0.49464600	-3.34139500	-2.03466400

F	-5.17355000	1.32896700	-1.46425200
F	-5.91914700	0.02950300	0.12535500
F	-5.60914400	-0.76810700	-1.90170500
F	-4.74045300	-1.77527900	2.06741000
F	-5.33118800	-2.67443500	0.15098700
F	-3.64615100	-3.49683500	1.27363100
H	-0.33207000	-4.72209400	-3.49291100
H	1.21024700	-6.60128700	-2.85116500
H	2.89763300	-6.25348000	-1.02061300
H	3.04418400	-4.06462200	0.15016400
H	4.25367800	-1.80336900	1.25462100
H	4.83939700	-2.64975700	3.50836700
H	3.03744500	-3.38675400	5.10004600
H	0.62693900	-3.25255000	4.38535900
H	0.03050800	-2.38012600	2.14457100
H	-0.29214200	0.34454100	2.50793900
H	0.62156200	0.19634600	4.82718400
H	2.64610300	1.53806100	5.47559200
H	3.73176600	3.04442000	3.78248500
H	2.78878900	3.24051000	1.48821200
H	-1.17004800	3.64664800	-1.62983700
H	-3.09204200	5.19148000	-1.31972500
H	-4.06761300	5.55839600	0.96908700
H	3.07635500	-2.07080800	-2.69487300
H	-3.08003100	4.36131000	2.94535000
H	-1.14763700	2.82626700	2.64688600
H	2.27054900	1.52739400	-2.11660600
H	3.74928300	3.06830600	-3.38245500
H	3.86515800	5.50458000	-2.76734400
H	2.47019500	6.37087600	-0.86230200
H	0.96237400	4.83517200	0.38420200
H	5.15808900	-1.13213800	-3.68516400
H	6.47693900	0.61351800	-2.44619200
H	5.64865400	1.44824800	-0.22358600
H	3.54275500	0.55172700	0.74758100
H	-0.19872000	-2.53268600	-2.30885600
O	0.50200800	0.21878800	-3.49974600
P	0.37848500	1.94635700	0.17499200
P	1.58809500	-1.47966500	-0.17967500
Ru	-0.36260800	-0.11820700	-0.63155900
S	-2.44081100	0.70120800	-1.29557700
S	-1.60182800	-1.71492600	0.45343100

Sum of electronic and zero-point Energies= -3827.793001
Sum of electronic and thermal Energies= -3827.743244
Sum of electronic and thermal Enthalpies= -3827.742300
Sum of electronic and thermal Free Energies= -3827.881839

$TS_{10'\text{-}5'}$

C	-0.63333000	0.20789900	-2.40445400
C	1.18437800	4.55204400	-2.58140400
C	0.76956200	5.80122600	-2.09445900
C	-0.07802400	5.86441500	-0.97208300
C	-0.50549100	4.68530900	-0.34425900
C	-0.35650500	2.42044800	1.78444000
C	-1.33812100	2.82223900	2.71662700
C	-0.96542400	3.27834600	3.99546400
C	0.38895100	3.35288700	4.35634000
C	1.37533600	2.97865700	3.42526600
C	1.00679400	2.51811400	2.15267100
C	-2.53821900	2.07875100	-0.16363800
C	-2.16390800	-1.64062900	1.55337100
C	-1.50402000	-1.10505700	2.68380800
C	-2.15054100	-1.05668800	3.93027400
C	-3.46818900	-1.53159300	4.06293100
C	-4.13226500	-2.06361100	2.94373900
C	-3.48505500	-2.12209100	1.69646000
C	-0.31911400	-3.29356200	0.08289000
C	0.60238900	-3.62391600	-0.93789800
C	1.32006300	-4.82863200	-0.88620400
C	1.13836100	-5.71453700	0.19199600
C	-3.05960100	2.76978700	-1.28296500
C	0.22711300	-5.39213100	1.21085700
C	-0.50410100	-4.19130100	1.15606000
C	-2.59649900	-2.16114800	-1.25519800
C	-3.45861900	-1.15890200	-1.75551300
C	-4.49515100	-1.48695800	-2.64411700
C	-4.68329700	-2.81862600	-3.05394600
C	-3.83008700	-3.82172600	-2.56461600
C	-2.79517800	-3.49833500	-1.66945600
C	3.52980000	-0.28338700	-0.83781200
C	3.25446700	-0.53695300	0.50044100
C	-4.44729100	2.84851500	-1.49389500
C	4.31108300	-0.84233700	1.56357600
C	4.92189900	-0.19440800	-1.45112000
C	-5.33863300	2.24916400	-0.58737900
C	-4.83129800	1.54935800	0.52173800
C	-3.44459800	1.45210500	0.72595300
C	-0.09771400	3.42019000	-0.83410200
C	0.75297600	3.36757100	-1.95483300
F	4.88836600	-0.33660400	-2.80738800
F	5.77042400	-1.15515900	-0.98503300
F	5.51338400	1.01736700	-1.20510300
F	4.78217400	-2.12044600	1.46271800
F	5.38464200	-0.00392700	1.48554500
F	3.81534300	-0.71290500	2.82764500
H	1.85453200	4.48943600	-3.45313500
H	1.11014200	6.72802900	-2.58304200
H	-0.40374200	6.84026700	-0.57786400
H	-1.15980200	4.75107400	0.53890700
H	-2.40395300	2.80065400	2.45122500
H	-1.74749300	3.58397100	4.70884200
H	0.67843100	3.70947700	5.35760700
H	2.44237500	3.04363300	3.68956300
H	1.78985100	2.23707800	1.43337600
H	-0.47571600	-0.72174100	2.59449700
H	-1.61990400	-0.63902000	4.80009500
H	-3.97674900	-1.48763900	5.03922600
H	-5.16333300	-2.44022900	3.03949200
H	-4.01408300	-2.54295900	0.82857800
H	0.76935600	-2.92329900	-1.77174000
H	2.03619400	-5.06982000	-1.68749900
H	1.71318700	-6.65298700	0.23963300
H	-2.37762600	3.25333200	-1.99763700
H	0.08159100	-6.07761400	2.06094500
H	-1.21665300	-3.95441400	1.95965200
H	-3.32277300	-0.11142700	-1.45183700
H	-5.15338200	-0.69030600	-3.02439000
H	-5.49108800	-3.07296200	-3.75850500
H	-3.96566300	-4.86819200	-2.88118100
H	-2.13699600	-4.29530000	-1.29441900
H	-4.83110100	3.39024900	-2.37294700
H	-6.42604600	2.32196000	-0.74747900
H	-5.51739200	1.06297600	1.23273300
H	-3.07036800	0.86911500	1.57886500
H	1.10020800	2.39424300	-2.33073600
O	-1.10971000	0.36898000	-3.45926400
P	-1.26196600	-1.70806500	-0.05880200
P	-0.71203100	1.89681600	0.03995700
Ru	0.25320400	-0.04793800	-0.76311100
S	2.21996500	0.01640300	-1.93912800
S	1.62242600	-0.57261200	1.06375700

Sum of electronic and zero-point Energies= -3827.798344
Sum of electronic and thermal Energies= -

3827.748599
Sum of electronic and thermal Enthalpies= -3827.747655
Sum of electronic and thermal Free Energies= -3827.886790

$TS_{2'-6'}$

C	0.46363200	0.24334500	-2.34150200
C	0.65502100	-4.30701600	-3.15226900
C	1.79747200	-5.12112500	-3.21103400
C	2.88449200	-4.85689100	-2.35776200
C	2.82819700	-3.78418700	-1.45346000
C	1.42075200	-2.42998800	1.46716200
C	1.08581800	-1.65624700	2.60204300
C	0.98519800	-2.25188000	3.87002900
C	1.19370300	-3.63378000	4.01990100
C	1.50272600	-4.41459400	2.89358000
C	1.61791200	-3.81919700	1.62540800
C	3.33517600	-0.99173700	-0.14963500
C	0.09006100	1.97020300	1.96691800
C	-1.24400200	1.79218500	2.40870300
C	-1.53401000	1.70454400	3.77869100
C	-0.49726200	1.77353500	4.72855500
C	0.83165600	1.92697300	4.29829300
C	1.12693100	2.02418200	2.92598500
C	-0.56893000	3.43847100	-0.47409900
C	-0.60588200	3.64400200	-1.87214900
C	-1.26245200	4.76117300	-2.41055400
C	-1.89151400	5.68947200	-1.56176700
C	4.03201800	-0.85642500	-1.37410000
C	-1.85251800	5.49569500	-0.17124100
C	-1.19150700	4.37993600	0.37302900
C	2.07688500	2.75830200	-0.04925400
C	2.95308500	2.30332800	-1.05210400
C	4.15452300	2.98605500	-1.31549800
C	4.49449700	4.12894300	-0.57551900
C	3.62103600	4.59705700	0.42423200
C	2.41608400	3.92578300	0.67853200
C	-3.53058400	-0.22606900	-0.63074100
C	-3.18129600	-1.38184400	0.04880600
C	5.36859700	-0.42627600	-1.39161300
C	-4.15499000	-2.37915600	0.66078500
C	-4.96498000	0.20460800	-0.93917600
C	6.02689800	-0.10869800	-0.18982500
C	5.33771300	-0.22489500	1.02872200
C	4.00297400	-0.66716300	1.05094100
C	1.67883400	-2.95799500	-1.38363100
C	0.59512900	-3.23394800	-2.24502500
F	-5.03710400	1.51691500	-1.30081100
F	-5.79622600	0.05508200	0.13291600
F	-5.49993300	-0.51186500	-1.97238600
F	-4.64745200	-1.94414100	1.86582200
F	-5.23011400	-2.63317300	-0.13894700
F	-3.56178000	-3.58318500	0.90363200
H	-0.20068700	-4.50176500	-3.81762600
H	1.84478700	-5.96015700	-3.92338300
H	3.78634900	-5.48850300	-2.39769100
H	3.69203000	-3.58542300	-0.80101700
H	0.88328600	-0.58054900	2.49270700
H	0.72334700	-1.63034900	4.74057800
H	1.10042000	-4.10433700	5.01157000
H	1.64794800	-5.50174100	2.99648000
H	1.84606400	-4.45032200	0.75486500
H	-2.05862900	1.70941900	1.67155400
H	-2.57725900	1.57055200	4.10492500
H	-0.72667400	1.70062900	5.80349300
H	1.65035600	1.97236400	5.03413400
H	2.17276300	2.13742500	2.60371700
H	-0.12087100	2.92538400	-2.55099600
H	-1.28766000	4.90236000	-3.50255700
H	-2.41345700	6.56204300	-1.98527000
H	3.53326500	-1.10727300	-2.32328700
H	-2.34174200	6.21743200	0.50223400
H	-1.16960300	4.24671600	1.46472900
H	2.69200400	1.41488400	-1.64161200
H	4.82501000	2.61667300	-2.10661400
H	5.43554100	4.66341700	-0.78138000
H	3.87261100	5.50169300	1.00051400
H	1.72588200	4.32750700	1.43602100
H	5.90030800	-0.34422500	-2.35319700
H	7.07651100	0.22502300	-0.20369500
H	5.84509900	0.01690300	1.97623000
H	3.48659600	-0.77928100	2.01617600
H	-0.30580800	-2.60413800	-2.20309600
O	0.82351700	0.34669100	-3.45547600
P	0.40798400	1.99523600	0.15504800
P	1.57620500	-1.56701300	-0.16242200
Ru	-0.24054000	-0.07449400	-0.66771600
S	-2.31210700	0.84331600	-1.23413900
S	-1.49627200	-1.73083300	0.32246800

Sum of electronic and zero-point Energies= -3827.797836
Sum of electronic and thermal Energies= -3827.748135
Sum of electronic and thermal Enthalpies= -3827.747191
Sum of electronic and thermal Free Energies= -3827.885593

$TS_{3'-7'}$

C	-0.62374900	0.43326500	-2.37826900
C	2.81663100	3.97973900	-2.10660600
C	3.54158000	4.69317300	-1.13365900
C	3.17239400	4.59340700	0.21646400
C	2.08206200	3.78913100	0.59809100
C	-0.19610100	2.25793000	1.91232900
C	-1.02278000	3.26274100	2.46867400
C	-1.02489300	3.49811900	3.85525600
C	-0.19382900	2.74750900	4.70416200
C	0.63776500	1.75298200	4.15842600
C	0.63171200	1.50532800	2.77595900
C	-1.51993400	3.00806200	-0.52821800
C	-1.84433800	-1.91663500	1.64114900
C	-1.91665200	-0.92752100	2.64927900
C	-1.97198700	-1.29135800	4.00476600
C	-1.93183800	-2.64751400	4.37388600
C	-1.83821400	-3.63577700	3.37970300
C	-1.79789700	-3.27587600	2.02138100
C	-1.76451500	-2.97440900	-1.06207000
C	-0.58348700	-3.44847700	-1.67263300
C	-0.57909900	-4.66947600	-2.37083700
C	-1.75384200	-5.43314200	-2.46635400
C	-1.35410200	4.22802300	-1.22106700
C	-2.93645400	-4.97091800	-1.85993600
C	-2.94428600	-3.75034500	-1.16613700
C	-3.50139600	-0.82059200	-0.46694400
C	-4.49214700	-0.70218200	0.53293000
C	-5.79934400	-0.30082200	0.19853700
C	-6.13701900	-0.02211800	-1.13642100
C	-5.15776700	-0.14517100	-2.13946600
C	-3.85196600	-0.53858300	-1.80883900
C	2.93690200	-1.42432600	0.42976500
C	3.34637300	-0.90723600	-0.79325600
C	-2.47488900	4.96375800	-1.64665500
C	4.78015500	-0.92245800	-1.31642000
C	3.84298100	-2.14486800	1.42381000
C	-3.77302300	4.50131500	-1.37587400
C	-3.94755100	3.29407200	-0.67548700

C	-2.83048800	2.55181600	-0.26171800
C	1.35697300	3.06058800	-0.36917400
C	1.74046600	3.16414400	-1.72725800
F	3.28800900	-2.20107100	2.67028800
F	5.05357100	-1.53435200	1.57094800
F	4.08468400	-3.44020900	1.05366600
F	5.54701900	0.05386700	-0.74101500
F	5.40897000	-2.11259900	-1.09276200
F	4.83051300	-0.70940500	-2.66266500
H	3.09982700	4.04597800	-3.16880900
H	4.39725000	5.32008900	-1.43038300
H	3.73553900	5.14280400	0.98748600
H	1.80433000	3.73019800	1.65993700
H	-1.66514000	3.87396800	1.81880900
H	-1.67867300	4.28183200	4.27027700
H	-0.19406700	2.93679100	5.78953100
H	1.29357200	1.15576900	4.81125500
H	1.26817200	0.70690800	2.36396600
H	-1.91966500	0.13899400	2.37726100
H	-2.03193600	-0.50653100	4.77488400
H	-1.96319700	-2.93302400	5.43735400
H	-1.79180100	-4.70009000	3.65994500
H	-1.72136600	-4.06067600	1.25510200
H	0.34323700	-2.85761400	-1.60505100
H	0.35187400	-5.01984000	-2.84360600
H	-1.75095000	-6.38802400	-3.01581400
H	-0.34640100	4.61492900	-1.42817500
H	-3.86290900	-5.56298400	-1.93079600
H	-3.87855200	-3.39829300	-0.70268700
H	-4.25115500	-0.93459200	1.58065100
H	-6.56017100	-0.21901600	0.99133400
H	-7.16246900	0.28461500	-1.39719500
H	-5.41080700	0.06569700	-3.19047400
H	-3.10474500	-0.63978500	-2.60961200
H	-2.32589600	5.91004100	-2.19071100
H	-4.64880900	5.08057500	-1.70915000
H	-4.95832600	2.91803200	-0.45380200
H	-2.98438200	1.60784900	0.27988100
H	1.19642000	2.60010300	-2.49975800
O	-1.04210500	0.75039900	-3.42482600
P	-1.76881200	-1.37504300	-0.11940500
P	-0.09618300	1.99952700	0.08022700
Ru	0.15886400	-0.12686600	-0.76757300
S	1.26700200	-1.34570800	0.88777700
S	2.19509800	-0.15310000	-1.84252200

Sum of electronic and zero-point Energies= -3827.799091
Sum of electronic and thermal Energies= -3827.749259
Sum of electronic and thermal Enthalpies= -3827.748315
Sum of electronic and thermal Free Energies= -3827.888734

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Ru	-0.49271300	-0.02485800	-0.36160200
S	-2.09444300	-1.64169300	-0.01177900
S	-2.25290800	1.44896900	-0.16915100
P	0.94249100	1.89222600	0.01825200
P	1.11896600	-1.79956900	-0.02583600
O	-0.22496000	-0.02998500	-3.33298200
C	-0.24611400	-0.01844300	-2.15743400
C	-3.71420600	0.51548300	-0.08466800
C	-3.64784500	-0.86403300	-0.00775500
C	-4.99914800	1.33549400	-0.03930600
C	-4.84094500	-1.80994100	0.04728800
F	-5.98476200	0.81006500	-0.82111700
F	-4.80387900	2.61504500	-0.46852700
F	-5.49942000	1.43057600	1.23272600
F	-4.48338400	-3.04783600	0.49844700
F	-5.40524900	-1.99635900	-1.18565700
F	-5.82792400	-1.36806900	0.87817100
C	1.20257500	-3.06025700	-1.38956800
C	0.05471200	-3.32151000	-2.17013100
C	0.07311300	-4.31169000	-3.16725100
C	1.23986500	-5.05571500	-3.40711100
C	2.39007000	-4.80473500	-2.63924900
C	2.37314200	-3.81826700	-1.63882100
C	0.79308000	-2.86380400	1.46746900
C	-0.03131200	-2.40714700	2.51869800
C	-0.23330600	-3.19000800	3.66993200
C	0.37943100	-4.44815500	3.78338400
C	1.19528000	-4.91876100	2.73873600
C	1.40154700	-4.13439400	1.59275200
C	2.90287200	-1.38611100	0.21384300
C	3.49229500	-1.38263200	1.49736200
C	4.85576300	-1.07750000	1.65707500
C	5.65120900	-0.78573400	0.53688300
C	5.07116500	-0.77815600	-0.74452500
C	3.70604400	-1.06230400	-0.90481700
C	1.39623800	2.17303000	1.78697200
C	1.87029400	3.42565600	2.24856000
C	2.19792000	3.60825600	3.60175900
C	2.05186300	2.54867300	4.51649900
C	1.57515800	1.30529000	4.07046600
C	1.25043600	1.12308300	2.71459400
C	0.14153700	3.51166700	-0.40576400
C	0.30273300	4.11611300	-1.67173700
C	-0.36986900	5.30911600	-1.98713500
C	-1.21340600	5.91893300	-1.04375500
C	-1.38426200	5.32474600	0.21784600
C	-0.71831000	4.12942000	0.53379700
C	2.55139300	2.04800400	-0.88889200
C	2.57780500	1.79214600	-2.28063300
C	3.74489400	2.01533100	-3.03111400
C	4.91303500	2.47891500	-2.40184800
C	4.90678700	2.70298400	-1.01504600
C	3.73791700	2.49050500	-0.26398400
H	-0.86925500	-2.75125000	-1.99713200
H	-0.83534400	-4.49478500	-3.76224700
H	1.25519900	-5.82734400	-4.19319000
H	3.31313000	-5.37883200	-2.81910100
H	3.28868700	-3.63379700	-1.05795400
H	-0.55288700	-1.44319000	2.42596000
H	-0.88846300	-2.81601400	4.47243200
H	0.21366200	-5.06739200	4.67925100
H	1.67108100	-5.90970200	2.81119300
H	2.03426300	-4.52721800	0.78367800
H	2.89043200	-1.64139900	2.38090900
H	5.29898700	-1.08480800	2.66557400
H	6.72319400	-0.56435500	0.66082600
H	5.68384200	-0.54606700	-1.62918700
H	3.26805200	-1.05602400	-1.91416600
H	1.96929600	4.26941300	1.54879200
H	2.56233600	4.58929600	3.94594700
H	2.30209100	2.69767900	5.57893100
H	1.44685000	0.47173100	4.77886300
H	0.86373500	0.15314500	2.36882500
H	0.96807800	3.66706300	-2.42280500
H	-0.22672000	5.76472600	-2.97974400
H	-1.73976400	6.85406200	-1.29217400
H	-2.04946400	5.78735900	0.96379000
H	-0.87199600	3.67580600	1.52398000
H	1.68221500	1.41540400	-2.79425200
H	3.73656300	1.82145400	-4.11550900
H	5.82754800	2.65683000	-2.98983100
H	5.82085700	3.04778100	-0.50583300
H	3.76146200	2.66572000	0.82054200

Sum of electronic and zero-point Energies= -3827.794537
Sum of electronic and thermal Energies= -3827.744110
Sum of electronic and thermal Enthalpies= -3827.743165
Sum of electronic and thermal Free Energies= -3827.883904

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Ru	-0.49055000	-0.02309900	-0.36900300
S	-2.09672100	-1.64887900	-0.06860700
S	-2.24580200	1.44530100	-0.12503600
P	0.94592200	1.89049100	0.01570400
P	1.11835300	-1.79995600	-0.02750400
O	-0.22191100	-0.00296900	-3.34030200
C	-0.24285000	-0.00236100	-2.16461200
C	-3.70946600	0.51365000	-0.04981400
C	-3.64796000	-0.86809600	-0.04950000
C	-4.99031700	1.33935800	-0.02784800
C	-4.84525800	-1.80797100	0.03339800
F	-5.92310200	0.84142800	0.83406800
F	-5.57784500	1.41102700	-1.26075300
F	-4.75505700	2.62650300	0.36326300
F	-4.52237300	-3.07724000	-0.34883000
F	-5.87821700	-1.41404300	-0.76432400
F	-5.33372700	-1.90449700	1.30949700
C	1.22234800	-3.05541800	-1.39430700
C	0.08898300	-3.30796200	-2.19851500
C	0.12273500	-4.29388400	-3.19950700
C	1.29058600	-5.04227700	-3.41948100
C	2.42643400	-4.80015900	-2.62772400
C	2.39414500	-3.81796200	-1.62353100
C	0.76742000	-2.86706100	1.45802900
C	-0.06627900	-2.40655000	2.50027300
C	-0.28751300	-3.19003600	3.64748900
C	0.31457200	-4.45297100	3.76542300
C	1.13929500	-4.92740800	2.72955400
C	1.36526600	-4.14209700	1.58785800
C	2.89883100	-1.39010600	0.24356000
C	3.46387700	-1.38544500	1.53805100
C	4.82460000	-1.08257000	1.72315400
C	5.64180600	-0.79429700	0.61780700
C	5.08630400	-0.78831200	-0.67441100
C	3.72393600	-1.07033500	-0.86013100
C	1.38148200	2.18036300	1.78732200
C	1.85422900	3.43408800	2.24730400
C	2.16766600	3.62312300	3.60299700
C	2.00884900	2.56886200	4.52170500
C	1.53360500	1.32436000	4.07718600
C	1.22277200	1.13574200	2.71895800
C	0.15117100	3.50698000	-0.42947100
C	0.31559400	4.09149500	-1.70455600
C	-0.35350100	5.28100100	-2.03930700
C	-1.19730500	5.90719800	-1.10673900
C	-1.37166700	5.33284400	0.16338100
C	-0.70877800	4.14098800	0.49902300
C	2.56492500	2.03743600	-0.87524500
C	2.60737000	1.77004300	-2.26441000
C	3.78301100	1.98691300	-3.00333700
C	4.94405600	2.45536800	-2.36468000
C	4.92205100	2.69049000	-0.97987800
C	3.74461000	2.48438500	-0.24055300
H	-0.83616000	-2.73517800	-2.04089800
H	-0.77466300	-4.47037100	-3.81298100
H	1.31797000	-5.81061100	-4.20845800
H	3.35016200	-5.37794900	-2.79161000
H	3.29876400	-3.64032200	-1.02372500
H	-0.58009300	-1.43876500	2.40317500
H	-0.94940300	-2.81284900	4.44293400
H	0.13349900	-5.07286700	4.65786600
H	1.60671000	-5.92207700	2.80544800
H	2.00476200	-4.53780500	0.78555300
H	2.84495500	-1.64172100	2.41046700
H	5.24850900	-1.08891700	2.73992600
H	6.71164000	-0.57462600	0.76175900
H	5.71616100	-0.55929200	-1.54773800
H	3.30531600	-1.06541000	-1.87761400
H	1.96318300	4.27382500	1.54418800
H	2.53097700	4.60502800	3.94587700
H	2.24795700	2.72289000	5.58597800
H	1.39547300	0.49502300	4.78867800
H	0.83699000	0.16491500	2.37449500
H	0.98061200	3.62918900	-2.44783100
H	-0.20761200	5.72100500	-3.03853700
H	-1.72100800	6.83964400	-1.37040500
H	-2.03720300	5.80805400	0.90101500
H	-0.86540200	3.70323900	1.49575800
H	1.71793400	1.38884800	-2.78529800
H	3.78694300	1.78411300	-4.08612300
H	5.86524900	2.62834900	-2.94363400
H	5.83037900	3.03898700	-0.46296600
H	3.75618400	2.66791400	0.84275900

Sum of electronic and zero-point Energies= -3827.794658
Sum of electronic and thermal Energies= -3827.744214
Sum of electronic and thermal Enthalpies= -3827.743270
Sum of electronic and thermal Free Energies= -3827.884172

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Ru	0.17011300	-0.23105100	-0.77745900
S	2.11666900	-0.52643800	-1.95838800
S	1.38547800	-1.05216500	1.04092900
P	-1.84864600	-1.28869800	-0.09249400
P	-0.01149300	1.89883100	0.06616600
O	-1.10016300	0.31717100	-3.49517300
C	-0.65303900	0.14975600	-2.42910300
C	3.01051400	-1.27034300	0.49131900
C	3.34116400	-1.03932700	-0.83918100
C	3.99993500	-1.70498000	1.57263200
C	4.72132000	-1.26158700	-1.44933500
F	4.84342000	-2.68753200	1.14580000
F	3.36428700	-2.19841000	2.67483300
F	4.77392500	-0.66537100	2.00709200
F	4.85651400	-0.62348200	-2.64789800
F	4.96970800	-2.58615600	-1.68963200
F	5.73125700	-0.80101300	-0.65458400
C	-0.52332400	3.20159600	-1.14055600
C	-1.73669200	3.05268000	-1.85105300
C	-2.16382700	4.03965100	-2.75320300
C	-1.38142800	5.18833200	-2.96871200
C	-0.17501100	5.34634700	-2.26711100
C	0.25088600	4.36444900	-1.35479400
C	1.61981600	2.53358600	0.66917400
C	1.74846800	3.20022000	1.90915500
C	2.99303400	3.71240400	2.31593000
C	4.12093800	3.57927900	1.48956300
C	3.99860100	2.92947100	0.24876700
C	2.76040600	2.40546400	-0.15587400
C	-1.10166000	2.23505600	1.51902500
C	-1.02301700	1.36694400	2.63240600
C	-1.78398500	1.61668700	3.78600200
C	-2.64767200	2.72587900	3.83712500
C	-2.73600600	3.59149700	2.73306600
C	-1.96257800	3.35477100	1.58230300

C	-2.29846000	-1.65816000	1.66823300
C	-1.36776900	-2.39814500	2.43778200
C	-1.65493600	-2.75206900	3.76556300
C	-2.88017400	-2.38145300	4.34905100
C	-3.81709600	-1.66207900	3.58913000
C	-3.53148300	-1.30373300	2.25909600
C	-1.84824100	-3.01583000	-0.77235200
C	-2.82873200	-3.94453400	-0.34831900
C	-2.84560900	-5.24819300	-0.86784400
C	-1.88125500	-5.64637300	-1.81278400
C	-0.90267200	-4.73262500	-2.23624300
C	-0.88639400	-3.42423700	-1.71923200
C	-3.39544200	-0.57671200	-0.80417900
C	-4.05165200	-1.18140800	-1.89949000
C	-5.19644200	-0.58979600	-2.46265800
C	-5.71079600	0.60627300	-1.93565600
C	-5.06133500	1.22052100	-0.84969300
C	-3.90629400	0.64245700	-0.29626500
H	-2.36117800	2.16024800	-1.69888000
H	-3.11108000	3.90214700	-3.29793500
H	-1.71120800	5.95726400	-3.68531900
H	0.44621600	6.24188300	-2.42733400
H	1.19441200	4.50815800	-0.80950400
H	0.87681800	3.32451800	2.56687200
H	3.07653900	4.21990400	3.29017600
H	5.09611400	3.97594100	1.81350700
H	4.87577000	2.81447500	-0.40689600
H	2.68046000	1.88579600	-1.12333300
H	-0.35189500	0.49459900	2.60012800
H	-1.70625900	0.93214300	4.64473600
H	-3.25123000	2.91610400	4.73888800
H	-3.40487900	4.46641100	2.76769700
H	-2.02568700	4.05025600	0.73249600
H	-0.41073000	-2.71018300	1.99342600
H	-0.91479000	-3.32698400	4.34427600
H	-3.10657600	-2.66190200	5.39011600
H	-4.78691900	-1.37885600	4.02862600
H	-4.28881400	-0.75595300	1.68113300
H	-3.58295300	-3.64807200	0.39699800
H	-3.61395000	-5.96067800	-0.52747300
H	-1.89165400	-6.67231500	-2.21408600
H	-0.13944000	-5.03540300	-2.97030100
H	-0.10821400	-2.71665700	-2.04875700
H	-3.66693600	-2.12144300	-2.32095400
H	-5.68964800	-1.07424800	-3.32025300
H	-6.61313000	1.06266700	-2.37257200
H	-5.45005900	2.16248800	-0.43116100
H	-3.39939600	1.14949100	0.53891600

Sum of electronic and zero-point Energies= -3827.800825

Sum of electronic and thermal Energies= -3827.750298

Sum of electronic and thermal Enthalpies= -3827.749354

Sum of electronic and thermal Free Energies= -3827.891349

14'

Ru	0.17080100	-0.23382000	-0.77223300
S	2.11181200	-0.54647300	-1.95669600
S	1.38935300	-1.03984400	1.05249800
P	-1.85126100	-1.28679700	-0.08756800
P	-0.00689800	1.89945100	0.06482000
O	-1.10211300	0.31877200	-3.48739600
C	-0.65304300	0.14962300	-2.42248400
C	3.01487000	-1.25360700	0.50063800
C	3.33166000	-1.07888500	-0.84132600
C	4.00347300	-1.70186200	1.57705200
C	4.71262400	-1.27848500	-1.45477700
F	5.21291900	-1.08219100	1.46779300
F	4.23083900	-3.05036200	1.53049700
F	3.54577100	-1.43456500	2.83349100
F	4.64310200	-1.46229300	-2.80467100
F	5.36659200	-2.36355100	-0.95253800
F	5.52737700	-0.19209500	-1.25696300
C	-0.49245400	3.19414900	-1.16055000
C	-1.71361500	3.06370700	-1.86180100
C	-2.11788600	4.04271300	-2.78280300
C	-1.30440600	5.16375700	-3.02745800
C	-0.08957400	5.30222100	-2.33647300
C	0.31359100	4.32885000	-1.40482100
C	1.61477800	2.53242500	0.69517700
C	1.71112500	3.24423900	1.91309700
C	2.94846500	3.75471500	2.34291000
C	4.10200000	3.57377800	1.56196000
C	4.01247800	2.87855500	0.34327200
C	2.78054500	2.35745400	-0.08428500
C	-1.11862200	2.24782000	1.49808600
C	-1.05166600	1.38937400	2.61969600
C	-1.82614400	1.64802600	3.76220700
C	-2.69134100	2.75682900	3.79400000
C	-2.76742500	3.61326800	2.68190300
C	-1.98057700	3.36757900	1.54207500
C	-2.30637600	-1.64679100	1.67333000
C	-1.37412600	-2.37538100	2.45167600
C	-1.66461200	-2.72223500	3.78059000
C	-2.89472400	-2.35554000	4.35631200
C	-3.83304600	-1.64731400	3.58765400
C	-3.54415300	-1.29614900	2.25640100
C	-1.84930900	-3.01693600	-0.75969200
C	-2.82637300	-3.94590200	-0.32847100
C	-2.84281000	-5.25152100	-0.84313300
C	-1.88158800	-5.65133200	-1.79051000
C	-0.90657400	-4.73720200	-2.22137100
C	-0.89061000	-3.42696500	-1.70914300
C	-3.39522700	-0.57781700	-0.80830700
C	-4.04694100	-1.18737700	-1.90356400
C	-5.18865800	-0.59759700	-2.47484400
C	-5.70428600	0.60154500	-1.95620900
C	-5.05956000	1.22030700	-0.86996800
C	-3.90775900	0.64384200	-0.30819400
H	-2.36159000	2.19189200	-1.68814300
H	-3.07175400	3.92056100	-3.31961000
H	-1.61663700	5.92610800	-3.75879400
H	0.55612000	6.17568500	-2.52004700
H	1.26436700	4.45684100	-0.86823000
H	0.81972400	3.40509700	2.53544400
H	3.00616300	4.29836000	3.29938700
H	5.07148200	3.96896600	1.90442200
H	4.90899600	2.72382500	-0.27667700
H	2.72549700	1.80335500	-1.03418500
H	-0.37862500	0.51807900	2.60268600
H	-1.75745700	0.97109000	4.62770900
H	-3.30529300	2.95417800	4.68717500
H	-3.43689800	4.48818600	2.70173900
H	-2.03379000	4.05632300	0.68612800
H	-0.41333700	-2.68411300	2.01297700
H	-0.92335000	-3.28839200	4.36647100
H	-3.12371400	-2.63031800	5.39831900
H	-4.80642000	-1.36727200	4.02130000
H	-4.30218200	-0.75678300	1.67141500
H	-3.57826300	-3.64816700	0.41865800
H	-3.60842400	-5.96417400	-0.49702700
H	-1.89164100	-6.67874600	-2.18802800
H	-0.14593300	-5.04114000	-2.95763500
H	-0.11537100	-2.71912300	-2.04490100
H	-3.66107900	-2.12977100	-2.31867900
H	-5.67836700	-1.08585000	-3.33228300

H -6.60408300 1.05666100 -2.39963600
H -5.44978700 2.16431300 -0.45743900
H -3.40506400 1.15373300 0.52770700
Sum of electronic and zero-point Energies= -3827.801164
Sum of electronic and thermal Energies= -3827.750655
Sum of electronic and thermal Enthalpies= -3827.749711
Sum of electronic and thermal Free Energies= -3827.891386