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Electronic Supplementary Information

for

Origin of Stereoselectivity in the Amination of Alcohols using Cooperative Asymmetric Dual Catalysis Involving Chiral Counter-ion

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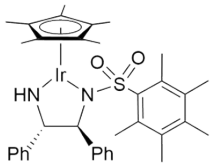
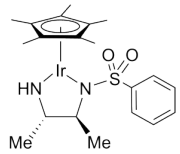
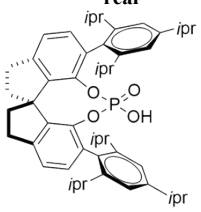
1. Model Systems of the Catalysts Used in the Preliminary Mechanistic Investigations



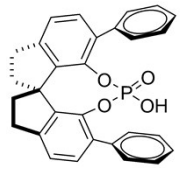
A$_{real}$



A$_{model}$



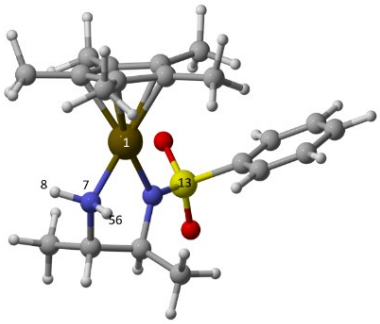
B$_{real}$



B$_{model}$

Fig. S1 The model catalysts used for our preliminary mechanistic study wherein the phenyl rings on the diamino backbone is replaced by methyl and pentamethyl aryl (C_6Me_5) of the $–NSO_2$ group is replaced by a phenyl ring. In the SPINOL phosphoric acid, the isopropyl substituents are replaced by hydrogens.

2. Natural Population Analysis of A$_{model}$



atom (number)	natural charge
Ir (1)	0.68
H (8, 56)	0.46
S (13)	2.41
N (7)	-0.90

Fig. S2 The NPA charges on some important atoms of the cationic Ir complex. The chiral phosphate was placed closer to the most positively charged centres in the cationic Ir complex in the initial guess geometries. We noted that the counter ion invariably moved closer to the $–NH_2$ hydrogen atoms in the converged minimum energy geometry when the phosphate oxygen atoms developed strong hydrogen bonding interaction.

3. Conformers and Configurations of the Metal Catalyst A_{model}

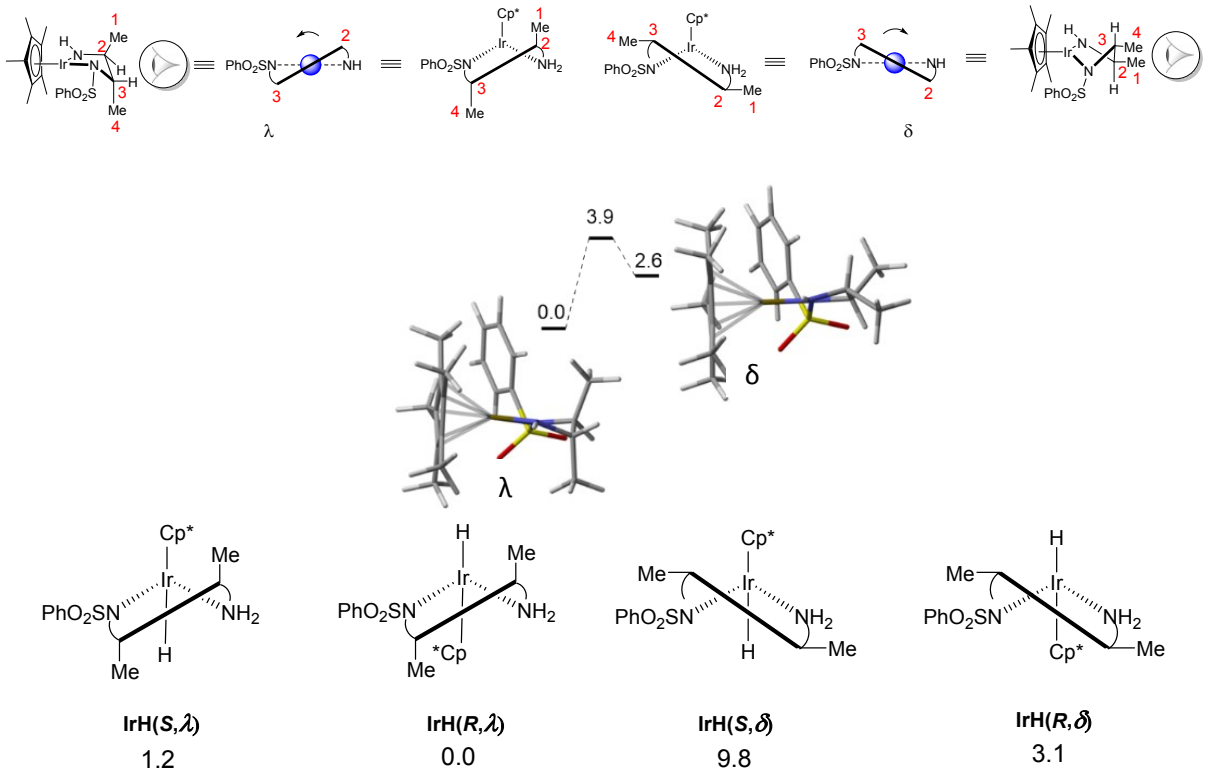


Fig. S3 The δ and λ conformers of the five-membered chelate bound to the Ir center and the four different stereoisomers of the corresponding [Ir]-H complex. The relative free energy (kcal/mol) profile for the interconversion of λ (left) and δ (right) conformers.

4. Active Catalysts Considered for the Alcohol Dehydrogenation Step

The (2*S*,3*S*) stereoisomer of alcohol **1** is used as a representative case for the evaluation of energetics using different possible catalyst complexes in the dehydrogenation step as summarized below.

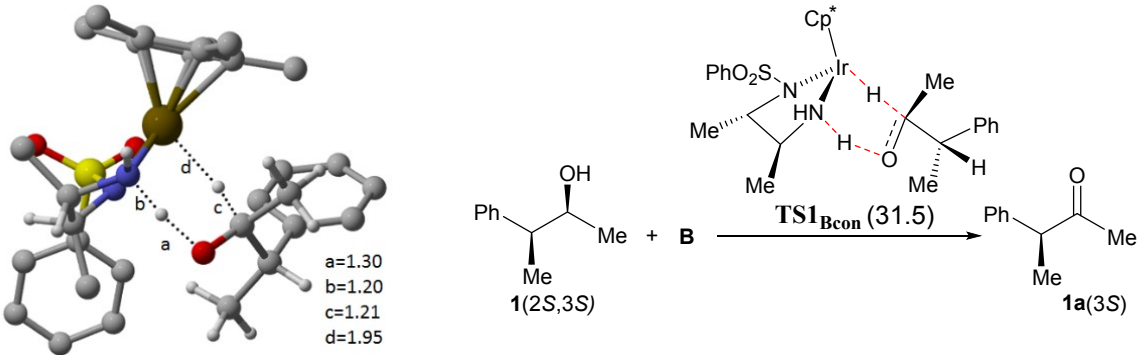
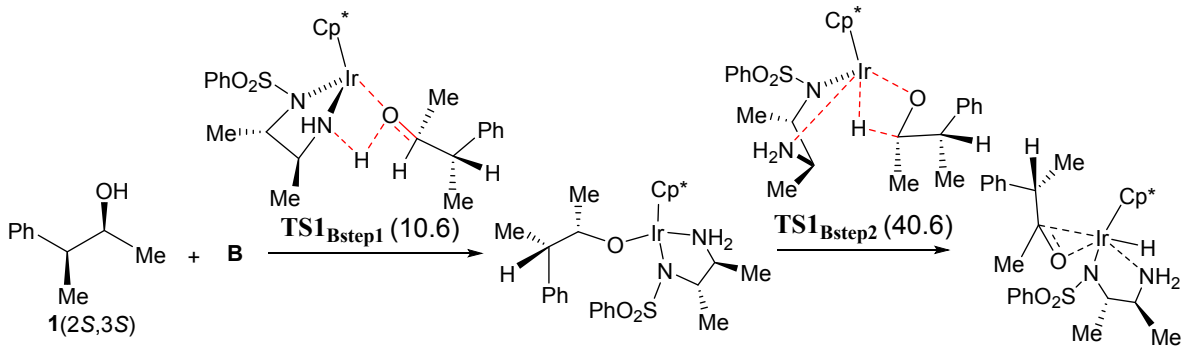
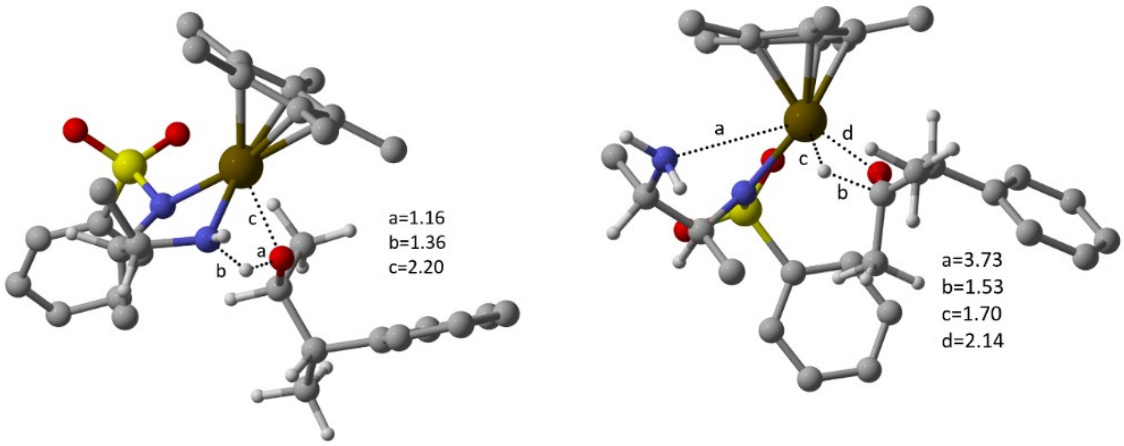


Fig. S4 The TS for concerted dehydrogenation of **1**(2*S*,3*S*) by catalyst $\mathbf{B_{model}}$. Relative free energy (in kcal/mol) of the most favored conformer of the TS given in parentheses is at the $SMD_{(toluene)}$/B3LYP-D3/6-31G**,SDD(Ir) Level of Theory. Distances are in Å.

Table S1. The Relative Free Energies (kcal/mol) of the Four Possible Stereoisomers of the Transition States of Concerted Dehydrogenation of Alcohol by Metal Catalyst $\mathbf{B_{model}}$ at the B3LYP-D3/6-31G**, SDD(Ir) Level of Theory

	Chirality on the metal	
Conformation of the five membered chelate	*R*	*S*
δ	15.9	18.7
λ	16.2	8.3





TS1$_{\mathbf{Bstep1}}$ **TS1$_{\mathbf{Bstep2}}$**

Fig. S5 The TS for stepwise dehydrogenation of **1**(2*S*,3*S*) by catalyst **B$_{\mathbf{model}}$**. Relative free energy (in kcal/mol) of the most favored conformer of the TS given in parentheses is obtained at the SMD$_{(toluene)}$/B3LYP-D3/6-31G**,SDD(Ir) Level of Theory. Distances are given in Å.

Table S2. The Relative Free Energies (kcal/mol) of the Four Possible Stereoisomers of the Transition States for the Stepwise Dehydrogenation of Alcohol by Metal Catalyst **B$_{\mathbf{model}}$** at the B3LYP-D3/6-31G**,SDD(Ir) Level of Theory

	Chirality on the metal	
Conformations of five membered chelate	*R*	*S*
δ	7.3	4.9
λ	8.9	4.8

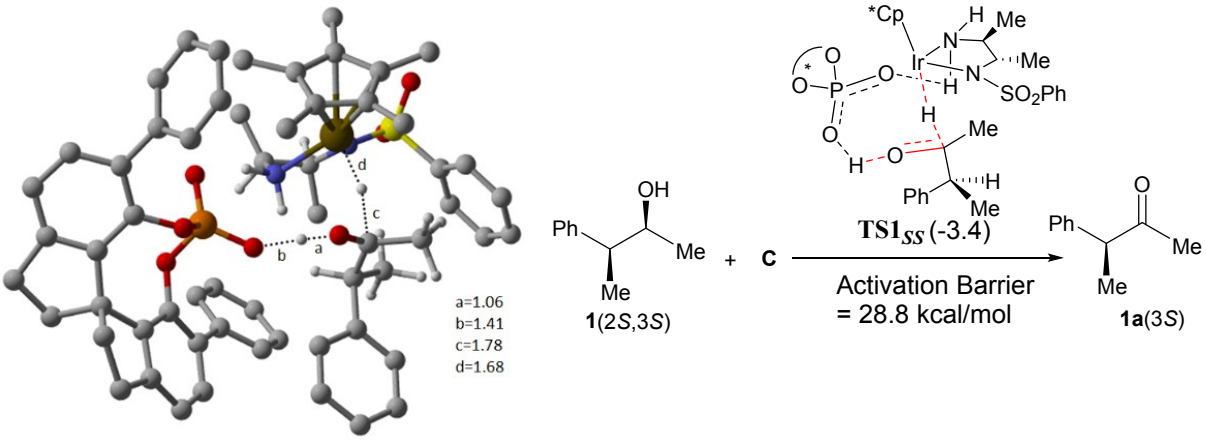


Fig. S6 The TS for concerted outer-sphere dehydrogenation of **1**(2*S*,3*S*) by catalyst $\mathbf{C_{model}}$. Relative free energy (in kcal/mol) of the most favored conformer of the TS given in parentheses is obtained through reoptimization at the $SMD_{(toluene)}$/B3LYP-D3/6-31G**,SDD(Ir) Level of Theory. Distances are given in Å.

Table S3. The Relative Free Energies (kcal/mol) of the Four Possible Stereoisomers of the TS of Concerted Outer-sphere Dehydrogenation of Alcohol by Catalyst Dyad $\mathbf{C_{model}}$ at the B3LYP-D3/6-31G**, SDD(Ir) Level of Theory[1]

	Chirality on the metal	
Conformations of five membered chelate	*R*	*S*
δ	-12.8	-13.3
λ	-10.1	-13.3

[1] See Fig. 1 in main text for catalyst dyad **C**. $\mathbf{A_{model}}$ and $\mathbf{B_{model}}$ form similar complex $\mathbf{C_{model}}$.

Based on the above free energies, the reaction is inferred to take place via concerted dehydrogenation by the ion pair complex $\mathbf{C_{model}}$. The concertedness of the process is verified by extended reaction coordinate plot in Fig. S7.

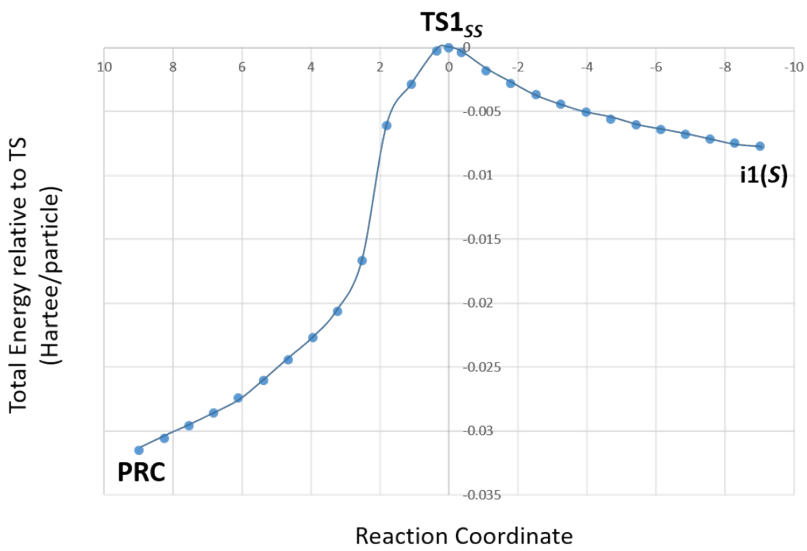


Fig. S7 Internal Reaction Coordinate extended up to 50 points for **TS1**$_{SS}$. The IRC plot suggests the absence of any intermediates between the TS and the two ends of the IRC that connects to the reactant/products. Hence, the mechanism is a concerted process.

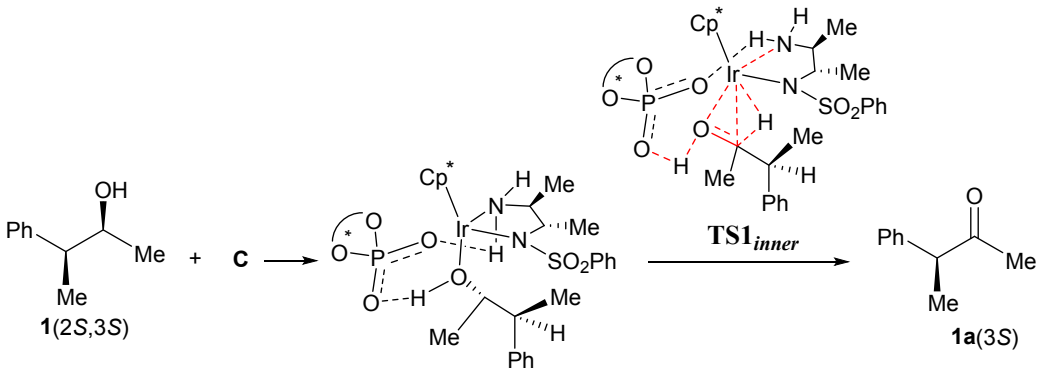


Fig. S8 The TS for concerted inner-sphere dehydrogenation of **1**(2*S*,3*S*) by **C**$_{\mathbf{model}}$. (The inner-sphere TS was not optimised in SMD as the gas phase energies were too high compared to the outer-sphere analogue.)

Table S4. The Relative Energies (kcal/mol) of the Four Possible Stereoisomers of the TS of Concerted Inner-sphere Dehydrogenation of Alcohol by **C**$_{\mathbf{model}}$ at the B3LYP-D3/6-31G**, SDD(Ir) Level of Theory

	Chirality on the metal	
Conformations of five membered chelate	*R*	*S*
δ	25.4	24.2
λ	23.6	23.4

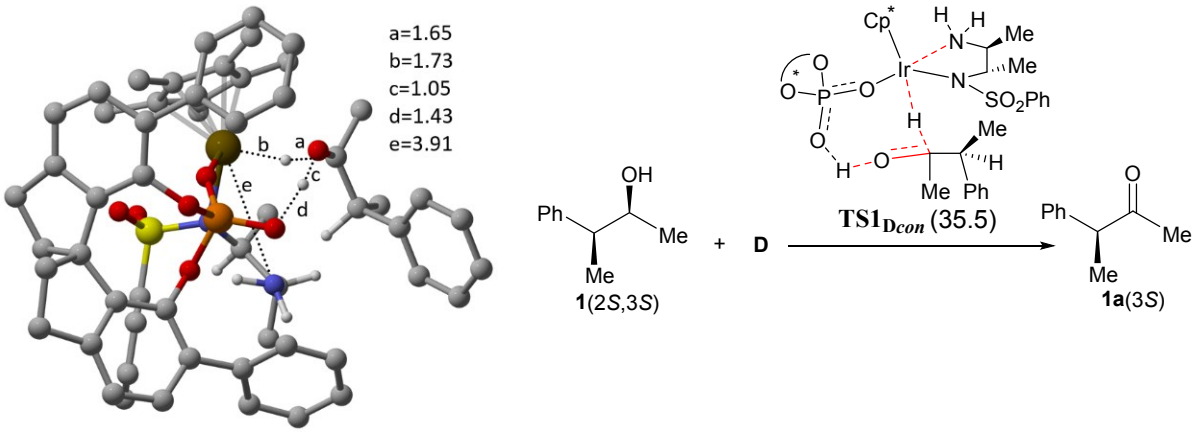


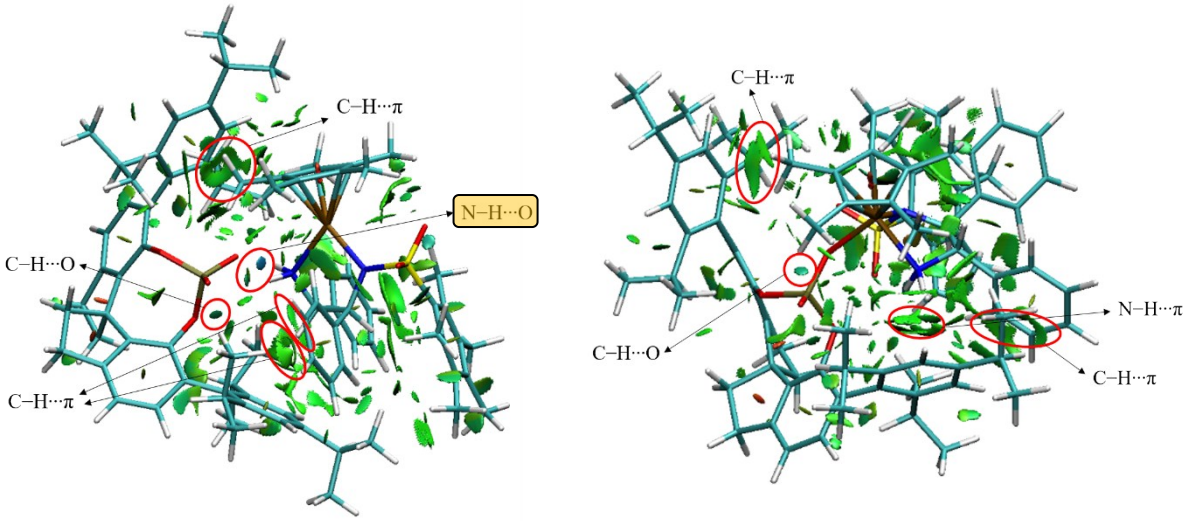
Fig. S9 The TS for concerted dehydrogenation of **1**(2*S*,3*S*) by catalyst dyad $\mathbf{D_{model}}$. Relative free energy given in parenthesis of the most favoured conformer of TS at the $SMD_{(toluene)}$/B3LYP-D3/6-31G**,SDD(Ir) Level of Theory. Distances are given in Å.

Table S5. The Relative Energies (kcal/mol) of Two Stereoisomers of the TS of Concerted Dehydrogenation of Alcohol by $\mathbf{D_{model}}$ at the B3LYP-D3/6-31G**, SDD(Ir) Level of Theory[2]

Chirality on the metal	
R	*S*
32.0	20.2

[2] See Fig. 1 in main text for catalyst dyad **D**. $\mathbf{A_{model}}$ and $\mathbf{B_{model}}$ form similar complex $\mathbf{D_{model}}$.

5. Noncovalent Interactions (NCI) Plots of Potential Active Catalysts C and D for the Full System



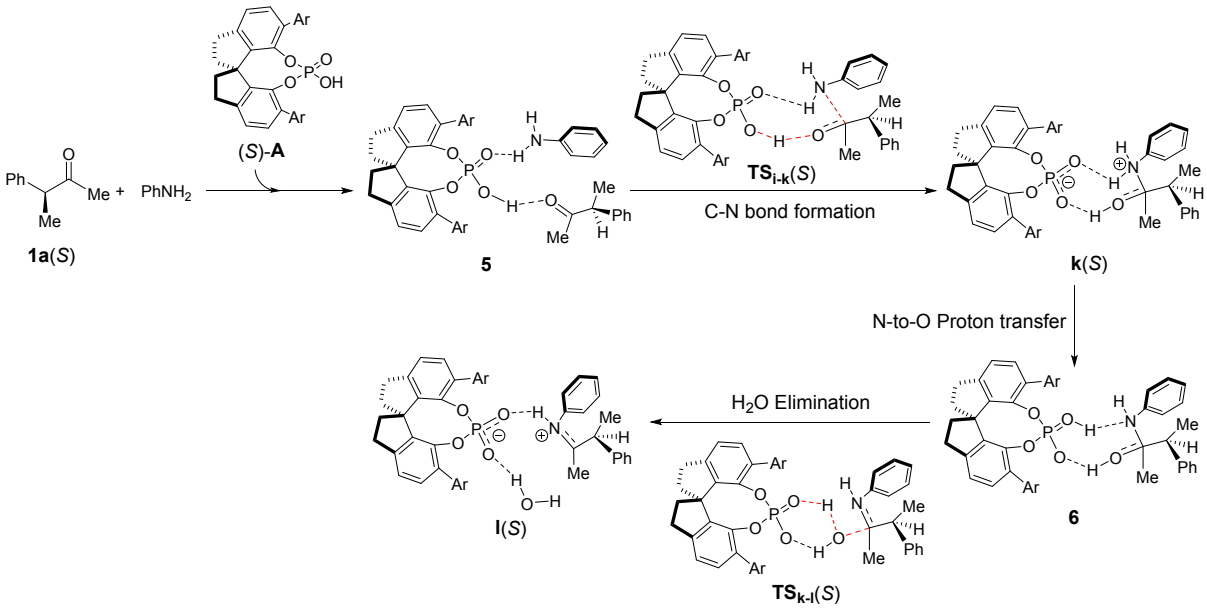
C **D**

Fig. S10 NCI plots for ion-pair catalyst dyad **C** and covalently bonded catalyst dyad **D** (blue: strongly attractive; green: weakly attractive).

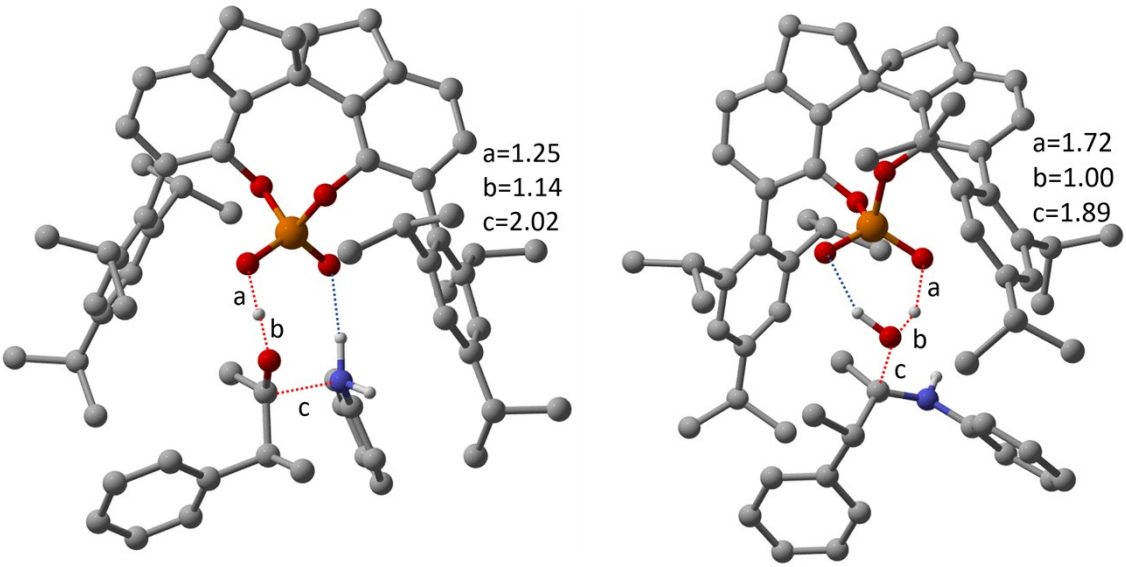
6. Chiral Phosphoric Acid Catalyzed Condensation of Ketone with Aryl Amine to Iminium

The condensation of enantiomeric ketones **1a**(3*S*) and **1a'**(3*R*) with aniline to form the enantiomeric iminiums is catalysed by the chiral phosphoric acid (*S*)-**A**. The mechanism of formation of iminium is shown in Scheme S1, using (*S*)-ketone as a representative substrate. The Lewis basic and Brønsted acidic sites on the phosphoric acid interact with the reacting partners, i.e., the amine and the ketone respectively, through hydrogen bonding and bring them closer as shown in **5**. The protonation of ketone facilitates easier nucleophilic attack of the amine on the carbonyl carbon. We noticed a concomittant protonation and C–N bond formation in the transition state $\mathbf{TS_{i\text{-}k}}$(*S*). For comparison, we have computed this step without the assistance of the phosphoric acid and found that the uncatalyzed pathway has a barrier of more than 40 kcal/mol. After the C–N bond formation, a proton transfer from the

amine nitrogen to the oxygen of the phosphate takes place. Elimination of a water molecule via **TS$_{k\text{-}l}$**(*S*) then results in the formation of complex **l**(*S*) where the iminium ion and water molecule are hydrogen-bonded with the chiral phosphate.



Scheme S1. Mechanism of chiral phosphoric acid catalysed condensation of ketone **1a**(*S*) with aniline.



TS(5-6) (6.5) **TS(7-8)** (23.0)

Fig. S11 The transition states for phosphoric acid catalyzed condensation of (*S*)-ketone and aniline to form iminium. The distances are in Å. The relative free energies (in kcal/mol) given in parentheses are calculated at the SMD$_{(toluene)}$/M06/6-31G**, SDD(Ir) level of theory.

7. Conformational Analysis of the Key Transition States

(i) Dehydrogenation of Alcohol with the Real Catalysts

A detailed conformational study is undertaken on the important transition states of dehydrogenation for the two isomers of alcohol at the $SMD_{toluene}$/B3LYP-D3/6-31G**,SDD(Ir) level of theory (Table S6). As discussed earlier (Fig. S3), the diamine ligand framework can assume two conformers λ or δ. Although with the model system, λ is found to be of lower energy, we have optimized some conformers of the full system in both λ and δ geometries. As such, it appears that they can interconvert from the initial guess geometries during optimization, indicating no apparent correlation of the conformation of the diamine framework with the corresponding change in free energies. The dihedral angles *Φ1* between the atoms O(1)-C(2)-Ir(3)-N(4) and *Φ2* between the atoms C(5)-S(6)-N(7)-Ir(3) were also varied. In addition to that, the groups on the β-C atom of the substrate were rotated along the C_α-C_β bond. The lowest energy conformation of $\mathbf{TS1}_{SS}$ is entry k, while that of $\mathbf{TS1}_{RS}$ is entry d in Table S6.

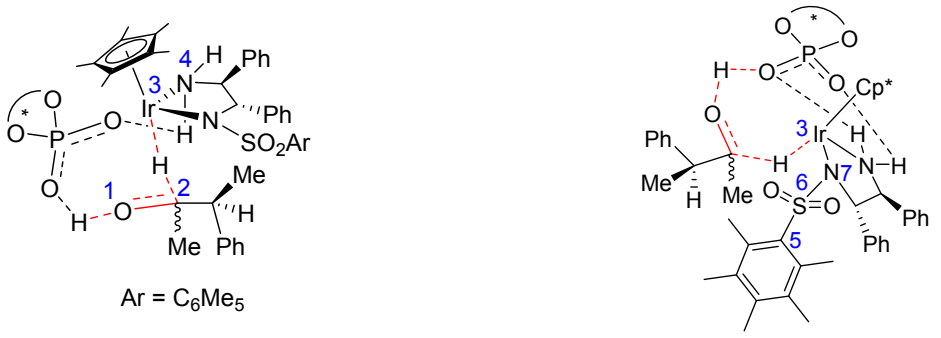
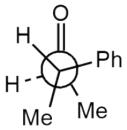
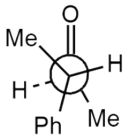
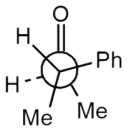
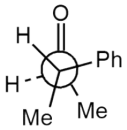
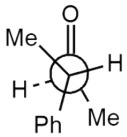
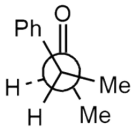
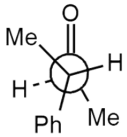
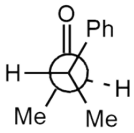
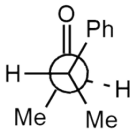
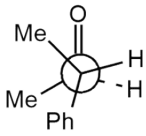
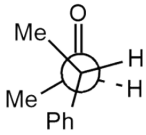
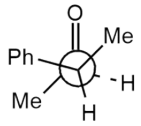


Fig. S12 The general representation of two different orientations of the transition state for dehydrogenation from **1**(2*X*,3*S*), *X* being the configuration (*S* or *R*). The transition states are shown in two different orientations to clearly represent the two dihedral angles *Φ1* and *Φ2*.

Table S6. The Conformational Analysis of Concerted Dehydrogenation of Alcohols **1**(2*S*,3*S*) and **1'**(2*R*,3*S*) by Ion-Pair Catalyst Dyad **C** at the $SMD_{(toluene)}$/B3LYP-D3/6-31G**,SDD(Ir) Level of Theory

TS1$_{SS}$							
Entry	Diamine ligand	*Φ1*(O1-C2-Ir3-N4)	*Φ2*(C5-S6-N7-Ir3)	Alcohol Newman projection	Dihedral angles in the alcohol		ΔG
					Front Carbon	Back Carbon	
a	Diaxial (*λ*)	-56.3	109.9		Ph-C-C-O =-72.6 Me-C-C-O =160.1 H-C-C-O =40.7	Me-C-C-Me =-48.9 Me-C-C-Ph =79.5 Angle H-C-O =102.6	14.2
b	Diequitorial (*δ*)	1.8	176.2		Ph-C-C-O =168.0 Me-C-C-O =37.5 H-C-C-O =-77.1	Me-C-C-H =68.6 Me-C-C-Ph =-49.4 Angle H-C-O =106.1	3.4
c	Diaxial (*λ*)	-52.2	177.1		Ph-C-C-O =-62.7 Me-C-C-O =169.8 H-C-C-O =51.9	Me-C-C-Me =-39.0 Me-C-C-Ph =88.4 Angle H-C-O =103.0	15.0
d	Diequitorial (*δ*)	-66.3	174.6		Ph-C-C-O =-71.0 Me-C-C-O =161.8 H-C-C-O =42.2	Me-C-C-Me =-45.8 Me-C-C-Ph =81.3 Angle H-C-O =104.1	2.4
e	Diequitorial (*δ*)	5.6	176.6		Ph-C-C-O =167.0 Me-C-C-O =36.1 H-C-C-O =-78.3	Me-C-C-H =65.6 Me-C-C-Ph =-49.1 Angle H-C-O =106.4	2.0
f	Diequitorial (*δ*)	46.0	164.0		Ph-C-C-O =6.3 Me-C-C-O =-119. H-C-C-O =125.3	Me-C-C-Me =35.8 Me-C-C-H =-79.3 Angle H-C-O =102.4	17.6
g	Diaxial (*λ*)	10.0	76.2		Ph-C-C-O =164.5 Me-C-C-O =31.1 H-C-C-O	Me-C-C-H =55.6 Me-C-C-Ph =-57.9 Angle H-C-O	17.2

					=-82.0	=106.0	
h	Diaxial (λ)	9.5	175.7		Ph-C-C-O =154.5 Me-C-C-O =22.0 H-C-C-O =-91.2	Me-C-C-H =50.0 Me-C-C-Ph =-64.3 Angle H-C-O =105.3	4.9
i	Diaxial (λ)	8.6	175.7		Ph-C-C-O =154.6 Me-C-C-O =21.9 H-C-C-O =-91.3	Me-C-C-H =50.0 Me-C-C-Ph =-64.1 Angle H-C-O =105.0	4.7
j	Diaxial (λ)	2.1	172.9		Ph-C-C-O =-75.6 Me-C-C-O =156.9 H-C-C-O =38.3	Me-C-C-Me =-54.8 Me-C-C-Ph =72.7 Angle H-C-O =105.0	0.9
k	Diaxial (λ)	-2.9	177.4		Ph-C-C-O =-65.5 Me-C-C-O =167.7 H-C-C-O =50.4	Me-C-C-Me =-41.7 Me-C-C-Ph =85.0 Angle H-C-O =106.0	0.0
	TS1$_{RS}$						
a	Diequitorial (δ)	-66.4	79.5		Ph-C-C-O =-20.7 Me-C-C-O =-156.1 H-C-C-O =91.6	Me-C-C-H =-55.9 Me-C-C-Me =56.4 Angle H-C-O =104.0	8.4
b	Diaxial (λ)	-79.5	132.5		Ph-C-C-O =-6.6 Me-C-C-O =-141.7 H-C-C-O =106.3	Me-C-C-H =-34.9 Me-C-C-Me =74.1 Angle H-C-O =106.3	4.8
c	Diaxial (λ)	-81.5	111.1		Ph-C-C-O =156.7 Me-C-C-O =30.4 H-C-C-O =-85.8	Me-C-C-Ph =10.7 Me-C-C-Me =-115.6 Angle H-C-O =104.3	1.8
d	Diaxial (λ)	-79.8	157.0		Ph-C-C-O =-169.7 Me-C-C-O =64.3 H-C-C-O	Me-C-C-Ph =42.4 Me-C-C-Me =-83.6 Angle H-C-O	0.0

					=-49.2	=103.8	
e	Diaxial (λ)	-96.0	122.4		Ph-C-C-O =86.6 Me-C-C-O =-39.3 H-C-C-O =-159.1	Me-C-C-Ph =-66.2 Me-C-C-H =48.0 Angle H-C-O =100.9	1.5

(ii) Hydride Addition to Iminium with Real Catalysts

In the next set of transition states for the conversion of (*S*)-iminium to two stereoisomeric amines, **3**(2*S*,3*S*) and **3'**(2*R*,3*S*), the dihedral angles *Φ3* between the atoms N(8)-C(2)-Ir(3)-N(4) and *Φ2* between the atoms C(5)-S(6)-N(7)-Ir(3) were varied along with the conformational changes to the diamine framework. In addition to that, the groups on the β-C atom of the substrate were also rotated along the C_α-C_β bond.

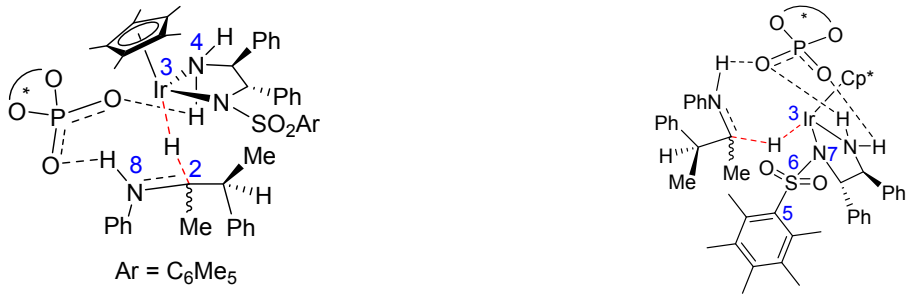
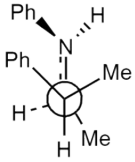
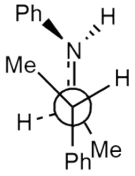
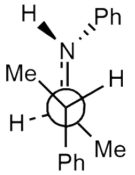
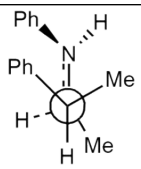
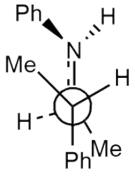
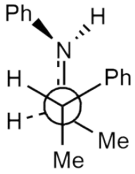
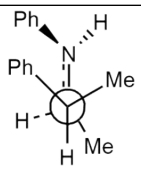
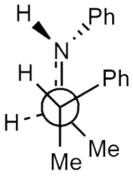
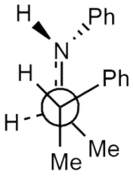
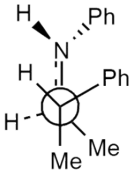
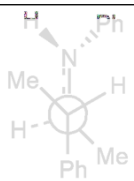
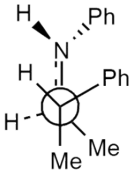
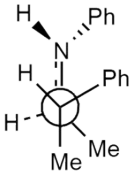
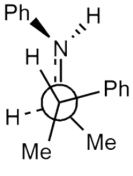
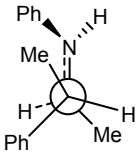
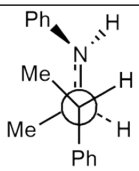
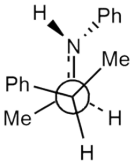
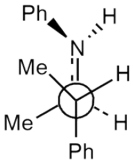
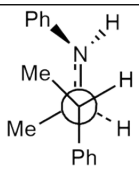
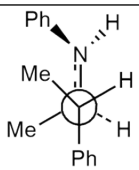
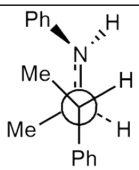


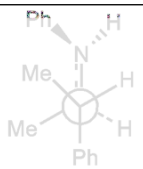
Fig. S13 The general representation of two different orientation of the transition state for asymmetric hydride addition to (*S*)-iminium. The transition states are shown in two different orientations to clearly represent the two dihedral angles *Φ3* and *Φ2*.

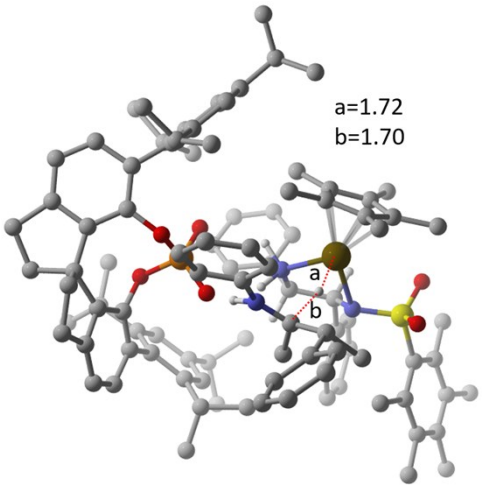
Table S7. The Conformational Analysis of Asymmetric Hydride Addition to (*S*)-Iminium to form **3**(2*S*,3*S*) and **3'**(2*R*,3*S*) at the $SMD_{(toluene)}$/B3LYP-D3/6-31G**,SDD(Ir) Level of Theory

TS2$_{SS}$							
Entry	Diamine ligand	*Φ3*(N8-C2-Ir3-N4)	*Φ2*(C5-S6-N7-Ir3)	Iminium Newman	Dihedral angles in the iminium		ΔG
					Front carbon	Back Carbon	
a	Diaxial (*λ*)	15.3	-57.3		Ph-C-C-N =52.7 Me-C-C-N =-76.9 H-C-C-N =170.1	Me-C-C-Me =57.3 Me-C-C-H =-55.7 Angle H-C-N =110.8	27.6
b	Diaxial (*λ*)	3.9	85.2		Ph-C-C-N =-173.7 Me-C-C-N =57.8 H-C-C-N =-60.1	Me-C-C-Ph =-31.7 Me-C-C-H =81.8 Angle H-C-N =111.0	23.6
c	Diequitorial (*δ*)	-43.3	176.8		Ph-C-C-N =-164.1 Me-C-C-N =62.9 H-C-C-N =-51.3	Me-C-C-Ph =-20.7 Me-C-C-H =92.1 Angle H-C-N =105.1	15.1
d	Diaxial (*λ*)	16.9	170.9		Ph-C-C-N =38.0 Me-C-C-N =-91.1 H-C-C-N =155.1	Me-C-C-Me =48.4 Me-C-C-H =-65.3 Angle H-C-N =110.5	20.4
e	Diaxial (*λ*)	2.6	-88.4		Ph-C-C-N =-165.0 Me-C-C-N =66.3 H-C-C-N =-50.8	Me-C-C-Ph =-22.5 Me-C-C-H =91.7 Angle H-C-N =110.0	23.8
f	Diequitorial (*δ*)	18.1	-59.8		Ph-C-C-N =-64.4 Me-C-C-N =170.3 H-C-C-N =53.1	Me-C-C-Ph =74.4 Me-C-C-Me =-50.8 Angle H-C-N =110.8	11.1
g	Diaxial (*λ*)	32.4	174.6		Ph-C-C-N =62.7 Me-C-C-N =-69.2 H-C-C-N	Me-C-C-Me =68.5 Me-C-C-H =-43.3 Angle H-C-N	9.3

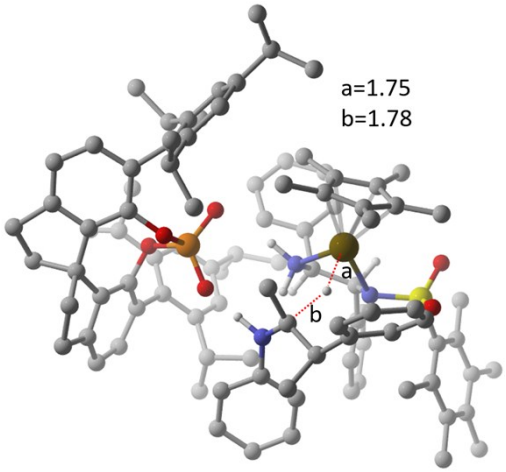
					=179.0	=110.1	
h	Diaxial (λ)	-61.6	-95.1		Ph-C-C-N =-172.5 Me-C-C-N =54.1 H-C-C-N =-59.5	Me-C-C-Ph =-28.9 Me-C-C-H =84.0 Angle H-C-N =103.4	27.7
i	Diaxial (λ)	-76.0	146.7		Ph-C-C-N =-61.8 Me-C-C-N =171.6 H-C-C-N =51.7	Me-C-C-Ph =86.5 Me-C-C-Me =-40.5 Angle H-C-N =106.9	4.7
j	Diequitorial (δ)	-75.0	178.3		Ph-C-C-N =-61.1 Me-C-C-N =172.7 H-C-C-N =52.6	Me-C-C-Ph =88.6 Me-C-C-Me =-37.5 Angle H-C-N =106.3	0.2
k	Diequitorial (δ)	-73.6	177.2		Ph-C-C-N =-63.0 Me-C-C-N =170.7 H-C-C-N =50.6	Me-C-C-Ph =85.3 Me-C-C-Me =-41.0 Angle H-C-N =106.8	0.1
l	Diaxial (λ)	2.1	179.8		Ph-C-C-N =178.4 Me-C-C-N =45.8 H-C-C-N =-68.6	Me-C-C-Ph =-39.2 Me-C-C-H =73.7 Angle H-C-N =105.9	20.5
m	Diaxial (λ)	-63.1	170.5		Ph-C-C-N =-58.9 Me-C-C-N =174.3 H-C-C-N =54.8	Me-C-C-Ph =88.7 Me-C-C-Me =-38.0 Angle H-C-N =105.5	15.2
n	Diaxial (λ)	3.4	162.9		Ph-C-C-N =-69.9 Me-C-C-N =163.2 H-C-C-N =44.3	Me-C-C-Ph =78.9 Me-C-C-Me =-47.9 Angle H-C-N =105.9	2.8
o	Diaxial (λ)	27.8	-60.9		Ph-C-C-N =-100.1 Me-C-C-N =130.4 H-C-C-N =13.4	Me-C-C-Ph =34.5 Me-C-C-Me =-94.9 Angle H-C-N =110.4	22.5

p	Diequitorial (δ)	-75.2	176.0		Ph-C-C-N =-60.9 Me-C-C-N =173.2 H-C-C-N =52.8	Me-C-C-Ph =89.4 Me-C-C-Me =-36.5 Angle H-C-N =106.1	0.0
q	Diequitorial (δ)	13.4	168.1		Ph-C-C-N =159.2 Me-C-C-N =25.0 H-C-C-N =-88.1	Me-C-C-Ph =-66.6 Me-C-C-H =46.2 Angle H-C-N =108.6	12.5
	TS2$_{RS}$						
a	Diequitorial (δ)	-69.5	178.5		Ph-C-C-N =-171.0 Me-C-C-N =63.5 H-C-C-N =-53.3	Me-C-C-Ph =48.1 Me-C-C-Me =-77.3 Angle H-C-N =108.2	1.5
b	Diequitorial (δ)	4.4	178.8		Ph-C-C-N =98.3 Me-C-C-N =-25.4 H-C-C-N =-147.0	Me-C-C-Ph =-55.6 Me-C-C-H =59.0 Angle H-C-N =105.8	0.0
c	Diaxial (λ)	-68.2	144.2		Ph-C-C-N =-171.4 Me-C-C-N =62.0 H-C-C-N =-53.9	Me-C-C-Ph =45.5 Me-C-C-Me =-81.1 Angle H-C-N =105.2	11.8
d	Diequitorial (δ)	-69.7	177.4		Ph-C-C-N =-170.5 Me-C-C-N =64.1 H-C-C-N =-52.6	Me-C-C-Ph =48.3 Me-C-C-Me =-77.0 Angle H-C-N =108.3	1.9
e	Diaxial (λ)	-74.6	-117.2		Ph-C-C-N =-174.4 Me-C-C-N =61.1 H-C-C-N =-56.4	Me-C-C-Ph =44.7 Me-C-C-Me =-79.8 Angle H-C-N =107.3	9.6
f	Diaxial (λ)	-66.5	159.0		Ph-C-C-N =-175.2 Me-C-C-N =61.1 H-C-C-N =-56.1	Me-C-C-Ph =44.1 Me-C-C-Me =-79.6 Angle H-C-N =107.3	5.4

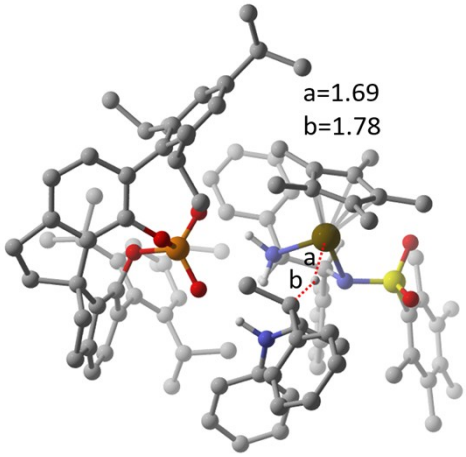
g	Diaxial (λ)	-61.2	172.8		Ph-C-C-N =-175.1 Me-C-C-N =58.6 H-C-C-N =-57.6	Me-C-C-Ph =42.3 Me-C-C-Me =-84.0 Angle H-C-N =105.3	3.3



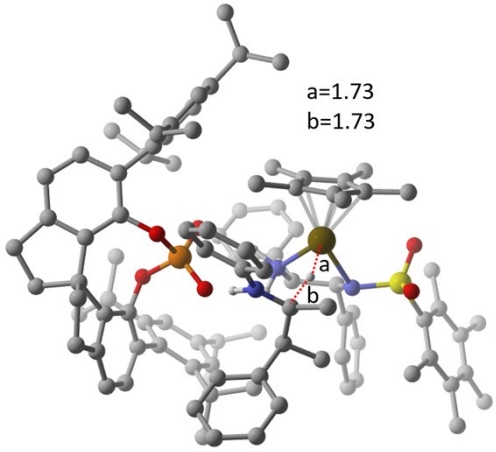
TS2$_{RR}$ (*0.9*)



TS2$_{SR}$ (*1.6*)



TS2$_{RS}$ (*3.6*)



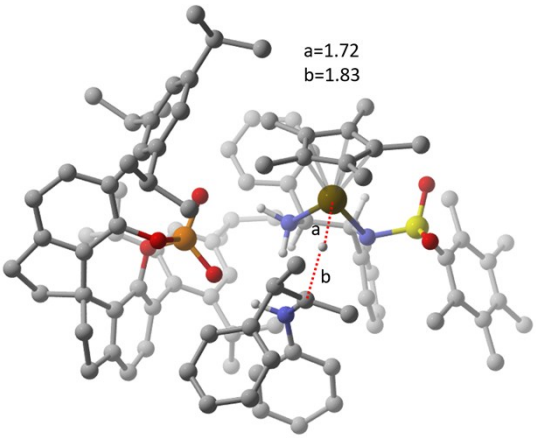
TS2$_{SS}$ (*0.0*)

Fig. S14 The transition states for asymmetric hydride addition to (*R*) and (*S*) iminium.

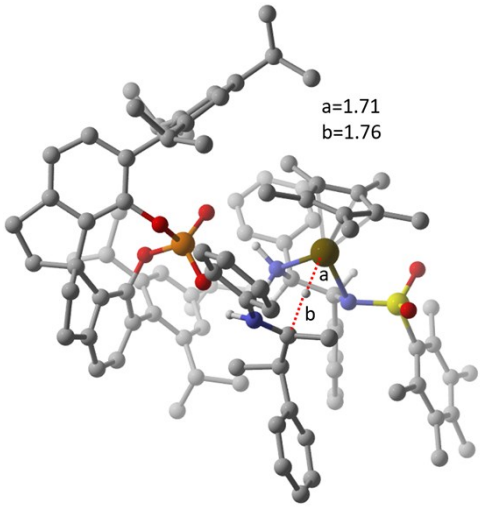
8. Hydride addition to (*Z*)-(*S*)-iminium and (*E*)-(*R*)-iminium intermediates

The lowest energy hydride addition transition state for the (*S*)-iminium involves the *E* configuration around the C=N bond irrespective of the prochiral face (*re*/*si*) to which hydride

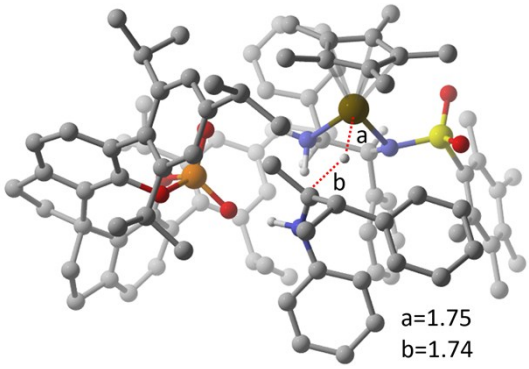
addition takes place. However, the preferred configuration of the lowest energy TS for the (*R*)-iminium around the C=N bond is *Z* (Fig. S14). The higher energy hydride addition TSs for (*Z*)-(*S*)-iminium and (*E*)-(*R*)-iminium are provided in Fig. S15.



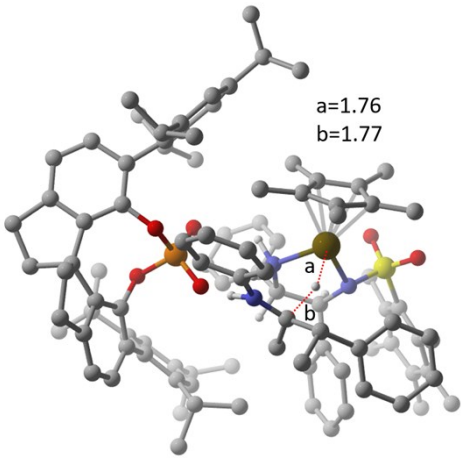
(*E*)-**TS2**$_{RR}$ (*4.7*)



(*E*)-**TS2**$_{SR}$ (*4.2*)



(*Z*)-**TS2**$_{SS}$ (*6.9*)

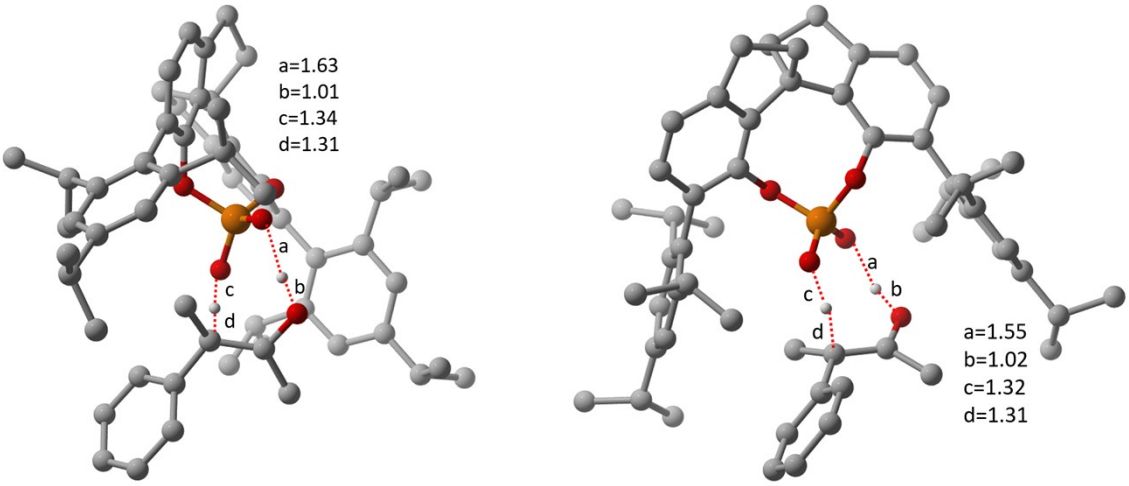


(*Z*)-**TS2**$_{RS}$ (*6.2*)

Fig. S15 The transition state geometries for the asymmetric hydride addition to (*E*)-(*R*)-iminium and (*Z*)-(*S*)-iminium. The free energies (in kcal/mol) given in parentheses are with respect to each lower energy transition state with iminium in its (*Z*)-(*R*) and (*E*)-(*S*) configurations. Distances are in Å.

9. Epimerization of (*R*)-ketone

Epimerization is considered for the (*E*)-enol intermediate (as the Boltzmann population (0.19% at 383 K) of the (*Z*)-enol is expected to be quite low). In **TS**$_{R\text{-j}}$, the Lewis basic oxygen of the phosphoric acid abstracts the β-C–H proton from the substrate while its acidic proton gets transferred to the carbonyl oxygen at the other end of the substrate to form the phosphoric acid-enol complex (**j**). In the next step, through **TS**$_{\text{j-}S}$, the proton abstraction from the enol end of the substrate and a concomitant protonation of the β-C through the other prochiral face leads to the (*S*) ketone.



TS$_{R\text{-j}}$ **TS**$_{\text{j-}S}$

Fig S16 The transition state geometries for phosphoric acid catalysed epimerization of (*R*)-ketone to (*S*)-ketone. Distances are in Å.

9. Epimerization of (*R*)-iminium intermediate

We note that the hydride addition to (*R*)-iminium is more preferred when the configuration (Figs. S14-S15) around the C=N bond is *Z*. The transition state for tautomerisation to form (*E*)-enamine is shown in Fig. S17 only for (*R*)-(*Z*)-iminium. Likewise, in the case of (*S*)-iminium, only the (*E*) configuration of the C=N bond is considered. In **TS**$_{R\text{-}m}$, Lewis basic

oxygen of the phosphate abstracts the β-C–H proton of (*R*)-iminium giving a complex of phosphoric acid and *E*-enamine (**m**). The phosphoric acid then transfers the proton to the prochiral face of the enamine such that the β-C of ensuing iminium assumes (*S*) configuration (Fig. S17).

TS$_{R\text{-}m}$ **TS$_{m\text{-}S}$**

Fig. S17 The transition state geometries for phosphoric acid catalysed epimerization of (*R*)-iminium to (*S*)-iminium intermediate. Distances are in Å.

This pathway for epimerization is less favoured over the direct hydride transfer to (*R*)-iminium to form the enantiomer **3''**(2*R*,3*R*). Therefore based on experimental observation and our calculations, we infer that the epimerization of (*R*)-ketone to form (*S*)-ketone is more likely than a direct condensation route to form (*R*)-iminium intermediate. Further, the epimerization of (*R*)-iminium to form (*S*)-iminium as shown in Fig. S18 will presumably not take place because of low percentage of (*R*)-iminium formed.

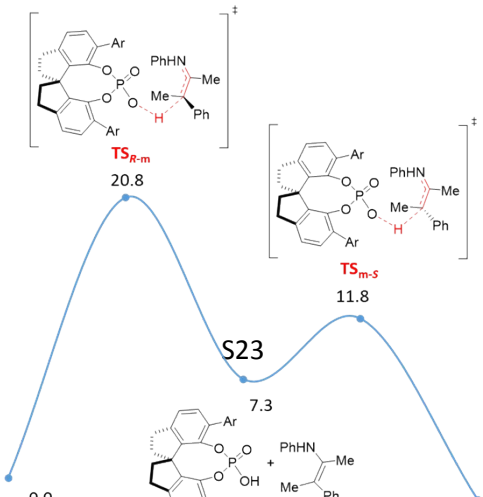
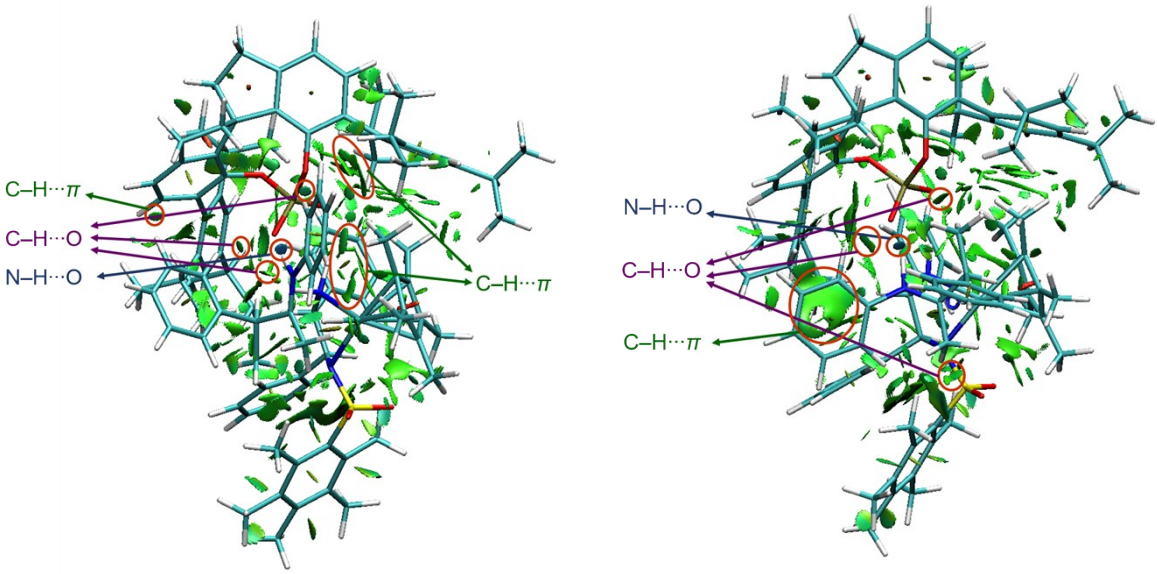


Fig. S18 The relative free energy (kcal/mol) profile for the epimerization of (*R*)-iminium to (*S*)-iminium. The energies are in kcal/mol.

9. NCI plots of TS2$_{SS}$ and TS2$_{RS}$

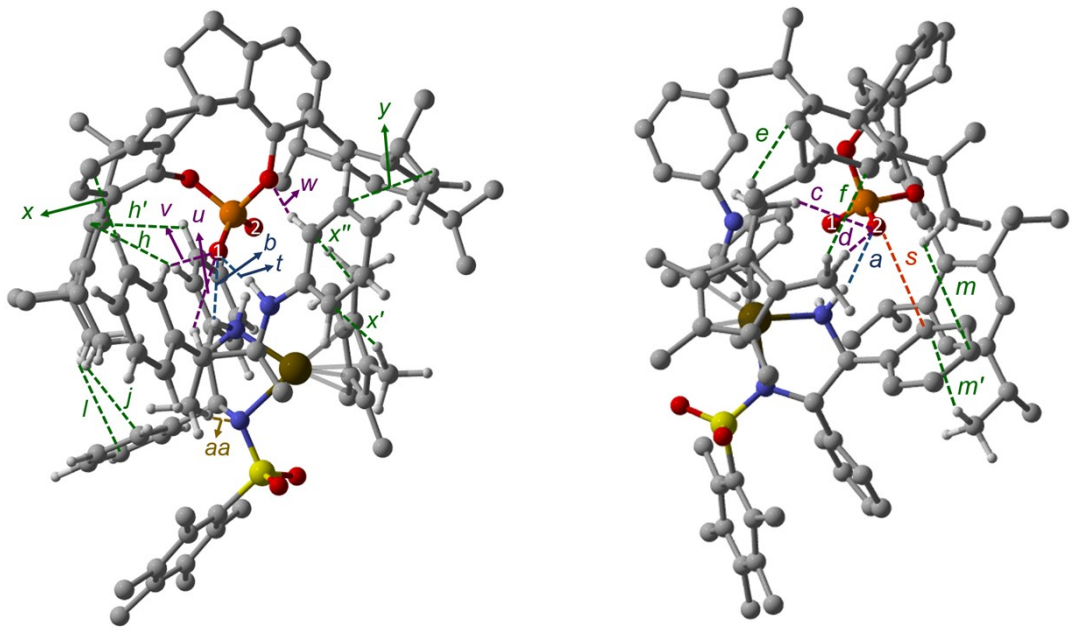


TS2$_{SS}$ **TS2$_{RS}$**

Fig. S19 NCI plots for diastereomeric transition states **TS2$_{SS}$** and **TS2$_{RS}$** with the interactions between substrate and catalyst dyad marked explicitly (blue: strongly attractive; green: weakly attractive).

10. Full Mapping of Noncovalent Interactions of TS2$_{SS}$ and TS2$_{RS}$ as Obtained Using the AIM Analysis

TS2$_{SS}$



TS2$_{RS}$

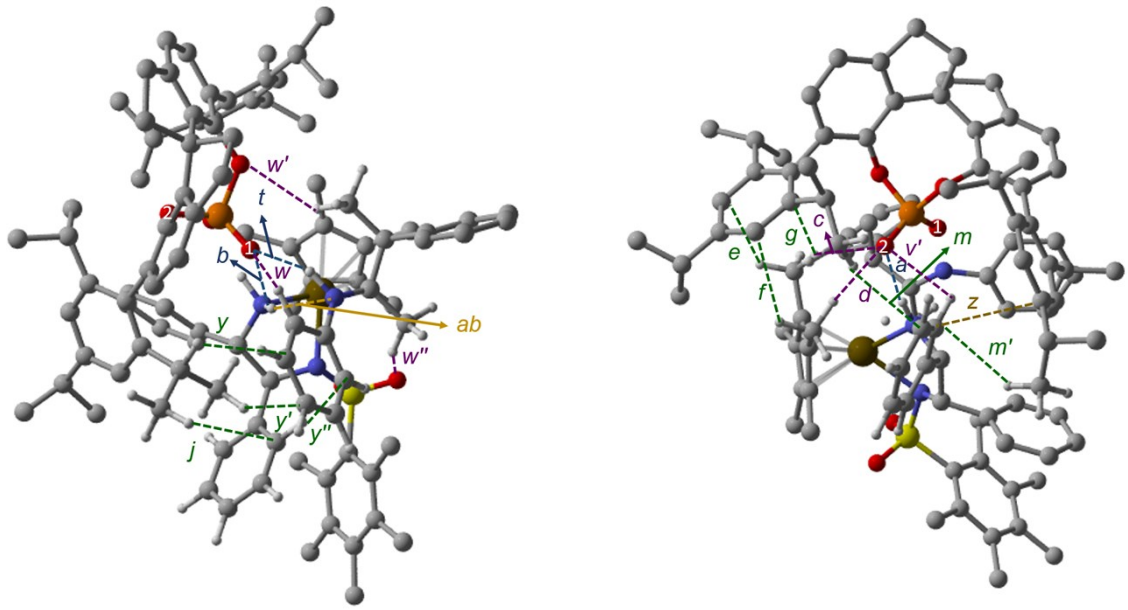


Fig. S20 Noncovalent interactions, as noted using the bond paths and bond critical points in atoms in molecule (AIM) formalism. Transition states (**TS2$_{SS}$** and **TS2$_{RS}$**) are shown in two orientations for representing all the interactions.

Table S8. The distances, angles and electron densities (ρ x 10^{-2} au) at the *bcps* of the noncovalent contacts

Label	type	**TS2$_{SS}$**			**TS2$_{RS}$**		
		distance (Å)	angle	ρ*10^{-2}	distance (Å)	angle	ρ*10^{-2}
a	N–H···O	2.05	157.6	2.22	1.98	162.9	2.53
b	N–H···O	2.40	124.1	1.19	2.46	120.5	1.06
t	N–H···O	1.82	165.1	3.30	1.85	152.3	3.01
c	C–H···O	2.55	157.9	0.93	2.63	155.6	0.76
d	C–H···O	2.24	163.5	1.46	2.31	169.0	1.22
u	C–H···O	2.45	136.2	1.04	-	-	-
v	C–H···O	2.40	146.3	1.10	-	-	-
w	C–H···O	2.15	167.9	1.83	2.54	122.4	0.86
w′	C–H···O	-	-	-	2.72	116.7	0.63
w″	C–H···O	-	-	-	2.59	136.9	0.79
v′	C–H···O	-	-	-	2.73	107.1	0.75
e	C–H···π	2.58	140.6	1.02	2.59	133.6	1.01
f	C–H···π	2.75	121.2	0.74	2.89	123.5	0.56
g	C–H···π	-	-	-	3.06	125.7	0.44
h	C–H···π	2.86	116.5	0.67	-	-	-
h′	C–H···π	3.07	109.7	0.42	-	-	-
j	C–H···π	2.89	121.3	0.58	2.74	104.8	0.85
l	C–H···π	3.00	114.4	0.51	-	-	-
m	C–H···π	2.85	108.3	0.61	2.83	119.2	0.60
m′	C–H···π	2.73	141.4	0.77	2.86	141.1	0.60
x	C–H···π	2.81	139.4	0.60	-	-	-
x′	C–H···π	3.06	157.6	0.44	-	-	-
x″	C–H···π	2.65	143.3	0.88	-	-	-
y	C–H···π	2.90	103.5	0.62	2.79	122.1	0.73
y′	C–H···π	-	-	-	2.71	145.4	0.84
y″	C–H···π	-	-	-	2.87	152.9	0.54
s	lp_O··· π	3.25	-	0.63	-	-	-
z	π···π	-	-	-	3.46	-	0.52
aa	C–H···N	2.26	169.7	1.80	-	-	-
ab	N–H···N	-	-	-	2.59	147.8	0.73

11. Relative Free Energies (in kcal/mol) of Stationary Points in the Favoured Pathway

Table S9. The relative free energies (in kcal/mol) of the important species involved in asymmetric amination of alcohol through the most favoured pathway

Level of theory	**PRC**	**TS1$_{SS}$**	**i1(*S*)**	**i2(*S*)**	**TS2$_{SS}$**	product	barrier **(TS2$_{SS}$-PRC)**
M06/6-31G**, def2-TZVP(Ir)	-3.5	22.1	17.6	20.9	32.6	-1.2	36.0
M06/6-31G**, def2-TZVPP(Ir)	-3.3	22.8	18.4	21.7	33.3	-1.1	36.6
M06/6-311G**, SDD(Ir)	-6.4	19.5	13.7	15.7	28.2	-5.9	34.6
M06/6-311G**, def2-TZVP(Ir)	-5.2	21.9	16.7	18.3	30.6	-4.9	35.8
M06/6-311G**, def2-TZVPP(Ir)	-4.9	22.7	17.6	19.1	31.4	-4.7	36.4
B3LYP-D3/6-31G**, def2-TZVP(Ir)	-19.8	1.5	-0.8	-0.8	9.7	-18.4	29.5
B3LYP-D3/6-31G**, def2-TZVPP(Ir)	-19.7	2.3	0.1	0.0	10.5	-18.2	30.2
B3LYP-D3/6-311G**, SDD(Ir)	-13.6	8.2	4.9	6.1	16.2	-11.4	29.9
B3LYP-D3/6-311G**, def2-TZVP(Ir)	-12.6	10.2	7.4	8.3	18.2	-10.5	30.8
B3LYP-D3/6-311G**, def2-TZVPP(Ir)	-12.4	11.0	8.3	9.1	19.1	-10.3	31.4
ω-B97XD/6-31G**, def2-TZVP(Ir)	-20.1	5.8	0.3	-0.6	13.4	-20.2	33.5
ω-B97XD/6-31G**, def2-TZVPP(Ir)	-19.9	6.7	1.3	0.4	14.4	-20.0	34.3
ω-B97XD/6-311G**, SDD(Ir)	-18.8	7.3	1.0	-0.3	13.7	-19.3	32.5
ω-B97XD/6-311G**, def2-TZVP(Ir)	-17.6	9.6	3.8	2.1	16.0	-18.2	33.6
ω-B97XD/6-311G**, def2-TZVPP(Ir)	-17.4	10.5	4.9	3.0	16.9	-17.9	34.3
M06L/6-31G**, def2-TZVP(Ir)	-3.9	21.7	18.3	22.9	32.2	-1.5	36.0
M06L/6-31G**, def2-TZVPP(Ir)	-3.7	22.6	19.4	23.9	33.1	-1.3	36.8
M06L/6-311G**, SDD(Ir)	-2.7	23.4	19.0	23.2	32.7	-0.8	35.3
M06L/6-311G**, def2-TZVP(Ir)	-1.6	25.6	21.6	25.5	34.9	0.1	36.5
M06L/6-311G**, def2-TZVPP(Ir)	-1.3	26.4	22.6	26.4	35.7	0.3	37.0

12. Cartesian Coordinates of the Optimized Geometries of Various Stationary Points Obtained at the M06 Level of Theory

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B

Number of imaginary frequencies : 0

Electronic energy : HF=-2120.9684483
Zero-point correction= 0.704449 (hartree/particle)
Thermal correction to Energy= 0.745695
Thermal correction to Enthalpy= 0.746639
Thermal correction to Gibbs Free Energy= 0.633705
Sum of electronic and zero-point Energies= -2120.264000
Sum of electronic and thermal Energies= -2120.222753
Sum of electronic and thermal Enthalpies= -2120.221809
Sum of electronic and thermal Free Energies= -2120.334743

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Cartesian Coordinates

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77	1.707726	-0.674659	0.212211
6	2.951698	-1.334749	-1.461697
6	2.254023	-2.504291	-1.035470
6	2.554422	-2.693220	0.358785
6	3.533753	-1.715015	0.772534
6	3.762546	-0.847884	-0.346927
7	1.493122	0.618864	1.690300
1	2.325492	0.843109	2.232901
6	-0.508950	1.379884	0.607245
1	-0.828360	2.217695	-0.031158
6	0.724838	1.827453	1.397378
1	0.371590	2.273611	2.344223
16	-0.852812	0.166782	-1.707662
8	-0.765773	1.480685	-2.359542
8	-0.317816	-0.967073	-2.468575
6	-2.587771	-0.173447	-1.297992
6	-5.160722	-0.541558	-0.285809
6	-2.850422	-1.283693	-0.469432
6	-3.608396	0.714425	-1.687845
6	-4.886610	0.549072	-1.121445
6	-4.141823	-1.444587	0.053544
6	-6.549472	-0.755652	0.248652
1	-6.685761	-0.281265	1.232784
1	-6.774453	-1.818958	0.373875
1	-7.313880	-0.347805	-0.418308
7	-0.091444	0.234258	-0.249546
6	2.946428	-0.762356	-2.833664
1	1.986363	-0.940535	-3.325621
1	3.742665	-1.213563	-3.442135
1	3.115426	0.320513	-2.818390
6	1.432661	-3.405640	-1.888167
1	2.081396	-4.103132	-2.436209
1	0.840524	-2.839465	-2.611733
1	0.739830	-4.009164	-1.291013
6	4.689908	0.314780	-0.404177
1	5.666549	0.014612	-0.807807
1	4.854184	0.752773	0.586439

1	4.290747	1.108995	-1.045168
6	2.008022	-3.772000	1.223902
1	2.624465	-4.678057	1.145029
1	0.986101	-4.038395	0.933572
1	1.990399	-3.471130	2.276883
6	4.158333	-1.629331	2.122580
1	4.949841	-2.380853	2.240908
1	3.419459	-1.796786	2.915238
1	4.610932	-0.646848	2.294459
6	1.614300	2.858594	0.724194
6	2.460044	3.615018	1.541231
6	1.706298	3.020830	-0.661619
6	3.387658	4.498270	0.999098
1	2.382600	3.507417	2.624778
6	2.629016	3.911399	-1.205032
1	1.057567	2.455268	-1.329236
6	3.477148	4.647074	-0.382036
1	4.032268	5.079712	1.655570
1	2.680678	4.031650	-2.285775
1	4.195155	5.341512	-0.813292
6	-1.672141	1.041433	1.519819
6	-2.855219	1.773903	1.426014
6	-1.593936	0.018466	2.472284
6	-3.944075	1.490714	2.245847
1	-2.932837	2.567562	0.680996
6	-2.680987	-0.270243	3.290189
1	-0.667833	-0.547837	2.562245
6	-3.862494	0.460781	3.176610
1	-4.861711	2.069302	2.146277
1	-2.606758	-1.072817	4.022364
1	-4.714020	0.227829	3.813699
6	-4.436235	-2.567014	1.011409
1	-5.153183	-2.257671	1.778766
1	-4.861453	-3.446943	0.505840
1	-3.541400	-2.901702	1.541630
6	-5.944813	1.595740	-1.354661
1	-6.637715	1.653178	-0.509909
1	-5.503927	2.592079	-1.461634
1	-6.546807	1.410860	-2.256439
6	-1.816010	-2.321901	-0.126426
1	-2.244924	-3.326530	-0.226499
1	-0.943472	-2.273014	-0.775211
1	-1.472035	-2.209150	0.911972
6	-3.435246	1.809056	-2.707833
1	-3.105219	2.755498	-2.257811
1	-2.692596	1.554519	-3.462033
1	-4.383473	1.997523	-3.219574

A

Number of imaginary frequencies : 0

Electronic energy : HF=-2467.4423333
Zero-point correction= 0.955558 (hartree/particle)
Thermal correction to Energy= 1.007402
Thermal correction to Enthalpy= 1.008346
Thermal correction to Gibbs Free Energy= 0.871582
Sum of electronic and zero-point Energies= -2466.486775
Sum of electronic and thermal Energies= -2466.434931

Sum of electronic and thermal Enthalpies= -2466.433987
Sum of electronic and thermal Free Energies= -2466.570751

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Cartesian Coordinates

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6	-1.130965	-4.935068	-1.613315
6	0.286449	-4.521700	-1.198185
6	0.071648	-3.576904	0.011067
6	-1.193893	-2.867242	-0.429612
6	-1.943330	-3.725234	-1.242786
6	-3.238780	-3.394750	-1.610227
6	-3.776151	-2.183830	-1.183134
6	-3.019900	-1.251847	-0.464058
6	-1.714102	-1.620132	-0.113059
6	1.347072	-2.870426	0.419553
6	2.043654	-3.647353	1.352594
6	1.209728	-4.824250	1.773212
6	-0.186559	-4.417215	1.291766
6	3.305990	-3.270453	1.785791
6	3.850014	-2.073812	1.328257
6	3.142714	-1.223960	0.472322
6	1.890490	-1.662341	0.014505
8	1.188127	-0.875177	-0.886500
15	0.061652	0.161168	-0.378680
8	0.726757	1.037063	0.770195
8	-0.908988	-0.705027	0.567918
8	-0.533374	0.840698	-1.535144
6	3.662655	0.127196	0.114784
1	4.835180	-1.760169	1.668960
1	3.857094	-3.888075	2.492713
1	-3.830845	-4.070284	-2.225312
1	-4.803493	-1.927448	-1.436004
6	-3.604388	0.063702	-0.076884
1	-1.209803	-5.177988	-2.679542
1	-1.465509	-5.826853	-1.063030
1	0.761080	-3.948396	-2.007013
1	0.940387	-5.368825	-0.959331
1	1.547791	-5.748453	1.281430
1	1.256515	-5.007393	2.853036
1	-0.663094	-3.768828	2.041225
1	-0.856289	-5.265747	1.110676
1	1.571627	1.438527	0.500272
6	-3.946829	1.012617	-1.066583
6	-4.549158	2.206948	-0.673480
6	-4.814357	2.503837	0.661413
6	-4.456553	1.560964	1.618873
6	-3.858120	0.346643	1.280505
1	-4.661540	1.779191	2.668277
6	3.974045	0.443552	-1.223979
6	4.423966	1.728897	-1.531056
6	4.572796	2.716091	-0.563920
6	4.262388	2.386106	0.754681
6	3.815885	1.115453	1.121975
1	4.670121	1.971665	-2.565779
6	-3.695733	0.785828	-2.547061
6	-2.993258	1.969172	-3.208270
6	-4.998709	0.481161	-3.286617
1	-3.029523	-0.080885	-2.648387
1	-2.077088	2.228618	-2.670791
1	-2.722728	1.714358	-4.241024

1	-3.639601	2.855867	-3.255608
1	-5.530341	-0.379331	-2.863470
1	-5.683702	1.339101	-3.244511
1	-4.802530	0.267998	-4.345421
6	-3.573058	-0.646366	2.392397
6	-4.877183	-1.246365	2.915862
6	-2.753982	-0.037102	3.525808
1	-2.985872	-1.475279	1.979044
1	-5.442181	-1.730915	2.109306
1	-4.679710	-1.998556	3.690603
1	-5.522513	-0.475229	3.357217
1	-1.830099	0.419390	3.151388
1	-3.314777	0.734938	4.068846
1	-2.480389	-0.809546	4.255799
1	-4.811573	2.935365	-1.441569
6	-5.449847	3.816052	1.064389
6	-6.790817	4.041597	0.372477
6	-4.506148	4.988564	0.805812
1	-5.634105	3.766436	2.149109
1	-7.485166	3.213392	0.556575
1	-7.261618	4.966125	0.729948
1	-6.667117	4.137279	-0.714269
1	-3.543041	4.846424	1.309901
1	-4.303504	5.103223	-0.267273
1	-4.943603	5.929927	1.162517
1	4.377397	3.143913	1.530266
6	3.897572	-0.579454	-2.340966
6	5.302630	-0.987345	-2.780385
6	3.070370	-0.088425	-3.525575
1	3.408474	-1.479802	-1.950742
1	5.883416	-1.386567	-1.939161
1	5.256334	-1.760545	-3.557732
1	5.856224	-0.133419	-3.193000
1	2.072362	0.239995	-3.211252
1	3.556833	0.748274	-4.044122
1	2.945051	-0.892752	-4.261152
6	5.039416	4.105535	-0.934886
6	6.287177	4.514642	-0.157793
6	3.923073	5.129662	-0.742163
1	5.297775	4.084915	-2.004874
1	7.097870	3.787510	-0.283826
1	6.651805	5.492485	-0.496045
1	6.077930	4.597632	0.916831
1	3.027669	4.861508	-1.315146
1	3.632675	5.202547	0.314508
1	4.247641	6.126754	-1.065130
6	3.537447	0.850124	2.594547
6	2.698264	1.938522	3.261684
6	4.849812	0.677373	3.360398
1	2.973377	-0.088067	2.674361
1	1.745130	2.103574	2.746781
1	2.466754	1.647108	4.293482
1	3.229959	2.897164	3.313922
1	5.477257	-0.115092	2.935520
1	5.438350	1.604574	3.341049
1	4.655725	0.428708	4.411339

1(2*S*,3*S*)

Number of imaginary frequencies : 0

Electronic energy : HF=-464.3914955
Zero-point correction= 0.217241 (hartree/particle)
Thermal correction to Energy= 0.228244
Thermal correction to Enthalpy= 0.229189
Thermal correction to Gibbs Free Energy= 0.180651
Sum of electronic and zero-point Energies= -464.174255
Sum of electronic and thermal Energies= -464.163251
Sum of electronic and thermal Enthalpies= -464.162307
Sum of electronic and thermal Free Energies= -464.210845

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Cartesian Coordinates

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6	1.882496	-0.336082	-0.481886
1	1.645721	0.122024	-1.463342
6	1.015882	0.361970	0.583128
1	1.230559	-0.150309	1.535413
6	1.626955	-1.823693	-0.556619
1	0.594176	-2.040460	-0.847016
1	2.300424	-2.283858	-1.286919
1	1.817794	-2.287939	0.420148
8	3.261706	-0.186448	-0.196313
1	3.496853	0.739806	-0.314026
6	1.405480	1.830070	0.736208
1	1.380004	2.360147	-0.226255
1	2.414670	1.932578	1.151794
1	0.721621	2.351471	1.414781
6	-0.454954	0.195661	0.284548
6	-1.244396	-0.662440	1.053769
6	-1.059946	0.874393	-0.778298
6	-2.597220	-0.834972	0.778984
1	-0.783996	-1.203226	1.880887
6	-2.411604	0.703512	-1.058513
1	-0.468296	1.549406	-1.396326
6	-3.186398	-0.150622	-0.279439
1	-3.193274	-1.504855	1.395459
1	-2.863391	1.241999	-1.889235
1	-4.244297	-0.281979	-0.496146

1(2*S*,3*R*)

Number of imaginary frequencies : 0

Electronic energy : HF=-464.3929492
Zero-point correction= 0.217692 (hartree/particle)
Thermal correction to Energy= 0.228490
Thermal correction to Enthalpy= 0.229434
Thermal correction to Gibbs Free Energy= 0.181569
Sum of electronic and zero-point Energies= -464.175257
Sum of electronic and thermal Energies= -464.164459
Sum of electronic and thermal Enthalpies= -464.163515
Sum of electronic and thermal Free Energies= -464.211381

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Cartesian Coordinates

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6	-1.839824	-0.346234	-0.509475
1	-1.615485	0.161713	-1.470687

6	-1.025557	0.366817	0.586626
1	-1.247200	-0.170004	1.523773
6	-3.331373	-0.297776	-0.266001
1	-3.725895	0.719840	-0.347390
1	-3.844240	-0.922179	-1.004982
1	-3.569058	-0.689881	0.731575
8	-1.498157	-1.714495	-0.584422
1	-0.542441	-1.774295	-0.707107
6	0.452672	0.211296	0.308507
6	1.187850	-0.795739	0.941310
6	1.108877	1.020162	-0.625842
6	2.538658	-0.984444	0.661497
1	0.688532	-1.434867	1.669697
6	2.458110	0.835738	-0.907041
1	0.559783	1.809449	-1.138162
6	3.178707	-0.166891	-0.263535
1	3.090875	-1.771441	1.170903
1	2.950429	1.479190	-1.633309
1	4.234623	-0.309304	-0.482574
6	-1.447587	1.823849	0.742563
1	-1.483230	2.343556	-0.224559
1	-2.444305	1.902347	1.189913
1	-0.750337	2.371168	1.386637

1(2*R*,3*R*)

Number of imaginary frequencies : 0

Electronic energy : HF=-464.3914955
Zero-point correction= 0.217241 (hartree/particle)
Thermal correction to Energy= 0.228244
Thermal correction to Enthalpy= 0.229189
Thermal correction to Gibbs Free Energy= 0.180651
Sum of electronic and zero-point Energies= -464.174255
Sum of electronic and thermal Energies= -464.163251
Sum of electronic and thermal Enthalpies= -464.162307
Sum of electronic and thermal Free Energies= -464.210845

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Cartesian Coordinates

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6	-1.882496	-0.336082	-0.481886
1	-1.645721	0.122024	-1.463342
6	-1.015882	0.361970	0.583128
1	-1.230559	-0.150309	1.535413
6	-1.626956	-1.823693	-0.556619
1	-0.594176	-2.040460	-0.847015
1	-2.300424	-2.283858	-1.286920
1	-1.817796	-2.287939	0.420148
8	-3.261706	-0.186448	-0.196313
1	-3.496855	0.739805	-0.314033
6	-1.405481	1.830070	0.736209
1	-1.380004	2.360147	-0.226254
1	-2.414671	1.932576	1.151794
1	-0.721622	2.351470	1.414783
6	0.454954	0.195661	0.284548
6	1.244396	-0.662440	1.053769
6	1.059947	0.874393	-0.778298
6	2.597220	-0.834973	0.778983
1	0.783995	-1.203228	1.880886

6	2.411604	0.703513	-1.058513
1	0.468297	1.549407	-1.396325
6	3.186398	-0.150622	-0.279439
1	3.193274	-1.504856	1.395457
1	2.863392	1.242000	-1.889234
1	4.244297	-0.281979	-0.496146

1(2*R*,3*S*)

Number of imaginary frequencies : 0

Electronic energy : HF=-464.3929492
Zero-point correction= 0.217692 (hartree/particle)
Thermal correction to Energy= 0.228490
Thermal correction to Enthalpy= 0.229434
Thermal correction to Gibbs Free Energy= 0.181569
Sum of electronic and zero-point Energies= -464.175257
Sum of electronic and thermal Energies= -464.164459
Sum of electronic and thermal Enthalpies= -464.163515
Sum of electronic and thermal Free Energies= -464.211381

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Cartesian Coordinates

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6	1.839824	-0.346234	-0.509475
1	1.615485	0.161713	-1.470687
6	1.025557	0.366817	0.586626
1	1.247200	-0.170004	1.523773
6	3.331373	-0.297776	-0.266001
1	3.725895	0.719840	-0.347390
1	3.844240	-0.922179	-1.004982
1	3.569058	-0.689881	0.731575
8	1.498157	-1.714495	-0.584422
1	0.542441	-1.774295	-0.707107
6	-0.452672	0.211296	0.308507
6	-1.187850	-0.795739	0.941310
6	-1.108877	1.020162	-0.625842
6	-2.538658	-0.984444	0.661497
1	-0.688532	-1.434867	1.669697
6	-2.458110	0.835738	-0.907041
1	-0.559783	1.809449	-1.138162
6	-3.178707	-0.166891	-0.263535
1	-3.090875	-1.771441	1.170903
1	-2.950429	1.479190	-1.633309
1	-4.234623	-0.309304	-0.482574
6	1.447587	1.823849	0.742563
1	1.483230	2.343556	-0.224559
1	2.444305	1.902347	1.189913
1	0.750337	2.371168	1.386637

Phenyl amine

Number of imaginary frequencies : 0

Electronic energy : HF=-287.3940519
Zero-point correction= 0.116735 (hartree/particle)
Thermal correction to Energy= 0.122580
Thermal correction to Enthalpy= 0.123524
Thermal correction to Gibbs Free Energy= 0.087580

Sum of electronic and zero-point Energies= -287.277317
Sum of electronic and thermal Energies= -287.271472
Sum of electronic and thermal Enthalpies= -287.270528
Sum of electronic and thermal Free Energies= -287.306472

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Cartesian Coordinates

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6	-0.221212	-1.205040	-0.005394
6	1.167162	-1.198810	0.003376
6	1.875885	0.000003	0.008035
6	1.167153	1.198819	0.003376
6	-0.221215	1.205034	-0.005391
6	-0.937341	-0.000009	-0.010554
1	-0.768340	-2.147461	-0.012062
1	1.702091	-2.146791	0.008908
1	2.962887	0.000004	0.016301
1	1.702077	2.146803	0.008909
1	-0.768363	2.147444	-0.012057
7	-2.323607	-0.000002	-0.072108
1	-2.773854	-0.839114	0.267058
1	-2.773837	0.839141	0.267006

Iridium hydride

Number of imaginary frequencies : 0

Electronic energy : HF=-2122.1682615
Zero-point correction= 0.725778 (hartree/particle)
Thermal correction to Energy= 0.767759
Thermal correction to Enthalpy= 0.768703
Thermal correction to Gibbs Free Energy= 0.655306
Sum of electronic and zero-point Energies= -2121.442484
Sum of electronic and thermal Energies= -2121.400502
Sum of electronic and thermal Enthalpies= -2121.399558
Sum of electronic and thermal Free Energies= -2121.512956

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Cartesian Coordinates

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77	1.556238	-0.818382	0.520109
6	2.893664	-1.409721	-1.341979
6	2.184201	-2.518256	-0.706924
6	2.690060	-2.644958	0.638680
6	3.567430	-1.532941	0.869826
6	3.740220	-0.816222	-0.393295
7	1.481916	0.976348	1.772407
1	2.402655	1.212277	2.140387
6	-0.368281	1.645109	0.353379
1	-0.612093	2.408620	-0.404072
6	0.917852	2.134565	1.026157
1	0.641964	2.915519	1.753477
16	-0.986520	0.076272	-1.619032
8	-0.983091	1.253354	-2.503281
7	-0.093578	0.363140	-0.292517
6	-2.712923	-0.208656	-1.096706
6	-3.697292	0.791228	-1.225321
6	-3.029064	-1.484756	-0.586830
6	-5.029297	0.469324	-0.897618
6	-4.367752	-1.785133	-0.286751
6	-5.359429	-0.800452	-0.405379

8	-0.535280	-1.172309	-2.240007
1	0.890064	0.776136	2.578956
1	0.463159	-1.344750	1.568351
6	1.378010	-3.540199	-1.431105
1	0.717270	-4.084933	-0.747285
1	0.751029	-3.073300	-2.193635
1	2.033555	-4.276685	-1.919170
6	2.700243	-1.005223	-2.759668
1	3.191789	-0.052397	-2.982786
1	3.119568	-1.764349	-3.434932
1	1.633235	-0.911083	-2.993388
6	4.681851	0.319832	-0.586867
1	4.618135	1.052095	0.228276
1	5.721159	-0.037575	-0.615951
1	4.486980	0.857494	-1.520102
6	4.365020	-1.280451	2.104753
1	4.620442	-0.218820	2.208999
1	3.818244	-1.583079	3.005138
1	5.313273	-1.835669	2.086861
6	2.395695	-3.756952	1.586114
1	3.078988	-4.600761	1.417123
1	2.509002	-3.437954	2.627895
1	1.371173	-4.125673	1.463958
6	1.971274	2.725319	0.116246
6	2.980386	3.490012	0.713123
6	1.974093	2.577579	-1.272097
6	3.976862	4.088193	-0.049964
1	2.967858	3.638788	1.794688
6	2.964326	3.189533	-2.037653
1	1.201223	1.989986	-1.764321
6	3.968295	3.939956	-1.434041
1	4.747651	4.684151	0.433927
1	2.945526	3.074273	-3.119664
1	4.736493	4.415666	-2.039708
6	-1.523558	1.637493	1.347794
6	-1.915967	0.488835	2.036233
6	-2.226576	2.824059	1.572660
6	-2.988323	0.525478	2.923224
1	-1.389896	-0.444735	1.846103
6	-3.304993	2.862065	2.449886
1	-1.937952	3.724559	1.027626
6	-3.689818	1.709257	3.129049
1	-3.287053	-0.383481	3.442450
1	-3.849797	3.792327	2.598602
1	-4.537701	1.732558	3.810345
6	-4.738823	-3.175750	0.156708
1	-4.074040	-3.929478	-0.273969
1	-4.693043	-3.295268	1.249831
1	-5.753675	-3.440487	-0.154514
6	-1.999359	-2.541877	-0.282099
1	-1.957551	-3.306703	-1.069349
1	-0.992859	-2.139027	-0.174815
1	-2.253014	-3.049059	0.657259
6	-6.768019	-1.090463	0.038219
1	-7.416466	-1.391076	-0.797692
1	-6.805523	-1.892698	0.779782
1	-7.229595	-0.214138	0.503817
6	-6.113380	1.496355	-1.095248
1	-7.094334	1.032679	-1.229405
1	-6.193327	2.186325	-0.241394

1	-5.933801	2.109022	-1.983983
6	-3.430062	2.213557	-1.645155
1	-2.408259	2.532546	-1.456255
1	-3.600728	2.358295	-2.720540
1	-4.096505	2.895731	-1.107845

(*R*) imine

Number of imaginary frequencies : 0

Electronic energy : HF=-674.1809181
Zero-point correction= 0.286969 (hartree/particle)
Thermal correction to Energy= 0.302022
Thermal correction to Enthalpy= 0.302967
Thermal correction to Gibbs Free Energy= 0.244229
Sum of electronic and zero-point Energies= -673.893949
Sum of electronic and thermal Energies= -673.878896
Sum of electronic and thermal Enthalpies= -673.877951
Sum of electronic and thermal Free Energies= -673.936689

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Cartesian Coordinates

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6	-0.551566	0.954705	-0.543911
1	0.241401	0.406371	-1.071107
6	-0.010012	1.313429	0.835570
7	1.120302	0.948726	1.305114
6	-0.867859	2.210452	-1.347541
1	-1.641235	2.827468	-0.875383
1	-1.216457	1.948286	-2.352980
1	0.027979	2.833222	-1.454153
6	-1.721198	-0.000579	-0.383808
6	-1.468799	-1.287418	0.104330
6	-3.037457	0.348881	-0.686972
6	-2.500061	-2.200445	0.280492
1	-0.441625	-1.571539	0.338106
6	-4.074038	-0.564955	-0.510512
1	-3.263464	1.341130	-1.072771
6	-3.810320	-1.840756	-0.026086
1	-2.281293	-3.197725	0.656365
1	-5.093754	-0.275262	-0.755972
1	-4.620009	-2.554169	0.110040
6	2.062738	0.218596	0.570572
6	2.337952	-1.106249	0.930981
6	2.809952	0.813600	-0.453144
6	3.319326	-1.825397	0.259902
1	1.773408	-1.553740	1.747427
6	3.798692	0.089954	-1.110545
1	2.612910	1.852539	-0.714015
6	4.056173	-1.232902	-0.762864
1	3.515376	-2.857314	0.544264
1	4.370707	0.566366	-1.904332
1	4.829591	-1.795727	-1.279970
6	-0.893665	2.151835	1.706145
1	-0.906096	3.190338	1.350156
1	-0.518608	2.148372	2.732429
1	-1.930093	1.793792	1.690450

(*S*) imine

Number of imaginary frequencies : 0

Electronic energy : HF=-674.1809181
Zero-point correction= 0.286969 (hartree/particle)
Thermal correction to Energy= 0.302022
Thermal correction to Enthalpy= 0.302967
Thermal correction to Gibbs Free Energy= 0.244229
Sum of electronic and zero-point Energies= -673.893949
Sum of electronic and thermal Energies= -673.878896
Sum of electronic and thermal Enthalpies= -673.877951
Sum of electronic and thermal Free Energies= -673.936689

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Cartesian Coordinates

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6	0.551566	0.954705	-0.543911
1	-0.241401	0.406371	-1.071107
6	0.010012	1.313429	0.835570
7	-1.120302	0.948726	1.305114
6	0.867859	2.210452	-1.347541
1	1.641235	2.827468	-0.875383
1	1.216457	1.948286	-2.352980
1	-0.027979	2.833222	-1.454153
6	1.721198	-0.000579	-0.383808
6	1.468799	-1.287418	0.104330
6	3.037457	0.348881	-0.686972
6	2.500061	-2.200445	0.280492
1	0.441625	-1.571539	0.338106
6	4.074038	-0.564955	-0.510512
1	3.263464	1.341130	-1.072771
6	3.810320	-1.840756	-0.026086
1	2.281293	-3.197725	0.656365
1	5.093754	-0.275262	-0.755972
1	4.620009	-2.554169	0.110040
6	-2.062738	0.218596	0.570572
6	-2.337952	-1.106249	0.930981
6	-2.809952	0.813600	-0.453144
6	-3.319326	-1.825397	0.259902
1	-1.773408	-1.553740	1.747427
6	-3.798692	0.089954	-1.110545
1	-2.612910	1.852539	-0.714015
6	-4.056173	-1.232902	-0.762864
1	-3.515376	-2.857314	0.544264
1	-4.370707	0.566366	-1.904332
1	-4.829591	-1.795727	-1.279970
6	0.893665	2.151835	1.706145
1	0.906096	3.190338	1.350156
1	0.518608	2.148372	2.732429
1	1.930093	1.793792	1.690450

C

Number of imaginary frequencies : 0

Electronic energy : HF=-4588.4706189
Zero-point correction= 1.667111 (hartree/particle)
Thermal correction to Energy= 1.758961
Thermal correction to Enthalpy= 1.759905
Thermal correction to Gibbs Free Energy= 1.548452

Sum of electronic and zero-point Energies= -4586.803508
Sum of electronic and thermal Energies= -4586.711658
Sum of electronic and thermal Enthalpies= -4586.710714
Sum of electronic and thermal Free Energies= -4586.922167

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Cartesian Coordinates

.....

77	1.155190	-2.512659	-0.580550
6	-0.309381	-3.932299	0.174256
6	0.929778	-4.651121	-0.108785
6	1.211299	-4.513476	-1.495662
6	0.147928	-3.695078	-2.074216
6	-0.813589	-3.390574	-1.048882
7	0.598107	-0.450795	-0.405030
1	-0.272600	-0.334887	0.148382
6	3.020268	-0.195151	-0.397787
1	3.812184	0.180059	0.267339
6	1.695655	0.350623	0.173894
1	1.581825	1.402888	-0.143913
16	4.367922	-2.530265	-0.518946
8	4.197474	-3.842780	0.111136
7	2.938355	-1.665533	-0.281099
6	5.562056	-1.530154	0.396495
6	5.353157	-1.375736	1.784162
6	6.526929	-0.778094	-0.306924
6	6.127389	-0.426039	2.472995
6	7.218893	0.226737	0.394805
6	7.064784	0.359866	1.783196
8	4.690013	-2.557653	-1.945073
6	-6.739725	4.054958	1.378239
6	-5.488561	4.662459	0.744767
6	-5.091780	3.662836	-0.378054
6	-5.460007	2.357932	0.289664
6	-6.493464	2.583775	1.206093
6	-7.143671	1.527224	1.822823
6	-6.726401	0.235917	1.530936
6	-5.637122	-0.021744	0.689251
6	-4.991708	1.063906	0.075540
6	-3.720871	4.033632	-0.900160
6	-3.871701	5.067842	-1.827140
6	-5.307336	5.182302	-2.263451
6	-5.950526	3.938087	-1.636076
6	-2.785825	5.856405	-2.175749
6	-1.553906	5.574975	-1.599850
6	-1.335889	4.447847	-0.790281
6	-2.450363	3.644094	-0.482557
8	-2.314596	2.521852	0.297965
15	-2.369267	1.006899	-0.364080
8	-1.614228	0.941067	-1.652344
8	-3.954114	0.856081	-0.797768
8	-2.019934	0.090085	0.772962
6	0.040862	4.245190	-0.247271
1	-0.709974	6.235195	-1.793911
1	-2.898431	6.699227	-2.855766
1	-7.961981	1.703698	2.518942
1	-7.233850	-0.615433	1.982644
6	-5.255375	-1.447690	0.492218
1	-6.873743	4.338059	2.429378
1	-7.651623	4.371006	0.849219
1	-4.674415	4.688211	1.483272

1	-5.629526	5.682865	0.370122
1	-5.768243	6.108125	-1.888068
1	-5.406315	5.208337	-3.355672
1	-5.858107	3.078523	-2.315160
1	-7.014099	4.064849	-1.399608
6	-4.734862	-2.180288	1.583354
6	-4.561409	-3.559599	1.450371
6	-4.893899	-4.237199	0.276649
6	-5.375943	-3.488253	-0.791773
6	-5.564562	-2.106639	-0.712832
1	-5.634946	-4.008227	-1.716182
6	0.273244	4.271626	1.146403
6	1.587036	4.304709	1.616808
6	2.689516	4.310863	0.771379
6	2.447237	4.224551	-0.599860
6	1.153185	4.202540	-1.129294
1	1.756864	4.350623	2.694440
1	-4.184651	-4.125968	2.305297
1	3.293552	4.209217	-1.286301
1	0.312340	-0.054475	-1.308899
6	2.343206	-5.111650	-2.250147
1	2.670107	-4.455563	-3.064023
1	3.209454	-5.272685	-1.602608
1	2.040683	-6.071426	-2.689631
6	0.023114	-3.307665	-3.502895
1	0.994279	-3.294331	-4.008178
1	-0.618236	-4.024932	-4.033237
1	-0.435084	-2.317107	-3.607578
6	-2.056429	-2.597156	-1.245425
1	-1.884106	-1.720815	-1.884048
1	-2.826286	-3.217301	-1.723797
1	-2.463170	-2.222041	-0.298925
6	-0.933794	-3.839413	1.516755
1	-1.786409	-3.155317	1.502396
1	-1.292885	-4.825712	1.842195
1	-0.219512	-3.487360	2.273167
6	1.691035	-5.412063	0.914104
1	1.841966	-4.808495	1.817094
1	1.126187	-6.308580	1.204458
1	2.675203	-5.713338	0.551529
6	1.680241	0.302666	1.687088
6	2.552692	1.143700	2.382381
6	0.839754	-0.533558	2.423574
6	2.597074	1.142128	3.771489
1	3.195885	1.821802	1.820166
6	0.886911	-0.544917	3.816230
1	0.122109	-1.178420	1.921542
6	1.766766	0.288974	4.496765
1	3.279296	1.814648	4.289391
1	0.220145	-1.206716	4.366545
1	1.797852	0.285692	5.583887
6	3.356071	0.289526	-1.795765
6	2.865699	-0.314453	-2.954316
6	4.218895	1.377436	-1.925100
6	3.224607	0.164614	-4.209387
1	2.223971	-1.191324	-2.871223
6	4.581537	1.862454	-3.178035
1	4.615830	1.844534	-1.025133
6	4.083849	1.254014	-4.327098
1	2.836039	-0.320834	-5.102167

1	5.262548	2.709829	-3.252846
1	4.369103	1.622284	-5.309964
6	6.902636	-1.017355	-1.745630
1	6.888025	-2.078062	-1.993094
1	6.218719	-0.523399	-2.449036
1	7.911839	-0.645084	-1.938296
6	4.354462	-2.168355	2.583428
1	3.543165	-1.520009	2.938386
1	3.908988	-2.992176	2.030183
1	4.838906	-2.593524	3.470639
6	5.937285	-0.228375	3.952536
1	6.611800	-0.867783	4.541256
1	6.135268	0.806399	4.249352
1	4.917647	-0.457800	4.272681
6	7.930403	1.322694	2.548551
1	8.157819	0.943928	3.549219
1	8.888938	1.494181	2.051665
1	7.450092	2.303717	2.679323
6	8.093918	1.190086	-0.363149
1	8.201100	2.138924	0.169515
1	9.107537	0.804329	-0.544076
1	7.658225	1.428973	-1.339738
6	0.984448	4.083244	-2.638141
6	0.832303	2.614579	-3.021186
6	2.101179	4.738322	-3.442940
1	0.053375	4.581260	-2.925177
1	-0.062267	2.173287	-2.563522
1	0.753216	2.501620	-4.111405
1	1.711871	2.050333	-2.690778
1	2.288436	5.772770	-3.126671
1	3.045746	4.182391	-3.369620
1	1.828698	4.754458	-4.505545
6	4.068045	4.559996	1.351230
6	4.396002	6.049328	1.229805
6	5.197051	3.731034	0.750155
1	4.012899	4.317962	2.425848
1	3.619613	6.666584	1.696832
1	5.356208	6.286008	1.706144
1	4.461030	6.342394	0.173037
1	5.064361	2.651362	0.913513
1	5.303504	3.904477	-0.330061
1	6.152697	4.015877	1.209776
6	-0.829216	4.309779	2.189004
6	-0.731840	5.548196	3.078101
6	-0.821354	3.031171	3.025706
1	-1.795147	4.365623	1.677255
1	-0.733212	6.470578	2.484158
1	-1.585405	5.589103	3.766917
1	0.179452	5.546950	3.690400
1	-0.892502	2.137434	2.392994
1	0.097458	2.957435	3.624810
1	-1.671620	3.020192	3.720141
6	-6.123999	-1.377635	-1.920206
6	-7.421846	-2.006253	-2.422407
6	-5.092509	-1.298149	-3.044461
1	-6.359166	-0.349318	-1.616671
1	-8.164982	-2.095981	-1.620853
1	-7.858336	-1.392782	-3.220545
1	-7.257295	-3.008731	-2.839515
1	-4.191599	-0.765538	-2.718839

1	-4.804187	-2.301675	-3.389448
1	-5.505265	-0.760680	-3.908290
6	-4.803698	-5.743996	0.170004
6	-5.860075	-6.413919	1.046697
6	-3.417286	-6.283214	0.501895
1	-5.022458	-6.005151	-0.877470
1	-6.867997	-6.062161	0.797410
1	-5.839489	-7.504551	0.925377
1	-5.685300	-6.193919	2.108530
1	-2.644319	-5.817331	-0.123604
1	-3.161699	-6.098299	1.554083
1	-3.372119	-7.367928	0.342574
6	-4.425194	-1.523867	2.920066
6	-2.979134	-1.712353	3.368422
6	-5.381658	-2.021912	4.002883
1	-4.572207	-0.443206	2.805352
1	-2.289918	-1.284162	2.629987
1	-2.819630	-1.188718	4.320489
1	-2.735717	-2.771495	3.537641
1	-6.432637	-1.871612	3.727329
1	-5.242316	-3.095647	4.190038
1	-5.203549	-1.496290	4.949765

D

Number of imaginary frequencies : 0

Electronic energy : HF=-4588.4431835
Zero-point correction= 1.667238 (hartree/particle)
Thermal correction to Energy= 1.759750
Thermal correction to Enthalpy= 1.760694
Thermal correction to Gibbs Free Energy= 1.546512
Sum of electronic and zero-point Energies= -4586.775946
Sum of electronic and thermal Energies= -4586.683434
Sum of electronic and thermal Enthalpies= -4586.682489
Sum of electronic and thermal Free Energies= -4586.896671

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Cartesian Coordinates

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77	0.214910	-0.588165	-1.915887
6	-0.333811	-2.149386	-3.357714
6	0.858977	-1.454368	-3.803035
6	0.488485	-0.072253	-4.025799
6	-0.895800	0.087979	-3.719770
6	-1.395337	-1.197911	-3.273995
7	1.854651	0.552101	-1.032189
1	1.611233	0.744081	-0.051436
6	2.598537	-1.605016	-0.249479
6	2.996861	-0.400488	-1.126224
16	0.473856	-1.847993	1.157097
8	0.634331	-0.542835	1.815190
7	1.148419	-1.850542	-0.363926
8	-0.881993	-2.386041	1.080706
6	-2.839511	4.670261	4.237979
6	-3.328194	3.227325	4.093171
6	-2.101652	2.441381	3.551234
6	-1.482196	3.498820	2.669026
6	-1.817858	4.772957	3.140971
6	-1.233392	5.908125	2.600937

6	-0.267447	5.753464	1.610759
6	0.064222	4.496258	1.098237
6	-0.614696	3.370681	1.593576
6	-2.550301	1.074119	3.088857
6	-2.571320	0.208835	4.183039
6	-1.826757	0.810449	5.343577
6	-1.163109	2.044302	4.716687
6	-3.282370	-0.979033	4.110883
6	-3.986313	-1.265118	2.946967
6	-3.893798	-0.476333	1.789628
6	-3.085316	0.674043	1.871218
8	-2.907541	1.496026	0.779205
15	-1.505986	1.593108	-0.053225
8	-1.081929	0.169069	-0.374623
8	-0.398028	2.119164	1.051257
8	-1.718687	2.607604	-1.115323
1	-4.635604	-2.137203	2.927532
1	-3.338756	-1.651695	4.965117
1	-1.501180	6.899169	2.963837
1	0.273046	6.621742	1.235260
6	1.264069	4.335412	0.232529
1	-3.643154	5.409894	4.137606
1	-2.378333	4.839501	5.223048
1	-4.122316	3.182660	3.333112
1	-3.728895	2.797972	5.019233
1	-2.514350	1.089166	6.156216
1	-1.099042	0.113464	5.777192
1	-0.188710	1.765284	4.290483
1	-0.999583	2.865792	5.425702
6	1.227211	4.535010	-1.158457
6	2.393992	4.324207	-1.899048
6	3.593425	3.946943	-1.296155
6	3.617549	3.816668	0.091869
6	2.480174	4.014710	0.875180
1	4.564339	3.560243	0.569256
1	2.368254	4.486639	-2.977290
1	2.071839	1.448381	-1.477977
6	1.497699	-3.068923	2.065721
6	1.327901	-4.426470	1.721342
6	2.403050	-2.682368	3.079051
6	2.066999	-5.404769	2.405759
6	3.105212	-3.689300	3.771873
6	2.983356	-5.034104	3.399233
6	2.137450	-2.084747	-4.235781
1	2.949134	-1.351653	-4.306607
1	2.468249	-2.878971	-3.559360
1	2.019081	-2.526060	-5.235102
6	-0.441397	-3.610414	-3.089717
1	-1.219398	-4.056419	-3.722487
1	0.499601	-4.125290	-3.309198
1	-0.704833	-3.814940	-2.046724
6	-2.811954	-1.433768	-2.896736
6	-1.754530	1.278855	-3.956991
1	-2.637661	0.980114	-4.536972
1	-2.091563	1.738636	-3.018984
1	-1.222632	2.040818	-4.535115
6	1.402861	0.995148	-4.514693
1	2.437405	0.825634	-4.191708
1	1.407692	1.023749	-5.612502
1	1.093992	1.983398	-4.154652

1	3.038701	-0.718576	-2.175465
1	2.852419	-1.281952	0.771227
6	4.348990	0.148755	-0.758623
6	4.597740	0.654973	0.517727
6	5.402220	0.070707	-1.669504
6	5.873707	1.066631	0.881923
1	3.781835	0.712105	1.236812
6	6.682169	0.485978	-1.312693
1	5.220139	-0.341002	-2.663588
6	6.920763	0.982269	-0.034490
1	6.053112	1.450683	1.885247
1	7.495083	0.413485	-2.031806
1	1.787954	1.870072	2.444704
6	3.447261	-2.834977	-0.518847
6	4.724782	-2.942675	0.039701
6	2.962897	-3.902545	-1.274807
6	5.496805	-4.081864	-0.160836
1	5.111811	-2.133569	0.660444
6	3.736156	-5.040534	-1.485088
1	1.942682	-3.852189	-1.647281
6	5.007649	-5.134806	-0.928349
1	6.482841	-4.150698	0.293990
1	3.332174	-5.866406	-2.068758
1	5.609003	-6.028537	-1.080436
6	-0.016679	5.062846	-1.843004
6	-0.263586	4.421567	-3.200342
6	0.066432	6.582735	-1.984269
1	-0.876664	4.804990	-1.212995
1	-0.235107	3.331481	-3.109754
1	-1.259884	4.692967	-3.572537
1	0.467187	4.743272	-3.957004
1	0.169244	7.081724	-1.013098
1	0.931213	6.872308	-2.598304
1	-0.836001	6.977014	-2.469111
6	4.865681	3.771561	-2.096763
6	5.505903	5.130854	-2.374947
6	4.656690	3.001159	-3.394659
1	5.563623	3.187931	-1.474019
1	5.697536	5.678033	-1.444084
1	6.459169	5.019823	-2.907580
1	4.844454	5.752013	-2.994363
1	4.182541	2.028088	-3.205299
1	4.027268	3.555210	-4.104426
1	5.618070	2.811653	-3.889659
6	2.574078	3.924515	2.391740
6	3.777366	4.683205	2.944105
6	2.575793	2.484329	2.905500
1	1.678294	4.405757	2.804882
1	3.788529	5.726221	2.605805
1	3.752633	4.684209	4.041136
1	4.729425	4.225129	2.643917
1	7.921780	1.298634	0.249901
1	3.547469	2.007282	2.716127
1	2.425852	2.465552	3.993301
6	2.741840	-1.260275	3.455687
1	3.818395	-1.167268	3.645280
1	2.459346	-0.537864	2.695487
1	2.220242	-0.946428	4.371543
6	3.995057	-3.317950	4.929220
1	3.617647	-2.442574	5.465087

1	4.060278	-4.128485	5.660677
1	5.022790	-3.081806	4.614676
6	3.853426	-6.078954	4.042888
1	3.369686	-6.549993	4.911198
1	4.102316	-6.879510	3.339901
1	4.802176	-5.660628	4.390122
6	1.863451	-6.858803	2.075527
1	2.114279	-7.507289	2.919405
1	0.823268	-7.072449	1.811601
1	2.481049	-7.179885	1.222754
6	0.420912	-4.903761	0.619834
1	-0.497809	-5.341508	1.034773
1	0.118766	-4.105342	-0.053806
1	0.919288	-5.680916	0.027935
1	-3.473701	-1.120998	-3.715368
1	-3.005957	-2.488124	-2.685156
1	-3.088169	-0.853511	-2.005120
6	-4.713294	-0.817714	0.589999
6	-5.596466	0.143442	0.036406
6	-4.716730	-2.130296	0.052055
6	-6.390086	-0.205106	-1.057650
6	-5.550906	-2.425838	-1.027563
6	-6.390600	-1.481038	-1.608439
1	-7.068570	0.540736	-1.475686
1	-5.542531	-3.442118	-1.424970
6	-3.898707	-3.281007	0.617829
6	-3.006041	-3.937621	-0.427346
6	-4.813288	-4.325895	1.257739
1	-3.218092	-2.888535	1.379758
1	-2.254976	-3.219427	-0.769901
1	-2.469145	-4.785874	0.017484
1	-3.570506	-4.324036	-1.288499
1	-5.499665	-3.888590	1.994260
1	-5.433232	-4.824814	0.500141
1	-4.222488	-5.100446	1.763588
6	-7.270705	-1.813078	-2.792862
6	-8.090065	-3.082598	-2.582562
6	-6.447767	-1.914942	-4.075451
1	-7.975648	-0.975611	-2.914588
1	-8.662109	-3.044749	-1.648210
1	-8.797724	-3.227068	-3.408631
1	-7.450819	-3.974512	-2.546398
1	-5.899301	-0.984820	-4.269811
1	-5.715697	-2.732086	-4.005808
1	-7.089699	-2.117518	-4.942683
6	-5.834248	1.520126	0.634524
6	-7.256441	1.625173	1.186311
6	-5.552601	2.646674	-0.355962
1	-5.162739	1.653850	1.487556
1	-7.458831	0.836837	1.922070
1	-7.404705	2.594447	1.680530
1	-8.010410	1.541842	0.392366
1	-4.538027	2.578423	-0.763999
1	-6.266162	2.636895	-1.191491
1	-5.648892	3.621693	0.139972

5

Number of imaginary frequencies : 0

Electronic energy : HF=-3218.0835018
Zero-point correction= 1.272830 (hartree/particle)
Thermal correction to Energy= 1.341838
Thermal correction to Enthalpy= 1.342782
Thermal correction to Gibbs Free Energy= 1.173100
Sum of electronic and zero-point Energies= -3216.810672
Sum of electronic and thermal Energies= -3216.741664
Sum of electronic and thermal Enthalpies= -3216.740720
Sum of electronic and thermal Free Energies= -3216.910402

.....

Cartesian Coordinates

.....

7	-0.557086	3.107557	0.423928
1	0.000320	2.293749	0.677293
1	-0.100680	3.691858	-0.265516
6	-2.263660	1.539705	-1.025936
8	-1.434072	1.210833	-1.877094
1	-0.531002	-0.029995	-1.544767
6	-3.182168	2.718154	-1.260175
1	-3.115318	3.332804	-0.349347
6	-1.238023	3.766829	1.430238
6	-1.468220	3.149638	2.670760
6	-1.798344	5.034179	1.198769
6	-2.223999	3.789843	3.643682
1	-1.042085	2.163942	2.860149
6	-2.549157	5.665061	2.183478
1	-1.642278	5.511468	0.229990
6	-2.769870	5.051396	3.413707
1	-2.384411	3.294849	4.599800
1	-2.968684	6.649332	1.982983
1	-3.356782	5.548146	4.182238
6	5.254192	-3.561242	1.798892
6	3.924575	-4.223551	1.421063
6	3.488259	-3.504676	0.116265
6	3.976344	-2.103422	0.415352
6	5.069818	-2.160910	1.284843
6	5.796348	-1.016255	1.578112
6	5.393970	0.198305	1.031486
6	4.244528	0.311916	0.239729
6	3.552006	-0.870520	-0.056125
6	2.060655	-3.860504	-0.245832
6	2.055198	-5.037012	-1.003322
6	3.455479	-5.402759	-1.410890
6	4.234912	-4.121565	-1.094610
6	0.862843	-5.684112	-1.287803
6	-0.330584	-5.130193	-0.835759
6	-0.376077	-3.899434	-0.169007
6	0.851409	-3.274682	0.099426
8	0.859297	-2.046812	0.749776
15	0.987649	-0.695572	-0.116244
8	0.018686	-0.852733	-1.331653
8	2.415612	-0.821581	-0.854942
8	0.829213	0.471117	0.776939
6	-1.692680	-3.326935	0.237442
1	-1.269794	-5.646511	-1.023727
1	0.855969	-6.612206	-1.856808
1	6.662186	-1.060990	2.236483
1	5.957991	1.103582	1.250434
6	3.779601	1.648686	-0.225985

1	5.456442	-3.588600	2.876128
1	6.103407	-4.059041	1.307454
1	3.173050	-4.018322	2.197242
1	3.989460	-5.311109	1.299163
1	3.831602	-6.255420	-0.826248
1	3.519825	-5.694459	-2.465860
1	4.161984	-3.421051	-1.938923
1	5.298996	-4.289749	-0.890533
6	3.417915	2.636460	0.720387
6	3.031598	3.897097	0.265741
6	2.991965	4.221004	-1.089016
6	3.336140	3.229729	-2.001510
6	3.729029	1.951248	-1.601848
1	3.316758	3.471181	-3.065601
6	-2.002253	-3.145959	1.604182
6	-3.282672	-2.723156	1.960110
6	-4.279185	-2.478889	1.019592
6	-3.945997	-2.627205	-0.323680
6	-2.676761	-3.040512	-0.737050
1	-3.526180	-2.601982	3.017696
6	3.445837	2.403117	2.222119
6	2.099925	2.689469	2.881321
6	4.545827	3.233850	2.882397
1	3.668736	1.344788	2.404230
1	1.797560	3.739199	2.770436
1	1.321378	2.052761	2.449884
1	2.153446	2.479975	3.957576
1	5.530964	3.045497	2.437374
1	4.342540	4.308478	2.781548
1	4.610260	3.010077	3.954936
6	4.152188	0.968221	-2.678250
6	5.450153	1.426156	-3.340823
6	3.055115	0.742567	-3.714583
1	4.357793	-0.000267	-2.206815
1	6.250762	1.549729	-2.600528
1	5.787536	0.694882	-4.086603
1	5.319943	2.388329	-3.853795
1	2.118510	0.424363	-3.241596
1	2.850179	1.651083	-4.296026
1	3.355916	-0.036834	-4.426193
1	2.758655	4.656274	1.000637
6	2.595958	5.604515	-1.555908
6	3.468268	6.689434	-0.930315
6	1.119043	5.886582	-1.287829
1	2.749231	5.635102	-2.645830
1	4.533228	6.500678	-1.108756
1	3.222744	7.674498	-1.346497
1	3.317559	6.746431	0.155603
1	0.477038	5.157425	-1.801616
1	0.898817	5.850196	-0.210784
1	0.835306	6.884669	-1.645470
1	-4.698778	-2.408389	-1.081747
6	-1.025018	-3.447276	2.725768
6	-1.513870	-4.616952	3.577818
6	-0.756553	-2.214889	3.586882
1	-0.068411	-3.753637	2.286937
1	-1.673317	-5.514630	2.967509
1	-0.779320	-4.861719	4.355615
1	-2.461648	-4.383376	4.080231
1	-0.422495	-1.365300	2.978637

1	-1.653499	-1.905867	4.140218
1	0.024693	-2.427475	4.327832
6	-5.644840	-2.010280	1.472119
6	-6.784941	-2.491507	0.583663
6	-5.666689	-0.486042	1.575281
1	-5.803713	-2.421185	2.482020
1	-6.758022	-3.577031	0.431096
1	-7.751764	-2.235703	1.033984
1	-6.755767	-2.010062	-0.403191
1	-4.900110	-0.116916	2.268383
1	-5.477536	-0.035548	0.591080
1	-6.644399	-0.125110	1.921539
6	-2.423379	-3.156341	-2.230463
6	-2.816420	-1.885503	-2.980853
6	-3.165926	-4.348332	-2.834972
1	-1.347301	-3.306931	-2.382718
1	-2.357409	-0.993124	-2.541029
1	-2.494405	-1.947023	-4.027883
1	-3.905274	-1.738552	-2.985020
1	-2.903476	-5.295793	-2.350103
1	-4.252615	-4.222914	-2.736333
1	-2.939886	-4.444188	-3.904721
6	-2.495263	0.714901	0.198749
1	-3.117637	1.232828	0.935035
1	-3.001153	-0.218580	-0.093606
1	-1.538034	0.441390	0.654916
6	-4.607779	2.208873	-1.348437
6	-5.582039	2.666947	-0.460247
6	-4.962428	1.257981	-2.309968
6	-6.889797	2.196442	-0.538530
1	-5.305273	3.396867	0.301370
6	-6.265651	0.776663	-2.381041
1	-4.208716	0.889961	-3.007567
6	-7.233674	1.247575	-1.496348
1	-7.638947	2.564732	0.159223
1	-6.526734	0.032610	-3.131478
1	-8.253172	0.872225	-1.552986
6	-2.770743	3.551799	-2.461067
1	-3.423011	4.426569	-2.556398
1	-1.735159	3.896886	-2.354978
1	-2.828257	2.977910	-3.392482

$TS_{i\text{-}k}$(*S*)

Number of imaginary frequencies : 1
Imaginary Frequency : -213.4954 cm(-1)

Electronic energy : HF= -3218.0746117
Zero-point correction= 1.272308 (hartree/particle)
Thermal correction to Energy= 1.339713
Thermal correction to Enthalpy= 1.340657
Thermal correction to Gibbs Free Energy= 1.175418
Sum of electronic and zero-point Energies= -3216.802304
Sum of electronic and thermal Energies= -3216.734899
Sum of electronic and thermal Enthalpies= -3216.733954
Sum of electronic and thermal Free Energies= -3216.899194

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Cartesian Coordinates

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7	-0.491690	2.741294	0.542379
1	0.098187	1.903368	0.696932
1	0.024061	3.389696	-0.053889
6	-1.871925	1.912558	-0.682048
8	-1.134362	1.417054	-1.609414
1	-0.722877	0.380038	-1.368968
6	-2.650799	3.162308	-1.055641
1	-2.746090	3.764087	-0.140285
6	-0.918436	3.335428	1.755063
6	-1.065754	2.541956	2.896820
6	-1.256696	4.689760	1.804145
6	-1.533569	3.108707	4.075340
1	-0.797220	1.487614	2.848731
6	-1.724674	5.246985	2.989832
1	-1.145623	5.306630	0.913077
6	-1.864491	4.461031	4.128553
1	-1.635628	2.486811	4.961611
1	-1.979350	6.303962	3.019928
1	-2.228084	4.899008	5.054919
6	5.183457	-3.808942	1.405504
6	3.802181	-4.424628	1.148417
6	3.269231	-3.671782	-0.098846
6	3.823239	-2.289382	0.177801
6	4.996216	-2.394343	0.930623
6	5.781174	-1.274851	1.167031
6	5.354943	-0.037729	0.692387
6	4.129700	0.122851	0.033257
6	3.381420	-1.036695	-0.221938
6	1.804857	-3.977056	-0.354109
6	1.701443	-5.121916	-1.152330
6	3.055118	-5.527584	-1.664785
6	3.896102	-4.279196	-1.381100
6	0.467417	-5.705158	-1.395722
6	-0.675489	-5.108202	-0.873315
6	-0.624035	-3.905013	-0.160616
6	0.643893	-3.356065	0.089890
8	0.739212	-2.173640	0.800508
15	0.818214	-0.777827	-0.024145
8	-0.266200	-0.751618	-1.091578
8	2.180668	-0.942316	-0.895321
8	0.885907	0.314725	0.987518
6	-1.890083	-3.246937	0.276685
1	-1.649363	-5.562950	-1.045568
1	0.389781	-6.609421	-1.997148
1	6.709495	-1.355258	1.730210
1	5.962879	0.847239	0.874398
6	3.626462	1.481143	-0.321224
1	5.486038	-3.859416	2.458292
1	5.965290	-4.326099	0.829406
1	3.134008	-4.207717	1.994345
1	3.822400	-5.512007	1.008540
1	3.442192	-6.403216	-1.122373
1	3.035649	-5.800864	-2.726581
1	3.775538	-3.553841	-2.198687
1	4.967774	-4.482408	-1.268776
6	3.422939	2.442692	0.697413
6	2.994647	3.723464	0.346436
6	2.746234	4.091922	-0.974816
6	2.917826	3.122006	-1.956289
6	3.362038	1.830939	-1.662373

1	2.734838	3.394198	-2.997393
6	-2.195438	-3.105411	1.645148
6	-3.423693	-2.551113	2.017039
6	-4.368355	-2.141586	1.083791
6	-4.042010	-2.276415	-0.264692
6	-2.824613	-2.805150	-0.690369
1	-3.659047	-2.451359	3.078211
6	3.663959	2.165540	2.172424
6	2.424305	2.431234	3.021024
6	4.853420	2.972313	2.691293
1	3.899723	1.101964	2.291679
1	2.121488	3.487456	3.000543
1	1.588508	1.818215	2.668658
1	2.620396	2.172278	4.069747
1	5.764823	2.783411	2.109882
1	4.652370	4.051034	2.639809
1	5.063323	2.725881	3.740043
6	3.612879	0.891229	-2.827341
6	4.755430	1.406458	-3.701217
6	2.352627	0.657662	-3.655536
1	3.927904	-0.080090	-2.429139
1	5.673645	1.546264	-3.117247
1	4.972922	0.696956	-4.509869
1	4.505817	2.369906	-4.165224
1	1.530541	0.293248	-3.029401
1	2.020325	1.575599	-4.158527
1	2.540347	-0.090905	-4.436023
1	2.866912	4.464854	1.137015
6	2.407324	5.518133	-1.351736
6	3.651246	6.398242	-1.234287
6	1.263236	6.105697	-0.534744
1	2.097175	5.510639	-2.408830
1	4.476844	6.002435	-1.837286
1	3.444599	7.423301	-1.567413
1	3.995427	6.446772	-0.192293
1	0.334467	5.538076	-0.679320
1	1.488695	6.114901	0.540066
1	1.062058	7.141615	-0.834850
1	-4.758392	-1.944443	-1.018008
6	-1.257939	-3.552336	2.751264
6	-1.882493	-4.664090	3.592073
6	-0.833052	-2.376028	3.627001
1	-0.351289	-3.966631	2.293220
1	-2.172946	-5.520143	2.970528
1	-1.173563	-5.021592	4.349976
1	-2.780458	-4.315940	4.119465
1	-0.372735	-1.584602	3.023585
1	-1.689148	-1.947162	4.165379
1	-0.100428	-2.697702	4.378391
6	-5.713708	-1.599482	1.515270
6	-6.832663	-2.573954	1.152228
6	-5.998438	-0.217289	0.933884
1	-5.690371	-1.507530	2.612580
1	-6.652867	-3.568194	1.578230
1	-7.801704	-2.214667	1.521741
1	-6.915231	-2.689445	0.063169
1	-5.233224	0.511147	1.227967
1	-6.029723	-0.240547	-0.164380
1	-6.970584	0.159301	1.278024
6	-2.566242	-2.872009	-2.186537

6	-2.874559	-1.548885	-2.885152
6	-3.375764	-3.990713	-2.842942
1	-1.500010	-3.079166	-2.340549
1	-2.365709	-0.711050	-2.397339
1	-2.540867	-1.586060	-3.930012
1	-3.953033	-1.339127	-2.898239
1	-3.168075	-4.972463	-2.401484
1	-4.453776	-3.807085	-2.736821
1	-3.154824	-4.051520	-3.916505
6	-2.505179	0.993963	0.318319
1	-2.991924	1.550223	1.126407
1	-3.271358	0.407455	-0.207088
1	-1.785501	0.284807	0.738619
6	-4.058005	2.767098	-1.466099
6	-5.155103	3.203186	-0.722385
6	-4.280392	1.948806	-2.577545
6	-6.450516	2.845200	-1.085311
1	-4.988208	3.829521	0.154110
6	-5.573422	1.585153	-2.938582
1	-3.431626	1.580747	-3.154411
6	-6.662920	2.035613	-2.196504
1	-7.294519	3.196870	-0.495599
1	-5.730782	0.946875	-3.805726
1	-7.673683	1.753251	-2.482462
6	-1.956802	3.976740	-2.140432
1	-2.471506	4.933427	-2.280920
1	-0.905404	4.182419	-1.899985
1	-1.959109	3.445356	-3.097329

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k(*S*)

Number of imaginary frequencies : 0

Electronic energy : HF=-3218.0852318
Zero-point correction= 1.277722 (hartree/particle)
Thermal correction to Energy= 1.344928
Thermal correction to Enthalpy= 1.345872
Thermal correction to Gibbs Free Energy= 1.181526
Sum of electronic and zero-point Energies= -3216.807510
Sum of electronic and thermal Energies= -3216.740304
Sum of electronic and thermal Enthalpies= -3216.739360
Sum of electronic and thermal Free Energies= -3216.903706

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Cartesian Coordinates

.....

7	-0.570741	2.529438	0.653424
1	0.028827	1.652452	0.747168
1	0.018745	3.201764	0.146112
6	-1.740486	2.103327	-0.341088
8	-1.090496	1.710892	-1.472474
1	-0.809696	0.755702	-1.397435
6	-2.598196	3.343659	-0.639560
1	-2.890987	3.766986	0.333089
6	-0.900011	3.012714	1.982949
6	-0.992935	2.089761	3.020704
6	-1.092664	4.370628	2.211096
6	-1.280975	2.540712	4.303482
1	-0.804256	1.036259	2.822125
6	-1.375261	4.811548	3.499918

1	-1.021610	5.081296	1.389442
6	-1.469790	3.898419	4.545222
1	-1.346304	1.824203	5.118346
1	-1.520404	5.873023	3.684073
1	-1.687379	4.246373	5.551988
6	5.254055	-3.705089	1.299040
6	3.885259	-4.359286	1.068947
6	3.303197	-3.617244	-0.162806
6	3.824051	-2.220075	0.110649
6	5.016375	-2.293840	0.836186
6	5.774120	-1.152619	1.059725
6	5.299499	0.075598	0.606285
6	4.053731	0.202624	-0.020633
6	3.336174	-0.978850	-0.271526
6	1.842172	-3.961116	-0.399072
6	1.755782	-5.096480	-1.212774
6	3.113533	-5.466819	-1.740811
6	3.924611	-4.198213	-1.460456
6	0.530707	-5.695042	-1.464832
6	-0.622285	-5.120217	-0.938969
6	-0.589297	-3.927614	-0.207964
6	0.671646	-3.367535	0.059674
8	0.753969	-2.197302	0.785928
15	0.754715	-0.799074	-0.055145
8	-0.333286	-0.763795	-1.083850
8	2.129929	-0.917264	-0.925971
8	0.847179	0.275614	0.993341
6	-1.869329	-3.289398	0.224174
1	-1.589991	-5.582888	-1.125277
1	0.467107	-6.590744	-2.080678
1	6.718451	-1.209239	1.598842
1	5.885236	0.977170	0.781935
6	3.476539	1.540326	-0.339711
1	5.580791	-3.752161	2.344857
1	6.037802	-4.197075	0.703801
1	3.230282	-4.164671	1.930181
1	3.934221	-5.445154	0.923793
1	3.529441	-6.333610	-1.205303
1	3.090406	-5.736765	-2.803412
1	3.770082	-3.470584	-2.270306
1	5.003294	-4.372915	-1.368252
6	3.273956	2.486544	0.689449
6	2.734859	3.740114	0.373127
6	2.358066	4.081572	-0.923291
6	2.521464	3.113483	-1.913701
6	3.096167	1.870466	-1.662002
1	2.226360	3.359908	-2.935532
6	-2.204303	-3.191281	1.588788
6	-3.441321	-2.650177	1.954149
6	-4.364853	-2.209295	1.014698
6	-4.007317	-2.296638	-0.329751
6	-2.782131	-2.811285	-0.747641
1	-3.697741	-2.583462	3.013238
6	3.621525	2.226990	2.146763
6	2.412674	2.373282	3.065553
6	4.767850	3.124820	2.608507
1	3.953338	1.187110	2.240776
1	2.002497	3.393555	3.067217
1	1.624626	1.679000	2.757164
1	2.691349	2.135624	4.100601

1	5.654390	3.020601	1.970022
1	4.477485	4.184126	2.593298
1	5.061365	2.880305	3.637453
6	3.382658	0.974776	-2.853493
6	4.472930	1.598925	-3.724856
6	2.134586	0.670859	-3.676076
1	3.775006	0.020267	-2.485789
1	5.385438	1.792104	-3.146887
1	4.733816	0.932658	-4.557200
1	4.143461	2.554433	-4.155499
1	1.349234	0.224383	-3.056129
1	1.727742	1.573942	-4.150666
1	2.372802	-0.036651	-4.480641
1	2.619540	4.470535	1.174004
6	1.882079	5.464095	-1.323127
6	2.970730	6.173280	-2.131773
6	1.462618	6.345464	-0.157375
1	1.011176	5.328598	-1.986589
1	3.262245	5.597894	-3.017781
1	2.631732	7.162226	-2.465597
1	3.870125	6.312869	-1.516835
1	0.726240	5.858856	0.495135
1	2.324054	6.613841	0.468953
1	1.021516	7.280512	-0.522225
1	-4.707091	-1.937351	-1.085869
6	-1.278692	-3.652293	2.698574
6	-1.912402	-4.759273	3.538241
6	-0.849475	-2.477240	3.574858
1	-0.373797	-4.071645	2.241439
1	-2.212498	-5.611453	2.916201
1	-1.205197	-5.125032	4.293880
1	-2.805634	-4.404645	4.069259
1	-0.371644	-1.696790	2.970268
1	-1.708804	-2.035407	4.098445
1	-0.130198	-2.802635	4.337657
6	-5.717899	-1.671848	1.427598
6	-6.841014	-2.589578	0.948701
6	-5.946336	-0.245134	0.934148
1	-5.741958	-1.657990	2.528780
1	-6.696297	-3.617874	1.300561
1	-7.815743	-2.238781	1.311428
1	-6.886646	-2.617147	-0.148030
1	-5.197921	0.446392	1.339898
1	-5.890871	-0.181360	-0.161985
1	-6.938093	0.119171	1.233560
6	-2.492794	-2.825931	-2.239742
6	-2.813909	-1.490820	-2.910860
6	-3.264649	-3.943796	-2.941321
1	-1.417932	-3.001370	-2.372763
1	-2.302667	-0.664454	-2.408620
1	-2.481692	-1.508605	-3.957004
1	-3.892011	-1.278579	-2.920155
1	-3.043262	-4.932660	-2.522872
1	-4.348343	-3.786027	-2.850391
1	-3.023033	-3.970652	-4.011874
6	-2.515740	1.003917	0.355711
1	-3.080123	1.394463	1.210110
1	-3.224790	0.565073	-0.354717
1	-1.854340	0.201666	0.696402
6	-3.878262	2.933271	-1.338404

6	-5.105562	3.092526	-0.692228
6	-3.862725	2.367712	-2.617531
6	-6.293075	2.698153	-1.302037
1	-5.129111	3.524384	0.308869
6	-5.046979	1.963223	-3.224163
1	-2.912347	2.218775	-3.125600
6	-6.266006	2.128599	-2.570888
1	-7.239290	2.829682	-0.780833
1	-5.015915	1.514561	-4.215093
1	-7.190485	1.813149	-3.049636
6	-1.835729	4.404370	-1.429329
1	-2.494346	5.248229	-1.660276
1	-0.978990	4.808023	-0.870615
1	-1.451966	3.998716	-2.371356

6

Number of imaginary frequencies : 0

Electronic energy : HF=-3218.0718338
Zero-point correction= 1.275342 (hartree/particle)
Thermal correction to Energy= 1.343416
Thermal correction to Enthalpy= 1.344361
Thermal correction to Gibbs Free Energy= 1.177799
Sum of electronic and zero-point Energies= -3216.796491
Sum of electronic and thermal Energies= -3216.728417
Sum of electronic and thermal Enthalpies= -3216.727473
Sum of electronic and thermal Free Energies= -3216.894034

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Cartesian Coordinates

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6	7.414712	1.512887	0.238895
6	6.769563	0.788042	1.235573
6	5.427898	1.025948	1.523309
6	4.707654	2.009715	0.836691
6	5.370879	2.730081	-0.162897
6	6.705952	2.482032	-0.464579
6	3.260574	2.322575	1.156948
6	2.876818	1.971899	2.590590
6	2.282535	1.691267	0.115510
8	0.936750	1.833081	0.611543
7	2.320568	2.360094	-1.158596
1	3.145411	3.410263	1.051211
1	0.798379	1.159172	1.303013
1	-0.203669	1.113756	-0.446941
1	2.705770	1.820346	-1.920224
1	4.940789	0.439278	2.302860
1	4.836024	3.514948	-0.697483
1	7.313416	0.029304	1.795820
1	7.198831	3.061675	-1.242498
1	8.462975	1.326474	0.015661
1	3.628150	2.350635	3.292222
1	1.919485	2.429981	2.859490
1	2.788990	0.889157	2.758662
6	2.123784	3.707942	-1.419319
6	1.522420	4.588173	-0.506241
6	2.511696	4.209834	-2.673170
6	1.339238	5.924969	-0.842236
1	1.166533	4.211865	0.449026

6	2.302634	5.541636	-3.000996
1	2.976316	3.533696	-3.391254
6	1.720667	6.416773	-2.086694
1	0.879270	6.590992	-0.112225
1	2.608478	5.900652	-3.981871
1	1.566497	7.462390	-2.340958
6	2.575048	0.223004	-0.138042
1	3.567467	0.096667	-0.581466
1	2.536414	-0.360724	0.788634
1	1.832111	-0.191145	-0.830713
6	-5.135280	-3.048927	-2.491546
6	-3.969772	-3.863754	-1.917987
6	-3.689917	-3.220584	-0.532640
6	-3.970702	-1.771456	-0.857238
6	-4.892144	-1.685626	-1.905783
6	-5.421612	-0.458319	-2.275087
6	-5.007153	0.689512	-1.603174
6	-4.023397	0.651692	-0.609522
6	-3.512809	-0.607908	-0.264906
6	-2.384978	-3.721512	0.051097
6	-2.617800	-4.895098	0.776883
6	-4.095236	-5.127504	0.931574
6	-4.688238	-3.776364	0.515504
6	-1.557990	-5.652709	1.252075
6	-0.256263	-5.226699	1.004109
6	0.014292	-4.014452	0.359417
6	-1.082740	-3.261564	-0.080111
8	-0.852130	-2.023884	-0.679456
15	-0.988821	-0.727804	0.269333
8	-0.128664	-0.663208	1.470558
8	-2.532655	-0.701416	0.718355
8	-0.781867	0.391757	-0.817113
6	1.422887	-3.600386	0.100015
1	0.586219	-5.832256	1.334462
1	-1.738392	-6.572865	1.805231
1	-6.151524	-0.387609	-3.079706
1	-5.437813	1.654202	-1.864884
6	-3.559298	1.891318	0.074844
1	-5.152989	-3.039445	-3.587641
1	-6.104655	-3.454304	-2.164858
1	-3.078917	-3.729527	-2.548479
1	-4.171764	-4.939122	-1.848358
1	-4.441406	-5.937215	0.272139
1	-4.367624	-5.418306	1.953042
1	-4.703658	-3.093800	1.377631
1	-5.710100	-3.843658	0.123744
6	-2.862421	2.895886	-0.635122
6	-2.457333	4.045158	0.044782
6	-2.737321	4.246629	1.394709
6	-3.425431	3.245915	2.071836
6	-3.834986	2.068973	1.446591
1	-3.654690	3.394958	3.128648
6	1.912852	-3.596452	-1.225688
6	3.262342	-3.336506	-1.445149
6	4.153968	-3.068365	-0.406716
6	3.642889	-3.039458	0.886638
6	2.296647	-3.301948	1.163632
1	3.646233	-3.369533	-2.467053
6	-2.579982	2.802772	-2.125992
6	-1.152700	3.190934	-2.505521

6	-3.558533	3.682546	-2.907491
1	-2.731181	1.761267	-2.438375
1	-0.398373	2.623394	-1.949201
1	-0.985585	3.002537	-3.573861
1	-0.953320	4.257453	-2.335763
1	-4.606020	3.437395	-2.694274
1	-3.413974	4.741382	-2.652949
1	-3.400073	3.576218	-3.988469
6	-4.622714	1.060841	2.263425
6	-6.014531	1.602426	2.584062
6	-3.884192	0.643535	3.531723
1	-4.764880	0.155462	1.660857
1	-6.563690	1.853501	1.667427
1	-6.603329	0.861156	3.139736
1	-5.959216	2.511284	3.197782
1	-2.874448	0.283639	3.300979
1	-3.794898	1.473023	4.245329
1	-4.424771	-0.164295	4.041592
1	-1.904957	4.808384	-0.503992
6	-2.283938	5.485686	2.134075
6	-2.558408	6.774421	1.367352
6	-0.802604	5.380211	2.489416
1	-2.854296	5.522745	3.075552
1	-3.614129	6.862101	1.085044
1	-2.295036	7.649147	1.974988
1	-1.961809	6.827843	0.447025
1	-0.584635	4.453511	3.034598
1	-0.195358	5.376409	1.574610
1	-0.478589	6.228925	3.105374
1	4.309238	-2.818420	1.719889
6	1.044357	-3.917398	-2.427818
6	1.474291	-5.230604	-3.077849
6	1.037378	-2.774395	-3.439560
1	0.011423	-4.053314	-2.086214
1	1.444766	-6.057403	-2.356906
1	0.812381	-5.486993	-3.914955
1	2.497279	-5.168384	-3.472050
1	0.723352	-1.832852	-2.972249
1	2.029843	-2.620355	-3.883832
1	0.342430	-2.990797	-4.261095
6	5.612282	-2.818666	-0.737615
6	6.535505	-2.863894	0.469652
6	5.780740	-1.489216	-1.474083
1	5.917791	-3.621046	-1.429588
1	6.463411	-3.814641	1.011215
1	7.578280	-2.729890	0.156755
1	6.303372	-2.052153	1.172323
1	5.141026	-1.429822	-2.362853
1	5.524229	-0.652596	-0.810433
1	6.821037	-1.344762	-1.794107
6	1.840059	-3.274369	2.611981
6	2.197885	-1.965763	3.311949
6	2.407862	-4.461509	3.388686
1	0.744431	-3.345009	2.621569
1	1.719529	-1.121868	2.803978
1	1.837550	-1.980061	4.348485
1	3.283719	-1.798060	3.349309
1	2.160060	-5.420291	2.917094
1	3.502927	-4.403357	3.453023
1	2.017490	-4.478524	4.414200

$TS_{k\text{-}l}(S)$

Number of imaginary frequencies : 1
Imaginary Frequency : -213.4954 cm(-1)

Electronic energy : HF=-3218.0518799
Zero-point correction= 1.275577 (hartree/particle)
Thermal correction to Energy= 1.342818
Thermal correction to Enthalpy= 1.343762
Thermal correction to Gibbs Free Energy= 1.179011
Sum of electronic and zero-point Energies= -3216.776303
Sum of electronic and thermal Energies= -3216.709062
Sum of electronic and thermal Enthalpies= -3216.708118
Sum of electronic and thermal Free Energies= -3216.872869

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Cartesian Coordinates

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6	7.474713	0.941204	0.244299
6	6.775580	0.299296	1.260839
6	5.454710	0.645921	1.534239
6	4.819375	1.658227	0.810418
6	5.529409	2.289854	-0.214990
6	6.843291	1.933885	-0.499124
6	3.392831	2.102268	1.123905
6	2.975894	1.796744	2.556633
6	2.480521	1.497814	0.060040
8	0.800545	1.762671	0.890738
7	2.347502	2.151329	-1.113120
1	3.369697	3.191371	0.995697
1	0.579727	0.958470	1.430748
1	0.180411	1.585510	0.126253
1	2.027612	1.581427	-1.891294
1	4.923893	0.127469	2.331652
1	5.052108	3.086997	-0.785020
1	7.260206	-0.477878	1.848520
1	7.379475	2.445219	-1.295639
1	8.506705	0.670387	0.033024
1	3.763734	2.121695	3.243854
1	2.061274	2.335289	2.816915
1	2.800750	0.727860	2.734802
6	2.322391	3.552367	-1.352355
6	1.728541	4.442361	-0.458566
6	2.861135	4.015078	-2.552643
6	1.718484	5.801445	-0.753768
1	1.254310	4.060575	0.442872
6	2.817716	5.371432	-2.851710
1	3.313319	3.303983	-3.242270
6	2.256711	6.270124	-1.948335
1	1.272041	6.495782	-0.043711
1	3.233352	5.728322	-3.790953
1	2.234827	7.332533	-2.177626
6	2.488545	0.011334	-0.098165
1	3.428065	-0.274897	-0.583772
1	2.418978	-0.513029	0.857603
1	1.656909	-0.312357	-0.732156
6	-5.413215	-2.718293	-2.393941
6	-4.292716	-3.605568	-1.836372
6	-3.931113	-2.966794	-0.467313

6	-4.124268	-1.506347	-0.806908
6	-5.059136	-1.367309	-1.836046
6	-5.499208	-0.107628	-2.216030
6	-4.978155	1.014640	-1.574125
6	-3.981215	0.913122	-0.597536
6	-3.562903	-0.376618	-0.236156
6	-2.648180	-3.549098	0.094995
6	-2.944950	-4.696388	0.839042
6	-4.431534	-4.825427	1.028559
6	-4.937692	-3.439961	0.612983
6	-1.931940	-5.522772	1.303192
6	-0.609873	-5.189609	1.023725
6	-0.273562	-4.006390	0.356822
6	-1.319702	-3.172133	-0.067997
8	-1.014906	-1.982192	-0.689392
15	-1.033914	-0.599436	0.194250
8	-0.212346	-0.680127	1.447269
8	-2.583464	-0.540235	0.714862
8	-0.737996	0.479248	-0.812151
6	1.154463	-3.689261	0.068107
1	0.197118	-5.845407	1.348964
1	-2.165271	-6.421095	1.872610
1	-6.238282	0.008591	-3.007233
1	-5.332817	2.006511	-1.850026
6	-3.395554	2.121809	0.049824
1	-5.459821	-2.724447	-3.489534
1	-6.399312	-3.051617	-2.036108
1	-3.410852	-3.542194	-2.490578
1	-4.568292	-4.663583	-1.749398
1	-4.848740	-5.613344	0.383453
1	-4.700448	-5.089655	2.058466
1	-4.877327	-2.748978	1.466539
1	-5.973097	-3.436940	0.251227
6	-2.670919	3.070756	-0.704586
6	-2.175620	4.213730	-0.070110
6	-2.375767	4.452590	1.286317
6	-3.076928	3.495904	2.013645
6	-3.586023	2.336762	1.432462
1	-3.244929	3.674760	3.078099
6	1.615598	-3.677431	-1.269181
6	2.972376	-3.485595	-1.515314
6	3.905314	-3.306322	-0.494627
6	3.428975	-3.294799	0.811818
6	2.074984	-3.483152	1.114987
1	3.328095	-3.500891	-2.547986
6	-2.422580	2.918661	-2.196064
6	-0.959648	3.131374	-2.578250
6	-3.308029	3.873803	-2.996856
1	-2.678262	1.889497	-2.477621
1	-0.314942	2.453244	-2.008448
1	-0.816755	2.919814	-3.646346
1	-0.627055	4.164900	-2.408112
1	-4.374063	3.733638	-2.779953
1	-3.064731	4.920396	-2.767147
1	-3.162406	3.729175	-4.075407
6	-4.376021	1.392402	2.320406
6	-5.670720	2.050107	2.793487
6	-3.545542	0.894847	3.500643
1	-4.662303	0.513641	1.731351
1	-6.288216	2.367285	1.943580

1	-6.262557	1.353072	3.400927
1	-5.469853	2.937255	3.408849
1	-2.603906	0.447393	3.161233
1	-3.306942	1.707493	4.200152
1	-4.099395	0.133365	4.064993
1	-1.621117	4.939601	-0.665404
6	-1.843808	5.675560	2.002543
6	-1.719614	6.906158	1.115730
6	-0.508772	5.361022	2.676603
1	-2.565507	5.910384	2.801615
1	-2.663439	7.140378	0.609165
1	-1.427781	7.780595	1.710369
1	-0.952922	6.771525	0.340215
1	-0.587331	4.494309	3.343924
1	0.255548	5.125041	1.922940
1	-0.148249	6.215507	3.264075
1	4.128971	-3.156600	1.635701
6	0.704450	-3.898827	-2.464190
6	1.109822	-5.141000	-3.254572
6	0.662558	-2.666127	-3.364712
1	-0.314290	-4.071976	-2.097713
1	1.135278	-6.031384	-2.614442
1	0.396581	-5.328881	-4.067240
1	2.102794	-5.028556	-3.709636
1	0.334605	-1.781004	-2.806676
1	1.649256	-2.458910	-3.801945
1	-0.038735	-2.819199	-4.195374
6	5.365858	-3.129534	-0.860175
6	6.320610	-3.301062	0.310857
6	5.594792	-1.774822	-1.530987
1	5.599180	-3.908929	-1.604375
1	6.204476	-4.276416	0.798260
1	7.360328	-3.212098	-0.027691
1	6.160531	-2.522091	1.068849
1	4.932159	-1.630245	-2.393172
1	5.411561	-0.960799	-0.816406
1	6.631409	-1.675012	-1.878988
6	1.669416	-3.473576	2.578749
6	2.034140	-2.160523	3.268623
6	2.277881	-4.660287	3.323958
1	0.577638	-3.566051	2.632165
1	1.516685	-1.326788	2.780065
1	1.718628	-2.182709	4.319764
1	3.118743	-1.977378	3.259647
1	2.011957	-5.616461	2.855765
1	3.374557	-4.599338	3.342647
1	1.930926	-4.685501	4.364830

I(*S*)

Number of imaginary frequencies : 0

Electronic energy : HF=-3218.0686979
Zero-point correction= 1.274007 (hartree/particle)
Thermal correction to Energy= 1.342696
Thermal correction to Enthalpy= 1.343640
Thermal correction to Gibbs Free Energy= 1.175560
Sum of electronic and zero-point Energies= -3216.794691
Sum of electronic and thermal Energies= -3216.726002

Sum of electronic and thermal Enthalpies= -3216.725058
Sum of electronic and thermal Free Energies= -3216.893138

.....

Cartesian Coordinates

.....

6	6.984659	3.662671	-0.267337
6	6.590215	3.116988	0.949287
6	5.237682	2.992153	1.259134
6	4.263124	3.418898	0.356126
6	4.670837	3.957928	-0.867656
6	6.019474	4.080482	-1.179851
6	2.777088	3.342171	0.644230
6	2.402376	3.188605	2.125181
6	2.120499	2.190084	-0.059466
8	-0.720419	1.912492	1.944848
7	1.042849	2.354096	-0.763391
1	2.324433	4.272296	0.278111
1	-0.366007	1.007107	1.848193
1	-1.657777	1.822846	1.726483
1	0.483277	1.489130	-1.010020
1	4.947205	2.564401	2.217400
1	3.913568	4.302340	-1.573532
1	7.337971	2.785194	1.666614
1	6.318101	4.509426	-2.133698
1	8.041379	3.762189	-0.504656
1	2.835041	4.015469	2.698377
1	1.312941	3.194919	2.251533
1	2.770575	2.247121	2.549566
6	0.474170	3.629286	-1.106610
6	-0.439949	4.238959	-0.255848
6	0.851071	4.208669	-2.314539
6	-0.958852	5.477144	-0.624332
1	-0.719265	3.727410	0.667229
6	0.314607	5.440330	-2.673155
1	1.554730	3.688493	-2.961698
6	-0.586246	6.077303	-1.824019
1	-1.659663	5.982721	0.037857
1	0.603581	5.902350	-3.613836
1	-1.000850	7.044257	-2.098680
6	2.627307	0.820583	0.144801
1	2.681037	0.269149	-0.803641
1	3.610960	0.812868	0.619324
1	1.911357	0.262643	0.772754
6	-3.971202	-4.441469	-2.426472
6	-2.616098	-4.858389	-1.839911
6	-2.516606	-4.081240	-0.502385
6	-3.194251	-2.788038	-0.899253
6	-4.139523	-3.043295	-1.896670
6	-5.061559	-2.071189	-2.258204
6	-5.022785	-0.836115	-1.616554
6	-4.026346	-0.517540	-0.685855
6	-3.085560	-1.509667	-0.369968
6	-1.132976	-4.179498	0.102774
6	-1.054042	-5.315116	0.915420
6	-2.416459	-5.925954	1.091251
6	-3.338903	-4.808119	0.594825
6	0.161364	-5.719836	1.446926
6	1.298865	-4.967453	1.170264
6	1.240139	-3.779368	0.432552
6	-0.008253	-3.384842	-0.074355

8	-0.118554	-2.213910	-0.790030
15	-0.574193	-0.853723	0.006658
8	0.194659	-0.674568	1.280607
8	-2.082808	-1.231884	0.526418
8	-0.590794	0.211856	-1.051796
6	2.486170	-3.005474	0.173260
1	2.266537	-5.288179	1.554418
1	0.227836	-6.610915	2.069039
1	-5.813922	-2.271697	-3.019295
1	-5.769278	-0.078972	-1.853315
6	-3.996699	0.813432	-0.019535
1	-3.992710	-4.479536	-3.522352
1	-4.779435	-5.100476	-2.075409
1	-1.803310	-4.515960	-2.497117
1	-2.505177	-5.941435	-1.706924
1	-2.527409	-6.835427	0.481563
1	-2.615562	-6.218165	2.129365
1	-3.526118	-4.092221	1.409144
1	-4.310116	-5.162565	0.229481
6	-3.854750	1.997964	-0.771710
6	-3.888413	3.235574	-0.117055
6	-4.069883	3.340470	1.258178
6	-4.192489	2.155122	1.983290
6	-4.162625	0.898357	1.383540
1	-4.348209	2.223226	3.062145
6	2.974668	-2.877011	-1.148124
6	4.193526	-2.239171	-1.360757
6	4.957443	-1.708452	-0.321630
6	4.456798	-1.838542	0.968145
6	3.238764	-2.472870	1.239887
1	4.577410	-2.163559	-2.380024
6	-3.689169	1.992673	-2.281746
6	-2.369287	2.616708	-2.719817
6	-4.866893	2.682765	-2.967635
1	-3.669613	0.949821	-2.618143
1	-1.530451	2.075499	-2.268683
1	-2.265392	2.560609	-3.811586
1	-2.299358	3.675217	-2.434127
1	-5.829268	2.245928	-2.671660
1	-4.903317	3.751959	-2.717906
1	-4.780431	2.603108	-4.058860
6	-4.380024	-0.309596	2.277997
6	-5.784241	-0.292482	2.879362
6	-3.315309	-0.408866	3.367238
1	-4.307313	-1.216130	1.666437
1	-6.551987	-0.249387	2.096636
1	-5.960045	-1.196390	3.476565
1	-5.931941	0.572635	3.539201
1	-2.306906	-0.419046	2.937631
1	-3.378098	0.428253	4.075810
1	-3.443688	-1.334149	3.943533
1	-3.779703	4.139805	-0.716694
6	-4.138493	4.655332	2.007842
6	-4.527725	5.845511	1.143880
6	-2.829099	4.929159	2.748638
1	-4.921574	4.531730	2.773770
1	-5.464001	5.668570	0.601341
1	-4.659222	6.740522	1.763710
1	-3.753348	6.078763	0.400815
1	-2.546399	4.093635	3.399523

1	-2.002151	5.085473	2.042562
1	-2.909904	5.831005	3.369008
1	5.026909	-1.437716	1.805995
6	2.249259	-3.432048	-2.360673
6	3.067841	-4.523615	-3.046559
6	1.879360	-2.321437	-3.340882
1	1.313966	-3.896469	-2.026682
1	3.313552	-5.334236	-2.349329
1	2.507589	-4.957045	-3.884903
1	4.011651	-4.132752	-3.449659
1	1.283624	-1.544546	-2.847230
1	2.773331	-1.851556	-3.773823
1	1.285983	-2.722652	-4.172685
6	6.255979	-0.999322	-0.653013
6	7.105224	-0.654342	0.560270
6	5.982037	0.266527	-1.467714
1	6.838801	-1.682903	-1.292743
1	7.363256	-1.539224	1.154295
1	8.039982	-0.173546	0.245931
1	6.584837	0.056569	1.217738
1	5.371204	0.060307	-2.354683
1	5.448560	1.008532	-0.856678
1	6.920351	0.725756	-1.803957
6	2.804247	-2.564265	2.693014
6	2.671778	-1.190568	3.347567
6	3.761340	-3.447207	3.493040
1	1.811415	-3.028177	2.726345
1	1.892806	-0.604845	2.848225
1	2.385840	-1.300244	4.401724
1	3.617765	-0.629992	3.324653
1	3.876248	-4.441355	3.042628
1	4.762182	-2.998163	3.553294
1	3.398179	-3.581066	4.520010

TS2$_{SS}$

Number of imaginary frequencies : 1
Imaginary frequency: -658.9793 cm(-1)

Electronic energy : HF=-5263.8344477
Zero-point correction= 1.976969 (hartree/particle)
Thermal correction to Energy= 2.084607
Thermal correction to Enthalpy= 2.085552
Thermal correction to Gibbs Free Energy= 1.841676
Sum of electronic and zero-point Energies= -5261.857478
Sum of electronic and thermal Energies= -5261.749840
Sum of electronic and thermal Enthalpies= -5261.748896
Sum of electronic and thermal Free Energies= -5261.992772

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Cartesian Coordinates

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77	-1.404130	-2.132396	0.346331
6	-1.558681	-3.858202	-1.124225
6	-1.768085	-4.340323	0.231004
6	-0.581717	-4.078055	0.979581
6	0.354621	-3.379129	0.131495
6	-0.253989	-3.280319	-1.176944
7	-0.949709	-0.205090	-0.448370
1	-0.063935	-0.243289	-0.974872

6	-3.410115	-0.326380	-1.011047
6	-2.045957	0.359511	-1.292026
16	-4.615060	-2.039703	0.602453
8	-4.720817	-3.119486	-0.392446
7	-3.353055	-1.013772	0.296000
6	-6.209500	-1.141942	0.489615
6	-7.007546	-1.277028	-0.667721
6	-6.658850	-0.400925	1.600018
6	-8.295159	-0.706771	-0.665001
6	-7.935329	0.185370	1.560866
6	-8.738090	0.060802	0.420506
8	-4.459776	-2.499954	1.989951
6	7.692196	2.836708	0.162439
6	6.449257	3.636946	0.529903
6	5.457018	2.589794	1.122716
6	5.792081	1.390093	0.255738
6	7.091316	1.527085	-0.250321
6	7.657629	0.555901	-1.057494
6	6.892918	-0.553663	-1.386369
6	5.577077	-0.715588	-0.934378
6	5.032672	0.271354	-0.093572
6	4.095696	3.246035	1.177482
6	4.055378	4.082369	2.295213
6	5.154866	3.709538	3.256945
6	5.741279	2.428056	2.633701
6	3.102231	5.088676	2.371391
6	2.179499	5.219594	1.335429
6	2.092465	4.291266	0.288078
6	3.051213	3.263595	0.264285
8	2.949022	2.256695	-0.669862
15	2.396766	0.797331	-0.151718
8	1.491062	0.964146	1.039977
8	3.777334	0.114260	0.448756
8	1.924502	0.061795	-1.361313
1	1.474461	6.047457	1.354876
1	3.086389	5.784362	3.209635
1	8.668066	0.672072	-1.445563
1	7.306707	-1.326626	-2.033092
1	8.288191	3.299342	-0.633194
1	8.360304	2.711622	1.028239
1	6.001669	4.055200	-0.382872
1	6.638700	4.468811	1.217015
1	5.911628	4.503070	3.339430
1	4.768888	3.544321	4.271098
1	5.202513	1.544563	3.004766
1	6.807579	2.288095	2.850482
1	-0.733706	0.435291	0.316333
1	1.221938	-0.054054	2.523886
6	-0.458655	-0.730968	3.354537
1	-1.109644	-1.392801	1.888707
6	-2.897271	-5.176373	0.725596
1	-3.675747	-5.284633	-0.031173
1	-2.528394	-6.174631	1.000613
1	-3.370440	-4.724674	1.603682
6	-2.466948	-4.072439	-2.283782
1	-2.158577	-3.470489	-3.146267
1	-2.437924	-5.126777	-2.594946
1	-3.502691	-3.825705	-2.029135
6	0.428489	-2.711549	-2.368527
1	1.102629	-1.893921	-2.088408

1	1.050493	-3.488815	-2.836414
1	-0.271303	-2.341326	-3.126423
6	1.760763	-3.027086	0.457049
1	2.101362	-2.140080	-0.093453
1	1.891871	-2.835802	1.528594
1	2.431114	-3.851464	0.176091
6	-0.332896	-4.558669	2.364080
1	-0.010695	-5.609593	2.340098
1	0.460941	-3.988395	2.860776
1	-1.242306	-4.509834	2.974353
6	4.866934	-1.937851	-1.417902
6	4.995303	-3.148237	-0.706025
6	4.236709	-1.920828	-2.678784
6	4.508954	-4.323666	-1.277246
6	3.756604	-3.123803	-3.199911
6	3.881021	-4.332463	-2.521500
1	4.613067	-5.261710	-0.731044
1	3.270918	-3.123487	-4.176793
6	1.035808	4.399726	-0.758674
6	1.382340	4.471258	-2.129716
6	-0.332380	4.473148	-0.399804
6	0.371514	4.591516	-3.084195
6	-1.302620	4.580330	-1.398399
6	-0.977694	4.634524	-2.750664
1	0.648048	4.655957	-4.138501
1	-2.352714	4.624838	-1.104783
6	-1.166114	-1.687290	4.252758
1	-0.735759	-2.688205	4.206504
1	-1.112663	-1.327479	5.291547
1	-2.218127	-1.759351	3.966639
6	-1.068943	0.654451	3.155332
1	-0.667821	1.034697	2.205574
7	0.874308	-0.741291	3.218446
6	-0.525912	1.590922	4.230595
6	-1.109761	1.673193	5.496671
6	0.571192	2.410048	3.941653
6	-0.612973	2.555445	6.452129
1	-1.974306	1.057489	5.740669
6	1.059175	3.299181	4.892888
1	1.042000	2.345197	2.957864
6	0.470362	3.374109	6.152010
1	-1.082474	2.608792	7.432234
1	1.902750	3.938728	4.638593
1	0.852479	4.070703	6.895123
6	-2.581061	0.632005	3.101778
1	-2.916069	0.019956	2.256854
1	-3.024671	0.231374	4.020042
1	-2.971672	1.647090	2.977213
6	1.905519	-1.476923	3.837873
6	3.178556	-1.313864	3.272844
6	1.770539	-2.240429	5.003170
6	4.287925	-1.901063	3.860107
1	3.288806	-0.719124	2.366721
6	2.891545	-2.843231	5.566422
1	0.816511	-2.348577	5.502801
6	4.152659	-2.680127	5.006333
1	5.266816	-1.748131	3.407509
1	2.769445	-3.433445	6.471764
1	5.022200	-3.147548	5.462295
6	-8.426932	0.974856	2.743501

1	-8.052873	0.574227	3.689687
1	-8.104138	2.026514	2.693629
1	-9.518123	0.973763	2.812264
6	-5.824097	-0.127606	2.818179
1	-6.235099	-0.629617	3.704448
1	-4.801821	-0.470979	2.714671
1	-5.812155	0.950319	3.033146
6	-10.051288	0.790874	0.341625
1	-10.887231	0.192711	0.733025
1	-10.028118	1.722897	0.913838
1	-10.303582	1.061498	-0.687650
6	-9.209006	-0.916247	-1.843475
1	-10.261233	-0.863312	-1.550324
1	-9.053494	-0.164345	-2.632906
1	-9.063404	-1.897713	-2.303884
6	-6.582876	-1.934677	-1.956658
1	-5.504655	-1.998221	-2.083948
1	-6.955436	-2.965804	-2.023168
1	-6.991741	-1.378570	-2.807160
6	5.699839	-3.201658	0.638886
6	7.188719	-3.498885	0.453951
6	5.108322	-4.220287	1.608103
1	5.598484	-2.205404	1.099690
1	7.686451	-2.748080	-0.169076
1	7.705581	-3.529985	1.422103
1	7.321386	-4.477161	-0.028745
1	4.036084	-4.065299	1.777229
1	5.255008	-5.249828	1.255784
1	5.610161	-4.147152	2.581342
6	3.354360	-5.616840	-3.123018
6	2.334824	-6.298419	-2.213441
6	4.489327	-6.577224	-3.470942
1	2.841547	-5.348740	-4.060829
1	1.489256	-5.636604	-1.982659
1	1.933747	-7.204564	-2.685087
1	2.790365	-6.598867	-1.260273
1	5.219250	-6.108627	-4.141487
1	5.026447	-6.899264	-2.568869
1	4.103792	-7.478800	-3.963991
6	4.151460	-0.655247	-3.515524
6	2.853651	-0.517639	-4.303724
6	5.337871	-0.575404	-4.477729
1	4.199094	0.203678	-2.829381
1	1.980990	-0.519879	-3.643532
1	2.857078	0.438593	-4.845714
1	2.735831	-1.304157	-5.062410
1	6.300162	-0.607891	-3.954333
1	5.314097	-1.413784	-5.188374
1	5.301413	0.356906	-5.057253
6	-0.814767	4.472487	1.038539
6	-1.930265	3.467437	1.281880
6	-1.286285	5.863090	1.465723
1	0.017857	4.177183	1.689525
1	-1.625288	2.456750	0.976561
1	-2.175634	3.444435	2.351466
1	-2.851363	3.714794	0.737712
1	-0.527652	6.635667	1.291890
1	-2.182516	6.160391	0.904463
1	-1.542332	5.873422	2.533180
6	2.813701	4.462681	-2.637449

6	3.164833	5.779936	-3.327001
6	3.074979	3.275178	-3.565171
1	3.488070	4.366291	-1.779798
1	3.022217	6.635055	-2.655033
1	4.213507	5.775903	-3.651546
1	2.546217	5.950034	-4.217878
1	2.715916	2.339147	-3.119400
1	2.581299	3.415170	-4.537946
1	4.150323	3.164647	-3.762573
6	-2.037758	4.785982	-3.819064
6	-2.617064	6.199825	-3.797321
6	-3.150324	3.748315	-3.704067
1	-1.538616	4.638162	-4.790563
1	-1.832264	6.958286	-3.905277
1	-3.342950	6.341210	-4.608273
1	-3.137008	6.392403	-2.848934
1	-2.756905	2.726116	-3.769727
1	-3.695307	3.836999	-2.753812
1	-3.885166	3.879766	-4.509213
1	-3.592841	-1.076075	-1.796649
1	-2.143344	1.415784	-0.995136
6	-4.462167	0.765292	-1.145480
6	-5.135995	0.955858	-2.350816
6	-4.701502	1.658996	-0.098816
6	-6.055277	1.992867	-2.499767
1	-4.942377	0.282875	-3.185541
6	-5.613034	2.697700	-0.243514
1	-4.181082	1.517369	0.847551
6	-6.300223	2.865299	-1.445065
1	-6.575270	2.119823	-3.447592
1	-5.795400	3.374086	0.590925
1	-7.020363	3.673016	-1.557304
6	-1.612705	0.362885	-2.746707
6	-0.568725	1.229169	-3.095794
6	-2.159939	-0.445264	-3.746968
6	-0.089564	1.283441	-4.397934
1	-0.115012	1.869666	-2.335884
6	-1.679691	-0.390922	-5.054408
1	-2.968745	-1.139328	-3.527498
6	-0.642460	0.471689	-5.384724
1	0.726487	1.962932	-4.636088
1	-2.123898	-1.031135	-5.813829
1	-0.264624	0.513407	-6.404091

TS2$_{RS}$

Number of imaginary frequencies : 1
Imaginary frequency : -416.3092 cm(-1)

Electronic energy : HF=-5263.8298974
Zero-point correction= 1.977584 (hartree/particle)
Thermal correction to Energy= 2.085018
Thermal correction to Enthalpy= 2.085962
Thermal correction to Gibbs Free Energy= 1.844046
Sum of electronic and zero-point Energies= -5261.852313
Sum of electronic and thermal Energies= -5261.744880
Sum of electronic and thermal Enthalpies= -5261.743935

Sum of electronic and thermal Free Energies= -5261.985851

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Cartesian Coordinates

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77	-1.351378	-2.180951	-0.500984
6	-1.482709	-3.336892	-2.475627
6	-1.837738	-4.198254	-1.361254
6	-0.707479	-4.300190	-0.499791
6	0.341024	-3.452812	-1.018973
6	-0.147815	-2.886022	-2.257333
7	-0.802099	-0.118926	-0.544607
1	0.153976	0.009507	-0.914031
6	-3.212878	0.126341	-1.176470
1	-3.502357	-0.275313	-2.158345
6	-1.780392	0.713705	-1.301582
1	-1.782414	1.703192	-0.823130
16	-4.556454	-1.947220	-0.312127
8	-4.673526	-2.567100	-1.642164
7	-3.223252	-0.974070	-0.188117
6	-6.094664	-0.970235	-0.115886
6	-6.882767	-0.639729	-1.236232
6	-6.526424	-0.673907	1.189713
6	-8.153755	-0.072209	-1.015896
6	-7.797418	-0.115159	1.384583
6	-8.597703	0.215406	0.282096
8	-4.508194	-2.882632	0.820379
6	7.697026	2.414206	1.878358
6	6.430468	3.213502	2.149631
6	5.308787	2.142837	2.326425
6	5.776184	1.104367	1.320904
6	7.151330	1.254623	1.101926
6	7.840347	0.427751	0.231373
6	7.122886	-0.532865	-0.462467
6	5.739615	-0.699626	-0.303215
6	5.067383	0.116918	0.627649
6	3.988640	2.873301	2.235563
6	3.745142	3.501114	3.458505
6	4.613863	2.889235	4.529228
6	5.269798	1.696989	3.805001
6	2.820437	4.534670	3.532166
6	2.139994	4.908473	2.374492
6	2.242628	4.182513	1.177886
6	3.145951	3.106341	1.157767
8	3.172453	2.252820	0.076689
15	2.475860	0.773666	0.301907
8	1.436548	0.855242	1.384053
8	3.739163	-0.089437	0.928646
8	2.115626	0.244517	-1.049605
1	1.470291	5.766207	2.404361
1	2.645643	5.066269	4.466756
1	8.910715	0.549154	0.074515
1	7.632326	-1.189111	-1.167732
1	8.458305	2.976486	1.324568
1	8.168425	2.077873	2.814734
1	6.187016	3.819907	1.265682
1	6.502272	3.892331	3.006322
1	5.366364	3.599503	4.901506
1	4.026767	2.579825	5.403063
1	4.634055	0.803978	3.887825
1	6.262201	1.443070	4.197902

1	-0.741483	0.227552	0.415981
1	0.345670	-0.066721	2.564233
6	-0.888055	-1.625923	2.893333
1	-1.160901	-1.971169	1.165231
6	-3.055632	-5.047098	-1.240212
1	-3.546839	-4.908130	-0.271073
1	-3.791642	-4.801611	-2.007012
1	-2.779997	-6.106678	-1.342507
6	-2.316369	-3.107423	-3.686719
1	-1.875778	-2.344599	-4.337407
1	-2.396276	-4.033903	-4.273312
1	-3.329952	-2.799293	-3.410070
6	0.679387	-2.018083	-3.137748
1	1.259899	-1.302432	-2.543517
1	1.406275	-2.632675	-3.689813
1	0.081284	-1.460390	-3.866660
6	1.741689	-3.360658	-0.528955
1	2.383063	-4.085387	-1.048458
1	2.172796	-2.362857	-0.695870
1	1.805982	-3.578688	0.541715
6	-0.618639	-5.241647	0.650880
1	-0.592304	-6.277353	0.283521
1	0.295305	-5.089226	1.235178
1	-1.486430	-5.156297	1.316994
6	5.131705	-1.753886	-1.173600
6	5.274641	-3.114143	-0.815633
6	4.643285	-1.411331	-2.449458
6	4.884713	-4.099019	-1.721333
6	4.264293	-2.438150	-3.319681
6	4.372154	-3.781397	-2.979215
1	4.991181	-5.148204	-1.444580
1	3.898983	-2.183163	-4.315183
6	1.430654	4.533253	-0.022162
6	2.055366	4.790847	-1.267558
6	0.023171	4.636842	0.063513
6	1.267711	5.101787	-2.374796
6	-0.716843	4.947919	-1.079849
6	-0.120732	5.167691	-2.315012
1	1.754723	5.294691	-3.333527
1	-1.802660	5.005720	-1.000771
6	-2.217324	-2.151721	3.315346
1	-2.439672	-1.846386	4.347463
1	-3.017263	-1.823221	2.649879
1	-2.199432	-3.244819	3.280941
6	0.273636	-2.591630	3.045442
1	0.035389	-3.462322	2.424814
7	-0.582730	-0.329265	2.941130
6	0.275040	-3.057853	4.495877
6	0.480486	-2.158384	5.546178
6	0.076439	-4.406620	4.792637
6	0.491406	-2.604193	6.862960
1	0.632735	-1.099153	5.335537
6	0.095157	-4.855351	6.109518
1	-0.092800	-5.113201	3.979536
6	0.300714	-3.953789	7.148187
1	0.649710	-1.893096	7.670724
1	-0.056035	-5.911199	6.323066
1	0.311354	-4.300300	8.179001
6	1.635010	-2.050288	2.655083
1	1.648731	-1.677820	1.626263

1	1.968575	-1.235504	3.309701
1	2.373128	-2.853685	2.747069
6	-1.264230	0.780119	3.499384
6	-2.633146	0.840144	3.765890
6	-0.439478	1.856447	3.853034
6	-3.155220	1.949068	4.425371
1	-3.299431	0.047806	3.451045
6	-0.973665	2.953371	4.511747
1	0.617250	1.823111	3.585902
6	-2.333006	3.000811	4.814895
1	-4.223437	1.982985	4.630476
1	-0.320188	3.782117	4.778970
1	-2.750122	3.860085	5.334559
6	-1.271926	0.960623	-2.710783
6	-0.119003	1.748549	-2.825977
6	-1.858247	0.477011	-3.882253
6	0.440745	2.025733	-4.065989
1	0.355696	2.141691	-1.924846
6	-1.303401	0.761731	-5.129396
1	-2.754956	-0.137980	-3.847964
6	-0.150212	1.531616	-5.226643
1	1.341270	2.636398	-4.117522
1	-1.779581	0.372135	-6.027223
1	0.283907	1.750303	-6.199886
6	-4.145272	1.286308	-0.866263
6	-4.436364	1.666891	0.442938
6	-4.649253	2.057328	-1.914283
6	-5.247813	2.765309	0.700810
1	-4.018608	1.089103	1.266840
6	-5.445054	3.172160	-1.660820
1	-4.423734	1.777292	-2.944124
6	-5.753841	3.526003	-0.350294
1	-5.473106	3.036242	1.732501
1	-5.827882	3.761579	-2.492002
1	-6.384702	4.389204	-0.149206
6	-8.294749	0.135774	2.782920
1	-7.881801	-0.582409	3.497250
1	-8.029598	1.141024	3.145323
1	-9.383360	0.047999	2.846744
6	-5.636367	-0.835035	2.388596
1	-5.837751	-1.755714	2.951126
1	-4.591512	-0.863058	2.085845
1	-5.767180	0.015733	3.070592
6	-9.910864	0.919452	0.489988
1	-10.756444	0.218094	0.542287
1	-9.917669	1.501368	1.415654
1	-10.125215	1.621267	-0.321454
6	-9.046208	0.230186	-2.190038
1	-10.102886	0.220680	-1.909709
1	-8.833890	1.218408	-2.626286
1	-8.929968	-0.505211	-2.991393
6	-6.455048	-0.783034	-2.674640
1	-5.376491	-0.844817	-2.806290
1	-6.868556	-1.693155	-3.129543
1	-6.819060	0.071542	-3.255133
6	5.832824	-3.505497	0.541082
6	6.509398	-4.870129	0.571598
6	4.732760	-3.443324	1.598183
1	6.591458	-2.758463	0.814303
1	7.258876	-4.979261	-0.221487

1	7.014181	-5.013785	1.534750
1	5.785872	-5.689937	0.468203
1	4.266703	-2.451686	1.633656
1	3.946583	-4.178401	1.367133
1	5.128211	-3.674968	2.596255
6	3.964390	-4.865028	-3.953647
6	2.803425	-5.703065	-3.421591
6	5.143931	-5.760674	-4.322326
1	3.621078	-4.362183	-4.871909
1	1.931690	-5.082229	-3.174363
1	2.485902	-6.447095	-4.163297
1	3.092663	-6.248586	-2.512669
1	5.982575	-5.176558	-4.718942
1	5.508795	-6.313333	-3.446387
1	4.854166	-6.499413	-5.080351
6	4.670470	0.020519	-2.956230
6	3.520155	0.379424	-3.887803
6	6.001360	0.283045	-3.664784
1	4.602162	0.691210	-2.086627
1	2.555256	0.275706	-3.382061
1	3.621979	1.426226	-4.204097
1	3.516383	-0.223374	-4.806339
1	6.860560	0.109789	-3.006383
1	6.107733	-0.376325	-4.537872
1	6.052568	1.320774	-4.020448
6	-0.748503	4.442617	1.353711
6	-1.860636	3.417959	1.206705
6	-1.317825	5.770914	1.851177
1	-0.062342	4.052787	2.114291
1	-1.439193	2.424862	0.999237
1	-2.444512	3.344866	2.132262
1	-2.558966	3.670046	0.399642
1	-0.545564	6.545162	1.943861
1	-2.078727	6.155561	1.158612
1	-1.798342	5.648753	2.831421
6	3.558844	4.778094	-1.475287
6	4.077657	6.165526	-1.848196
6	3.967935	3.741229	-2.520556
1	4.041132	4.502190	-0.531063
1	3.822560	6.908604	-1.082710
1	5.170060	6.151706	-1.955574
1	3.658407	6.513390	-2.801680
1	3.518735	2.765638	-2.297869
1	3.658203	4.046544	-3.530700
1	5.059387	3.618577	-2.538242
6	-0.924088	5.506195	-3.550035
6	-1.141956	7.016099	-3.638933
6	-2.255442	4.767580	-3.624984
1	-0.318313	5.199302	-4.418341
1	-0.189721	7.560548	-3.641333
1	-1.692997	7.286128	-4.549127
1	-1.723455	7.368649	-2.775805
1	-2.129259	3.689133	-3.461280
1	-2.966162	5.139953	-2.874829
1	-2.720113	4.913482	-4.608130

TS2$_{RR}$

Number of imaginary frequencies : 1

Imaginary Frequency : -538.4262 cm(-1)

Electronic energy : HF=-5263.8330246
Zero-point correction= 1.976194 (hartree/particle)
Thermal correction to Energy= 2.083511
Thermal correction to Enthalpy= 2.084455
Thermal correction to Gibbs Free Energy= 1.842982
Sum of electronic and zero-point Energies= -5261.856830
Sum of electronic and thermal Energies= -5261.749514
Sum of electronic and thermal Enthalpies= -5261.748570
Sum of electronic and thermal Free Energies= -5261.990043

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Cartesian Coordinates

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77	-1.364639	-2.187087	-0.663161
6	-1.528994	-3.248532	-2.658689
6	-1.901488	-4.168559	-1.600787
6	-0.783409	-4.319895	-0.728667
6	0.289241	-3.467196	-1.200362
6	-0.185166	-2.825916	-2.407803
7	-0.703114	-0.160276	-0.796031
1	0.089528	-0.085622	-1.444764
6	-3.134244	0.120792	-1.355282
6	-1.763452	0.810145	-1.221627
16	-4.568174	-1.881680	-0.450876
8	-4.777206	-2.350919	-1.832297
7	-3.206147	-0.950097	-0.332968
6	-6.044345	-0.908372	0.021226
6	-7.062553	-0.620311	-0.911209
6	-6.182505	-0.568495	1.381740
6	-8.248011	-0.020023	-0.439015
6	-7.363731	0.048348	1.819231
6	-8.379168	0.357425	0.903596
8	-4.470664	-2.936401	0.566410
6	7.453238	3.226726	1.083211
6	6.184268	3.728552	1.767058
6	5.310128	2.456057	1.962868
6	5.660143	1.698454	0.699402
6	6.921864	2.100194	0.246382
6	7.509101	1.500169	-0.854719
6	6.802845	0.505430	-1.516505
6	5.516153	0.109661	-1.125989
6	4.946932	0.723339	0.003263
6	3.912486	2.894461	2.338876
6	3.877385	3.152352	3.711506
6	5.089073	2.564342	4.385089
6	5.739237	1.737906	3.263655
6	2.839366	3.896577	4.250395
6	1.846079	4.371745	3.398506
6	1.779721	4.017534	2.043648
6	2.818289	3.209273	1.542371
8	2.770223	2.734957	0.248926
15	2.334679	1.157301	0.040799
8	1.324646	0.785932	1.101195
8	3.708000	0.346765	0.472674
8	2.031436	0.962165	-1.401624
1	1.077799	5.027141	3.799451
1	2.814121	4.138759	5.311651
1	8.492842	1.810352	-1.202942
1	7.241422	0.014052	-2.384515

1	7.959229	3.995878	0.487681
1	8.186641	2.861681	1.818673
1	5.649673	4.409194	1.089214
1	6.362438	4.265414	2.705961
1	5.766147	3.351022	4.749273
1	4.823217	1.957655	5.259599
1	5.326847	0.717694	3.255436
1	6.828833	1.653487	3.357344
1	-0.272997	0.164512	0.077940
1	1.117133	-0.630384	2.076198
6	-0.470306	-1.727073	2.587330
1	-1.050633	-2.072040	1.024682
6	-3.135032	-4.998257	-1.566639
1	-3.365550	-5.340017	-0.553271
1	-4.003681	-4.448310	-1.936428
1	-2.986846	-5.886524	-2.198374
6	-2.355181	-2.917958	-3.851097
1	-1.936949	-2.069144	-4.405117
1	-2.390920	-3.773187	-4.541463
1	-3.383067	-2.678933	-3.558649
6	0.609385	-1.888376	-3.248626
1	1.440237	-1.435296	-2.692875
1	1.049324	-2.426428	-4.099667
1	-0.005356	-1.076796	-3.659649
6	1.663687	-3.377953	-0.637660
1	2.059321	-2.352975	-0.668011
1	1.680966	-3.699530	0.410005
1	2.367000	-4.009897	-1.199258
6	-0.721451	-5.270966	0.414700
1	-0.588272	-6.298411	0.048271
1	0.124036	-5.049955	1.075178
1	-1.644614	-5.250180	1.007115
6	4.875764	-0.946664	-1.965152
6	5.027578	-2.303916	-1.614034
6	4.306174	-0.596491	-3.205615
6	4.617594	-3.285588	-2.516683
6	3.908908	-1.618130	-4.070604
6	4.056591	-2.964137	-3.751465
1	4.752311	-4.335542	-2.254622
1	3.470459	-1.355963	-5.035243
6	0.680058	4.526624	1.172033
6	0.986234	5.274548	0.008984
6	-0.681802	4.332628	1.514738
6	-0.052111	5.767605	-0.784010
6	-1.677136	4.839220	0.677458
6	-1.392109	5.561418	-0.477584
1	0.194677	6.353622	-1.671869
1	-2.720232	4.671455	0.944031
6	-1.241570	-0.441460	2.653202
1	-0.652739	0.379085	2.232121
1	-2.200851	-0.503999	2.132384
1	-1.440072	-0.202087	3.708831
6	-1.047708	-2.951624	3.273239
1	-0.748192	-3.824619	2.678619
7	0.854287	-1.547086	2.486901
6	-0.518730	-3.163698	4.687120
6	-0.560666	-4.464217	5.200827
6	-0.042036	-2.141736	5.507978
6	-0.130834	-4.741117	6.491331
1	-0.926435	-5.272209	4.564937

6	0.391546	-2.417034	6.802676
1	0.026668	-1.120218	5.138584
6	0.350045	-3.713903	7.299260
1	-0.165390	-5.761983	6.865631
1	0.769177	-1.607261	7.423126
1	0.693674	-3.925540	8.309157
6	-2.572444	-2.944051	3.304157
1	-2.928327	-3.893570	3.719869
1	-2.948258	-2.146878	3.957194
1	-3.005038	-2.832812	2.303419
6	1.987920	-2.329417	2.794887
6	3.185198	-1.606781	2.888368
6	2.002603	-3.705067	3.043760
6	4.358151	-2.236181	3.276715
1	3.179549	-0.541996	2.662331
6	3.182235	-4.322848	3.444689
1	1.105618	-4.304242	2.947734
6	4.359667	-3.595591	3.578402
1	5.275267	-1.653020	3.348422
1	3.171341	-5.389434	3.656602
1	5.274525	-4.087491	3.900593
6	-7.535538	0.380072	3.277298
1	-7.000921	-0.323301	3.921575
1	-7.159114	1.385635	3.520655
1	-8.585491	0.345697	3.581707
6	-5.095662	-0.782002	2.396066
1	-5.340570	-1.608298	3.077009
1	-4.142190	-1.021210	1.934021
1	-4.958758	0.119505	3.009324
6	-9.588288	1.131149	1.354967
1	-10.423595	0.476180	1.642808
1	-9.362888	1.763274	2.218289
1	-9.957062	1.796165	0.568127
6	-9.390822	0.221357	-1.389679
1	-10.348500	0.280264	-0.865740
1	-9.270180	1.158292	-1.954806
1	-9.486379	-0.584417	-2.123766
6	-6.974350	-0.861634	-2.395784
1	-5.953083	-0.847560	-2.765684
1	-7.389139	-1.841117	-2.670536
1	-7.539306	-0.097540	-2.937961
6	5.716580	-2.709262	-0.322043
6	7.223115	-2.845659	-0.551053
6	5.184499	-4.000010	0.286884
1	5.549045	-1.908905	0.416152
1	7.669717	-1.913925	-0.915836
1	7.737384	-3.125875	0.377521
1	7.423935	-3.628178	-1.296170
1	4.107148	-3.953205	0.485935
1	5.382422	-4.871468	-0.351152
1	5.684447	-4.190233	1.244272
6	3.649812	-4.040649	-4.734970
6	2.702728	-5.069277	-4.122887
6	4.876380	-4.731906	-5.326570
1	3.115868	-3.539755	-5.558929
1	1.815116	-4.595957	-3.681512
1	2.361200	-5.783889	-4.882367
1	3.198748	-5.648637	-3.332481
1	5.552547	-4.010447	-5.800131
1	5.444083	-5.255130	-4.545383

1	4.586021	-5.474749	-6.080655
6	4.181903	0.846526	-3.659786
6	2.851117	1.155589	-4.338686
6	5.333997	1.215609	-4.595577
1	4.240035	1.481198	-2.765131
1	2.007226	0.886526	-3.696163
1	2.783182	2.234363	-4.533856
1	2.749143	0.649521	-5.309489
1	6.312482	1.103078	-4.113653
1	5.327665	0.578738	-5.491538
1	5.242910	2.258047	-4.927735
6	-1.138430	3.656204	2.796990
6	-2.283848	2.675054	2.574958
6	-1.590323	4.697946	3.825228
1	-0.293062	3.092060	3.214324
1	-2.051517	1.965712	1.772610
1	-2.487653	2.108332	3.492808
1	-3.215510	3.190125	2.306897
1	-0.837449	5.471667	4.012869
1	-2.493013	5.213562	3.470344
1	-1.834253	4.222027	4.784027
6	2.401823	5.651477	-0.391133
6	2.603982	7.164271	-0.316027
6	2.774612	5.121432	-1.774137
1	3.095711	5.206256	0.329339
1	2.373035	7.549800	0.684735
1	3.644791	7.425552	-0.547473
1	1.964180	7.695458	-1.032869
1	2.568961	4.046853	-1.856085
1	2.221418	5.646665	-2.566205
1	3.843431	5.278469	-1.970234
6	-2.492835	6.095926	-1.366504
6	-3.609918	6.773931	-0.577833
6	-3.072905	4.986631	-2.243720
1	-2.036257	6.851207	-2.025806
1	-3.222878	7.519741	0.126920
1	-4.306331	7.278095	-1.259336
1	-4.196804	6.041752	-0.006523
1	-2.329163	4.589499	-2.944436
1	-3.425944	4.148548	-1.625714
1	-3.928262	5.356331	-2.825018
1	-3.212580	-0.336803	-2.355636
1	-1.845423	1.555755	-0.414751
6	-4.195263	1.206222	-1.271269
6	-4.859215	1.640420	-2.417762
6	-4.486293	1.831626	-0.056544
6	-5.814452	2.652922	-2.350702
1	-4.636994	1.171248	-3.376008
6	-5.436549	2.842125	0.017336
1	-3.978735	1.491394	0.844477
6	-6.109894	3.253628	-1.132047
1	-6.329019	2.969703	-3.255924
1	-5.664564	3.300056	0.979736
1	-6.857260	4.042660	-1.075700
6	-1.305132	1.535729	-2.468600
6	-0.453855	2.633293	-2.321698
6	-1.613938	1.101877	-3.762190
6	0.051676	3.295641	-3.434328
1	-0.179574	2.974575	-1.321434
6	-1.108565	1.764057	-4.877899

1	-2.258015	0.236771	-3.914390
6	-0.278771	2.868240	-4.716435
1	0.706822	4.152336	-3.291230
1	-1.369170	1.414889	-5.874884
1	0.117013	3.388492	-5.586313

TS2$_{SR}$

Number of imaginary frequencies : 1
Imaginary Frequency : -646.8657 cm(-1)

Electronic energy : HF=-5263.833089
Zero-point correction= 1.977560 (hartree/particle)
Thermal correction to Energy= 2.085021
Thermal correction to Enthalpy= 2.085965
Thermal correction to Gibbs Free Energy= 1.844544
Sum of electronic and zero-point Energies= -5261.855529
Sum of electronic and thermal Energies= -5261.748068
Sum of electronic and thermal Enthalpies= -5261.747124
Sum of electronic and thermal Free Energies= -5261.988545

.....

Cartesian Coordinates

.....

77	-1.423906	-2.000699	-0.569379
6	-1.479012	-3.017198	-2.598321
6	-1.962914	-3.928914	-1.576011
6	-0.895855	-4.174548	-0.662944
6	0.225340	-3.352606	-1.044862
6	-0.134091	-2.676791	-2.267832
7	-0.732208	0.022539	-0.514704
1	0.255282	0.096843	-0.801208
6	-3.068708	0.469120	-1.305481
1	-3.346080	0.156342	-2.322337
6	-1.585572	0.931341	-1.337453
1	-1.533083	1.918039	-0.857806
16	-4.634977	-1.514807	-0.677788
8	-4.799767	-1.850755	-2.103845
7	-3.232412	-0.688508	-0.395414
6	-6.048989	-0.458478	-0.214542
6	-6.874847	0.133957	-1.189696
6	-6.329691	-0.328971	1.159584
6	-8.030785	0.815572	-0.760143
6	-7.482321	0.362265	1.561282
6	-8.311813	0.965083	0.604665
8	-4.684515	-2.656770	0.240910
6	7.910979	1.981756	2.307688
6	6.709284	2.907814	2.442218
6	5.490904	1.954142	2.629874
6	5.909983	0.810152	1.723167
6	7.304348	0.813323	1.590786
6	7.961292	-0.149871	0.843721
6	7.197884	-1.094255	0.177121
6	5.796895	-1.103431	0.235973
6	5.152712	-0.153361	1.048743
6	4.241354	2.781540	2.436996
6	3.982189	3.479231	3.618339
6	4.764765	2.875045	4.756210
6	5.355933	1.599481	4.128067
6	3.122233	4.568878	3.604196

6	2.522905	4.932370	2.400494
6	2.638228	4.152585	1.239728
6	3.480039	3.029567	1.303561
8	3.532068	2.142358	0.247705
15	2.691924	0.738592	0.447530
8	1.572201	0.961389	1.425026
8	3.790500	-0.201316	1.245048
8	2.398152	0.185819	-0.907083
1	1.903947	5.827083	2.363361
1	2.937383	5.150160	4.506459
1	9.046507	-0.146484	0.758354
1	7.683199	-1.856517	-0.431593
1	8.747414	2.428946	1.757481
1	8.300861	1.685096	3.293531
1	6.567737	3.461820	1.503123
1	6.795515	3.642396	3.250796
1	5.555185	3.553259	5.109929
1	4.130009	2.663006	5.625575
1	4.650200	0.763320	4.230650
1	6.309035	1.292962	4.576681
1	-0.745008	0.353230	0.452887
1	0.446355	0.167112	2.326478
6	-0.662426	-1.474893	2.742568
1	-1.405789	-1.866848	1.174737
6	-3.247447	-4.675830	-1.629180
1	-3.592690	-4.948474	-0.627356
1	-4.037230	-4.081505	-2.097470
1	-3.111518	-5.599404	-2.211495
6	-2.216099	-2.667935	-3.842063
1	-1.720820	-1.859900	-4.391238
1	-2.263338	-3.543766	-4.505520
1	-3.243632	-2.364738	-3.614542
6	0.826018	-1.848188	-3.043717
1	1.460131	-1.250911	-2.377269
1	1.501003	-2.511573	-3.606299
1	0.333286	-1.178244	-3.756249
6	1.599795	-3.389036	-0.484822
1	2.065065	-2.394320	-0.450296
1	1.618782	-3.814852	0.521902
1	2.242700	-4.015030	-1.113450
6	-0.892219	-5.223184	0.386899
1	-0.632072	-6.187777	-0.073487
1	-0.152936	-5.033445	1.171786
1	-1.871794	-5.334298	0.859611
6	5.146312	-2.149611	-0.611964
6	5.075596	-3.478475	-0.136462
6	4.862251	-1.867265	-1.962040
6	4.727190	-4.497108	-1.021493
6	4.496882	-2.922584	-2.803903
6	4.439167	-4.240523	-2.363342
1	4.680506	-5.524054	-0.658148
1	4.289563	-2.716861	-3.855149
6	1.888569	4.503379	0.000689
6	2.566773	4.680740	-1.230376
6	0.487211	4.696007	0.039145
6	1.834464	5.011059	-2.369506
6	-0.195939	5.017952	-1.136046
6	0.452392	5.168242	-2.355806
1	2.360435	5.146770	-3.317244
1	-1.278467	5.142938	-1.093222

6	0.580410	-2.262682	2.480622
1	1.204584	-1.773589	1.726294
1	1.161780	-2.302139	3.414845
1	0.350910	-3.281881	2.169046
6	-1.712909	-2.079248	3.662415
1	-2.657246	-1.552279	3.497877
7	-0.445926	-0.156176	2.762309
6	-2.021007	-3.549907	3.462928
6	-3.183860	-3.910195	2.779060
6	-1.247355	-4.561575	4.039805
6	-3.583805	-5.241160	2.701752
1	-3.777947	-3.145634	2.281669
6	-1.636603	-5.895002	3.951049
1	-0.337845	-4.311916	4.584076
6	-2.814798	-6.238690	3.293995
1	-4.501301	-5.492524	2.172464
1	-1.024343	-6.666007	4.414187
1	-3.129190	-7.278864	3.242891
6	-1.266710	-1.799124	5.109600
1	-1.975244	-2.261740	5.803979
1	-0.274099	-2.214665	5.317598
1	-1.231711	-0.726502	5.323054
6	-1.169864	0.900493	3.366278
6	-2.560277	0.967493	3.408527
6	-0.403905	1.928012	3.927548
6	-3.180276	2.022476	4.070013
1	-3.153531	0.214349	2.901216
6	-1.033280	2.981762	4.577062
1	0.680904	1.895241	3.835155
6	-2.423371	3.025871	4.667652
1	-4.268477	2.061906	4.101578
1	-0.428506	3.776473	5.009507
1	-2.913412	3.848454	5.182936
6	-0.971127	1.130098	-2.712333
6	0.276953	1.766330	-2.755767
6	-1.560615	0.759825	-3.922330
6	0.933564	1.978997	-3.960723
1	0.748929	2.094584	-1.828156
6	-0.911951	0.988782	-5.135455
1	-2.535542	0.278431	-3.945808
6	0.341435	1.588617	-5.159378
1	1.907475	2.465848	-3.958234
1	-1.394776	0.688319	-6.063397
1	0.850400	1.760408	-6.105339
6	-3.919328	1.684211	-0.968774
6	-4.263739	2.006589	0.343458
6	-4.313512	2.545987	-1.993331
6	-5.029062	3.132541	0.622058
1	-3.941579	1.350262	1.149938
6	-5.066945	3.684844	-1.717779
1	-4.043226	2.314908	-3.024930
6	-5.437192	3.976201	-0.408222
1	-5.305444	3.352032	1.653153
1	-5.372298	4.339351	-2.532203
1	-6.038266	4.856708	-0.190887
6	-7.824782	0.459636	3.024110
1	-7.470226	-0.409164	3.585548
1	-7.382771	1.351017	3.497000
1	-8.905378	0.514125	3.183701
6	-5.410367	-0.830375	2.240316

1	-5.767431	-1.771589	2.679691
1	-4.399935	-1.012640	1.870706
1	-5.353177	-0.094023	3.052645
6	-9.478815	1.809401	1.039518
1	-10.420293	1.241413	1.064582
1	-9.329920	2.230055	2.037666
1	-9.632057	2.655806	0.363192
6	-8.980925	1.386006	-1.779574
1	-9.994447	1.481858	-1.381094
1	-8.669212	2.384198	-2.122683
1	-9.052900	0.751028	-2.667625
6	-6.596748	0.139693	-2.670301
1	-5.541682	0.028247	-2.910005
1	-7.114301	-0.683371	-3.181611
1	-6.946431	1.076797	-3.114119
6	5.361093	-3.792149	1.321646
6	5.930217	-5.184790	1.562207
6	4.100823	-3.587655	2.164481
1	6.109130	-3.068395	1.674721
1	6.797125	-5.391057	0.923130
1	6.249956	-5.282953	2.606872
1	5.184933	-5.971585	1.383485
1	3.682609	-2.582486	2.026213
1	3.332951	-4.322493	1.879766
1	4.316380	-3.728123	3.232166
6	4.079830	-5.360895	-3.316348
6	2.749988	-6.022895	-2.958167
6	5.187900	-6.408076	-3.394844
1	3.968225	-4.910467	-4.315383
1	1.920292	-5.303957	-2.966566
1	2.507600	-6.819149	-3.673491
1	2.787788	-6.477997	-1.958647
1	6.152181	-5.954465	-3.652164
1	5.310551	-6.927355	-2.435074
1	4.956196	-7.168165	-4.151569
6	5.086851	-0.485330	-2.553051
6	4.070992	-0.080635	-3.614972
6	6.494458	-0.401856	-3.148897
1	5.008034	0.246910	-1.735886
1	3.050686	-0.098233	-3.222039
1	4.283133	0.945139	-3.946711
1	4.124351	-0.716938	-4.509182
1	7.274427	-0.594600	-2.403695
1	6.613694	-1.137202	-3.957314
1	6.676502	0.593515	-3.575107
6	-0.342435	4.579099	1.304652
6	-1.475357	3.577302	1.151764
6	-0.895478	5.936880	1.734843
1	0.297757	4.204312	2.111284
1	-1.063249	2.575124	0.973253
1	-2.078201	3.532603	2.067181
1	-2.153573	3.829180	0.326158
1	-0.107245	6.693563	1.837490
1	-1.619202	6.319194	1.002410
1	-1.415275	5.851332	2.698874
6	4.072558	4.566564	-1.388843
6	4.689432	5.909292	-1.775395
6	4.449301	3.480992	-2.396846
1	4.508771	4.282482	-0.424997
1	4.463517	6.683084	-1.031466

1	5.781046	5.823494	-1.853796
1	4.316685	6.262888	-2.745820
1	3.928538	2.541440	-2.173357
1	4.201405	3.782619	-3.424856
1	5.529913	3.285995	-2.368353
6	-0.286902	5.530230	-3.623585
6	-0.430934	7.047574	-3.734583
6	-1.647218	4.852794	-3.741500
1	0.336270	5.187162	-4.465494
1	0.544861	7.547661	-3.703762
1	-0.932030	7.332204	-4.668919
1	-1.029416	7.436615	-2.899197
1	-1.575071	3.770623	-3.569925
1	-2.363364	5.262292	-3.016245
1	-2.072174	5.014293	-4.740042

(*Z*)-**TS2**$_{SS}$

Number of imaginary frequencies : 1
Imaginary Frequency : -706.7492 cm(-1)

Electronic energy : HF=-5263.824471
Zero-point correction= 1.977135 (hartree/particle)
Thermal correction to Energy= 2.084284
Thermal correction to Enthalpy= 2.085228
Thermal correction to Gibbs Free Energy= 1.844120
Sum of electronic and zero-point Energies= -5261.847336
Sum of electronic and thermal Energies= -5261.740187
Sum of electronic and thermal Enthalpies= -5261.739243
Sum of electronic and thermal Free Energies= -5261.980351

.....

Cartesian Coordinates

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77	-1.592800	-1.834099	-1.469458
6	-2.180798	-2.232914	-3.656541
6	-2.625947	-3.325976	-2.815037
6	-1.479365	-3.933194	-2.226223
6	-0.312768	-3.199819	-2.648770
6	-0.761044	-2.150381	-3.527563
7	-0.647781	0.014562	-0.877158
1	0.298678	0.155209	-1.257391
6	-2.956618	0.903379	-0.756055
1	-3.602158	1.289691	-1.559944
6	-1.495449	1.203021	-1.179648
1	-1.117934	2.035203	-0.557012
16	-4.690543	-1.060775	-0.871747
8	-5.056409	-0.915579	-2.292761
7	-3.149880	-0.558074	-0.579883
6	-5.830345	0.006811	0.067660
6	-5.918082	-0.204314	1.457052
6	-6.628432	0.972160	-0.581902
6	-6.820149	0.566268	2.207036
6	-7.553547	1.701214	0.190212
6	-7.597923	1.549738	1.582579
8	-4.831433	-2.419039	-0.334261
6	8.171916	2.565765	0.374315
6	6.992669	3.432961	0.812293
6	6.026760	2.447219	1.529298
6	6.221480	1.221264	0.669945

6	7.509080	1.242646	0.119795
6	8.020446	0.139780	-0.544413
6	7.221206	-0.989924	-0.655442
6	5.902307	-1.014310	-0.186993
6	5.389451	0.128255	0.449233
6	4.712181	3.146868	1.779438
6	4.843316	3.924641	2.934693
6	6.050738	3.493019	3.724052
6	6.501158	2.224259	2.985753
6	3.965686	4.969290	3.177823
6	2.951553	5.210495	2.256573
6	2.698098	4.348133	1.181969
6	3.576563	3.264584	0.986939
8	3.369322	2.384628	-0.052072
15	2.825174	0.849722	0.202098
8	1.748271	0.819086	1.250801
8	4.110909	0.127338	0.953148
8	2.566363	0.286615	-1.159809
1	2.321203	6.089751	2.373340
1	4.090917	5.617317	4.043790
1	9.028336	0.152129	-0.955782
1	7.609571	-1.889318	-1.131937
1	8.689133	2.954340	-0.511346
1	8.928302	2.485026	1.169801
1	6.476746	3.828950	-0.074625
1	7.275230	4.285603	1.440529
1	6.834412	4.264700	3.714609
1	5.811152	3.308441	4.778620
1	5.978997	1.343941	3.388571
1	7.579020	2.034371	3.054881
1	-0.510497	-0.003919	0.136735
1	0.748590	-0.487511	1.854044
6	0.087105	-2.334359	1.425045
1	-1.115509	-2.195581	0.175179
6	-3.996105	-3.903194	-2.806116
1	-4.218456	-4.416388	-1.865855
1	-4.758104	-3.134670	-2.948397
1	-4.075972	-4.634639	-3.624436
6	-3.037193	-1.516725	-4.638093
1	-2.519849	-0.656895	-5.073352
1	-3.292633	-2.202198	-5.459821
1	-3.973788	-1.175386	-4.185539
6	0.160810	-1.215969	-4.228128
1	0.925498	-0.820131	-3.546078
1	0.690569	-1.744468	-5.033815
1	-0.369251	-0.366690	-4.671963
6	1.100806	-3.642657	-2.534392
1	1.785802	-2.823781	-2.290563
1	1.228347	-4.430118	-1.783119
1	1.429348	-4.066053	-3.496236
6	-1.482553	-5.206154	-1.455630
1	-1.473724	-6.058060	-2.150158
1	-0.600787	-5.305654	-0.811281
1	-2.373961	-5.306655	-0.828069
6	5.140582	-2.282403	-0.321558
6	4.868789	-3.058632	0.824530
6	4.812561	-2.773442	-1.600509
6	4.258044	-4.304418	0.670685
6	4.210619	-4.028118	-1.700721
6	3.917072	-4.807828	-0.584701

1	4.062924	-4.907738	1.560063
1	3.958820	-4.417073	-2.690052
6	1.585020	4.633595	0.234069
6	1.878333	4.909866	-1.119702
6	0.245210	4.688746	0.683684
6	0.831735	5.181314	-1.997597
6	-0.769290	4.928501	-0.249091
6	-0.499355	5.172987	-1.594220
1	1.058453	5.407516	-3.042158
1	-1.804627	4.933285	0.087039
6	1.264825	-2.359092	0.490845
1	1.348520	-1.473350	-0.142032
1	2.183264	-2.396030	1.092953
1	1.243991	-3.243357	-0.142045
6	-0.302613	-3.728871	1.927979
1	-0.224064	-4.340511	1.017198
7	0.072136	-1.217912	2.167720
6	-1.682490	-4.032262	2.487032
6	-2.795969	-3.978555	1.643580
6	-1.874151	-4.449071	3.807057
6	-4.061193	-4.325214	2.103599
1	-2.691692	-3.616439	0.621258
6	-3.141243	-4.786733	4.273026
1	-1.035684	-4.491847	4.497868
6	-4.240851	-4.729454	3.422959
1	-4.903967	-4.244737	1.420301
1	-3.265249	-5.098555	5.308162
1	-5.230823	-4.998202	3.785914
6	0.832959	-4.183240	2.857241
1	1.798060	-4.162815	2.341803
1	0.912003	-3.551231	3.750765
1	0.653717	-5.214750	3.178985
6	-0.539566	-0.895338	3.406521
6	0.222249	-0.095351	4.265172
6	-1.831520	-1.270613	3.765811
6	-0.288837	0.274540	5.501647
1	1.210598	0.231490	3.944964
6	-2.325885	-0.910807	5.016276
1	-2.456304	-1.818641	3.067953
6	-1.558364	-0.147757	5.890766
1	0.312116	0.892673	6.164393
1	-3.331343	-1.224046	5.293452
1	-1.953770	0.132830	6.864101
6	-1.260230	1.625838	-2.617135
6	0.019922	2.097484	-2.936627
6	-2.227508	1.600400	-3.621129
6	0.325996	2.512694	-4.226576
1	0.791117	2.142969	-2.162795
6	-1.929156	2.038883	-4.910497
1	-3.229461	1.228537	-3.414783
6	-0.651026	2.491229	-5.219448
1	4.069646	-1.010426	-4.498388
1	-2.702678	2.013547	-5.675757
1	-0.417141	2.828966	-6.226736
6	-3.345481	1.669850	0.498699
6	-2.932608	1.236810	1.755357
6	-4.177689	2.788621	0.420008
6	-3.362752	1.878907	2.912996
1	-2.294283	0.357111	1.827862
6	-4.627527	3.425840	1.572985

1	-4.522806	3.132967	-0.555925
6	-4.231237	2.962822	2.826135
1	-3.019244	1.515042	3.882191
1	-5.309241	4.271955	1.492051
1	-4.588079	3.455241	3.729391
6	-8.486652	2.679675	-0.474475
1	-8.031556	3.674553	-0.602570
1	-8.796914	2.337986	-1.466269
1	-9.403226	2.817163	0.106108
6	-6.510920	1.356313	-2.035156
1	-5.502776	1.227151	-2.425385
1	-7.161402	0.748813	-2.677317
1	-6.789281	2.405005	-2.175129
6	-8.413803	2.494011	2.422801
1	-8.558694	3.457525	1.925924
1	-9.411093	2.099689	2.665958
1	-7.909772	2.707068	3.371828
6	-6.930014	0.345093	3.690713
1	-6.135010	0.874895	4.239861
1	-7.888111	0.690603	4.088326
1	-6.843162	-0.714970	3.950049
6	-5.058274	-1.177645	2.208632
1	-5.617306	-2.092244	2.448643
1	-4.173085	-1.488732	1.656172
1	-4.730963	-0.735604	3.155910
6	5.304116	-2.618950	2.211909
6	6.405482	-3.537029	2.739104
6	4.149625	-2.528342	3.204790
1	5.736051	-1.614668	2.130969
1	7.259386	-3.567420	2.050339
1	6.770072	-3.189324	3.714214
1	6.043986	-4.566251	2.866849
1	3.361418	-1.852323	2.844222
1	3.704209	-3.512922	3.402750
1	4.505826	-2.136192	4.166083
6	3.311710	-6.183588	-0.764337
6	2.216362	-6.507759	0.245136
6	4.403871	-7.251833	-0.722685
1	2.859212	-6.206081	-1.769725
1	1.435158	-5.734103	0.269368
1	1.734881	-7.462168	-0.001476
1	2.619037	-6.605308	1.262235
1	5.172604	-7.066708	-1.482337
1	4.900349	-7.256574	0.257249
1	3.987671	-8.252988	-0.893733
6	5.106258	-1.995231	-2.870949
6	3.832591	-1.640794	-3.631043
6	6.081000	-2.748059	-3.773737
1	5.575881	-1.046141	-2.586286
1	3.325723	-2.539608	-4.008497
1	7.013885	-3.000861	-3.254453
1	5.644367	-3.688114	-4.137718
1	6.338131	-2.144221	-4.653337
6	-0.115536	4.497441	2.151113
6	-0.037345	3.030552	2.559081
6	-1.462787	5.096833	2.528854
1	0.633516	5.028542	2.748889
1	0.970154	2.620590	2.438772
1	-0.350446	2.904459	3.605417
1	-0.709510	2.425017	1.936129

1	-1.530608	6.157731	2.255869
1	-2.297607	4.568870	2.053895
1	-1.613692	5.015848	3.613204
6	3.295309	4.995774	-1.657093
6	3.627820	6.427551	-2.072463
6	3.539234	4.022820	-2.807289
1	3.987697	4.728852	-0.850795
1	3.493756	7.126396	-1.237357
1	4.669051	6.500996	-2.412601
1	2.986325	6.766428	-2.896999
1	3.266537	2.997720	-2.526132
1	2.966471	4.310346	-3.700660
1	4.600038	4.023434	-3.090927
6	-1.576871	5.504348	-2.604198
6	-1.671675	7.019453	-2.787322
6	-2.946813	4.933297	-2.268224
1	-1.256715	5.064096	-3.563332
1	-0.711865	7.453542	-3.092001
1	-2.420001	7.280559	-3.546909
1	-1.967348	7.498004	-1.843305
1	-2.895832	3.857200	-2.058844
1	-3.636286	5.079608	-3.109255
1	-3.390454	5.429485	-1.393281
1	3.148185	-1.082307	-2.980247
1	1.329874	2.869283	-4.448500

(*Z*)-**TS2**$_{RS}$

Number of imaginary frequencies : 1
Imaginary Frequency : -739.8541 cm(-1)

Electronic energy : HF=-5263.8190373
Zero-point correction= 1.976545 (hartree/particle)
Thermal correction to Energy= 2.084165
Thermal correction to Enthalpy= 2.085109
Thermal correction to Gibbs Free Energy= 1.843407
Sum of electronic and zero-point Energies= -5261.842492
Sum of electronic and thermal Energies= -5261.734872
Sum of electronic and thermal Enthalpies= -5261.733928
Sum of electronic and thermal Free Energies= -5261.975631

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Cartesian Coordinates

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77	-1.427684	-2.283763	0.000409
6	-1.527445	-4.057430	-1.471195
6	-1.699362	-4.494797	-0.104663
6	-0.486917	-4.175932	0.601969
6	0.375144	-3.432958	-0.275368
6	-0.282426	-3.374725	-1.571180
7	-0.611611	-0.348888	-0.435507
1	0.082742	-0.440373	-1.184133
6	-3.035320	0.323563	-0.746094
1	-3.404319	0.500459	-1.765288
6	-1.540481	0.760437	-0.811579
1	-1.376815	1.567598	-0.081631
16	-4.274093	-1.789769	-1.474019
8	-3.707113	-1.814846	-2.834125
7	-3.227150	-1.099624	-0.401587
6	-5.718956	-0.677970	-1.491775

6	-6.544806	-0.686658	-0.352096
6	-5.914424	0.258780	-2.531526
6	-7.612405	0.223900	-0.279701
6	-6.867873	1.276689	-2.336997
6	-7.753654	1.225288	-1.250564
8	-4.696142	-3.096477	-0.952906
6	7.764782	2.810008	0.328121
6	6.596912	3.474131	1.053399
6	5.685591	2.296848	1.507504
6	5.880672	1.346607	0.347973
6	7.104853	1.605988	-0.276723
6	7.554705	0.810442	-1.317258
6	6.755669	-0.246756	-1.730004
6	5.503451	-0.512656	-1.158115
6	5.065418	0.313644	-0.109361
6	4.347547	2.866035	1.919506
6	4.439266	3.323976	3.235472
6	5.671660	2.765006	3.896129
6	6.184379	1.747267	2.863793
6	3.491435	4.207859	3.726915
6	2.479395	4.642325	2.874381
6	2.295200	4.116458	1.588094
6	3.218467	3.142489	1.159973
8	3.034661	2.476879	-0.034218
15	2.506501	0.917855	0.045924
8	1.544456	0.793540	1.202862
8	3.863138	0.097551	0.530303
8	2.110893	0.495327	-1.323213
1	1.800210	5.415844	3.220142
1	3.558580	4.597652	4.741364
1	8.509520	1.008296	-1.801434
1	7.094578	-0.903671	-2.530472
1	8.234944	3.458815	-0.420466
1	8.557345	2.513455	1.032180
1	6.029880	4.089757	0.339959
1	6.896573	4.121241	1.885912
1	6.415050	3.553346	4.085520
1	5.452214	2.308021	4.869032
1	5.715595	0.766925	3.034670
1	7.272115	1.607095	2.888518
1	-0.021170	-0.026859	0.339542
1	1.021121	-0.291163	2.464704
6	-0.712611	-0.997995	3.145955
1	-1.381641	-1.709004	1.666115
6	-2.814153	-5.356011	0.381900
1	-2.760957	-5.506190	1.466381
1	-3.784159	-4.906883	0.139428
1	-2.770614	-6.349555	-0.087560
6	-2.389845	-4.443965	-2.614651
1	-2.047661	-5.426189	-2.976285
1	-3.439877	-4.524578	-2.325607
1	-2.325465	-3.729805	-3.438219
6	0.278899	-2.775151	-2.811994
1	1.088568	-2.069318	-2.594631
1	0.708006	-3.557569	-3.454804
1	-0.490175	-2.255696	-3.396338
6	1.741373	-2.926457	0.022023
1	1.964280	-1.992002	-0.512167
1	1.883115	-2.737968	1.093306
1	2.496744	-3.656692	-0.294047

6	-0.138111	-4.671905	1.958528
1	-0.962726	-4.562202	2.672348
1	0.096033	-5.744114	1.901566
1	0.742983	-4.165898	2.361947
6	4.784744	-1.707715	-1.692231
6	4.972789	-2.954215	-1.059072
6	4.105101	-1.635579	-2.924099
6	4.504223	-4.108894	-1.684291
6	3.635759	-2.820555	-3.497074
6	3.826759	-4.063963	-2.902256
1	4.661544	-5.074329	-1.200639
1	3.112211	-2.774000	-4.453479
6	1.247014	4.656519	0.671500
6	1.637951	5.202876	-0.575426
6	-0.122107	4.712630	1.038792
6	0.667192	5.733795	-1.425309
6	-1.051945	5.242572	0.141315
6	-0.683565	5.753582	-1.100885
1	0.981625	6.157863	-2.381284
1	-2.103702	5.261160	0.429514
6	-1.270219	0.357741	2.855781
1	-1.166367	0.962390	3.770505
1	-0.697574	0.874567	2.079105
1	-2.325047	0.321121	2.582826
6	-1.446464	-1.856513	4.157728
1	-1.087603	-2.884268	4.028079
7	0.629614	-1.034282	3.071964
6	-1.052938	-1.369750	5.564285
1	0.028360	-1.397905	5.726177
1	-1.382284	-0.339540	5.735543
1	-1.529863	-2.002117	6.320458
6	1.667064	-1.836489	3.602178
6	2.959886	-1.378178	3.295480
6	1.532780	-2.976382	4.405362
6	4.077679	-2.038371	3.780322
1	3.077692	-0.495442	2.668902
6	2.666088	-3.632226	4.878456
1	0.563993	-3.379820	4.671809
6	3.941055	-3.171864	4.577267
1	5.067105	-1.663986	3.524100
1	2.536680	-4.516532	5.498031
1	4.818260	-3.691678	4.954805
6	-1.140721	1.286560	-2.171129
6	-0.443998	2.487957	-2.280773
6	-1.393222	0.536981	-3.327423
6	-0.025256	2.949583	-3.526746
1	-0.223806	3.068654	-1.383849
6	-0.958527	0.991029	-4.568039
1	-1.950426	-0.399209	-3.257865
6	-0.279435	2.203439	-4.671841
1	0.506002	3.898150	-3.590029
1	-1.161522	0.399164	-5.458725
1	0.053366	2.562616	-5.643662
6	-3.855267	1.263750	0.123217
6	-4.365889	0.895615	1.366835
6	-4.158879	2.533853	-0.375448
6	-5.149216	1.781984	2.103214
1	-4.177141	-0.111344	1.738734
6	-4.954699	3.415338	0.348955
1	-3.776562	2.825000	-1.357271

6	-5.454959	3.040988	1.594572
1	-5.540109	1.473089	3.072655
1	-5.198759	4.391692	-0.069323
1	-6.084249	3.724548	2.161313
6	-6.893465	2.462988	-3.267436
1	-5.928140	2.614524	-3.757454
1	-7.653978	2.386200	-4.057969
1	-7.095121	3.383555	-2.709075
6	-5.183811	0.246578	-3.851030
1	-4.226087	0.790116	-3.817850
1	-4.952629	-0.766485	-4.171741
1	-5.796492	0.717133	-4.624709
6	-8.849308	2.244129	-1.100061
1	-8.706246	2.861064	-0.202086
1	-8.926844	2.918246	-1.954284
1	-9.828426	1.761034	-0.995534
6	-8.538588	0.184052	0.904325
1	-9.494485	0.674439	0.705293
1	-8.765994	-0.839674	1.218673
1	-8.090961	0.697743	1.769808
6	-6.327551	-1.596381	0.823221
1	-5.293253	-1.924104	0.925025
1	-6.598973	-1.083464	1.750489
1	-6.943516	-2.504440	0.751403
6	5.724817	-3.067969	0.255450
6	7.200284	-3.375362	-0.002459
6	5.141928	-4.106968	1.207971
1	5.662384	-2.092040	0.758916
1	7.672556	-2.609065	-0.628446
1	7.761427	-3.435060	0.939220
1	7.305049	-4.340309	-0.517764
1	4.080131	-3.926743	1.421448
1	5.244770	-5.127621	0.816294
1	5.680015	-4.080261	2.164247
6	3.319510	-5.330242	-3.557070
6	2.328521	-6.076650	-2.665314
6	4.470653	-6.249160	-3.958838
1	2.790165	-5.032812	-4.476569
1	1.465754	-5.451417	-2.396966
1	1.949686	-6.975102	-3.169036
1	2.805084	-6.400506	-1.730003
1	5.183676	-5.734813	-4.613700
1	5.022859	-6.599028	-3.076526
1	4.099544	-7.135868	-4.488390
6	3.945015	-0.327317	-3.680973
6	2.551318	-0.118773	-4.267002
6	4.991974	-0.229532	-4.791795
1	4.108296	0.490103	-2.965118
1	1.790322	-0.107108	-3.480577
1	2.509055	0.856492	-4.769573
1	2.291269	-0.877552	-5.019650
1	6.016013	-0.304697	-4.406341
1	4.855284	-1.032376	-5.530066
1	4.903753	0.727564	-5.321923
6	-0.633295	4.293139	2.406404
6	-1.952436	3.529681	2.355827
6	-0.839884	5.522811	3.298447
1	0.120558	3.639278	2.868391
1	-1.942520	2.723719	1.614318
1	-2.178699	3.092936	3.337463

1	-2.795879	4.184400	2.102669
1	0.038050	6.175471	3.352152
1	-1.663851	6.134385	2.906218
1	-1.105953	5.225056	4.321160
6	3.082401	5.323518	-1.030530
6	3.495381	6.791157	-1.138485
6	3.347485	4.586361	-2.341294
1	3.726509	4.877663	-0.266579
1	3.344703	7.319976	-0.189093
1	4.557426	6.871797	-1.405134
1	2.921338	7.320759	-1.910177
1	3.008137	3.544771	-2.293729
1	2.848293	5.079109	-3.187287
1	4.423474	4.580188	-2.561691
6	-1.695556	6.353273	-2.051171
6	-2.214875	7.687716	-1.519638
6	-2.854055	5.406133	-2.345741
1	-1.170206	6.547004	-3.000148
1	-1.395799	8.391621	-1.329806
1	-2.906728	8.153273	-2.233241
1	-2.757218	7.546598	-0.574701
1	-2.494559	4.442585	-2.729318
1	-3.442647	5.210824	-1.438979
1	-3.532676	5.840607	-3.090688
6	-2.955239	-1.928923	4.015249
6	-3.812364	-1.000520	4.612083
6	-3.523564	-3.033118	3.375251
6	-5.191528	-1.195132	4.602289
1	-3.407784	-0.122687	5.113656
6	-4.898253	-3.232882	3.362329
1	-2.871220	-3.756154	2.888621
6	-5.737614	-2.319876	3.993193
1	-5.839784	-0.469849	5.090479
1	-5.313064	-4.104179	2.858450
1	-6.814027	-2.478658	3.998503

(*E*)-**TS2$_{RR}$**

Number of imaginary frequencies : 1
Imaginary Frequency : -416.8164 cm(-1)

Electronic energy : HF=-5263.8278301
Zero-point correction= 1.978058 (hartree/particle)
Thermal correction to Energy= 2.085009
Thermal correction to Enthalpy= 2.085953
Thermal correction to Gibbs Free Energy= 1.846148
Sum of electronic and zero-point Energies= -5261.849772
Sum of electronic and thermal Energies= -5261.742821
Sum of electronic and thermal Enthalpies= -5261.741877
Sum of electronic and thermal Free Energies= -5261.981682

.....

Cartesian Coordinates

.....

77	1.403548	2.332265	0.065542
6	1.571007	3.882155	-1.612095
6	1.963873	4.500203	-0.364882
6	0.859390	4.464840	0.528451
6	-0.224604	3.754684	-0.117785
6	0.221774	3.432244	-1.453470

7	0.844442	0.358201	-0.516029
1	-0.092214	0.346446	-0.945810
6	3.282043	0.210527	-1.050231
6	1.852296	-0.290431	-1.402860
16	4.571672	2.049801	0.284806
8	4.751955	2.879616	-0.918167
7	3.246718	1.065308	0.158492
6	6.111615	1.066642	0.408219
6	6.971756	0.934088	-0.699939
6	6.469224	0.562318	1.671799
6	8.240453	0.355534	-0.496021
6	7.737826	-0.007448	1.850884
6	8.613028	-0.135941	0.762591
8	4.445952	2.777072	1.555055
6	-7.718914	-2.839895	0.665793
6	-6.444311	-3.671590	0.748612
6	-5.386873	-2.711714	1.372903
6	-5.809345	-1.404302	0.732611
6	-7.164393	-1.474975	0.385485
6	-7.820528	-0.394216	-0.178021
6	-7.083948	0.747648	-0.452756
6	-5.710824	0.834260	-0.186276
6	-5.079655	-0.246342	0.452992
6	-4.026989	-3.343589	1.187856
6	-3.840112	-4.302845	2.183721
6	-4.842626	-4.098469	3.290862
6	-5.514245	-2.765838	2.911305
6	-2.869735	-5.283552	2.023840
6	-2.099432	-5.280860	0.863547
6	-2.160508	-4.240841	-0.078696
6	-3.110197	-3.231748	0.149878
8	-3.130037	-2.109943	-0.648888
15	-2.492428	-0.732481	-0.005072
8	-1.435580	-1.082413	1.003013
8	-3.768274	-0.157570	0.870795
8	-2.172891	0.174918	-1.146488
1	-1.397253	-6.094483	0.693228
1	-2.735181	-6.066566	2.768888
1	-8.879222	-0.449234	-0.425499
1	-7.566568	1.612190	-0.908121
1	-8.412726	-3.182264	-0.111225
1	-8.272713	-2.858760	1.616940
1	-6.113907	-3.934781	-0.266009
1	-6.551058	-4.603755	1.315040
1	-5.574556	-4.918388	3.327896
1	-4.366506	-4.071897	4.280032
1	-4.963487	-1.915148	3.338722
1	-6.554569	-2.691244	3.250940
1	0.740445	-0.207268	0.329731
1	-0.264724	-0.805032	2.237673
6	0.688798	0.711096	3.117974
1	1.084973	1.703149	1.630936
6	3.201345	5.285276	-0.111376
1	3.610028	5.075944	0.882311
1	3.983877	5.056413	-0.835684
1	2.964785	6.358303	-0.168298
6	2.374185	3.902464	-2.863883
1	1.939182	3.254308	-3.630898
1	2.408969	4.922524	-3.273758
1	3.405829	3.585836	-2.676446

6	-0.640549	2.794681	-2.483238
1	-1.287829	2.027966	-2.041281
1	-1.298437	3.551903	-2.935049
1	-0.056600	2.332452	-3.286636
6	-1.605024	3.546902	0.391544
1	-2.281435	4.340795	0.053334
1	-2.024930	2.596204	0.033361
1	-1.632675	3.539874	1.484547
6	0.830788	5.228366	1.810178
1	1.071657	6.281624	1.609998
1	-0.158280	5.208261	2.276748
1	1.570629	4.863152	2.533626
6	-5.068671	2.111177	-0.619229
6	-5.119966	3.230773	0.233319
6	-4.652703	2.259117	-1.957832
6	-4.777669	4.486396	-0.270789
6	-4.311025	3.534926	-2.410787
6	-4.382127	4.662509	-1.596194
1	-4.820676	5.352483	0.392478
1	-4.011359	3.665955	-3.451891
6	-1.261714	-4.217540	-1.268481
6	-1.789695	-4.099856	-2.579496
6	0.138680	-4.349843	-1.113421
6	-0.918567	-4.095581	-3.667785
6	0.964286	-4.326191	-2.240722
6	0.461536	-4.190213	-3.528387
1	-1.332243	-4.001735	-4.674273
1	2.043097	-4.409231	-2.104640
6	1.868748	1.209831	3.874777
1	2.778535	1.151806	3.272990
1	1.737828	2.257521	4.152571
1	2.009426	0.611064	4.787043
6	-0.694979	1.313614	3.367747
1	-1.285051	1.156818	2.450994
7	0.623957	-0.561167	2.713685
6	-1.319527	0.466539	4.475714
6	-2.299182	-0.485084	4.177761
6	-0.873958	0.582007	5.795977
6	-2.821635	-1.291232	5.185307
1	-2.640333	-0.606128	3.147733
6	-1.395305	-0.228136	6.799001
1	-0.108845	1.313886	6.052156
6	-2.373751	-1.168498	6.496173
1	-3.585958	-2.026069	4.940682
1	-1.033343	-0.122857	7.819511
1	-2.783767	-1.804501	7.277462
6	-0.678047	2.783952	3.725737
1	-1.699919	3.180177	3.729416
1	-0.259570	2.969075	4.720923
1	-0.083366	3.338642	3.000522
6	1.322207	-1.702499	3.181525
6	2.673706	-1.735202	3.521617
6	0.536714	-2.852525	3.325628
6	3.223369	-2.908529	4.030733
1	3.304699	-0.867380	3.372325
6	1.095505	-4.013106	3.839985
1	-0.513449	-2.820463	3.030802
6	2.441527	-4.046427	4.200318
1	4.279873	-2.925392	4.292704
1	0.471988	-4.898493	3.947950

1	2.878910	-4.957149	4.602194
6	8.155030	-0.483916	3.216513
1	7.921490	-1.547997	3.375919
1	9.230997	-0.363458	3.374569
1	7.658360	0.075673	4.014050
6	5.506438	0.508849	2.824329
1	5.671950	1.308133	3.558014
1	4.478231	0.602875	2.476461
1	5.605390	-0.453554	3.344813
6	9.928725	-0.844278	0.936297
1	10.752993	-0.146456	1.144050
1	9.898392	-1.561979	1.760355
1	10.204078	-1.409250	0.040637
6	9.208811	0.264807	-1.645588
1	10.245946	0.228471	-1.302074
1	9.036921	-0.632223	-2.259810
1	9.132405	1.128102	-2.313279
6	6.625041	1.305440	-2.118483
1	5.554293	1.354223	-2.302831
1	7.028306	2.290212	-2.389224
1	7.051698	0.570661	-2.809410
6	-5.539061	3.094745	1.685285
6	-6.630642	4.084636	2.078355
6	-4.329053	3.214505	2.609468
1	-5.951107	2.086144	1.821952
1	-7.495643	4.011801	1.407266
1	-6.977849	3.887836	3.100497
1	-6.273571	5.122569	2.051838
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1	-3.872849	4.212733	2.534962
1	-4.615134	3.052666	3.657289
6	-4.025949	6.027475	-2.146369
6	-2.696154	6.536129	-1.591992
6	-5.130169	7.051983	-1.903987
1	-3.906738	5.911201	-3.235287
1	-1.876321	5.834200	-1.795313
1	-2.430876	7.501968	-2.040849
1	-2.751567	6.682694	-0.503966
1	-6.093836	6.705700	-2.295495
1	-5.259748	7.254095	-0.832450
1	-4.888817	8.006532	-2.388404
6	-4.696471	1.102085	-2.942994
6	-3.510040	1.054172	-3.899832
6	-5.996686	1.149274	-3.747795
1	-4.680018	0.167376	-2.363195
1	-2.569005	0.921140	-3.357198
1	-3.627555	0.203540	-4.585752
1	-3.443224	1.954627	-4.526268
1	-6.884558	1.131050	-3.105328
1	-6.042132	2.064340	-4.355075
1	-6.058704	0.291697	-4.430797
6	0.821669	-4.536745	0.228244
6	1.933464	-3.524099	0.441268
6	1.375384	-5.954892	0.366273
1	0.087866	-4.374329	1.026611
1	1.526548	-2.503129	0.445156
1	2.431611	-3.690226	1.403881
1	2.704668	-3.581126	-0.335393
1	0.607674	-6.721878	0.201648
1	2.173608	-6.134933	-0.366329

1	1.804796	-6.110983	1.365079
6	-3.270733	-3.997538	-2.896824
6	-3.749391	-5.197915	-3.711772
6	-3.591562	-2.686296	-3.616382
1	-3.834885	-4.007325	-1.958826
1	-3.549482	-6.142458	-3.191074
1	-4.830433	-5.133032	-3.891407
1	-3.256921	-5.248407	-4.691835
1	-3.171843	-1.827543	-3.076887
1	-3.189637	-2.686736	-4.640416
1	-4.678140	-2.542539	-3.694910
6	1.352935	-4.193900	-4.748912
6	1.593230	-5.628290	-5.218879
6	2.677318	-3.472680	-4.530582
1	0.806892	-3.663632	-5.546111
1	0.649584	-6.145453	-5.431882
1	2.208232	-5.651246	-6.127941
1	2.117797	-6.201815	-4.442164
1	2.524681	-2.471288	-4.107196
1	3.332726	-4.026759	-3.844499
1	3.217839	-3.366299	-5.479471
1	3.640356	0.815734	-1.895867
1	1.810191	-1.368392	-1.186377
6	4.191980	-1.002125	-0.930354
6	4.737799	-1.583632	-2.076063
6	4.450817	-1.592404	0.304785
6	5.548936	-2.712906	-1.982502
1	4.538743	-1.143166	-3.054355
6	5.273415	-2.707782	0.406427
1	3.993625	-1.162400	1.193779
6	5.829557	-3.272233	-0.738466
1	5.971540	-3.148539	-2.886317
1	5.467871	-3.141243	1.387731
1	6.475324	-4.144624	-0.664309
6	1.419687	-0.158900	-2.853362
6	0.220739	-0.792742	-3.210181
6	2.120834	0.527201	-3.846816
6	-0.276984	-0.710107	-4.503961
1	-0.340912	-1.355830	-2.461476
6	1.630417	0.598567	-5.150221
1	3.060418	1.027529	-3.623375
6	0.426681	-0.011278	-5.482044
1	-1.216640	-1.205172	-4.744485
1	2.196751	1.140726	-5.904925
1	0.041523	0.049642	-6.497551

(*E*)-**TS2**$_{SR}$

Number of imaginary frequencies : 1
Imaginary Frequency : -499.3944 cm(-1)

Electronic energy : HF=-5263.8264451
Zero-point correction= 1.977556 (hartree/particle)
Thermal correction to Energy= 2.084958
Thermal correction to Enthalpy= 2.085903
Thermal correction to Gibbs Free Energy= 1.843680
Sum of electronic and zero-point Energies= -5261.848889
Sum of electronic and thermal Energies= -5261.741487
Sum of electronic and thermal Enthalpies= -5261.740542

Sum of electronic and thermal Free Energies= -5261.982765

.....

Cartesian Coordinates

.....

77	-1.174574	-2.064705	-0.456330
6	-1.027187	-3.414432	-2.296585
6	-1.430804	-4.195675	-1.143053
6	-0.391413	-4.116484	-0.169578
6	0.640458	-3.239604	-0.674663
6	0.245425	-2.841518	-2.009874
7	-0.715438	0.003738	-0.669360
1	0.242546	0.093488	-1.040979
6	-3.113730	0.077393	-1.432403
1	-3.328872	-0.368566	-2.414958
6	-1.701050	0.733652	-1.512960
1	-1.780399	1.752498	-1.100516
16	-4.368633	-2.080791	-0.616314
8	-4.420371	-2.611773	-1.990795
7	-3.132675	-0.996509	-0.415395
6	-5.985421	-1.275011	-0.336154
6	-6.789620	-0.873490	-1.421390
6	-6.441492	-1.168940	0.992877
6	-8.089549	-0.402300	-1.153167
6	-7.742016	-0.696750	1.232214
6	-8.547359	-0.272943	0.164987
8	-4.235680	-3.085206	0.444773
6	7.398014	3.017485	1.991712
6	6.028834	3.631962	2.257097
6	5.071961	2.416175	2.453820
6	5.682416	1.444553	1.456241
6	7.026324	1.775574	1.238828
6	7.826480	1.026243	0.392305
6	7.257985	-0.049018	-0.276944
6	5.908869	-0.389989	-0.124219
6	5.127129	0.363558	0.769357
6	3.656963	2.950875	2.378397
6	3.328778	3.523592	3.607016
6	4.282276	3.040378	4.670111
6	5.117225	1.973538	3.934098
6	2.279439	4.428995	3.682356
6	1.581033	4.751768	2.519708
6	1.789314	4.082930	1.302239
6	2.805011	3.105730	1.294488
8	2.976713	2.291171	0.200741
15	2.506364	0.718350	0.342220
8	1.431805	0.569416	1.377679
8	3.826702	0.000869	1.021970
8	2.291479	0.249295	-1.058124
1	0.836781	5.542379	2.564006
1	2.027831	4.919443	4.621444
1	8.870804	1.290388	0.234752
1	7.860343	-0.643438	-0.963299
1	8.067405	3.673836	1.422954
1	7.915990	2.772133	2.931647
1	5.698631	4.185782	1.366285
1	6.006001	4.325751	3.104854
1	4.913316	3.857644	5.048277
1	3.754178	2.632448	5.540858
1	4.640216	0.987478	4.026596
1	6.142179	1.885817	4.315606

1	-0.659467	0.416877	0.261587
1	0.580809	-0.377169	2.832956
6	-1.197117	-1.278696	2.923924
1	-1.186038	-1.618517	1.191739
6	-2.597008	-5.116179	-1.101461
1	-2.986817	-5.232323	-0.086802
1	-3.416307	-4.743931	-1.721513
1	-2.293993	-6.104935	-1.476437
6	-1.753476	-3.351557	-3.594021
1	-1.365877	-2.547503	-4.230185
1	-1.632390	-4.296748	-4.143395
1	-2.824405	-3.186861	-3.437888
6	1.065731	-2.016133	-2.937360
1	1.718961	-1.331959	-2.386940
1	1.710043	-2.673918	-3.540588
1	0.448795	-1.425155	-3.626896
6	1.955485	-2.980814	-0.031068
1	2.385025	-2.028367	-0.361552
1	1.859360	-2.947262	1.060343
1	2.673836	-3.773028	-0.285422
6	-0.324331	-4.902079	1.090998
1	0.146406	-5.877161	0.899893
1	0.275967	-4.396974	1.857935
1	-1.323271	-5.097282	1.498504
6	5.381588	-1.509675	-0.961364
6	5.411425	-2.834378	-0.478366
6	4.969177	-1.250107	-2.283424
6	5.032878	-3.872894	-1.327785
6	4.572133	-2.323585	-3.084090
6	4.592329	-3.637177	-2.628993
1	5.057262	-4.898685	-0.958990
1	4.242614	-2.131982	-4.106176
6	1.037900	4.422331	0.053351
6	1.752313	4.697892	-1.144077
6	-0.378933	4.520026	0.021540
6	1.049804	4.975627	-2.316017
6	-1.026755	4.789185	-1.188140
6	-0.337323	5.000680	-2.376083
1	1.610422	5.185348	-3.229252
1	-2.115439	4.840750	-1.199792
6	-2.004358	-2.509844	3.178069
1	-1.448026	-3.412892	2.922199
1	-2.311358	-2.566943	4.230386
1	-2.907168	-2.484462	2.558915
6	-1.944936	0.048897	2.925922
1	-2.619858	0.035490	2.053594
7	0.103662	-1.203773	3.221682
6	-2.800130	0.172289	4.183865
6	-4.033321	0.821609	4.101467
6	-2.328813	-0.204264	5.444186
6	-4.796927	1.053758	5.240655
1	-4.392723	1.160083	3.128338
6	-3.093362	0.019977	6.584935
1	-1.348171	-0.671163	5.543624
6	-4.333221	0.643542	6.486701
1	-5.758468	1.555821	5.151072
1	-2.712940	-0.289208	7.556045
1	-4.930225	0.818928	7.378584
6	-1.070043	1.302911	2.894008
1	-1.724128	2.173568	2.978324

1	-0.394808	1.334168	3.759546
1	-0.452722	1.411593	1.996159
6	1.018311	-2.174647	3.686659
6	2.363072	-1.950334	3.370356
6	0.667249	-3.242803	4.517743
6	3.339994	-2.803919	3.858758
1	2.624307	-1.110290	2.727995
6	1.657613	-4.103377	4.980369
1	-0.360696	-3.399015	4.826293
6	2.992979	-3.894012	4.653028
1	4.381551	-2.615713	3.605100
1	1.376610	-4.937561	5.618943
1	3.760074	-4.569336	5.025029
6	-1.114537	0.900881	-2.904427
6	0.021460	1.716174	-3.009662
6	-1.603292	0.299962	-4.065832
6	0.653319	1.913038	-4.229977
1	0.431454	2.200495	-2.120502
6	-0.971320	0.499145	-5.293179
1	-2.482851	-0.340270	-4.039151
6	0.159707	1.302088	-5.380552
1	1.533965	2.553035	-4.272624
1	-1.371345	0.017438	-6.183239
1	0.651539	1.455277	-6.338686
6	-4.137082	1.183056	-1.216661
6	-4.685157	1.465019	0.033616
6	-4.509734	1.982890	-2.298770
6	-5.610688	2.489978	0.195977
1	-4.393684	0.850276	0.882571
6	-5.422325	3.022932	-2.139808
1	-4.094934	1.776081	-3.286691
6	-5.984840	3.274414	-0.891424
1	-6.040715	2.674474	1.180290
1	-5.704544	3.627504	-3.000022
1	-6.712022	4.074117	-0.768067
6	-8.278630	-0.665741	2.639767
1	-7.912793	-1.511443	3.229974
1	-7.993440	0.249537	3.181569
1	-9.370173	-0.724471	2.658760
6	-5.577986	-1.472023	2.185853
1	-5.647728	-2.522892	2.493066
1	-4.523561	-1.277893	1.982342
1	-5.867713	-0.853452	3.039392
6	-9.889735	0.352817	0.433791
1	-10.703973	-0.386451	0.436970
1	-9.913991	0.862699	1.401001
1	-10.140457	1.104246	-0.320520
6	-9.001853	-0.046315	-2.297396
1	-10.055254	-0.144958	-2.021804
1	-8.850556	0.986385	-2.646444
1	-8.843551	-0.700596	-3.159733
6	-6.352589	-0.859083	-2.862707
1	-5.273622	-0.817108	-2.986967
1	-6.687340	-1.760507	-3.393351
1	-6.781161	0.008233	-3.374767
6	5.885235	-3.145156	0.930111
6	7.403838	-3.325007	0.961405
6	5.227507	-4.377587	1.542456
1	5.627170	-2.277574	1.559532
1	7.932619	-2.430088	0.616191

1	7.752046	-3.550921	1.977833
1	7.697361	-4.161395	0.311854
1	4.132709	-4.341328	1.482855
1	5.564781	-5.301725	1.054551
1	5.506247	-4.465406	2.600710
6	4.140085	-4.776479	-3.515151
6	2.950889	-5.520311	-2.909489
6	5.282532	-5.743595	-3.813633
1	3.810296	-4.334807	-4.469343
1	2.110918	-4.842620	-2.704428
1	2.594319	-6.307571	-3.586060
1	3.226749	-6.001248	-1.960951
1	6.135419	-5.228373	-4.270912
1	5.640114	-6.225693	-2.893913
1	4.957449	-6.537803	-4.497693
6	5.038430	0.141356	-2.887683
6	3.861823	0.487018	-3.792982
6	6.346421	0.310216	-3.662839
1	5.038057	0.867790	-2.061461
1	2.916433	0.417530	-3.247029
1	3.972383	1.517217	-4.159143
1	3.812588	-0.156983	-4.682319
1	7.227103	0.113446	-3.040858
1	6.382475	-0.381430	-4.516442
1	6.432872	1.332111	-4.056086
6	-1.259137	4.450661	1.258226
6	-2.521728	3.622157	1.060754
6	-1.656961	5.864780	1.692089
1	-0.685421	3.987705	2.070493
1	-2.294306	2.595113	0.748895
1	-3.096909	3.565106	1.996802
1	-3.197431	4.049133	0.309163
1	-0.793456	6.532686	1.795998
1	-2.323184	6.319935	0.946784
1	-2.192152	5.845669	2.650453
6	3.266404	4.774272	-1.247742
6	3.721224	6.200434	-1.555572
6	3.809266	3.790929	-2.285558
1	3.705685	4.515167	-0.280445
1	3.367719	6.907233	-0.794691
1	4.817506	6.254596	-1.583396
1	3.350429	6.547341	-2.529247
1	3.358891	2.798537	-2.160837
1	3.608330	4.139331	-3.309222
1	4.899053	3.684983	-2.188975
6	-1.040981	5.323553	-3.674713
6	-1.354624	6.817920	-3.741531
6	-2.303781	4.500868	-3.898685
1	-0.336287	5.088493	-4.488607
1	-0.447552	7.424300	-3.629359
1	-1.826972	7.082314	-4.696421
1	-2.044701	7.100890	-2.934752
1	-2.106164	3.424276	-3.809208
1	-3.086057	4.760366	-3.172661
1	-2.713777	4.691337	-4.898470

PRC

Number of imaginary frequencies : 0

Electronic energy : HF=-5052.879778
Zero-point correction= 1.887712 (hartree/particle)
Thermal correction to Energy= 1.991861
Thermal correction to Enthalpy= 1.992806
Thermal correction to Gibbs Free Energy= 1.754837
Sum of electronic and zero-point Energies= -5050.992066
Sum of electronic and thermal Energies= -5050.887917
Sum of electronic and thermal Enthalpies= -5050.886972
Sum of electronic and thermal Free Energies= -5051.124941

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Cartesian Coordinates

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77	-1.365941	-2.267255	0.213173
6	-0.969681	-4.277669	-0.487283
6	-1.507393	-4.422197	0.831369
6	-0.616006	-3.734945	1.725948
6	0.477702	-3.175014	0.977558
6	0.266675	-3.513642	-0.398988
7	-0.743047	-0.335053	-0.421108
1	0.264908	-0.296033	-0.654432
6	-3.061434	-0.249099	-1.287456
6	-1.578046	0.072613	-1.586421
16	-4.479341	-2.318200	-0.322647
8	-4.426485	-3.123264	-1.551520
7	-3.113823	-1.334845	-0.262633
6	-5.925041	-1.239954	-0.347211
6	-6.740369	-1.135406	-1.491487
6	-6.232412	-0.573583	0.857453
6	-7.909621	-0.358211	-1.398635
6	-7.399653	0.202080	0.913437
6	-8.199944	0.356091	-0.228087
8	-4.530070	-3.065917	0.932135
6	8.074827	2.792513	-0.639673
6	6.857428	3.699759	-0.500802
6	5.959167	2.985613	0.548983
6	6.197819	1.541526	0.161302
6	7.468646	1.437395	-0.422621
6	8.019634	0.208935	-0.742534
6	7.256485	-0.926010	-0.518531
6	5.946682	-0.855073	-0.029216
6	5.410971	0.397849	0.322088
6	4.617899	3.676999	0.565933
6	4.733736	4.833142	1.343002
6	5.973394	4.771001	2.194783
6	6.465671	3.332834	1.969419
6	3.794391	5.844161	1.225174
6	2.719070	5.655026	0.363449
6	2.481550	4.437364	-0.289629
6	3.455682	3.430811	-0.151978
8	3.284737	2.210414	-0.764705
15	2.777555	0.917146	0.120793
8	1.837709	1.342875	1.204356
8	4.169172	0.483734	0.906860
8	2.371434	-0.125751	-0.878105
1	0.107839	7.099963	0.124913
1	3.897454	6.775626	1.779602
1	9.017987	0.137584	-1.170942
1	7.655865	-1.910511	-0.760118
1	8.573525	2.877652	-1.612830

1	8.833556	3.018683	0.124970
1	6.308190	3.730990	-1.452881
1	7.096673	4.731961	-0.221829
1	6.723185	5.509722	1.875372
1	5.757639	4.985849	3.248688
1	5.987977	2.650224	2.685991
1	7.551857	3.219471	2.071277
1	-0.870999	0.313266	0.376981
1	0.242901	1.278930	1.845576
8	-0.708167	1.143915	2.079906
6	-0.817998	0.184948	3.116044
1	-0.783253	-0.830685	2.663595
6	-2.653574	-5.287277	1.212513
1	-3.156762	-4.925969	2.112741
1	-3.404756	-5.327401	0.419507
1	-2.292843	-6.308291	1.402243
6	-1.551000	-4.873869	-1.715857
1	-1.066169	-4.492074	-2.619459
1	-1.416168	-5.964156	-1.692423
1	-2.624639	-4.662381	-1.780104
6	1.157487	-3.181442	-1.533960
1	1.784787	-2.313506	-1.303852
1	1.818491	-4.034318	-1.742422
1	0.588066	-2.964169	-2.445366
6	1.619901	-2.415194	1.546094
1	2.126540	-1.810919	0.783353
1	1.293569	-1.740369	2.347086
1	2.360689	-3.105331	1.968677
6	-0.737433	-3.716254	3.202611
1	-0.279818	-2.826995	3.646860
1	-1.777923	-3.785403	3.533775
1	-0.205416	-4.591908	3.602752
6	5.220547	-2.152035	0.046732
6	5.091765	-2.823950	1.277153
6	4.852511	-2.792547	-1.153589
6	4.600876	-4.130013	1.286925
6	4.367234	-4.099997	-1.089940
6	4.234705	-4.788949	0.113298
1	4.521902	-4.657198	2.240297
1	4.104544	-4.611817	-2.018935
6	1.231277	4.220096	-1.069861
6	1.282028	3.808847	-2.421330
6	-0.033870	4.442178	-0.463931
6	0.090459	3.580513	-3.116979
6	-1.187068	4.177480	-1.197820
6	-1.155500	3.745780	-2.522903
1	0.144818	3.272915	-4.161743
1	-2.162124	4.326689	-0.728833
6	0.335150	0.319414	4.089374
1	1.289578	0.199185	3.560443
1	0.338117	1.314920	4.548692
1	0.286000	-0.433338	4.886680
6	-2.225151	0.312992	3.726190
1	-2.890943	0.402613	2.852733
6	-2.630290	-0.960393	4.460869
1	-1.914808	-1.242848	5.244904
1	-3.609997	-0.838840	4.937600
1	-2.706152	-1.799862	3.757776
6	-2.434242	1.551747	4.566324
6	-2.034951	1.620857	5.905971

6	-3.079959	2.661273	4.020298
6	-2.256372	2.767762	6.661248
1	-1.546429	0.766388	6.372473
6	-3.307163	3.811153	4.769964
1	-3.412823	2.611029	2.984599
6	-2.890936	3.870164	6.095513
1	-1.934287	2.798655	7.700215
1	-3.809545	4.662254	4.312028
1	-3.065737	4.766140	6.687174
6	-5.355769	-0.600239	2.080769
1	-5.722006	-1.327852	2.817588
1	-4.321857	-0.865300	1.860549
1	-5.346684	0.384933	2.563154
6	-7.792366	0.868710	2.203291
1	-7.300121	1.843179	2.338356
1	-8.870950	1.039513	2.258860
1	-7.525498	0.256689	3.070038
6	-9.334100	1.342995	-0.210275
1	-9.505744	1.775138	-1.200800
1	-10.283100	0.895235	0.118311
1	-9.119221	2.178055	0.463769
6	-8.847695	-0.268881	-2.573324
1	-8.541379	0.504340	-3.295075
1	-8.904132	-1.214406	-3.120920
1	-9.867249	-0.029962	-2.259148
6	-6.403591	-1.717759	-2.839719
1	-6.836454	-1.107320	-3.637010
1	-5.330910	-1.777986	-3.017586
1	-6.789421	-2.738437	-2.958373
6	5.574139	-2.197100	2.572472
6	6.839673	-2.901101	3.059632
6	4.509772	-2.171621	3.664161
1	5.841159	-1.154170	2.361882
1	7.623054	-2.884053	2.291447
1	7.237709	-2.414972	3.959606
1	6.641070	-3.952405	3.308990
1	3.626838	-1.601618	3.349277
1	4.184996	-3.182357	3.948235
1	4.906329	-1.693920	4.568963
6	5.043370	-2.142273	-2.514775
6	3.750880	-2.006671	-3.314087
6	6.097291	-2.895463	-3.325897
1	5.415042	-1.122908	-2.352195
1	3.027070	-1.378969	-2.780906
1	3.967146	-1.530637	-4.280626
1	3.289554	-2.981131	-3.531034
1	7.050187	-2.973396	-2.787370
1	5.765623	-3.916611	-3.558826
1	6.289473	-2.386464	-4.279140
6	3.728436	-6.214873	0.138956
6	2.370442	-6.318053	0.830045
6	4.732070	-7.165060	0.786054
1	3.592759	-6.528776	-0.908499
1	1.621133	-5.694246	0.325672
1	2.005893	-7.353447	0.830224
1	2.431214	-5.987956	1.877077
1	5.712948	-7.104613	0.300554
1	4.873424	-6.930962	1.849506
1	4.383971	-8.203789	0.723029
6	-0.210972	5.061905	0.912226

6	-1.256334	4.381119	1.785142
6	-0.585382	6.540424	0.764543
1	0.741283	4.994666	1.449999
1	-1.084569	3.304178	1.878137
1	-1.226942	4.813024	2.793799
1	-2.273251	4.538610	1.398384
1	2.011580	6.466880	0.219794
1	-1.581437	6.636163	0.309841
1	-0.618757	7.033981	1.744766
6	2.578638	3.712278	-3.209763
6	2.627624	4.805094	-4.277822
6	2.797018	2.336423	-3.835132
1	3.415455	3.899392	-2.528213
1	2.497734	5.800983	-3.836085
1	3.591864	4.790521	-4.802543
1	1.839908	4.670117	-5.031023
1	2.780460	1.545036	-3.074717
1	2.033264	2.115768	-4.594496
1	3.772276	2.297761	-4.338545
6	-2.466514	3.555116	-3.252076
6	-2.395350	2.635068	-4.461034
6	-3.059362	4.906666	-3.649218
1	-3.156946	3.100767	-2.527295
1	-1.968941	1.652910	-4.214596
1	-3.401039	2.472897	-4.870504
1	-1.787482	3.067980	-5.267496
1	-3.182117	5.564153	-2.779777
1	-2.406734	5.420618	-4.368821
1	-4.045169	4.778003	-4.116620
1	-1.469875	1.163016	-1.707737
1	-3.489903	-0.636102	-2.224605
6	-1.024386	-0.578276	-2.837767
6	-1.615939	-1.668598	-3.480824
6	0.163166	-0.053238	-3.357845
6	-1.033293	-2.215109	-4.623297
1	-2.530895	-2.117111	-3.093272
6	0.742573	-0.598328	-4.497159
1	0.640753	0.791481	-2.857298
6	0.145880	-1.683089	-5.134269
1	-1.510113	-3.061933	-5.113669
1	1.667621	-0.174271	-4.883561
1	0.596592	-2.108129	-6.028565
6	-3.869636	0.992166	-0.958490
6	-3.611573	1.784956	0.161628
6	-4.881239	1.383643	-1.839599
6	-4.380936	2.922015	0.402401
1	-2.795166	1.527677	0.841896
6	-5.652824	2.515415	-1.597005
1	-5.074250	0.782000	-2.728663
6	-5.405339	3.288069	-0.467444
1	-4.173039	3.538763	1.275839
1	-6.447806	2.788837	-2.289435
1	-6.004052	4.173318	-0.263745

TS1$_{SS}$

Number of imaginary frequencies : 1
Imaginary frequency : -396.0837 cm(-1)

Electronic energy : HF=-5052.8389141
Zero-point correction= 1.883477 (hartree/particle)
Thermal correction to Energy= 1.986145
Thermal correction to Enthalpy= 1.987089
Thermal correction to Gibbs Free Energy= 1.755547
Sum of electronic and zero-point Energies= -5050.955437
Sum of electronic and thermal Energies= -5050.852769
Sum of electronic and thermal Enthalpies= -5050.851825
Sum of electronic and thermal Free Energies= -5051.083367

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Cartesian Coordinates

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77	-1.366212	-2.142101	0.589055
6	-1.324029	-4.181880	-0.442661
6	-1.828147	-4.333732	0.906095
6	-0.819842	-3.907841	1.817630
6	0.312057	-3.429852	1.050333
6	-0.016528	-3.612432	-0.344788
7	-0.790426	-0.381087	-0.467530
1	0.171344	-0.440263	-0.821537
6	-3.187735	-0.251418	-1.128805
6	-1.719478	-0.013286	-1.567233
16	-4.567490	-2.016014	0.210628
8	-4.546627	-3.060944	-0.832475
7	-3.238743	-1.049125	0.121622
6	-6.057245	-1.005289	-0.088504
6	-6.825507	-1.161297	-1.259676
6	-6.474076	-0.155494	0.954739
6	-8.067404	-0.501358	-1.337020
6	-7.695383	0.525069	0.832671
6	-8.475849	0.375479	-0.322526
8	-4.680865	-2.507110	1.587369
6	8.262672	2.653607	-0.588884
6	7.064098	3.585291	-0.455555
6	6.150055	2.894682	0.598512
6	6.362823	1.444358	0.217137
6	7.621664	1.312957	-0.388527
6	8.121450	0.076038	-0.755237
6	7.316703	-1.038581	-0.576197
6	6.017524	-0.939499	-0.065249
6	5.559766	0.314523	0.362599
6	4.815846	3.602267	0.589514
6	4.941817	4.774417	1.341252
6	6.172269	4.711262	2.206255
6	6.647671	3.261486	2.016148
6	4.012045	5.791421	1.197782
6	2.934395	5.596971	0.340443
6	2.678459	4.366591	-0.282295
6	3.647197	3.364188	-0.117244
8	3.430236	2.106216	-0.672650
15	2.964968	0.876207	0.263743
8	2.178929	1.467250	1.476645
8	4.327526	0.412719	1.001924
8	2.289923	-0.156690	-0.557358
1	0.347801	7.079429	0.262501
1	4.123282	6.732914	1.732928
1	9.111931	-0.016071	-1.197265
1	7.674414	-2.025492	-0.865501
1	8.772595	2.734858	-1.555981

1	9.017108	2.856127	0.186224
1	6.518089	3.623042	-1.409079
1	7.322629	4.613549	-0.180847
1	6.935048	5.433738	1.882096
1	5.946888	4.949010	3.252914
1	6.157027	2.600673	2.743982
1	7.731456	3.137767	2.127906
1	-0.769392	0.376611	0.233243
1	1.179626	1.289351	1.550557
8	-0.374611	1.102542	1.840466
6	-0.742030	0.250817	2.712625
1	-1.185789	-1.053845	1.907200
6	-3.087627	-5.036312	1.268758
1	-3.512112	-4.657808	2.202395
1	-3.849961	-4.907318	0.496135
1	-2.880807	-6.110544	1.385812
6	-1.983555	-4.734317	-1.655413
1	-1.461848	-4.438290	-2.570462
1	-1.975174	-5.833292	-1.609693
1	-3.027788	-4.410442	-1.718284
6	0.902554	-3.298303	-1.468318
1	1.520357	-2.421996	-1.237339
1	1.591867	-4.138951	-1.632109
1	0.366341	-3.111356	-2.406126
6	1.642617	-3.031718	1.580255
1	2.095639	-2.219043	0.994168
1	1.576363	-2.714000	2.625230
1	2.340493	-3.877096	1.540672
6	-0.892488	-4.057110	3.296559
1	-0.217219	-3.370029	3.816640
1	-1.907702	-3.885111	3.670661
1	-0.604531	-5.078734	3.582282
6	5.231598	-2.205536	-0.066862
6	5.218865	-3.029628	1.072782
6	4.723323	-2.674347	-1.294470
6	4.728191	-4.330513	0.958120
6	4.248788	-3.985208	-1.357539
6	4.252185	-4.833658	-0.252544
1	4.728735	-4.975857	1.839161
1	3.886204	-4.373383	-2.311287
6	1.413717	4.147730	-1.039956
6	1.432173	3.698581	-2.380572
6	0.163998	4.422697	-0.422055
6	0.224897	3.514667	-3.062046
6	-1.004705	4.207707	-1.146868
6	-1.006855	3.760201	-2.466577
1	0.257292	3.183166	-4.100056
1	-1.966700	4.402805	-0.670679
6	0.347167	-0.381380	3.539585
1	1.179674	-0.679760	2.895206
1	0.735978	0.381041	4.229286
1	0.008593	-1.239870	4.125961
6	-2.140693	0.424482	3.317154
1	-2.799716	0.516072	2.443955
6	-2.630799	-0.752070	4.151617
1	-2.032424	-0.895484	5.060748
1	-3.663652	-0.569678	4.470690
1	-2.623308	-1.678635	3.564623
6	-2.254217	1.719344	4.100848
6	-1.465404	1.985409	5.223441

6	-3.222296	2.658541	3.737726
6	-1.625029	3.164034	5.944986
1	-0.724070	1.258518	5.552168
6	-3.395168	3.832424	4.464062
1	-3.847104	2.461325	2.866515
6	-2.591470	4.093059	5.568985
1	-0.995494	3.354327	6.811811
1	-4.156636	4.547880	4.157968
1	-2.718708	5.012087	6.136845
6	-5.650092	0.091758	2.186581
1	-5.998014	-0.517941	3.031333
1	-4.599627	-0.148081	2.030740
1	-5.718441	1.143971	2.485919
6	-8.171196	1.402019	1.959415
1	-7.761416	2.421128	1.888826
1	-9.260784	1.489420	1.979285
1	-7.871875	1.005610	2.933989
6	-9.731584	1.187182	-0.490069
1	-9.940884	1.398545	-1.542672
1	-10.616634	0.679332	-0.079624
1	-9.653289	2.155037	0.013836
6	-8.972277	-0.741771	-2.517637
1	-8.768354	-0.057510	-3.355368
1	-8.872371	-1.759945	-2.904891
1	-10.024661	-0.613982	-2.248228
6	-6.387806	-1.926318	-2.482457
1	-6.786813	-1.452953	-3.385303
1	-5.305020	-1.975316	-2.582680
1	-6.738302	-2.966290	-2.469660
6	5.766152	-2.544446	2.401648
6	6.903762	-3.430907	2.900366
6	4.665469	-2.415105	3.450931
1	6.180034	-1.539473	2.244532
1	7.701326	-3.515584	2.151417
1	7.342976	-3.019518	3.817980
1	6.555307	-4.446413	3.130618
1	3.888196	-1.715431	3.116429
1	4.192987	-3.384477	3.662074
1	5.074990	-2.035313	4.395786
6	4.769307	-1.830366	-2.558660
6	3.444855	-1.781854	-3.314655
6	5.878661	-2.317440	-3.491058
1	5.000692	-0.795119	-2.264770
1	2.646362	-1.357604	-2.696127
1	3.555546	-1.148103	-4.205199
1	3.125897	-2.772566	-3.669026
1	6.860739	-2.310749	-3.004344
1	5.682464	-3.344339	-3.828683
1	5.941388	-1.681655	-4.383445
6	3.752144	-6.257907	-0.373219
6	2.453437	-6.479916	0.401056
6	4.808534	-7.269576	0.062709
1	3.536848	-6.433617	-1.439388
1	1.660285	-5.793542	0.075338
1	2.088158	-7.505034	0.259097
1	2.602801	-6.332338	1.479923
1	5.749955	-7.130476	-0.481358
1	5.027247	-7.177859	1.134702
1	4.461519	-8.295492	-0.112923
6	0.014136	5.013488	0.970793

6	-1.028916	4.308384	1.830117
6	-0.349656	6.498384	0.877976
1	0.972908	4.921588	1.494613
1	-0.879826	3.224269	1.853595
1	-0.975427	4.682858	2.860777
1	-2.048584	4.507013	1.472337
1	2.232170	6.410207	0.181292
1	-1.344652	6.618315	0.427310
1	-0.382087	6.952788	1.876751
6	2.710466	3.489765	-3.175978
6	2.815913	4.511606	-4.307724
6	2.831376	2.066938	-3.719905
1	3.567462	3.666146	-2.516644
1	2.754777	5.538191	-3.926276
1	3.772094	4.402999	-4.835899
1	2.014759	4.383205	-5.047337
1	2.721448	1.320976	-2.922593
1	2.071646	1.868656	-4.489911
1	3.813373	1.918316	-4.189086
6	-2.330713	3.631091	-3.185964
6	-2.300252	2.763640	-4.433892
6	-2.887002	5.014662	-3.524880
1	-3.026656	3.164793	-2.473458
1	-1.899890	1.759987	-4.238178
1	-3.317245	2.644557	-4.829187
1	-1.695008	3.217029	-5.231436
1	-2.980505	5.647314	-2.633781
1	-2.227601	5.533039	-4.235293
1	-3.881004	4.931594	-3.984387
1	-1.587200	1.067377	-1.743454
1	-3.675489	-0.792818	-1.954285
6	-1.280719	-0.709709	-2.837513
6	-1.911767	-1.829292	-3.377557
6	-0.144825	-0.204048	-3.482552
6	-1.429067	-2.419315	-4.544986
1	-2.776719	-2.266027	-2.880602
6	0.338678	-0.792535	-4.644474
1	0.358004	0.673641	-3.066864
6	-0.305426	-1.904714	-5.181921
1	-1.937107	-3.291585	-4.952614
1	1.220944	-0.381318	-5.131710
1	0.065869	-2.364011	-6.095397
6	-3.925094	1.071717	-1.010523
6	-3.645663	1.974198	0.017561
6	-4.888719	1.416229	-1.959827
6	-4.349754	3.171913	0.115496
1	-2.861536	1.741599	0.741584
6	-5.590883	2.614866	-1.868662
1	-5.096036	0.730037	-2.781746
6	-5.330085	3.493590	-0.821870
1	-4.128600	3.862765	0.929650
1	-6.346518	2.857491	-2.613735

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i1(*S*)

Number of imaginary frequencies : 0

Electronic energy : HF=-5052.8500173
Zero-point correction= 1.886961 (hartree/particle)

Thermal correction to Energy= 1.990128
Thermal correction to Enthalpy= 1.991072
Thermal correction to Gibbs Free Energy= 1.757679
Sum of electronic and zero-point Energies= -5050.963056
Sum of electronic and thermal Energies= -5050.859889
Sum of electronic and thermal Enthalpies= -5050.858945
Sum of electronic and thermal Free Energies= -5051.092338

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Cartesian Coordinates

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77	-1.575111	-2.256568	0.577941
6	-1.301749	-4.387961	-0.439291
6	-1.868524	-4.447683	0.900581
6	-0.903759	-3.924085	1.818746
6	0.196886	-3.402381	1.049165
6	-0.055503	-3.742668	-0.348158
7	-0.966558	-0.411831	-0.378779
1	0.027380	-0.437603	-0.635199
6	-3.291382	-0.345323	-1.254251
6	-1.794822	-0.120023	-1.582988
16	-4.750077	-2.195844	-0.112458
8	-4.786642	-3.096375	-1.283792
7	-3.415170	-1.261688	-0.104453
6	-6.146740	-1.038329	-0.200555
6	-6.965885	-0.932224	-1.340006
6	-6.361461	-0.239281	0.942645
6	-8.030659	-0.010257	-1.314409
6	-7.413201	0.689809	0.929091
6	-8.206290	0.844067	-0.218017
8	-4.873004	-2.867105	1.184454
6	8.347295	2.615546	-0.743611
6	7.155108	3.560332	-0.639954
6	6.246951	2.921845	0.450928
6	6.449495	1.454312	0.132427
6	7.702029	1.288057	-0.477151
6	8.190183	0.031644	-0.791653
6	7.381294	-1.070264	-0.556158
6	6.087241	-0.940464	-0.039265
6	5.644730	0.335453	0.333008
6	4.913794	3.632817	0.429706
6	5.042405	4.828577	1.143327
6	6.289523	4.801878	1.985842
6	6.761537	3.345674	1.847001
6	4.094100	5.828049	0.997244
6	2.996148	5.597529	0.174225
6	2.746120	4.350231	-0.415331
6	3.734225	3.367337	-0.246915
8	3.516153	2.090935	-0.759687
15	3.054829	0.902316	0.223553
8	2.298284	1.562090	1.434067
8	4.415343	0.466969	0.971684
8	2.330343	-0.142994	-0.530753
1	0.384761	7.017019	0.111429
1	4.205076	6.783844	1.506510
1	9.175743	-0.086321	-1.238573
1	7.730352	-2.070772	-0.806917
1	8.847430	2.651106	-1.718469
1	9.110933	2.848376	0.013819
1	6.601058	3.562390	-1.589549
1	7.422750	4.597209	-0.409352

1	7.045221	5.509870	1.616104
1	6.085277	5.083445	3.025915
1	6.278948	2.715464	2.606740
1	7.846288	3.224509	1.950711
1	-1.056066	0.351881	0.296341
1	1.347740	1.304583	1.560694
8	-0.249797	1.051351	2.096659
6	-0.556738	0.535713	3.171436
1	-1.870097	-1.321876	1.839540
6	-3.091074	-5.221661	1.249212
1	-3.499083	-4.925388	2.219215
1	-3.885315	-5.065811	0.514005
1	-2.853020	-6.295559	1.285630
6	-1.951751	-4.982975	-1.638809
1	-1.392060	-4.758039	-2.552107
1	-2.000506	-6.077404	-1.542898
1	-2.981056	-4.618718	-1.758367
6	0.891227	-3.429462	-1.449773
1	1.406930	-2.478565	-1.263952
1	1.673523	-4.200172	-1.510850
1	0.395048	-3.366791	-2.425157
6	1.477754	-2.862169	1.586162
1	1.885897	-2.065021	0.950042
1	1.343272	-2.451574	2.593847
1	2.243623	-3.647117	1.649880
6	-1.001186	-3.996749	3.303811
1	-0.423750	-3.204398	3.793933
1	-2.040211	-3.911285	3.641345
1	-0.609555	-4.957468	3.667638
6	5.278169	-2.190444	0.020811
6	5.201199	-2.932428	1.212948
6	4.792640	-2.730305	-1.186540
6	4.683406	-4.226399	1.169635
6	4.294739	-4.034169	-1.179368
6	4.243903	-4.805462	-0.020453
1	4.639732	-4.807236	2.093283
1	3.946506	-4.474612	-2.115553
6	1.473506	4.086935	-1.146222
6	1.483922	3.599984	-2.474401
6	0.225878	4.344555	-0.517190
6	0.272752	3.373113	-3.135159
6	-0.947279	4.081922	-1.219161
6	-0.955648	3.606506	-2.528775
1	0.298693	3.015041	-4.164604
1	-1.909690	4.264191	-0.737501
6	0.470490	-0.136675	4.016898
1	1.472254	0.016331	3.606715
1	0.429604	0.213722	5.054413
1	0.246199	-1.211583	4.043935
6	-1.996147	0.608739	3.654837
1	-2.605025	0.512052	2.743857
6	-2.400299	-0.505366	4.613486
1	-1.826124	-0.481451	5.547841
1	-3.458641	-0.389352	4.872876
1	-2.278195	-1.490490	4.145893
6	-2.271099	1.981518	4.244834
6	-1.566566	2.466719	5.350054
6	-3.286961	2.770160	3.702123
6	-1.867454	3.712371	5.891731
1	-0.778048	1.867794	5.804423

6	-3.595143	4.012788	4.246154
1	-3.842315	2.399027	2.840712
6	-2.882935	4.489693	5.341813
1	-1.307426	4.075038	6.750887
1	-4.394517	4.608752	3.809133
1	-3.119326	5.461527	5.769040
6	-5.495416	-0.289744	2.175445
1	-5.954204	-0.917771	2.951552
1	-4.502664	-0.698462	1.984582
1	-5.378173	0.715068	2.598411
6	-7.678346	1.537451	2.144441
1	-7.022507	2.422738	2.184114
1	-8.710118	1.898229	2.173940
1	-7.514427	0.978981	3.071155
6	-9.203786	1.968416	-0.289329
1	-9.372713	2.292939	-1.320342
1	-10.183498	1.698156	0.131039
1	-8.847575	2.846804	0.258551
6	-8.975906	0.079729	-2.483699
1	-8.603570	0.750253	-3.274565
1	-9.143886	-0.897658	-2.945547
1	-9.958287	0.452618	-2.180830
6	-6.738737	-1.689033	-2.624186
1	-7.107121	-1.115123	-3.479449
1	-5.687789	-1.917681	-2.796463
1	-7.259740	-2.655759	-2.626526
6	5.702113	-2.374868	2.530322
6	6.836823	-3.219542	3.103313
6	4.564379	-2.218791	3.535199
1	6.107762	-1.371935	2.342324
1	7.662101	-3.313660	2.386136
1	7.234993	-2.767410	4.020584
1	6.499184	-4.233379	3.355798
1	3.780514	-1.563513	3.133759
1	4.106466	-3.186910	3.780902
1	4.930428	-1.778271	4.471557
6	4.859530	-1.960080	-2.495481
6	3.526256	-1.913391	-3.236859
6	5.945271	-2.526888	-3.409476
1	5.123388	-0.917605	-2.261280
1	2.739398	-1.460773	-2.621724
1	3.635875	-1.308683	-4.147605
1	3.188344	-2.910190	-3.554465
1	6.932222	-2.515634	-2.932385
1	5.722080	-3.566498	-3.685423
1	6.013417	-1.945294	-4.337703
6	3.728272	-6.228143	-0.056771
6	2.424580	-6.386733	0.723984
6	4.775283	-7.216908	0.449666
1	3.517352	-6.468339	-1.111133
1	1.633309	-5.731366	0.337240
1	2.060946	-7.420564	0.665117
1	2.566652	-6.148789	1.787619
1	5.719768	-7.121652	-0.098804
1	4.990752	-7.053713	1.514102
1	4.420753	-8.249633	0.341884
6	0.077609	4.963001	0.863992
6	-0.964989	4.269107	1.734319
6	-0.302592	6.441925	0.742935
1	1.039177	4.889785	1.386972

1	-0.804567	3.188116	1.793264
1	-0.936895	4.677247	2.753046
1	-1.980625	4.438489	1.352867
1	2.277359	6.396326	0.015868
1	-1.300874	6.540927	0.294781
1	-0.334589	6.917437	1.731802
6	2.755081	3.389309	-3.280423
6	2.836865	4.391855	-4.431152
6	2.882146	1.957602	-3.800511
1	3.618780	3.585748	-2.635920
1	2.781195	5.424785	-4.066150
1	3.782989	4.275816	-4.975559
1	2.021730	4.249246	-5.152626
1	2.755153	1.222646	-2.995271
1	2.138330	1.749544	-4.582891
1	3.872254	1.800182	-4.249107
6	-2.285856	3.444776	-3.227390
6	-2.278696	2.496016	-4.414993
6	-2.832386	4.809806	-3.646472
1	-2.978638	3.035772	-2.478984
1	-1.906990	1.497099	-4.150271
1	-3.298534	2.378398	-4.803524
1	-1.662117	2.877497	-5.240750
1	-2.904521	5.497116	-2.794445
1	-2.180009	5.275267	-4.398708
1	-3.835238	4.707111	-4.082062
1	-1.655187	0.946700	-1.825945
1	-3.741402	-0.780456	-2.162296
6	-1.271823	-0.893712	-2.772875
6	-1.891947	-2.030245	-3.293021
6	-0.113333	-0.413170	-3.395274
6	-1.369982	-2.661946	-4.420559
1	-2.785660	-2.437447	-2.819462
6	0.404598	-1.041689	-4.521185
1	0.372896	0.483416	-2.999634
6	-0.224724	-2.171057	-5.038853
1	-1.868425	-3.545437	-4.815847
1	1.298126	-0.644324	-4.999151
1	0.172979	-2.661204	-5.924925
6	-3.989562	0.993978	-1.060862
6	-3.704383	1.835038	0.017593
6	-4.909685	1.432325	-2.015695
6	-4.335435	3.070645	0.140947
1	-2.982291	1.519572	0.774266
6	-5.554827	2.659979	-1.889323
1	-5.126297	0.797129	-2.875655
6	-5.267567	3.487053	-0.808159
1	-4.097612	3.715786	0.987040
1	-6.281152	2.969286	-2.639870
1	-5.763306	4.450054	-0.703625
1	-5.880423	4.428563	-0.739813

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i2(*S*)

Number of imaginary frequencies : 0

Electronic energy : HF=-5263.8574822
Zero-point correction= 1.980448 (hartree/particle)

Thermal correction to Energy= 2.087805
Thermal correction to Enthalpy= 2.088749
Thermal correction to Gibbs Free Energy= 1.848170
Sum of electronic and zero-point Energies= -5261.877034
Sum of electronic and thermal Energies= -5261.769677
Sum of electronic and thermal Enthalpies= -5261.768733
Sum of electronic and thermal Free Energies= -5262.009312

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Cartesian Coordinates

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77	-1.407550	-2.038146	1.087160
6	-1.479802	-4.346846	0.713707
6	-1.687702	-3.994780	2.114035
6	-0.503574	-3.346393	2.588963
6	0.391530	-3.180007	1.470330
6	-0.219771	-3.848284	0.324643
7	-0.981814	-0.693725	-0.513515
1	-0.099277	-0.959306	-0.970743
6	-3.382095	-1.277541	-0.979799
6	-2.093593	-0.598316	-1.507935
16	-4.602372	-1.817361	1.310677
8	-4.954049	-3.152406	0.786409
7	-3.347734	-1.151073	0.488696
6	-6.048786	-0.712852	1.141353
6	-7.233190	-1.121159	0.499884
6	-5.957542	0.534671	1.793728
6	-8.348923	-0.259894	0.542401
6	-7.075278	1.382755	1.798863
6	-8.252737	1.006102	1.134513
8	-4.295892	-1.763261	2.744174
6	7.133737	2.839989	-1.922971
6	5.837765	3.612848	-1.693456
6	5.147666	2.871828	-0.512437
6	5.522725	1.441005	-0.848445
6	6.712945	1.439117	-1.586977
6	7.322565	0.253054	-1.958326
6	6.698731	-0.941652	-1.626251
6	5.468266	-0.984144	-0.957192
6	4.888595	0.233714	-0.554935
6	3.731183	3.384883	-0.388796
6	3.738036	4.567367	0.355781
6	5.057039	4.728007	1.063968
6	5.739415	3.372951	0.824010
6	2.641761	5.417649	0.314309
6	1.550184	5.072630	-0.481262
6	1.470215	3.844607	-1.150635
6	2.570466	2.977771	-1.031606
8	2.513470	1.717180	-1.579829
15	2.239254	0.476241	-0.531749
8	1.366436	0.963495	0.602660
8	3.715367	0.256743	0.172339
8	1.846272	-0.694670	-1.360589
1	0.723788	5.773573	-0.581127
1	2.650752	6.365484	0.852160
1	8.252949	0.256179	-2.523603
1	7.149601	-1.889427	-1.918598
1	7.518564	2.929571	-2.945782
1	7.932330	3.191882	-1.252245
1	5.192427	3.520864	-2.579992
1	5.981866	4.681123	-1.493645

1	5.638736	5.558939	0.638416
1	4.932732	4.950805	2.132203
1	5.451550	2.664587	1.610473
1	6.834668	3.428845	0.808598
1	-0.770924	0.221234	-0.111322
1	1.858759	1.258135	2.101472
6	1.112151	1.493868	3.981291
1	-1.361028	-0.700953	1.971516
6	-2.822860	-4.485787	2.942965
1	-3.760830	-4.465549	2.378828
1	-2.633368	-5.520092	3.267499
1	-2.971454	-3.865418	3.831192
6	-2.456278	-5.113166	-0.109876
1	-2.182860	-5.105529	-1.171409
1	-2.497384	-6.164605	0.210088
1	-3.465969	-4.696148	-0.006083
6	0.412188	-3.931143	-1.021633
1	0.969631	-3.015601	-1.257044
1	1.140590	-4.754237	-1.058828
1	-0.324089	-4.098196	-1.816649
6	1.785550	-2.657379	1.520578
1	2.091398	-2.229603	0.557442
1	1.885727	-1.868525	2.279633
1	2.502667	-3.456009	1.763672
6	-0.218379	-2.963414	4.000322
1	0.245312	-3.797653	4.545882
1	0.474820	-2.113640	4.049716
1	-1.135125	-2.684257	4.532141
6	4.866026	-2.338514	-0.764828
6	5.104927	-3.054432	0.426170
6	4.210391	-2.966897	-1.842895
6	4.690399	-4.381699	0.518065
6	3.804086	-4.295237	-1.695007
6	4.032577	-5.021273	-0.530634
1	4.887818	-4.936609	1.436013
1	3.300792	-4.791696	-2.526346
6	0.317682	3.518647	-2.042530
6	0.544990	3.331513	-3.427747
6	-1.006398	3.469713	-1.551293
6	-0.544042	3.107087	-4.269873
6	-2.060308	3.235234	-2.439401
6	-1.857136	3.065801	-3.807259
1	-0.367529	2.971310	-5.339335
1	-3.077597	3.202649	-2.046310
6	1.311269	1.488627	5.449075
1	2.357131	1.442699	5.751452
1	0.835579	2.369078	5.896956
1	0.789528	0.611304	5.853397
6	-0.277143	1.685158	3.445695
1	-0.266504	1.399962	2.381619
7	2.093708	1.396315	3.136072
6	-0.510158	3.197788	3.540968
6	-1.558596	3.737442	4.289932
6	0.354879	4.072738	2.872458
6	-1.735824	5.116369	4.371446
1	-2.260592	3.084294	4.802704
6	0.180681	5.449473	2.961512
1	1.161846	3.678034	2.250390
6	-0.861246	5.977656	3.718219
1	-2.564281	5.515410	4.952292

1	0.858596	6.108111	2.422272
1	-0.997464	7.054281	3.787618
6	-1.313769	0.847596	4.178352
1	-1.068889	-0.217496	4.114098
1	-1.410555	1.124185	5.234575
1	-2.292119	0.964147	3.700528
6	3.477635	1.533917	3.479391
6	4.373485	0.521195	3.158419
6	3.904073	2.709461	4.096483
6	5.713546	0.678827	3.499186
1	4.019079	-0.365244	2.634807
6	5.244013	2.851926	4.436791
1	3.183943	3.503171	4.293322
6	6.146971	1.833351	4.145097
1	6.425735	-0.106523	3.253134
1	5.582769	3.763827	4.922454
1	7.195728	1.945037	4.408681
6	-7.017341	2.691151	2.543528
1	-6.416950	2.610805	3.454897
1	-6.575477	3.499433	1.941188
1	-8.010505	3.026794	2.854961
6	-4.699867	1.031219	2.458357
1	-4.724838	0.839075	3.539943
1	-3.802174	0.552076	2.062876
1	-4.594367	2.113513	2.316569
6	-9.401733	1.973446	1.031142
1	-10.116857	1.872625	1.860850
1	-9.056142	3.011257	1.028536
1	-9.963479	1.830490	0.103351
6	-9.662666	-0.710337	-0.041005
1	-10.508546	-0.186471	0.412603
1	-9.720371	-0.544130	-1.127292
1	-9.832659	-1.778091	0.127706
6	-7.385813	-2.409307	-0.265009
1	-6.451100	-2.735532	-0.713903
1	-7.721501	-3.228933	0.384817
1	-8.120395	-2.293392	-1.066756
6	5.872720	-2.429197	1.574863
6	7.367512	-2.723158	1.445095
6	5.381718	-2.871861	2.949933
1	5.742416	-1.338919	1.497474
1	7.774440	-2.347318	0.499007
1	7.933635	-2.259607	2.264892
1	7.548353	-3.806152	1.482281
1	4.297166	-2.749643	3.064348
1	5.618228	-3.925808	3.145296
1	5.874220	-2.291008	3.740775
6	3.607329	-6.469382	-0.419100
6	2.678850	-6.709216	0.768826
6	4.819970	-7.394724	-0.343888
1	3.050746	-6.716238	-1.337421
1	1.782231	-6.077357	0.722366
1	2.350394	-7.755833	0.800535
1	3.185600	-6.496515	1.719913
1	5.488810	-7.250701	-1.200637
1	5.402481	-7.205012	0.567717
1	4.511032	-8.447619	-0.325440
6	4.022361	-2.291418	-3.190468
6	2.639426	-2.494068	-3.801816
6	5.088187	-2.785835	-4.171522

1	4.157818	-1.209044	-3.053191
1	1.853478	-2.090897	-3.156373
1	2.587155	-1.962657	-4.761694
1	2.423184	-3.551028	-4.013347
1	6.106363	-2.620116	-3.800535
1	4.975030	-3.863406	-4.355327
1	4.994276	-2.272839	-5.137449
6	-1.340455	3.731479	-0.095544
6	-2.299947	2.715446	0.511229
6	-1.945074	5.125022	0.085977
1	-0.406287	3.683493	0.478888
1	-1.979163	1.674763	0.374225
1	-2.395189	2.895416	1.590958
1	-3.308479	2.809934	0.086066
1	-1.305318	5.920488	-0.313904
1	-2.909837	5.195831	-0.435057
1	-2.120869	5.332066	1.150553
6	1.919749	3.437528	-4.065546
6	1.981473	4.610261	-5.042763
6	2.344575	2.138632	-4.746810
1	2.652561	3.644557	-3.277328
1	1.702663	5.552143	-4.554222
1	2.996410	4.724266	-5.445210
1	1.304812	4.463791	-5.894613
1	2.297855	1.288867	-4.053331
1	1.710664	1.918799	-5.617514
1	3.377504	2.218610	-5.111379
6	-3.000219	2.837438	-4.774991
6	-4.238761	3.657729	-4.433718
6	-3.362938	1.355229	-4.871282
1	-2.642370	3.161018	-5.765702
1	-4.007073	4.722863	-4.311888
1	-4.991200	3.559789	-5.226143
1	-4.706692	3.301155	-3.506655
1	-2.516499	0.747852	-5.214338
1	-3.676174	0.967519	-3.891487
1	-4.197179	1.206497	-5.569496
1	-3.375905	-2.348096	-1.249071
1	-2.321385	0.474395	-1.617992
6	-4.565733	-0.633657	-1.680436
6	-5.272001	-1.322386	-2.665326
6	-4.945043	0.679867	-1.387126
6	-6.329916	-0.719147	-3.343749
1	-4.994416	-2.350286	-2.899653
6	-6.011057	1.279871	-2.044446
1	-4.407685	1.218500	-0.608530
6	-6.705253	0.582509	-3.032564
1	-6.864905	-1.274152	-4.111800
1	-6.307810	2.293643	-1.777541
1	-7.536177	1.053929	-3.553765
6	-1.595322	-1.080889	-2.853719
6	-0.635412	-0.289860	-3.497853
6	-1.999234	-2.264008	-3.472757
6	-0.117599	-0.657286	-4.731866
1	-0.292871	0.632718	-3.023779
6	-1.477498	-2.637283	-4.710720
1	-2.730863	-2.912391	-2.996572
6	-0.542349	-1.832179	-5.348314
1	0.621713	-0.019412	-5.212547
1	-1.812620	-3.561991	-5.176123

1	-0.137071	-2.121550	-6.315909

---

product

Number of imaginary frequencies : 0

Electronic energy : HF=-5263.889633
Zero-point correction= 1.981739 (hartree/particle)
Thermal correction to Energy= 2.090172
Thermal correction to Enthalpy= 2.091116
Thermal correction to Gibbs Free Energy= 1.843907
Sum of electronic and zero-point Energies= -5261.907894
Sum of electronic and thermal Energies= -5261.799461
Sum of electronic and thermal Enthalpies= -5261.798517
Sum of electronic and thermal Free Energies= -5262.045726

.....

Cartesian Coordinates

.....

77	2.082983	2.055951	-0.210724
6	2.107833	4.089517	-0.977480
6	2.375790	4.178965	0.418826
6	1.239155	3.603893	1.112873
6	0.244069	3.228870	0.157834
6	0.789852	3.476914	-1.146452
7	1.244263	0.124702	-0.590332
1	0.300311	0.207980	-1.012388
6	3.601781	-0.430796	-0.997709
6	2.159828	-0.635804	-1.492010
16	5.273597	1.610290	-0.696226
8	5.673814	1.464159	-2.098476
7	3.733499	0.959440	-0.504023
6	6.374082	0.650843	0.370696
6	7.310604	-0.248411	-0.174501
6	6.306296	0.909958	1.755798
6	8.251556	-0.830788	0.696170
6	7.248312	0.303257	2.599200
6	8.195933	-0.589252	2.075823
8	5.242273	2.972623	-0.170535
6	-7.700215	-2.046757	-1.088854
6	-6.562080	-3.034660	-0.866645
6	-5.591148	-2.295573	0.101838
6	-5.707368	-0.883912	-0.450236
6	-6.967114	-0.739321	-1.053052
6	-7.392401	0.470974	-1.571039
6	-6.519900	1.548355	-1.525930
6	-5.227708	1.427941	-1.005466
6	-4.820217	0.196214	-0.463074
6	-4.316459	-3.102109	0.180062
6	-4.521992	-4.173297	1.056677
6	-5.764492	-3.936102	1.876295
6	-6.100042	-2.472674	1.552608
6	-3.665851	-5.265166	1.039389
6	-2.608111	-5.270480	0.133257
6	-2.305399	-4.156725	-0.661382
6	-3.154726	-3.041503	-0.574728
8	-2.856243	-1.904757	-1.288596
15	-2.230575	-0.598731	-0.506982
8	-1.414723	-0.990319	0.690399
8	-3.583935	0.099807	0.127537

8	-1.621678	0.253393	-1.579201
1	-1.971642	-6.151368	0.053847
1	-3.832893	-6.117126	1.696581
1	-8.378533	0.568069	-2.022073
1	-6.822001	2.515469	-1.926673
1	-8.235513	-2.201177	-2.033397
1	-8.448531	-2.111728	-0.284443
1	-6.033968	-3.204489	-1.816017
1	-6.882780	-4.010195	-0.485759
1	-6.577216	-4.614113	1.576894
1	-5.605425	-4.108555	2.948182
1	-5.516465	-1.813659	2.212189
1	-7.162277	-2.225697	1.671458
1	1.082657	-0.395007	0.279122
1	-1.637468	0.114151	2.397164
6	-0.149211	0.270834	3.783082
1	0.500071	0.658860	2.971168
6	3.496042	4.890259	1.087739
1	4.323403	5.082262	0.403181
1	3.127725	5.851404	1.473293
1	3.892645	4.323106	1.935955
6	2.989377	4.544054	-2.082086
1	2.769916	4.003099	-3.009224
1	2.831761	5.613971	-2.275611
1	4.043765	4.385346	-1.832924
6	0.118249	3.199368	-2.440739
1	-0.700148	2.485103	-2.302194
1	-0.303319	4.124569	-2.860353
1	0.816034	2.778980	-3.177656
6	-1.097500	2.690200	0.478048
1	-1.562376	2.197281	-0.380506
1	-1.076026	1.976552	1.311489
1	-1.745149	3.523614	0.773928
6	1.109917	3.512764	2.589079
1	1.003976	4.520297	3.014985
1	0.227521	2.931809	2.878749
1	1.998679	3.057934	3.046325
6	-4.373576	2.646430	-1.090875
6	-4.303400	3.524078	0.009446
6	-3.807382	3.006985	-2.328637
6	-3.705146	4.770985	-0.162151
6	-3.187106	4.254976	-2.438923
6	-3.137780	5.155484	-1.378151
1	-3.671497	5.459357	0.683681
1	-2.751956	4.550830	-3.395952
6	-1.154415	-4.171576	-1.605321
6	-1.373456	-3.991978	-2.991509
6	0.158978	-4.401603	-1.138073
6	-0.282573	-4.018360	-3.857445
6	1.218954	-4.410263	-2.051324
6	1.022136	-4.215339	-3.416449
1	-0.453195	-3.883490	-4.927605
1	2.229516	-4.582937	-1.676297
6	0.266583	1.016780	5.042606
1	-0.121612	2.041845	5.042076
1	-0.072138	0.518248	5.957528
1	1.360311	1.074700	5.094638
6	0.159438	-1.251189	3.829559
1	0.110178	-1.571205	2.778306
7	-1.506541	0.547249	3.316307

6	-0.903904	-2.032873	4.560243
6	-0.913471	-2.180035	5.949854
6	-1.961347	-2.579302	3.826373
6	-1.964889	-2.827525	6.592102
1	-0.091801	-1.783506	6.545675
6	-3.013254	-3.222662	4.466465
1	-1.968332	-2.462254	2.739904
6	-3.024049	-3.343274	5.852644
1	-1.957320	-2.925913	7.676011
1	-3.828102	-3.630502	3.870537
1	-3.850245	-3.842750	6.354458
6	1.571579	-1.517238	4.329478
1	2.298826	-0.902182	3.779520
1	1.693278	-1.291727	5.395603
1	1.844867	-2.569555	4.183325
6	-2.696513	0.549264	4.046211
6	-3.881071	0.263777	3.336826
6	-2.828847	0.892210	5.401764
6	-5.125408	0.343518	3.942156
1	-3.802600	-0.025299	2.288238
6	-4.083248	0.941845	6.003932
1	-1.961209	1.125584	6.006248
6	-5.246168	0.682094	5.289327
1	-6.013339	0.135626	3.343403
1	-4.141742	1.203803	7.059445
1	-6.220952	0.736837	5.768075
6	7.238949	0.610579	4.072131
1	6.872738	1.620679	4.275258
1	6.598185	-0.084094	4.636312
1	8.241571	0.547810	4.504507
6	5.235400	1.746797	2.405985
1	5.614557	2.738411	2.688359
1	4.367486	1.905325	1.767297
1	4.886137	1.256039	3.324163
6	9.122943	-1.325343	3.003136
1	10.075397	-0.795042	3.147419
1	8.678405	-1.465618	3.992112
1	9.363616	-2.322529	2.623510
6	9.327285	-1.724762	0.140268
1	10.217376	-1.725938	0.774991
1	8.992084	-2.768814	0.047211
1	9.652168	-1.401701	-0.852996
6	7.346810	-0.682945	-1.615740
1	6.381486	-0.605777	-2.112176
1	8.044992	-0.077957	-2.209279
1	7.673281	-1.724828	-1.683528
6	-4.913025	3.145159	1.347275
6	-6.339203	3.681837	1.458274
6	-4.090430	3.590397	2.551752
1	-4.964685	2.047845	1.389874
1	-6.968726	3.332691	0.630313
1	-6.801949	3.354101	2.398806
1	-6.342874	4.780883	1.443377
1	-3.070073	3.186052	2.523903
1	-4.029197	4.684528	2.631812
1	-4.555975	3.222842	3.475127
6	-2.473677	6.505924	-1.536790
6	-1.199816	6.604611	-0.698363
6	-3.423256	7.652421	-1.200839
1	-2.185502	6.603854	-2.595945

1	-0.472767	5.830851	-0.980164
1	-0.718349	7.582891	-0.826512
1	-1.419626	6.480492	0.371453
1	-4.345742	7.596199	-1.790172
1	-3.705882	7.637134	-0.139845
1	-2.950666	8.622755	-1.399152
6	-3.930300	2.119996	-3.558098
6	-2.604691	1.839472	-4.261347
6	-4.931909	2.721155	-4.544890
1	-4.323134	1.147331	-3.230683
1	-1.910215	1.310814	-3.598572
1	-2.786405	1.200101	-5.136445
1	-2.124818	2.756646	-4.632211
1	-5.907346	2.907888	-4.079333
1	-4.567336	3.678202	-4.943200
1	-5.088531	2.046818	-5.396540
6	0.478517	-4.591282	0.334136
6	1.122352	-3.333806	0.901456
6	1.343345	-5.819069	0.600089
1	-0.459587	-4.728366	0.879712
1	0.444706	-2.478419	0.764899
1	1.322839	-3.453302	1.975452
1	2.079412	-3.124920	0.407362
1	0.902143	-6.728862	0.172851
1	2.353710	-5.710940	0.183481
1	1.458540	-5.972812	1.680539
6	-2.749311	-3.820049	-3.610226
6	-3.088548	-5.000722	-4.518786
6	-2.879273	-2.497426	-4.364454
1	-3.494020	-3.815485	-2.806690
1	-3.027911	-5.952632	-3.977004
1	-4.107153	-4.901518	-4.915651
1	-2.406216	-5.061853	-5.377022
1	-2.624446	-1.644591	-3.722543
1	-2.230930	-2.478231	-5.252559
1	-3.910332	-2.357045	-4.715586
6	2.149012	-4.283724	-4.423271
6	2.485791	-5.741276	-4.734735
6	3.399046	-3.526974	-3.994226
1	1.776892	-3.815605	-5.348642
1	1.604041	-6.287790	-5.090401
1	3.266631	-5.814342	-5.502640
1	2.851053	-6.252687	-3.833436
1	3.170397	-2.481013	-3.745745
1	3.868721	-3.998719	-3.119876
1	4.143939	-3.526986	-4.799431
1	4.246602	-0.560490	-1.881410
1	1.907638	-1.706795	-1.413010
6	4.039409	-1.469367	0.016513
6	4.624724	-2.649370	-0.447343
6	3.887413	-1.290802	1.390121
6	5.044110	-3.636397	0.437942
1	4.763950	-2.785020	-1.520591
6	4.326911	-2.266380	2.280719
1	3.451089	-0.364289	1.765532
6	4.901228	-3.442909	1.809690
1	5.496050	-4.550092	0.056862
1	4.221486	-2.104938	3.352413
1	5.243643	-4.202183	2.509053
6	1.890412	-0.212464	-2.920865

6	0.708917	-0.676959	-3.508931
6	2.741845	0.606646	-3.667577
6	0.377294	-0.320331	-4.810409
1	0.037595	-1.322131	-2.939227
6	2.407820	0.959444	-4.974008
1	3.677356	0.975408	-3.248687
6	1.224597	0.503669	-5.546384
1	-0.548460	-0.691097	-5.246957
1	3.083642	1.592693	-5.545436
1	0.967752	0.780168	-6.566801

TS1$_{RS}$

Number of imaginary frequencies : 1
Imaginary frequency : -676.9615 cm(-1)

Electronic energy : HF=-5052.828668
Zero-point correction= 1.880467 (hartree/particle)
Thermal correction to Energy= 1.983572
Thermal correction to Enthalpy= 1.984516
Thermal correction to Gibbs Free Energy= 1.750496
Sum of electronic and zero-point Energies= -5050.948201
Sum of electronic and thermal Energies= -5050.845096
Sum of electronic and thermal Enthalpies= -5050.844152
Sum of electronic and thermal Free Energies= -5051.078172

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Cartesian Coordinates

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77	-1.364111	-1.904695	-0.015467
6	-1.326370	-3.689524	-1.396734
6	-1.680929	-4.094574	-0.047210
6	-0.557830	-3.792850	0.793732
6	0.444117	-3.133040	0.014793
6	-0.032996	-3.087939	-1.354687
7	-0.613315	0.085200	-0.462672
1	0.360372	0.015096	-0.791234
6	-2.925132	0.527406	-1.242801
6	-1.429833	0.829809	-1.461218
16	-4.415702	-1.574314	-1.455699
8	-4.369433	-1.530763	-2.928385
7	-3.118031	-0.850243	-0.774030
6	-5.877174	-0.628969	-0.927924
6	-6.551591	0.254424	-1.793540
6	-6.324346	-0.852099	0.389090
6	-7.729941	0.873284	-1.330686
6	-7.506378	-0.230467	0.819891
6	-8.186970	0.659097	-0.023720
8	-4.564215	-2.918086	-0.890181
6	8.061399	2.409325	1.248621
6	6.829640	3.267150	1.515092
6	5.754579	2.265761	2.031903
6	6.090678	1.055690	1.182243
6	7.441901	1.113801	0.815871
6	8.047910	0.076184	0.128430
6	7.273216	-1.017204	-0.227715
6	5.904182	-1.085367	0.058560
6	5.314304	-0.031749	0.778513
6	4.425201	2.986312	2.042968
6	4.365691	3.777111	3.193463
6	5.402314	3.326743	4.189242

6	5.957929	2.043566	3.548960
6	3.462080	4.825483	3.261966
6	2.606852	5.043761	2.185849
6	2.520695	4.166368	1.094724
6	3.437715	3.097563	1.075121
8	3.375919	2.157552	0.069242
15	2.761572	0.678232	0.387799
8	1.681335	0.808640	1.445384
8	3.986912	-0.093417	1.159063
8	2.434631	0.065467	-0.929848
1	1.960133	5.914929	2.202238
1	3.435418	5.488101	4.125536
1	9.102753	0.123121	-0.136415
1	7.722825	-1.856381	-0.756949
1	8.729800	2.831536	0.488733
1	8.663883	2.276994	2.160183
1	6.468744	3.699628	0.570727
1	7.002291	4.093320	2.213470
1	6.187840	4.084000	4.326807
1	4.967875	3.151194	5.181221
1	5.362765	1.173043	3.858787
1	7.004726	1.843456	3.807899
1	-0.547223	0.635812	0.391765
1	1.069529	-0.168487	2.290096
8	0.543258	-0.854859	2.892673
6	-0.689894	-0.538336	3.092554
1	-1.558625	-1.201132	1.587977
6	-2.843360	-4.926696	0.375067
1	-2.525556	-5.966828	0.538557
1	-3.278032	-4.555665	1.311732
1	-3.640551	-4.911345	-0.368919
6	-2.112837	-3.958556	-2.629211
1	-1.945756	-3.192346	-3.393404
1	-1.802118	-4.924978	-3.051985
1	-3.186360	-3.993894	-2.426521
6	0.750554	-2.559168	-2.501110
1	1.352906	-1.695587	-2.196935
1	1.452729	-3.327476	-2.859726
1	0.112473	-2.257076	-3.339152
6	1.803901	-2.790125	0.500946
1	2.377471	-2.216112	-0.232179
1	1.765397	-2.215164	1.431335
1	2.363178	-3.711284	0.710053
6	-0.383104	-4.237338	2.198832
1	0.060090	-5.244320	2.201799
1	0.298465	-3.581120	2.752128
1	-1.339601	-4.303821	2.729674
6	5.192139	-2.304799	-0.423440
6	5.151716	-3.454715	0.394435
6	4.742346	-2.368342	-1.756304
6	4.613163	-4.627891	-0.128330
6	4.200005	-3.568491	-2.228220
6	4.117164	-4.705819	-1.430510
1	4.578092	-5.524961	0.493075
1	3.865933	-3.613723	-3.264191
6	1.510436	4.376768	0.014829
6	1.903657	4.410861	-1.348996
6	0.143790	4.594077	0.328275
6	0.940904	4.605216	-2.339866
6	-0.773118	4.791054	-0.708008

6	-0.407206	4.794865	-2.048405
1	1.264826	4.627149	-3.381712
1	-1.821062	4.958766	-0.456454
6	-1.081632	0.883111	2.911492
1	-2.143430	1.008450	2.694565
1	-0.856508	1.397726	3.859656
1	-0.462665	1.373301	2.154739
6	-2.851723	-1.325428	4.326975
6	-3.503816	-0.160108	4.747247
6	-3.594538	-2.506846	4.260568
6	-4.853412	-0.182814	5.087264
1	-2.956998	0.776601	4.840102
6	-4.938955	-2.537792	4.617063
1	-3.100429	-3.425621	3.944829
6	-5.572591	-1.373935	5.037723
1	-5.339272	0.733747	5.416992
1	-5.490749	-3.473924	4.563706
1	-6.622126	-1.391769	5.323101
6	-1.355802	-1.409469	4.131627
1	-1.109329	-2.439552	3.852109
6	-0.643024	-1.128069	5.472427
1	-1.048459	-1.796930	6.238409
1	0.434298	-1.300323	5.391721
1	-0.808019	-0.097968	5.810872
6	-5.562452	-1.659969	1.404916
1	-6.016108	-2.648811	1.563316
1	-4.521636	-1.836180	1.134806
1	-5.572555	-1.140295	2.369812
6	-8.032168	-0.504884	2.203079
1	-9.123774	-0.440567	2.242066
1	-7.759685	-1.506517	2.548993
1	-7.636873	0.208829	2.943692
6	-9.376474	1.421395	0.493828
1	-10.326039	0.904733	0.290513
1	-9.319204	1.574738	1.575227
1	-9.447222	2.414441	0.040094
6	-8.509856	1.774201	-2.251406
1	-9.567918	1.813775	-1.978475
1	-8.130493	2.807550	-2.237198
1	-8.467692	1.433167	-3.289935
6	-6.092910	0.633652	-3.178263
1	-5.037211	0.444488	-3.357755
1	-6.632945	0.063994	-3.947272
1	-6.290297	1.695058	-3.361734
6	5.681124	-3.430013	1.817851
6	6.355191	-4.731943	2.237800
6	4.577390	-3.069139	2.813242
1	6.441412	-2.637992	1.872381
1	7.107478	-5.059188	1.510236
1	6.854587	-4.600343	3.205596
1	5.631212	-5.548030	2.363435
1	4.981455	-3.009496	3.832484
1	4.111511	-2.105915	2.574108
1	3.790451	-3.837755	2.813454
6	4.962224	-1.218488	-2.726394
6	3.783471	-0.918493	-3.644806
6	6.209651	-1.498834	-3.568178
1	5.143340	-0.309159	-2.135381
1	2.912973	-0.588458	-3.071464
1	4.059375	-0.108765	-4.334308

1	3.498844	-1.779388	-4.266424
1	7.096524	-1.678199	-2.949291
1	6.059560	-2.387737	-4.196785
1	6.428110	-0.653297	-4.233056
6	3.496915	-6.006352	-1.899962
6	3.420196	-6.152738	-3.412391
6	2.105721	-6.185391	-1.287717
1	4.132680	-6.819273	-1.512566
1	4.394818	-6.002236	-3.891541
1	3.063221	-7.154400	-3.679991
1	2.714014	-5.433590	-3.849903
1	2.132694	-6.137355	-0.191399
1	1.424094	-5.397068	-1.640171
1	1.673447	-7.153068	-1.573177
6	3.349922	4.344997	-1.814835
6	3.779950	5.687613	-2.405563
6	3.588104	3.210760	-2.810860
1	3.995980	4.162655	-0.949961
1	3.648781	6.502185	-1.682396
1	4.838501	5.659875	-2.695080
1	3.199034	5.942033	-3.302019
1	3.239308	2.249294	-2.412269
1	3.077942	3.401162	-3.766202
1	4.659489	3.114668	-3.031291
6	-0.404876	4.694045	1.742561
6	-1.730032	3.957792	1.920346
6	-0.630842	6.156827	2.139626
1	0.324984	4.249536	2.432235
1	-1.738622	2.983773	1.420795
1	-1.945931	3.803394	2.986356
1	-2.570961	4.529274	1.510627
1	0.259605	6.785059	2.029178
1	-1.411567	6.600484	1.507298
1	-0.969456	6.228045	3.181618
6	-1.429920	5.081274	-3.125556
6	-1.452461	4.030050	-4.230454
6	-1.208550	6.473318	-3.715350
1	-2.418651	5.079027	-2.636434
1	-1.624747	3.018622	-3.838714
1	-2.244589	4.253320	-4.956243
1	-0.502926	4.005599	-4.781935
1	-1.222519	7.245699	-2.937104
1	-0.237280	6.532989	-4.224883
1	-1.985049	6.716014	-4.451957
1	-1.275981	1.907439	-1.273383
6	-0.884883	0.561025	-2.847325
6	0.353965	1.131271	-3.163322
6	-1.553187	-0.182506	-3.820847
6	0.913426	0.963542	-4.423179
1	0.882414	1.723666	-2.412570
6	-0.992657	-0.344047	-5.087553
1	-2.510462	-0.651875	-3.598076
6	0.239113	0.224947	-5.392902
1	1.876500	1.419867	-4.646407
1	-1.528477	-0.923200	-5.837334
1	0.671405	0.099292	-6.383545
1	-3.379689	0.657679	-2.237754
6	-3.610737	1.562551	-0.363530
6	-3.989936	1.289120	0.948139
6	-3.961124	2.796698	-0.918588

6	-4.715041	2.220353	1.688291
1	-3.753922	0.312056	1.365864
6	-4.693790	3.726370	-0.188767
1	-3.685778	3.009413	-1.954440
6	-5.079928	3.436364	1.119276
1	-5.013809	1.974978	2.707886
1	-4.976541	4.673289	-0.646428
1	-5.666053	4.155120	1.688303

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i1'(*R*)

Number of imaginary frequencies : 0

Electronic energy : HF=-2930.6630097
Zero-point correction= 1.152856 (hartree/particle)
Thermal correction to Energy= 1.215557
Thermal correction to Enthalpy= 1.216502
Thermal correction to Gibbs Free Energy= 1.059316
Sum of electronic and zero-point Energies= -2929.510153
Sum of electronic and thermal Energies= -2929.447452
Sum of electronic and thermal Enthalpies= -2929.446508
Sum of electronic and thermal Free Energies= -2929.603694

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Cartesian Coordinates

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6	0.168251	5.978725	1.069655
6	1.426794	5.255536	0.578653
6	0.909238	4.260714	-0.492366
6	-0.416212	3.867756	0.128938
6	-0.890259	4.922305	0.917637
6	-2.170380	4.886284	1.448700
6	-2.972414	3.777256	1.200594
6	-2.501428	2.661970	0.497812
6	-1.196430	2.728266	-0.011499
6	1.986279	3.278673	-0.894872
6	2.743050	3.807031	-1.945097
6	2.103660	5.065410	-2.462492
6	0.703098	4.999753	-1.841403
6	3.893222	3.161707	-2.374651
6	4.264726	1.964975	-1.768678
6	3.480639	1.358487	-0.779915
6	2.332521	2.046722	-0.364232
8	1.515152	1.496666	0.618904
15	0.274958	0.600902	0.115105
8	0.597958	-0.555057	-0.738796
8	-0.679030	1.626080	-0.684447
8	-0.427769	0.335515	1.499483
6	3.865035	0.033853	-0.216293
1	5.173688	1.456408	-2.085395
1	4.496641	3.578958	-3.178961
1	-2.546352	5.713692	2.047995
1	-3.993332	3.750496	1.576631
6	-3.406495	1.494325	0.290623
1	0.255226	6.337777	2.101998
1	-0.056420	6.859452	0.449683
1	1.869867	4.677154	1.402358
1	2.199658	5.928303	0.188376
1	2.650393	5.957868	-2.123453
1	2.084718	5.107409	-3.557869

1	0.044707	4.386861	-2.473862
1	0.228228	5.979770	-1.714477
6	-3.879111	0.755468	1.399864
6	-4.840825	-0.233410	1.195912
6	-5.337530	-0.540145	-0.069186
6	-4.832814	0.173978	-1.149748
6	-3.879775	1.183935	-1.001008
1	-5.201583	-0.062255	-2.149518
6	4.215491	-0.084078	1.146025
6	4.598202	-1.329564	1.645644
6	4.650166	-2.464067	0.840068
6	4.316339	-2.321254	-0.502802
6	3.908989	-1.104939	-1.050260
1	4.868931	-1.412493	2.698616
1	-5.202321	-0.796023	2.058001
1	4.346596	-3.208009	-1.138959
6	-1.107995	-3.038890	-0.633614
1	-0.518835	-2.683531	-1.492284
6	-0.188866	-2.902083	0.562399
6	1.158624	-3.551653	0.480560
1	1.434342	-3.828474	-0.542088
1	1.909175	-2.868401	0.896149
1	1.150369	-4.460642	1.096345
6	-2.365955	-2.200701	-0.500886
1	-3.010672	-2.336500	-1.377397
1	-2.940486	-2.473276	0.392584
1	-2.129879	-1.132766	-0.425341
6	-1.404298	-4.510749	-0.841358
6	-0.963884	-5.179366	-1.983943
6	-2.121339	-5.223909	0.124230
6	-1.246418	-6.529331	-2.169129
1	-0.397712	-4.629556	-2.736582
6	-2.402618	-6.573520	-0.057820
1	-2.458524	-4.712813	1.026832
6	-1.967655	-7.228924	-1.206689
1	-0.902314	-7.035728	-3.068475
1	-2.961449	-7.116393	0.701510
1	-2.189557	-8.284070	-1.350568
1	-0.568140	-0.628909	1.655881
6	-3.422572	1.916212	-2.249313
6	-4.582337	2.660190	-2.907697
6	-2.745575	0.967981	-3.236923
1	-2.680549	2.670675	-1.959671
1	-5.055867	3.358421	-2.206326
1	-4.232534	3.235693	-3.774272
1	-5.356710	1.967732	-3.263524
1	-1.892807	0.452681	-2.778100
1	-3.444017	0.205483	-3.607996
1	-2.374816	1.522604	-4.108663
6	-6.395678	-1.603517	-0.265298
6	-7.723229	-1.168575	0.352952
6	-5.971274	-2.963495	0.283582
1	-6.548499	-1.711775	-1.350618
1	-8.055374	-0.202799	-0.046174
1	-8.509672	-1.908034	0.155306
1	-7.634619	-1.063951	1.442681
1	-5.049341	-3.327139	-0.187304
1	-5.797918	-2.919864	1.367352
1	-6.755042	-3.711423	0.109064
6	-3.356699	0.965162	2.810304

6	-2.950757	-0.356176	3.466208
6	-4.377879	1.675278	3.698391
1	-2.458211	1.593190	2.747701
1	-2.373985	-0.998661	2.790473
1	-2.343651	-0.166655	4.360042
1	-3.827817	-0.932491	3.790194
1	-4.644911	2.668270	3.318472
1	-5.305512	1.091347	3.771821
1	-3.984169	1.800883	4.715358
6	3.518718	-1.077322	-2.518099
6	2.490570	-2.152035	-2.866664
6	4.745300	-1.213917	-3.419405
1	3.047625	-0.109020	-2.727844
1	1.625694	-2.079083	-2.198849
1	2.141137	-2.018854	-3.898649
1	2.911745	-3.164540	-2.798056
1	5.492381	-0.434011	-3.227113
1	5.239491	-2.183171	-3.267053
1	4.458618	-1.152918	-4.477180
6	5.072376	-3.814087	1.375686
6	4.486210	-4.126183	2.747594
6	6.595929	-3.922258	1.404791
1	4.691867	-4.568997	0.667895
1	3.397403	-3.992648	2.765345
1	4.707269	-5.162196	3.032475
1	4.913559	-3.481544	3.526634
1	7.029079	-3.754918	0.411212
1	7.020704	-3.169743	2.083324
1	6.917714	-4.910947	1.756273
6	4.269082	1.113064	2.078135
6	5.721355	1.507868	2.343465
6	3.516887	0.882070	3.384913
1	3.791016	1.965442	1.580715
1	6.253058	1.722379	1.407445
1	5.774247	2.403677	2.975700
1	6.264855	0.703798	2.857678
1	2.480157	0.573946	3.203872
1	3.994727	0.112644	4.005428
1	3.495128	1.804602	3.978740
8	-0.532949	-2.331547	1.592346

$TS_{R\text{-}j}$

Number of imaginary frequencies : 1
Imaginary Frequency : -1590.5197 cm(-1)

Electronic energy : HF=-2930.6249982
Zero-point correction= 1.149289 (hartree/particle)
Thermal correction to Energy= 1.210631
Thermal correction to Enthalpy= 1.211576
Thermal correction to Gibbs Free Energy= 1.058808
Sum of electronic and zero-point Energies= -2929.475709
Sum of electronic and thermal Energies= -2929.414367
Sum of electronic and thermal Enthalpies= -2929.413423
Sum of electronic and thermal Free Energies= -2929.566190

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Cartesian Coordinates

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6	-0.444678	5.920543	0.419463

6	0.847804	5.247914	-0.056513
6	0.369351	4.060270	-0.932379
6	-0.869243	3.650245	-0.163316
6	-1.400213	4.761826	0.498584
6	-2.641034	4.687441	1.114281
6	-3.346059	3.488102	1.071248
6	-2.808329	2.332528	0.492673
6	-1.539105	2.436715	-0.093330
6	1.517800	3.135935	-1.271005
6	2.159249	3.582453	-2.430858
6	1.354762	4.676057	-3.078680
6	0.007599	4.567321	-2.353313
6	3.358499	3.013310	-2.833889
6	3.904489	1.978108	-2.078217
6	3.242185	1.444940	-0.967318
6	2.024696	2.036613	-0.597886
8	1.326200	1.532865	0.485171
15	0.127815	0.475171	0.223612
8	0.572292	-0.621238	-0.736360
8	-0.954732	1.314556	-0.649647
8	-0.379747	0.080897	1.578208
6	3.806507	0.302765	-0.194689
1	4.859707	1.542804	-2.367067
1	3.870394	3.369299	-3.726412
1	-3.064764	5.555165	1.617215
1	-4.339847	3.427411	1.511392
6	-3.599790	1.068011	0.470726
1	-0.330139	6.436367	1.380286
1	-0.793706	6.674329	-0.302100
1	1.394207	4.839609	0.806387
1	1.526529	5.919293	-0.595874
1	1.818235	5.660984	-2.917319
1	1.267920	4.546259	-4.164075
1	-0.617206	3.805710	-2.842594
1	-0.561929	5.504155	-2.333161
6	-3.935064	0.412325	1.676587
6	-4.776909	-0.700745	1.633948
6	-5.289333	-1.199716	0.438577
6	-4.908715	-0.566456	-0.739575
6	-4.077540	0.554669	-0.754133
1	-5.284126	-0.960918	-1.685847
6	4.157495	0.476327	1.163717
6	4.654560	-0.607556	1.884029
6	4.821909	-1.864639	1.308456
6	4.500270	-2.007451	-0.037024
6	3.986255	-0.957196	-0.802211
1	4.916234	-0.464051	2.933226
1	-5.036868	-1.196913	2.570010
1	4.640154	-2.984752	-0.503787
6	-0.569055	-2.901783	-0.055730
1	0.059719	-1.825870	-0.469166
6	0.424806	-3.096110	0.926493
6	1.552835	-4.051427	0.801175
1	1.494698	-4.668730	-0.095875
1	2.491068	-3.478287	0.806100
1	1.567259	-4.697735	1.687969
6	-1.929246	-2.336414	0.343875
1	-2.432837	-1.921600	-0.539021
1	-2.563263	-3.144427	0.731481
1	-1.885602	-1.537676	1.087679

6	-0.702962	-3.888461	-1.176984
6	-0.632991	-3.443805	-2.499557
6	-1.011077	-5.230362	-0.934256
6	-0.834996	-4.325898	-3.555923
1	-0.414499	-2.393685	-2.695002
6	-1.210139	-6.115078	-1.989122
1	-1.094166	-5.580111	0.095844
6	-1.119927	-5.664272	-3.303107
1	-0.770069	-3.964918	-4.580082
1	-1.442214	-7.158099	-1.784161
1	-1.277024	-6.355553	-4.128073
1	0.015666	-1.465582	1.920039
6	-3.745584	1.168562	-2.102588
6	-5.003669	1.592180	-2.858246
6	-2.898701	0.216072	-2.946583
1	-3.152272	2.076505	-1.935673
1	-5.627870	2.262388	-2.254888
1	-4.736281	2.119727	-3.782703
1	-5.619777	0.729078	-3.143214
1	-1.958985	-0.031312	-2.438033
1	-3.435928	-0.719582	-3.156598
1	-2.647425	0.675359	-3.911787
6	-6.190170	-2.414783	0.394872
6	-7.302336	-2.368802	1.437323
6	-5.380717	-3.703068	0.537069
1	-6.662118	-2.426423	-0.600141
1	-7.872741	-1.434254	1.381466
1	-8.000950	-3.202151	1.292430
1	-6.904226	-2.456907	2.456758
1	-4.614036	-3.789783	-0.244083
1	-4.873714	-3.734262	1.512109
1	-6.031334	-4.584865	0.472758
6	-3.415792	0.873341	3.028203
6	-2.787653	-0.265135	3.828350
6	-4.524644	1.529278	3.850651
1	-2.624063	1.613150	2.851847
1	-1.983272	-0.749021	3.264717
1	-2.355393	0.122854	4.759315
1	-3.526311	-1.027963	4.107538
1	-4.984077	2.378480	3.330448
1	-5.325428	0.809643	4.069680
1	-4.135112	1.893879	4.809833
6	3.643622	-1.235624	-2.254369
6	2.771308	-2.477623	-2.417525
6	4.907193	-1.374790	-3.102878
1	3.069548	-0.384074	-2.640123
1	1.900700	-2.435726	-1.754255
1	2.406511	-2.554815	-3.450097
1	3.324431	-3.402782	-2.204920
1	5.546583	-0.485494	-3.047280
1	5.511708	-2.230747	-2.772906
1	4.650456	-1.540009	-4.157302
6	5.341192	-3.037768	2.108351
6	4.557598	-3.243805	3.401783
6	6.832385	-2.890038	2.401663
1	5.206869	-3.936758	1.484527
1	3.476077	-3.286311	3.220832
1	4.861340	-4.174991	3.896235
1	4.736112	-2.426398	4.112379
1	7.414571	-2.782960	1.478782

1	7.021387	-2.001376	3.018723
1	7.215177	-3.761647	2.947924
6	4.065082	1.817724	1.868841
6	5.462499	2.384174	2.114639
6	3.261877	1.743943	3.164132
1	3.547959	2.524067	1.208528
1	6.018297	2.490296	1.174136
1	5.404871	3.373248	2.587355
1	6.049267	1.732631	2.776064
1	2.274583	1.297831	2.995414
1	3.776656	1.154122	3.934057
1	3.113900	2.750287	3.576797
8	0.534065	-2.331868	1.973894

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Number of imaginary frequencies : 0

Electronic energy : HF=-2930.6421126
Zero-point correction= 1.152823 (hartree/particle)
Thermal correction to Energy= 1.215548
Thermal correction to Enthalpy= 1.216492
Thermal correction to Gibbs Free Energy= 1.059428
Sum of electronic and zero-point Energies= -2929.489289
Sum of electronic and thermal Energies= -2929.426565
Sum of electronic and thermal Enthalpies= -2929.425621
Sum of electronic and thermal Free Energies= -2929.582685

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Cartesian Coordinates

.....

6	-0.518127	5.933288	0.593605
6	0.784292	5.286582	0.104770
6	0.318640	4.134205	-0.822251
6	-0.922232	3.686806	-0.082292
6	-1.473582	4.771703	0.606297
6	-2.729704	4.666928	1.185547
6	-3.426130	3.466439	1.080576
6	-2.865483	2.330155	0.484150
6	-1.584249	2.469509	-0.064258
6	1.465002	3.223672	-1.203255
6	2.087641	3.706687	-2.359767
6	1.285841	4.832469	-2.951024
6	-0.053468	4.698642	-2.219527
6	3.272157	3.143793	-2.810060
6	3.825914	2.078177	-2.106142
6	3.189388	1.514706	-0.995167
6	1.987660	2.103951	-0.577270
8	1.323062	1.574124	0.526240
15	0.085845	0.573842	0.331696
8	0.555818	-0.547689	-0.675344
8	-0.951358	1.355914	-0.616821
8	-0.418475	0.143173	1.651918
6	3.787404	0.354694	-0.276603
1	4.771846	1.648267	-2.430216
1	3.766398	3.529523	-3.700011
1	-3.172899	5.512276	1.709039
1	-4.429090	3.384425	1.495516
6	-3.635503	1.055286	0.418618
1	-0.417696	6.402647	1.579375

1	-0.858332	6.720583	-0.095311
1	1.327076	4.847993	0.955112
1	1.462608	5.983356	-0.401682
1	1.758106	5.805322	-2.747903
1	1.189523	4.752794	-4.040241
1	-0.684397	3.959312	-2.733929
1	-0.620699	5.634564	-2.155632
6	-4.038862	0.399492	1.603143
6	-4.853408	-0.732063	1.511533
6	-5.278543	-1.244121	0.288960
6	-4.833570	-0.606976	-0.865684
6	-4.029204	0.531160	-0.833489
1	-5.150107	-1.006448	-1.831332
6	4.259448	0.513833	1.044213
6	4.819176	-0.579643	1.702723
6	4.933369	-1.828428	1.098840
6	4.489053	-1.956069	-0.213531
6	3.906433	-0.898894	-0.914026
1	5.174986	-0.449099	2.725586
1	-5.165614	-1.224530	2.433195
1	4.575979	-2.929530	-0.699710
6	-0.594410	-3.206931	0.320175
1	0.409025	-1.463626	-0.338991
6	0.512424	-3.179234	1.108163
6	1.739076	-4.006632	0.916456
1	1.708829	-4.612517	0.008965
1	2.614672	-3.345423	0.881493
1	1.872514	-4.674309	1.778194
6	-1.857993	-2.451307	0.636093
1	-2.157196	-1.767777	-0.175210
1	-2.683328	-3.165573	0.753073
1	-1.802816	-1.858503	1.551921
6	-0.720627	-4.122943	-0.844720
6	-1.030922	-3.604471	-2.108888
6	-0.624881	-5.512449	-0.707475
6	-1.212413	-4.442745	-3.202941
1	-1.115257	-2.524042	-2.234126
6	-0.806201	-6.353790	-1.800618
1	-0.418388	-5.934908	0.275193
6	-1.098433	-5.822324	-3.052671
1	-1.441122	-4.015538	-4.177281
1	-0.727210	-7.431213	-1.670322
1	-1.242492	-6.480299	-3.906804
1	0.074077	-1.600521	2.161365
6	-3.659289	1.165946	-2.162159
6	-4.900467	1.602327	-2.938910
6	-2.792173	0.230602	-3.002994
1	-3.075037	2.073469	-1.967307
1	-5.532266	2.269959	-2.340564
1	-4.613557	2.137007	-3.853366
1	-5.515070	0.744233	-3.241226
1	-1.878390	-0.050593	-2.465352
1	-3.334053	-0.688419	-3.266256
1	-2.494788	0.717294	-3.940967
6	-6.158289	-2.470548	0.172897
6	-7.196885	-2.585096	1.281651
6	-5.312403	-3.741549	0.106031
1	-6.696329	-2.381001	-0.784286
1	-7.786967	-1.666938	1.385723
1	-7.888014	-3.410694	1.072955

1	-6.730687	-2.797404	2.252790
1	-4.574955	-3.698358	-0.706399
1	-4.766926	-3.888757	1.049069
1	-5.943128	-4.625358	-0.054284
6	-3.634355	0.877392	2.987905
6	-2.967799	-0.222989	3.809030
6	-4.833013	1.443358	3.748884
1	-2.894584	1.679731	2.871752
1	-2.069757	-0.596343	3.306741
1	-2.663235	0.167620	4.788305
1	-3.644124	-1.068165	3.991620
1	-5.329665	2.253501	3.200536
1	-5.586879	0.666217	3.933561
1	-4.520991	1.838672	4.723969
6	3.426204	-1.153594	-2.332404
6	2.598194	-2.430907	-2.455310
6	4.603532	-1.221268	-3.305833
1	2.780583	-0.316089	-2.627821
1	1.799301	-2.471488	-1.707791
1	2.131707	-2.491280	-3.446682
1	3.212337	-3.333247	-2.334224
1	5.213132	-0.310100	-3.289650
1	5.265235	-2.061295	-3.054215
1	4.251005	-1.373212	-4.334155
6	5.520710	-3.013027	1.832245
6	4.912249	-3.194819	3.219388
6	7.041495	-2.902729	1.917885
1	5.280134	-3.909432	1.237553
1	3.815593	-3.195593	3.185300
1	5.244909	-4.140192	3.665723
1	5.219627	-2.390628	3.900641
1	7.494146	-2.816832	0.922670
1	7.334623	-2.014326	2.493779
1	7.474035	-3.780232	2.415336
6	4.219405	1.841855	1.778554
6	5.632932	2.360720	2.035840
6	3.421311	1.756382	3.077179
1	3.724686	2.581063	1.136151
1	6.196889	2.460711	1.099950
1	5.602721	3.345168	2.520331
1	6.196388	1.685948	2.693709
1	2.413202	1.362138	2.903114
1	3.914451	1.107968	3.813077
1	3.324140	2.750321	3.532864
8	0.661694	-2.380668	2.189013

$TS_{j\text{-}s}$

Number of imaginary frequencies : 1
Imaginary Frequency : -1609.3111 cm(-1)

Electronic energy : HF=-2930.6257827
Zero-point correction= 1.149094 (hartree/particle)
Thermal correction to Energy= 1.210054
Thermal correction to Enthalpy= 1.210999
Thermal correction to Gibbs Free Energy= 1.061019
Sum of electronic and zero-point Energies= -2929.476689
Sum of electronic and thermal Energies= -2929.415728
Sum of electronic and thermal Enthalpies= -2929.414784

Sum of electronic and thermal Free Energies= -2929.564763

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Cartesian Coordinates

.....

6	-2.099317	5.663246	0.575254
6	-0.620843	5.348183	0.323150
6	-0.644348	4.192143	-0.711944
6	-1.857786	3.429432	-0.219093
6	-2.745747	4.317950	0.396139
6	-4.012161	3.898704	0.774743
6	-4.362841	2.565599	0.591106
6	-3.458950	1.619044	0.091637
6	-2.203281	2.089272	-0.324058
6	0.738515	3.598677	-0.905630
6	1.421222	4.332988	-1.881937
6	0.487023	5.289337	-2.569247
6	-0.886659	4.773897	-2.129417
6	2.770511	4.116298	-2.116167
6	3.427282	3.120772	-1.401598
6	2.752946	2.287585	-0.500200
6	1.394286	2.552817	-0.267862
8	0.699254	1.771520	0.639405
15	-0.193616	0.524515	0.128370
8	0.595531	-0.390330	-0.799455
8	-1.282597	1.204264	-0.858938
8	-0.803939	-0.060653	1.367220
6	3.466927	1.141541	0.131387
1	4.488321	2.943234	-1.570884
1	3.307200	4.706734	-2.856896
1	-4.716813	4.595217	1.225945
1	-5.352542	2.222570	0.887870
6	-3.834122	0.175366	0.086591
1	-2.284289	6.085172	1.570342
1	-2.483116	6.394401	-0.151796
1	-0.156717	4.975474	1.247542
1	-0.037038	6.210558	-0.019574
1	0.653604	6.323682	-2.233817
1	0.617588	5.289169	-3.657979
1	-1.207223	3.955091	-2.789168
1	-1.671852	5.539042	-2.141153
6	-4.183390	-0.456468	1.303822
6	-4.617557	-1.782495	1.283497
6	-4.679235	-2.527374	0.112421
6	-4.312322	-1.895684	-1.072299
6	-3.898201	-0.564517	-1.114498
1	-4.366391	-2.464823	-2.003648
6	3.636882	1.069998	1.532035
6	4.348902	0.002837	2.079950
6	4.903421	-1.002490	1.291152
6	4.724549	-0.915616	-0.085623
6	4.020728	0.130324	-0.686918
1	4.481578	-0.034596	3.162176
1	-4.885373	-2.254748	2.228648
1	5.159399	-1.692627	-0.716978
6	0.731473	-2.833294	0.121050
1	0.578949	-1.658591	-0.438769
6	-0.636651	-3.171786	0.306827
6	-1.374474	-4.222407	-0.441270
1	-0.726768	-5.000314	-0.846851
1	-2.132855	-4.655652	0.220144

1	-1.919077	-3.746061	-1.269545
6	1.496611	-2.339582	1.350129
1	1.761311	-3.168798	2.019178
1	2.418070	-1.839279	1.025995
1	0.928899	-1.610172	1.933654
6	1.524490	-3.656481	-0.849371
6	1.145053	-3.726142	-2.196304
6	2.686006	-4.329898	-0.460357
6	1.878091	-4.469068	-3.113594
1	0.273779	-3.162761	-2.534427
6	3.428002	-5.068052	-1.378144
1	3.020761	-4.276438	0.573919
6	3.024192	-5.146609	-2.706824
1	1.562990	-4.502474	-4.154290
1	4.326750	-5.585963	-1.049052
1	3.604710	-5.722685	-3.423833
1	-1.078552	-1.591149	1.367489
6	-3.572101	0.023931	-2.473930
6	-4.810415	0.065288	-3.366895
6	-2.434376	-0.737089	-3.152219
1	-3.240909	1.059075	-2.336894
1	-5.620546	0.637455	-2.898330
1	-4.578234	0.534585	-4.331567
1	-5.192395	-0.943390	-3.573428
1	-1.562199	-0.817187	-2.490663
1	-2.745786	-1.751030	-3.441028
1	-2.115781	-0.223374	-4.067982
6	-5.156809	-3.962497	0.086530
6	-6.647135	-4.017483	-0.247998
6	-4.878455	-4.721889	1.377498
1	-4.611206	-4.466104	-0.729378
1	-6.864281	-3.531463	-1.206747
1	-7.005181	-5.053726	-0.301399
1	-7.228170	-3.498671	0.526786
1	-3.841242	-4.595216	1.715604
1	-5.531126	-4.380899	2.192099
1	-5.069372	-5.793426	1.242945
6	-4.095956	0.220609	2.662854
6	-3.190136	-0.541335	3.628392
6	-5.482637	0.401749	3.279300
1	-3.649855	1.213140	2.530392
1	-2.171269	-0.607148	3.236232
1	-3.145540	-0.020055	4.593486
1	-3.555116	-1.558307	3.823258
1	-6.161429	0.956659	2.619720
1	-5.952300	-0.569378	3.487212
1	-5.417027	0.945149	4.230615
6	3.905168	0.116244	-2.202326
6	3.227368	-1.151138	-2.710383
6	5.273192	0.296820	-2.857684
1	3.271218	0.955095	-2.512242
1	2.221520	-1.236550	-2.288918
1	3.137711	-1.124320	-3.804781
1	3.783684	-2.061499	-2.449043
1	5.777306	1.209463	-2.515280
1	5.936637	-0.548204	-2.629859
1	5.175059	0.353311	-3.949336
6	5.705076	-2.135741	1.892662
6	4.980755	-2.829211	3.041358
6	7.078102	-1.643052	2.345924

1	5.858999	-2.879394	1.093830
1	3.985542	-3.181185	2.741073
1	5.555197	-3.695099	3.393632
1	4.848587	-2.156980	3.898970
1	7.627489	-1.174015	1.520998
1	6.979307	-0.895911	3.145086
1	7.686203	-2.469524	2.735480
6	3.117061	2.131961	2.483244
6	4.265720	2.831350	3.208430
6	2.115360	1.552772	3.479982
1	2.597254	2.899678	1.897959
1	4.982895	3.263336	2.499563
1	3.885313	3.642842	3.842066
1	4.816701	2.138587	3.858071
1	1.275552	1.068530	2.967139
1	2.589520	0.813545	4.139810
1	1.707111	2.345787	4.119842
8	-1.405117	-2.524944	1.124963

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i1'(*S*)

Number of imaginary frequencies : 0

Electronic energy : HF=-2930.6612667
Zero-point correction= 1.153246 (hartree/particle)
Thermal correction to Energy= 1.215768
Thermal correction to Enthalpy= 1.216712
Thermal correction to Gibbs Free Energy= 1.061153
Sum of electronic and zero-point Energies= -2929.508020
Sum of electronic and thermal Energies= -2929.445499
Sum of electronic and thermal Enthalpies= -2929.444555
Sum of electronic and thermal Free Energies= -2929.600114

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Cartesian Coordinates

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6	-2.820133	5.149092	1.455061
6	-1.370284	5.077927	0.964912
6	-1.412188	4.090615	-0.232241
6	-2.453268	3.115061	0.270579
6	-3.328717	3.769588	1.143245
6	-4.468864	3.130955	1.606305
6	-4.706095	1.814303	1.224972
6	-3.801797	1.094477	0.434520
6	-2.671320	1.779894	-0.034056
6	-0.011949	3.704780	-0.658484
6	0.469766	4.646084	-1.573710
6	-0.639625	5.560901	-2.014625
6	-1.889656	4.832303	-1.506752
6	1.801466	4.633687	-1.959429
6	2.645087	3.657417	-1.439612
6	2.175809	2.637720	-0.602353
6	0.821863	2.675885	-0.242640
8	0.294323	1.658505	0.548260
15	-0.428865	0.455794	-0.251408
8	0.332399	-0.180238	-1.340722
8	-1.765576	1.124167	-0.856264
8	-0.844939	-0.427453	0.980392
6	3.127052	1.594725	-0.119887
1	3.700223	3.655495	-1.706735

1	2.185550	5.375850	-2.657250
1	-5.165327	3.645443	2.266153
1	-5.602735	1.304146	1.572613
6	-4.045760	-0.345483	0.140647
1	-2.901558	5.395429	2.520379
1	-3.389143	5.917393	0.910560
1	-0.733939	4.641396	1.748445
1	-0.944267	6.050582	0.691938
1	-0.541570	6.556382	-1.556539
1	-0.645649	5.715682	-3.100057
1	-2.210828	4.082135	-2.243695
1	-2.740549	5.495867	-1.311718
6	-4.100589	-1.280925	1.198800
6	-4.382389	-2.616479	0.908340
6	-4.589591	-3.066128	-0.391202
6	-4.524236	-2.129396	-1.418520
6	-4.261726	-0.781106	-1.184796
1	-4.694032	-2.468809	-2.442540
6	3.495062	1.544019	1.241137
6	4.504579	0.665902	1.643007
6	5.145490	-0.182849	0.746445
6	4.737722	-0.146816	-0.584801
6	3.750987	0.725338	-1.043722
1	4.788316	0.644503	2.695335
1	-4.419099	-3.331710	1.729733
1	5.220173	-0.826016	-1.290639
6	1.659561	-2.715639	0.422467
1	1.293868	-1.873163	-0.185438
6	0.449647	-3.580093	0.716486
6	0.650491	-5.038490	0.976347
1	1.572529	-5.216561	1.542447
1	-0.212160	-5.450664	1.504075
1	0.768969	-5.564662	0.020905
6	2.122895	-2.150237	1.767118
1	2.452295	-2.938747	2.457555
1	2.951189	-1.447692	1.616487
1	1.303718	-1.603346	2.248520
6	2.717566	-3.432565	-0.382463
6	2.399693	-3.824613	-1.688134
6	3.997228	-3.703502	0.100021
6	3.332392	-4.468892	-2.490058
1	1.406239	-3.598250	-2.080016
6	4.938221	-4.345983	-0.703360
1	4.273523	-3.407689	1.111081
6	4.610572	-4.728047	-1.999272
1	3.066921	-4.758129	-3.504627
1	5.932964	-4.546854	-0.309132
1	5.347023	-5.225768	-2.626208
1	-0.838332	-1.409067	0.796795
6	-4.285952	0.166238	-2.369452
6	-5.702352	0.286664	-2.929329
6	-3.298536	-0.244746	-3.458372
1	-3.994577	1.164860	-2.024232
1	-6.407160	0.623239	-2.158392
1	-5.734612	1.008086	-3.756035
1	-6.064850	-0.675761	-3.314682
1	-2.281253	-0.343391	-3.061272
1	-3.578366	-1.201853	-3.918363
1	-3.278280	0.505798	-4.258852
6	-4.933961	-4.504417	-0.708023

6	-6.451743	-4.684463	-0.736676
6	-4.300266	-5.508168	0.245521
1	-4.552074	-4.708535	-1.720962
1	-6.924447	-4.008655	-1.459483
1	-6.724699	-5.714136	-1.001763
1	-6.879937	-4.465695	0.251398
1	-3.222645	-5.338931	0.350979
1	-4.748216	-5.449995	1.246664
1	-4.455355	-6.531961	-0.115934
6	-3.875817	-0.908799	2.656187
6	-2.810493	-1.769460	3.332802
6	-5.181320	-0.997526	3.447543
1	-3.524272	0.129565	2.697255
1	-1.846310	-1.702060	2.819592
1	-2.663174	-1.436535	4.368296
1	-3.099038	-2.827930	3.369381
1	-5.978103	-0.387003	3.005936
1	-5.547988	-2.032258	3.483621
1	-5.033652	-0.663103	4.482475
6	3.404446	0.698852	-2.522341
6	3.035994	-0.702625	-2.999386
6	4.549769	1.257268	-3.366881
1	2.519621	1.328898	-2.677194
1	2.186264	-1.088010	-2.427383
1	2.747990	-0.676170	-4.058598
1	3.873787	-1.407190	-2.905843
1	4.837916	2.271519	-3.064262
1	5.444444	0.625210	-3.283786
1	4.267822	1.290076	-4.427124
6	6.283906	-1.090865	1.155357
6	6.185122	-1.599317	2.587475
6	7.618973	-0.379435	0.936755
1	6.249363	-1.962609	0.481037
1	5.206233	-2.049693	2.799454
1	6.955612	-2.356212	2.778971
1	6.341958	-0.791732	3.314968
1	7.735127	-0.056026	-0.104560
1	7.681669	0.515341	1.571451
1	8.464517	-1.032222	1.189192
6	2.844652	2.404142	2.309430
6	3.862248	3.265221	3.054145
6	2.048450	1.536068	3.283432
1	2.138375	3.090091	1.824631
1	4.456529	3.875051	2.363077
1	3.352905	3.942523	3.751295
1	4.558143	2.655976	3.645387
1	1.282523	0.953779	2.756971
1	2.705741	0.834917	3.816327
1	1.546169	2.156630	4.036883
8	-0.667896	-3.080276	0.797747

$TS_{i\text{-}k}(R)$

Number of imaginary frequencies : 1
Imaginary Frequency : -269.4379 cm(-1)

Electronic energy : HF=-3218.066904
Zero-point correction= 1.272488 (hartree/particle)
Thermal correction to Energy= 1.339234

Thermal correction to Enthalpy= 1.340178
Thermal correction to Gibbs Free Energy= 1.178549
Sum of electronic and zero-point Energies= -3216.794416
Sum of electronic and thermal Energies= -3216.727670
Sum of electronic and thermal Enthalpies= -3216.726726
Sum of electronic and thermal Free Energies= -3216.888355

.....

Cartesian Coordinates

.....

7	1.363879	-2.499462	0.024147
1	1.020062	-1.621759	-0.400463
1	2.262208	-2.269030	0.459297
6	0.274556	-2.521859	1.803308
6	-1.183604	-2.701055	1.388803
1	-1.546280	-1.694563	1.133963
6	-1.939548	-3.146301	2.652948
1	-1.687573	-2.518274	3.516028
1	-1.725104	-4.190879	2.908006
1	-3.017023	-3.062673	2.474346
6	-1.536731	-3.586563	0.219145
6	-1.375076	-4.974772	0.229924
6	-2.164755	-2.998540	-0.881395
6	-1.806064	-5.747500	-0.843418
1	-0.916193	-5.466208	1.087124
6	-2.618511	-3.770910	-1.946306
1	-2.325670	-1.918790	-0.891325
6	-2.435282	-5.149367	-1.932195
1	-1.658485	-6.825173	-0.824033
1	-3.117350	-3.288762	-2.785785
1	-2.782882	-5.758530	-2.763837
8	0.601139	-1.365272	2.245154
1	0.003808	-0.483824	1.792814
6	1.022256	-3.664263	2.413532
1	1.004187	-4.561272	1.787930
1	2.055697	-3.356581	2.606478
1	0.567151	-3.905911	3.382176
6	1.501723	-3.535113	-0.935071
6	0.795373	-3.467273	-2.137719
6	2.335264	-4.626942	-0.686617
6	0.917478	-4.485566	-3.072695
1	0.160350	-2.604700	-2.334380
6	2.455714	-5.641395	-1.631517
1	2.898238	-4.674188	0.243911
6	1.747103	-5.577656	-2.826310
1	0.363507	-4.420184	-4.006965
1	3.112870	-6.484620	-1.429494
1	1.844587	-6.369918	-3.564772
6	1.347652	5.572325	-2.701029
6	-0.075955	5.282101	-2.206831
6	0.120780	4.698197	-0.783837
6	1.389197	3.901614	-1.006560
6	2.152036	4.504945	-2.010749
6	3.448247	4.076078	-2.258478
6	3.959274	3.007283	-1.526539
6	3.181174	2.302886	-0.599422
6	1.881994	2.777734	-0.362187
6	-1.167476	4.129858	-0.218171
6	-1.872204	5.141610	0.443687
6	-1.031244	6.382494	0.550871
6	0.367541	5.852677	0.223645

6	-3.155631	4.918320	0.918799
6	-3.720896	3.657066	0.764744
6	-3.011970	2.592876	0.195906
6	-1.724018	2.859105	-0.292868
8	-1.010686	1.839594	-0.890514
15	0.061781	0.982400	-0.030092
8	-0.597811	0.457619	1.244210
8	1.072443	2.121572	0.541902
8	0.705188	0.033666	-0.978110
6	-3.630971	1.236784	0.139878
1	-4.731316	3.469366	1.123414
1	-3.709894	5.713319	1.414904
1	4.057980	4.559195	-3.020153
1	4.981598	2.675492	-1.702559
6	3.708614	1.086143	0.082505
1	1.439761	5.522411	-3.792600
1	1.677351	6.579450	-2.405010
1	-0.538803	4.507837	-2.835633
1	-0.734091	6.159249	-2.215614
1	-1.350834	7.144900	-0.175469
1	-1.095356	6.847667	1.541819
1	0.825344	5.428040	1.128917
1	1.050648	6.614760	-0.169300
6	4.149854	-0.023606	-0.678067
6	4.681798	-1.135725	-0.018328
6	4.811349	-1.185639	1.369289
6	4.348538	-0.094371	2.097611
6	3.802520	1.037015	1.491181
1	4.451079	-0.114685	3.183935
6	-3.960925	0.649520	-1.099134
6	-4.648983	-0.564887	-1.112350
6	-5.009465	-1.233508	0.053100
6	-4.642537	-0.655483	1.267562
6	-3.965628	0.564619	1.338476
1	-4.926705	-1.006467	-2.072125
6	4.116406	-0.059619	-2.197426
6	3.317718	-1.239958	-2.738067
6	5.532803	-0.060518	-2.771704
1	3.613218	0.846478	-2.553020
1	3.755166	-2.210013	-2.461935
1	2.290031	-1.202700	-2.365317
1	3.281041	-1.202727	-3.834576
1	6.124738	0.790484	-2.410996
1	6.074431	-0.975257	-2.494593
1	5.505778	-0.013464	-3.867855
6	3.419598	2.194574	2.395875
6	4.654642	2.772026	3.086112
6	2.358608	1.793273	3.417590
1	2.996486	2.997431	1.781498
1	5.410495	3.084811	2.354964
1	4.384919	3.647982	3.689968
1	5.123045	2.040520	3.757720
1	1.467861	1.381700	2.928827
1	2.738779	1.041714	4.122508
1	2.048335	2.665429	4.007643
1	5.029281	-1.978984	-0.618567
6	5.549309	-2.304184	2.073577
6	7.056708	-2.104017	1.913640
6	5.152141	-3.699711	1.613157
1	5.311317	-2.223496	3.146066

1	7.369119	-1.116291	2.272751
1	7.618214	-2.864599	2.471097
1	7.345861	-2.179787	0.856586
1	4.083326	-3.887715	1.778038
1	5.364965	-3.856823	0.547280
1	5.709506	-4.463010	2.170045
1	-4.912567	-1.157006	2.198431
6	-3.638846	1.295763	-2.433083
6	-4.914522	1.678623	-3.180312
6	-2.748027	0.397324	-3.288266
1	-3.085520	2.223464	-2.246734
1	-5.543972	2.343861	-2.576008
1	-4.675023	2.197497	-4.117345
1	-5.513578	0.794574	-3.436454
1	-1.836670	0.107343	-2.749735
1	-3.274315	-0.518270	-3.592522
1	-2.444222	0.917409	-4.205760
6	-5.838163	-2.497901	-0.024318
6	-7.307268	-2.173042	0.245160
6	-5.360911	-3.610608	0.900640
1	-5.757644	-2.870688	-1.057970
1	-7.682868	-1.408876	-0.446044
1	-7.936307	-3.066503	0.141483
1	-7.436449	-1.788423	1.266207
1	-4.310730	-3.869037	0.713956
1	-5.465146	-3.331571	1.958311
1	-5.961597	-4.516076	0.748835
6	-3.650256	1.134647	2.712350
6	-2.907542	0.152417	3.613588
6	-4.924089	1.611283	3.411706
1	-2.989914	2.000266	2.577938
1	-1.975694	-0.184813	3.146688
1	-2.649328	0.638949	4.562983
1	-3.518893	-0.726728	3.858368
1	-5.485507	2.334683	2.807917
1	-5.598539	0.769198	3.619304
1	-4.685570	2.087180	4.371629

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k(*R*)

Number of imaginary frequencies : 0

Electronic energy : HF=-3218.0823428
Zero-point correction= 1.277661 (hartree/particle)
Thermal correction to Energy= 1.344737
Thermal correction to Enthalpy= 1.345681
Thermal correction to Gibbs Free Energy= 1.183037
Sum of electronic and zero-point Energies= -3216.804682
Sum of electronic and thermal Energies= -3216.737606
Sum of electronic and thermal Enthalpies= -3216.736662
Sum of electronic and thermal Free Energies= -3216.899306

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Cartesian Coordinates

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7	1.424489	-2.348290	0.182958
1	1.068655	-1.422573	-0.207856
1	2.372153	-2.116276	0.522565
6	0.618155	-2.637407	1.516535
6	-0.900546	-2.733757	1.242749

1	-1.189683	-1.708729	0.965057
6	-1.631814	-3.064043	2.547872
1	-1.267220	-2.457959	3.384425
1	-1.533911	-4.123765	2.813688
1	-2.700246	-2.855919	2.418761
6	-1.405048	-3.635973	0.139634
6	-1.249532	-5.025862	0.157312
6	-2.151538	-3.065978	-0.895393
6	-1.787778	-5.815729	-0.852976
1	-0.702175	-5.503506	0.969235
6	-2.699524	-3.854197	-1.902737
1	-2.317330	-1.985971	-0.904635
6	-2.515640	-5.232857	-1.887567
1	-1.646330	-6.894182	-0.826472
1	-3.274357	-3.386338	-2.700581
1	-2.941712	-5.852933	-2.673243
8	0.895102	-1.542709	2.298202
1	0.321688	-0.777956	2.032779
6	1.263205	-3.832675	2.177194
1	1.208251	-4.741396	1.572043
1	2.314103	-3.598029	2.391804
1	0.774544	-4.019019	3.137367
6	1.521690	-3.306192	-0.914833
6	0.791914	-3.057833	-2.071643
6	2.378110	-4.396846	-0.830116
6	0.899678	-3.933254	-3.144441
1	0.163034	-2.171721	-2.125721
6	2.481011	-5.268047	-1.910460
1	2.964020	-4.569738	0.068366
6	1.740457	-5.039947	-3.065527
1	0.324631	-3.743190	-4.047282
1	3.149097	-6.123354	-1.847425
1	1.823605	-5.721654	-3.908436
6	1.304031	5.589952	-2.647270
6	-0.125511	5.273046	-2.187132
6	0.050370	4.684536	-0.763618
6	1.334019	3.907566	-0.964005
6	2.110505	4.532817	-1.943414
6	3.422811	4.134749	-2.156484
6	3.930631	3.064759	-1.424707
6	3.137161	2.331664	-0.532669
6	1.826003	2.784455	-0.315406
6	-1.238287	4.095656	-0.220638
6	-1.965056	5.095746	0.435897
6	-1.145563	6.349730	0.554781
6	0.265051	5.839354	0.251293
6	-3.246215	4.851052	0.905265
6	-3.785301	3.578622	0.752546
6	-3.053859	2.527096	0.189132
6	-1.769739	2.813202	-0.301523
8	-1.029404	1.807299	-0.887668
15	-0.000614	0.961532	0.056970
8	-0.651793	0.460660	1.311009
8	1.020921	2.125314	0.579681
8	0.681689	0.000587	-0.878820
6	-3.655072	1.163093	0.145145
1	-4.792200	3.370010	1.109939
1	-3.816554	5.636230	1.398921
1	4.046051	4.640221	-2.892328
1	4.963102	2.753128	-1.577729

6	3.658086	1.093720	0.116049
1	1.422171	5.546278	-3.736718
1	1.609680	6.601383	-2.340422
1	-0.561400	4.495106	-2.830274
1	-0.797731	6.139317	-2.205868
1	-1.463694	7.106682	-0.178027
1	-1.232790	6.814975	1.544017
1	0.711334	5.417364	1.163417
1	0.945987	6.610689	-0.127358
6	4.134072	0.025949	-0.683232
6	4.672548	-1.107393	-0.063578
6	4.764930	-1.221976	1.324568
6	4.255893	-0.176282	2.089476
6	3.716028	0.978538	1.523638
1	4.328376	-0.247995	3.175992
6	-3.994862	0.568254	-1.086691
6	-4.672188	-0.653273	-1.088706
6	-5.013507	-1.318112	0.084940
6	-4.641870	-0.728059	1.291488
6	-3.973521	0.496103	1.350183
1	-4.956777	-1.101142	-2.043634
6	4.137653	0.062013	-2.203520
6	3.336653	-1.077669	-2.819543
6	5.565738	0.076776	-2.746295
1	3.647158	0.986361	-2.525843
1	3.736736	-2.067275	-2.556434
1	2.293533	-1.022310	-2.492969
1	3.350732	-1.003046	-3.914832
1	6.158570	0.896718	-2.321441
1	6.091437	-0.859770	-2.514783
1	5.563681	0.190609	-3.837787
6	3.301355	2.088862	2.472900
6	4.515170	2.629153	3.228869
6	2.209821	1.639650	3.441566
1	2.898411	2.921043	1.884817
1	5.299404	2.964319	2.538630
1	4.228555	3.483446	3.855434
1	4.954328	1.870212	3.889933
1	1.317946	1.290208	2.907714
1	2.557289	0.830575	4.098245
1	1.909210	2.475847	4.086091
1	5.073350	-1.902039	-0.696067
6	5.539421	-2.333832	2.002012
6	7.033092	-2.008713	1.944903
6	5.285242	-3.724366	1.438901
1	5.236962	-2.339897	3.061280
1	7.243246	-1.023801	2.378215
1	7.622544	-2.756328	2.490648
1	7.384163	-1.995438	0.904046
1	4.238246	-4.026720	1.567069
1	5.533674	-3.789385	0.371086
1	5.902236	-4.467135	1.959109
1	-4.898447	-1.225975	2.227867
6	-3.685584	1.217010	-2.422447
6	-4.964168	1.556940	-3.184323
6	-2.756983	0.342378	-3.260588
1	-3.159743	2.160915	-2.234285
1	-5.621167	2.202762	-2.588483
1	-4.731182	2.081674	-4.119790
1	-5.532322	0.654313	-3.445838

1	-1.837390	0.109990	-2.708698
1	-3.242164	-0.601686	-3.546194
1	-2.472341	0.856834	-4.187575
6	-5.824290	-2.595118	0.036934
6	-7.290602	-2.296282	0.348399
6	-5.296298	-3.689130	0.957613
1	-5.770918	-2.974174	-0.996199
1	-7.702158	-1.547627	-0.339320
1	-7.904364	-3.203339	0.274086
1	-7.396820	-1.902716	1.368592
1	-4.240751	-3.911438	0.756753
1	-5.390878	-3.408724	2.015481
1	-5.868538	-4.615076	0.819283
6	-3.654432	1.069757	2.720463
6	-2.884076	0.090692	3.600857
6	-4.928269	1.522294	3.435505
1	-3.011173	1.946719	2.581365
1	-1.972560	-0.239771	3.093469
1	-2.595626	0.577408	4.541601
1	-3.485700	-0.790350	3.864090
1	-5.500130	2.252185	2.848927
1	-5.593540	0.670368	3.632713
1	-4.687203	1.983039	4.402302

$TS_{k\text{-}l}(R)$

Number of imaginary frequencies : 1
Imaginary Frequency : -207.8940 cm(-1)

Electronic energy : HF=-3218.0491277
Zero-point correction= 1.276402 (hartree/particle)
Thermal correction to Energy= 1.343243
Thermal correction to Enthalpy= 1.344187
Thermal correction to Gibbs Free Energy= 1.181654
Sum of electronic and zero-point Energies= -3216.772725
Sum of electronic and thermal Energies= -3216.705885
Sum of electronic and thermal Enthalpies= -3216.704941
Sum of electronic and thermal Free Energies= -3216.867474

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Cartesian Coordinates

.....

6	7.396725	-0.402858	0.737012
6	6.487502	-0.816742	1.704986
6	5.211692	-0.261336	1.746846
6	4.834654	0.732287	0.841004
6	5.756793	1.144773	-0.124536
6	7.025311	0.576184	-0.180351
6	3.478620	1.399858	0.993225
6	3.647875	2.828859	1.502047
6	2.619935	1.181036	-0.247451
8	1.005599	1.665437	0.557385
7	2.710028	1.961221	-1.346193
1	2.949445	0.833371	1.773947
1	0.699662	0.900294	1.119894
1	0.328295	1.568521	-0.171823
1	2.322857	1.542947	-2.187942
1	4.499214	-0.591163	2.503675
1	5.486668	1.931574	-0.827646
1	6.770058	-1.575562	2.432005

1	7.731607	0.908271	-0.938249
1	8.391799	-0.840275	0.697502
1	2.681640	3.315649	1.667915
1	4.179691	2.790096	2.459486
1	4.241483	3.450278	0.823207
6	2.966194	3.365606	-1.451221
6	2.095043	4.298678	-0.892485
6	4.070995	3.786303	-2.187750
6	2.367660	5.654958	-1.032486
1	1.216663	3.957554	-0.345793
6	4.330208	5.145202	-2.333338
1	4.721316	3.041465	-2.643505
6	3.483923	6.080854	-1.747091
1	1.698309	6.385366	-0.581110
1	5.196547	5.470754	-2.903994
1	3.688718	7.143373	-1.853930
6	2.365169	-0.255654	-0.600151
1	3.277537	-0.662713	-1.052090
1	2.106957	-0.872049	0.267121
1	1.545788	-0.329563	-1.324375
6	-5.803232	-2.049698	-2.301358
6	-4.781050	-3.061625	-1.761626
6	-4.311619	-2.460155	-0.411294
6	-4.339641	-0.990955	-0.759424
6	-5.288214	-0.745352	-1.754237
6	-5.601327	0.559631	-2.109528
6	-4.938198	1.612381	-1.479277
6	-3.919323	1.394474	-0.545544
6	-3.629762	0.062875	-0.211440
6	-3.094464	-3.178226	0.142061
6	-3.507472	-4.255019	0.934879
6	-4.995904	-4.211394	1.142359
6	-5.344623	-2.787292	0.699213
6	-2.588395	-5.171602	1.423184
6	-1.239954	-4.996117	1.126019
6	-0.782435	-3.884784	0.410715
6	-1.734991	-2.967875	-0.060006
8	-1.311040	-1.862024	-0.763863
15	-1.126736	-0.454862	0.056175
8	-0.230108	-0.593859	1.252537
8	-2.621688	-0.220077	0.679478
8	-0.796818	0.562578	-1.000698
6	0.670366	-3.750017	0.099955
1	-0.508934	-5.729424	1.463254
1	-2.914048	-6.018454	2.025218
1	-6.350520	0.764297	-2.872756
1	-5.192984	2.639224	-1.737117
6	-3.163192	2.514974	0.084317
1	-5.868815	-2.051380	-3.395995
1	-6.814864	-2.267262	-1.926684
1	-3.914755	-3.110527	-2.437651
1	-5.180689	-4.077517	-1.654480
1	-5.506397	-4.960483	0.518220
1	-5.281426	-4.421146	2.180257
1	-5.183085	-2.089111	1.533750
1	-6.380341	-2.668717	0.358555
6	-2.362447	3.380234	-0.694714
6	-1.667130	4.416439	-0.064527
6	-1.737984	4.631026	1.310083
6	-2.524238	3.761629	2.057891

6	-3.236336	2.711670	1.480766
1	-2.593793	3.919740	3.136047
6	1.117420	-3.967054	-1.220909
6	2.486869	-3.979897	-1.477304
6	3.437302	-3.786276	-0.477409
6	2.975718	-3.526077	0.810392
6	1.611787	-3.499971	1.119976
1	2.835478	-4.178485	-2.493579
6	-2.259421	3.264373	-2.205688
6	-0.822017	3.268225	-2.719242
6	-3.052030	4.382836	-2.884299
1	-2.697236	2.303686	-2.501673
1	-0.253779	2.447206	-2.269473
1	-0.815002	3.125520	-3.807824
1	-0.304501	4.216458	-2.518092
1	-4.095375	4.415835	-2.547233
1	-2.610586	5.365480	-2.667295
1	-3.052897	4.254585	-3.974558
6	-4.102638	1.863166	2.393770
6	-5.235608	2.693804	2.993887
6	-3.281500	1.185785	3.488758
1	-4.570179	1.071190	1.796758
1	-5.850215	3.155941	2.211277
1	-5.890155	2.066805	3.613162
1	-4.849190	3.499097	3.632785
1	-2.444653	0.620552	3.063088
1	-2.875845	1.917457	4.200714
1	-3.907884	0.489378	4.061336
1	-1.061447	5.086263	-0.677097
6	-0.982730	5.739203	2.011519
6	-0.918672	7.033989	1.212050
6	0.419123	5.272762	2.402339
1	-1.529221	5.951552	2.944197
1	-1.917538	7.384353	0.926397
1	-0.434632	7.825665	1.797070
1	-0.336833	6.913915	0.288119
1	0.383638	4.340895	2.980415
1	1.029216	5.084264	1.507868
1	0.937120	6.031715	3.002894
1	3.697338	-3.346405	1.608328
6	0.170053	-4.234478	-2.376519
6	0.362229	-5.644893	-2.928122
6	0.316077	-3.183696	-3.474041
1	-0.859798	-4.171786	-2.004877
1	0.227183	-6.399194	-2.142479
1	-0.362961	-5.852989	-3.725238
1	1.366735	-5.779936	-3.350816
1	0.151134	-2.174623	-3.076357
1	1.313298	-3.214734	-3.933627
1	-0.417712	-3.354805	-4.272268
6	4.906717	-3.835488	-0.841219
6	5.815781	-4.213625	0.318685
6	5.350111	-2.505497	-1.450680
1	5.012058	-4.609167	-1.619131
1	5.508718	-5.155015	0.789733
1	6.850488	-4.327308	-0.027834
1	5.820567	-3.433531	1.090791
1	4.746812	-2.243844	-2.329666
1	5.252662	-1.698003	-0.711906
1	6.402712	-2.542085	-1.761996

6	1.193659	-3.222859	2.553321
6	1.920079	-2.026094	3.162147
6	1.406090	-4.450815	3.438683
1	0.125531	-2.972958	2.543338
1	1.817042	-1.139973	2.525099
1	1.485530	-1.782493	4.139685
1	2.987282	-2.232054	3.327518
1	0.839386	-5.320033	3.084935
1	2.467018	-4.736441	3.462929
1	1.093596	-4.245344	4.470756

I(*R*)

Number of imaginary frequencies : 0

Electronic energy : HF=-3218.0628793
Zero-point correction= 1.276002 (hartree/particle)
Thermal correction to Energy= 1.344167
Thermal correction to Enthalpy= 1.345111
Thermal correction to Gibbs Free Energy= 1.179247
Sum of electronic and zero-point Energies= -3216.786877
Sum of electronic and thermal Energies= -3216.718712
Sum of electronic and thermal Enthalpies= -3216.717768
Sum of electronic and thermal Free Energies= -3216.883633

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Cartesian Coordinates

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6	6.280757	4.276325	-2.061930
6	6.353271	4.441280	-0.681329
6	5.344241	3.948972	0.136731
6	4.240004	3.286442	-0.408007
6	4.177975	3.125003	-1.793809
6	5.190728	3.615705	-2.614606
6	3.184724	2.730017	0.538748
6	2.681867	3.748662	1.564649
6	2.116423	1.952820	-0.183687
8	-1.763851	1.609250	2.322688
7	0.927169	2.387174	-0.461784
1	3.689261	1.929360	1.113596
1	-1.136912	0.882439	2.141827
1	-2.549859	1.383972	1.809149
1	0.236850	1.634302	-0.766898
1	5.423960	4.072055	1.215467
1	3.338046	2.603068	-2.252728
1	7.203469	4.953044	-0.235974
1	5.121736	3.477640	-3.691143
1	7.071294	4.660049	-2.702338
1	1.831705	3.351366	2.129832
1	3.477570	3.953044	2.287783
1	2.387634	4.700555	1.113017
6	0.435052	3.729592	-0.373070
6	-0.628478	4.001165	0.481948
6	0.983321	4.707391	-1.198290
6	-1.100472	5.308346	0.545230
1	-1.051181	3.201120	1.100650
6	0.484852	6.003506	-1.134628
1	1.795018	4.453720	-1.876741
6	-0.550127	6.306281	-0.255685
1	-1.907805	5.552138	1.232784

1	0.907958	6.774684	-1.773446
1	-0.934033	7.322043	-0.197113
6	2.423943	0.547981	-0.527354
1	1.839374	0.199898	-1.382801
1	3.495398	0.404863	-0.701281
1	2.144974	-0.078597	0.334966
6	-3.060205	-4.547619	-2.950891
6	-1.807747	-4.849316	-2.116958
6	-2.044590	-4.109927	-0.774302
6	-2.775055	-2.885717	-1.272487
6	-3.476284	-3.194634	-2.441261
6	-4.407505	-2.304465	-2.955861
6	-4.638271	-1.107606	-2.281658
6	-3.895795	-0.737982	-1.154590
6	-2.919603	-1.635237	-0.693495
6	-0.791369	-4.076036	0.071948
6	-0.741103	-5.213654	0.883722
6	-2.038355	-5.969512	0.806110
6	-2.970549	-4.951252	0.142956
6	0.398188	-5.507831	1.617514
6	1.495710	-4.659823	1.513215
6	1.457685	-3.483404	0.755105
6	0.267249	-3.174787	0.076328
8	0.150834	-2.000742	-0.636156
15	-0.615768	-0.720776	0.067740
8	-0.017245	-0.421234	1.404162
8	-2.119664	-1.300332	0.378092
8	-0.665057	0.321324	-1.017182
6	2.719962	-2.698448	0.617081
1	2.421269	-4.902562	2.034049
1	0.441884	-6.393670	2.248940
1	-4.967082	-2.543305	-3.858909
1	-5.405670	-0.423136	-2.641210
6	-4.189570	0.520698	-0.416658
1	-2.864347	-4.548814	-4.030054
1	-3.847201	-5.296588	-2.775894
1	-0.922475	-4.408225	-2.599137
1	-1.616011	-5.920665	-1.980470
1	-1.931544	-6.874895	0.189728
1	-2.393309	-6.301008	1.789403
1	-3.390661	-4.282221	0.908673
1	-3.807396	-5.402187	-0.404100
6	-4.007251	1.783795	-1.013335
6	-4.299499	2.936538	-0.275001
6	-4.776546	2.879772	1.029453
6	-4.984365	1.618536	1.586592
6	-4.698601	0.441286	0.901978
1	-5.380151	1.555197	2.602251
6	3.456622	-2.781084	-0.586534
6	4.709355	-2.173262	-0.652373
6	5.275238	-1.498920	0.429501
6	4.522659	-1.407627	1.596120
6	3.254411	-1.988117	1.710587
1	5.287512	-2.246822	-1.575752
6	-3.527249	1.952254	-2.443461
6	-2.320347	2.878113	-2.551314
6	-4.660521	2.448401	-3.341096
1	-3.209169	0.969823	-2.813393
1	-1.516535	2.522604	-1.900829
1	-1.945170	2.895959	-3.582598

1	-2.556160	3.914400	-2.271656
1	-5.533588	1.784363	-3.308379
1	-4.998730	3.447697	-3.034645
1	-4.327796	2.517411	-4.384899
6	-4.978818	-0.870885	1.611627
6	-6.472525	-1.036698	1.882627
6	-4.167546	-1.001047	2.899541
1	-4.680477	-1.693382	0.951435
1	-7.055480	-0.979349	0.954863
1	-6.674805	-2.009053	2.349916
1	-6.848424	-0.259934	2.561652
1	-3.097988	-0.850574	2.713745
1	-4.484479	-0.266798	3.653089
1	-4.300846	-1.998729	3.338030
1	-4.149681	3.907417	-0.745806
6	-5.022345	4.100452	1.889950
6	-5.093153	5.406392	1.113916
6	-3.950222	4.180095	2.979077
1	-5.993311	3.951060	2.390591
1	-5.855713	5.376167	0.326316
1	-5.336326	6.237728	1.786366
1	-4.131120	5.642632	0.638074
1	-3.907526	3.266485	3.583010
1	-2.953896	4.294948	2.531318
1	-4.129235	5.031602	3.648160
1	4.933560	-0.880555	2.457418
6	2.944630	-3.513665	-1.815548
6	3.972453	-4.491340	-2.379594
6	2.499496	-2.525485	-2.895046
1	2.065150	-4.102855	-1.523058
1	4.340224	-5.181507	-1.610965
1	3.525703	-5.087848	-3.184651
1	4.840325	-3.972231	-2.807160
1	1.675324	-1.891871	-2.545601
1	3.332984	-1.875449	-3.198526
1	2.156063	-3.060673	-3.790265
6	6.649808	-0.880089	0.276515
6	7.372985	-0.643925	1.594790
6	6.568238	0.424864	-0.515750
1	7.249805	-1.589216	-0.316440
1	7.408829	-1.547749	2.214371
1	8.404013	-0.319394	1.410321
1	6.888503	0.148438	2.181659
1	6.098422	0.281816	-1.496941
1	5.978203	1.174310	0.032339
1	7.565768	0.852990	-0.679963
6	2.497315	-1.832217	3.017229
6	2.376589	-0.368855	3.437041
6	3.139551	-2.656787	4.131159
1	1.476438	-2.201616	2.856473
1	1.874182	0.215937	2.657325
1	1.767062	-0.287207	4.345816
1	3.354835	0.079655	3.660347
1	3.194437	-3.721386	3.871774
1	4.162584	-2.315549	4.341496
1	2.563553	-2.567662	5.061011

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i2'(*R*)

Number of imaginary frequencies : 0

Electronic energy : HF=-3141.6563473
Zero-point correction= 1.246387 (hartree/particle)
Thermal correction to Energy= 1.312687
Thermal correction to Enthalpy= 1.313631
Thermal correction to Gibbs Free Energy= 1.151716
Sum of electronic and zero-point Energies= -3140.409960
Sum of electronic and thermal Energies= -3140.343660
Sum of electronic and thermal Enthalpies= -3140.342716
Sum of electronic and thermal Free Energies= -3140.504631

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Cartesian Coordinates

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6	3.442014	-4.927493	2.098626
6	2.033716	-5.119889	1.527542
6	2.024097	-4.278816	0.223411
6	2.890648	-3.115445	0.654164
6	3.775655	-3.530808	1.654168
6	4.767742	-2.679540	2.116023
6	4.843434	-1.393120	1.592587
6	3.919349	-0.915645	0.655807
6	2.935599	-1.805717	0.192654
6	0.617465	-4.135399	-0.317450
6	0.322054	-5.225979	-1.140502
6	1.563614	-6.032975	-1.404023
6	2.674863	-5.090531	-0.926158
6	-0.968068	-5.425690	-1.608178
6	-1.953627	-4.503912	-1.270350
6	-1.669555	-3.346012	-0.535003
6	-0.355542	-3.173579	-0.072228
8	-0.020369	-2.046018	0.641924
15	0.585552	-0.775854	-0.206340
8	-0.217778	-0.456336	-1.416029
8	2.014542	-1.395398	-0.742541
8	0.858993	0.270202	0.846315
6	-2.761747	-2.362793	-0.285529
1	-2.976298	-4.657820	-1.611640
1	-1.208986	-6.285079	-2.231990
1	5.470028	-3.005197	2.881746
1	5.622860	-0.715548	1.938263
6	4.010279	0.499400	0.196762
1	3.484841	-5.043905	3.188271
1	4.147202	-5.659590	1.676293
1	1.291936	-4.692569	2.217728
1	1.764998	-6.169086	1.355334
1	1.560977	-6.971724	-0.829922
1	1.663378	-6.313200	-2.459697
1	2.944331	-4.391727	-1.731294
1	3.589233	-5.607714	-0.610391
6	3.842539	1.556734	1.121854
6	4.042071	2.869087	0.693539
6	4.412114	3.179375	-0.613123
6	4.532058	2.129074	-1.516261
6	4.336980	0.796634	-1.142309
1	4.802330	2.356577	-2.549904
6	-3.215143	-2.100815	1.025805
6	-4.345339	-1.299898	1.213234
6	-5.058721	-0.763483	0.144209
6	-4.565741	-0.994983	-1.137137

6	-3.427268	-1.763732	-1.378891
1	-4.701381	-1.132498	2.231475
1	3.922326	3.676393	1.417052
1	-5.106400	-0.572221	-1.987231
6	-1.022588	4.025044	-1.678598
1	-0.965245	3.822252	-2.759804
6	-0.115917	2.979157	-1.077593
7	-0.225595	2.507011	0.120203
6	0.946297	2.408933	-1.939450
1	1.820721	2.089506	-1.360435
1	0.524445	1.505637	-2.410809
1	1.248771	3.109378	-2.724555
6	-0.415782	5.413454	-1.468183
1	-1.008159	6.160736	-2.006126
1	-0.388828	5.692012	-0.408874
1	0.607327	5.455266	-1.855706
6	-2.482532	3.888827	-1.299171
6	-3.161608	2.740137	-1.713897
6	-3.183417	4.868098	-0.597209
6	-4.511962	2.576961	-1.438085
1	-2.621926	1.953048	-2.245202
6	-4.534941	4.699702	-0.308377
1	-2.675998	5.768105	-0.256467
6	-5.205059	3.558812	-0.734785
1	-5.022717	1.675241	-1.770163
1	-5.065029	5.470040	0.247389
1	-6.264754	3.432114	-0.520586
6	-1.176608	2.854928	1.131449
6	-0.996221	4.012697	1.879808
6	-2.186043	1.943933	1.427819
6	-1.883766	4.293729	2.913466
1	-0.155785	4.668825	1.657781
6	-3.059841	2.232994	2.467969
1	-2.295344	1.036385	0.831906
6	-2.917708	3.408597	3.202618
1	-1.757327	5.199255	3.501813
1	-3.850862	1.523811	2.703980
1	-3.605857	3.625635	4.016098
1	0.363907	1.641320	0.382612
6	4.518168	-0.271369	-2.204844
6	5.937307	-0.263499	-2.769029
6	3.482653	-0.121918	-3.317568
1	4.359077	-1.252213	-1.739996
1	6.684586	-0.378179	-1.974232
1	6.073378	-1.086605	-3.482026
1	6.159097	0.670565	-3.302261
1	2.464854	-0.198428	-2.916555
1	3.585420	0.843296	-3.834041
1	3.607169	-0.910917	-4.070570
6	4.624897	4.609597	-1.056587
6	5.450164	5.428851	-0.070857
6	3.279212	5.283109	-1.317301
1	5.173403	4.576006	-2.011013
1	6.400676	4.937634	0.167130
1	5.673519	6.419344	-0.486097
1	4.911818	5.588632	0.872500
1	2.731344	4.761404	-2.112967
1	2.656447	5.264506	-0.409705
1	3.402815	6.331032	-1.620610
6	3.487596	1.337644	2.583232

6	2.257065	2.130348	3.017651
6	4.671604	1.683128	3.487291
1	3.249081	0.276916	2.721688
1	1.379941	1.830460	2.436736
1	2.039043	1.935537	4.075648
1	2.405918	3.214138	2.914305
1	5.581242	1.137300	3.209252
1	4.908033	2.754951	3.437281
1	4.442301	1.445149	4.533966
6	-2.968251	-1.918255	-2.818625
6	-2.666968	-0.567032	-3.462747
6	-3.986821	-2.688823	-3.656733
1	-2.026119	-2.478287	-2.818279
1	-1.908671	-0.039150	-2.873092
1	-2.273459	-0.710704	-4.477796
1	-3.568441	0.056812	-3.550438
1	-4.208735	-3.676666	-3.234376
1	-4.937697	-2.143127	-3.728342
1	-3.614950	-2.836034	-4.678871
6	-6.377750	-0.046857	0.334912
6	-6.371995	0.959177	1.478416
6	-7.498641	-1.067983	0.526561
1	-6.585114	0.505549	-0.597113
1	-5.561836	1.690785	1.367234
1	-7.322428	1.507615	1.513640
1	-6.255306	0.464469	2.452554
1	-7.546189	-1.771127	-0.313481
1	-7.331381	-1.654225	1.440347
1	-8.474934	-0.574361	0.617265
6	-2.563421	-2.700648	2.258502
6	-3.525573	-3.629590	2.996801
6	-2.017818	-1.618366	3.186830
1	-1.712342	-3.312947	1.939251
1	-3.903130	-4.418751	2.334538
1	-3.023234	-4.112188	3.845082
1	-4.392900	-3.085950	3.394156
1	-1.309859	-0.965257	2.661759
1	-2.824113	-0.995441	3.599309
1	-1.489893	-2.071454	4.036035

$TS_{R\text{-}m}$

Number of imaginary frequencies : 1
Imaginary Frequency : -1618.7893 cm(-1)

Electronic energy : HF=-3141.6228658
Zero-point correction= 1.244564 (hartree/particle)
Thermal correction to Energy= 1.309851
Thermal correction to Enthalpy= 1.310795
Thermal correction to Gibbs Free Energy= 1.152508
Sum of electronic and zero-point Energies= -3140.378302
Sum of electronic and thermal Energies= -3140.313015
Sum of electronic and thermal Enthalpies= -3140.312071
Sum of electronic and thermal Free Energies= -3140.470358

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Cartesian Coordinates

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6	-0.491198	6.258395	-1.299249
6	-1.750208	5.413336	-1.076799

6	-1.394703	4.507697	0.131288
6	0.063418	4.233519	-0.168437
6	0.602364	5.323589	-0.861321
6	1.968171	5.416011	-1.080141
6	2.787122	4.375999	-0.652994
6	2.266782	3.213530	-0.073510
6	0.884861	3.166026	0.169119
6	-2.451249	3.444863	0.365937
6	-3.460334	3.980235	1.176346
6	-3.044038	5.314398	1.728596
6	-1.540827	5.323885	1.442583
6	-4.639058	3.286114	1.399142
6	-4.774921	2.013793	0.858683
6	-3.738493	1.394896	0.149644
6	-2.573929	2.139545	-0.102345
8	-1.566572	1.581976	-0.858992
15	-0.255654	0.863472	-0.192330
8	-0.693477	-0.199973	0.815416
8	0.335565	2.049221	0.762921
8	0.630792	0.471288	-1.315602
6	-3.887281	-0.040359	-0.221185
1	-5.687434	1.445020	1.032701
1	-5.434574	3.718704	2.003592
1	2.393808	6.277826	-1.591727
1	3.861969	4.431287	-0.815963
6	3.155492	2.046097	0.183366
1	-0.369335	6.580837	-2.340409
1	-0.508992	7.173624	-0.688772
1	-1.928256	4.769777	-1.949701
1	-2.657005	6.005975	-0.907155
1	-3.556461	6.141624	1.214893
1	-3.280524	5.414329	2.794815
1	-1.005853	4.790863	2.241379
1	-1.109310	6.328652	1.364086
6	3.763053	1.393769	-0.915939
6	4.592744	0.304361	-0.673343
6	4.847755	-0.177350	0.612096
6	4.255225	0.488728	1.677385
6	3.404263	1.582963	1.488126
1	4.424928	0.132733	2.693454
6	-3.968683	-0.454837	-1.567507
6	-4.205235	-1.800586	-1.852856
6	-4.366198	-2.755300	-0.849651
6	-4.259593	-2.329361	0.469781
6	-4.027747	-0.995034	0.810112
1	-4.280095	-2.109530	-2.897617
1	5.040815	-0.217292	-1.521300
1	-4.377268	-3.065106	1.267216
6	0.654055	-2.451004	0.533268
1	-0.035066	-1.330766	0.601970
6	0.474633	-2.604390	-0.878309
7	1.477588	-2.704114	-1.755068
6	-0.871809	-2.442188	-1.490571
1	-1.658933	-2.356971	-0.736779
1	-0.855620	-1.499821	-2.058853
1	-1.106220	-3.252482	-2.191640
6	2.762902	-3.277514	-1.577496
6	3.804141	-2.838699	-2.393263
6	2.970529	-4.324664	-0.678195
6	5.060686	-3.423312	-2.287343

1	3.622455	-2.033179	-3.101439
6	4.235014	-4.891033	-0.567394
1	2.143260	-4.698474	-0.077750
6	5.284194	-4.443493	-1.366638
1	5.870844	-3.069186	-2.921252
1	4.394288	-5.700390	0.140992
1	6.270579	-4.892121	-1.275427
1	1.258805	-2.436534	-2.712006
6	2.776783	2.219025	2.714158
6	3.837679	2.788494	3.653407
6	1.868010	1.235402	3.451944
1	2.151019	3.057909	2.383050
1	4.483953	3.509670	3.138275
1	3.368312	3.301207	4.502923
1	4.481315	1.998199	4.062189
1	1.096596	0.830864	2.783973
1	2.443731	0.398601	3.872788
1	1.360859	1.733455	4.288742
6	5.682912	-1.431651	0.765061
6	5.662734	-2.038289	2.158508
6	7.121871	-1.208281	0.304362
1	5.238016	-2.171673	0.079934
1	4.640352	-2.227609	2.510006
1	6.197636	-2.996701	2.157681
1	6.158159	-1.388362	2.893113
1	7.167611	-0.819680	-0.720219
1	7.632608	-0.486404	0.956172
1	7.688778	-2.148712	0.331571
6	3.544795	1.830397	-2.354299
6	3.181729	0.671640	-3.277638
6	4.774497	2.556971	-2.900224
1	2.697538	2.525851	-2.374045
1	2.368343	0.083437	-2.838122
1	2.847225	1.056749	-4.249550
1	4.048116	0.024026	-3.473220
1	5.046758	3.431480	-2.297142
1	5.647131	1.889225	-2.915964
1	4.600371	2.899187	-3.928898
6	-3.964121	-0.648604	2.288086
6	-2.863388	-1.421395	3.002827
6	-5.313968	-0.883242	2.964871
1	-3.719863	0.415276	2.386912
1	-1.889306	-1.196837	2.556897
1	-2.828117	-1.144620	4.065618
1	-3.018597	-2.507528	2.953513
1	-6.125299	-0.333158	2.471430
1	-5.585151	-1.947733	2.952402
1	-5.280428	-0.565429	4.014887
6	-4.697792	-4.196322	-1.171279
6	-3.641967	-4.858307	-2.049918
6	-6.077080	-4.305109	-1.817988
1	-4.725049	-4.741895	-0.214825
1	-2.659961	-4.855493	-1.560190
1	-3.908173	-5.901129	-2.264302
1	-3.540989	-4.340111	-3.013509
1	-6.851290	-3.852932	-1.187172
1	-6.097365	-3.789586	-2.787565
1	-6.348790	-5.353814	-1.993870
6	-3.862981	0.520908	-2.725502
6	-5.142303	0.534045	-3.559798

6	-2.645847	0.229224	-3.600164
1	-3.736073	1.528666	-2.310906
1	-6.022467	0.746574	-2.940833
1	-5.084747	1.302460	-4.341198
1	-5.311291	-0.429104	-4.059297
1	-1.715473	0.317212	-3.025152
1	-2.699877	-0.779784	-4.033983
1	-2.589597	0.940916	-4.434194
6	-0.121074	-3.348526	1.448388
6	-0.851499	-4.451342	0.984446
6	-0.078017	-3.132249	2.832186
6	-1.539977	-5.282963	1.861975
1	-0.860733	-4.687482	-0.079340
6	-0.743910	-3.976686	3.711527
1	0.471299	-2.278871	3.227193
6	-1.486494	-5.052804	3.232692
1	-2.099906	-6.129801	1.468413
1	-0.693332	-3.781591	4.780832
6	2.007542	-1.999673	1.040826
1	1.869079	-1.352877	1.916199
1	2.676767	-2.820127	1.336113
1	2.510870	-1.383874	0.286718
1	-2.010323	-5.710520	3.922474

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Number of imaginary frequencies : 0

Electronic energy : HF=-3141.645743
Zero-point correction= 1.247843 (hartree/particle)
Thermal correction to Energy= 1.314572
Thermal correction to Enthalpy= 1.315517
Thermal correction to Gibbs Free Energy= 1.152896
Sum of electronic and zero-point Energies= -3140.397900
Sum of electronic and thermal Energies= -3140.331171
Sum of electronic and thermal Enthalpies= -3140.330226
Sum of electronic and thermal Free Energies= -3140.492847

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Cartesian Coordinates

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6	-1.395369	5.586896	2.115893
6	-0.014682	5.289132	1.519889
6	-0.318426	4.476395	0.234760
6	-1.503605	3.664449	0.709432
6	-2.196424	4.389971	1.685405
6	-3.433531	3.958439	2.136528
6	-3.955068	2.769813	1.636546
6	-3.239380	1.957712	0.749046
6	-1.999032	2.435787	0.299561
6	0.942359	3.894867	-0.372353
6	1.513427	4.839958	-1.232245
6	0.578297	5.996911	-1.441947
6	-0.742473	5.443124	-0.902698
6	2.769876	4.631397	-1.778549
6	3.426281	3.436856	-1.511054
6	2.837632	2.413094	-0.756352
6	1.585516	2.678510	-0.179902
8	0.998021	1.725859	0.642630
15	-0.136512	0.710977	0.127462

8	0.448169	-0.027766	-1.141102
8	-1.235168	1.659454	-0.573854
8	-0.612943	-0.126000	1.240728
6	3.545270	1.105281	-0.653233
1	4.415202	3.258614	-1.929887
1	3.229686	5.381499	-2.419498
1	-3.987054	4.532533	2.877552
1	-4.931092	2.424967	1.972716
6	-3.794998	0.639467	0.331921
1	-1.374883	5.701747	3.206109
1	-1.816013	6.519361	1.711175
1	0.559816	4.650963	2.206160
1	0.582495	6.186421	1.319978
1	0.902383	6.883242	-0.876612
1	0.521208	6.300253	-2.494018
1	-1.247843	4.855323	-1.682604
1	-1.441405	6.214403	-0.559386
6	-4.032545	-0.367872	1.297679
6	-4.585272	-1.579834	0.886409
6	-4.943715	-1.826929	-0.437410
6	-4.720516	-0.814934	-1.364802
6	-4.138975	0.405518	-1.014905
1	-5.024532	-0.977489	-2.400762
6	3.975119	0.598843	0.592220
6	4.721647	-0.580280	0.626235
6	5.093261	-1.258465	-0.531723
6	4.654565	-0.745904	-1.748972
6	3.868432	0.403442	-1.838962
1	5.055983	-0.956446	1.594471
1	-4.755165	-2.355782	1.634235
1	4.912498	-1.282867	-2.664015
6	0.674478	-3.042539	-1.060296
1	0.468593	-1.008296	-1.007455
6	0.438505	-3.068227	0.292632
7	1.521621	-2.954703	1.147674
6	-0.909440	-3.305316	0.897039
1	-1.454921	-2.368240	1.063812
1	-1.514279	-3.925534	0.228161
1	-0.824369	-3.818414	1.860937
6	2.099493	-2.942269	-1.542721
1	2.692229	-3.850890	-1.334877
1	2.145617	-2.772266	-2.622094
1	2.624377	-2.099700	-1.071418
6	-0.358436	-3.308720	-2.084322
6	-0.065584	-4.187761	-3.141753
6	-1.612310	-2.678795	-2.098500
6	-0.981517	-4.439823	-4.153823
1	0.898005	-4.694992	-3.157639
6	-2.527652	-2.927965	-3.116766
1	-1.875955	-1.962036	-1.318196
6	-2.222798	-3.809483	-4.147945
1	-0.724412	-5.133858	-4.951724
1	-3.484243	-2.407754	-3.099705
1	-2.941339	-3.996548	-4.942767
6	1.570279	-2.943342	2.553080
6	0.729114	-2.141062	3.328797
6	2.563015	-3.704259	3.181843
6	0.864663	-2.133813	4.712228
1	0.026733	-1.475843	2.833620
6	2.706402	-3.669897	4.563285

1	3.214516	-4.331751	2.573494
6	1.850098	-2.892570	5.338304
1	0.207123	-1.500119	5.304455
1	3.485041	-4.264532	5.036529
1	1.956658	-2.870783	6.420281
1	2.432383	-3.066569	0.720973
6	-3.961417	1.444161	-2.105833
6	-5.315226	1.915366	-2.633543
6	-3.078112	0.930081	-3.239832
1	-3.465723	2.321728	-1.673513
1	-5.939592	2.316859	-1.825567
1	-5.186243	2.703928	-3.386043
1	-5.870314	1.094900	-3.107421
1	-2.110832	0.572987	-2.865233
1	-3.556609	0.102628	-3.781108
1	-2.886341	1.727134	-3.969665
6	-5.589661	-3.133907	-0.841629
6	-6.983273	-3.266865	-0.230824
6	-4.725313	-4.338415	-0.479595
1	-5.702215	-3.116192	-1.937566
1	-7.619266	-2.412357	-0.491037
1	-7.478851	-4.180834	-0.582028
1	-6.929408	-3.319921	0.864728
1	-3.741147	-4.284975	-0.962172
1	-4.566538	-4.403405	0.605476
1	-5.207176	-5.271859	-0.797022
6	-3.765470	-0.179777	2.782063
6	-2.934988	-1.307842	3.383288
6	-5.081404	-0.037230	3.548778
1	-3.187508	0.742788	2.916799
1	-1.970160	-1.382247	2.875368
1	-2.748973	-1.114301	4.447811
1	-3.438469	-2.281531	3.314269
1	-5.715373	0.762974	3.147250
1	-5.665404	-0.966519	3.501058
1	-4.892242	0.180282	4.607837
6	3.388211	0.824553	-3.219659
6	2.533578	-0.249533	-3.891136
6	4.558103	1.199292	-4.128081
1	2.751056	1.709738	-3.110654
1	1.664162	-0.518175	-3.279279
1	2.159597	0.118796	-4.855084
1	3.110372	-1.161728	-4.095564
1	5.190763	1.979614	-3.687813
1	5.201501	0.331419	-4.326224
1	4.194399	1.565689	-5.096436
6	5.962510	-2.495489	-0.481512
6	5.412330	-3.565237	0.456927
6	7.395386	-2.133673	-0.093761
1	5.983043	-2.918495	-1.498514
1	4.408177	-3.890923	0.152542
1	6.058338	-4.452116	0.457492
1	5.354225	-3.203147	1.492158
1	7.815423	-1.382174	-0.772532
1	7.433074	-1.720680	0.923250
1	8.045865	-3.017176	-0.118266
6	3.725541	1.312930	1.907810
6	5.038936	1.755362	2.550651
6	2.908014	0.450514	2.865048
1	3.147151	2.222320	1.705421

1	5.625710	2.387070	1.872273
1	4.844347	2.330006	3.465197
1	5.663133	0.896258	2.829674
1	1.958616	0.143521	2.410228
1	3.450295	-0.458949	3.160620
1	2.675419	1.003738	3.784464

$TS_{m\text{-}s}$

Number of imaginary frequencies : 1
Imaginary Frequency : -1295.7344 cm(-1)

Electronic energy : HF=-3141.6352802
Zero-point correction= 1.243467 (hartree/particle)
Thermal correction to Energy= 1.309330
Thermal correction to Enthalpy= 1.310275
Thermal correction to Gibbs Free Energy= 1.150019
Sum of electronic and zero-point Energies= -3140.391814
Sum of electronic and thermal Energies= -3140.325950
Sum of electronic and thermal Enthalpies= -3140.325006
Sum of electronic and thermal Free Energies= -3140.485262

.....

Cartesian Coordinates

.....

6	-1.075977	5.582211	2.242821
6	0.279242	5.239179	1.614509
6	-0.082833	4.480354	0.311570
6	-1.294846	3.706901	0.784621
6	-1.937048	4.434688	1.793296
6	-3.185015	4.049779	2.256665
6	-3.770916	2.903183	1.730501
6	-3.105949	2.087509	0.808374
6	-1.846925	2.509555	0.349476
6	1.140960	3.861802	-0.331486
6	1.744844	4.804767	-1.170439
6	0.860545	6.009072	-1.332321
6	-0.477405	5.500171	-0.789573
6	2.985707	4.557251	-1.736578
6	3.589783	3.327401	-1.506914
6	2.961516	2.313639	-0.772113
6	1.724745	2.610005	-0.174227
8	1.106666	1.673175	0.626837
15	-0.057378	0.680851	0.063223
8	0.465193	-0.063278	-1.170964
8	-1.147756	1.728317	-0.555050
8	-0.572123	-0.100047	1.214211
6	3.607543	0.973764	-0.700229
1	4.565997	3.116013	-1.940816
1	3.472828	5.303830	-2.361441
1	-3.697556	4.627809	3.023888
1	-4.759224	2.596843	2.069150
6	-3.721535	0.810980	0.352385
1	-1.032908	5.666243	3.335413
1	-1.459914	6.543721	1.870290
1	0.833189	4.552843	2.270875
1	0.915440	6.113275	1.431920
1	1.232493	6.862388	-0.745758
1	0.803028	6.347104	-2.373940
1	-1.020101	4.960701	-1.579462

1	-1.134840	6.292859	-0.413842
6	-3.985236	-0.223175	1.280184
6	-4.555176	-1.411628	0.823891
6	-4.899152	-1.610189	-0.511700
6	-4.670008	-0.562951	-1.397957
6	-4.077564	0.636889	-1.000820
1	-4.967007	-0.685691	-2.441413
6	4.017783	0.424695	0.533122
6	4.675737	-0.807358	0.546535
6	4.975082	-1.500878	-0.623904
6	4.574374	-0.935180	-1.830810
6	3.875071	0.271000	-1.898311
1	4.993282	-1.219133	1.506214
1	-4.743458	-2.210013	1.543623
1	4.783278	-1.478241	-2.754832
6	0.415693	-2.677729	-1.078030
1	0.354232	-1.317081	-1.057788
6	0.258125	-2.915417	0.312724
7	1.334833	-2.868927	1.106215
6	-1.080491	-3.203873	0.890678
1	-1.746419	-2.346890	0.723076
1	-1.514926	-4.066096	0.370789
1	-1.042890	-3.410548	1.961965
6	1.819588	-2.863053	-1.630497
1	2.230533	-3.865601	-1.427624
1	1.819109	-2.720607	-2.714911
1	2.516002	-2.118726	-1.226520
6	-0.679200	-3.140070	-1.997654
6	-0.603986	-4.405946	-2.593704
6	-1.756780	-2.315232	-2.328259
6	-1.568304	-4.832346	-3.499477
1	0.230385	-5.061325	-2.344066
6	-2.716713	-2.736873	-3.245116
1	-1.850015	-1.331573	-1.863850
6	-2.626820	-3.992437	-3.835801
1	-1.489528	-5.820403	-3.948816
1	-3.545545	-2.075734	-3.492353
1	-3.377977	-4.316822	-4.552869
6	1.405532	-2.963104	2.529447
6	0.710026	-2.071933	3.343304
6	2.254936	-3.919532	3.083067
6	0.849522	-2.163594	4.724146
1	0.110999	-1.292624	2.874968
6	2.400978	-3.989943	4.464162
1	2.789932	-4.606019	2.428761
6	1.693481	-3.116944	5.286190
1	0.309819	-1.466728	5.361605
1	3.064786	-4.734086	4.897908
1	1.806411	-3.176413	6.366182
1	2.230591	-2.707674	0.650110
6	-3.891940	1.721713	-2.045113
6	-5.242680	2.213719	-2.561585
6	-3.000271	1.263241	-3.196550
1	-3.398406	2.577960	-1.569703
1	-5.874810	2.577838	-1.742104
1	-5.109842	3.034720	-3.277901
1	-5.791998	1.413496	-3.075454
1	-2.032367	0.897630	-2.831043
1	-3.475683	0.462642	-3.779773
1	-2.807563	2.094385	-3.887260

6	-5.531235	-2.904702	-0.973382
6	-6.957715	-3.037403	-0.444647
6	-4.695957	-4.122070	-0.586697
1	-5.580586	-2.868397	-2.073839
1	-7.575297	-2.179550	-0.736449
1	-7.435510	-3.948430	-0.827238
1	-6.966140	-3.093993	0.652130
1	-3.673408	-4.041599	-0.976218
1	-4.635625	-4.236415	0.504436
1	-5.140339	-5.041937	-0.987960
6	-3.713883	-0.091891	2.769518
6	-2.900898	-1.253204	3.329433
6	-5.025211	0.051452	3.542906
1	-3.116531	0.813071	2.932137
1	-1.951252	-1.334180	2.794473
1	-2.686964	-1.086750	4.393598
1	-3.432565	-2.211857	3.252876
1	-5.638693	0.882855	3.174313
1	-5.632217	-0.860455	3.458163
1	-4.831358	0.221668	4.609901
6	3.420135	0.750633	-3.267691
6	2.495287	-0.249065	-3.959035
6	4.611915	1.073082	-4.167494
1	2.839185	1.669930	-3.135879
1	1.618192	-0.472019	-3.340069
1	2.138904	0.168334	-4.909676
1	3.012664	-1.189479	-4.194348
1	5.285374	1.810655	-3.713626
1	5.206744	0.173709	-4.377745
1	4.271930	1.474074	-5.130822
6	5.719191	-2.817885	-0.594401
6	5.097909	-3.822503	0.372312
6	7.193650	-2.598902	-0.261034
1	5.658645	-3.246280	-1.607685
1	4.039007	-4.007454	0.141298
1	5.619830	-4.786175	0.319202
1	5.164877	-3.475158	1.412130
1	7.661577	-1.901403	-0.965530
1	7.307010	-2.177162	0.746875
1	7.752108	-3.543042	-0.292796
6	3.831851	1.140657	1.858093
6	5.178692	1.505377	2.479225
6	2.985322	0.315285	2.821689
1	3.295978	2.079167	1.673483
1	5.781458	2.119800	1.799071
1	5.033428	2.071668	3.408068
1	5.764554	0.610695	2.727853
1	2.020177	0.058419	2.368703
1	3.490781	-0.616671	3.114682
1	2.783155	0.876818	3.743374

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i2'(*S*)

Number of imaginary frequencies : 0

Electronic energy : HF=-3141.6614691
Zero-point correction= 1.247976 (hartree/particle)
Thermal correction to Energy= 1.313689
Thermal correction to Enthalpy= 1.314633

Thermal correction to Gibbs Free Energy= 1.154885
Sum of electronic and zero-point Energies= -3140.413493
Sum of electronic and thermal Energies= -3140.347781
Sum of electronic and thermal Enthalpies= -3140.346836
Sum of electronic and thermal Free Energies= -3140.506584

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Cartesian Coordinates

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6	-0.788452	4.594005	2.782803
6	0.482980	4.406175	1.946565
6	-0.028820	4.021033	0.532910
6	-1.239379	3.200656	0.907244
6	-1.737219	3.615250	2.146021
6	-2.940106	3.111112	2.618880
6	-3.627249	2.178786	1.845049
6	-3.113192	1.678607	0.643148
6	-1.891083	2.205394	0.193652
6	1.103879	3.508341	-0.327965
6	1.702868	4.575238	-1.003416
6	0.886493	5.826778	-0.832231
6	-0.431106	5.289474	-0.261881
6	2.890107	4.392369	-1.696593
6	3.483421	3.133438	-1.684769
6	2.877642	2.033033	-1.066806
6	1.643657	2.231521	-0.429083
8	0.963921	1.171487	0.133125
15	-0.245362	0.501970	-0.798343
8	0.255688	0.139465	-2.145931
8	-1.305788	1.742846	-0.964403
8	-0.859546	-0.505576	0.140526
6	3.645076	0.756522	-0.983086
1	4.448973	2.983036	-2.166929
1	3.364014	5.220445	-2.221160
1	-3.347369	3.440430	3.573815
1	-4.588632	1.799434	2.187426
6	-3.871644	0.637013	-0.107340
1	-0.631876	4.400382	3.851346
1	-1.168759	5.623743	2.705204
1	1.063299	3.556260	2.341289
1	1.141027	5.283632	1.932084
1	1.373227	6.522490	-0.131914
1	0.752734	6.374182	-1.773099
1	-1.094292	4.982106	-1.083483
1	-0.976531	6.015163	0.353726
6	-4.069310	-0.645201	0.455153
6	-4.868209	-1.565090	-0.221303
6	-5.471069	-1.270861	-1.443152
6	-5.238986	-0.015412	-1.992217
6	-4.450098	0.944503	-1.353944
1	-5.697442	0.229388	-2.952156
6	4.304249	0.442031	0.224085
6	5.160487	-0.661743	0.268591
6	5.403083	-1.451840	-0.853347
6	4.721558	-1.136080	-2.027149
6	3.841649	-0.056807	-2.117444
1	5.681289	-0.882650	1.202194
1	-5.020634	-2.549308	0.224595
1	4.889983	-1.759095	-2.908023
6	1.495128	-2.902902	-0.259929
1	1.504467	-1.923058	-0.773687

6	1.585812	-2.589181	1.220937
7	0.638420	-1.848978	1.701030
6	2.713864	-3.084944	2.039964
1	3.647037	-2.787497	1.541847
1	2.709226	-2.686850	3.056146
1	2.718475	-4.182045	2.081070
6	0.341766	-1.489651	3.042803
6	0.355979	-2.430573	4.071597
6	-0.117157	-0.188523	3.263309
6	-0.056887	-2.050759	5.343417
1	0.635903	-3.461312	3.863482
6	-0.527713	0.174788	4.538997
1	-0.161176	0.513419	2.429630
6	-0.493512	-0.750470	5.579658
1	-0.056265	-2.781800	6.148049
1	-0.889220	1.184930	4.715381
1	-0.823754	-0.462061	6.574604
1	-0.026382	-1.367971	0.986861
6	-4.286202	2.294501	-2.027266
6	-5.621459	3.030923	-2.112465
6	-3.641467	2.163334	-3.404579
1	-3.619235	2.911845	-1.412982
1	-6.069242	3.158494	-1.118603
1	-5.489260	4.026824	-2.555073
1	-6.343024	2.486022	-2.735736
1	-2.683632	1.634142	-3.346077
1	-4.289598	1.617519	-4.103396
1	-3.456354	3.154618	-3.838590
6	-6.392964	-2.257198	-2.126144
6	-7.711457	-2.375085	-1.363219
6	-5.760169	-3.632754	-2.308899
1	-6.618199	-1.853078	-3.125625
1	-8.191454	-1.396644	-1.241937
1	-8.413158	-3.037766	-1.886211
1	-7.546865	-2.790034	-0.359449
1	-4.830724	-3.575759	-2.888523
1	-5.525610	-4.094336	-1.340104
1	-6.445805	-4.308537	-2.835836
6	-3.439063	-1.069862	1.770688
6	-2.774864	-2.441267	1.675869
6	-4.447674	-1.071705	2.917856
1	-2.645487	-0.349078	2.006392
1	-2.119743	-2.494692	0.800518
1	-2.175786	-2.631664	2.579237
1	-3.509464	-3.255036	1.602142
1	-4.923203	-0.094611	3.062453
1	-5.248031	-1.802739	2.736087
1	-3.953005	-1.346610	3.860003
6	3.151124	0.224921	-3.437796
6	2.464993	-1.015249	-4.003288
6	4.135115	0.795785	-4.457807
1	2.363374	0.965140	-3.248651
1	1.761973	-1.436941	-3.276662
1	1.887486	-0.749584	-4.897599
1	3.187425	-1.788633	-4.299467
1	4.602477	1.722866	-4.103771
1	4.940903	0.080048	-4.673331
1	3.626501	1.017841	-5.404626
6	6.424171	-2.571603	-0.854260
6	6.419475	-3.431682	0.404222

6	7.818894	-1.991832	-1.090056
1	6.180531	-3.224541	-1.708082
1	5.439422	-3.890365	0.590496
1	7.149785	-4.244655	0.310130
1	6.699940	-2.854298	1.295174
1	7.854664	-1.401107	-2.013040
1	8.102985	-1.329268	-0.261076
1	8.573496	-2.785468	-1.161540
6	4.138963	1.278173	1.480720
6	5.470263	1.835464	1.975703
6	3.425806	0.484931	2.571305
1	3.501827	2.138668	1.240031
1	5.972485	2.415834	1.191797
1	5.313800	2.496188	2.837768
1	6.156910	1.039748	2.294106
1	2.470653	0.098089	2.195338
1	4.034243	-0.364442	2.914399
1	3.213558	1.114071	3.445991
6	0.169526	-3.583215	-0.569231
6	-0.672263	-3.072876	-1.556617
6	-0.202640	-4.743147	0.116150
6	-1.870683	-3.716199	-1.851454
1	-0.403913	-2.147648	-2.066798
6	-1.400617	-5.384319	-0.179594
1	0.449826	-5.152014	0.890690
6	-2.237946	-4.869827	-1.166577
1	-2.523639	-3.299845	-2.616092
1	-1.681756	-6.284543	0.362944
6	2.649971	-3.735600	-0.805195
1	2.684839	-4.734914	-0.352338
1	2.504586	-3.872286	-1.882682
1	3.616870	-3.242145	-0.667338
1	-3.178468	-5.366394	-1.398520