

Electronic Supplementary Information
for

**Insights into the Role of Noncovalent Interactions in Distal Functionalization
of Aryl C(sp²)-H Bond**

*Anju Unnikrishnan and Raghavan B. Sunoj**

Department of Chemistry

Indian Institute of Technology Bombay

Powai, Mumbai 400076

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

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1. Model Systems used for Initial Investigations

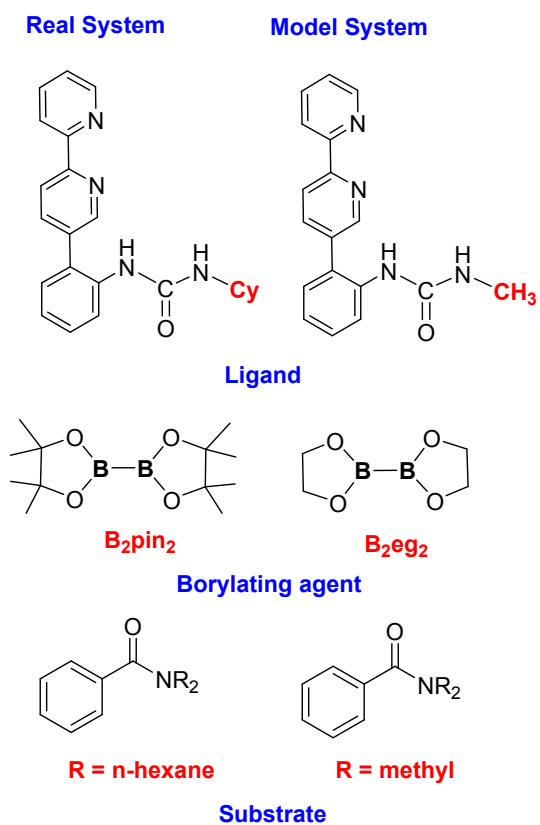


Fig. S1 Comparison of the real and model system used for the preliminary mechanistic study focusing on conformationally and configurationally different possibilities.

2. The Configurational Study for the Active Catalyst



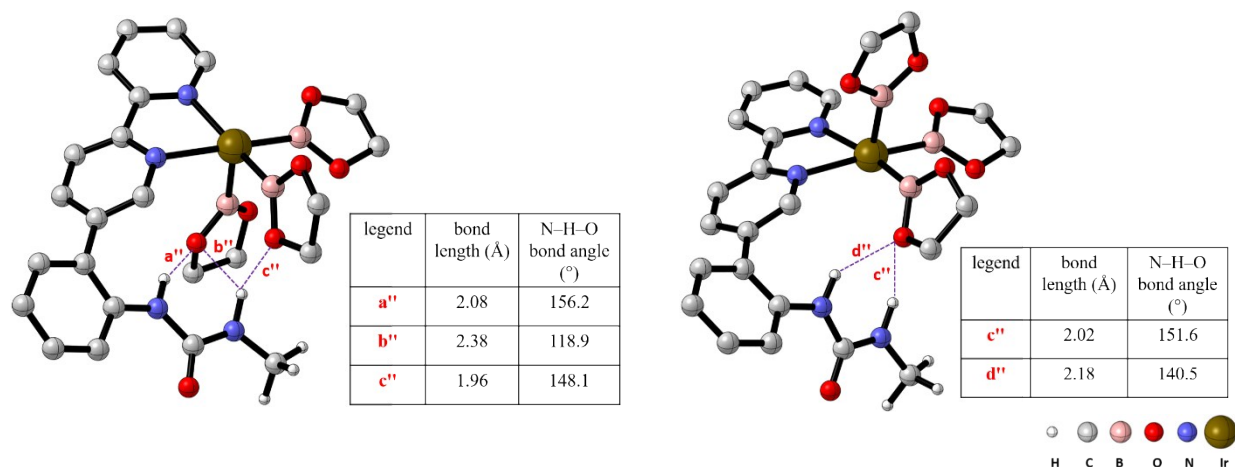


Fig. S2 The two possible configurations for the active catalyst with the N-H $\cdots$ O hydrogen bonding. Selected hydrogen atoms are removed for improved clarity. The relative Gibbs free energies in kcal/mol are provided in parentheses. The distances are in Å and the bond angles in degrees.

3. Different Binding Modes of the Substrate with the Catalyst in the Catalyst-Substrate Complex

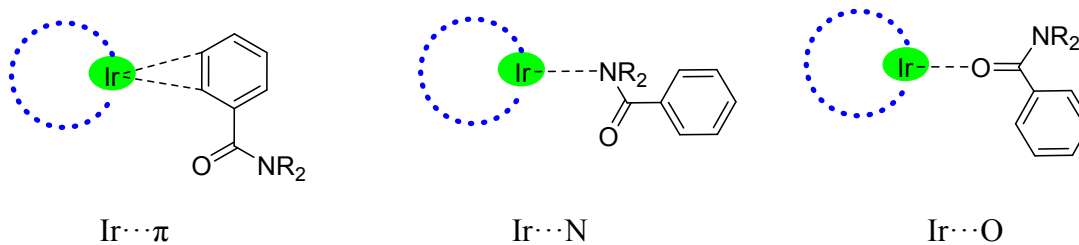


Fig. S3 Different modes of substrate coordination in the catalyst-substrate complex (The catalyst part is depicted using a dotted circle to convey the site of substrate coordination more clear).

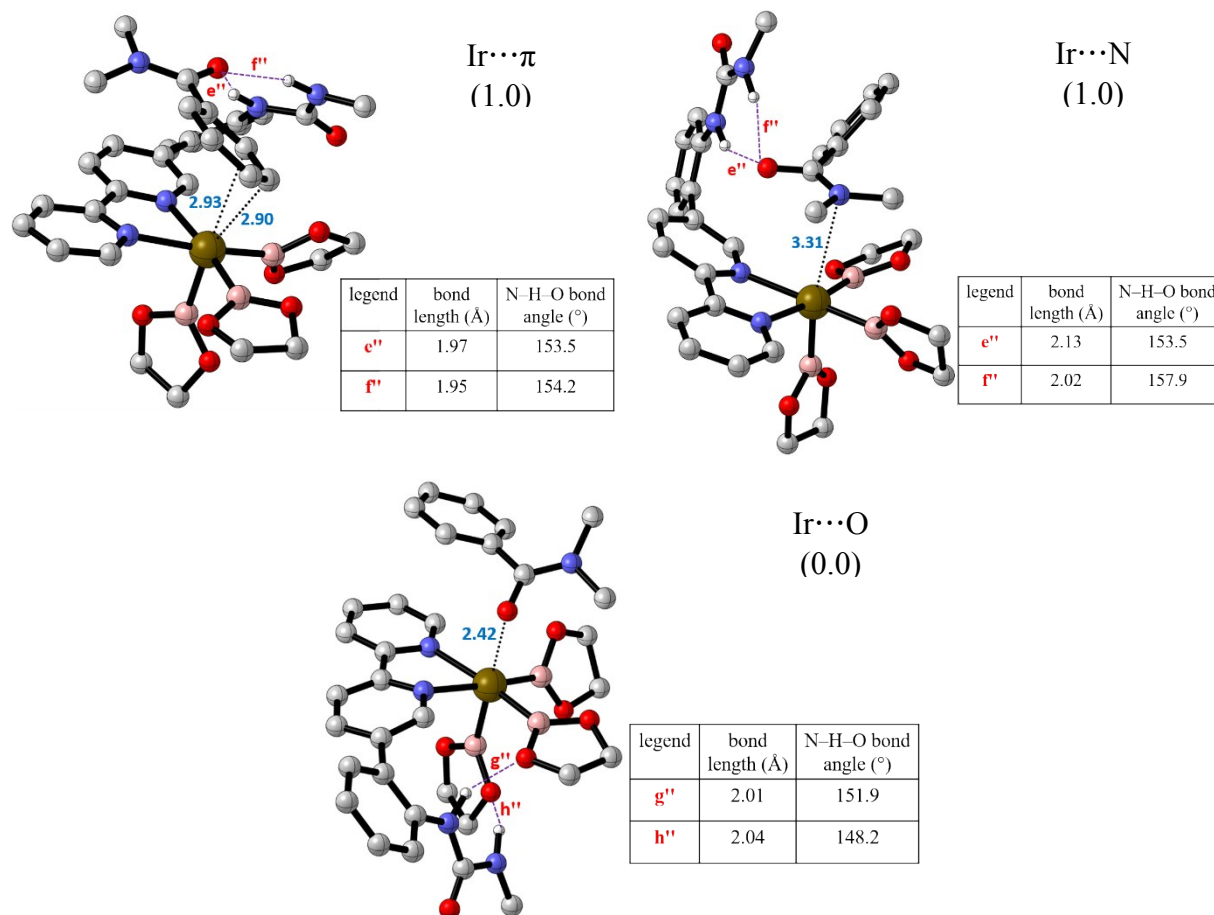


Fig. S4 Optimized geometries of different binding modes in the catalyst-substrate complex for *N,N*-dimethylbenzamide and the corresponding relative Gibbs free energies (in kcal/mol in parentheses) with respect to the lowest energy structure. For improved clarity, only a few hydrogen atoms are shown. Color code: brown-Ir, red-O, blue-N, white-C, and orange-B.

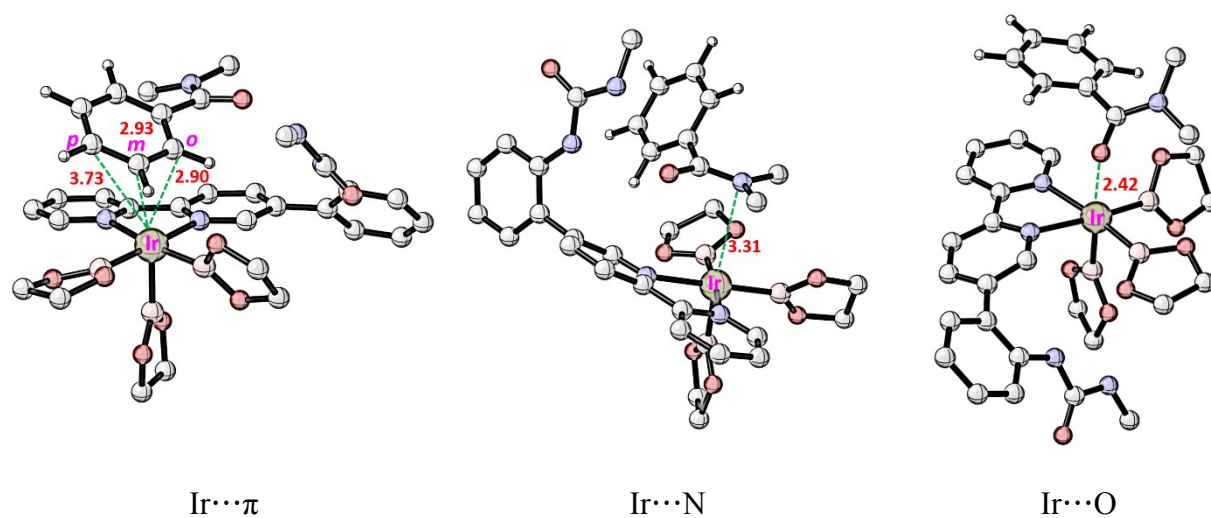
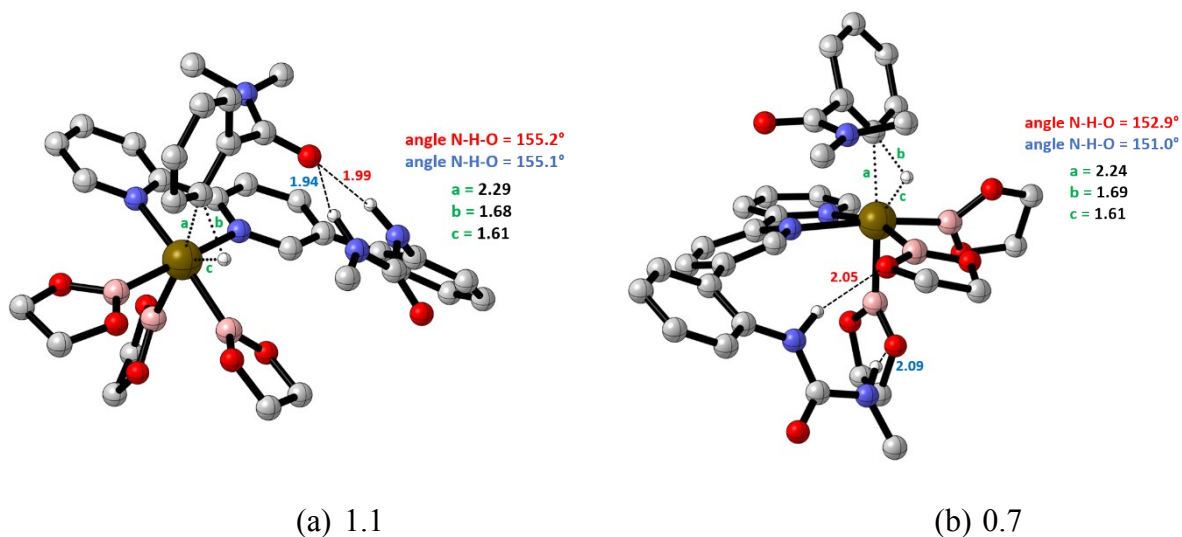
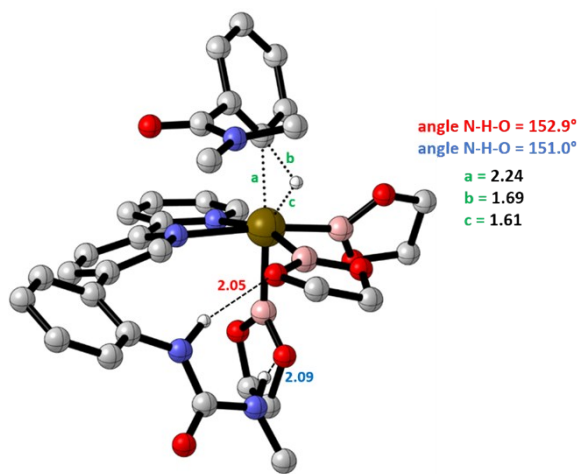


Fig. S5 Optimized geometries of the catalyst-substrate complex for *N,N*-dimethylbenzamide in different binding modes to depict the proximity of the aryl $\text{C}(\text{sp}^2)\text{-H}$ bonds towards the metal in each binding mode.





(c) 0.0

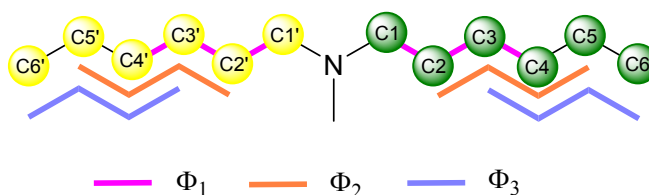
Fig. S6 The optimized TS geometries for the *ortho* C–H activation with different binding modes (a) Ir $\cdots\pi$, b) Ir $\cdots$ N, and (c) Ir $\cdots$ O for the model system and the corresponding relative Gibbs free energies (in kcal/mol in parentheses) with respect to the lowest energy structure. The distances are in Å and the bond angles in degrees. Color code: brown-Ir, red-O, blue-N, white-C, and orange-B. The non-interacting hydrogen atoms are removed for improved clarity.

4. Conformational Analysis of Important Transition States

The presence of the dihexyl chains on the substrate gives way to numerous conformers. A detailed conformational search is thus undertaken to identify the most favorable geometry for both the C–H activation (**TS1**) and the reductive elimination (**TS2**) TSs. Here, certain key dihedral angles (Φ_1 , Φ_2 , Φ_3) as shown in Table S1 are changed and the corresponding TS geometries are re-optimized. The initial guess values of the dihedral angles are made in such a way that it belongs either to an *anti* (*a*) or a *gauche* (*g*) conformer along the hexyl chain. Thus, for a hexyl chain, three major combinations of the primary dihedral angles Φ_1 , Φ_2 , Φ_3 are considered. Within a primary dihedral, say Φ_1 , other combinations of *a* and *g* that differ in Φ_2 and/or Φ_3 values are likely. Further combinations of the *a* and *g* conformers are also possible. We have therefore considered *aaa*, *ggg*, *aga*, *agg*, *aag*, *gag*, *gaa* and *gga* conformers of both the hexyl chains of *N,N*-dihexyl substituent, to access the energetically most favorable geometries of

the transition states for C–H activation and reductive elimination leading to *meta*, *ortho* and *para* borylated products. Tables S1-S3 provide a compilation of the optimized dihedral angles and their corresponding energies.

Table S1 Conformational Sampling for the *meta* C–H Activation TSs by Varying the Dihedrals Φ_1 , Φ_2 and Φ_3 of the *N,N*-dihexyl Chains of the Substrate at the SMD_(p-xylene)/B3LYP-D3/6-31G**//B3LYP-D3/6-31G** Level of Theory (The lowest energy conformer is highlighted)



conformer	dihedral angle	the values defined by the carbon centers on both sides of the hexyl chain		E (kcal/mol)
<i>aaa</i>	Φ_1	-178.9	173.3	2.6
	Φ_2	-176.5	171.3	
	Φ_3	-174.2	179.5	
<i>ggg</i>	Φ_1	-59.2	63.8	7.6
	Φ_2	-51.8	51.7	
	Φ_3	-56.2	57.6	
<i>aga</i>	Φ_1	-170.7	174.3	3.9
	Φ_2	66.8	62.8	
	Φ_3	-178.9	175.9	
<i>agg</i>	Φ_1	177.4	-179.6	5.5
	Φ_2	56.2	-55.7	
	Φ_3	57.3	-56.6	
<i>aag</i>	Φ_1	178.3	172.8	4.9
	Φ_2	-173.5	169.9	
	Φ_3	-64.3	63.3	
<i>gag</i>	Φ_1	-68.8	65.1	3.3
	Φ_2	178.1	-176.3	
	Φ_3	66.9	-61.5	
<i>gaa</i>	Φ_1	-78.7	-73.4	0.0
	Φ_2	-173.6	-179.8	
	Φ_3	-175.0	178.3	
<i>gga</i>	Φ_1	62.8	-63.4	11.9
	Φ_2	54.9	-59.3	
	Φ_3	173.4	-173.0	

Table S2 Conformational Sampling for the *ortho* C–H Activation TSs by Varying the Dihedrals Φ_1 , Φ_2 and Φ_3 of the *N,N*-dihexyl Chains of the Substrate at the SMD_(p-xylene)/B3LYP-D3/6-31G**//B3LYP-D3/6-31G** Level of Theory (The lowest energy conformer is highlighted)

conformer	dihedral angle	the values defined by the carbon centers on both sides of the hexyl chain		E (kcal/mol)
aaa	Φ_1	176.3	-178.2	3.1
	Φ_2	178.1	-179.2	
	Φ_3	179.9	-179.8	
ggg	Φ_1	58.8	-56.8	4.9
	Φ_2	49.5	-52.7	
	Φ_3	60.2	-59.6	
aga	Φ_1	-175.8	172.1	5.9
	Φ_2	-64.9	64.0	
	Φ_3	-176.3	176.7	
agg	Φ_1	-177.9	175.1	7.4
	Φ_2	-60.2	58.9	
	Φ_3	-57.9	58.2	
aag	Φ_1	-178.4	-179.9	4.5
	Φ_2	-177.8	177.4	
	Φ_3	-64.1	64.3	
gag	Φ_1	70.6	-63.1	2.7
	Φ_2	-163.6	178.9	
	Φ_3	-61.6	65.1	
gaa	Φ_1	71.7	-62.3	0.0
	Φ_2	-164.9	179.6	
	Φ_3	-175.7	-178.4	
gga	Φ_1	56.8	-54.1	3.2
	Φ_2	51.9	-56.8	
	Φ_3	176.6	-177.2	

Table S3 Conformational Sampling for the *para* C–H Activation TSs by Varying the Dihedrals Φ_1 , Φ_2 and Φ_3 of the *N,N*-dihexyl Chains of the Substrate at the SMD_(p-xylene)/B3LYP-D3/6-31G**//B3LYP-D3/6-31G** Level of Theory (The lowest energy conformer is highlighted)

conformer	dihedral angle	the values defined by the carbon centers on both sides of the hexyl chain		E (kcal/mol)
aaa	Φ_1	-175.7	-179.2	3.4
	Φ_2	-178.1	-174.6	
	Φ_3	179.4	179.4	
ggg	Φ_1	-58.4	-57.8	6.2
	Φ_2	-55.6	-56.2	
	Φ_3	-58.9	-58.8	
aga	Φ_1	179.5	-176.0	5.3

	Φ_2	-65.2	-66.1	
	Φ_3	-170.5	-176.2	
<i>agg</i>	Φ_1	-162.5	-179.3	6.7
	Φ_2	75.9	61.2	
	Φ_3	65.9	58.3	
<i>aag</i>	Φ_1	-172.4	-174.6	4.3
	Φ_2	-174.1	171.4	
	Φ_3	-59.9	-59.2	
<i>gag</i>	Φ_1	-69.3	-67.3	3.2
	Φ_2	174.7	170.3	
	Φ_3	61.1	67.3	
<i>gaa</i>	Φ_1	-67.5	-67.3	0.0
	Φ_2	175.4	167.9	
	Φ_3	-174.9	-179.9	
<i>gga</i>	Φ_1	-52.8	-50.0	4.5
	Φ_2	-56.7	-56.2	
	Φ_3	178.9	176.3	

Table S4 Conformational Sampling^a for the *meta* Reductive Elimination TSs by Varying the Dihedrals Φ_1 , Φ_2 and Φ_3 of the *N,N*-dihexyl Chains of the Substrate. (The lowest energy conformer is highlighted)

conformer	dihedral angle	the values defined by the carbon centers on both sides of the hexyl chain		E (kcal/mol)
<i>aaa</i>	Φ_1	-179.3	-175.9	0.0
	Φ_2	-179.3	-172.9	
	Φ_3	179.8	178.0	
<i>gag</i>	Φ_1	-75.9	-58.5	2.4
	Φ_2	-172.4	173.2	
	Φ_3	-62.2	-69.1	
<i>gaa</i>	Φ_1	73.4	57.4	1.1
	Φ_2	-177.3	163.9	
	Φ_3	-178.7	177.7	
<i>gga</i>	Φ_1	58.5	52.2	0.4
	Φ_2	54.2	58.4	
	Φ_3	173.5	-177.5	
	Φ_2	-56.7	-56.2	
	Φ_3	178.9	176.3	

^a On the basis of results of the conformational analysis on the C–H activation TSs, we have considered only the lower energy possibilities such as *gaa*, *aaa*, *gag*, and *gga* for the reductive elimination **TS2**.

Table S5 Conformational Sampling for the *para* and *ortho*^a Reductive Elimination TSs by Varying the Dihedrals Φ_1 , Φ_2 and Φ_3 of the *N,N*-dihexyl Chains of the Substrate (The lowest energy conformer is highlighted)

isomer	conformer	dihedral angle	the values defined by the carbon centers on both sides of the hexyl chain		E (kcal/mol)
<i>para</i>	<i>aaa</i>	Φ_1	-178.3	178.8	0.0
		Φ_2	179.8	-176.0	
		Φ_3	-179.3	-179.8	
	<i>gag</i>	Φ_1	64.3	55.9	2.3
		Φ_2	177.2	171.4	
		Φ_3	-65.9	-71.4	
	<i>gaa</i>	Φ_1	64.5	59.1	0.4
		Φ_2	175.5	177.1	
		Φ_3	179.5	177.7	
	<i>gga</i>	Φ_1	58.2	79.6	0.8
		Φ_2	53.5	67.2	
		Φ_3	175.9	176.1	
<i>ortho</i>	<i>aaa</i>	Φ_1	171.9	-170.7	
		Φ_2	177.6	-178.9	
		Φ_3	178.4	-179.3	

^a In the case of reductive elimination TSs for the *ortho* borylation, conformers other than *aaa* could not be identified even after repeated attempts. Since *aaa* is found to be the most preferred conformer of the reductive elimination TS for the *meta* and *para* positions, we have considered the *aaa* conformer for *ortho* borylation as well.

5. Transition State Geometries of the Different Steps in the Mechanistic Cycle for the *meta* C–H Borylation

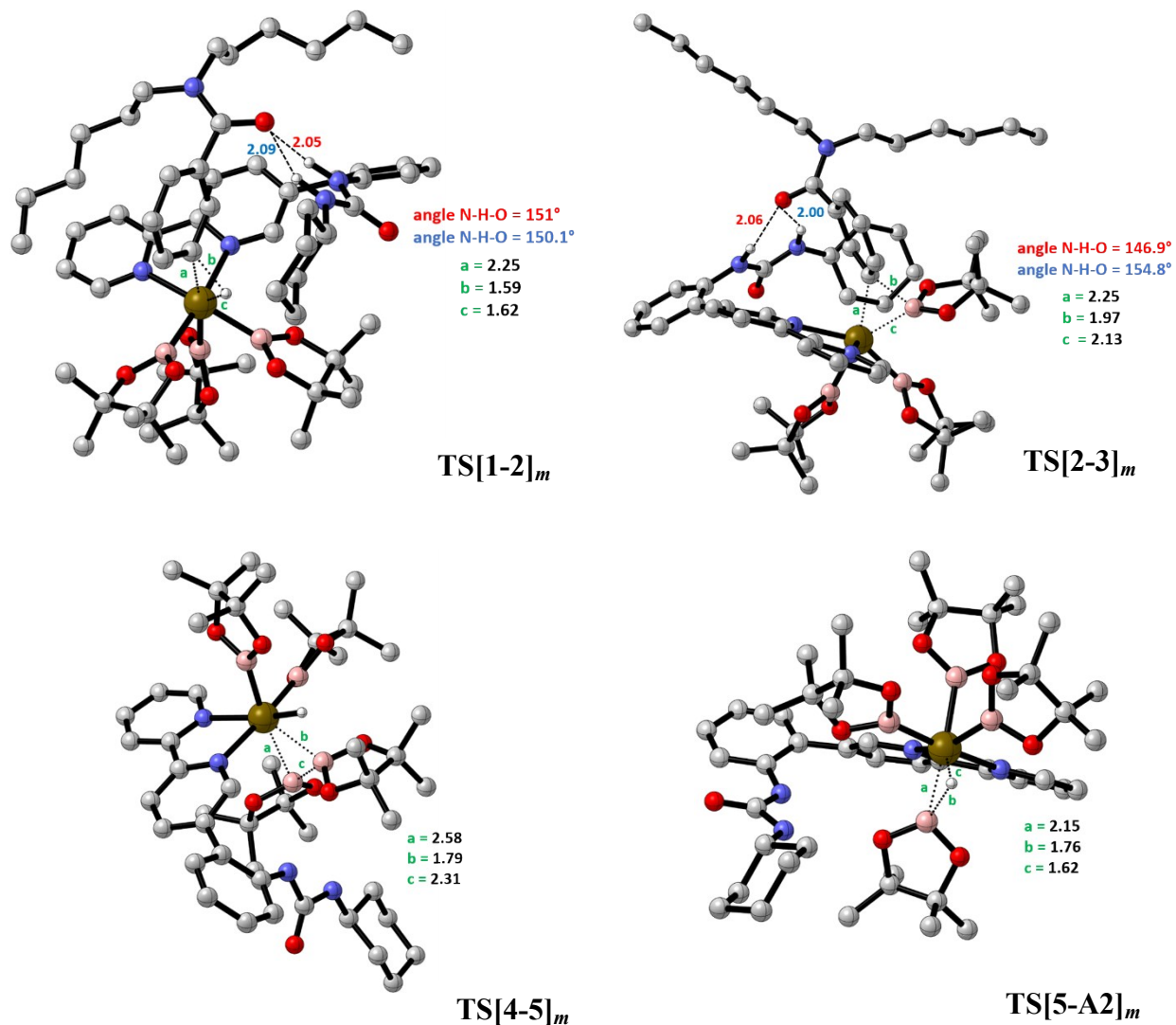


Fig. S7 Optimized geometries for the important TSs involved in the formation of *meta* borylated product. The distances are in Å and the bond angles in degrees. Color code: brown-Ir, red-O, blue-N, white-C, and orange-B. The non-interacting hydrogen atoms are removed for improved clarity.

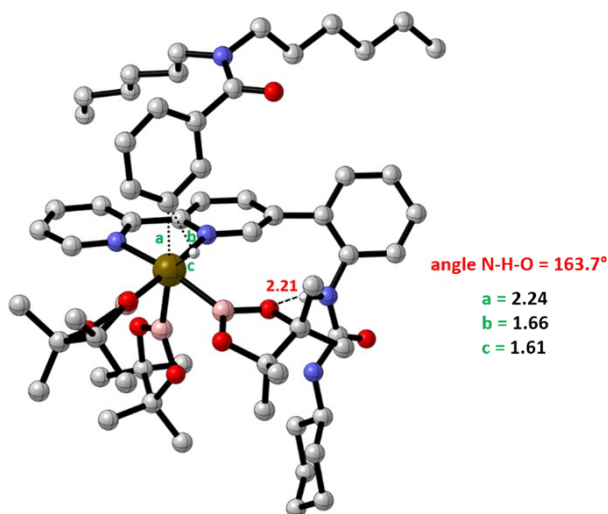


Fig. S8 The optimized *meta* C–H activation obtained from the active catalyst **A1**. The distances are in Å and the bond angles in degrees. Color code: brown-Ir, red-O, blue-N, white-C, and orange-B. The non-interacting hydrogen atoms are removed for improved clarity.

6. Energetic Span Model

The energies of various stationary points are considered for the evaluation of the turnover frequency (TOF) of a catalytic cycle. The TOF in turn is determined by identifying the turnover determining intermediate (TDI) and turnover determining transition state (TDTS).¹ The energy span (δE) can then be calculated using the following equations:

$$\delta E = T_{\text{TDTS}} - I_{\text{TDI}} \quad (1), \text{ if the TDTS is after the TDI}$$

$$\delta E = T_{\text{TDTS}} - I_{\text{TDI}} + \Delta G_r \quad (2), \text{ if the TDTS is before the TDI}$$

where ΔG_r is the free energy of the reaction.

Table S6 The Energetic Span Calculation (δE , in kcal/mol) using Different Likely Combinations of TDI and TDTS for the *meta* C–H activation. For easier comprehension, the combination of TDI-TDTS that gives the maximum span is highlighted

TDI	TDTS	δE
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1) Kozuch, S.; Shaik, S. How to Conceptualize Catalytic Cycles? The Energetic Span Model. *Acc. Chem. Res.* **2011**, *44*, 101-110.

1	TS[1-2]	21.6
	TS[2-3]	21.5
	TS[4-5]	10.9
	TS[5-A2]	7.4
2	TS[1-2]	1.2
	TS[2-3]	8.4
	TS[4-5]	-2.2
	TS[5-A2]	-5.7
3	TS[1-2]	9.2
	TS[2-3]	9.1
	TS[4-5]	5.8
	TS[5-A2]	2.3
4	TS[1-2]	9.0
	TS[2-3]	8.9
	TS[4-5]	5.6
	TS[5-A2]	2.1
5	TS[1-2]	9.0
	TS[2-3]	8.9
	TS[4-5]	-1.7
	TS[5-A2]	2.1
A2+HBpin	TS[1-2]	18.5
	TS[2-3]	18.4
	TS[4-5]	7.8
	TS[5-A2]	4.3

7. Evaluation of Relative Strengths of Noncovalent Interactions using the Espinosa's Formulation

Table S7 Estimated Strengths of the Important Noncovalent Interactions in the *meta* and *para* C–H Activation Transition States for ubpy-**S0** and ubpy-**S1** Catalyst-Substrate Combinations.

The Topological Quantities are Derived from the Atoms In Molecule (AIM) Analysis^a

ubpy- S0					
C–H⋯π	ρ	∇ ² ρ	G	V=1/4∇ ² ρ-2G	E = 1/2(V) (kcal/mol)
<i>meta</i> (a)	0.006	-0.004	0.003	-0.008	-2.5
(b)	0.005	-0.004	0.003	-0.007	-2.3
(c)	0.005	-0.004	0.003	-0.007	-2.3
(d)	0.005	-0.003	0.003	-0.006	-1.9
(e)	0.006	-0.004	0.003	-0.008	-2.5
(f)	0.009	-0.007	0.006	-0.013	-4.0
<i>para</i>	-	-	-	-	-
C–H⋯O					

<i>meta</i>	(g)	0.019	-0.014	0.014	-0.032	-10.1
	(h)	0.012	-0.010	0.009	-0.020	-6.2
	(i)	0.013	-0.011	0.010	-0.023	-7.1
	(j)	0.011	-0.009	0.008	-0.019	-5.9
	(k)	0.006	-0.005	0.004	-0.010	-3.2
	(l)	0.009	-0.008	0.007	-0.016	-4.9
<i>para</i>	(g)	0.017	-0.013	0.013	-0.028	-8.9
	(i)	0.015	-0.012	0.011	-0.025	-7.9
	(m)	0.007	-0.006	0.005	-0.012	-3.8
	(n)	0.015	-0.012	0.011	-0.026	-8.1
	(o)	0.010	-0.008	0.007	-0.016	-5.1
	(p)	0.007	-0.007	0.006	-0.014	-4.3
C–H···N						
<i>meta</i>	(q)	0.006	-0.005	0.004	-0.010	-3.1
	(r)	0.014	-0.013	0.011	-0.026	-8.1
<i>para</i>	(s)	0.011	-0.010	0.008	-0.019	-5.8
	(u)	0.009	-0.008	0.007	-0.015	-4.7
N–H···O						
<i>meta</i>	(v)	0.021	-0.014	0.015	-0.034	-10.6
	(w)	0.020	-0.015	0.015	-0.035	-10.9
<i>para</i>	(v)	0.027	-0.019	0.019	-0.043	-13.6
ubpy-S1						
C–H··· π						
<i>meta</i>	(f)	0.009	-0.007	0.006	-0.013	-4.1
<i>para</i>		-	-	-	-	-
C–H···O						
<i>meta</i>	(g)	0.017	-0.013	0.013	-0.029	-9.1
	(h)	0.012	-0.010	0.009	-0.020	-6.2
	(i)	0.013	-0.011	0.010	-0.023	-7.2
	(j)	0.011	-0.009	0.008	-0.018	-5.7
	(k)	0.009	-0.007	0.007	-0.015	-4.7
	(l)	0.006	-0.005	0.004	-0.010	-3.1
	(m)	0.005	-0.005	0.004	-0.009	-2.9
<i>para</i>	(g)	0.017	-0.013	0.013	-0.029	-9.0
	(i)	0.017	-0.013	0.013	-0.028	-8.9
	(m)	0.007	-0.006	0.005	-0.012	-3.7
	(n)	0.013	-0.010	0.010	-0.022	-7.0
	(o)	0.010	-0.008	0.007	-0.016	-5.1
	(p)	0.008	-0.007	0.006	-0.014	-4.3
C–H···N						
<i>meta</i>	(r)	0.013	-0.012	0.010	-0.023	-7.3
<i>para</i>	(s)	0.011	-0.010	0.008	-0.019	-5.8
	(t)	0.005	-0.004	0.004	-0.008	-2.6
	(u)	0.008	-0.007	0.006	-0.014	-4.3
N–H···O						
<i>meta</i>	(v)	0.018	-0.014	0.014	-0.031	-9.7
	(w)	0.022	-0.015	0.016	-0.035	-11.0
<i>para</i>	(v)	0.025	-0.017	0.018	-0.041	-12.8

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

8. Noncovalent Interactions (NCI) Plots for the *meta* and *para* C–H Activation TSs

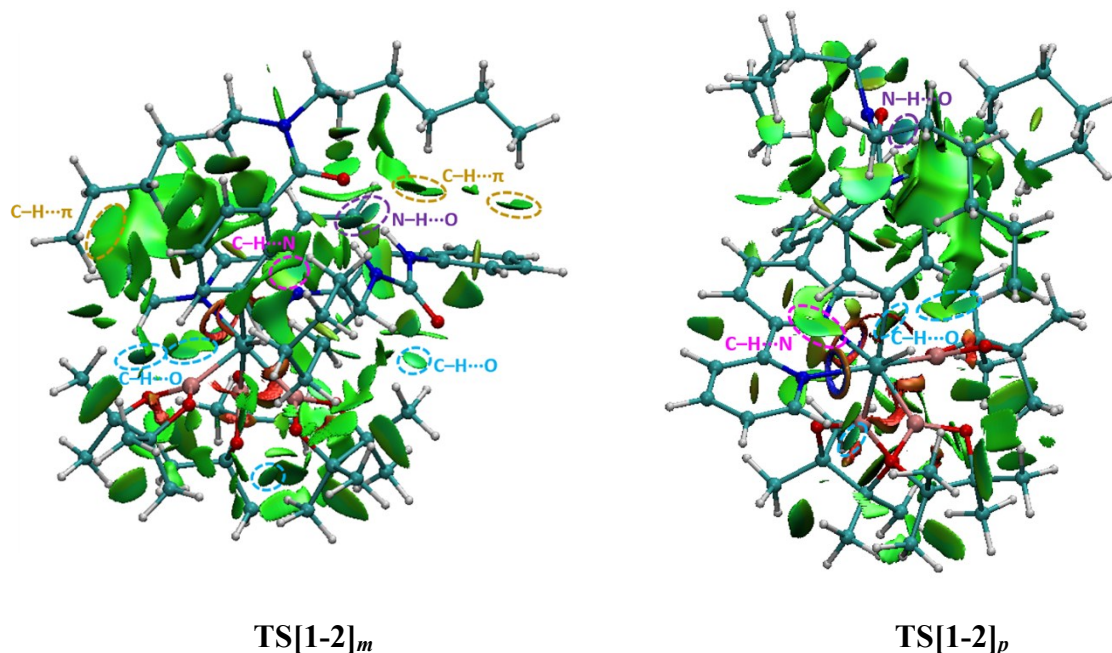


Fig. S9 The NCI plots depicting the noncovalent interactions in the case of *meta* and *para* C–H activation TSs. The green regions represent attractive interactions.

9. Distortion-Interaction/Activation-Strain (DI-AS) Analysis

The barrier height for an elementary step, calculated as the energy difference between the respective pre-reacting complex and the transition state is described in terms of the extent of distortion experienced by the reactants and the interaction between such distorted reacting partners (also referred to as fragments), both at the TS geometry. The destabilizing distortion energy $\Delta E_{\text{dis}}(\zeta)$ and the stabilizing interaction energy $\Delta E_{\text{int}}(\zeta)$ between the distorted fragments is equated to the activation energy as shown in equation (3). The DI-AS analysis includes calculation of the extent of distortion and interaction along the respective IRC trajectories.

$$\Delta E^\ddagger = \Delta E(\zeta^{\text{TS}}) = \Delta E_{\text{dis}}(\zeta) + \Delta E_{\text{int}}(\zeta) \quad (3)$$

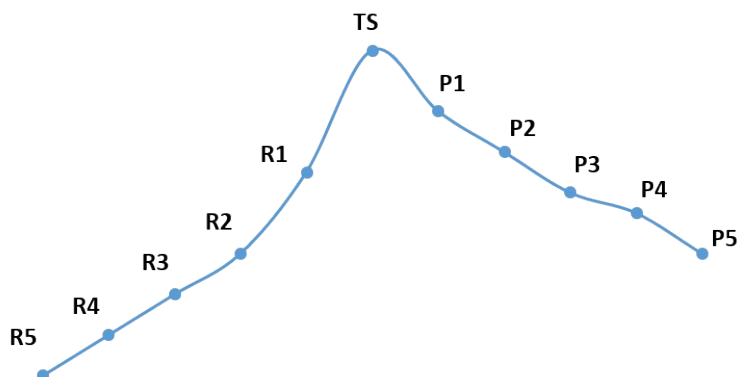


Fig. S10 The IRC trajectory and the points at which the distortion ($\Delta E_{\text{dis}}(\zeta)$) and interaction ($\Delta E_{\text{int}}(\zeta)$) energies are evaluated.

Table S8 Distortion and Interaction Energies (in kcal/mol) along the IRC points for the *meta* and *para* C–H Activation TSs for ubpy-S0 and ubpy-S1

IRC points ^a	total distortion energy ($\Delta E_{\text{dis}}(\zeta)$)			
	<i>meta</i>		<i>para</i>	
	ubpy-S0	ubpy-S1	ubpy-S0	ubpy-S1
R1	107.8	100.0	109.2	107.3
R2	95.8	88.2	97.4	95.5
R3	84.7	77.1	85.7	83.7
R4	74.3	67.0	74.7	72.6
R5	67.9	61.1	64.9	62.7
TS	107.8	100.0	109.2	107.3
P1	107.8	100.0	109.2	107.3
P2	119.8	111.8	120.5	118.7
P3	131.0	123.1	130.9	129.2
P4	141.3	133.4	140.5	138.9
P5	150.5	142.7	149.2	147.5
	total interaction energy ($\Delta E_{\text{int}}(\zeta)$)			
	ubpy-S0	ubpy-S1	ubpy-S0	ubpy-S1
R1	-89.8	-76.9	-80.5	-74.7
R2	-77.0	-64.4	-69.1	-63.2
R3	-64.9	-52.4	-58.5	-52.5
R4	-53.3	-41.1	-49.1	-43.1
R5	-46.0	-34.4	-41.5	-35.5
TS	-85.6	-72.9	-80.5	-74.7
P1	-85.6	-72.9	-83.8	-77.9
P2	-97.9	-85.1	-94.6	-88.7
P3	-109.9	-97.1	-104.2	-98.5
P4	-121.1	-108.4	-112.9	-107.2

P5	-131.1	-118.6	-120.9	-115.2
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^a See Fig. S10 for the details of IRC trajectory.

10. Full Details of Calculations on Different Combinations of Modified Systems

Table S9 Relative Enthalpy and Gibbs Free Energy Differences (in kcal/mol) between the *meta* and *para* C–H Activation Transition States

system	$\Delta\Delta H$		$\Delta\Delta G$	
	<i>meta</i>	<i>para</i>	<i>meta</i>	<i>para</i>
ubpy-S0	0.0	6.8	0.0	6.6
ubpy-S1	0.0	7.4	0.0	7.4
bpy-S0	0.0	1.6	0.0	0.0
ubpy-S0-B1	0.0	1.7	0.0	2.6
dtbpy-S0	0.0	-0.9	0.0	0.4

11. The *meta* and *para* C–H Activation TSs for the Ir-dtbpy catalyst

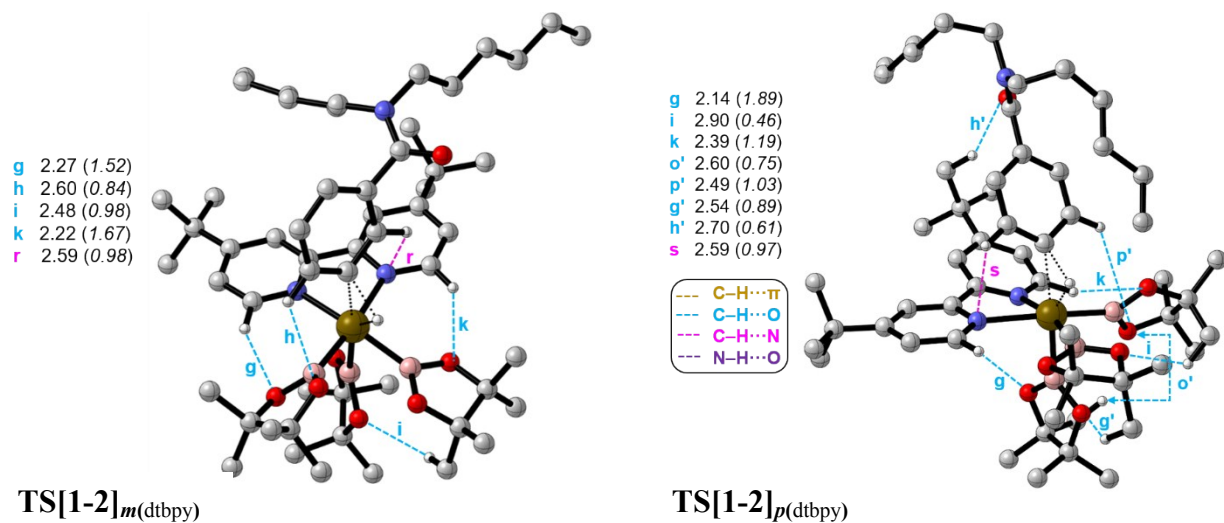


Fig. S11 Optimized transition state geometries for the *meta* and *para* C–H activation transition state for Ir-dtbpy catalyst. The distances are in Å and electron densities ($\rho \times 10^{-2}$ au) at the

bond critical points are given in parentheses. The hydrogen atoms that are not involved in any noticeable interaction are removed for improved clarity.

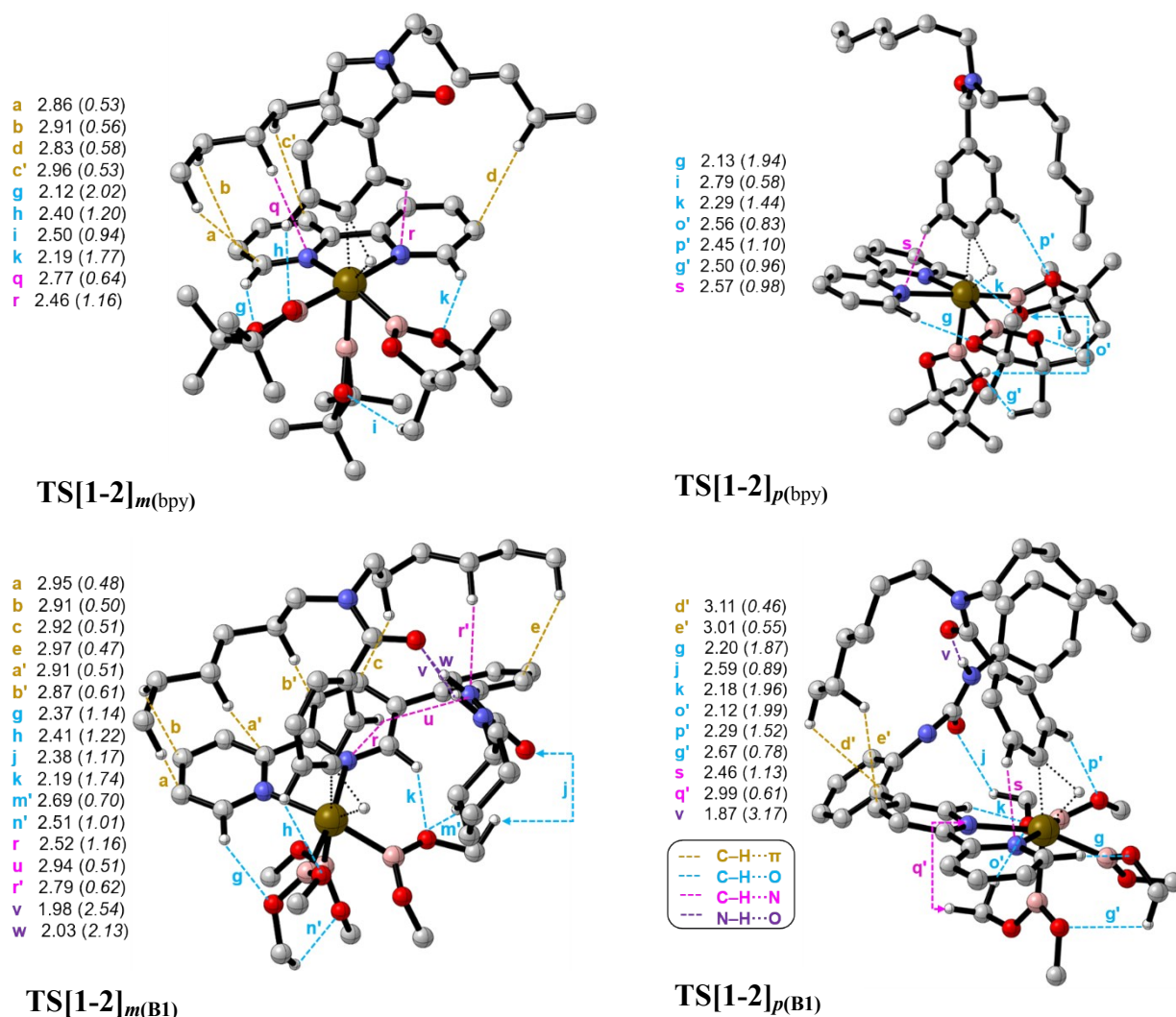


Fig. S12 Optimized geometries of the transition state for the *meta* and *para* C–H activation for Ir-bpy catalyst and **B1** as the borylating agent. The distances are in Å and electron densities ($\rho \times 10^{-2}$ au) at the bond critical points are given in parentheses. The hydrogen atoms that are not involved in any noticeable interaction are removed for improved clarity.

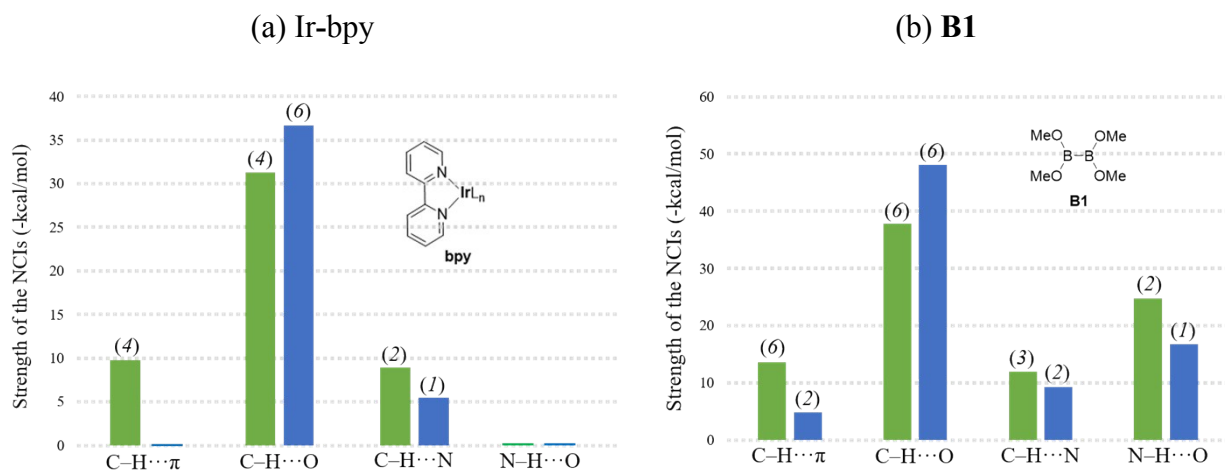


Fig. S13 Comparison of the sum of interaction energies of the NCIs in the *meta* (green) and *para* (blue) C–H activation TSs for (a) ligand Ir-bpy and (b) and borylating agent **B1** in the optimized geometries. Values in parentheses above the bar diagrams are the number of noncovalent interactions.

Table S10 Estimated Strengths of the Important Noncovalent Interactions in the *meta* and *para* C–H Activation Transition States for bpy and **B1** Catalyst-Substrate Combinations. The Topological Quantities are Derived from the Atoms In Molecule (AIM) Analysis^a

bpy					
C–H... π	ρ	$\nabla^2\rho$	G	$V=1/4\nabla^2\rho-2G$	$E = 1/2(V)$ (kcal/mol)
<i>meta</i> (a)	0.005	-0.004	0.003	-0.008	-2.4
(b)	0.006	-0.004	0.003	-0.008	-2.5
(d)	0.006	-0.005	0.004	-0.009	-2.7
(c2)	0.005	-0.004	0.003	-0.007	-2.3
<i>para</i>	-	-	-	-	-
C–H...O					
<i>meta</i> (g)	0.020	-0.015	0.015	-0.034	-10.5
(h)	0.012	-0.010	0.009	-0.021	-6.4
(i)	0.009	-0.008	0.007	-0.016	-5.0
(k)	0.018	-0.013	0.013	-0.030	-9.3
<i>para</i> (g)	0.019	-0.014	0.015	-0.033	-10.2
(i)	0.006	-0.006	0.004	-0.010	-3.2
(k)	0.014	-0.011	0.011	-0.024	-7.5
(o2)	0.008	-0.007	0.006	-0.014	-4.4
(p2)	0.011	-0.010	0.009	-0.019	-6.1

(g ₂)	0.010	-0.008	0.007	-0.017	-5.2
C–H···N					
<i>meta</i> (q)	0.006	-0.005	0.004	-0.010	-3.2
(r)	0.012	-0.011	0.009	-0.018	-5.7
<i>para</i> (s)	0.010	-0.009	0.008	-0.017	-5.5
B1					
C–H··· π					
<i>meta</i> (a)	0.005	-0.004	0.003	-0.006	-2.0
(b)	0.005	-0.004	0.003	-0.007	-2.2
(c)	0.005	-0.004	0.003	-0.008	-2.4
(e)	0.005	-0.004	0.003	-0.007	-2.1
(a ₂)	0.005	-0.004	0.003	-0.007	-2.2
(b ₂)	0.006	-0.005	0.004	-0.009	-2.7
<i>para</i> (d ₂)	0.005	-0.004	0.003	-0.007	-2.1
(e ₂)	0.006	-0.005	0.004	-0.009	-2.7
C–H···O					
<i>meta</i> (g)	0.011	-0.010	0.009	-0.020	-6.4
(h)	0.012	-0.011	0.010	-0.022	-6.8
(j)	0.012	-0.009	0.008	-0.019	-6.0
(k)	0.017	-0.013	0.013	-0.029	-9.3
(m ₂)	0.007	-0.007	0.005	-0.012	-3.9
(n ₂)	0.010	-0.009	0.008	-0.018	-5.5
<i>para</i> (g)	0.019	-0.013	0.014	-0.031	-9.7
(j)	0.009	-0.008	0.007	-0.015	-4.8
(k)	0.020	-0.014	0.015	-0.033	-10.2
(o ₂)	0.020	-0.014	0.015	-0.033	-10.5
(p ₂)	0.015	-0.012	0.012	-0.026	-8.3
(g ₂)	0.008	-0.008	0.006	-0.015	-4.7
C–H···N					
<i>meta</i> (r)	0.012	-0.010	0.009	-0.020	-6.2
(u)	0.005	-0.005	0.004	-0.008	-2.7
(r ₂)	0.006	-0.005	0.004	-0.010	-3.0
<i>para</i> (s)	0.011	-0.010	0.009	-0.020	-6.2
(q ₂)	0.006	-0.005	0.004	-0.010	-3.1
N–H···O					
<i>meta</i> (v)	0.025	-0.018	0.019	-0.042	-13.2
(w)	0.021	-0.016	0.016	-0.037	-11.6
<i>para</i> (v)	0.032	-0.024	0.024	-0.053	-16.7

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

12. Distortion-Interaction-Activation-Strain (DI-AS) Analysis for dtbpy, bpy and B1 systems

Table S11 Distortion and Interaction Energies (in kcal/mol) for the *meta* and *para* C–H activation TSs for ubpy-**S0** and dtbpy

IRC points	total distortion energy ($\Delta E_{\text{dis}}(\zeta)$)			
	<i>meta</i>		<i>para</i>	
	ubpy- S0	dtbpy	ubpy- S0	dtbpy
R1	107.8	96.9	109.2	101.1
R2	95.8	85.0	97.4	89.3
R3	84.7	73.3	85.7	77.6
R4	74.3	62.4	74.7	66.5
R5	67.9	53.5	64.9	56.4
TS	107.8	96.9	109.2	101.1
P1	107.8	96.9	109.2	101.1
P2	119.8	108.5	120.5	112.3
P3	131.0	119.2	130.9	122.7
P4	141.3	128.9	140.5	132.1
P5	150.5	137.6	149.2	140.4
	total interaction energy ($\Delta E_{\text{int}}(\zeta)$)			
	<i>meta</i>		<i>para</i>	
	ubpy- S0	dtbpy	ubpy- S0	dtbpy
R1	-89.8	-70.3	-80.5	-72.0
R2	-77.0	-58.7	-69.1	-60.4
R3	-64.9	-48.0	-58.5	-49.9
R4	-53.3	-38.7	-49.1	-40.5
R5	-46.0	-31.4	-41.5	-32.6
TS	-85.6	-70.3	-80.5	-72.0
P1	-85.6	-73.6	-83.8	-74.7
P2	-97.9	-84.5	-94.6	-85.5
P3	-109.9	-94.4	-104.2	-95.3
P4	-121.1	-103.3	-112.9	-104.0
P5	-131.1	-111.3	-120.9	-111.6

Table S12 Distortion and Interaction Energies (in kcal/mol) for the *meta* and *para* C–H activation TSs for ubpy-**S0** and bpy

IRC points	total distortion energy ($\Delta E_{\text{dis}}(\zeta)$)			
	<i>meta</i>		<i>para</i>	
	ubpy- S0	bpy	ubpy- S0	bpy
R1	107.8	93.4	109.2	94.8
R2	95.8	81.5	97.4	83.1
R3	84.7	69.8	85.7	71.6
R4	74.3	59.0	74.7	61.0
R5	67.9	50.1	64.9	52.2
TS	107.8	93.4	109.2	94.8
P1	107.8	93.4	109.2	94.8

P2	119.8	105.0	120.5	106.3
P3	131.0	115.7	130.9	116.9
P4	141.3	125.5	140.5	126.6
P5	150.5	134.3	149.2	135.3
	total interaction energy ($\Delta E_{\text{int}}(\zeta)$)			
R1	-89.8	-76.8	-80.5	-66.0
R2	-77.0	-63.9	-69.1	-54.6
R3	-64.9	-50.6	-58.5	-44.1
R4	-53.3	-38.4	-49.1	-34.9
R5	-46.0	-28.5	-41.5	-27.6
TS	-85.6	-71.5	-80.5	-66.0
P1	-85.6	-71.5	-83.8	-69.3
P2	-97.9	-83.4	-94.6	-80.2
P3	-109.9	-94.8	-104.2	-90.1
P4	-121.1	-105.5	-112.9	-98.9
P5	-131.1	-115.1	-120.9	-106.8

Table S13 Distortion and Interaction Energies (in kcal/mol) for the *meta* and *para* C–H activation TSs for ubpy-**S0** and **B1**

IRC points	total distortion energy ($\Delta E_{\text{dis}}(\zeta)$)			
	<i>meta</i>		<i>para</i>	
	ubpy- S0	B1	ubpy- S0	B1
R1	107.8	108.0	109.2	84.5
R2	95.8	96.1	97.4	72.5
R3	84.7	85.0	85.7	60.9
R4	74.3	74.8	74.7	50.1
R5	67.9	68.3	64.9	41.4
TS	107.8	108.0	109.2	84.5
P1	107.8	108.0	109.2	84.5
P2	119.8	119.8	120.5	96.2
P3	131.0	131.1	130.9	107.1
P4	141.3	141.4	140.5	117.2
P5	150.5	150.9	149.2	126.3
	total interaction energy ($\Delta E_{\text{int}}(\zeta)$)			
R1	-89.8	-87.4	-80.5	-85.0
R2	-77.0	-74.7	-69.1	-72.0
R3	-64.9	-62.4	-58.5	-58.6
R4	-53.3	-50.7	-49.1	-46.1
R5	-46.0	-43.2	-41.5	-36.4
TS	-85.6	-82.5	-80.5	-79.0
P1	-85.6	-82.5	-83.8	-79.0
P2	-97.9	-94.7	-94.6	-91.0
P3	-109.9	-106.9	-104.2	-102.8
P4	-121.1	-118.5	-112.9	-114.0
P5	-131.1	-129.3	-120.9	-124.2

13. Free Energy Barriers for the C–H Activation Step

Table S14 Comparison of the Free Energy Barriers (in kcal/mol) with respect to the Preceding Intermediates for the C–H Activation Step Obtained using Different Functionals with 6-311++G** Basis Set for the Lighter Elements and Different ECP Basis Sets for Iridium^a

level of theory	<i>meta</i>	<i>ortho</i>	<i>para</i>
B3LYP-D3/bs-1	19.0	19.9	21.9
B3PW91-D3/bs-1	12.9	12.6	16.8
ωB97XD/bs-1	14.5	15.8	20.2
M06/bs-1	17.7	20.3	21.8
M06-D3/bs-1	14.4	18.2	23.1
M06L/bs-1	22.9	22.1	23.7
M052X-D3/bs-1	18.7	20.8	21.4
M062X-D3/bs-1	23.7	23.1	24.9
ωB97XD/bs-2	18.3	19.9	23.8
M06/bs-2	21.4	24.4	25.3
M06L/bs-2	26.5	26.1	27.1
ωB97XD/bs-3	17.9	19.4	23.8
M06/bs-3	20.8	23.8	25.3
M06L/bs-3	26.1	25.7	27.1

^a ECP basis sets are bs-1 = LANL2TZ(f), bs-2 = SDD, bs-3 = def2-TZVP

14. Gibbs Free Energy Profiles for *para* and *ortho* Borylations

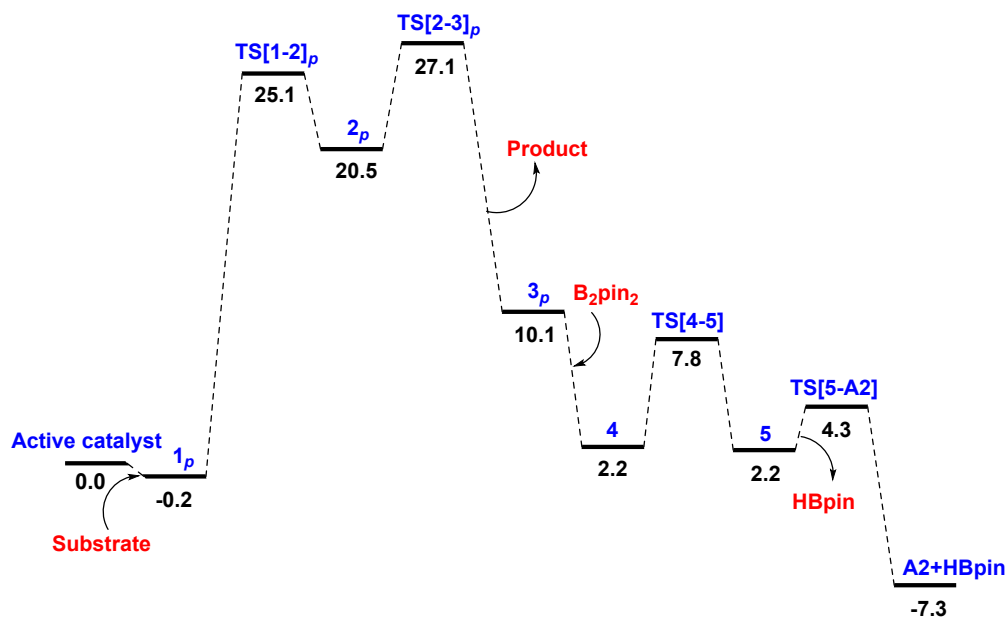


Fig. S14 Free energy profile for the Ir(III) catalyzed *para* C–H activation reaction. The subscript *p* in TS notation indicates the *para* isomer.

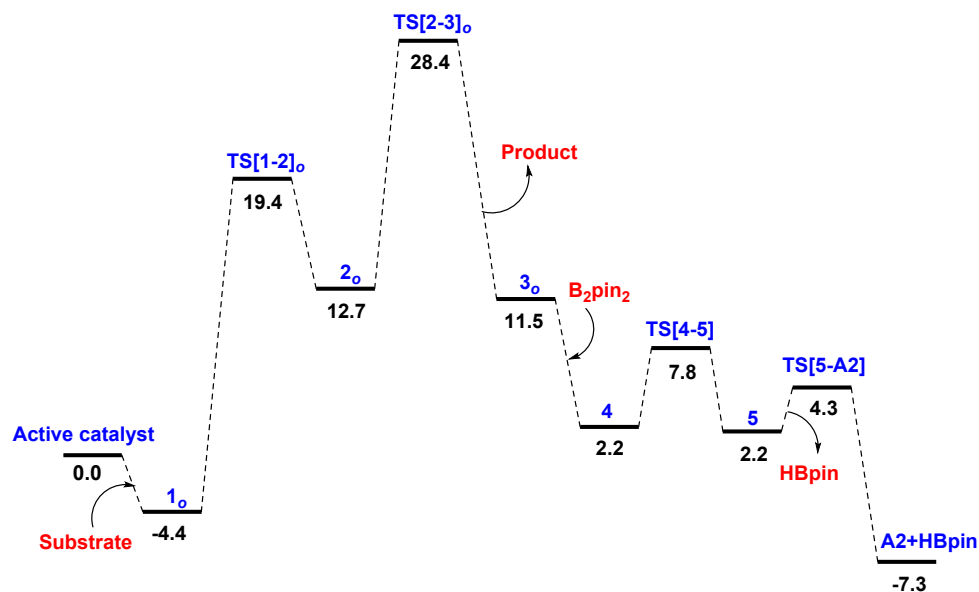


Fig. S15 Free energy profile for the Ir(III) catalyzed *ortho* C–H activation reaction. The subscript *o* in TS notation indicates the *ortho* isomer.

15. Energy Span - *para* and *ortho* C–H Activation

Table S15 The Energetic Span Calculation (δE , in kcal/mol) using Different Likely Combinations of TDI and TDTS for the *para* C–H activation. The subscript *p* used in the notation of TSs and intermediates denotes the *para* isomer. For easier comprehension the maximum span is highlighted

TDI	TDTS	δE
1_p	TS[1-2] _p	25.3
	TS[2-3] _p	27.3
	TS[4-5]	8.0
	TS[5-A2]	4.5
2_p	TS[1-2] _p	-2.7
	TS[2-3] _p	-0.7
	TS[4-5]	-12.7
	TS[5-A2]	-16.2
3_p	TS[1-2] _p	7.7
	TS[2-3] _p	9.7
	TS[4-5]	-2.3
	TS[5-A2]	-5.8
4	TS[1-2] _p	15.6
	TS[2-3] _p	17.6
	TS[4-5]	5.6
	TS[5-A2]	2.1
5	TS[1-2] _p	15.6
	TS[2-3] _p	22.0
	TS[4-5]	-1.7
	TS[5-A2]	2.1
A2+HBpin	TS[1-2] _p	25.1
	TS[2-3] _p	27.1
	TS[4-5]	7.8
	TS[5-A2]	4.3

Table S16 The Energetic Span Calculation (δE , in kcal/mol) using Different Likely Combinations of TDI and TDTS for the *ortho* C–H activation. For easier comprehension the maximum span is highlighted

TDI	TDTS	δE
1_o	TS[1-2] _o	23.8
	TS[2-3] _o	32.8
	TS[4-5]	12.2
	TS[5-A2]	8.7
2_o	TS[1-2] _o	-0.6
	TS[2-3] _o	8.4

	TS[4-5]	-4.9
	TS[5-A2]	-8.4
3 _o	TS[1-2] _o	14.1
	TS[2-3] _o	25.6
	TS[4-5]	5.8
	TS[5-A2]	2.3
4	TS[1-2] _o	9.9
	TS[2-3] _o	18.9
	TS[4-5]	5.6
	TS[5-A2]	2.1
5	TS[1-2] _o	9.9
	TS[2-3] _o	29.8
	TS[4-5]	-1.7
	TS[5-A2]	2.1
A2+HBpin	TS[1-2] _o	19.4
	TS[2-3] _o	34.9
	TS[4-5]	7.8
	TS[5-A2]	4.3

16. Comparison of Enthalpy and Free Energies

Table S17. Enthalpies and Gibbs Free Energies (in kcal/mol) (a) Associated with Various Steps Involved in the Reaction via *meta*, *ortho* and *para* Pathways, and (b) for the Overall Formation of the Borylated Products

(a) for elementary steps ^a		
transition states	ΔH	ΔG
TS[1-2]	20.4	21.6
TS[1-2] _o	22.7	23.8
TS[1-2] _p	25.2	25.3
TS[2-3]	21.5	21.5
TS[2-3] _o	32.0	32.8
TS[2-3] _p	26.7	27.3
TS[4-5]	11.7	10.9
TS[4-5] _o	14.1	12.2
TS[4-5] _p	9.6	8.0
TS[5-A2]	8.6	7.4
TS[5-A2] _o	11.0	8.7
TS[5-A2] _p	6.6	4.5
(b) for overall reaction		
<i>meta</i>	-15.0	-13.4
<i>ortho</i>	-14.6	-13.7
<i>para</i>	-12.0	-12.8

^aΔH and ΔG are calculated with respect to the turn-over determining intermediate (i.e., **1**) in the respective pathways. (Thank you Sir. The text is very appropriate)

17. Comparison of Free Energy Profiles

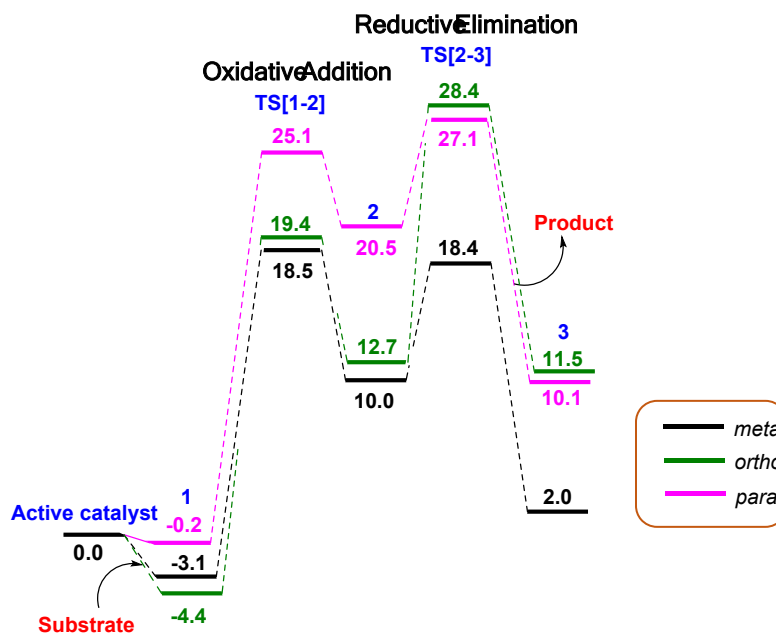


Fig. S16 A comparison of the free energy profiles for the Ir(III)-catalyzed C–H activation and reductive elimination steps for the three isomers (values are in kcal/mol).

Table S18 Comparison of the Free Energy Barriers (in kcal/mol) with respect to the Preceding Intermediates for the Reductive Elimination Step Obtained using Different Functionals with 6-311++G** Basis Set for the Lighter Elements and Different ECP Basis Sets for Iridium^a

level of theory	<i>meta</i>	<i>ortho</i>	<i>para</i>
wB97XD/bs-1	12.0	23.5	18.6
M06L/bs-1	16.0	26.4	22.3
M06/bs-1	13.0	25.2	21.5
M06L/bs-2	19.5	29.7	33.3
wB97XD/bs-2	15.9	27.1	30.2
M06/bs-2	16.5	28.5	31.6
M06L/bs-3	19.1	29.5	24.7
wB97XD/bs-3	15.4	26.8	22.2
M06/bs-3	15.9	28.1	25.6

^a ECP basis sets are bs-1 = LANL2TZ(f), bs-2 = SDD, bs-3 = def2-TZVP

Cartesian Coordinates of the Optimized Geometries of Various Stationary Points Obtained at the B3LYP-D3 Level of Theory

A2

Number of imaginary frequencies : 0

Electronic energy : HF=-2523.7732231
Zero-point correction= 0.985732 (Hartree/Particle)
Thermal correction to Energy= 1.041518
Thermal correction to Enthalpy= 1.042463
Thermal correction to Gibbs Free Energy= 0.898279
Sum of electronic and zero-point Energies= -2522.787491
Sum of electronic and thermal Energies= -2522.731705
Sum of electronic and thermal Enthalpies= -2522.730761
Sum of electronic and thermal Free Energies= -2522.874944

Cartesian Coordinates

77	-0.443239	0.376809	-0.296504
7	1.476183	1.551271	-0.577422
7	-0.760186	1.800649	-2.058572
6	1.560852	2.318890	-1.690300
6	0.281783	2.606495	-2.379333
6	0.141340	3.636618	-3.316389
6	-1.086802	3.827150	-3.942786
6	-2.146900	2.980692	-3.621022
6	-1.941296	1.980911	-2.673469
6	2.802978	2.739078	-2.175777
6	3.965847	2.305131	-1.547609
6	3.881188	1.491863	-0.412233
6	2.595787	1.192514	0.058730
1	0.977242	4.289033	-3.540143
1	-1.211980	4.625271	-4.668106
1	-3.119330	3.087092	-4.089845
1	-2.717980	1.280426	-2.386522
1	2.866816	3.339768	-3.075687
1	4.936852	2.557820	-1.961427
1	2.457071	0.606710	0.957440
5	-1.414644	1.552264	0.990056
8	-2.714649	1.411279	1.476081
8	-0.842070	2.734628	1.468731
6	-3.084639	2.633374	2.155618
6	-1.684289	3.236429	2.536179
5	-0.035025	-0.805466	1.302875
8	0.467029	-2.128071	1.209263
8	-0.174932	-0.484079	2.657064
6	0.640910	-2.698182	2.529666
6	-0.137361	-1.683714	3.457375
5	-2.141560	-0.742768	-0.389936
8	-2.623456	-1.685299	0.525140
8	-3.041649	-0.676501	-1.476819
6	-4.271713	-1.342874	-1.103164
6	-3.769923	-2.365789	-0.023820
6	5.078859	0.937094	0.259810

6	6.161049	1.774127	0.567425
6	5.154994	-0.430517	0.619846
6	7.273203	1.301121	1.261974
1	6.103889	2.822883	0.289596
6	6.273028	-0.896048	1.322108
6	7.319442	-0.037494	1.654190
1	8.089309	1.974716	1.504851
1	6.321205	-1.948598	1.588318
1	8.175547	-0.420175	2.202209
7	4.102788	-1.324150	0.330594
1	3.928557	-2.048575	1.011702
6	-1.617650	4.759901	2.540011
1	-0.604310	5.085001	2.795708
1	-1.865235	5.176050	1.561305
1	-2.304567	5.180239	3.282805
6	-1.126768	2.669107	3.846966
1	-0.086562	2.991299	3.955694
1	-1.688561	3.022243	4.717710
1	-1.132650	1.576852	3.823114
6	-3.855085	3.491373	1.143794
1	-4.708883	2.917767	0.771084
1	-4.230388	4.417204	1.591300
1	-3.222255	3.746379	0.288577
6	-3.979157	2.281354	3.339836
1	-4.216563	3.172299	3.931574
1	-4.920723	1.854335	2.980151
1	-3.504832	1.544351	3.990308
6	-3.267601	-3.683383	-0.627017
1	-2.563518	-3.495719	-1.440609
1	-2.740433	-4.248946	0.146955
1	-4.087815	-4.300798	-1.007403
6	-4.759175	-2.648574	1.104105
1	-5.691798	-3.070824	0.713745
1	-4.329423	-3.374120	1.802210
1	-4.990161	-1.741829	1.666206
6	-4.890797	-1.966650	-2.349157
1	-5.786281	-2.544314	-2.095262
1	-5.185540	-1.179012	-3.050193
1	-4.185423	-2.623805	-2.862034
6	-5.197382	-0.269519	-0.516507
1	-5.366972	0.505552	-1.271138
1	-6.169744	-0.680537	-0.226803
1	-4.728075	0.202125	0.350881
6	2.146560	-2.750616	2.814234
1	2.363136	-3.183948	3.795036
1	2.626708	-3.384681	2.060070
1	2.588616	-1.751443	2.772525
6	0.073750	-4.116260	2.502616
1	0.642622	-4.724293	1.791705
1	0.141527	-4.591878	3.486985
1	-0.968694	-4.117513	2.181486
6	-1.594447	-2.087674	3.715417
1	-1.669038	-2.992643	4.327449
1	-2.094679	-1.273113	4.247934
1	-2.121104	-2.232300	2.770560
6	0.556463	-1.358366	4.778922
1	-0.041014	-0.627529	5.332139
1	0.659351	-2.251897	5.404025
1	1.546134	-0.923966	4.622192
6	3.588979	-1.542690	-0.958492
8	4.120113	-1.085004	-1.967005

7	2.451826	-2.303254	-0.947306
1	1.870512	-2.280616	-0.106437
6	1.720298	-2.551260	-2.191046
6	0.656581	-3.631773	-1.946435
6	1.060049	-1.272859	-2.728457
1	2.444360	-2.906193	-2.934760
6	-0.178862	-3.893774	-3.209403
1	-0.000002	-3.290865	-1.134791
1	1.139964	-4.553616	-1.601021
6	0.240738	-1.523148	-3.997457
1	0.361986	-0.931419	-1.943301
1	1.814731	-0.497160	-2.872576
6	-0.819586	-2.604786	-3.749138
1	-0.951311	-4.641018	-2.991408
1	0.465504	-4.329124	-3.986729
1	-0.233408	-0.589307	-4.322405
1	0.913953	-1.837094	-4.808397
1	-1.376059	-2.816338	-4.670691
1	-1.543579	-2.215501	-3.021596

substrate

Number of imaginary frequencies : 0

Electronic energy : HF=-872.8007809
 Zero-point correction= 0.470198 (Hartree/Particle)
 Thermal correction to Energy= 0.493963
 Thermal correction to Enthalpy= 0.494907
 Thermal correction to Gibbs Free Energy= 0.412679
 Sum of electronic and zero-point Energies= -872.330583
 Sum of electronic and thermal Energies= -872.306818
 Sum of electronic and thermal Enthalpies= -872.305874
 Sum of electronic and thermal Free Energies= -872.388102

Cartesian Coordinates

6	3.129931	-3.915083	0.720076
6	2.128482	-3.505827	1.603740
6	1.077671	-2.707546	1.149483
6	1.017062	-2.320317	-0.195746
6	2.008802	-2.755349	-1.083186
6	3.068138	-3.538311	-0.624090
1	3.950785	-4.531299	1.075866
1	2.163658	-3.809736	2.646142
1	0.294487	-2.393286	1.834098
1	1.940418	-2.480085	-2.131394
1	3.840263	-3.861711	-1.316465
6	-0.151479	-1.540641	-0.743081
8	-0.864395	-2.046969	-1.612756
7	-0.388975	-0.290983	-0.235907
6	-1.558300	0.436747	-0.745898
1	-1.325462	1.506803	-0.736135
1	-1.725261	0.140442	-1.784455
6	0.573783	0.466998	0.571540
1	1.076761	-0.199438	1.272783
6	-2.814102	0.154945	0.085360
1	-2.620462	0.419994	1.133956
1	-3.004568	-0.924656	0.060748
6	-4.043972	0.912689	-0.424771
1	-3.838793	1.993213	-0.419155

1	-4.226311	0.641734	-1.474231
6	-5.306883	0.632897	0.398237
1	-5.126893	0.912441	1.446532
1	-5.504330	-0.448484	0.401779
6	-6.548157	1.371773	-0.115718
1	-6.735759	1.081259	-1.158541
1	-6.346387	2.451806	-0.131248
6	-7.798229	1.096718	0.724091
1	-7.654344	1.409836	1.765210
1	-8.671417	1.631949	0.334850
1	-8.041324	0.027427	0.733176
1	0.004392	1.181956	1.175765
6	1.619969	1.197651	-0.279201
1	2.171230	0.449146	-0.863036
1	1.112762	1.848656	-1.003342
6	2.595174	2.019741	0.569602
1	2.034153	2.764677	1.152268
1	3.081673	1.361418	1.303304
6	3.669417	2.730280	-0.262131
1	4.230510	1.984141	-0.842681
1	3.184196	3.386480	-0.998745
6	4.648833	3.554269	0.582358
1	5.136967	2.896514	1.314535
1	4.087867	4.297304	1.166072
6	5.713787	4.263629	-0.258306
1	6.398697	4.846193	0.367671
1	6.314765	3.544288	-0.827357
1	5.256150	4.952081	-0.978716

B₂pin₂

Number of imaginary frequencies : 0

Electronic energy : HF=-822.6241979
 Zero-point correction= 0.365234 (Hartree/Particle)
 Thermal correction to Energy= 0.384556
 Thermal correction to Enthalpy= 0.385500
 Thermal correction to Gibbs Free Energy= 0.319288
 Sum of electronic and zero-point Energies= -822.258964
 Sum of electronic and thermal Energies= -822.239642
 Sum of electronic and thermal Enthalpies= -822.238698
 Sum of electronic and thermal Free Energies= -822.304909

Cartesian Coordinates

5	0.851181	0.000002	0.000001
5	-0.851181	0.000002	0.000000
8	-1.612651	1.057065	0.440142
8	-1.612649	-1.057062	-0.440142
8	1.612650	-1.057058	0.440153
8	1.612651	1.057060	-0.440152
6	-2.998791	-0.603518	-0.502649
6	-2.998793	0.603518	0.502648
6	2.998792	-0.603513	0.502655
6	2.998793	0.603512	-0.502655
6	3.254103	-0.182937	1.953976
1	4.296182	0.109953	2.113145
1	2.608756	0.651659	2.242533
6	3.254102	0.182936	-1.953976
1	3.028769	1.025999	-2.613046

1	4.296179	-0.109963	-2.113143
1	2.608749	-0.651654	-2.242534
6	3.909682	1.764590	-0.119258
1	4.954082	1.437917	-0.075791
1	3.834259	2.557738	-0.869159
1	3.635649	2.190504	0.847522
6	-3.254105	0.182958	1.953973
1	-3.028771	1.026027	2.613035
1	-4.296183	-0.109937	2.113143
1	-2.608754	-0.651631	2.242542
6	-3.909677	-1.764595	-0.119239
1	-4.954078	-1.437926	-0.075779
1	-3.834248	-2.557752	-0.869130
1	-3.635644	-2.190496	0.847547
6	-3.254105	-0.182958	-1.953973
1	-3.028765	-1.026025	-2.613035
1	-4.296184	0.109931	-2.113144
1	-2.608758	0.651634	-2.242540
6	-3.909680	1.764593	0.119238
1	-4.954081	1.437921	0.075778
1	-3.834253	2.557750	0.869130
1	-3.635648	2.190494	-0.847548
1	3.028762	-1.025997	2.613047
6	3.909679	-1.764592	0.119257
1	4.954079	-1.437921	0.075791
1	3.834254	-2.557741	0.869158
1	3.635645	-2.190504	-0.847523

substrate-Bpin

Number of imaginary frequencies : 0

Electronic energy : HF=-1283.5334965
 Zero-point correction= 0.643157 (Hartree/Particle)
 Thermal correction to Energy= 0.676783
 Thermal correction to Enthalpy= 0.677727
 Thermal correction to Gibbs Free Energy= 0.573969
 Sum of electronic and zero-point Energies= -1282.890339
 Sum of electronic and thermal Energies= -1282.856714
 Sum of electronic and thermal Enthalpies= -1282.855770
 Sum of electronic and thermal Free Energies= -1282.959527

Cartesian Coordinates

6	-2.227797	-0.368092	1.375422
6	-2.628500	0.268348	2.562670
6	-0.855270	-0.444320	1.088212
6	-1.685000	0.794117	3.445899
6	0.098747	0.093695	1.958654
6	-0.325081	0.693998	3.152089
5	-3.274923	-0.961429	0.393789
8	-2.935068	-1.629908	-0.757157
8	-4.630893	-0.855722	0.583325
6	-4.161196	-1.799334	-1.529094
6	-5.269564	-1.707046	-0.414224
1	-3.687907	0.340538	2.792987
1	-2.005223	1.273789	4.366614
1	0.420409	1.073994	3.843941
1	-0.530663	-0.943451	0.179203
6	1.579491	-0.050224	1.724510

7	2.100704	0.355474	0.522519
6	3.545875	0.156771	0.333401
1	3.885929	0.869456	-0.424169
6	1.427480	1.279382	-0.398849
1	0.360105	1.062824	-0.426635
8	2.286634	-0.545314	2.606652
1	4.062917	0.392138	1.268826
1	1.811444	1.081241	-1.405885
6	-4.094835	-3.132136	-2.265290
1	-5.034753	-3.329836	-2.790830
1	-3.291701	-3.104998	-3.007809
1	-3.894231	-3.960476	-1.583545
6	-4.210516	-0.637729	-2.527205
1	-3.297378	-0.647897	-3.129001
1	-5.068320	-0.718946	-3.201228
1	-4.262953	0.325107	-2.010548
6	-6.571945	-1.048003	-0.852880
1	-7.040175	-1.617090	-1.662598
1	-7.272050	-1.017138	-0.012702
1	-6.410064	-0.023832	-1.193497
6	-5.550156	-3.048669	0.270165
1	-6.160374	-2.872695	1.160431
1	-6.091650	-3.733160	-0.389337
1	-4.621308	-3.531101	0.587776
6	1.638546	2.752092	-0.026505
6	0.966052	3.709255	-1.015850
1	2.713912	2.966766	0.026372
1	1.237448	2.913999	0.982526
6	1.166474	5.185885	-0.656236
1	1.357944	3.525312	-2.026626
1	-0.109871	3.488369	-1.060905
6	0.494641	6.150569	-1.640487
1	0.776724	5.369453	0.355102
1	2.242774	5.405602	-0.611270
1	0.879627	5.962237	-2.652241
1	-0.582126	5.935735	-1.679254
6	3.883581	-1.274249	-0.096258
6	5.389228	-1.487083	-0.283628
1	3.351652	-1.506070	-1.028893
1	3.503425	-1.959726	0.669139
6	5.749537	-2.916886	-0.702441
1	5.770637	-0.781318	-1.036321
1	5.907935	-1.243054	0.654227
6	7.256447	-3.139816	-0.877195
1	5.362894	-3.621747	0.047237
1	5.235297	-3.161451	-1.643189
1	7.643248	-2.430818	-1.622404
1	7.768661	-2.901186	0.065023
6	0.710577	7.621787	-1.276651
1	0.305987	7.847709	-0.282888
1	1.777636	7.874260	-1.262375
1	0.221497	8.290194	-1.993850
6	7.604849	-4.569025	-1.301010
1	8.685763	-4.703305	-1.419446
1	7.259410	-5.297560	-0.557780
1	7.131796	-4.825204	-2.256642

TS1-meta-aaa (Refer to Table S1)

Number of imaginary frequencies : 1

Imaginary frequency : -826.7943 cm(-1)

Electronic energy : HF=-3396.5262348
Zero-point correction= 1.454878 (Hartree/Particle)
Thermal correction to Energy= 1.535317
Thermal correction to Enthalpy= 1.536261
Thermal correction to Gibbs Free Energy= 1.336789
Sum of electronic and zero-point Energies= -3395.071356
Sum of electronic and thermal Energies= -3394.990918
Sum of electronic and thermal Enthalpies= -3394.989973
Sum of electronic and thermal Free Energies= -3395.189446

.....
Cartesian Coordinates

.....
77 -1.434036 0.341586 0.040278
5 -2.716060 0.562437 -1.621474
8 -2.457876 1.514725 -2.606960
8 -3.897451 -0.116863 -1.909601
6 -3.359420 1.274195 -3.716359
6 -4.559311 0.559857 -3.005620
5 -1.799188 -1.587864 -0.643309
8 -1.360006 -1.966447 -1.911719
8 -2.416695 -2.643558 -0.003353
6 -1.616253 -3.381041 -2.112261
6 -2.647778 -3.707582 -0.959685
5 -3.169343 0.284297 1.101994
8 -3.498376 -0.632032 2.097650
8 -4.199764 1.234613 0.981828
6 -4.905944 -0.497127 2.390365
6 -5.166058 1.007585 2.036021
6 -0.120936 2.946698 -0.945437
6 0.847795 1.906762 -1.356903
7 -1.169039 2.540857 -0.186878
7 0.451042 0.622435 -1.192954
6 0.005386 4.287155 -1.330886
6 -0.928053 5.221121 -0.895948
6 -1.981552 4.793792 -0.088587
6 -2.073181 3.442878 0.229997
6 2.121283 2.198120 -1.860043
6 2.985381 1.158152 -2.196473
6 2.566943 -0.169340 -2.043236
6 1.270888 -0.372922 -1.544810
6 -0.159690 0.379681 1.885243
6 -0.672699 0.611142 3.176837
6 1.235333 0.359923 1.762090
6 0.169448 0.874528 4.261741
6 2.087982 0.644508 2.832546
6 1.556241 0.910906 4.099066
1 -0.927815 -0.766127 1.108636
1 1.695880 0.108583 0.816938
1 2.212171 1.108247 4.942275
1 -0.260296 1.041157 5.246242
1 -1.742525 0.542671 3.337929
1 -2.902971 3.038456 0.798510
1 -2.736364 5.484007 0.272158
1 -0.837292 6.261023 -1.192948
1 0.810389 4.591352 -1.987906
1 2.452719 3.224973 -1.960121
1 3.984085 1.372267 -2.564332
1 0.874616 -1.372602 -1.428339
6 3.548232 0.542358 2.525966

8	3.997942	-0.525820	2.066290
7	4.363315	1.616855	2.687472
6	3.382291	-1.341014	-2.448771
6	3.852642	-1.420030	-3.769401
6	3.604427	-2.427846	-1.570623
6	4.473624	-2.572545	-4.242537
1	3.679162	-0.580459	-4.436919
6	4.215838	-3.592089	-2.060455
6	4.634976	-3.665191	-3.385364
1	4.813302	-2.624937	-5.272235
1	4.345374	-4.429090	-1.386274
1	5.106222	-4.574700	-3.746305
7	3.253080	-2.312690	-0.215558
6	2.625341	-3.321944	0.527059
8	2.243449	-4.375876	0.018455
7	2.467639	-3.002497	1.842750
1	3.468738	-1.446819	0.265430
1	2.812822	-2.097565	2.152136
6	3.850072	2.981234	2.846790
1	4.562045	3.543307	3.462204
1	2.911844	2.939332	3.400328
6	5.753124	1.443849	2.232276
1	6.321728	2.294050	2.618713
1	6.138680	0.541177	2.712820
6	1.460892	-3.675356	2.660964
6	1.735550	-3.390387	4.143701
6	0.042563	-3.217473	2.281233
1	1.551670	-4.751472	2.471652
6	0.656792	-4.015403	5.042589
1	1.739158	-2.299931	4.293420
1	2.733314	-3.755033	4.414806
6	-1.039115	-3.841269	3.167975
1	0.004130	-2.130624	2.397670
1	-0.146730	-3.431330	1.227376
6	-0.753049	-3.545150	4.647861
1	0.862909	-3.774505	6.092656
1	0.707871	-5.110300	4.957018
1	-2.016867	-3.448847	2.869290
1	-1.064992	-4.929758	3.011303
1	-1.504505	-4.018872	5.291539
1	-0.829784	-2.460747	4.813191
6	3.620905	3.695386	1.508127
6	2.900155	5.036748	1.674860
1	3.022751	3.039232	0.863213
1	4.581160	3.845055	0.998402
6	2.818650	5.823291	0.362831
1	1.885949	4.850903	2.054554
1	3.407258	5.646741	2.435858
6	1.926143	7.065621	0.441820
1	3.830653	6.113579	0.046981
1	2.434666	5.159963	-0.422814
1	0.917148	6.758922	0.747626
1	2.296325	7.732562	1.231786
6	5.909555	1.314805	0.691978
6	6.657775	0.044883	0.270372
1	6.422341	2.199802	0.292934
1	4.914597	1.305101	0.233610
6	6.838348	-0.075991	-1.245458
1	7.645049	0.022255	0.753937
1	6.101990	-0.819061	0.652803
6	7.509967	-1.386916	-1.672048

1	5.858012	-0.010060	-1.737482
1	7.427812	0.777124	-1.613562
1	8.439578	-1.520827	-1.101574
1	6.854342	-2.224281	-1.401783
6	1.851250	7.827974	-0.884422
1	1.199565	8.704749	-0.811318
1	2.842227	8.174226	-1.198840
1	1.461691	7.188103	-1.685863
6	7.814696	-1.439522	-3.171799
1	8.265751	-2.396299	-3.455434
1	6.898469	-1.319949	-3.757975
1	8.510006	-0.642458	-3.461516
6	-5.141570	-0.873899	3.849384
1	-6.185861	-0.705620	4.134422
1	-4.913775	-1.933980	3.992461
1	-4.497747	-0.300115	4.519018
6	-5.643371	-1.465716	1.455772
1	-5.234119	-2.467135	1.608803
1	-6.719772	-1.486521	1.654496
1	-5.472765	-1.194850	0.410403
6	-6.560733	1.314212	1.499216
1	-7.324936	1.080239	2.248266
1	-6.637979	2.377569	1.252413
1	-6.770611	0.743480	0.594027
6	-4.817753	1.964927	3.183523
1	-4.832127	2.992236	2.806368
1	-5.533659	1.891649	4.007777
1	-3.815946	1.758886	3.570184
6	-5.559075	1.540509	-2.379909
1	-6.142170	2.069124	-3.140530
1	-6.246012	0.979852	-1.741308
1	-5.042179	2.267463	-1.748913
6	-5.292782	-0.474456	-3.853794
1	-6.086895	-0.938856	-3.261870
1	-5.750413	-0.003234	-4.730436
1	-4.621126	-1.264270	-4.193675
6	-2.612337	0.359828	-4.695918
1	-3.202752	0.151576	-5.593752
1	-1.684651	0.854398	-4.998055
1	-2.347544	-0.582652	-4.210069
6	-3.695375	2.610188	-4.370362
1	-2.795338	3.032460	-4.827218
1	-4.448658	2.482794	-5.155407
1	-4.069455	3.326813	-3.636838
6	-2.418706	-5.043622	-0.257381
1	-2.570203	-5.877151	-0.951429
1	-1.413358	-5.116333	0.159030
1	-3.133063	-5.146664	0.564483
6	-4.112964	-3.581918	-1.397164
1	-4.387422	-4.352057	-2.124662
1	-4.751661	-3.694359	-0.517041
1	-4.300962	-2.593368	-1.821413
6	-0.275058	-4.104506	-1.979426
1	0.426873	-3.692325	-2.711010
1	0.175088	-3.981674	-0.994595
1	-0.372912	-5.177260	-2.171980
6	-2.162910	-3.561570	-3.527728
1	-1.397914	-3.268060	-4.252688
1	-2.425736	-4.608178	-3.713887
1	-3.045516	-2.943231	-3.696169

TS1-meta-ggg (Refer to Table S1)

Number of imaginary frequencies : 1
 Imaginary frequency : -804.7658 cm(-1)
 Electronic energy : HF=-3396.5209732
 Zero-point correction= 1.456750 (Hartree/Particle)
 Thermal correction to Energy= 1.536413
 Thermal correction to Enthalpy= 1.537357
 Thermal correction to Gibbs Free Energy= 1.340309
 Sum of electronic and zero-point Energies= -3395.064223
 Sum of electronic and thermal Energies= -3394.984560
 Sum of electronic and thermal Enthalpies= -3394.983616
 Sum of electronic and thermal Free Energies= -3395.180665

Cartesian Coordinates

77	1.358350	-0.607949	0.042696
5	2.562220	-1.321429	-1.536766
8	2.037341	-2.141246	-2.535372
8	3.923927	-1.120127	-1.748521
6	3.029327	-2.265114	-3.585511
6	4.361778	-2.013796	-2.800020
5	2.427303	1.046279	-0.624702
8	2.210115	1.536864	-1.912818
8	3.358151	1.817980	0.042394
6	2.955857	2.769515	-2.090509
6	4.000517	2.703818	-0.908202
5	2.929221	-1.145062	1.216555
8	3.490223	-0.383590	2.238223
8	3.566208	-2.397591	1.160496
6	4.740662	-0.994517	2.622597
6	4.482737	-2.502388	2.276979
6	-0.785427	-2.592090	-0.950784
6	-1.274431	-1.291996	-1.459550
7	0.318797	-2.566625	-0.164226
7	-0.436786	-0.238592	-1.308461
6	-1.410742	-3.805531	-1.265721
6	-0.915746	-4.993457	-0.740045
6	0.206269	-4.947930	0.086677
6	0.800490	-3.715791	0.338315
6	-2.540075	-1.118521	-2.031755
6	-2.946337	0.150636	-2.437263
6	-2.080724	1.238958	-2.280193
6	-0.819496	0.972395	-1.723687
6	0.050072	-0.157838	1.801486
6	0.334586	-0.577942	3.115300
6	-1.235427	0.340214	1.570565
6	-0.648940	-0.573329	4.110295
6	-2.242530	0.301692	2.539629
6	-1.954082	-0.161901	3.826740
1	1.246617	0.629816	1.079209
1	-1.493319	0.757496	0.608383
1	-2.716983	-0.164872	4.599779
1	-0.393968	-0.892652	5.117586
1	1.344321	-0.885452	3.363781
1	1.707030	-3.621807	0.925657
1	0.631423	-5.848033	0.517117
1	-1.394623	-5.937769	-0.979944
1	-2.263155	-3.821480	-1.933033
1	-3.222379	-1.954857	-2.127632

1	-3.937076	0.302885	-2.854654
1	-0.089645	1.761753	-1.605469
6	-3.568327	0.802889	2.062758
8	-3.644078	1.939484	1.556845
7	-4.653177	-0.017819	2.103584
6	-2.399544	2.620873	-2.715472
6	-2.748850	2.860770	-4.053013
6	-2.253072	3.715956	-1.830942
6	-2.880684	4.159972	-4.536050
1	-2.864459	2.013568	-4.723822
6	-2.356372	5.021829	-2.331941
6	-2.656135	5.237562	-3.674165
1	-3.131421	4.331043	-5.578487
1	-2.196874	5.849948	-1.653177
1	-2.734107	6.255563	-4.045184
7	-2.060528	3.467887	-0.461646
6	-1.190069	4.182129	0.368394
8	-0.425918	5.048971	-0.055719
7	-1.260813	3.792384	1.674369
1	-2.631356	2.750838	-0.025939
1	-1.927983	3.064806	1.910194
6	-4.562514	-1.460680	2.390635
1	-5.591663	-1.816252	2.484475
1	-4.089649	-1.614987	3.363322
6	-5.885416	0.489074	1.478920
1	-6.728108	-0.043376	1.929260
1	-5.977506	1.546636	1.736039
6	-0.165269	4.052254	2.610908
6	-0.577524	3.540736	3.998520
6	1.140510	3.381346	2.148848
1	-0.005859	5.137655	2.656228
6	0.559406	3.690185	5.020437
1	-0.838463	2.476701	3.913620
1	-1.479402	4.066943	4.334736
6	2.274656	3.515558	3.169830
1	0.933716	2.319468	1.992318
1	1.434888	3.796685	1.184511
6	1.837930	2.983509	4.541934
1	0.237896	3.291758	5.990541
1	0.772177	4.757854	5.174686
1	3.148794	2.969034	2.800816
1	2.566180	4.572033	3.264848
1	2.640518	3.108620	5.279354
1	1.644206	1.904859	4.459622
6	-3.813210	-2.280953	1.328487
6	-3.883716	-3.794479	1.582550
1	-2.765316	-1.969414	1.314812
1	-4.213106	-2.041846	0.338046
6	-5.294334	-4.411977	1.512219
1	-3.231900	-4.289232	0.854630
1	-3.448597	-4.014713	2.566489
6	-6.087452	-4.081175	0.237507
1	-5.197797	-5.502404	1.600303
1	-5.883547	-4.096114	2.382775
1	-7.067438	-4.571000	0.295391
1	-6.297173	-3.005750	0.201936
6	-5.881027	0.333613	-0.048625
6	-7.089269	0.980756	-0.739237
1	-5.833080	-0.731019	-0.304452
1	-4.960844	0.789481	-0.427042
6	-8.463697	0.442085	-0.298390

1	-7.062001	2.063930	-0.564571
1	-6.977206	0.849783	-1.822706
6	-8.618291	-1.087273	-0.353522
1	-8.677666	0.778641	0.724261
1	-9.233688	0.902538	-0.931381
1	-7.960120	-1.551229	0.392076
1	-9.639482	-1.345521	-0.046536
6	-5.390595	-4.497265	-1.061752
1	-6.017443	-4.282871	-1.933205
1	-4.444328	-3.962554	-1.193119
1	-5.163918	-5.569857	-1.064907
6	-8.334374	-1.702317	-1.728513
1	-8.512439	-2.782668	-1.721430
1	-8.977469	-1.260844	-2.498480
1	-7.295590	-1.543355	-2.036972
6	4.997842	-0.697896	4.096126
1	5.896396	-1.215323	4.449195
1	5.145548	0.377327	4.230850
1	4.151600	-0.999530	4.716540
6	5.827655	-0.360225	1.743729
1	5.781482	0.724055	1.870286
1	6.829078	-0.708876	2.015996
1	5.643075	-0.577389	0.688254
6	5.714615	-3.283194	1.829658
1	6.464238	-3.315623	2.627577
1	5.433193	-4.311475	1.582574
1	6.165248	-2.836305	0.942847
6	3.750427	-3.259759	3.392627
1	3.428965	-4.233065	3.008926
1	4.392446	-3.428883	4.262388
1	2.861395	-2.710553	3.714356
6	4.902489	-3.274237	-2.112877
1	5.296545	-3.995036	-2.836109
1	5.707942	-2.984750	-1.433497
1	4.121929	-3.750471	-1.514656
6	5.465498	-1.329157	-3.600030
1	6.337740	-1.167395	-2.959927
1	5.773663	-1.949584	-4.448615
1	5.140914	-0.358222	-3.977414
6	2.721420	-1.165951	-4.610569
1	3.395670	-1.209171	-5.471714
1	1.695408	-1.296706	-4.966377
1	2.792096	-0.179618	-4.145144
6	2.902756	-3.646878	-4.218225
1	1.942755	-3.728746	-4.736664
1	3.700962	-3.815371	-4.949244
1	2.947008	-4.433383	-3.462527
6	4.271424	4.038411	-0.219345
1	4.738675	4.744447	-0.914131
1	3.356486	4.486095	0.169472
1	4.954317	3.880574	0.620471
6	5.321499	2.029308	-1.299853
1	5.891106	2.632814	-2.013337
1	5.925611	1.895902	-0.398381
1	5.131951	1.041011	-1.723160
6	1.953093	3.919554	-1.981195
1	1.177736	3.791644	-2.742922
1	1.452367	3.946435	-1.013659
1	2.429128	4.891245	-2.143889
6	3.572757	2.748551	-3.488100
1	2.776156	2.752287	-4.237931

1	4.198682	3.632339	-3.650470
1	4.180582	1.855899	-3.642932

TS1-meta-aga (Refer to Table S1)

Number of imaginary frequencies : 1
Imaginary frequency : -784.1984 cm(-1)

Electronic energy : HF=-3396.5226388
Zero-point correction= 1.455053 (Hartree/Particle)
Thermal correction to Energy= 1.535488
Thermal correction to Enthalpy= 1.536432
Thermal correction to Gibbs Free Energy= 1.334379
Sum of electronic and zero-point Energies= -3395.067586
Sum of electronic and thermal Energies= -3394.987151
Sum of electronic and thermal Enthalpies= -3394.986207
Sum of electronic and thermal Free Energies= -3395.188260

Cartesian Coordinates

77	1.361400	0.530990	-0.066979
5	2.559704	1.146439	1.556901
8	2.112044	2.118344	2.451558
8	3.851525	0.747372	1.891452
6	3.040100	2.173331	3.563388
6	4.361290	1.647201	2.904710
5	2.085312	-1.211660	0.810531
8	1.684877	-1.553560	2.102533
8	2.941984	-2.164583	0.295923
6	2.217218	-2.860168	2.444853
6	3.344820	-3.064743	1.358019
5	3.082001	0.680701	-1.141312
8	3.557895	-0.260432	-2.052771
8	3.943419	1.791324	-1.123437
6	4.929057	0.065406	-2.363787
6	4.945716	1.619855	-2.154687
6	-0.419526	2.918710	0.681601
6	-1.196085	1.756263	1.166258
7	0.701962	2.652136	-0.032656
7	-0.563375	0.559108	1.132545
6	-0.790134	4.238402	0.964907
6	-0.018348	5.289372	0.483692
6	1.118938	5.000246	-0.269437
6	1.450211	3.668133	-0.494164
6	-2.518827	1.848652	1.614729
6	-3.188923	0.698633	2.023848
6	-2.531219	-0.537584	1.998937
6	-1.198818	-0.538117	1.556294
6	0.125457	0.153499	-1.911037
6	0.605790	0.327611	-3.224911
6	-1.244133	-0.109025	-1.780733
6	-0.252836	0.294566	-4.327590
6	-2.118891	-0.126709	-2.873062
6	-1.623910	0.077833	-4.165158
1	1.071968	-0.739354	-1.035463
1	-1.665334	-0.330069	-0.810600
1	-2.284296	0.030635	-5.026531
1	0.154715	0.421065	-5.327403
1	1.671489	0.441873	-3.385749
1	2.353617	3.378766	-1.019686

1	1.754993	5.786197	-0.661951
1	-0.299296	6.315452	0.699888
1	-1.663883	4.439875	1.571752
1	-3.035533	2.801598	1.615143
1	-4.221977	0.752842	2.349907
1	-0.620052	-1.451387	1.539476
6	-3.527117	-0.502280	-2.526519
8	-3.727963	-1.591253	-1.952822
7	-4.559575	0.353675	-2.738715
6	-3.150539	-1.795919	2.481947
6	-3.733579	-1.821324	3.759819
6	-3.087260	-2.994510	1.730418
6	-4.190096	-3.011411	4.319235
1	-3.773543	-0.899690	4.333792
6	-3.517247	-4.194959	2.315402
6	-4.054837	-4.202022	3.599061
1	-4.621469	-3.014448	5.315470
1	-3.421539	-5.109688	1.744189
1	-4.386581	-5.140965	4.032920
7	-2.648855	-2.949380	0.396330
6	-1.842611	-3.913672	-0.216514
8	-1.297826	-4.821682	0.410626
7	-1.706256	-3.721154	-1.563656
1	-3.038100	-2.229655	-0.204742
1	-2.179999	-2.916185	-1.963708
6	-4.418076	1.699124	-3.296990
1	-5.204695	1.839426	-4.049738
1	-3.462828	1.759753	-3.818081
6	-5.859658	-0.038947	-2.167297
1	-6.627387	0.597450	-2.618964
1	-6.056200	-1.071864	-2.466910
6	-0.528986	-4.228194	-2.268877
6	-0.773742	-4.174589	-3.782991
6	0.721323	-3.412969	-1.900796
1	-0.386606	-5.269268	-1.956972
6	0.473217	-4.615090	-4.567167
1	-1.022716	-3.138377	-4.059193
1	-1.641136	-4.792702	-4.042732
6	1.970419	-3.843677	-2.673918
1	0.509757	-2.366821	-2.139664
1	0.894556	-3.464237	-0.824316
6	1.708220	-3.781637	-4.185773
1	0.278407	-4.544751	-5.644331
1	0.675106	-5.674681	-4.354111
1	2.804256	-3.193535	-2.389777
1	2.246937	-4.870185	-2.391443
1	2.585536	-4.125844	-4.747378
1	1.537683	-2.733812	-4.472214
6	-4.491448	2.815877	-2.249083
6	-4.270756	4.196035	-2.881420
1	-3.737776	2.612817	-1.479328
1	-5.468668	2.796761	-1.750058
6	-4.467490	5.367986	-1.908770
1	-3.257211	4.240659	-3.303995
1	-4.961391	4.315179	-3.727340
6	-3.476798	5.374802	-0.739042
1	-4.369490	6.311069	-2.462856
1	-5.494700	5.349608	-1.517151
1	-3.608575	4.465103	-0.139933
1	-2.453898	5.325698	-1.133168
6	-5.895288	0.059244	-0.632667

6	-7.124953	-0.625280	-0.023289
1	-5.846701	1.111021	-0.331902
1	-4.996569	-0.423841	-0.238888
6	-7.062502	-0.734782	1.508166
1	-8.040602	-0.094382	-0.321809
1	-7.203268	-1.636739	-0.442828
6	-7.127476	0.607344	2.249066
1	-7.890080	-1.366198	1.857690
1	-6.140416	-1.261684	1.791981
1	-6.318455	1.265180	1.904946
1	-8.061265	1.123103	1.985713
6	-3.623842	6.601639	0.164809
1	-2.906447	6.581893	0.992855
1	-3.456814	7.527770	-0.396671
1	-4.628614	6.656292	0.598972
6	-7.035558	0.441669	3.769463
1	-7.067262	1.406719	4.286099
1	-7.863540	-0.168309	4.147752
1	-6.105659	-0.065003	4.051396
6	5.235771	-0.407253	-3.780977
1	6.246528	-0.112122	-4.083263
1	5.170710	-1.498350	-3.821854
1	4.521636	-0.002796	-4.501104
6	5.799141	-0.681887	-1.343893
1	5.556120	-1.745571	-1.398786
1	6.867627	-0.548971	-1.541880
1	5.572465	-0.345289	-0.328926
6	6.268897	2.189967	-1.653118
1	7.068814	2.010444	-2.379641
1	6.175659	3.270330	-1.506087
1	6.554255	1.743827	-0.699840
6	4.465476	2.398045	-3.386768
1	4.312268	3.445248	-3.108167
1	5.194781	2.362493	-4.201787
1	3.513963	2.001052	-3.751089
6	5.145799	2.740874	2.168991
1	5.613585	3.445341	2.863871
1	5.928004	2.267103	1.571107
1	4.493818	3.287620	1.483762
6	5.283860	0.868497	3.837113
1	6.156110	0.514267	3.279942
1	5.636242	1.504846	4.656191
1	4.780349	-0.000781	4.262743
6	2.488656	1.229434	4.639485
1	3.107270	1.230991	5.542413
1	1.480405	1.556893	4.908943
1	2.417219	0.210718	4.250526
6	3.101405	3.607007	4.079423
1	2.133797	3.886448	4.506816
1	3.861789	3.706819	4.861583
1	3.330549	4.308177	3.274766
6	3.429110	-4.476783	0.782983
1	3.705093	-5.196846	1.560680
1	2.483911	-4.789636	0.337981
1	4.194859	-4.504178	0.002491
6	4.731291	-2.595919	1.817770
1	5.128236	-3.224932	2.620672
1	5.416846	-2.646787	0.967767
1	4.691009	-1.556979	2.150500
6	1.060283	-3.855709	2.345463
1	0.254390	-3.535392	3.012863

1	0.641469	-3.914948	1.341652
1	1.365333	-4.863685	2.642624
6	2.723206	-2.799315	3.885542
1	1.881764	-2.608584	4.558169
1	3.183665	-3.749199	4.176705
1	3.454208	-2.000994	4.020875

TS1-meta-agg (Refer to Table S1)

Number of imaginary frequencies : 1
Imaginary frequency : -791.2229 cm(-1)

Electronic energy : HF=-3396.5225991
Zero-point correction= 1.455988 (Hartree/Particle)
Thermal correction to Energy= 1.536000
Thermal correction to Enthalpy= 1.536944
Thermal correction to Gibbs Free Energy= 1.337971
Sum of electronic and zero-point Energies= -3395.066611
Sum of electronic and thermal Energies= -3394.986599
Sum of electronic and thermal Enthalpies= -3394.985655
Sum of electronic and thermal Free Energies= -3395.184629

Cartesian Coordinates

77	1.291427	-0.589104	0.072424
5	2.467092	-1.345897	-1.506419
8	1.940362	-2.236885	-2.440610
8	3.812930	-1.107819	-1.776958
6	2.899616	-2.382425	-3.517601
6	4.247634	-2.041488	-2.795068
5	2.241396	1.063823	-0.759277
8	1.950519	1.444155	-2.070009
8	3.150756	1.932532	-0.189028
6	2.614250	2.701568	-2.364268
6	3.706344	2.778034	-1.227467
5	2.941051	-0.968120	1.205285
8	3.548169	-0.092303	2.102115
8	3.603160	-2.209085	1.243732
6	4.832261	-0.640340	2.470864
6	4.582927	-2.179450	2.309651
6	-0.722755	-2.756206	-0.771502
6	-1.321012	-1.516944	-1.312321
7	0.372964	-2.615074	0.015699
7	-0.564725	-0.396678	-1.216660
6	-1.233703	-4.026018	-1.066522
6	-0.634827	-5.154258	-0.518861
6	0.471747	-4.991863	0.313950
6	0.950789	-3.706631	0.544952
6	-2.603117	-1.463425	-1.871248
6	-3.105080	-0.248064	-2.327823
6	-2.322018	0.909038	-2.234991
6	-1.040433	0.763609	-1.679901
6	0.056725	-0.016857	1.865368
6	0.477180	-0.163689	3.202895
6	-1.276723	0.361413	1.670496
6	-0.408890	0.013001	4.270145
6	-2.181598	0.512102	2.726574
6	-1.749095	0.339984	4.045107
1	1.138092	0.725900	1.010280
1	-1.648614	0.559071	0.675515

1	-2.429815	0.492883	4.877713
1	-0.046562	-0.089881	5.289847
1	1.521916	-0.370117	3.407140
1	1.843879	-3.519163	1.129469
1	0.973590	-5.841557	0.763879
1	-1.024826	-6.142303	-0.742545
1	-2.081355	-4.130665	-1.731454
1	-3.222087	-2.351991	-1.921481
1	-4.106757	-0.191001	-2.740463
1	-0.369683	1.608595	-1.607475
6	-3.556228	0.919491	2.292476
8	-3.692574	1.953538	1.610790
7	-4.620558	0.113028	2.550746
6	-2.755343	2.227594	-2.756334
6	-3.227238	2.319355	-4.075707
6	-2.618984	3.409969	-1.989312
6	-3.490373	3.554707	-4.660503
1	-3.333597	1.407703	-4.657515
6	-2.855175	4.652615	-2.595950
6	-3.275852	4.721422	-3.920849
1	-3.834349	3.608611	-5.688865
1	-2.703493	5.550325	-2.010407
1	-3.456019	5.692808	-4.372465
7	-2.305610	3.311211	-0.623662
6	-1.458960	4.181429	0.068216
8	-0.787671	5.046848	-0.493104
7	-1.438957	3.951894	1.415928
1	-2.790626	2.607974	-0.075315
1	-2.005492	3.185630	1.765581
6	-4.481920	-1.230059	3.134866
1	-5.470109	-1.517623	3.509165
1	-3.822115	-1.179537	4.002341
6	-5.881723	0.457616	1.870992
1	-6.693872	-0.063004	2.388694
1	-6.040861	1.532447	1.985756
6	-0.295669	4.376939	2.222561
6	-0.673093	4.339854	3.709391
6	0.931265	3.488017	1.956995
1	-0.060928	5.406967	1.930596
6	0.524153	4.710673	4.599458
1	-1.003841	3.320574	3.960104
1	-1.522429	5.007982	3.894155
6	2.130483	3.855343	2.836000
1	0.643980	2.454970	2.171681
1	1.199039	3.530503	0.899208
6	1.739089	3.810214	4.320464
1	0.234773	4.649921	5.655761
1	0.801407	5.757670	4.410749
1	2.954513	3.165368	2.625147
1	2.481987	4.865893	2.580756
1	2.583793	4.106076	4.954728
1	1.486684	2.774065	4.587865
6	-3.964352	-2.293722	2.157455
6	-3.965252	-3.693911	2.777175
1	-2.952831	-2.021755	1.833506
1	-4.591599	-2.287145	1.262232
6	-3.443162	-4.784386	1.827432
1	-3.348699	-3.691112	3.685651
1	-4.984149	-3.943489	3.103384
6	-4.175819	-4.875823	0.477116
1	-2.377221	-4.610520	1.636443

1	-3.513079	-5.755810	2.334982
1	-3.984600	-3.965160	-0.104438
1	-3.732220	-5.695716	-0.102157
6	-5.867758	0.095032	0.379055
6	-7.153892	0.483428	-0.353013
1	-5.703281	-0.981646	0.277390
1	-5.010955	0.592600	-0.087248
6	-7.101999	0.172486	-1.859999
1	-8.008134	-0.033390	0.105032
1	-7.340411	1.556763	-0.220481
6	-6.795181	-1.294074	-2.216571
1	-8.062287	0.452101	-2.312875
1	-6.345260	0.818186	-2.326591
1	-6.795084	-1.392642	-3.309644
1	-5.778516	-1.550615	-1.891928
6	-5.688201	-5.093994	0.591979
1	-6.145548	-5.229264	-0.393617
1	-5.915045	-5.982421	1.192415
1	-6.184524	-4.240335	1.065880
6	-7.778465	-2.305364	-1.616718
1	-7.559931	-3.322002	-1.959730
1	-7.731627	-2.313245	-0.522556
1	-8.810278	-2.069780	-1.901549
6	5.175890	-0.179878	3.883621
1	6.105830	-0.643275	4.230504
1	5.310254	0.905497	3.890295
1	4.378250	-0.423128	4.588519
6	5.849009	-0.091844	1.460163
1	5.792798	0.999178	1.476384
1	6.872016	-0.399063	1.700295
1	5.599037	-0.421115	0.447900
6	5.801022	-2.991157	1.880282
1	6.596127	-2.926214	2.630931
1	5.524572	-4.043872	1.766078
1	6.191609	-2.640262	0.924560
6	3.927723	-2.813485	3.543646
1	3.598971	-3.826249	3.290703
1	4.622085	-2.877889	4.386822
1	3.050771	-2.238707	3.853821
6	4.857629	-3.242982	-2.061786
1	5.255312	-3.986252	-2.759818
1	5.673475	-2.889003	-1.426615
1	4.116208	-3.716142	-1.413264
6	5.298599	-1.363433	-3.668310
1	6.186599	-1.141517	-3.069188
1	5.598060	-2.016455	-4.495239
1	4.929844	-0.423520	-4.082140
6	2.516597	-1.350556	-4.585847
1	3.167310	-1.409627	-5.463901
1	1.487227	-1.540371	-4.903287
1	2.558065	-0.340730	-4.170129
6	2.801068	-3.799988	-4.071215
1	1.825258	-3.942589	-4.545052
1	3.575613	-3.980053	-4.824625
1	2.903037	-4.542691	-3.277725
6	3.928160	4.171509	-0.645817
1	4.318603	4.852178	-1.409855
1	3.005931	4.592106	-0.242996
1	4.657274	4.113396	0.167440
6	5.045032	2.145432	-1.627754
1	5.551789	2.722999	-2.407113

1	5.692193	2.109074	-0.747482
1	4.892084	1.120073	-1.970446
6	1.552419	3.799312	-2.287312
1	0.745016	3.568479	-2.988869
1	1.106013	3.880827	-1.296959
1	1.960578	4.779332	-2.551840
6	3.173544	2.618880	-3.783663
1	2.347803	2.528877	-4.495649
1	3.740336	3.522454	-4.031527
1	3.824929	1.752481	-3.907834

TS1-meta-aag (Refer to Table S1)

Number of imaginary frequencies : 1
Imaginary frequency : -786.4960 cm(-1)

Electronic energy : HF=-3396.5226872
Zero-point correction= 1.454891 (Hartree/Particle)
Thermal correction to Energy= 1.535345
Thermal correction to Enthalpy= 1.536289
Thermal correction to Gibbs Free Energy= 1.336129
Sum of electronic and zero-point Energies= -3395.067797
Sum of electronic and thermal Energies= -3394.987343
Sum of electronic and thermal Enthalpies= -3394.986398
Sum of electronic and thermal Free Energies= -3395.186558

Cartesian Coordinates

77	-1.446288	0.348822	-0.028189
5	-2.819102	0.401719	-1.629526
8	-2.641665	1.263900	-2.710733
8	-4.002921	-0.318031	-1.780814
6	-3.601037	0.907041	-3.737252
6	-4.741504	0.238137	-2.895034
5	-1.835888	-1.639986	-0.497665
8	-1.465152	-2.137076	-1.747491
8	-2.402793	-2.632491	0.275996
6	-1.711939	-3.566059	-1.792969
6	-2.673583	-3.786624	-0.558676
5	-3.129402	0.421272	1.114914
8	-3.439947	-0.416352	2.182791
8	-4.133897	1.397925	0.979037
6	-4.826229	-0.210670	2.531667
6	-5.052262	1.276724	2.092518
6	-0.150751	2.818886	-1.326154
6	0.796602	1.730821	-1.652772
7	-1.181273	2.507920	-0.501538
7	0.392118	0.473516	-1.351309
6	-0.021261	4.109182	-1.854754
6	-0.934271	5.095248	-1.498791
6	-1.972687	4.767176	-0.627910
6	-2.069067	3.458875	-0.165168
6	2.061431	1.957042	-2.208088
6	2.911001	0.880346	-2.451315
6	2.488958	-0.420464	-2.148792
6	1.199661	-0.560042	-1.610908
6	-0.097568	0.565180	1.754160
6	-0.560852	0.896227	3.043505
6	1.291918	0.538453	1.579001
6	0.321006	1.237588	4.073113

6	2.183756	0.895035	2.594647
6	1.701049	1.254134	3.857487
1	-0.891231	-0.639758	1.130864
1	1.716637	0.220784	0.637036
1	2.388481	1.509436	4.659032
1	-0.071763	1.478598	5.057654
1	-1.622929	0.838851	3.251776
1	-2.889966	3.125571	0.460031
1	-2.713221	5.500025	-0.326453
1	-0.840648	6.097488	-1.904338
1	0.770044	4.330964	-2.559842
1	2.399109	2.965456	-2.416575
1	3.903850	1.047474	-2.856743
1	0.800420	-1.538136	-1.379713
6	3.631988	0.759635	2.244397
8	4.070360	-0.353356	1.892737
7	4.440724	1.850025	2.243191
6	3.299973	-1.630237	-2.431287
6	3.795300	-1.834773	-3.729159
6	3.516229	-2.623409	-1.446693
6	4.426836	-3.025284	-4.077643
1	3.635076	-1.063349	-4.477409
6	4.124205	-3.833172	-1.814324
6	4.562970	-4.034293	-3.119599
1	4.786553	-3.174747	-5.090975
1	4.242517	-4.601324	-1.060609
1	5.035209	-4.975931	-3.384140
7	3.170755	-2.361576	-0.109696
6	2.573674	-3.289463	0.750841
8	2.159750	-4.381646	0.361468
7	2.479668	-2.848855	2.039141
1	3.435194	-1.465541	0.286095
1	2.834417	-1.918284	2.241421
6	3.925296	3.220467	2.307488
1	4.657892	3.834988	2.843819
1	3.011080	3.221205	2.901522
6	5.807471	1.640971	1.736674
1	6.379312	2.539574	1.983301
1	6.237571	0.809637	2.301307
6	1.478011	-3.411990	2.943799
6	1.805392	-3.009078	4.387655
6	0.065086	-2.940487	2.562864
1	1.530741	-4.502672	2.847330
6	0.733157	-3.516859	5.365327
1	1.848237	-1.910569	4.442435
1	2.798281	-3.383221	4.663613
6	-1.011270	-3.444301	3.528601
1	0.067050	-1.847001	2.584455
1	-0.163187	-3.238941	1.537724
6	-0.671650	-3.032727	4.968996
1	0.977842	-3.195288	6.385069
1	0.745690	-4.616232	5.372317
1	-1.982421	-3.042096	3.221225
1	-1.080308	-4.540364	3.467925
1	-1.418744	-3.422376	5.671497
1	-0.707641	-1.936035	5.041645
6	3.636892	3.821731	0.925508
6	2.935330	5.180261	1.021514
1	3.006281	3.120111	0.364915
1	4.573550	3.921046	0.361780
6	2.801731	5.870017	-0.342124

1	1.936453	5.035465	1.456984
1	3.483816	5.830268	1.716155
6	1.897221	7.110571	-0.337317
1	3.801123	6.143845	-0.709222
1	2.400921	5.143132	-1.059168
1	1.788556	7.473707	-1.368047
1	0.891952	6.813950	-0.009340
6	5.878163	1.324530	0.217728
6	6.649031	0.034121	-0.083443
1	6.330896	2.167222	-0.320977
1	4.858737	1.224930	-0.170859
6	6.688027	-0.307715	-1.577045
1	7.670037	0.122896	0.310453
1	6.166620	-0.781656	0.468259
6	7.317032	-1.672969	-1.894565
1	5.661524	-0.309706	-1.962877
1	7.226434	0.481981	-2.122704
1	6.747910	-2.453125	-1.373688
1	7.188523	-1.877987	-2.964309
6	2.409734	8.253269	0.546667
1	1.761557	9.132453	0.473412
1	2.449083	7.960902	1.600876
1	3.420036	8.557244	0.248564
6	8.801496	-1.778398	-1.528119
1	9.214775	-2.747695	-1.826097
1	9.387555	-0.997779	-2.028522
1	8.961460	-1.671631	-0.450168
6	-5.002784	-0.484754	4.021533
1	-6.026590	-0.263148	4.342231
1	-4.801252	-1.540442	4.223896
1	-4.309868	0.108537	4.621521
6	-5.641016	-1.208161	1.696584
1	-5.269465	-2.214309	1.904874
1	-6.708465	-1.167438	1.936237
1	-5.500420	-1.018252	0.628924
6	-6.461685	1.600877	1.607038
1	-7.193474	1.436775	2.405367
1	-6.518169	2.650619	1.302681
1	-6.735241	0.987511	0.748195
6	-4.612390	2.293092	3.154601
1	-4.605287	3.292213	2.708092
1	-5.290075	2.305448	4.013600
1	-3.601808	2.073440	3.508981
6	-5.731445	1.250656	-2.305744
1	-6.363862	1.700883	-3.077175
1	-6.373961	0.732913	-1.589061
1	-5.200877	2.038033	-1.765221
6	-5.491621	-0.887581	-3.599565
1	-6.235864	-1.314045	-2.920585
1	-6.012889	-0.512085	-4.486700
1	-4.816431	-1.688376	-3.904049
6	-2.890441	-0.079308	-4.673291
1	-3.524948	-0.376899	-5.514056
1	-1.991803	0.401493	-5.070516
1	-2.578190	-0.970092	-4.122019
6	-4.007207	2.171165	-4.487185
1	-3.147483	2.566404	-5.036382
1	-4.804022	1.957637	-5.207704
1	-4.353490	2.944584	-3.799032
6	-2.387706	-5.046970	0.254055
1	-2.562798	-5.943727	-0.349836

1	-1.360235	-5.070020	0.619459
1	-3.055782	-5.079546	1.119474
6	-4.162773	-3.712113	-0.920165
1	-4.472293	-4.551262	-1.550999
1	-4.747297	-3.739658	0.003360
1	-4.384872	-2.770493	-1.426652
6	-0.355386	-4.260353	-1.662086
1	0.300690	-3.915444	-2.467467
1	0.141661	-4.037468	-0.718012
1	-0.447446	-5.347703	-1.742905
6	-2.331877	-3.891969	-3.150928
1	-1.613239	-3.661853	-3.943115
1	-2.585658	-4.954992	-3.218578
1	-3.233616	-3.304852	-3.329666

TS1-meta-gag (Refer to Table S1)

Number of imaginary frequencies : 1
Imaginary frequency : -787.7987 cm(-1)

Electronic energy : HF=-3396.526555
Zero-point correction= 1.455628 (Hartree/Particle)
Thermal correction to Energy= 1.535698
Thermal correction to Enthalpy= 1.536643
Thermal correction to Gibbs Free Energy= 1.337588
Sum of electronic and zero-point Energies= -3395.070927
Sum of electronic and thermal Energies= -3394.990857
Sum of electronic and thermal Enthalpies= -3394.989912
Sum of electronic and thermal Free Energies= -3395.188967

Cartesian Coordinates

77	-1.331448	0.328630	-0.092462
5	-2.788349	0.096199	-1.600658
8	-2.568236	0.542526	-2.902924
8	-4.058463	-0.466293	-1.494643
6	-3.616136	0.001935	-3.747020
6	-4.782646	-0.203651	-2.720599
5	-1.949267	-1.652743	0.050950
8	-1.716776	-2.535061	-1.005802
8	-2.549833	-2.305524	1.108649
6	-2.061750	-3.881689	-0.585649
6	-2.987507	-3.612670	0.661759
5	-2.925556	0.906673	1.039120
8	-3.281249	0.431010	2.298175
8	-3.811565	1.934182	0.661747
6	-4.612198	0.903637	2.602782
6	-4.675635	2.237051	1.782045
6	0.089959	2.214299	-2.076132
6	0.851558	0.953345	-2.206041
7	-0.885084	2.246490	-1.133272
7	0.376929	-0.106595	-1.507699
6	0.335136	3.328770	-2.889595
6	-0.414695	4.486440	-2.718635
6	-1.400802	4.509969	-1.732899
6	-1.608795	3.366652	-0.969018
6	2.013758	0.832390	-2.976669
6	2.688279	-0.384346	-3.024660
6	2.196928	-1.476671	-2.299979
6	1.020750	-1.275761	-1.564189

6	0.156451	0.825035	1.509628
6	-0.187240	1.455181	2.722333
6	1.524806	0.679178	1.241297
6	0.789168	1.957494	3.587365
6	2.508477	1.212375	2.077610
6	2.143561	1.856454	3.265661
1	-0.798997	-0.407899	1.248552
1	1.857312	0.152158	0.356989
1	2.905806	2.244537	3.935560
1	0.490977	2.423185	4.523236
1	-1.232241	1.512306	3.006538
1	-2.395885	3.300761	-0.227181
1	-2.011979	5.389556	-1.562784
1	-0.232693	5.353879	-3.345103
1	1.092485	3.284671	-3.662519
1	2.412331	1.685064	-3.513124
1	3.601483	-0.484307	-3.601831
1	0.574881	-2.087173	-1.006440
6	3.934005	1.004586	1.666874
8	4.361112	-0.152102	1.492617
7	4.713267	2.107530	1.484126
6	2.828036	-2.817299	-2.308836
6	3.066783	-3.463943	-3.531067
6	3.143992	-3.481535	-1.100567
6	3.543336	-4.771407	-3.568339
1	2.830336	-2.940824	-4.453589
6	3.596541	-4.808150	-1.145416
6	3.782902	-5.446914	-2.367853
1	3.705462	-5.265701	-4.521222
1	3.797910	-5.317814	-0.211930
1	4.136996	-6.473672	-2.383055
7	3.065998	-2.782296	0.116680
6	2.564367	-3.321291	1.307891
8	2.050296	-4.438267	1.361478
7	2.684127	-2.480906	2.373140
1	3.385873	-1.821477	0.137602
1	3.133974	-1.579477	2.234370
6	4.126992	3.446173	1.293480
1	4.953460	4.160238	1.335688
1	3.466557	3.681438	2.130593
6	6.152765	1.948496	1.239008
1	6.669570	2.705124	1.842090
1	6.436698	0.968179	1.622200
6	1.877646	-2.685681	3.574705
6	2.438345	-1.828123	4.716803
6	0.397503	-2.351112	3.316954
1	1.956305	-3.745927	3.844507
6	1.582678	-1.957177	5.986440
1	2.444234	-0.777126	4.394259
1	3.479476	-2.109697	4.914661
6	-0.458284	-2.481940	4.581368
1	0.344374	-1.320063	2.955648
1	0.012457	-2.991750	2.519873
6	0.109966	-1.611584	5.712177
1	1.988711	-1.311972	6.775098
1	1.646761	-2.988522	6.361856
1	-1.491354	-2.198187	4.351955
1	-0.479557	-3.532493	4.906505
1	-0.483645	-1.728475	6.627173
1	0.038188	-0.555141	5.417112
6	3.341365	3.598924	-0.023898

6	2.399078	4.809770	-0.018965
1	2.743521	2.695826	-0.176824
1	4.038879	3.659891	-0.868732
6	3.109597	6.168118	0.059375
1	1.783308	4.768069	-0.922906
1	1.702152	4.710277	0.825930
6	2.155599	7.369507	0.154445
1	3.776434	6.186647	0.931276
1	3.757015	6.284947	-0.822398
1	1.553386	7.276235	1.068535
1	2.749999	8.284302	0.272551
6	6.566886	2.097988	-0.232487
6	6.014880	1.010762	-1.165884
1	7.664741	2.088777	-0.270239
1	6.261426	3.089789	-0.588847
6	6.627454	-0.374741	-0.916114
1	4.924464	0.948863	-1.051983
1	6.199554	1.320172	-2.202207
6	6.050091	-1.477144	-1.812514
1	7.717863	-0.318297	-1.049778
1	6.440952	-0.656788	0.124532
1	6.402534	-2.453533	-1.459182
1	4.964258	-1.494548	-1.682362
6	1.222158	7.527847	-1.052083
1	0.626688	8.443288	-0.973249
1	1.793589	7.580923	-1.986973
1	0.526864	6.687212	-1.134843
6	6.375359	-1.341221	-3.303358
1	5.920886	-2.157222	-3.874950
1	6.005783	-0.396930	-3.719944
1	7.457548	-1.369327	-3.476380
6	-4.745711	1.064915	4.113129
1	-5.712303	1.509632	4.374032
1	-4.678837	0.084759	4.593607
1	-3.949577	1.692161	4.519097
6	-5.586988	-0.161586	2.082342
1	-5.334493	-1.116058	2.550295
1	-6.626810	0.085258	2.319829
1	-5.479779	-0.282673	1.000839
6	-6.057155	2.605976	1.250572
1	-6.763102	2.756537	2.074392
1	-5.998356	3.535912	0.676569
1	-6.445846	1.828824	0.591650
6	-4.054034	3.429021	2.522500
1	-3.947919	4.264788	1.823827
1	-4.674776	3.759586	3.360816
1	-3.060200	3.173870	2.900454
6	-5.608467	1.066754	-2.481301
1	-6.227417	1.321236	-3.347343
1	-6.263704	0.900716	-1.622425
1	-4.955621	1.909940	-2.242695
6	-5.699963	-1.387369	-3.011364
1	-6.461551	-1.463786	-2.229697
1	-6.207962	-1.259190	-3.973298
1	-5.144480	-2.326307	-3.031585
6	-3.081772	-1.319402	-4.315159
1	-3.796393	-1.788766	-4.998495
1	-2.157890	-1.116610	-4.864578
1	-2.844263	-2.014115	-3.505380
6	-3.905207	0.995602	-4.866660
1	-3.030018	1.080677	-5.517627

1	-4.751999	0.661246	-5.475918
1	-4.128685	1.987340	-4.469094
6	-2.812958	-4.596906	1.814867
1	-3.091783	-5.610115	1.506132
1	-1.784176	-4.612598	2.177613
1	-3.459940	-4.300808	2.645674
6	-4.470591	-3.470292	0.296679
1	-4.901180	-4.419160	-0.038129
1	-5.017286	-3.134741	1.181787
1	-4.599978	-2.713933	-0.480564
6	-0.753255	-4.596769	-0.243372
1	-0.095050	-4.586177	-1.117360
1	-0.216736	-4.112743	0.572687
1	-0.922515	-5.640000	0.039285
6	-2.750022	-4.580004	-1.756474
1	-2.042552	-4.687564	-2.584018
1	-3.091177	-5.579358	-1.466709
1	-3.607409	-4.007859	-2.114402

TS1-meta-gaa (Refer to Table S1)

Number of imaginary frequencies : 1
Imaginary frequency : -770.1699 cm(-1)

Electronic energy : HF=-3396.5327936
Zero-point correction= 1.455507 (Hartree/Particle)
Thermal correction to Energy= 1.535670
Thermal correction to Enthalpy= 1.536614
Thermal correction to Gibbs Free Energy= 1.338060
Sum of electronic and zero-point Energies= -3395.077287
Sum of electronic and thermal Energies= -3394.997124
Sum of electronic and thermal Enthalpies= -3394.996180
Sum of electronic and thermal Free Energies= -3395.194734

Cartesian Coordinates

77	-1.339681	0.141536	-0.260115
5	-2.667520	-0.694584	-1.668853
8	-2.558129	-0.414605	-3.030050
8	-3.755559	-1.534410	-1.438406
6	-3.434497	-1.318213	-3.749461
6	-4.515815	-1.652406	-2.664936
5	-1.481316	-1.870989	0.251449
8	-1.021099	-2.844441	-0.635987
8	-1.947199	-2.450886	1.414192
6	-1.086151	-4.147590	0.000996
6	-2.063924	-3.881521	1.211944
5	-3.042694	0.534352	0.785254
8	-3.274969	0.249374	2.127947
8	-4.153268	1.215199	0.253126
6	-4.684275	0.425511	2.390824
6	-5.077052	1.509913	1.329300
6	-0.260412	1.974590	-2.489853
6	0.788468	0.937914	-2.373532
7	-1.313763	1.879712	-1.640322
7	0.500163	-0.116317	-1.571828
6	-0.199863	3.003632	-3.439301
6	-1.228415	3.935241	-3.515049
6	-2.310213	3.815275	-2.643475
6	-2.316297	2.770224	-1.726870

6	2.026797	1.019811	-3.021178
6	2.973221	0.015056	-2.834728
6	2.676407	-1.071331	-2.004016
6	1.403749	-1.088162	-1.410917
6	-0.050557	1.257226	1.214510
6	-0.545712	2.025084	2.287215
6	1.325861	1.340480	0.973792
6	0.292252	2.854525	3.039152
6	2.167368	2.197743	1.688014
6	1.653455	2.961674	2.740359
1	-0.699282	-0.173694	1.195164
1	1.787431	0.726842	0.214456
1	2.302694	3.605613	3.326749
1	-0.119750	3.418766	3.871857
1	-1.591041	1.935216	2.560140
1	-3.140572	2.605330	-1.042427
1	-3.139438	4.513499	-2.666680
1	-1.188724	4.735075	-4.247875
1	0.635197	3.063743	-4.126158
1	2.271013	1.874942	-3.639777
1	3.945096	0.081641	-3.313601
1	1.096636	-1.914880	-0.784733
6	3.598752	2.152829	1.247505
8	4.204420	1.064107	1.273611
7	4.180375	3.272896	0.736468
6	3.593378	-2.214882	-1.774610
6	4.063563	-2.953443	-2.871280
6	3.913442	-2.642219	-0.463664
6	4.766261	-4.141204	-2.686218
1	3.822358	-2.611330	-3.874063
6	4.591650	-3.857129	-0.284710
6	4.999312	-4.602778	-1.386982
1	5.105871	-4.713230	-3.544080
1	4.792548	-4.194527	0.723563
1	5.527968	-5.538414	-1.229439
7	3.592090	-1.813888	0.622525
6	3.145542	-2.265892	1.868379
8	2.886946	-3.447751	2.095116
7	3.005413	-1.264610	2.786481
1	3.721626	-0.813563	0.511451
1	3.210008	-0.318003	2.481627
6	3.394570	4.466936	0.392463
1	4.089861	5.310208	0.330677
1	2.718611	4.682615	1.217909
6	5.502015	3.099275	0.120166
1	6.015389	4.065546	0.146923
1	6.060395	2.408358	0.753020
6	2.115622	-1.439590	3.935104
6	2.352473	-0.306733	4.942156
6	0.642683	-1.474839	3.493149
1	2.370073	-2.399403	4.399997
6	1.383219	-0.404231	6.131460
1	2.195113	0.654630	4.431339
1	3.394709	-0.323666	5.282368
6	-0.327371	-1.574240	4.674388
1	0.437460	-0.549903	2.947806
1	0.488248	-2.298123	2.792862
6	-0.082460	-0.428687	5.667421
1	1.555242	0.432498	6.819559
1	1.597170	-1.322847	6.696413
1	-1.355252	-1.553870	4.296798

1	-0.189651	-2.537750	5.186819
1	-0.752035	-0.514548	6.532096
1	-0.318877	0.524474	5.173541
6	2.587780	4.343823	-0.917611
6	1.418548	5.340912	-0.983756
1	2.189944	3.325419	-0.990496
1	3.258003	4.480993	-1.773705
6	0.254396	4.957669	-0.060351
1	1.775997	6.352139	-0.739421
1	1.049949	5.389872	-2.016027
6	-0.925353	5.932489	-0.111382
1	-0.093331	3.951595	-0.322582
1	0.599666	4.879007	0.976536
1	-0.586574	6.935890	0.181597
1	-1.280188	6.019821	-1.147035
6	5.440553	2.553228	-1.325110
6	6.658277	1.686982	-1.685167
1	5.344946	3.390322	-2.026568
1	4.531280	1.951530	-1.431850
6	6.568042	0.263165	-1.117004
1	6.759959	1.630236	-2.777113
1	7.576279	2.174749	-1.325820
6	7.841372	-0.559859	-1.336138
1	6.325637	0.296941	-0.047907
1	5.720645	-0.253633	-1.588800
1	8.108763	-0.539583	-2.402403
1	8.675640	-0.079657	-0.805888
6	-2.080083	5.489079	0.792390
1	-2.920893	6.189887	0.753604
1	-2.448763	4.501822	0.497319
1	-1.754024	5.410378	1.835570
6	7.692920	-2.011676	-0.873206
1	8.626650	-2.570676	-0.997168
1	7.409446	-2.060814	0.184120
1	6.913303	-2.527513	-1.441321
6	-4.865143	0.844508	3.845948
1	-5.915450	1.070694	4.059669
1	-4.549829	0.028545	4.502321
1	-4.260998	1.721364	4.087315
6	-5.352681	-0.931664	2.131114
1	-4.868215	-1.679301	2.763693
1	-6.422547	-0.911190	2.362153
1	-5.211131	-1.236450	1.090528
6	-6.501891	1.405793	0.795287
1	-7.229305	1.531312	1.604466
1	-6.679059	2.189505	0.052197
1	-6.672649	0.442111	0.314532
6	-4.786583	2.941847	1.797220
1	-4.886718	3.622812	0.946716
1	-5.481236	3.264411	2.578704
1	-3.765698	3.027043	2.178660
6	-5.638392	-0.610159	-2.590200
1	-6.294599	-0.652793	-3.465118
1	-6.236763	-0.805105	-1.696574
1	-5.223457	0.396317	-2.497733
6	-5.102440	-3.058266	-2.747406
1	-5.816564	-3.207239	-1.932199
1	-5.630505	-3.204224	-3.695920
1	-4.327228	-3.820816	-2.658910
6	-2.582389	-2.533524	-4.138206
1	-3.150399	-3.259360	-4.728433

1	-1.733274	-2.188689	-4.735184
1	-2.187609	-3.023120	-3.244056
6	-3.960275	-0.606341	-4.991214
1	-3.132570	-0.403711	-5.677408
1	-4.693364	-1.228773	-5.515731
1	-4.427407	0.346755	-4.735698
6	-1.680655	-4.584478	2.511652
1	-1.733956	-5.672126	2.393947
1	-0.673673	-4.318823	2.835811
1	-2.378391	-4.290430	3.301042
6	-3.536653	-4.149668	0.875797
1	-3.730049	-5.214808	0.715226
1	-4.153277	-3.807907	1.711260
1	-3.834181	-3.585317	-0.010623
6	0.338770	-4.517145	0.416526
1	0.983313	-4.512264	-0.467972
1	0.763708	-3.813201	1.131814
1	0.385175	-5.515412	0.861964
6	-1.604111	-5.149664	-1.028973
1	-0.882900	-5.237629	-1.846939
1	-1.731379	-6.139574	-0.578528
1	-2.558611	-4.831391	-1.450350

TS1-meta-gga (Refer to Table S1)

Number of imaginary frequencies : 1
Imaginary frequency : -765.5662 cm(-1)

Electronic energy : HF=-3396.5341341
Zero-point correction= 1.456803 (Hartree/Particle)
Thermal correction to Energy= 1.536363
Thermal correction to Enthalpy= 1.537307
Thermal correction to Gibbs Free Energy= 1.341738
Sum of electronic and zero-point Energies= -3395.077331
Sum of electronic and thermal Energies= -3394.997771
Sum of electronic and thermal Enthalpies= -3394.996827
Sum of electronic and thermal Free Energies= -3395.192396

Cartesian Coordinates

77	-1.373529	0.258745	-0.232427
5	-2.832728	-0.329823	-1.636524
8	-2.779609	0.094392	-2.963163
8	-3.967333	-1.113169	-1.429044
6	-3.760024	-0.659760	-3.719041
6	-4.802343	-1.035538	-2.609434
5	-1.632368	-1.786326	0.055439
8	-1.295205	-2.671636	-0.969271
8	-2.071392	-2.472167	1.169714
6	-1.415955	-4.035496	-0.487803
6	-2.295091	-3.859510	0.811590
5	-2.986904	0.646540	0.944615
8	-3.180581	0.216614	2.254756
8	-4.062456	1.468352	0.558776
6	-4.557424	0.464736	2.613242
6	-4.906427	1.699607	1.713417
6	-0.291054	2.220548	-2.345389
6	0.730445	1.150248	-2.319316
7	-1.312521	2.115640	-1.459634
7	0.394917	0.024851	-1.642430

6	-0.246517	3.273512	-3.268679
6	-1.266224	4.218372	-3.285826
6	-2.314900	4.091686	-2.375674
6	-2.300663	3.026257	-1.482111
6	1.982534	1.263502	-2.934237
6	2.887990	0.207150	-2.857054
6	2.533079	-0.962863	-2.175493
6	1.254922	-0.997113	-1.594771
6	0.063491	1.127497	1.275597
6	-0.337204	1.819692	2.436015
6	1.434176	1.141365	0.988774
6	0.579333	2.529512	3.217026
6	2.359550	1.868788	1.744136
6	1.933403	2.575504	2.873247
1	-0.669281	-0.249661	1.137782
1	1.823623	0.570213	0.159609
1	2.643782	3.118706	3.489875
1	0.235302	3.045978	4.109281
1	-1.373861	1.769488	2.748246
1	-3.099762	2.861363	-0.768146
1	-3.135906	4.799900	-2.353208
1	-1.246131	5.032064	-4.004182
1	0.560946	3.330685	-3.988566
1	2.267801	2.180403	-3.436610
1	3.872773	0.293945	-3.305528
1	0.911389	-1.875975	-1.065795
6	3.778658	1.720256	1.285083
8	4.269011	0.574584	1.231786
7	4.479801	2.799929	0.852665
6	3.399560	-2.163737	-2.086757
6	3.870860	-2.763361	-3.264228
6	3.677599	-2.774218	-0.840409
6	4.540059	-3.984120	-3.228612
1	3.660343	-2.282942	-4.215975
6	4.313925	-4.024141	-0.815137
6	4.731655	-4.623356	-2.000347
1	4.883785	-4.444657	-4.149618
1	4.474029	-4.504154	0.141756
1	5.229811	-5.587791	-1.961220
7	3.366101	-2.080659	0.339216
6	2.922421	-2.663264	1.528377
8	2.595669	-3.847098	1.612441
7	2.863431	-1.778901	2.569943
1	3.573236	-1.086941	0.367841
1	3.119526	-0.816401	2.375678
6	3.868311	4.125469	0.683847
1	4.671666	4.868033	0.738370
1	3.212423	4.312554	1.532214
6	5.794010	2.531177	0.244367
1	6.367068	3.463867	0.257118
1	6.305008	1.812217	0.886818
6	1.954610	-2.025749	3.690852
6	2.274060	-1.055990	4.835719
6	0.488691	-1.878331	3.252141
1	2.126997	-3.055336	4.025521
6	1.290179	-1.231402	6.004240
1	2.195827	-0.026674	4.454272
1	3.309075	-1.198578	5.168177
6	-0.499272	-2.054672	4.408459
1	0.366597	-0.872136	2.842520
1	0.271748	-2.579089	2.444270

6	-0.169656	-1.076674	5.545896
1	1.523089	-0.510219	6.797211
1	1.425689	-2.231297	6.440800
1	-1.516376	-1.896005	4.034885
1	-0.448478	-3.086440	4.786143
1	-0.849764	-1.223240	6.394094
1	-0.326186	-0.049720	5.185865
6	3.078332	4.293221	-0.623295
6	2.333110	5.636500	-0.700367
1	2.371813	3.461017	-0.712009
1	3.763101	4.212445	-1.474616
6	1.239138	5.845404	0.362349
1	3.062289	6.456391	-0.639947
1	1.870663	5.712581	-1.693556
6	0.131821	4.786715	0.318110
1	1.678463	5.872644	1.368795
1	0.796723	6.838991	0.207404
1	-0.237044	4.712953	-0.710599
1	0.538461	3.803206	0.569144
6	5.691805	1.972099	-1.184027
6	7.028039	1.469417	-1.753221
1	5.289895	2.746638	-1.846804
1	4.962270	1.158160	-1.175590
6	7.666067	0.288398	-0.999880
1	6.857291	1.167097	-2.795605
1	7.743191	2.302929	-1.794341
6	6.751400	-0.934146	-0.846263
1	8.578773	-0.005139	-1.536194
1	8.000872	0.610579	-0.004400
1	5.899567	-0.672475	-0.210561
1	6.337901	-1.212124	-1.825781
6	-1.036764	5.088766	1.257252
1	-1.793750	4.300747	1.204201
1	-0.698769	5.147302	2.297733
1	-1.516983	6.041940	1.004794
6	7.473256	-2.138605	-0.236421
1	6.794665	-2.989725	-0.134112
1	8.318253	-2.454440	-0.859983
1	7.866224	-1.897866	0.758295
6	-4.636933	0.711349	4.116134
1	-5.655718	0.981038	4.414794
1	-4.352365	-0.199578	4.650335
1	-3.957296	1.507330	4.426986
6	-5.344137	-0.795581	2.228153
1	-4.891026	-1.650398	2.735896
1	-6.396947	-0.725685	2.520074
1	-5.275803	-0.976390	1.151872
6	-6.358223	1.776298	1.252575
1	-7.033632	1.864997	2.110325
1	-6.499877	2.654121	0.614449
1	-6.635695	0.893326	0.676067
6	-4.471980	3.035396	2.330730
1	-4.544591	3.819444	1.570958
1	-5.103046	3.318148	3.178782
1	-3.433278	2.988278	2.668377
6	-5.832619	0.070790	-2.351660
1	-6.532963	0.176482	-3.185871
1	-6.399398	-0.180791	-1.451616
1	-5.335098	1.027042	-2.173166
6	-5.502646	-2.376223	-2.807420
1	-6.180553	-2.565054	-1.969803

1	-6.091642	-2.373882	-3.730917
1	-4.786752	-3.198175	-2.852433
6	-3.025951	-1.879885	-4.289187
1	-3.678377	-2.493861	-4.917893
1	-2.187000	-1.529979	-4.897555
1	-2.621331	-2.492353	-3.479452
6	-4.298532	0.223261	-4.839514
1	-3.498295	0.442135	-5.552774
1	-5.108060	-0.280655	-5.378738
1	-4.673254	1.171564	-4.449831
6	-1.876334	-4.737859	1.987734
1	-2.019069	-5.796708	1.746920
1	-0.831913	-4.582306	2.260384
1	-2.493399	-4.496639	2.857904
6	-3.801190	-3.996883	0.553240
1	-4.076412	-5.020825	0.282211
1	-4.337985	-3.724396	1.465881
1	-4.115942	-3.310863	-0.236060
6	0.002873	-4.543581	-0.222576
1	0.586254	-4.465014	-1.145304
1	0.519821	-3.964834	0.542876
1	0.007325	-5.591620	0.091655
6	-2.067441	-4.867956	-1.590764
1	-1.407224	-4.897745	-2.462564
1	-2.235678	-5.896283	-1.254209
1	-3.021808	-4.441059	-1.901705

TS1-ortho-aaa (Refer to Table S2)

Number of imaginary frequencies : 1
Imaginary frequency : -735.3945 cm(-1)

Electronic energy : HF=-3396.5240348
Zero-point correction= 1.455556 (Hartree/Particle)
Thermal correction to Energy= 1.535888
Thermal correction to Enthalpy= 1.536833
Thermal correction to Gibbs Free Energy= 1.336805
Sum of electronic and zero-point Energies= -3395.068479
Sum of electronic and thermal Energies= -3394.988146
Sum of electronic and thermal Enthalpies= -3394.987202
Sum of electronic and thermal Free Energies= -3395.187229

Cartesian Coordinates

77	1.000485	-0.724647	-0.058529
5	2.818160	-0.716701	-1.140094
8	2.841262	-0.666405	-2.530493
8	4.117205	-0.748466	-0.639899
6	4.188182	-0.326487	-2.945550
6	5.039512	-0.879564	-1.750326
5	2.146365	0.761437	0.865589
8	2.611671	1.849308	0.126327
8	2.494889	0.895529	2.195396
6	3.156780	2.836957	1.042812
6	3.475199	1.959277	2.305601
5	2.024430	-2.131090	1.023994
8	2.484649	-2.065724	2.333868
8	2.358838	-3.384416	0.477273
6	3.374877	-3.178104	2.575474
6	2.866329	-4.232548	1.533382

6	-0.071340	-1.370041	-2.858208
6	-0.080479	0.103667	-2.822852
7	0.300474	-2.011952	-1.717873
7	0.177493	0.670199	-1.620300
6	-0.455837	-2.098818	-3.992721
6	-0.464076	-3.487669	-3.956990
6	-0.084621	-4.131060	-2.779070
6	0.295309	-3.357065	-1.689109
6	-0.356080	0.903952	-3.937225
6	-0.402887	2.285698	-3.799539
6	-0.163720	2.873657	-2.548612
6	0.138636	1.998670	-1.496041
6	-0.839886	-0.964273	1.306275
6	-2.153327	-0.559362	0.979463
6	-0.689979	-1.605190	2.557128
6	-3.231002	-0.766955	1.855875
6	-1.763545	-1.846951	3.415291
6	-3.045536	-1.414471	3.074941
1	0.413088	0.008804	1.254965
1	0.306219	-1.880195	2.883441
1	-3.883834	-1.564279	3.748890
1	-4.219077	-0.409124	1.576062
1	0.645407	-3.798523	-0.765490
1	-0.074513	-5.212480	-2.698744
1	-0.764063	-4.055877	-4.832082
1	-0.753895	-1.581103	-4.895712
1	-0.541809	0.458316	-4.906876
1	-0.638950	2.910739	-4.655154
1	0.378424	2.381913	-0.517649
6	-0.152818	4.341206	-2.343490
6	0.486754	5.151893	-3.297150
6	-0.717247	4.952597	-1.192524
6	0.615234	6.524687	-3.116511
1	0.932184	4.679119	-4.168093
6	-0.577153	6.339477	-1.015413
6	0.090407	7.110427	-1.961411
1	1.131900	7.126766	-3.857628
1	-0.993317	6.786249	-0.123160
1	0.189253	8.180096	-1.799476
7	-1.439708	4.182494	-0.268028
6	-1.302930	4.299814	1.128144
8	-0.819804	5.289355	1.674398
7	-1.743992	3.189535	1.785111
1	-1.798160	3.293071	-0.596288
1	-2.080465	2.400383	1.236526
6	-2.509545	0.150875	-0.296496
8	-2.516627	1.393448	-0.348184
7	-2.911141	-0.611672	-1.348485
1	-1.588362	-2.342653	4.366637
6	-2.922785	-2.078947	-1.291775
1	-2.639015	-2.444465	-2.283843
1	-2.136125	-2.392268	-0.605519
6	-3.386672	0.055590	-2.565918
1	-2.915678	1.038457	-2.593815
1	-3.014577	-0.516538	-3.423087
6	-4.913151	0.213050	-2.655055
1	-5.126274	0.806887	-3.554446
1	-5.386201	-0.763416	-2.817414
6	-5.538291	0.887409	-1.429569
1	-5.356443	0.260278	-0.547117
1	-5.025110	1.835793	-1.231465

6	-7.045288	1.118998	-1.571836
1	-7.545155	0.162540	-1.785196
1	-7.238114	1.762275	-2.442532
6	-7.673906	1.751756	-0.324728
1	-7.479116	1.106006	0.542697
1	-7.170401	2.704175	-0.111817
6	-9.181214	1.984346	-0.464838
1	-9.710383	1.041849	-0.648003
1	-9.604719	2.434839	0.438740
1	-9.399844	2.653413	-1.305136
6	-4.248029	-2.720810	-0.866074
1	-4.573932	-2.279378	0.081372
1	-5.030434	-2.508497	-1.603555
6	-4.087978	-4.235666	-0.697566
1	-3.696325	-4.669785	-1.629483
1	-3.327420	-4.430093	0.071846
6	-5.389864	-4.946103	-0.314090
1	-6.150015	-4.757078	-1.085747
1	-5.782899	-4.506260	0.613518
6	-5.222216	-6.458367	-0.126427
1	-4.821993	-6.894623	-1.052167
1	-4.465706	-6.643106	0.648331
6	-6.528306	-7.163712	0.251035
1	-6.381360	-8.240996	0.380088
1	-6.933014	-6.767331	1.189375
1	-7.291273	-7.020944	-0.522962
6	-1.690878	3.052209	3.233790
6	-3.105798	2.892246	3.817150
6	-0.809751	1.854937	3.626862
1	-1.245751	3.977484	3.613734
6	-3.070443	2.682471	5.338895
1	-3.578314	2.020873	3.340521
1	-3.709181	3.768801	3.554793
6	-0.770257	1.642677	5.145858
1	-1.220971	0.956513	3.156336
1	0.200915	1.977433	3.226158
6	-2.186428	1.484394	5.718168
1	-4.088600	2.546412	5.723701
1	-2.673808	3.589298	5.817735
1	-0.160762	0.761240	5.376867
1	-0.278551	2.502032	5.624604
1	-2.150773	1.366471	6.808204
1	-2.630934	0.565590	5.310761
6	4.230673	1.203471	-3.057482
1	5.202019	1.561608	-3.412271
1	3.461934	1.521173	-3.768183
1	4.002581	1.662214	-2.092123
6	4.463606	-0.978319	-4.295938
1	3.811534	-0.537092	-5.055615
1	5.502412	-0.814989	-4.602187
1	4.270327	-2.052253	-4.266224
6	6.300258	-0.082930	-1.431294
1	6.803861	-0.523381	-0.565841
1	6.995918	-0.098109	-2.277170
1	6.063221	0.954455	-1.191186
6	5.366607	-2.372182	-1.883168
1	6.083471	-2.561381	-2.688023
1	5.803122	-2.723533	-0.944306
1	4.457845	-2.950600	-2.068018
6	3.942083	-5.143729	0.950575
1	4.706866	-4.564694	0.431212

1	4.420140	-5.737402	1.737162
1	3.492452	-5.833292	0.229345
6	4.795487	-2.679650	2.279695
1	5.011653	-1.834147	2.937177
1	5.545588	-3.457806	2.453072
1	4.864774	-2.321794	1.249959
6	1.680847	-5.061043	2.047815
1	1.256478	-5.628265	1.213439
1	1.981355	-5.769785	2.825508
1	0.899027	-4.408543	2.446869
6	3.249168	-3.598476	4.036648
1	3.850531	-4.491664	4.238243
1	3.608522	-2.791009	4.680605
1	2.211863	-3.805459	4.306359
6	3.281463	2.662907	3.644918
1	3.970579	3.508976	3.739089
1	2.261264	3.030632	3.764201
1	3.485604	1.961066	4.458452
6	4.853086	1.288298	2.243214
1	5.663893	2.015975	2.348279
1	4.924211	0.566682	3.061115
1	4.971376	0.742695	1.303816
6	4.368052	3.485798	0.380574
1	4.045894	4.041271	-0.505056
1	4.854461	4.187888	1.065761
1	5.098858	2.738386	0.067886
6	2.061161	3.877725	1.283361
1	1.755577	4.314434	0.328928
1	1.181189	3.424228	1.741491
1	2.398465	4.690913	1.931149

TS1-ortho-ggg (Refer to Table S2)

Number of imaginary frequencies : 1
Imaginary frequency : -754.6791 cm(-1)

Electronic energy : HF=-3396.5254905
Zero-point correction= 1.457468 (Hartree/Particle)
Thermal correction to Energy= 1.536855
Thermal correction to Enthalpy= 1.537799
Thermal correction to Gibbs Free Energy= 1.340404
Sum of electronic and zero-point Energies= -3395.068023
Sum of electronic and thermal Energies= -3394.988636
Sum of electronic and thermal Enthalpies= -3394.987692
Sum of electronic and thermal Free Energies= -3395.185086

Cartesian Coordinates

77	-1.154082	0.429464	0.007192
5	-2.491759	0.079617	-1.596204
8	-2.155057	0.383803	-2.911124
8	-3.771228	-0.466618	-1.542274
6	-3.107219	-0.275804	-3.783398
6	-4.370262	-0.374740	-2.859376
5	-1.762209	-1.553039	0.265117
8	-1.543999	-2.498479	-0.737646
8	-2.330061	-2.147580	1.374928
6	-1.836327	-3.819556	-0.205919
6	-2.775601	-3.476635	1.005811
5	-2.896133	1.028034	0.904116

8	-3.591815	0.448316	1.958010
8	-3.572986	2.186991	0.481770
6	-4.889081	1.075435	2.067233
6	-4.624209	2.483493	1.430216
6	0.172620	2.195973	-2.126116
6	0.763444	0.868696	-2.373489
7	-0.673236	2.305608	-1.066223
7	0.493770	-0.082595	-1.449280
6	0.487506	3.318888	-2.905311
6	-0.064856	4.555814	-2.596964
6	-0.925144	4.652700	-1.502966
6	-1.201003	3.506341	-0.767046
6	1.589814	0.580881	-3.466099
6	2.183459	-0.670105	-3.570214
6	1.933403	-1.648325	-2.595416
6	1.047035	-1.292265	-1.568884
6	0.026794	0.944946	1.906972
6	1.417717	1.182446	1.961397
6	-0.671063	1.116169	3.123395
6	2.059579	1.568012	3.149308
6	-0.041673	1.512875	4.304112
6	1.335661	1.735343	4.326968
1	-0.628904	-0.392528	1.290991
1	-1.729535	0.886285	3.151559
1	1.840830	2.019283	5.245508
1	3.136868	1.715697	3.148150
1	-1.889208	3.511163	0.067503
1	-1.378070	5.595742	-1.217750
1	0.179627	5.429098	-3.193578
1	1.168239	3.226305	-3.742177
1	1.787318	1.329392	-4.223896
1	2.855272	-0.886864	-4.394809
1	0.760696	-2.010207	-0.817625
6	2.519007	-3.008398	-2.666115
6	2.549508	-3.665482	-3.908468
6	3.015981	-3.687218	-1.521056
6	3.013756	-4.970325	-4.031763
1	2.153507	-3.150856	-4.779546
6	3.480045	-5.006816	-1.654850
6	3.467783	-5.640625	-2.892856
1	3.007710	-5.462720	-4.999339
1	3.835749	-5.515635	-0.769720
1	3.827498	-6.662875	-2.968879
7	3.079384	-3.031932	-0.280497
6	2.667685	-3.621852	0.933152
8	2.595207	-4.837269	1.097685
7	2.336240	-2.692811	1.873566
1	3.030461	-2.020344	-0.304454
1	2.391552	-1.706429	1.627031
6	2.314091	0.943222	0.783276
8	2.689556	-0.212943	0.521490
7	2.739557	2.016730	0.067199
1	-0.627297	1.619220	5.213724
6	2.224258	3.369565	0.318471
1	2.032388	3.824087	-0.657442
1	1.258166	3.275892	0.816441
6	3.632798	1.808520	-1.079797
1	3.560960	0.755680	-1.349777
1	3.227131	2.389382	-1.915981
6	5.103845	2.195075	-0.865918
1	5.614111	2.008263	-1.819629

1	5.181121	3.274970	-0.696705
6	5.833046	1.455796	0.265778
1	6.852110	1.859237	0.320073
1	5.357421	1.712091	1.221565
6	5.888444	-0.080429	0.143677
1	4.901277	-0.491236	0.363597
1	6.560131	-0.457693	0.926641
6	6.358117	-0.626058	-1.213929
1	6.310911	-1.721338	-1.176504
1	5.649648	-0.330915	-2.000166
6	7.772797	-0.188825	-1.609568
1	8.500304	-0.483165	-0.844069
1	8.082401	-0.643636	-2.556388
1	7.843981	0.898334	-1.727028
6	3.141985	4.270053	1.153983
1	3.412334	3.742528	2.073679
1	4.076728	4.454781	0.615591
6	2.472549	5.604581	1.518725
1	1.619435	5.403162	2.180020
1	3.180241	6.197012	2.110562
6	1.978173	6.435697	0.319054
1	1.606317	7.398300	0.695139
1	1.114270	5.937440	-0.136952
6	3.027028	6.701522	-0.773154
1	3.340706	5.752228	-1.227846
1	2.551081	7.274158	-1.579909
6	4.263530	7.459677	-0.277773
1	4.950731	7.680864	-1.100866
1	3.979953	8.411497	0.186167
1	4.819232	6.882631	0.468663
6	1.851679	-3.042171	3.201668
6	2.945675	-2.847415	4.267277
6	0.615240	-2.193273	3.535923
1	1.577544	-4.102191	3.166257
6	2.415063	-3.136703	5.679981
1	3.296431	-1.806476	4.212942
1	3.801711	-3.488424	4.028327
6	0.083560	-2.479332	4.945672
1	0.895701	-1.135421	3.475739
1	-0.170203	-2.351758	2.790453
6	1.181512	-2.278441	6.000426
1	3.205172	-2.967770	6.421719
1	2.142007	-4.199409	5.750755
1	-0.774203	-1.828567	5.150922
1	-0.285527	-3.514060	4.995984
1	0.802070	-2.514012	7.002299
1	1.471683	-1.217872	6.010356
6	-2.503061	-1.644622	-4.124052
1	-3.135875	-2.210413	-4.814856
1	-1.527704	-1.487789	-4.594098
1	-2.344652	-2.227755	-3.213330
6	-3.285554	0.568099	-5.040678
1	-2.348012	0.588674	-5.604275
1	-4.062032	0.145115	-5.687086
1	-3.554891	1.596991	-4.794859
6	-5.241537	-1.606105	-3.084256
1	-6.073833	-1.603904	-2.374300
1	-5.655721	-1.609258	-4.098200
1	-4.674176	-2.526035	-2.935460
6	-5.225699	0.898082	-2.872343
1	-5.747814	1.026289	-3.825455

1	-5.972417	0.830394	-2.076701
1	-4.608350	1.779358	-2.680169
6	-5.804428	3.087750	0.675967
1	-6.112234	2.445803	-0.150637
1	-6.659221	3.238478	1.343992
1	-5.521086	4.059815	0.260411
6	-5.864443	0.220034	1.248387
1	-5.859207	-0.795293	1.652084
1	-6.886456	0.609490	1.294183
1	-5.537147	0.162136	0.207832
6	-4.050426	3.495762	2.431281
1	-3.708658	4.380577	1.885082
1	-4.796738	3.813487	3.165537
1	-3.192809	3.070008	2.959858
6	-5.299528	1.096655	3.536602
1	-6.242449	1.637834	3.670296
1	-5.439091	0.071717	3.891459
1	-4.534745	1.565453	4.158837
6	-2.624466	-4.389733	2.218263
1	-2.896608	-5.419663	1.964290
1	-1.602679	-4.383074	2.601243
1	-3.286749	-4.045633	3.017672
6	-4.250458	-3.343346	0.606865
1	-4.686122	-4.308310	0.329654
1	-4.805537	-2.942805	1.458974
1	-4.358511	-2.641012	-0.223636
6	-2.482123	-4.649082	-1.311282
1	-1.760217	-4.810981	-2.117109
1	-2.791731	-5.627280	-0.928813
1	-3.354567	-4.145279	-1.730777
6	-0.501664	-4.438244	0.214151
1	0.172742	-4.475437	-0.645401
1	-0.021256	-3.840467	0.989807
1	-0.619487	-5.457187	0.592038

TS1-ortho-aga (Refer to Table S2)

Number of imaginary frequencies : 1
Imaginary frequency : -763.4338 cm(-1)

Electronic energy : HF=-3396.5222044
Zero-point correction= 1.456708 (Hartree/Particle)
Thermal correction to Energy= 1.536397
Thermal correction to Enthalpy= 1.537341
Thermal correction to Gibbs Free Energy= 1.339801
Sum of electronic and zero-point Energies= -3395.065496
Sum of electronic and thermal Energies= -3394.985808
Sum of electronic and thermal Enthalpies= -3394.984864
Sum of electronic and thermal Free Energies= -3395.182404

Cartesian Coordinates

77	1.194504	-0.721737	-0.081008
5	2.833854	-0.436823	-1.388067
8	2.668756	-0.414170	-2.769717
8	4.172013	-0.233157	-1.062401
6	3.870708	0.144732	-3.356210
6	4.952117	-0.228884	-2.284013
5	2.202183	0.931761	0.707533
8	2.374406	2.080944	-0.065515

8	2.710911	1.122515	1.977463
6	2.876310	3.146356	0.785951
6	3.507455	2.335195	1.974109
5	2.565008	-1.941741	0.829489
8	3.149198	-1.829044	2.085464
8	3.055227	-3.095430	0.189669
6	4.246338	-2.764613	2.178661
6	3.825243	-3.863780	1.143047
6	-0.089025	-1.573355	-2.732826
6	-0.314002	-0.116896	-2.701712
7	0.478534	-2.129680	-1.628690
7	-0.009873	0.504242	-1.537693
6	-0.469685	-2.375093	-3.818183
6	-0.279112	-3.750529	-3.765248
6	0.283587	-4.307987	-2.616907
6	0.651736	-3.462225	-1.577249
6	-0.837768	0.611045	-3.776428
6	-1.085091	1.970562	-3.632608
6	-0.797067	2.611038	-2.417524
6	-0.237446	1.813236	-1.410090
6	-0.394576	-1.263239	1.488304
6	-1.789527	-1.105131	1.327190
6	0.017856	-1.862347	2.700900
6	-2.698018	-1.505266	2.321106
6	-0.882341	-2.285722	3.678957
6	-2.253276	-2.097294	3.499908
1	0.663458	-0.088390	1.306538
1	1.079056	-1.953350	2.899669
1	-2.963675	-2.393155	4.266335
1	-3.760566	-1.345387	2.163121
1	1.134404	-3.830236	-0.682206
1	0.445260	-5.376238	-2.523349
1	-0.572253	-4.375986	-4.602798
1	-0.918415	-1.926027	-4.695300
1	-1.066171	0.123928	-4.716589
1	-1.517899	2.534761	-4.452809
1	0.054666	2.245169	-0.467017
6	-1.003184	4.064188	-2.211523
6	-0.633089	4.950676	-3.237841
6	-1.516012	4.597296	-0.998492
6	-0.717012	6.329094	-3.075244
1	-0.225584	4.541486	-4.158155
6	-1.592061	5.991654	-0.841518
6	-1.186811	6.843329	-1.863845
1	-0.405182	6.993102	-3.875604
1	-1.964529	6.380870	0.095882
1	-1.251018	7.917656	-1.715898
7	-1.977192	3.739638	0.013063
6	-1.674247	3.907554	1.379694
8	-1.316950	4.980527	1.860817
7	-1.799050	2.745754	2.081075
1	-2.208819	2.793035	-0.265047
1	-2.048369	1.896806	1.576433
6	-2.408546	-0.432655	0.134921
8	-2.502245	0.806581	0.096266
7	-2.943014	-1.207498	-0.847125
1	-0.506656	-2.732799	4.595756
6	-2.788401	-2.668218	-0.900263
1	-2.211782	-2.915686	-1.797248
1	-2.191451	-2.971595	-0.040843
6	-3.583770	-0.542812	-1.992335

1	-3.081335	0.413631	-2.141075
1	-3.384702	-1.162766	-2.873593
6	-5.095923	-0.303002	-1.853522
1	-5.428733	0.143551	-2.799092
1	-5.624258	-1.259538	-1.767186
6	-5.495077	0.602259	-0.680831
1	-5.067389	0.202261	0.244570
1	-5.037011	1.590513	-0.809073
6	-7.013838	0.742415	-0.504091
1	-7.210011	1.302669	0.419872
1	-7.456053	-0.254189	-0.354088
6	-7.733005	1.442809	-1.664736
1	-7.258711	2.417601	-1.843620
1	-7.602644	0.865147	-2.588785
6	-9.229414	1.637625	-1.400359
1	-9.394501	2.247612	-0.504871
1	-9.726374	2.135177	-2.239708
1	-9.728786	0.675012	-1.239352
6	-4.108106	-3.450392	-0.931018
1	-4.654221	-3.216727	-1.854251
1	-3.842598	-4.512011	-1.003343
6	-5.016511	-3.211781	0.280343
1	-4.517910	-3.583424	1.185098
1	-5.135907	-2.132277	0.422312
6	-6.408168	-3.845308	0.150766
1	-6.907877	-3.438083	-0.740868
1	-7.020074	-3.533211	1.007899
6	-6.410821	-5.377844	0.074473
1	-5.852482	-5.708638	-0.810596
1	-5.872141	-5.780674	0.943358
6	-7.825471	-5.963750	0.026504
1	-7.807524	-7.057116	-0.028396
1	-8.398545	-5.682876	0.917584
1	-8.374644	-5.594446	-0.847417
6	-1.530573	2.641192	3.508420
6	-2.825055	2.351514	4.290503
6	-0.490631	1.538546	3.766370
1	-1.130561	3.611198	3.821456
6	-2.550624	2.155985	5.789469
1	-3.275673	1.435841	3.880283
1	-3.540485	3.164756	4.123375
6	-0.213802	1.340861	5.261724
1	-0.878159	0.600877	3.355119
1	0.437166	1.752388	3.227171
6	-1.512309	1.048757	6.027760
1	-3.485016	1.927398	6.316589
1	-2.175622	3.098846	6.212832
1	0.505346	0.524387	5.395182
1	0.255261	2.246807	5.672370
1	-1.311320	0.938014	7.100446
1	-1.920027	0.089942	5.677275
6	3.632637	1.656907	-3.468367
1	4.472554	2.168900	-3.948034
1	2.734471	1.823526	-4.070472
1	3.458072	2.090404	-2.480154
6	4.079724	-0.476943	-4.732254
1	3.270057	-0.169831	-5.401030
1	5.027414	-0.144256	-5.168981
1	4.080240	-1.567154	-4.678985
6	6.087476	0.778347	-2.134375
1	6.769334	0.450382	-1.344318

1	6.657778	0.863369	-3.065619
1	5.709274	1.765293	-1.864445
6	5.511382	-1.646256	-2.458825
1	6.141071	-1.729058	-3.349968
1	6.119011	-1.894797	-1.584534
1	4.699833	-2.375566	-2.522038
6	4.978344	-4.539640	0.408066
1	5.562628	-3.814099	-0.159500
1	5.640615	-5.055469	1.111669
1	4.586200	-5.280156	-0.296030
6	5.511127	-2.002003	1.763897
1	5.637637	-1.150296	2.436498
1	6.405647	-2.630144	1.823002
1	5.402069	-1.608399	0.750608
6	2.879365	-4.915754	1.738875
1	2.473877	-5.528590	0.927670
1	3.393751	-5.576787	2.442907
1	2.042663	-4.434857	2.253967
6	4.359860	-3.243584	3.622929
1	5.135039	-4.011624	3.719677
1	4.629884	-2.401256	4.265924
1	3.414440	-3.652125	3.985136
6	3.387580	2.998544	3.342350
1	3.931000	3.949289	3.358926
1	2.346569	3.187942	3.608610
1	3.818214	2.343192	4.104685
6	4.955044	1.904344	1.707236
1	5.639896	2.758078	1.710829
1	5.261713	1.209543	2.493168
1	5.027902	1.381338	0.750576
6	3.861388	3.982681	-0.024481
1	3.331634	4.482807	-0.840620
1	4.324157	4.751332	0.603260
1	4.648603	3.363460	-0.457436
6	1.672073	3.995036	1.198553
1	1.167497	4.374838	0.306308
1	0.951050	3.403230	1.763811
1	1.961132	4.853503	1.810238

TS1-ortho-agg (Refer to Table S2)

Number of imaginary frequencies : 1

Imaginary frequency : -750.2175 cm(-1)

Electronic energy : HF=-3396.5218397

Zero-point correction= 1.457653 (Hartree/Particle)

Thermal correction to Energy= 1.536882

Thermal correction to Enthalpy= 1.537826

Thermal correction to Gibbs Free Energy= 1.341653

Sum of electronic and zero-point Energies= -3395.064186

Sum of electronic and thermal Energies= -3394.984957

Sum of electronic and thermal Enthalpies= -3394.984013

Sum of electronic and thermal Free Energies= -3395.180187

Cartesian Coordinates

77	1.186311	-0.633805	-0.128172
5	2.807180	-0.138603	-1.394959
8	2.653588	-0.048631	-2.775213
8	4.122112	0.149579	-1.039573

6	3.812725	0.636443	-3.312271
6	4.910595	0.287376	-2.248337
5	2.042571	1.048342	0.771927
8	2.142257	2.249661	0.070038
8	2.506196	1.202171	2.063966
6	2.550863	3.296541	0.992332
6	3.215025	2.464482	2.147447
5	2.651451	-1.783811	0.724305
8	3.236830	-1.675012	1.980106
8	3.217078	-2.876040	0.040392
6	4.392841	-2.539401	2.038334
6	4.040674	-3.626253	0.963277
6	-0.010565	-1.423742	-2.837402
6	-0.355273	0.004501	-2.721290
7	0.598050	-1.997076	-1.764259
7	-0.108600	0.577631	-1.519461
6	-0.323222	-2.187548	-3.970887
6	-0.023058	-3.543945	-3.998246
6	0.581487	-4.121373	-2.881470
6	0.879365	-3.312052	-1.791575
6	-0.934364	0.749449	-3.755254
6	-1.298718	2.070971	-3.531418
6	-1.071288	2.659043	-2.277453
6	-0.446363	1.853095	-1.315624
6	-0.353441	-1.403846	1.391784
6	-1.756162	-1.354101	1.233470
6	0.108007	-2.040980	2.566611
6	-2.628338	-1.893378	2.193863
6	-0.753174	-2.600330	3.510820
6	-2.135143	-2.518777	3.335564
1	0.602401	-0.126397	1.288620
1	1.173018	-2.053272	2.765323
1	-2.818107	-2.922398	4.077377
1	-3.700668	-1.814607	2.040571
1	1.391921	-3.691912	-0.918293
1	0.829124	-5.176717	-2.850309
1	-0.263916	-4.140012	-4.873063
1	-0.806678	-1.724752	-4.822004
1	-1.115544	0.303129	-4.725509
1	-1.776838	2.644539	-4.319292
1	-0.192030	2.251217	-0.346808
6	-1.409025	4.072664	-1.987118
6	-1.122520	5.048527	-2.957725
6	-1.971132	4.483678	-0.748831
6	-1.336613	6.401032	-2.716136
1	-0.676563	4.733951	-3.897220
6	-2.179942	5.852880	-0.512384
6	-1.855811	6.797295	-1.480803
1	-1.087447	7.136928	-3.474485
1	-2.589500	6.149618	0.443208
1	-2.022345	7.850255	-1.271733
7	-2.347619	3.530042	0.211095
6	-2.041025	3.645680	1.582469
8	-1.793396	4.719552	2.126230
7	-2.017651	2.436320	2.210591
1	-2.488934	2.583079	-0.121313
1	-2.216863	1.599360	1.665348
6	-2.425894	-0.657245	0.083981
8	-2.617816	0.570537	0.126850
7	-2.895744	-1.405838	-0.949851
1	-0.341261	-3.070849	4.399928

6	-2.618579	-2.840914	-1.101108
1	-2.025214	-2.977646	-2.010753
1	-1.996399	-3.148841	-0.261384
6	-3.583801	-0.720155	-2.053993
1	-3.154058	0.278761	-2.139023
1	-3.338381	-1.265732	-2.972029
6	-5.108804	-0.601801	-1.907182
1	-5.471707	-0.114332	-2.821333
1	-5.568045	-1.597401	-1.890937
6	-5.569905	0.190851	-0.678481
1	-5.146803	-0.263487	0.223768
1	-5.145625	1.199821	-0.714459
6	-7.097973	0.249920	-0.526969
1	-7.333849	0.796361	0.395937
1	-7.481494	-0.770682	-0.385287
6	-7.852352	0.906951	-1.696027
1	-7.732580	0.301602	-2.604073
1	-8.925767	0.892112	-1.468378
6	-7.415730	2.348392	-1.982282
1	-6.372610	2.398145	-2.312033
1	-8.031093	2.800848	-2.766801
1	-7.504528	2.971835	-1.085200
6	-3.865573	-3.729732	-1.188173
1	-4.438385	-3.479602	-2.090574
1	-3.506274	-4.755357	-1.338560
6	-4.776693	-3.665751	0.040795
1	-4.217600	-4.007910	0.919694
1	-5.033567	-2.619295	0.239100
6	-6.079560	-4.466892	-0.108493
1	-6.675017	-4.026037	-0.920413
1	-6.672764	-4.342427	0.807339
6	-5.898581	-5.969589	-0.383151
1	-6.891306	-6.428657	-0.471264
1	-5.416001	-6.112707	-1.358590
6	-5.095386	-6.704398	0.696231
1	-5.058234	-7.780632	0.498813
1	-4.062453	-6.343885	0.748862
1	-5.543971	-6.561277	1.686225
6	-1.757107	2.284664	3.635123
6	-3.045881	1.932837	4.400359
6	-0.688010	1.202950	3.855115
1	-1.385339	3.252622	3.987634
6	-2.771058	1.692360	5.892652
1	-3.470656	1.020775	3.955698
1	-3.781597	2.732773	4.258986
6	-0.411914	0.958409	5.343848
1	-1.046401	0.270066	3.407029
1	0.235561	1.465628	3.330049
6	-1.703566	0.606028	6.095737
1	-3.700338	1.420185	6.407930
1	-2.423100	2.629646	6.350245
1	0.327919	0.156609	5.450771
1	0.032948	1.860753	5.788107
1	-1.501451	0.464086	7.164530
1	-2.085705	-0.351172	5.712921
6	3.456936	2.129206	-3.342568
1	4.258299	2.731460	-3.781626
1	2.553794	2.259173	-3.946219
1	3.240285	2.491538	-2.334297
6	4.082726	0.113936	-4.718761
1	3.255805	0.392480	-5.378858

1	5.003465	0.546636	-5.124656
1	4.172088	-0.973842	-4.728112
6	5.959718	1.371471	-2.024248
1	6.657631	1.052935	-1.244385
1	6.530632	1.555602	-2.940625
1	5.500377	2.307607	-1.703677
6	5.583712	-1.067773	-2.498352
1	6.226682	-1.045323	-3.383528
1	6.200762	-1.320308	-1.631909
1	4.834129	-1.854160	-2.617473
6	5.233238	-4.194939	0.201274
1	5.765243	-3.409395	-0.336818
1	5.931525	-4.691637	0.883429
1	4.888739	-4.932238	-0.530598
6	5.605855	-1.683603	1.652420
1	5.683246	-0.852037	2.357022
1	6.537711	-2.256899	1.685759
1	5.469047	-1.258515	0.655667
6	3.168645	-4.759387	1.521344
1	2.802862	-5.368518	0.688673
1	3.726832	-5.409635	2.201677
1	2.302902	-4.353216	2.052293
6	4.540360	-3.062781	3.464103
1	5.363563	-3.782334	3.532326
1	4.757045	-2.228965	4.137664
1	3.624011	-3.544295	3.811039
6	3.021990	3.037390	3.547811
1	3.496722	4.020709	3.632114
1	1.965034	3.138184	3.799194
1	3.481939	2.369402	4.281544
6	4.693436	2.147546	1.890322
1	5.319019	3.043051	1.957373
1	5.029862	1.430186	2.643148
1	4.818232	1.685347	0.907932
6	3.491612	4.243129	0.253961
1	2.945609	4.753909	-0.544674
1	3.889325	5.002880	0.934969
1	4.327328	3.702824	-0.193639
6	1.281382	4.032891	1.424367
1	0.765232	4.422380	0.542672
1	0.595952	3.361740	1.943805
1	1.497484	4.876425	2.085233

TS1-ortho-aag (Refer to Table S2)

Number of imaginary frequencies : 1
Imaginary frequency : -767.4469 cm(-1)

Electronic energy : HF=-3396.5221415
Zero-point correction= 1.456223 (Hartree/Particle)
Thermal correction to Energy= 1.536346
Thermal correction to Enthalpy= 1.537291
Thermal correction to Gibbs Free Energy= 1.337830
Sum of electronic and zero-point Energies= -3395.065919
Sum of electronic and thermal Energies= -3394.985795
Sum of electronic and thermal Enthalpies= -3394.984851
Sum of electronic and thermal Free Energies= -3395.184311

Cartesian Coordinates

77	-1.172235	0.356291	-0.197076
5	-2.443473	-0.391272	-1.713002
8	-2.048962	-0.428446	-3.046858
8	-3.729783	-0.907385	-1.579182
6	-2.971000	-1.286311	-3.765097
6	-4.273052	-1.147324	-2.901620
5	-1.826089	-1.488965	0.538183
8	-1.568382	-2.661328	-0.172165
8	-2.467739	-1.773925	1.727384
6	-1.917132	-3.799780	0.661633
6	-2.916869	-3.152570	1.686702
5	-2.943461	1.179316	0.419346
8	-3.680752	0.924087	1.569513
8	-3.596834	2.166749	-0.341888
6	-4.976302	1.551225	1.447032
6	-4.678702	2.718929	0.443103
6	0.272566	1.460593	-2.669154
6	0.860118	0.118837	-2.505850
7	-0.611170	1.864328	-1.717240
7	0.542943	-0.531931	-1.361453
6	0.622879	2.315078	-3.724219
6	0.074062	3.589452	-3.796817
6	-0.818947	3.994271	-2.804443
6	-1.138035	3.099866	-1.789845
6	1.721396	-0.469735	-3.438708
6	2.290119	-1.707769	-3.166155
6	1.987431	-2.370675	-1.966799
6	1.080327	-1.728065	-1.111977
6	-0.062046	1.337933	1.557794
6	1.333878	1.537569	1.623903
6	-0.807345	1.854372	2.641733
6	1.936388	2.209865	2.700309
6	-0.216678	2.539294	3.704284
6	1.167125	2.714088	3.745806
1	-0.740554	-0.084367	1.294609
1	-1.875280	1.672986	2.670618
1	1.641563	3.222433	4.580125
1	3.017735	2.324899	2.715960
1	-1.859705	3.338755	-1.020313
1	-1.270073	4.980387	-2.812593
1	0.344218	4.256187	-4.609909
1	1.329985	1.988359	-4.476298
1	1.961772	0.035063	-4.366523
1	2.983014	-2.155160	-3.871855
1	0.757003	-2.198675	-0.197840
6	2.533041	-3.708476	-1.636370
6	2.589379	-4.682637	-2.648684
6	2.957510	-4.058099	-0.326593
6	3.008347	-5.982284	-2.386742
1	2.247448	-4.418843	-3.645619
6	3.375251	-5.375109	-0.070736
6	3.388970	-6.325061	-1.086635
1	3.022687	-6.721656	-3.181642
1	3.675765	-5.629397	0.936233
1	3.711805	-7.337709	-0.861943
7	2.993888	-3.089932	0.690046
6	2.497039	-3.311769	1.990030
8	2.358011	-4.433588	2.472327
7	2.159568	-2.151262	2.620609
1	3.022454	-2.120224	0.395601
1	2.300980	-1.270311	2.129433

6	2.293208	1.020518	0.591187
8	2.783313	-0.119681	0.685256
7	2.685331	1.868932	-0.391682
1	-0.838797	2.910235	4.514837
6	2.151912	3.226317	-0.534069
1	1.961295	3.399452	-1.598130
1	1.185868	3.261118	-0.030794
6	3.747771	1.420973	-1.299338
1	3.513417	0.402723	-1.615986
1	3.713715	2.060680	-2.187597
6	5.145335	1.437206	-0.670305
1	5.415657	2.460485	-0.381939
1	5.110362	0.840456	0.247274
6	6.199711	0.860353	-1.620429
1	5.895924	-0.154149	-1.909170
1	6.224932	1.449928	-2.549366
6	7.603688	0.828110	-1.003845
1	7.581235	0.208753	-0.096092
1	7.869188	1.842220	-0.675154
6	8.698036	0.304546	-1.947242
1	8.734255	0.937534	-2.844996
1	9.671593	0.420790	-1.454288
6	8.518882	-1.161501	-2.360295
1	7.606523	-1.311286	-2.946621
1	9.360505	-1.506266	-2.969917
1	8.455046	-1.811635	-1.480007
6	3.061737	4.329752	0.011661
1	3.285040	4.119819	1.064038
1	4.019489	4.326017	-0.524315
6	2.398869	5.705843	-0.113511
1	2.151237	5.899890	-1.167832
1	1.443065	5.684263	0.425636
6	3.275210	6.845502	0.420258
1	4.246549	6.815150	-0.092008
1	3.485272	6.667682	1.484575
6	2.664102	8.245491	0.251896
1	3.407012	8.992766	0.558283
1	2.470689	8.428344	-0.814387
6	1.374016	8.465707	1.051285
1	1.016100	9.495291	0.948272
1	0.569220	7.803474	0.716329
1	1.536455	8.273933	2.118391
6	1.630566	-2.109094	3.976818
6	2.680212	-1.574051	4.967966
6	0.364161	-1.239156	4.013301
1	1.380902	-3.141213	4.244536
6	2.106860	-1.452788	6.388286
1	3.007018	-0.583215	4.619703
1	3.560185	-2.227135	4.952308
6	-0.210303	-1.113358	5.429712
1	0.624787	-0.239029	3.650932
1	-0.390601	-1.633556	3.325929
6	0.844721	-0.576629	6.407987
1	2.866770	-1.049225	7.068561
1	1.854541	-2.455943	6.761029
1	-1.088343	-0.457350	5.410075
1	-0.558644	-2.097959	5.774282
1	0.435356	-0.518817	7.424029
1	1.112186	0.447917	6.112184
6	-2.370061	-2.697389	-3.723441
1	-2.975307	-3.416416	-4.284087

1	-1.370504	-2.663086	-4.166993
1	-2.265294	-3.036866	-2.689886
6	-3.087789	-0.786290	-5.200417
1	-2.127457	-0.907421	-5.710536
1	-3.841197	-1.358756	-5.752068
1	-3.357485	0.270935	-5.231795
6	-5.150231	-2.393860	-2.849585
1	-6.009387	-2.212120	-2.197243
1	-5.524990	-2.647751	-3.846960
1	-4.601783	-3.249818	-2.453503
6	-5.110443	0.083818	-3.268302
1	-5.583987	-0.024078	-4.248838
1	-5.896057	0.212032	-2.518860
1	-4.492134	0.985036	-3.263742
6	-5.827674	3.078090	-0.493347
1	-6.114026	2.224253	-1.108545
1	-6.702155	3.415758	0.073108
1	-5.521237	3.888249	-1.162435
6	-5.927510	0.493443	0.872861
1	-5.949338	-0.360302	1.554506
1	-6.946396	0.877664	0.761642
1	-5.560170	0.135192	-0.091505
6	-4.134731	3.977977	1.132734
1	-3.772309	4.672378	0.368119
1	-4.903584	4.487776	1.721207
1	-3.296969	3.726380	1.789294
6	-5.439556	1.991057	2.832654
1	-6.385797	2.539605	2.771696
1	-5.593793	1.110095	3.461920
1	-4.697030	2.625560	3.320558
6	-2.851618	-3.723628	3.099604
1	-3.128074	-4.783361	3.101768
1	-1.853180	-3.622986	3.527928
1	-3.551923	-3.184038	3.743470
6	-4.364216	-3.123794	1.180894
1	-4.800157	-4.126984	1.143054
1	-4.958732	-2.510961	1.863054
1	-4.412879	-2.665836	0.190042
6	-2.516260	-4.880753	-0.232933
1	-1.753752	-5.244279	-0.927996
1	-2.864839	-5.729092	0.365362
1	-3.354943	-4.496053	-0.815564
6	-0.621888	-4.298710	1.304204
1	0.099708	-4.555337	0.524010
1	-0.172968	-3.529845	1.934267
1	-0.781949	-5.189496	1.917246

TS1-ortho-gag (Refer to Table S2)

Number of imaginary frequencies : 1
Imaginary frequency : -733.0016 cm(-1)

Electronic energy : HF=-3396.5289474
Zero-point correction= 1.457035 (Hartree/Particle)
Thermal correction to Energy= 1.536607
Thermal correction to Enthalpy= 1.537551
Thermal correction to Gibbs Free Energy= 1.340948
Sum of electronic and zero-point Energies= -3395.071912
Sum of electronic and thermal Energies= -3394.992340
Sum of electronic and thermal Enthalpies= -3394.991396

Sum of electronic and thermal Free Energies= -3395.187999

Cartesian Coordinates			
77	-1.168336	-0.138385	0.038350
5	-2.378413	-1.414385	-1.138157
8	-2.395980	-1.334400	-2.527047
8	-3.230882	-2.426142	-0.703961
6	-3.035469	-2.532012	-3.037923
6	-3.972979	-2.926320	-1.844513
5	-0.738529	-2.054352	0.763615
8	-0.226435	-3.033983	-0.087249
8	-0.826727	-2.534329	2.055946
6	0.198836	-4.170778	0.713142
6	-0.647687	-3.972964	2.021284
5	-2.861570	-0.136783	1.193610
8	-3.058547	-0.651586	2.469184
8	-4.057072	0.451853	0.740538
6	-4.471981	-0.642335	2.768506
6	-4.993315	0.509495	1.841138
6	-1.086538	1.446134	-2.591945
6	0.031290	0.496745	-2.740634
7	-1.749581	1.433941	-1.403873
7	0.329793	-0.242958	-1.646826
6	-1.447598	2.353330	-3.598605
6	-2.481854	3.255614	-3.383095
6	-3.139397	3.242815	-2.152515
6	-2.743925	2.315786	-1.195858
6	0.777848	0.355731	-3.916658
6	1.857481	-0.518471	-3.948233
6	2.181249	-1.270110	-2.808993
6	1.351706	-1.099791	-1.692123
6	-0.132356	1.287256	1.501757
6	0.976711	2.101634	1.186705
6	-0.667404	1.453668	2.798963
6	1.507142	3.019561	2.109018
6	-0.154608	2.374392	3.713467
6	0.947481	3.161188	3.375953
1	-0.165884	-0.311741	1.290219
1	-1.481454	0.810538	3.111255
1	1.372541	3.862892	4.087648
1	2.374792	3.612604	1.830036
1	-3.243117	2.226628	-0.240862
1	-3.946398	3.932475	-1.931105
1	-2.763145	3.961482	-4.158361
1	-0.917016	2.357634	-4.542411
1	0.533343	0.932369	-4.800470
1	2.460880	-0.608479	-4.846199
1	1.507101	-1.684201	-0.800016
6	3.303330	-2.237772	-2.776766
6	3.489097	-3.103481	-3.867256
6	4.172654	-2.347222	-1.657949
6	4.470679	-4.089031	-3.853826
1	2.813918	-3.024849	-4.714965
6	5.156531	-3.350016	-1.649105
6	5.292602	-4.214728	-2.730685
1	4.582358	-4.759974	-4.699988
1	5.794728	-3.432696	-0.780218
1	6.058098	-4.984975	-2.699625
7	4.068240	-1.429914	-0.602391
6	4.162882	-1.761963	0.761573

8	4.724207	-2.773804	1.174073
7	3.532326	-0.846405	1.552523
1	3.570621	-0.570051	-0.798704
1	3.079967	-0.049638	1.107101
6	1.720716	2.006818	-0.113588
8	2.572133	1.117786	-0.288298
7	1.506158	2.974905	-1.042476
1	-0.600899	2.454156	4.701423
6	0.427439	3.961168	-0.909042
1	-0.092824	4.003960	-1.869879
1	-0.286459	3.573855	-0.181888
6	2.343340	3.001671	-2.250202
1	2.599713	1.971039	-2.496555
1	1.722889	3.389003	-3.065727
6	3.618932	3.855048	-2.117991
1	4.114005	3.855621	-3.099195
1	3.332177	4.893162	-1.917084
6	4.609890	3.378619	-1.044230
1	5.347691	4.172653	-0.878113
1	4.079362	3.257183	-0.092438
6	5.333181	2.068112	-1.392741
1	6.080583	2.267234	-2.174608
1	4.615892	1.360183	-1.819102
6	6.005113	1.395430	-0.187358
1	5.230994	1.150879	0.549370
1	6.426776	0.434900	-0.506218
6	7.098075	2.240069	0.476147
1	6.696883	3.174725	0.883225
1	7.566790	1.697331	1.303743
1	7.886249	2.503012	-0.239955
6	0.874658	5.365628	-0.481287
1	1.571188	5.269366	0.357361
1	1.423345	5.852777	-1.296797
6	-0.311219	6.246298	-0.057199
1	-0.829382	5.762617	0.783452
1	0.082087	7.193340	0.329554
6	-1.320950	6.526124	-1.180167
1	-1.702294	5.576257	-1.572692
1	-0.802835	7.018828	-2.016378
6	-2.520844	7.384251	-0.747625
1	-3.242025	7.422385	-1.574567
1	-3.036727	6.883615	0.083561
6	-2.157540	8.815965	-0.336585
1	-3.053803	9.398686	-0.100321
1	-1.512622	8.834413	0.547583
1	-1.626842	9.332557	-1.145077
6	3.557602	-0.890735	3.006647
6	4.504956	0.184846	3.570603
6	2.134593	-0.699395	3.554898
1	3.933476	-1.881413	3.283300
6	4.479763	0.217015	5.105778
1	4.185267	1.161530	3.178498
1	5.519055	0.005706	3.195041
6	2.107198	-0.667162	5.088016
1	1.746470	0.253001	3.177939
1	1.469957	-1.479035	3.168538
6	3.050652	0.414282	5.635020
1	5.141072	1.009220	5.477345
1	4.879729	-0.731362	5.492388
1	1.081105	-0.491501	5.431570
1	2.410134	-1.647762	5.482926

1	3.045687	0.410939	6.731902
1	2.680444	1.399135	5.316227
6	-1.914846	-3.550917	-3.284548
1	-2.296387	-4.479566	-3.720333
1	-1.192019	-3.112169	-3.978837
1	-1.389410	-3.775232	-2.352983
6	-3.750375	-2.187165	-4.339565
1	-3.013914	-1.913181	-5.100893
1	-4.319787	-3.046268	-4.710083
1	-4.431179	-1.344084	-4.208222
6	-4.193057	-4.424318	-1.661949
1	-4.832110	-4.599060	-0.791468
1	-4.684689	-4.856059	-2.540326
1	-3.249019	-4.945564	-1.496999
6	-5.314482	-2.183412	-1.862762
1	-5.956543	-2.523044	-2.681210
1	-5.833212	-2.367759	-0.918209
1	-5.155962	-1.105850	-1.953148
6	-6.404087	0.315261	1.294416
1	-6.474026	-0.596724	0.700077
1	-7.134443	0.263704	2.109067
1	-6.671323	1.158768	0.650282
6	-5.016709	-2.021883	2.375988
1	-4.483564	-2.782454	2.951380
1	-6.087336	-2.113362	2.584856
1	-4.829025	-2.217877	1.317794
6	-4.851252	1.900155	2.475508
1	-5.048679	2.659856	1.712548
1	-5.557518	2.049595	3.297751
1	-3.835014	2.050960	2.850945
6	-4.653255	-0.401933	4.264467
1	-5.714648	-0.310630	4.519704
1	-4.238206	-1.246129	4.822085
1	-4.135131	0.501945	4.590627
6	0.043720	-4.406722	3.309633
1	0.255083	-5.481209	3.292649
1	0.980992	-3.869644	3.463898
1	-0.609326	-4.198424	4.161835
6	-2.051629	-4.583014	1.928046
1	-2.019575	-5.676930	1.920863
1	-2.629349	-4.256934	2.796552
1	-2.564477	-4.224948	1.031899
6	-0.104331	-5.444415	-0.069018
1	0.512847	-5.475482	-0.971760
1	0.124004	-6.331360	0.531154
1	-1.152268	-5.485714	-0.370809
6	1.705591	-4.025652	0.936894
1	2.217528	-3.985106	-0.028230
1	1.934372	-3.105658	1.477371
1	2.120489	-4.865879	1.499840

TS1-ortho-gaa (Refer to Table S2)

Number of imaginary frequencies : 1
Imaginary frequency : -778.4005 cm(-1)

Electronic energy : HF=-3396.5324955
Zero-point correction= 1.456558 (Hartree/Particle)
Thermal correction to Energy= 1.536335
Thermal correction to Enthalpy= 1.537280

Thermal correction to Gibbs Free Energy=	1.339078
Sum of electronic and zero-point Energies=	-3395.075938
Sum of electronic and thermal Energies=	-3394.996160
Sum of electronic and thermal Enthalpies=	-3394.995216
Sum of electronic and thermal Free Energies=	-3395.193417

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Cartesian Coordinates

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77	-1.122063	-0.261751	0.075405
5	-2.190619	-1.591509	-1.171744
8	-2.280162	-1.392736	-2.546144
8	-2.871850	-2.749505	-0.807944
6	-2.760670	-2.621656	-3.147484
6	-3.578211	-3.255529	-1.968100
5	-0.400235	-2.141218	0.636316
8	0.188932	-2.978715	-0.311331
8	-0.337803	-2.713771	1.892310
6	0.813398	-4.096218	0.376995
6	0.032982	-4.107719	1.739580
5	-2.754775	-0.592707	1.269053
8	-2.833786	-1.238515	2.497573
8	-4.035364	-0.138008	0.901037
6	-4.224132	-1.451584	2.829058
6	-4.927829	-0.303178	2.027613
6	-1.359539	1.508142	-2.424185
6	-0.120942	0.746531	-2.666753
7	-1.971380	1.318637	-1.223921
7	0.317820	-0.013481	-1.635791
6	-1.884770	2.414543	-3.356679
6	-3.034603	3.133487	-3.055139
6	-3.642859	2.937876	-1.814804
6	-3.080801	2.022412	-0.933348
6	0.598682	0.794599	-3.866670
6	1.788392	0.086784	-3.987477
6	2.254560	-0.685807	-2.913093
6	1.450606	-0.707035	-1.765509
6	-0.219931	1.165439	1.642684
6	0.755076	2.150164	1.375257
6	-0.726889	1.141436	2.961035
6	1.184606	3.052091	2.363062
6	-0.314894	2.044582	3.941567
6	0.653952	3.005590	3.649648
1	-0.049065	-0.369803	1.277592
1	-1.431684	0.364417	3.232209
1	1.001557	3.697825	4.410892
1	1.953655	3.781050	2.119731
1	-3.531207	1.797522	0.023912
1	-4.537461	3.479979	-1.528573
1	-3.443583	3.839483	-3.771159
1	-1.393247	2.559568	-4.310482
1	0.245235	1.388404	-4.700817
1	2.365817	0.143291	-4.905007
1	1.719918	-1.319454	-0.920897
6	3.496075	-1.492268	-2.982306
6	3.753178	-2.243710	-4.141391
6	4.413548	-1.566707	-1.899676
6	4.856753	-3.085000	-4.233431
1	3.041246	-2.195711	-4.960795
6	5.523149	-2.423144	-1.999051
6	5.732312	-3.178494	-3.148391
1	5.023191	-3.671043	-5.132026

1	6.200270	-2.483398	-1.158421
1	6.595359	-3.836275	-3.199854
7	4.231490	-0.754437	-0.771148
6	4.443757	-1.166840	0.558922
8	5.113033	-2.151843	0.860478
7	3.805092	-0.357115	1.450404
1	3.622176	0.047445	-0.881125
1	3.222384	0.396992	1.090478
6	1.467768	2.259665	0.058076
8	2.445164	1.530279	-0.184785
7	1.073774	3.229269	-0.807323
1	-0.732048	1.976116	4.942982
6	-0.132119	4.034274	-0.580071
1	-0.663258	4.092552	-1.534028
1	-0.775502	3.479879	0.104150
6	1.854041	3.444712	-2.033746
1	2.305288	2.489776	-2.302950
1	1.147415	3.708292	-2.828330
6	2.935486	4.535047	-1.913625
1	3.440506	4.603179	-2.887077
1	2.449591	5.503506	-1.751599
6	3.972664	4.290459	-0.806977
1	4.530610	5.219751	-0.633621
1	3.446447	4.082313	0.132562
6	4.967263	3.156490	-1.092993
1	5.677331	3.483086	-1.866270
1	4.437945	2.288823	-1.499229
6	5.726408	2.713391	0.163250
1	6.185034	3.590192	0.642452
1	4.999173	2.311133	0.879780
6	6.797306	1.655833	-0.117809
1	7.569255	2.043455	-0.793335
1	7.290719	1.334096	0.805341
1	6.355978	0.769306	-0.583554
6	0.107305	5.442761	-0.017313
1	0.804558	5.370379	0.822812
1	0.583599	6.077689	-0.773946
6	-1.201074	6.093979	0.457369
1	-1.641199	5.467413	1.246216
1	-0.971215	7.059264	0.926373
6	-2.234444	6.308102	-0.656263
1	-2.477901	5.347950	-1.126742
1	-1.793428	6.932633	-1.447263
6	-3.536268	6.950444	-0.164831
1	-3.961031	6.331159	0.637040
1	-3.315430	7.925929	0.288981
6	-4.569759	7.121962	-1.282504
1	-5.493349	7.579510	-0.913742
1	-4.179866	7.756537	-2.086723
1	-4.832214	6.153909	-1.726615
6	3.826711	-0.572272	2.889260
6	4.587014	0.562769	3.599022
6	2.388487	-0.671310	3.424629
1	4.352970	-1.518054	3.055828
6	4.552525	0.400188	5.126102
1	4.114612	1.517056	3.322766
1	5.617434	0.596739	3.226888
6	2.350422	-0.836320	4.948835
1	1.859394	0.250057	3.157546
1	1.851881	-1.488310	2.932263
6	3.109434	0.302469	5.645725

1	5.078858	1.234274	5.605953
1	5.097285	-0.513963	5.402605
1	1.308403	-0.869326	5.287515
1	2.804134	-1.799082	5.225653
1	3.104583	0.160176	6.733357
1	2.587455	1.249023	5.444684
6	-1.515627	-3.436676	-3.522229
1	-1.777360	-4.373545	-4.023753
1	-0.899075	-2.839895	-4.200927
1	-0.919043	-3.654320	-2.632609
6	-3.574340	-2.273294	-4.388758
1	-2.920926	-1.819515	-5.139907
1	-4.022690	-3.172154	-4.825475
1	-4.368584	-1.561181	-4.157322
6	-3.564380	-4.779742	-1.916537
1	-4.129279	-5.123165	-1.044906
1	-4.026459	-5.204747	-2.813956
1	-2.546544	-5.163100	-1.830942
6	-5.015123	-2.726667	-1.879063
1	-5.634116	-3.088484	-2.705696
1	-5.459504	-3.068480	-0.940557
1	-5.022468	-1.633744	-1.875490
6	-6.320817	-0.634703	1.502017
1	-6.291390	-1.487126	0.821963
1	-7.004886	-0.862618	2.326399
1	-6.723331	0.221634	0.951970
6	-4.591565	-2.850953	2.319454
1	-3.940519	-3.580994	2.806447
1	-5.631988	-3.107046	2.543475
1	-4.417244	-2.920510	1.243476
6	-4.942981	1.032347	2.784440
1	-5.259246	1.824636	2.098586
1	-5.635595	1.016467	3.631351
1	-3.942378	1.279069	3.150854
6	-4.382997	-1.376330	4.344696
1	-5.437173	-1.457508	4.631569
1	-3.837282	-2.202148	4.809539
1	-3.981767	-0.443130	4.744617
6	0.857672	-4.526985	2.952099
1	1.200649	-5.561671	2.846689
1	1.728423	-3.883957	3.088377
1	0.241589	-4.458637	3.853121
6	-1.277231	-4.902454	1.675650
1	-1.095120	-5.978228	1.588936
1	-1.840421	-4.717322	2.593831
1	-1.888824	-4.568174	0.833715
6	0.636778	-5.343815	-0.482927
1	1.194302	-5.226724	-1.416902
1	1.020096	-6.229404	0.034652
1	-0.413008	-5.509656	-0.730851
6	2.297689	-3.756108	0.527827
1	2.732321	-3.569718	-0.457779
1	2.434079	-2.856757	1.130423
1	2.863074	-4.566737	0.994866

TS1-ortho-gga (Refer to Table S2)

Number of imaginary frequencies : 1
Imaginary frequency : -752.2393 cm(-1)

Electronic energy : HF=-3396.5293366
 Zero-point correction= 1.457426 (Hartree/Particle)
 Thermal correction to Energy= 1.536783
 Thermal correction to Enthalpy= 1.537727
 Thermal correction to Gibbs Free Energy= 1.341990
 Sum of electronic and zero-point Energies= -3395.071911
 Sum of electronic and thermal Energies= -3394.992553
 Sum of electronic and thermal Enthalpies= -3394.991609
 Sum of electronic and thermal Free Energies= -3395.187347

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 Cartesian Coordinates

77	-1.170944	-0.008298	0.027827
5	-2.329995	-0.864898	-1.521217
8	-2.189341	-0.469225	-2.847474
8	-3.298836	-1.859219	-1.417091
6	-2.850179	-1.452901	-3.683251
6	-3.939681	-2.019772	-2.707766
5	-0.961602	-2.069963	0.303469
8	-0.427170	-2.867364	-0.709009
8	-1.224717	-2.828351	1.427585
6	-0.173836	-4.195222	-0.174135
6	-1.138436	-4.229999	1.065170
5	-2.977396	-0.104319	0.990127
8	-3.353186	-0.883935	2.077137
8	-4.065655	0.693772	0.591212
6	-4.787178	-0.807144	2.236870
6	-5.113566	0.579503	1.581762
6	-0.687361	2.073980	-2.176222
6	0.364889	1.072095	-2.424474
7	-1.479292	1.879022	-1.087636
7	0.510781	0.116337	-1.477269
6	-0.857872	3.204739	-2.987998
6	-1.843988	4.135396	-2.685341
6	-2.647183	3.921530	-1.564932
6	-2.431964	2.783194	-0.796826
6	1.205962	1.095704	-3.543125
6	2.233120	0.167917	-3.652054
6	2.409538	-0.803579	-2.654919
6	1.486353	-0.787803	-1.599608
6	-0.214590	0.949332	1.886102
6	0.991282	1.685129	1.888801
6	-0.887093	0.873931	3.126461
6	1.486688	2.294357	3.052731
6	-0.411595	1.495993	4.281603
6	0.789430	2.205402	4.254958
1	-0.349906	-0.537203	1.312831
1	-1.783016	0.268752	3.195728
1	1.185386	2.668545	5.153954
1	2.434914	2.824723	3.013252
1	-3.049340	2.541497	0.058104
1	-3.428043	4.619346	-1.283903
1	-1.978485	5.013699	-3.308763
1	-0.218142	3.357570	-3.847931
1	1.076550	1.841085	-4.318563
1	2.911661	0.203963	-4.498569
1	1.523193	-1.536770	-0.825500
6	3.473376	-1.833255	-2.732533
6	3.722456	-2.454397	-3.969016
6	4.229816	-2.238218	-1.601175
6	4.659127	-3.474034	-4.096845

1	3.130854	-2.156551	-4.830197
6	5.174171	-3.268790	-1.739420
6	5.376245	-3.884667	-2.970037
1	4.818246	-3.951063	-5.059054
1	5.729920	-3.573766	-0.863453
1	6.108689	-4.682865	-3.050460
7	4.067469	-1.585681	-0.366835
6	3.926018	-2.273824	0.857331
8	4.326418	-3.422057	1.030476
7	3.270547	-1.532999	1.794446
1	3.638692	-0.667933	-0.395968
1	2.955624	-0.597746	1.544697
6	1.863216	1.800826	0.673594
8	2.670555	0.893492	0.405129
7	1.780986	2.937922	-0.065858
1	-0.967372	1.397421	5.210575
6	0.785588	3.977919	0.230129
1	0.397077	4.336582	-0.727657
1	-0.049489	3.502374	0.745492
6	2.642635	3.101831	-1.242207
1	3.041481	2.116580	-1.480187
1	2.000745	3.404897	-2.077194
6	3.786392	4.115886	-1.096221
1	4.316181	4.125972	-2.057133
1	3.371565	5.123018	-0.975482
6	4.782484	3.843767	0.041734
1	5.540202	4.638324	0.013595
1	4.262145	3.954232	1.002189
6	5.481117	2.471986	0.012867
1	4.759630	1.690038	0.264941
1	6.237158	2.457942	0.809581
6	6.157318	2.109525	-1.315899
1	5.403816	2.051876	-2.113060
1	6.851783	2.909106	-1.611458
6	6.899746	0.770362	-1.239634
1	6.218980	-0.039640	-0.956075
1	7.355066	0.505977	-2.199802
1	7.697911	0.807428	-0.489277
6	1.303652	5.153425	1.072325
1	1.932957	4.760564	1.875854
1	1.944717	5.800194	0.464488
6	0.158741	5.970005	1.693920
1	-0.340890	5.347479	2.447839
1	0.590211	6.823178	2.233221
6	-0.895060	6.481409	0.696948
1	-1.646113	7.062221	1.249065
1	-1.436550	5.630860	0.263167
6	-0.335497	7.344986	-0.440056
1	0.236829	8.181054	-0.015616
1	0.378760	6.760800	-1.035074
6	-1.433199	7.884430	-1.362782
1	-1.018650	8.489645	-2.175629
1	-2.001582	7.062625	-1.813932
1	-2.143608	8.508735	-0.809334
6	3.002349	-2.013469	3.143191
6	3.976072	-1.393746	4.162236
6	1.547712	-1.693980	3.519419
1	3.152278	-3.098413	3.124127
6	3.644203	-1.827902	5.598197
1	3.903280	-0.299169	4.084028
1	5.002540	-1.668062	3.893997

6	1.214363	-2.123592	4.953214
1	1.400256	-0.611493	3.436015
1	0.858213	-2.160282	2.808946
6	2.188617	-1.493485	5.959239
1	4.335533	-1.353284	6.305099
1	3.797861	-2.912647	5.690901
1	0.181227	-1.841419	5.186726
1	1.268246	-3.219229	5.031064
1	1.961066	-1.828651	6.978593
1	2.054681	-0.402199	5.944609
6	-1.782250	-2.488383	-4.059423
1	-2.178805	-3.259512	-4.727135
1	-0.962366	-1.974166	-4.569749
1	-1.374334	-2.958648	-3.161198
6	-3.391632	-0.754630	-4.925479
1	-2.558754	-0.379252	-5.527480
1	-3.970996	-1.450281	-5.541952
1	-4.026763	0.092348	-4.659989
6	-4.278180	-3.494249	-2.902154
1	-5.020840	-3.802518	-2.160469
1	-4.696326	-3.669993	-3.899093
1	-3.396084	-4.123803	-2.776638
6	-5.219705	-1.175123	-2.677660
1	-5.788815	-1.267582	-3.607658
1	-5.849959	-1.517913	-1.852664
1	-4.982815	-0.122288	-2.504568
6	-6.463311	0.662685	0.875732
1	-6.526476	-0.061581	0.062398
1	-7.283317	0.478685	1.578078
1	-6.597882	1.661500	0.448934
6	-5.381848	-1.990866	1.463175
1	-4.974513	-2.916400	1.877240
1	-6.473194	-2.023278	1.541679
1	-5.087720	-1.943521	0.412194
6	-4.941899	1.756126	2.552467
1	-4.990999	2.692555	1.987935
1	-5.725988	1.774829	3.315339
1	-3.967858	1.708650	3.047635
6	-5.122620	-0.915530	3.721303
1	-6.196523	-0.778412	3.888315
1	-4.842181	-1.906999	4.087612
1	-4.578978	-0.174489	4.310386
6	-0.616403	-5.008215	2.268591
1	-0.476349	-6.064541	2.015732
1	0.332999	-4.606226	2.625991
1	-1.339819	-4.943198	3.086255
6	-2.562292	-4.673651	0.708300
1	-2.603809	-5.735627	0.446950
1	-3.206398	-4.502177	1.574467
1	-2.950412	-4.076822	-0.120832
6	-0.481826	-5.215674	-1.265454
1	0.221431	-5.087884	-2.093619
1	-0.376509	-6.236237	-0.882875
1	-1.493525	-5.090856	-1.655125
6	1.307030	-4.251854	0.205607
1	1.920705	-4.029873	-0.671558
1	1.542408	-3.514153	0.973789
1	1.599752	-5.237011	0.578041

TS1-para-aaa (Refer to Table S3)

Number of imaginary frequencies : 1
Imaginary frequency : -819.2349 cm(-1)

Electronic energy : HF=-3396.5087807
Zero-point correction= 1.454489 (Hartree/Particle)
Thermal correction to Energy= 1.534991
Thermal correction to Enthalpy= 1.535935
Thermal correction to Gibbs Free Energy= 1.335376
Sum of electronic and zero-point Energies= -3395.054292
Sum of electronic and thermal Energies= -3394.973790
Sum of electronic and thermal Enthalpies= -3394.972846
Sum of electronic and thermal Free Energies= -3395.173405

Cartesian Coordinates

77	1.897020	-0.282093	-0.806411
5	3.666158	0.402917	0.129645
8	3.928013	1.768012	0.244990
8	4.643438	-0.329413	0.794746
6	4.906864	1.944867	1.300220
6	5.673281	0.577443	1.257678
5	1.651295	-1.215286	0.995530
8	1.837512	-0.537022	2.210187
8	1.232667	-2.515597	1.246432
6	1.374572	-1.382608	3.294887
6	1.466333	-2.806523	2.644729
5	3.266959	-1.775998	-1.268241
8	3.359477	-3.046244	-0.727977
8	4.245677	-1.600345	-2.254155
6	4.585060	-3.664527	-1.176559
6	4.893443	-2.872260	-2.500064
6	1.905405	2.389733	-2.400850
6	1.146682	2.688170	-1.165996
7	2.302361	1.106159	-2.574087
7	1.053660	1.699892	-0.243268
6	2.216467	3.373683	-3.349848
6	2.924569	3.025271	-4.494316
6	3.318657	1.698789	-4.664989
6	2.993724	0.774851	-3.676412
6	0.545692	3.929753	-0.930153
6	-0.104712	4.163710	0.273128
6	-0.159910	3.156236	1.245902
6	0.426414	1.925738	0.918389
6	-0.724890	0.132185	-2.473214
6	-0.186935	-0.661062	-1.443316
6	-2.089472	0.409600	-2.536978
6	-1.098487	-1.323203	-0.598383
6	-2.970483	-0.148836	-1.599450
6	-2.462775	-1.057202	-0.662458
1	-2.463237	1.115122	-3.275167
1	-3.133407	-1.521614	0.049103
1	-0.722871	-2.004874	0.156592
1	3.314355	-0.258471	-3.725287
1	3.877549	1.380297	-5.538311
1	3.170986	3.779834	-5.235030
1	1.922842	4.403883	-3.191529
1	0.576093	4.710608	-1.680031
1	-0.568973	5.125297	0.466998
1	0.446188	1.108337	1.627477
6	-4.343239	0.409512	-1.420526

8	-4.710770	0.760172	-0.284552
7	-5.121417	0.651786	-2.518924
6	-0.681456	3.430403	2.607813
6	-0.133545	4.531167	3.289130
6	-1.655793	2.631709	3.256116
6	-0.492366	4.834348	4.596999
1	0.617514	5.128924	2.780041
6	-2.009220	2.943226	4.583453
6	-1.428111	4.021760	5.240475
1	-0.040138	5.677994	5.108830
1	-2.735674	2.322240	5.086661
1	-1.721224	4.232581	6.265114
7	-2.296514	1.599486	2.555738
6	-2.992125	0.525936	3.138256
8	-2.899982	0.238774	4.331291
7	-3.748285	-0.177943	2.252338
1	-2.257740	1.626923	1.545746
1	-3.989918	0.221565	1.344147
6	-6.255761	1.574222	-2.369356
1	-6.611384	1.516047	-1.338820
1	-7.065042	1.238261	-3.024416
6	-5.046826	-0.140825	-3.750843
1	-5.274577	0.519363	-4.595520
1	-4.024389	-0.494441	-3.884232
6	-4.497942	-1.344159	2.715595
6	-5.635263	-1.674322	1.738736
6	-3.580286	-2.563823	2.922184
1	-4.936715	-1.094769	3.691777
6	-6.437279	-2.887496	2.232431
1	-5.213604	-1.899965	0.750067
1	-6.279893	-0.798681	1.605389
6	-4.377630	-3.783721	3.404061
1	-3.083563	-2.799304	1.970477
1	-2.800472	-2.297104	3.640253
6	-5.530743	-4.110797	2.443006
1	-7.239791	-3.120477	1.522285
1	-6.927216	-2.633775	3.182911
1	-3.712799	-4.648321	3.514784
1	-4.788048	-3.574102	4.401955
1	-6.116854	-4.958211	2.818517
1	-5.114656	-4.419889	1.473571
6	-5.851571	3.018198	-2.715657
6	-4.702368	3.552069	-1.850752
1	-6.737031	3.658374	-2.602490
1	-5.564274	3.069807	-3.775555
6	-4.296581	4.994632	-2.165449
1	-4.969183	3.460101	-0.791015
1	-3.823941	2.910856	-1.991580
6	-3.062186	5.430554	-1.365702
1	-4.083827	5.093066	-3.240267
1	-5.133387	5.676202	-1.956887
1	-3.271454	5.322765	-0.292528
1	-2.239703	4.735119	-1.580052
6	-5.996931	-1.350180	-3.737086
6	-5.716193	-2.321364	-2.584177
1	-5.890468	-1.869708	-4.698981
1	-7.039662	-1.009662	-3.685511
6	-6.586457	-3.580954	-2.619444
1	-4.655180	-2.606684	-2.595955
1	-5.879549	-1.805385	-1.629491
6	-6.322987	-4.515526	-1.432636

1	-7.647463	-3.291848	-2.625422
1	-6.413666	-4.123739	-3.559780
1	-5.262399	-4.801823	-1.427327
1	-6.490823	-3.962450	-0.500124
6	-2.614061	6.864125	-1.662366
1	-1.726026	7.138279	-1.081196
1	-2.369869	6.990250	-2.723722
1	-3.403044	7.584357	-1.418380
6	-7.196830	-5.772509	-1.445986
1	-6.988376	-6.413061	-0.582911
1	-8.261308	-5.512046	-1.419621
1	-7.024132	-6.364479	-2.352149
6	4.330484	-5.158508	-1.363328
1	5.215754	-5.658160	-1.771652
1	4.099955	-5.609756	-0.394200
1	3.483362	-5.341953	-2.026351
6	5.630625	-3.440739	-0.076739
1	5.264574	-3.892614	0.848713
1	6.592383	-3.897202	-0.331315
1	5.761757	-2.374061	0.109348
6	6.372848	-2.612993	-2.770158
1	6.921777	-3.554593	-2.877170
1	6.485288	-2.045268	-3.699012
1	6.822491	-2.031951	-1.963528
6	4.222094	-3.480207	-3.738385
1	4.323544	-2.783656	-4.576359
1	4.679898	-4.431698	-4.025006
1	3.156046	-3.643994	-3.558088
6	6.797089	0.552449	0.213631
1	7.639276	1.186971	0.506418
1	7.161356	-0.472899	0.105946
1	6.423376	0.882136	-0.759374
6	6.179972	0.076715	2.606597
1	6.680145	-0.887620	2.476864
1	6.898679	0.780262	3.040476
1	5.354792	-0.062158	3.306837
6	4.114320	2.148985	2.599298
1	4.772850	2.330837	3.454435
1	3.459455	3.017076	2.476897
1	3.483061	1.280289	2.802652
6	5.753879	3.173266	0.985712
1	5.130242	4.071034	1.031759
1	6.563980	3.283521	1.714837
1	6.187357	3.114030	-0.014363
6	0.413078	-3.802479	3.119175
1	0.507391	-3.985477	4.194939
1	-0.597047	-3.442106	2.914657
1	0.547197	-4.753804	2.596090
6	2.872966	-3.412192	2.737726
1	3.113728	-3.723080	3.759424
1	2.921532	-4.282549	2.078834
1	3.620491	-2.692865	2.392890
6	-0.058955	-0.957849	3.617247
1	-0.079947	0.100750	3.886406
1	-0.708128	-1.098772	2.749235
1	-0.479781	-1.517641	4.456078
6	2.281962	-1.159004	4.500950
1	2.160604	-0.135039	4.866948
1	2.022212	-1.844173	5.314981
1	3.331615	-1.305434	4.239768
1	-0.065505	0.612421	-3.188468

1 1.229515 -1.556361 -1.556971

TS1-para-ggg (Refer to Table S3)

Number of imaginary frequencies : 1

Imaginary frequency : -801.4344 cm(-1)

Electronic energy : HF=-3396.5060458
Zero-point correction= 1.455865 (Hartree/Particle)
Thermal correction to Energy= 1.535789
Thermal correction to Enthalpy= 1.536733
Thermal correction to Gibbs Free Energy= 1.335306
Sum of electronic and zero-point Energies= -3395.050181
Sum of electronic and thermal Energies= -3394.970257
Sum of electronic and thermal Enthalpies= -3394.969313
Sum of electronic and thermal Free Energies= -3395.170739

Cartesian Coordinates

77	1.940326	-0.599382	-0.618926
5	3.722452	0.534017	-0.487051
8	3.887466	1.689575	-1.250796
8	4.794446	0.380487	0.384885
6	4.915490	2.495469	-0.621244
6	5.779890	1.403124	0.100463
5	1.904623	-0.237332	1.393001
8	2.120010	1.044441	1.923567
8	1.592121	-1.118919	2.420076
6	1.778055	1.034857	3.333310
6	1.916034	-0.488285	3.681341
5	3.379963	-2.046561	-0.231365
8	3.599890	-2.742611	0.944062
8	4.277282	-2.472536	-1.218653
6	4.838751	-3.476905	0.835116
6	5.006227	-3.621218	-0.722674
6	1.595520	0.513454	-3.503720
6	0.953277	1.521373	-2.630877
7	2.078030	-0.596001	-2.894778
7	1.006692	1.303194	-1.294673
6	1.716856	0.682362	-4.890203
6	2.324985	-0.307794	-5.653229
6	2.811311	-1.447664	-5.014247
6	2.673209	-1.546262	-3.633177
6	0.321076	2.664767	-3.132000
6	-0.216731	3.597226	-2.255569
6	-0.127717	3.387280	-0.873208
6	0.484560	2.200323	-0.449563
6	-0.839505	-1.384136	-1.891337
6	-0.158746	-1.294350	-0.662965
6	-2.225392	-1.230621	-1.968727
6	-0.943826	-1.217001	0.501764
6	-2.974835	-1.006085	-0.806145
6	-2.320398	-1.042016	0.430553
1	-2.718898	-1.231749	-2.938162
1	-2.885529	-0.901871	1.341445
1	-0.464118	-1.242362	1.472687
1	3.072220	-2.381920	-3.071871
1	3.298509	-2.244156	-5.566234
1	2.423153	-0.186121	-6.727599
1	1.351058	1.581385	-5.370275

1	0.246478	2.831014	-4.199465
1	-0.697068	4.494590	-2.633196
1	0.617624	1.986461	0.602524
6	-4.389639	-0.522480	-0.865232
8	-4.660590	0.584124	-0.360786
7	-5.332802	-1.264107	-1.513220
6	-0.522790	4.435382	0.100518
6	0.065150	5.702497	-0.049946
6	-1.411745	4.207858	1.180009
6	-0.171790	6.729696	0.856253
1	0.749042	5.856294	-0.880225
6	-1.639787	5.251415	2.097669
6	-1.021001	6.486357	1.937539
1	0.308510	7.694878	0.730047
1	-2.298254	5.072475	2.934926
1	-1.216591	7.269436	2.664725
7	-2.093030	2.985857	1.276821
6	-2.733370	2.490160	2.424559
8	-2.551272	2.956958	3.548481
7	-3.548952	1.428532	2.175644
1	-2.135614	2.411324	0.445944
1	-3.849724	1.216391	1.224110
6	-6.640689	-0.658106	-1.790622
1	-6.637341	0.319483	-1.310463
1	-7.427818	-1.250558	-1.312226
6	-5.141141	-2.670354	-1.884472
1	-5.205624	-2.773834	-2.975053
1	-4.129994	-2.955675	-1.598464
6	-4.239380	0.766867	3.281838
6	-5.374920	-0.116409	2.743609
6	-3.268764	-0.057503	4.150189
1	-4.673562	1.545272	3.925385
6	-6.117315	-0.818998	3.889834
1	-4.957142	-0.878211	2.073227
1	-6.060115	0.484327	2.135614
6	-4.011586	-0.754064	5.298637
1	-2.778361	-0.811684	3.519092
1	-2.488210	0.605641	4.532117
6	-5.154171	-1.632968	4.768696
1	-6.901738	-1.467171	3.480463
1	-6.623793	-0.066468	4.510264
1	-3.310391	-1.352027	5.892372
1	-4.424738	0.007426	5.975105
1	-5.698841	-2.100046	5.597975
1	-4.727431	-2.450944	4.170527
6	-6.920957	-0.530494	-3.296308
6	-5.833581	0.228331	-4.073440
1	-7.890039	-0.029417	-3.408470
1	-7.049107	-1.526918	-3.737909
6	-5.557315	1.662321	-3.582617
1	-4.897579	-0.342321	-4.020190
1	-6.115473	0.246013	-5.133185
6	-6.784188	2.588822	-3.556783
1	-5.118754	1.628671	-2.579310
1	-4.793798	2.104843	-4.237320
1	-7.516192	2.214957	-2.828831
1	-6.468543	3.569590	-3.179794
6	-6.152776	-3.615529	-1.213800
6	-6.220424	-3.491481	0.316742
1	-5.874670	-4.637192	-1.499470
1	-7.152419	-3.452979	-1.634179

6	-4.895037	-3.747108	1.055380
1	-6.571847	-2.486244	0.581426
1	-6.986140	-4.185303	0.683693
6	-4.224552	-5.100093	0.768522
1	-4.182756	-2.950464	0.818367
1	-5.086340	-3.666988	2.133789
1	-3.928032	-5.152435	-0.287525
1	-3.289144	-5.147074	1.339384
6	-7.464023	2.765096	-4.919395
1	-8.283505	3.489163	-4.864763
1	-6.750053	3.124134	-5.670233
1	-7.882576	1.822729	-5.288849
6	-5.094651	-6.313167	1.115500
1	-4.548776	-7.249969	0.963546
1	-5.414689	-6.279047	2.163569
1	-5.997947	-6.355070	0.497041
6	4.687603	-4.795228	1.591013
1	5.580286	-5.418539	1.470035
1	4.556278	-4.589022	2.656906
1	3.816073	-5.356345	1.249582
6	5.927890	-2.616038	1.487961
1	5.645875	-2.430326	2.527730
1	6.902809	-3.113414	1.473833
1	5.996223	-1.648057	0.989835
6	6.443072	-3.532458	-1.228972
1	7.056979	-4.335384	-0.807306
1	6.458227	-3.627501	-2.319102
1	6.889554	-2.571909	-0.967844
6	4.312987	-4.865433	-1.292638
1	4.311471	-4.802093	-2.385254
1	4.824944	-5.787950	-1.002824
1	3.275042	-4.918477	-0.952590
6	6.835124	0.770570	-0.815636
1	7.643383	1.470780	-1.047928
1	7.267921	-0.099130	-0.313615
1	6.378539	0.429925	-1.748605
6	6.406669	1.842057	1.420347
1	6.976026	1.013399	1.851953
1	7.089548	2.684745	1.268032
1	5.639521	2.134861	2.139071
6	4.196909	3.434094	0.358093
1	4.895589	4.112740	0.857366
1	3.470555	4.033612	-0.199275
1	3.649394	2.857865	1.107901
6	5.642332	3.293267	-1.698282
1	4.951109	4.009803	-2.152101
1	6.480155	3.853556	-1.269248
1	6.022561	2.643573	-2.488693
6	0.948349	-0.996779	4.745158
1	1.111968	-0.482114	5.698098
1	-0.090527	-0.848325	4.443353
1	1.106525	-2.067708	4.901938
6	3.357102	-0.897389	4.014552
1	3.672922	-0.517377	4.991357
1	3.415170	-1.988638	4.021230
1	4.044020	-0.533902	3.245668
6	0.344387	1.559215	3.453279
1	0.282241	2.564187	3.029102
1	-0.352186	0.919870	2.904609
1	0.009072	1.621107	4.491552
6	2.744613	1.958284	4.069232

1	2.584799	2.990866	3.744758
1	2.578774	1.912518	5.150823
1	3.782829	1.693027	3.861064
1	-0.277882	-1.506473	-2.812097
1	1.304059	-2.065319	-0.340130

TS1-para-aga (Refer to Table S3)

Number of imaginary frequencies : 1
Imaginary frequency : -817.2529 cm(-1)

Electronic energy : HF=-3396.5056027
Zero-point correction= 1.455000 (Hartree/Particle)
Thermal correction to Energy= 1.535324
Thermal correction to Enthalpy= 1.536268
Thermal correction to Gibbs Free Energy= 1.335184
Sum of electronic and zero-point Energies= -3395.050603
Sum of electronic and thermal Energies= -3394.970279
Sum of electronic and thermal Enthalpies= -3394.969335
Sum of electronic and thermal Free Energies= -3395.170419

Cartesian Coordinates

77	1.966750	0.309052	-0.792885
5	3.816547	0.488694	0.213841
8	4.102191	1.614411	0.985769
8	4.842709	-0.443206	0.327727
6	5.179924	1.269894	1.892687
6	5.923146	0.143502	1.093248
5	1.880024	-1.418728	0.297195
8	2.144451	-1.438210	1.675813
8	1.498790	-2.686545	-0.122166
6	1.766249	-2.734945	2.207187
6	1.826772	-3.631968	0.922773
5	3.280894	-0.678486	-2.064756
8	3.399034	-2.039567	-2.284067
8	4.179661	0.019766	-2.881270
6	4.575823	-2.289714	-3.083270
6	4.783076	-0.911515	-3.811185
6	1.837765	3.414947	-0.792908
6	1.192488	3.009007	0.474791
7	2.209010	2.416909	-1.630126
7	1.169696	1.684065	0.758677
6	2.068060	4.757093	-1.126149
6	2.666604	5.071150	-2.340751
6	3.034724	4.034827	-3.197900
6	2.795095	2.723562	-2.798741
6	0.621448	3.928683	1.361432
6	0.064564	3.485307	2.552735
6	0.071860	2.118120	2.860334
6	0.626640	1.255964	1.905261
6	-0.812227	1.366762	-1.854712
6	-0.167636	0.211645	-1.375307
6	-2.191663	1.541009	-1.719538
6	-0.984073	-0.827377	-0.891819
6	-2.970767	0.541130	-1.125178
6	-2.355594	-0.655435	-0.744921
1	-2.656955	2.472312	-2.036149
1	-2.951728	-1.447877	-0.312852
1	-0.531191	-1.763878	-0.588164

1	3.105174	1.874433	-3.394808
1	3.509714	4.229698	-4.153359
1	2.849373	6.107454	-2.607942
1	1.796870	5.549451	-0.439746
1	0.604656	4.985327	1.124606
1	-0.370799	4.191450	3.252992
1	0.689409	0.191345	2.084842
6	-4.394322	0.773879	-0.727983
8	-4.697818	0.718076	0.477306
7	-5.318566	1.077251	-1.684394
6	-0.345997	1.621815	4.194932
6	0.265927	2.211696	5.314338
6	-1.279362	0.573929	4.389398
6	0.009639	1.768281	6.606314
1	0.984926	3.008808	5.146370
6	-1.527554	0.126514	5.701477
6	-0.885013	0.711538	6.786714
1	0.509578	2.227098	7.453517
1	-2.222080	-0.687071	5.851248
1	-1.097572	0.340565	7.785420
7	-1.987418	0.052023	3.295767
6	-2.665847	-1.177963	3.278492
8	-2.469248	-2.059926	4.114063
7	-3.540263	-1.312483	2.243429
1	-2.034143	0.616791	2.458462
1	-3.831591	-0.507018	1.689251
6	-6.674908	1.447129	-1.256213
1	-6.838139	1.023847	-0.263480
1	-7.388937	0.981908	-1.943019
6	-5.117751	0.847582	-3.121560
1	-5.633826	1.649940	-3.660750
1	-4.056094	0.937104	-3.352277
6	-4.274500	-2.567457	2.083832
6	-5.530661	-2.343601	1.230967
6	-3.388724	-3.679299	1.487835
1	-4.584110	-2.899063	3.084078
6	-6.316169	-3.650841	1.055556
1	-5.235311	-1.963624	0.244967
1	-6.153449	-1.564403	1.683759
6	-4.178089	-4.983415	1.307691
1	-3.005838	-3.349649	0.512761
1	-2.525326	-3.826696	2.142840
6	-5.436016	-4.757373	0.454397
1	-7.197404	-3.476011	0.426862
1	-6.692225	-3.981576	2.033851
1	-3.538914	-5.750410	0.855069
1	-4.475852	-5.365569	2.294273
1	-6.008146	-5.687756	0.355917
1	-5.135001	-4.464214	-0.561671
6	-6.880767	2.968446	-1.231399
6	-5.975874	3.690218	-0.223738
1	-7.934033	3.163923	-0.986789
1	-6.719959	3.368058	-2.240874
6	-6.236168	5.199654	-0.116410
1	-6.100991	3.222631	0.759751
1	-4.926053	3.526038	-0.499422
6	-5.895915	5.997894	-1.382775
1	-7.289332	5.373652	0.148171
1	-5.645319	5.600170	0.718643
1	-4.856372	5.786286	-1.670493
1	-6.518525	5.657054	-2.219596

6	-5.632161	-0.524998	-3.591691
6	-4.873068	-1.700878	-2.966296
1	-5.537221	-0.562347	-4.685451
1	-6.703798	-0.607099	-3.374691
6	-5.362987	-3.088749	-3.400067
1	-3.805478	-1.599361	-3.195895
1	-4.951990	-1.636531	-1.874708
6	-6.792596	-3.422844	-2.949700
1	-5.290026	-3.188855	-4.492430
1	-4.679275	-3.839708	-2.981342
1	-6.891429	-3.195637	-1.879859
1	-7.510523	-2.773964	-3.467080
6	-6.083116	7.507161	-1.198138
1	-5.836398	8.060015	-2.110636
1	-7.120090	7.744878	-0.934055
1	-5.444035	7.887579	-0.392805
6	-7.162170	-4.888491	-3.195192
1	-8.189955	-5.102338	-2.884025
1	-7.073220	-5.146100	-4.256951
1	-6.497598	-5.556474	-2.635586
6	4.290086	-3.469918	-4.008872
1	5.131613	-3.646584	-4.687772
1	4.139064	-4.372313	-3.409883
1	3.387275	-3.306863	-4.599801
6	5.710480	-2.642411	-2.112869
1	5.412831	-3.521563	-1.535337
1	6.641816	-2.870541	-2.640797
1	5.873518	-1.827405	-1.406515
6	6.238153	-0.504677	-4.023948
1	6.759618	-1.233707	-4.653251
1	6.281479	0.468905	-4.521945
1	6.763419	-0.420393	-3.071504
6	3.997247	-0.796783	-5.124068
1	4.036020	0.240314	-5.471573
1	4.412642	-1.437249	-5.907888
1	2.948514	-1.065763	-4.970300
6	6.939755	0.693094	0.084316
1	7.817314	1.119404	0.580027
1	7.273744	-0.122436	-0.562896
1	6.478364	1.457534	-0.546331
6	6.552514	-0.951050	1.949093
1	7.029431	-1.695043	1.303993
1	7.315474	-0.536076	2.616495
1	5.797593	-1.460754	2.549811
6	4.519689	0.755455	3.179844
1	5.260896	0.496761	3.942587
1	3.872657	1.541891	3.580145
1	3.894971	-0.116138	2.967634
6	6.005485	2.521311	2.171059
1	5.395767	3.248716	2.715265
1	6.880392	2.283036	2.785644
1	6.343706	2.990308	1.245228
6	0.814826	-4.772907	0.883804
1	0.979773	-5.468915	1.713287
1	-0.209778	-4.399753	0.941154
1	0.922632	-5.325301	-0.054149
6	3.239704	-4.147608	0.617157
1	3.551563	-4.923098	1.324129
1	3.245033	-4.563931	-0.393237
1	3.960449	-3.325991	0.640515
6	0.354133	-2.593086	2.780837

1	0.344032	-1.816719	3.549493
1	-0.355650	-2.303139	2.001533
1	-0.003190	-3.516097	3.244103
6	2.753374	-3.108954	3.308547
1	2.648003	-2.413804	4.146807
1	2.557967	-4.120977	3.678913
1	3.783632	-3.057998	2.951531
1	-0.227364	2.173219	-2.285849
1	1.237587	-0.426882	-2.040618

TS1-para-agg (Refer to Table S3)

Number of imaginary frequencies : 1

Imaginary frequency : -813.8796 cm(-1)

Electronic energy : HF=-3396.5034323
 Zero-point correction= 1.455072 (Hartree/Particle)
 Thermal correction to Energy= 1.535424
 Thermal correction to Enthalpy= 1.536368
 Thermal correction to Gibbs Free Energy= 1.333771
 Sum of electronic and zero-point Energies= -3395.048360
 Sum of electronic and thermal Energies= -3394.968008
 Sum of electronic and thermal Enthalpies= -3394.967064
 Sum of electronic and thermal Free Energies= -3395.169661

Cartesian Coordinates

77	-1.947028	0.146550	-0.835359
5	-3.733100	-0.788640	-0.193039
8	-3.918722	-2.159577	-0.369918
8	-4.793188	-0.250848	0.527622
6	-4.944806	-2.592043	0.558724
6	-5.788748	-1.281259	0.737609
5	-1.896439	0.745282	1.117244
8	-2.115380	-0.153772	2.172526
8	-1.585531	1.998549	1.629579
6	-1.777405	0.500745	3.422795
6	-1.924547	2.012899	3.036009
5	-3.373493	1.627758	-1.137954
8	-3.588599	2.772997	-0.392106
8	-4.264668	1.582521	-2.217260
6	-4.817369	3.396872	-0.824557
6	-4.976508	2.841313	-2.287647
6	-1.698426	-2.209731	-2.845914
6	-0.992516	-2.673334	-1.631303
7	-2.138899	-0.928833	-2.839197
7	-1.004811	-1.848269	-0.556574
6	-1.917135	-3.040809	-3.953350
6	-2.573620	-2.537976	-5.070791
6	-3.008052	-1.213106	-5.057335
6	-2.777041	-0.447933	-3.918232
6	-0.331427	-3.904881	-1.565079
6	0.275828	-4.299424	-0.381555
6	0.229172	-3.462184	0.741777
6	-0.414133	-2.227105	0.584329
6	0.825020	0.205225	-2.326021
6	0.145023	0.756123	-1.224119
6	2.216511	0.091216	-2.341405
6	0.927665	1.329353	-0.205412
6	2.972814	0.562583	-1.260868

6	2.313785	1.213482	-0.212296
1	2.714131	-0.400679	-3.174541
1	2.884472	1.607641	0.617526
1	0.440697	1.828520	0.624564
1	-3.136182	0.569266	-3.824825
1	-3.527889	-0.777394	-5.903739
1	-2.749308	-3.173612	-5.933245
1	-1.593904	-4.074203	-3.938054
1	-0.282399	-4.551541	-2.432597
1	0.781983	-5.257593	-0.316386
1	-0.509655	-1.538517	1.412779
6	4.427299	0.234050	-1.115545
8	4.792240	-0.458006	-0.149161
7	5.308087	0.660259	-2.067590
6	0.706499	-3.925873	2.068526
6	0.197496	-5.150688	2.534877
6	1.602117	-3.194247	2.887007
6	0.519011	-5.645283	3.793080
1	-0.494408	-5.695472	1.898454
6	1.919947	-3.702064	4.161591
6	1.377962	-4.902554	4.605764
1	0.096911	-6.583912	4.138078
1	2.587749	-3.136687	4.794954
1	1.641493	-5.263881	5.595805
7	2.209328	-2.027123	2.400023
6	2.787014	-1.020449	3.192090
8	2.596828	-0.934702	4.404785
7	3.547923	-0.136439	2.489467
1	2.211207	-1.883751	1.399409
1	3.880616	-0.361080	1.551548
6	6.706440	0.223461	-1.975910
1	6.889625	-0.083057	-0.944323
1	7.349102	1.083357	-2.190196
6	5.007781	1.742270	-3.012124
1	5.406452	1.467314	-3.995613
1	3.925680	1.812316	-3.110972
6	4.140007	1.009321	3.181154
6	5.259249	1.621963	2.328092
6	3.075782	2.065094	3.539615
1	4.573476	0.648835	4.124517
6	5.883858	2.841389	3.020503
1	4.847051	1.934691	1.362455
1	6.016033	0.861947	2.104609
6	3.705474	3.277606	4.237043
1	2.573192	2.392942	2.619379
1	2.319022	1.596805	4.173836
6	4.820850	3.891981	3.378265
1	6.652927	3.280087	2.372881
1	6.393910	2.517380	3.938481
1	2.934700	4.025136	4.458397
1	4.124041	2.963376	5.203612
1	5.283502	4.741872	3.894166
1	4.381051	4.286230	2.450687
6	7.029026	-0.929885	-2.936013
6	6.205531	-2.194848	-2.664532
1	8.100602	-1.144928	-2.840488
1	6.872165	-0.604258	-3.974277
6	6.528729	-3.364378	-3.608149
1	6.341118	-2.496501	-1.619631
1	5.141123	-1.950410	-2.762685
6	7.977386	-3.880425	-3.551434

1	5.851139	-4.196932	-3.374156
1	6.299532	-3.064828	-4.640491
1	8.078475	-4.706721	-4.266680
1	8.665863	-3.099850	-3.900193
6	5.559294	3.113535	-2.568884
6	5.304779	3.404301	-1.082395
1	5.078690	3.870787	-3.200234
1	6.634488	3.188339	-2.775784
6	5.442373	4.884134	-0.693599
1	4.303847	3.052697	-0.812364
1	5.999923	2.802353	-0.486139
6	4.254105	5.763894	-1.121827
1	5.551049	4.955414	0.396721
1	6.371565	5.286537	-1.120106
1	4.506069	6.813111	-0.922256
1	4.108268	5.692929	-2.208153
6	8.412035	-4.359951	-2.161827
1	9.417512	-4.792510	-2.188587
1	8.425896	-3.540283	-1.435876
1	7.728039	-5.126182	-1.778439
6	2.940950	5.418970	-0.405829
1	2.140337	6.106481	-0.697156
1	2.596466	4.404879	-0.633869
1	3.059148	5.488734	0.682104
6	-4.651814	4.911484	-0.725797
1	-5.535552	5.426929	-1.117416
1	-4.527611	5.195197	0.323056
1	-3.771391	5.255806	-1.270946
6	-5.921095	2.922748	0.129274
1	-5.651738	3.217906	1.146670
1	-6.890597	3.366291	-0.118245
1	-5.994518	1.834663	0.112776
6	-6.412358	2.557008	-2.719509
1	-7.015601	3.470821	-2.698755
1	-6.421246	2.165761	-3.741565
1	-6.875675	1.813024	-2.069596
6	-4.259933	3.696711	-3.340629
1	-4.252259	3.155644	-4.291845
1	-4.758897	4.658016	-3.495982
1	-3.223314	3.882809	-3.046345
6	-6.858722	-1.103492	-0.347131
1	-7.673047	-1.826115	-0.236528
1	-7.280015	-0.097325	-0.271155
1	-6.418779	-1.211539	-1.342078
6	-6.392148	-1.085223	2.125065
1	-6.938890	-0.138104	2.157782
1	-7.091082	-1.893500	2.366184
1	-5.613731	-1.051532	2.889031
6	-4.217720	-3.018978	1.841902
1	-4.912241	-3.399169	2.597536
1	-3.508383	-3.814155	1.593172
1	-3.650463	-2.181827	2.256677
6	-5.695817	-3.769795	-0.053009
1	-5.018938	-4.623559	-0.153358
1	-6.532889	-4.072129	0.585667
1	-6.081035	-3.526137	-1.044849
6	-0.972273	2.960607	3.758478
1	-1.142671	2.934164	4.840102
1	0.070706	2.703024	3.563843
1	-1.140042	3.983791	3.409764
6	-3.371220	2.516750	3.129172

1	-3.696934	2.632307	4.167941
1	-3.432507	3.485027	2.626417
1	-4.047652	1.831351	2.611657
6	-0.339109	0.105247	3.765129
1	-0.259444	-0.982100	3.838676
1	0.349396	0.441592	2.985711
1	-0.008134	0.523490	4.718818
6	-2.739092	0.007887	4.499389
1	-2.572797	-1.058540	4.678903
1	-2.574808	0.541378	5.441728
1	-3.778415	0.143514	4.194702
1	0.260560	-0.201836	-3.158944
1	-1.317585	1.565239	-1.305610

TS1-para-aag (Refer to Table S3)

Number of imaginary frequencies : 1
Imaginary frequency: -828.2067 cm(-1)

Electronic energy : HF=-3396.5118664
Zero-point correction= 1.455948 (Hartree/Particle)
Thermal correction to Energy= 1.535697
Thermal correction to Enthalpy= 1.536641
Thermal correction to Gibbs Free Energy= 1.340424
Sum of electronic and zero-point Energies= -3395.055919
Sum of electronic and thermal Energies= -3394.976170
Sum of electronic and thermal Enthalpies= -3394.975225
Sum of electronic and thermal Free Energies= -3395.171443

Cartesian Coordinates

77	1.921019	-0.338011	-0.722417
5	3.620871	0.648123	0.062222
8	3.817674	2.011125	-0.156294
8	4.608833	0.151800	0.905843
6	4.760200	2.491081	0.835896
6	5.584890	1.194038	1.147371
5	1.641414	-0.790200	1.249628
8	1.740466	0.190538	2.248248
8	1.285441	-2.005209	1.820325
6	1.290657	-0.375161	3.506465
6	1.488205	-1.909643	3.250510
5	3.368931	-1.830234	-0.754941
8	3.494012	-2.922231	0.084840
8	4.377242	-1.852392	-1.726581
6	4.760591	-3.569927	-0.165369
6	5.084388	-3.112910	-1.634945
6	1.922840	1.853058	-2.928953
6	1.074389	2.402434	-1.848781
7	2.352443	0.577940	-2.773686
7	0.966357	1.673367	-0.711824
6	2.279246	2.600492	-4.060141
6	3.061621	2.017141	-5.050325
6	3.480536	0.697322	-4.887680
6	3.110525	0.018936	-3.730296
6	0.396843	3.620675	-1.971635
6	-0.351719	4.102828	-0.908369
6	-0.424437	3.371609	0.286581
6	0.248365	2.142351	0.318264
6	-0.655532	-0.460783	-2.491004

6	-0.114530	-0.984435	-1.302313
6	-2.030765	-0.304664	-2.656868
6	-1.018350	-1.519220	-0.363935
6	-2.915230	-0.726318	-1.654163
6	-2.392721	-1.377011	-0.528636
1	-2.416959	0.204314	-3.536641
1	-3.065765	-1.732449	0.241438
1	-0.635116	-1.995297	0.531760
1	3.448285	-0.987860	-3.519736
1	4.093683	0.200306	-5.631648
1	3.344759	2.587604	-5.929611
1	1.965544	3.632200	-4.159837
1	0.441620	4.185730	-2.894362
1	-0.879217	5.046935	-0.992111
1	0.262785	1.533380	1.212724
6	-4.340037	-0.284212	-1.648029
8	-4.814060	0.215766	-0.612174
7	-5.067767	-0.321984	-2.807071
6	-1.068751	3.951565	1.490737
6	-0.671163	5.249277	1.859808
6	-2.038674	3.280187	2.274859
6	-1.178359	5.878025	2.990207
1	0.079980	5.748643	1.254281
6	-2.546514	3.925242	3.419123
6	-2.115171	5.198250	3.771667
1	-0.840309	6.872734	3.263019
1	-3.276951	3.409247	4.025117
1	-2.526477	5.665784	4.661791
7	-2.539920	2.033882	1.871419
6	-3.163227	1.097926	2.719346
8	-3.100093	1.167043	3.945823
7	-3.809140	0.104550	2.051510
1	-2.412777	1.767330	0.904605
1	-4.060466	0.222587	1.068382
6	-6.325729	0.442202	-2.841660
1	-6.772545	0.425645	-1.844552
1	-7.011836	-0.065410	-3.525586
6	-4.877015	-1.364291	-3.824557
1	-5.179425	-0.951080	-4.792885
1	-3.815490	-1.602750	-3.893274
6	-4.481129	-0.951881	2.806931
6	-5.550718	-1.636073	1.942913
6	-3.475944	-1.982467	3.352041
1	-4.974971	-0.485471	3.670705
6	-6.269251	-2.735479	2.738537
1	-5.075354	-2.085658	1.060833
1	-6.258497	-0.891502	1.563030
6	-4.187394	-3.090427	4.139867
1	-2.926022	-2.420608	2.507143
1	-2.749077	-1.462336	3.980878
6	-5.274143	-3.767904	3.291557
1	-7.017585	-3.226334	2.104596
1	-6.818212	-2.278056	3.573619
1	-3.458372	-3.829604	4.492100
1	-4.649087	-2.653495	5.036753
1	-5.802431	-4.528951	3.878373
1	-4.798708	-4.291173	2.450796
6	-6.100499	1.894705	-3.298023
6	-5.121852	2.673403	-2.408849
1	-7.076917	2.398542	-3.308445
1	-5.737235	1.897409	-4.335423

6	-4.987269	4.155226	-2.772704
1	-5.429347	2.566990	-1.364636
1	-4.130423	2.206548	-2.475704
6	-3.853024	4.859699	-2.008062
1	-4.805603	4.253763	-3.852361
1	-5.938215	4.669968	-2.573809
1	-2.898034	4.393527	-2.288913
1	-3.794167	5.904695	-2.339800
6	-5.659006	-2.652581	-3.511981
6	-5.265116	-3.271465	-2.164834
1	-5.463812	-3.366733	-4.323642
1	-6.738910	-2.453701	-3.529046
6	-5.888678	-4.646803	-1.908510
1	-4.172385	-3.344157	-2.113952
1	-5.561724	-2.594027	-1.353660
6	-5.605025	-5.192168	-0.499004
1	-6.975506	-4.584703	-2.057653
1	-5.516197	-5.359990	-2.657827
1	-6.052921	-4.517177	0.242831
1	-6.116408	-6.156047	-0.382536
6	-4.003293	4.818703	-0.481628
1	-3.219116	5.396414	0.017642
1	-4.969457	5.233591	-0.171425
1	-3.944421	3.797461	-0.093273
6	-4.113627	-5.369698	-0.185914
1	-3.969493	-5.854920	0.784723
1	-3.622947	-5.991227	-0.944393
1	-3.585544	-4.411102	-0.153247
6	4.577073	-5.075004	0.016065
1	5.497074	-5.613974	-0.235490
1	4.331640	-5.286626	1.060522
1	3.763045	-5.457678	-0.601898
6	5.753876	-3.030003	0.871560
1	5.371121	-3.255535	1.870235
1	6.742487	-3.487492	0.765143
1	5.834322	-1.945421	0.789591
6	6.560968	-2.858228	-1.922671
1	7.150820	-3.768667	-1.772569
1	6.686480	-2.538103	-2.961690
1	6.955191	-2.071333	-1.277859
6	4.482851	-4.037478	-2.701187
1	4.586965	-3.564133	-3.682393
1	4.987906	-5.007562	-2.732715
1	3.418193	-4.202267	-2.513630
6	6.739340	0.965561	0.162693
1	7.544437	1.693333	0.303340
1	7.149740	-0.035477	0.320948
1	6.381263	1.024333	-0.868475
6	6.074144	1.066794	2.586644
1	6.616346	0.124424	2.708810
1	6.751717	1.888100	2.843871
1	5.237437	1.066991	3.287018
6	3.926636	2.975008	2.030655
1	4.554625	3.391417	2.824502
1	3.242535	3.756375	1.685962
1	3.323469	2.157372	2.432907
6	5.561430	3.641211	0.235479
1	4.897792	4.489570	0.043480
1	6.345289	3.971595	0.925702
1	6.024336	3.353491	-0.710161
6	0.480624	-2.816143	3.949721

1	0.548893	-2.706869	5.037415
1	-0.541338	-2.590007	3.640387
1	0.689391	-3.859557	3.696047
6	2.923649	-2.378458	3.523440
1	3.146455	-2.397271	4.595109
1	3.043646	-3.385430	3.116341
1	3.641105	-1.728115	3.016348
6	-0.175416	0.023788	3.679012
1	-0.269715	1.112070	3.654410
1	-0.783380	-0.386029	2.868619
1	-0.592074	-0.318850	4.629437
6	2.141886	0.209833	4.629058
1	1.942813	1.281705	4.722069
1	1.901929	-0.265228	5.586207
1	3.206352	0.076989	4.427154
1	0.005831	-0.089623	-3.266473
1	1.346307	-1.789937	-1.162402

TS1-para-gag (Refer to Table S3)

Number of imaginary frequencies : 1
Imaginary frequency : -815.3260 cm(-1)

Electronic energy : HF=-3396.5146776
Zero-point correction= 1.456173 (Hartree/Particle)
Thermal correction to Energy= 1.535775
Thermal correction to Enthalpy= 1.536720
Thermal correction to Gibbs Free Energy= 1.340467
Sum of electronic and zero-point Energies= -3395.058505
Sum of electronic and thermal Energies= -3394.978902
Sum of electronic and thermal Enthalpies= -3394.977958
Sum of electronic and thermal Free Energies= -3395.174211

Cartesian Coordinates

77	1.939625	-0.343593	-0.687526
5	3.595633	0.755603	0.037053
8	3.757607	2.100120	-0.293806
8	4.579542	0.362078	0.937751
6	4.663190	2.690254	0.673023
6	5.519220	1.450692	1.107954
5	1.650095	-0.661356	1.309084
8	1.706606	0.385777	2.240371
8	1.321581	-1.846160	1.955081
6	1.262248	-0.110534	3.530356
6	1.506795	-1.651835	3.377240
5	3.438703	-1.781806	-0.592215
8	3.585318	-2.808247	0.323384
8	4.464854	-1.836477	-1.543564
6	4.876909	-3.428068	0.139099
6	5.213422	-3.061161	-1.352902
6	1.870171	1.669081	-3.058746
6	0.970643	2.251433	-2.039555
7	2.365713	0.436331	-2.798089
7	0.903998	1.626952	-0.838821
6	2.211418	2.349817	-4.235723
6	3.047876	1.739810	-5.163635
6	3.536057	0.462302	-4.892379
6	3.177500	-0.147673	-3.693879
6	0.203405	3.395277	-2.282738

6	-0.584236	3.924059	-1.271486
6	-0.603234	3.317220	-0.006843
6	0.151558	2.143819	0.142658
6	-0.606720	-0.689868	-2.478931
6	-0.069854	-1.082911	-1.239188
6	-1.981943	-0.554135	-2.666056
6	-0.976011	-1.521875	-0.255271
6	-2.869409	-0.865240	-1.625807
6	-2.348287	-1.393666	-0.437361
1	-2.363211	-0.139372	-3.595953
1	-3.021725	-1.663731	0.364620
1	-0.597470	-1.906781	0.684873
1	3.567075	-1.114125	-3.399811
1	4.194264	-0.052653	-5.583813
1	3.320315	2.258383	-6.077751
1	1.845443	3.352907	-4.416772
1	0.208263	3.864209	-3.259051
1	-1.183452	4.809603	-1.450765
1	0.197800	1.621607	1.089632
6	-4.295623	-0.428967	-1.656376
8	-4.764087	0.159285	-0.663595
7	-5.032942	-0.576073	-2.797772
6	-1.278563	3.976886	1.138677
6	-0.977813	5.333376	1.357959
6	-2.175870	3.322170	2.019134
6	-1.505567	6.037480	2.433476
1	-0.282059	5.822101	0.681736
6	-2.697122	4.039816	3.112951
6	-2.359942	5.372774	3.315866
1	-1.242298	7.078826	2.589583
1	-3.363104	3.533095	3.796518
1	-2.780040	5.897867	4.169062
7	-2.588053	2.011092	1.751538
6	-3.233760	1.150534	2.658301
8	-3.177639	1.297686	3.878084
7	-3.888049	0.128698	2.045266
1	-2.489883	1.678273	0.802183
1	-4.118696	0.195479	1.052848
6	-6.276028	0.200992	-2.918149
1	-6.689075	0.350227	-1.919654
1	-6.997269	-0.392046	-3.487152
6	-4.824705	-1.670790	-3.753773
1	-5.037574	-1.291272	-4.759775
1	-3.775297	-1.959563	-3.737413
6	-4.535801	-0.914223	2.835372
6	-5.595311	-1.631470	1.985947
6	-3.509190	-1.915486	3.397129
1	-5.032674	-0.434089	3.689667
6	-6.282146	-2.747403	2.785909
1	-5.114199	-2.068833	1.100939
1	-6.324627	-0.905621	1.609616
6	-4.196421	-3.030393	4.196902
1	-2.948523	-2.354055	2.559568
1	-2.792878	-1.369906	4.017674
6	-5.259329	-3.746230	3.349804
1	-7.012058	-3.264489	2.151552
1	-6.846954	-2.301506	3.616674
1	-3.450423	-3.745421	4.563021
1	-4.675282	-2.594412	5.085223
1	-5.767808	-4.517262	3.941007
1	-4.766479	-4.263495	2.515127

6	-6.044778	1.546644	-3.631564
6	-5.064872	2.503615	-2.930141
1	-7.021344	2.036861	-3.746414
1	-5.680565	1.339574	-4.646846
6	-5.562961	3.055865	-1.585942
1	-4.107574	1.988295	-2.775778
1	-4.849597	3.333430	-3.614933
6	-4.486786	3.814810	-0.794639
1	-6.426855	3.713889	-1.760318
1	-5.909748	2.224598	-0.966875
1	-4.860117	4.021238	0.215489
1	-3.621179	3.153973	-0.660972
6	-5.707806	-2.898718	-3.455736
6	-5.475925	-3.535482	-2.075817
1	-5.519989	-3.641158	-4.243307
1	-6.763039	-2.614668	-3.550430
6	-4.119922	-4.240430	-1.923152
1	-5.581941	-2.767672	-1.297523
1	-6.282454	-4.254863	-1.893334
6	-3.842311	-4.763102	-0.504706
1	-4.070478	-5.076292	-2.636194
1	-3.311382	-3.552660	-2.193728
1	-2.832041	-5.189857	-0.481495
1	-3.822975	-3.914040	0.190324
6	-4.028774	5.129808	-1.434025
1	-3.317424	5.650649	-0.783956
1	-3.544561	4.963583	-2.403135
1	-4.878154	5.802334	-1.602644
6	-4.846746	-5.807548	-0.005116
1	-4.547968	-6.207881	0.969067
1	-5.849883	-5.384074	0.111281
1	-4.920131	-6.649808	-0.703564
6	4.739334	-4.922924	0.418228
1	5.680658	-5.445697	0.216617
1	4.483448	-5.073455	1.470746
1	3.948944	-5.372476	-0.185099
6	5.832734	-2.787398	1.153728
1	5.441813	-2.963382	2.159154
1	6.838395	-3.214914	1.091174
1	5.877390	-1.707868	1.004127
6	6.685539	-2.773206	-1.631993
1	7.304172	-3.649097	-1.409492
1	6.820230	-2.520117	-2.688220
1	7.039013	-1.930336	-1.036187
6	4.665802	-4.077560	-2.363571
1	4.771227	-3.667692	-3.372789
1	5.205865	-5.028212	-2.321081
1	3.604406	-4.268800	-2.182609
6	6.699674	1.176364	0.166551
1	7.480684	1.937134	0.260742
1	7.134980	0.204677	0.415082
1	6.361398	1.139006	-0.872337
6	5.983703	1.460695	2.560879
1	6.548827	0.548032	2.772204
1	6.633848	2.320144	2.757167
1	5.134737	1.497314	3.245292
6	3.788910	3.243534	1.807613
1	4.386664	3.742821	2.576637
1	3.089530	3.972040	1.386505
1	3.202356	2.442243	2.264331
6	5.442045	3.812692	-0.004464

1	4.756903	4.620187	-0.279161
1	6.199131	4.224179	0.671845
1	5.935035	3.464360	-0.913898
6	0.518816	-2.540931	4.125219
1	0.569488	-2.357509	5.203807
1	-0.505665	-2.368633	3.790205
1	0.762668	-3.591841	3.944163
6	2.952361	-2.061070	3.689618
1	3.166714	-2.010659	4.761986
1	3.103880	-3.086293	3.343367
1	3.655573	-1.422092	3.149232
6	-0.216760	0.252971	3.666576
1	-0.344513	1.333922	3.573080
1	-0.803812	-0.224031	2.877770
1	-0.632337	-0.043670	4.632775
6	2.085703	0.572138	4.617971
1	1.856650	1.641878	4.635897
1	1.848445	0.156940	5.603242
1	3.155596	0.455855	4.435482
1	0.058468	-0.397510	-3.284484
1	1.413249	-1.842639	-1.016663

TS1-para-gaa (Refer to Table S3)

Number of imaginary frequencies : 1
Imaginary frequency : -813.8816 cm(-1)

Electronic energy : HF=-3396.5188278
Zero-point correction= 1.455546 (Hartree/Particle)
Thermal correction to Energy= 1.535345
Thermal correction to Enthalpy= 1.536290
Thermal correction to Gibbs Free Energy= 1.338186
Sum of electronic and zero-point Energies= -3395.063282
Sum of electronic and thermal Energies= -3394.983482
Sum of electronic and thermal Enthalpies= -3394.982538
Sum of electronic and thermal Free Energies= -3395.180641

Cartesian Coordinates

77	1.884496	-0.369920	-0.639803
5	3.554499	0.821039	-0.125834
8	3.718650	2.095805	-0.665233
8	4.545702	0.566734	0.815804
6	4.637384	2.825153	0.188359
6	5.491445	1.663461	0.807999
5	1.630396	-0.358641	1.387644
8	1.684873	0.830185	2.131379
8	1.318499	-1.420935	2.225961
6	1.244671	0.555572	3.486771
6	1.499747	-0.987911	3.595171
5	3.382834	-1.781908	-0.346852
8	3.534924	-2.651507	0.717827
8	4.392692	-1.998311	-1.292832
6	4.818944	-3.304869	0.615863
6	5.130354	-3.188081	-0.920627
6	1.741496	1.227791	-3.302756
6	0.863674	1.967359	-2.369546
7	2.260248	0.060797	-2.851911
7	0.831404	1.544655	-1.082178
6	2.039893	1.700706	-4.588246

6	2.858715	0.949271	-5.423469
6	3.372584	-0.258678	-4.953584
6	3.055058	-0.659748	-3.659383
6	0.082962	3.055394	-2.775021
6	-0.685911	3.737280	-1.843101
6	-0.673156	3.337265	-0.499558
6	0.094937	2.208623	-0.180394
6	-0.685310	-1.061798	-2.310951
6	-0.126180	-1.204041	-1.027596
6	-2.066297	-1.019071	-2.503315
6	-1.011162	-1.470880	0.033724
6	-2.935437	-1.165276	-1.413157
6	-2.387792	-1.425359	-0.151206
1	-2.468336	-0.814132	-3.492463
1	-3.044551	-1.562155	0.696082
1	-0.614442	-1.663762	1.023814
1	3.463991	-1.559974	-3.217767
1	4.018921	-0.877511	-5.566614
1	3.097756	1.306868	-6.420319
1	1.653103	2.653823	-4.926736
1	0.062988	3.362297	-3.813542
1	-1.295102	4.583127	-2.145070
1	0.166131	1.849737	0.838182
6	-4.387257	-0.834282	-1.512789
8	-4.876232	-0.046551	-0.680970
7	-5.129967	-1.312247	-2.554516
6	-1.328487	4.160513	0.547540
6	-0.986967	5.523790	0.590541
6	-2.248215	3.650958	1.495932
6	-1.495586	6.375295	1.564090
1	-0.278024	5.899622	-0.141963
6	-2.751018	4.518048	2.484544
6	-2.372289	5.854776	2.518459
1	-1.202376	7.420102	1.586740
1	-3.438163	4.125491	3.220092
1	-2.779717	6.497450	3.293749
7	-2.707033	2.330708	1.390585
6	-3.315186	1.595288	2.424115
8	-3.232145	1.916701	3.608795
7	-3.971364	0.487799	1.986791
1	-2.612753	1.873870	0.493628
1	-4.207918	0.379158	0.999830
6	-6.419007	-0.666984	-2.838994
1	-6.783912	-0.222027	-1.913358
1	-7.136050	-1.436544	-3.140091
6	-4.819977	-2.547814	-3.284091
1	-5.099172	-2.399941	-4.333488
1	-3.744852	-2.715926	-3.262801
6	-4.555680	-0.443055	2.950069
6	-5.578796	-1.353615	2.255588
6	-3.470130	-1.273589	3.661079
1	-5.074159	0.146924	3.718617
6	-6.194145	-2.349927	3.249621
1	-5.082439	-1.910930	1.450495
1	-6.352213	-0.745548	1.773464
6	-4.086924	-2.267172	4.653928
1	-2.888487	-1.820835	2.906173
1	-2.784058	-0.589757	4.167158
6	-5.112714	-3.177610	3.962378
1	-6.897245	-3.008807	2.726310
1	-6.779092	-1.798631	3.999211

1	-3.298271	-2.864847	5.125869
1	-4.583306	-1.709829	5.460884
1	-5.573283	-3.859530	4.687234
1	-4.595518	-3.805278	3.222866
6	-6.293526	0.391168	-3.953560
6	-5.248866	1.486821	-3.685389
1	-7.284013	0.841882	-4.102361
1	-6.041870	-0.118119	-4.893531
6	-5.576095	2.439391	-2.526616
1	-4.279596	1.008511	-3.493713
1	-5.111798	2.072047	-4.604453
6	-4.377610	3.307890	-2.124900
1	-6.422806	3.082173	-2.806931
1	-5.886507	1.864663	-1.649093
1	-3.548260	2.645362	-1.839710
1	-4.023675	3.877828	-2.996503
6	-5.549873	-3.779536	-2.713150
6	-5.188757	-4.110211	-1.256828
1	-5.311547	-4.634686	-3.360112
1	-6.633273	-3.626758	-2.794060
6	-3.745930	-4.589565	-1.046360
1	-5.374554	-3.226339	-0.632119
1	-5.878730	-4.880831	-0.889461
6	-3.397454	-4.800318	0.432134
1	-3.587096	-5.525836	-1.600484
1	-3.041932	-3.861328	-1.463936
1	-3.628605	-3.880147	0.983930
1	-4.046852	-5.579037	0.855590
6	-4.689445	4.261992	-0.968189
1	-3.826398	4.881578	-0.706724
1	-5.520730	4.929749	-1.222299
1	-4.971680	3.701813	-0.070381
6	-1.925720	-5.159789	0.654541
1	-1.706944	-5.313200	1.716324
1	-1.656727	-6.078686	0.120562
1	-1.273887	-4.356977	0.292770
6	4.677262	-4.732542	1.138407
1	5.612618	-5.288920	1.012856
1	4.436025	-4.705432	2.204688
1	3.875344	-5.269282	0.628718
6	5.796334	-2.514470	1.495167
1	5.417872	-2.511723	2.520595
1	6.796586	-2.958914	1.493193
1	5.849963	-1.476815	1.163523
6	6.600352	-2.971903	-1.268179
1	7.211085	-3.811176	-0.918849
1	6.717047	-2.893436	-2.353493
1	6.977565	-2.050924	-0.821017
6	4.549829	-4.344646	-1.744805
1	4.640684	-4.103766	-2.808498
1	5.077874	-5.284820	-1.559262
1	3.489699	-4.487081	-1.517408
6	6.664559	1.239768	-0.084600
1	7.447370	2.003685	-0.117345
1	7.100335	0.318716	0.312083
1	6.318802	1.038939	-1.102013
6	5.962088	1.896617	2.240300
1	6.519526	1.022678	2.590328
1	6.620344	2.770005	2.300410
1	5.114828	2.046766	2.911351
6	3.777828	3.557050	1.228000

1	4.386559	4.166778	1.902996
1	3.078870	4.215123	0.702983
1	3.191639	2.841295	1.809857
6	5.417049	3.819224	-0.665556
1	4.733917	4.575127	-1.064321
1	6.179504	4.330589	-0.068039
1	5.904231	3.325973	-1.508728
6	0.515736	-1.745151	4.481216
1	0.560812	-1.380517	5.513044
1	-0.508714	-1.639941	4.119379
1	0.767911	-2.809621	4.481881
6	2.947283	-1.329909	3.973100
1	3.157407	-1.102269	5.023037
1	3.106072	-2.397194	3.800662
1	3.648372	-0.783020	3.337115
6	-0.236915	0.928096	3.563912
1	-0.371355	1.979001	3.296541
1	-0.823084	0.326369	2.865070
1	-0.649138	0.789452	4.566215
6	2.063748	1.418008	4.442038
1	1.835335	2.474035	4.269796
1	1.820962	1.182834	5.483757
1	3.134612	1.272195	4.288798
1	-0.037743	-0.904011	-3.167209
1	1.364081	-1.903024	-0.701414

TS1-para-gga (Refer to Table S3)

Number of imaginary frequencies : 1
Imaginary frequency : -810.4849 cm(-1)

Electronic energy : HF=-3396.5100086
Zero-point correction= 1.455397 (Hartree/Particle)
Thermal correction to Energy= 1.535462
Thermal correction to Enthalpy= 1.536406
Thermal correction to Gibbs Free Energy= 1.335980
Sum of electronic and zero-point Energies= -3395.054611
Sum of electronic and thermal Energies= -3394.974547
Sum of electronic and thermal Enthalpies= -3394.973603
Sum of electronic and thermal Free Energies= -3395.174029

Cartesian Coordinates

77	1.904122	-0.461342	-0.645511
5	3.588255	0.738407	-0.200347
8	3.720491	2.010252	-0.755940
8	4.617933	0.499181	0.702046
6	4.656881	2.755552	0.063405
6	5.547809	1.608770	0.656545
5	1.736192	-0.485297	1.391129
8	1.833755	0.690105	2.150817
8	1.453333	-1.559724	2.224356
6	1.459818	0.395206	3.521467
6	1.705308	-1.152292	3.590642
5	3.431656	-1.855942	-0.435576
8	3.646188	-2.730738	0.613793
8	4.397923	-2.050691	-1.430279
6	4.931320	-3.367839	0.444981
6	5.170137	-3.231825	-1.103617
6	1.650097	1.188599	-3.269220

6	0.817700	1.915220	-2.285217
7	2.186953	0.014072	-2.861935
7	0.827649	1.463035	-1.007390
6	1.890353	1.681174	-4.559651
6	2.670287	0.943160	-5.442684
6	3.205065	-0.271461	-5.015480
6	2.945259	-0.693004	-3.714943
6	0.042537	3.026444	-2.633476
6	-0.672061	3.702343	-1.655175
6	-0.616774	3.270655	-0.322505
6	0.137304	2.116475	-0.062264
6	-0.715778	-1.101707	-2.229246
6	-0.116622	-1.289598	-0.970534
6	-2.097062	-0.974028	-2.362265
6	-0.970993	-1.566008	0.113918
6	-2.929719	-1.091817	-1.239555
6	-2.350389	-1.447807	-0.013563
1	-2.522220	-0.709717	-3.326352
1	-2.979728	-1.578102	0.856315
1	-0.543141	-1.803842	1.081266
1	3.373411	-1.599877	-3.306279
1	3.823284	-0.880123	-5.666506
1	2.863751	1.316339	-6.443713
1	1.489215	2.638976	-4.866513
1	-0.011689	3.360692	-3.662213
1	-1.267274	4.572081	-1.913699
1	0.239561	1.729871	0.943359
6	-4.328533	-0.572861	-1.264480
8	-4.706936	0.180643	-0.346788
7	-5.121620	-0.807113	-2.352435
6	-1.203681	4.090615	0.767579
6	-0.829937	5.445569	0.813249
6	-2.078959	3.585628	1.760037
6	-1.263059	6.290998	1.827615
1	-0.153036	5.818738	0.049712
6	-2.508627	4.447577	2.787058
6	-2.097901	5.774857	2.821016
1	-0.943736	7.328155	1.850710
1	-3.161465	4.056383	3.554105
1	-2.446288	6.413405	3.627895
7	-2.560473	2.272855	1.670419
6	-3.106510	1.526204	2.732247
8	-2.956860	1.831821	3.914161
7	-3.781712	0.425826	2.310010
1	-2.548730	1.832370	0.760072
1	-4.060526	0.352128	1.330966
6	-6.255637	0.091357	-2.589281
1	-6.329683	0.730087	-1.710282
1	-7.184293	-0.486733	-2.645958
6	-4.993505	-2.005131	-3.186169
1	-4.888199	-1.712893	-4.238684
1	-4.071728	-2.509884	-2.900093
6	-4.344165	-0.523124	3.264854
6	-5.414541	-1.378011	2.568794
6	-3.249102	-1.405877	3.893527
1	-4.817468	0.046629	4.076701
6	-6.005262	-2.422547	3.525691
1	-4.964681	-1.896521	1.711969
1	-6.196704	-0.729564	2.158010
6	-3.845533	-2.449888	4.846524
1	-2.699221	-1.914063	3.089026

1	-2.537341	-0.758363	4.412719
6	-4.906209	-3.305498	4.137251
1	-6.740953	-3.038343	2.994111
1	-6.548784	-1.911571	4.332937
1	-3.049460	-3.083291	5.255079
1	-4.308336	-1.937336	5.701846
1	-5.343795	-4.031843	4.832534
1	-4.424357	-3.884723	3.335768
6	-6.091629	0.940171	-3.864279
6	-4.733270	1.652884	-4.017143
1	-6.906387	1.674790	-3.862891
1	-6.254760	0.315488	-4.752119
6	-4.236736	2.467716	-2.809617
1	-3.969194	0.903027	-4.257652
1	-4.798815	2.308911	-4.895694
6	-5.187595	3.558669	-2.304736
1	-4.016352	1.799563	-1.973586
1	-3.276062	2.928297	-3.078932
1	-5.365049	4.296954	-3.099343
1	-6.166450	3.120033	-2.072866
6	-6.173892	-2.983075	-3.031860
6	-6.562094	-3.304050	-1.577155
1	-5.896897	-3.901174	-3.564204
1	-7.055950	-2.592409	-3.553560
6	-5.426440	-3.790615	-0.662874
1	-7.003032	-2.408073	-1.122756
1	-7.358525	-4.059407	-1.599220
6	-4.667188	-5.033709	-1.140092
1	-4.700353	-2.985970	-0.512016
1	-5.848163	-3.991804	0.331331
1	-5.367368	-5.871715	-1.261646
1	-4.235702	-4.849863	-2.132927
6	-4.645069	4.250012	-1.047984
1	-5.324123	5.028439	-0.685714
1	-4.503089	3.526348	-0.237651
1	-3.673519	4.721101	-1.236596
6	-3.543573	-5.417730	-0.170608
1	-3.001114	-6.306254	-0.509273
1	-2.821040	-4.599351	-0.071795
1	-3.942167	-5.629210	0.828753
6	4.829886	-4.802458	0.957803
1	5.764473	-5.346944	0.783411
1	4.637803	-4.789448	2.034302
1	4.011283	-5.342958	0.479607
6	5.939117	-2.575492	1.287253
1	5.610075	-2.591448	2.329460
1	6.943730	-3.006263	1.231666
1	5.963266	-1.533059	0.967398
6	6.619135	-2.989606	-1.516023
1	7.257652	-3.822967	-1.204253
1	6.684418	-2.898843	-2.604708
1	7.003484	-2.067470	-1.077411
6	4.570194	-4.389580	-1.911953
1	4.610440	-4.138269	-2.976344
1	5.119166	-5.323491	-1.758456
1	3.523252	-4.549074	-1.639305
6	6.694687	1.197480	-0.275241
1	7.465356	1.971821	-0.338459
1	7.156813	0.284374	0.109730
1	6.316450	0.987687	-1.279194
6	6.065013	1.855355	2.070379

1	6.650712	0.993166	2.402904
1	6.708682	2.741002	2.103871
1	5.239501	1.992296	2.770618
6	3.821321	3.477024	1.130295
1	4.441990	4.100799	1.781167
1	3.091932	4.119480	0.627789
1	3.269403	2.753548	1.736093
6	5.390704	3.759352	-0.819103
1	4.682126	4.503914	-1.194127
1	6.166149	4.283828	-0.250253
1	5.854426	3.272352	-1.679074
6	0.758923	-1.915684	4.511535
1	0.853341	-1.563714	5.544443
1	-0.280249	-1.800423	4.198265
1	1.004483	-2.981452	4.488137
6	3.166115	-1.514020	3.891043
1	3.429297	-1.311537	4.934288
1	3.306575	-2.578490	3.688071
1	3.841178	-0.959571	3.233970
6	-0.011933	0.779413	3.679665
1	-0.148558	1.836524	3.439533
1	-0.637942	0.196616	2.999478
1	-0.375421	0.625680	4.698469
6	2.333650	1.233525	4.449472
1	2.109074	2.294481	4.304310
1	2.137301	0.984718	5.497825
1	3.394439	1.079038	4.243881
1	-0.095357	-0.954230	-3.106801
1	1.394997	-1.998426	-0.709520

TS1-meta_{AI} (Refer to Figure S8)

Number of imaginary frequencies : 1
Imaginary frequency : -802.6137 cm(-1)

Electronic energy : HF=-3396.5581536
Zero-point correction= 1.453902 (Hartree/Particle)
Thermal correction to Energy= 1.534553
Thermal correction to Enthalpy= 1.535497
Thermal correction to Gibbs Free Energy= 1.335420
Sum of electronic and zero-point Energies= -3395.104251
Sum of electronic and thermal Energies= -3395.023601
Sum of electronic and thermal Enthalpies= -3395.022657
Sum of electronic and thermal Free Energies= -3395.222734

Cartesian Coordinates

77	-0.789159	-1.394226	-0.367273
5	-2.284824	-0.624677	0.924148
8	-2.148991	-0.758771	2.307553
8	-3.486611	0.018301	0.630582
6	-3.211730	-0.022980	2.958172
6	-4.301330	0.029126	1.834103
5	-1.693305	0.025282	-1.582798
8	-1.250653	1.366969	-1.706624
8	-2.727134	-0.201496	-2.471932
6	-1.746592	1.846202	-2.999492
6	-3.079697	1.041352	-3.121733
5	-2.244273	-2.702335	-0.957233
8	-2.413434	-3.215469	-2.240709

8	-3.165249	-3.305552	-0.085954
6	-3.675568	-3.919248	-2.291788
6	-3.860697	-4.360281	-0.797770
6	0.788028	-1.809784	2.260236
6	1.247497	-0.481364	1.800146
7	-0.096515	-2.452518	1.459658
7	0.778945	-0.074543	0.598907
6	1.228439	-2.394465	3.454084
6	0.753088	-3.647611	3.823994
6	-0.161628	-4.293268	2.994050
6	-0.562795	-3.656327	1.825101
6	2.126403	0.332892	2.527422
6	2.513572	1.564339	2.012547
6	2.030939	1.977668	0.763400
6	1.180201	1.095098	0.094076
6	0.846420	-2.424653	-1.490466
6	0.781886	-3.788166	-1.829584
6	2.070268	-1.770722	-1.695903
6	1.910367	-4.475746	-2.285995
6	3.210266	-2.452025	-2.136614
6	3.133193	-3.817703	-2.431262
1	-0.421405	-1.458483	-1.935616
1	2.157898	-0.706859	-1.504388
1	4.011760	-4.352257	-2.782392
1	1.833618	-5.531083	-2.537705
1	-0.165978	-4.310306	-1.754335
1	-1.304051	-4.089681	1.167140
1	-0.567872	-5.267445	3.243110
1	1.090364	-4.106774	4.747870
1	1.938584	-1.881969	4.089134
1	2.490302	0.025211	3.499282
1	3.170964	2.213984	2.581805
1	0.793925	1.321103	-0.891079
6	4.461069	-1.635065	-2.329015
8	4.516356	-0.789031	-3.225694
7	5.500338	-1.822707	-1.455303
6	2.380345	3.287811	0.172986
6	3.731142	3.660838	0.086048
6	1.384490	4.193880	-0.267332
6	4.107603	4.904392	-0.411849
1	4.488808	2.952320	0.407664
6	1.776442	5.442486	-0.772904
6	3.121287	5.796440	-0.838534
1	5.157898	5.171564	-0.467676
1	1.009182	6.136364	-1.091012
1	3.398372	6.769895	-1.232844
7	0.008999	3.872858	-0.169585
6	-0.940640	4.754704	0.335811
8	-0.673540	5.895475	0.710486
7	-2.214718	4.245444	0.364497
1	-0.314233	2.973622	-0.507648
1	-2.380282	3.274866	0.131730
6	5.456658	-2.718084	-0.298953
1	6.385826	-3.303130	-0.280262
1	4.640729	-3.426368	-0.441187
6	6.658508	-0.931861	-1.597631
1	7.489091	-1.377042	-1.039072
1	6.940256	-0.906804	-2.654766
6	-3.344729	5.081876	0.766001
6	-4.603199	4.696090	-0.025218
6	-3.586275	5.041175	2.285415

1	-3.070032	6.109105	0.503166
6	-5.812025	5.545917	0.394950
1	-4.831520	3.636115	0.143237
1	-4.408004	4.810102	-1.097582
6	-4.796162	5.896783	2.686121
1	-3.753720	4.002172	2.592766
1	-2.677309	5.383077	2.791205
6	-6.053157	5.476631	1.910269
1	-6.703620	5.217971	-0.152301
1	-5.633603	6.591538	0.107516
1	-4.967642	5.823083	3.766564
1	-4.578695	6.953376	2.475094
1	-6.904315	6.110227	2.187273
1	-6.322370	4.446973	2.186807
6	5.270042	-2.004803	1.046840
6	5.030485	-3.000899	2.187150
1	4.417571	-1.318660	0.968352
1	6.150804	-1.389762	1.270430
6	4.925744	-2.328677	3.559517
1	4.104792	-3.557661	1.984261
1	5.838826	-3.745771	2.206167
6	4.571019	-3.297806	4.692276
1	5.870880	-1.819230	3.794733
1	4.165290	-1.538487	3.507685
1	3.654982	-3.840645	4.423935
1	5.358718	-4.057978	4.781324
6	6.393669	0.502909	-1.117136
6	7.603664	1.420197	-1.318584
1	6.109260	0.489843	-0.057818
1	5.537132	0.892296	-1.676264
6	7.328667	2.869122	-0.899683
1	8.463406	1.031921	-0.752826
1	7.899898	1.402438	-2.376750
6	8.524628	3.806975	-1.099695
1	6.469404	3.249298	-1.468624
1	7.027037	2.891028	0.158209
1	9.375140	3.443645	-0.506467
1	8.844595	3.765805	-2.149818
6	4.377357	-2.598510	6.040299
1	4.124676	-3.310875	6.833160
1	5.286572	-2.068803	6.347948
1	3.569536	-1.856770	5.993989
6	8.216384	5.257561	-0.718559
1	9.090359	5.904538	-0.852399
1	7.408474	5.665558	-1.337612
1	7.904320	5.336297	0.329918
6	-3.561653	-5.061643	-3.295734
1	-4.476518	-5.664206	-3.311086
1	-3.408601	-4.654040	-4.299606
1	-2.716307	-5.714856	-3.069834
6	-4.733341	-2.907494	-2.750459
1	-4.427698	-2.494541	-3.715108
1	-5.718406	-3.371527	-2.864162
1	-4.802672	-2.075130	-2.046439
6	-5.305471	-4.413188	-0.311223
1	-5.884917	-5.140958	-0.889664
1	-5.334713	-4.718398	0.739671
1	-5.790878	-3.439351	-0.389911
6	-3.144766	-5.675032	-0.464577
1	-3.143888	-5.816183	0.621075
1	-3.641448	-6.538631	-0.917524

1	-2.106040	-5.653053	-0.807175
6	-5.181260	-1.224929	1.786337
1	-5.861622	-1.276345	2.642384
1	-5.781812	-1.194941	0.872631
1	-4.568817	-2.127999	1.749175
6	-5.166100	1.282383	1.837386
1	-5.878351	1.249666	1.007248
1	-5.735527	1.362115	2.769770
1	-4.561304	2.181191	1.727922
6	-2.640654	1.354540	3.314791
1	-3.353830	1.963391	3.878648
1	-1.746466	1.216607	3.930142
1	-2.344267	1.902958	2.416202
6	-3.621142	-0.773936	4.220375
1	-2.795769	-0.768283	4.939575
1	-4.487433	-0.302259	4.696920
1	-3.867039	-1.814032	3.998190
6	-3.517313	0.737550	-4.550022
1	-3.681068	1.662274	-5.114004
1	-2.775468	0.131995	-5.074195
1	-4.458202	0.179301	-4.537446
6	-4.230243	1.665385	-2.324178
1	-4.589903	2.591254	-2.783126
1	-5.059420	0.953581	-2.285490
1	-3.923994	1.862066	-1.295252
6	-0.701360	1.441203	-4.046766
1	0.267421	1.865911	-3.767141
1	-0.590854	0.354484	-4.100076
1	-0.962351	1.813856	-5.041563
6	-1.902964	3.359641	-2.979026
1	-0.926245	3.842323	-2.882488
1	-2.352683	3.698118	-3.918390
1	-2.529219	3.700667	-2.155722

TS2-meta-aaa (Refer to Table S4)

Number of imaginary frequencies : 1

Imaginary frequency : -173.0392 cm(-1)

Electronic energy : HF=-3396.5788599

Zero-point correction= 1.456098 (Hartree/Particle)

Thermal correction to Energy= 1.536082

Thermal correction to Enthalpy= 1.537027

Thermal correction to Gibbs Free Energy= 1.336130

Sum of electronic and zero-point Energies= -3395.122762

Sum of electronic and thermal Energies= -3395.042778

Sum of electronic and thermal Enthalpies= -3395.041833

Sum of electronic and thermal Free Energies= -3395.242730

Cartesian Coordinates

77	1.734035	-0.172912	0.531197
6	1.868183	-1.579331	3.254947
6	0.842170	-2.344787	2.512146
7	2.511929	-0.603363	2.565777
7	0.610319	-1.962112	1.235737
6	2.186709	-1.843070	4.592905
6	3.172604	-1.093773	5.225524
6	3.828935	-0.097754	4.504378
6	3.468613	0.112394	3.176854
6	0.154300	-3.442595	3.041972

6	-0.695605	-4.180002	2.229027
6	-0.863402	-3.836828	0.877402
6	-0.204420	-2.673977	0.450304
5	2.817057	-1.693177	-0.438571
8	3.268238	-2.803179	0.270655
8	2.972446	-1.889676	-1.801966
6	3.894710	-3.729517	-0.654156
6	3.278224	-3.290181	-2.033628
5	3.472536	0.648405	-0.225350
8	3.676846	1.378186	-1.392398
8	4.698421	0.449870	0.428063
6	5.101227	1.450676	-1.652669
6	5.705698	1.265639	-0.216152
6	0.084637	0.969590	1.552609
6	0.090543	1.247017	2.932266
6	-1.166033	0.757284	0.950262
6	-1.089232	1.280373	3.679809
6	-2.353661	0.778634	1.686240
6	-2.317287	1.037420	3.063692
5	1.440571	1.938367	0.517043
8	0.749424	2.652638	-0.472102
8	2.180709	2.833807	1.318388
6	1.107220	4.049146	-0.392106
6	1.685529	4.172314	1.068331
1	1.085757	-0.004688	-0.892031
1	-0.292872	-2.318090	-0.566220
1	-1.218243	-5.039119	2.637212
1	0.291259	-3.737134	4.075235
1	1.668537	-2.622019	5.138235
1	3.423650	-1.287745	6.263761
1	4.606446	0.510588	4.953612
1	3.944711	0.863926	2.562603
1	1.035463	1.451463	3.424417
1	-1.052087	1.493023	4.745350
1	-3.237580	1.040527	3.641515
1	-1.208127	0.559058	-0.114743
6	-1.568411	-4.732591	-0.073432
6	-2.353074	-4.264792	-1.156174
6	-1.366563	-6.120422	0.056791
6	-2.861072	-5.183337	-2.088018
6	-1.883882	-7.023803	-0.865067
1	-0.746400	-6.486299	0.869782
6	-2.623685	-6.546401	-1.950003
1	-3.439767	-4.804155	-2.920257
1	-1.694389	-8.086703	-0.749460
1	-3.024997	-7.237005	-2.686209
6	-3.616068	0.404279	0.974188
7	-4.649690	1.280878	0.924445
6	-5.865752	0.852836	0.211435
1	-6.410679	1.753291	-0.085159
6	-4.531468	2.703668	1.275093
1	-3.802261	2.818660	2.076641
1	-5.498322	3.031397	1.672770
8	-3.695613	-0.712009	0.420685
7	-2.644955	-2.898047	-1.291216
1	-2.785542	-2.350015	-0.447442
6	-2.477131	-2.191774	-2.488352
8	-2.135400	-2.725241	-3.542633
1	-5.571946	0.323607	-0.699917
6	-0.145265	4.885401	-0.645890
1	0.053061	5.950557	-0.484829

1	-0.469585	4.758646	-1.682193
1	-0.966472	4.579448	0.003935
6	0.606175	4.480982	2.115982
1	1.031098	4.350572	3.115792
1	0.245987	5.511055	2.029708
1	-0.245309	3.804586	2.025297
6	2.150848	4.316460	-1.478272
1	3.024268	3.688584	-1.316227
1	1.730697	4.042690	-2.449764
1	2.447170	5.369982	-1.512511
6	2.836406	5.162352	1.222831
1	2.501432	6.182719	1.007072
1	3.207710	5.139718	2.252439
1	3.670005	4.928267	0.560114
6	5.430338	2.780664	-2.324980
1	4.898464	2.850984	-3.278471
1	5.141431	3.639279	-1.717726
1	6.504349	2.850450	-2.529408
6	5.785652	2.573002	0.579513
1	4.815373	3.073563	0.583824
1	6.044655	2.340804	1.617447
1	6.545465	3.254348	0.184256
6	5.437606	0.294955	-2.602010
1	5.164330	-0.659897	-2.153118
1	4.845081	0.402731	-3.514800
1	6.497798	0.283628	-2.873946
6	7.039038	0.527913	-0.164653
1	7.810418	1.074946	-0.717485
1	7.371506	0.432475	0.873966
1	6.957187	-0.477399	-0.581232
6	5.406148	-3.498554	-0.561670
1	5.966203	-4.194991	-1.193565
1	5.662333	-2.476464	-0.849978
1	5.724810	-3.639583	0.475447
6	3.550775	-5.151673	-0.220588
1	3.940361	-5.884452	-0.935384
1	4.001265	-5.358552	0.755407
1	2.472030	-5.293396	-0.129247
6	1.949487	-3.987224	-2.352003
1	1.463564	-3.474271	-3.186558
1	2.096303	-5.035509	-2.629445
1	1.264973	-3.952620	-1.501265
6	4.219028	-3.395899	-3.229837
1	4.507533	-4.437901	-3.405192
1	3.711535	-3.029457	-4.127228
1	5.124265	-2.802398	-3.092060
6	-4.118748	3.564803	0.075970
1	-3.170854	3.177709	-0.316414
1	-4.858054	3.455700	-0.728041
6	-3.951818	5.044493	0.434515
1	-4.862242	5.418358	0.924272
1	-3.143653	5.144811	1.172959
6	-3.635950	5.912863	-0.788983
1	-4.491727	5.894068	-1.478599
1	-2.795735	5.469039	-1.337515
6	-3.293151	7.365163	-0.440248
1	-2.451944	7.376020	0.266566
1	-4.140647	7.825165	0.086394
6	-2.934522	8.200646	-1.671801
1	-2.698698	9.236335	-1.403358
1	-2.061729	7.783799	-2.188299

1	-3.762145	8.223346	-2.390844
6	-6.751446	-0.049493	1.075191
1	-6.158271	-0.917381	1.383189
1	-7.032418	0.490326	1.989542
6	-8.008085	-0.517484	0.334056
1	-8.592434	0.355664	0.009206
1	-7.710716	-1.045308	-0.582730
6	-8.895779	-1.435831	1.181450
1	-8.306785	-2.303624	1.510516
1	-9.196638	-0.907355	2.097660
6	-10.148708	-1.924834	0.445232
1	-9.847114	-2.457190	-0.467054
1	-10.735281	-1.057492	0.112148
6	-11.028406	-2.837769	1.303359
1	-11.917632	-3.170408	0.756714
1	-10.480040	-3.732767	1.620560
1	-11.369084	-2.322216	2.209348
7	-2.714396	-0.853930	-2.349347
1	-2.968331	-0.523749	-1.425270
6	-2.210839	0.123759	-3.313304
6	-2.746816	1.506894	-2.918736
6	-0.671791	0.129106	-3.373063
1	-2.598243	-0.145569	-4.304472
6	-2.204651	2.614353	-3.832361
1	-2.429341	1.716081	-1.887334
1	-3.843980	1.495903	-2.921763
6	-0.137848	1.228588	-4.299243
1	-0.281158	0.297747	-2.362016
1	-0.323566	-0.857646	-3.691746
6	-0.668738	2.602420	-3.866894
1	-2.576927	3.588018	-3.489469
1	-2.595465	2.470212	-4.849709
1	0.957883	1.220948	-4.279224
1	-0.442154	1.023029	-5.336312
1	-0.298185	3.390855	-4.534431
1	-0.284108	2.814582	-2.862206

TS2-*meta*-gag (Refer to Table S4)

Number of imaginary frequencies : 1
Imaginary frequency : -170.0903 cm(-1)

Electronic energy : HF=-3396.5781268
Zero-point correction= 1.457100 (Hartree/Particle)
Thermal correction to Energy= 1.536460
Thermal correction to Enthalpy= 1.537404
Thermal correction to Gibbs Free Energy= 1.340599
Sum of electronic and zero-point Energies= -3395.121027
Sum of electronic and thermal Energies= -3395.041667
Sum of electronic and thermal Enthalpies= -3395.040723
Sum of electronic and thermal Free Energies= -3395.237528

Cartesian Coordinates

77	1.578360	-0.381316	0.425048
6	1.596707	-1.265538	3.365795
6	0.365329	-1.883459	2.823782
7	2.408184	-0.649542	2.469876
7	0.113708	-1.680786	1.510557
6	1.930655	-1.308968	4.725349

6	3.111388	-0.718398	5.162374
6	3.941467	-0.099580	4.229149
6	3.551181	-0.088203	2.893715
6	-0.493532	-2.688400	3.580352
6	-1.556938	-3.331501	2.962352
6	-1.770264	-3.187861	1.581584
6	-0.907162	-2.305138	0.913376
5	2.153316	-2.254569	-0.338147
8	2.268230	-3.348429	0.516418
8	2.257530	-2.660314	-1.660886
6	2.635788	-4.514053	-0.264672
6	2.153634	-4.108712	-1.702517
5	3.400480	-0.188944	-0.527854
8	3.698837	0.323290	-1.785377
8	4.576131	-0.643479	0.090618
6	5.076924	0.009076	-2.106242
6	5.711808	-0.189572	-0.684047
6	0.388894	1.301152	1.351335
6	0.630113	1.839782	2.628303
6	-0.942538	1.287234	0.912237
6	-0.410860	2.307041	3.436229
6	-1.998155	1.724110	1.718543
6	-1.733461	2.239124	2.993887
5	1.808902	1.690407	0.007431
8	1.162776	2.391049	-1.019222
8	2.854005	2.472621	0.536093
6	1.845739	3.640498	-1.258905
6	2.698492	3.830088	0.057757
1	0.859907	-0.267780	-0.970633
1	-1.004151	-2.118548	-0.146707
1	-2.214582	-3.966012	3.547872
1	-0.323627	-2.838333	4.639477
1	1.270942	-1.786915	5.438863
1	3.376050	-0.741231	6.214999
1	4.873167	0.372525	4.521501
1	4.150988	0.375002	2.122657
1	1.650426	1.901417	2.992177
1	-0.192078	2.714183	4.420275
1	-2.547944	2.563495	3.635551
1	-1.169841	0.902442	-0.075474
6	-2.750420	-4.036527	0.855829
6	-3.530973	-3.579839	-0.234134
6	-2.845902	-5.392573	1.223843
6	-4.336114	-4.488545	-0.938364
6	-3.653440	-6.284392	0.526382
1	-2.232881	-5.757606	2.042287
6	-4.392334	-5.827564	-0.567988
1	-4.910009	-4.121887	-1.779789
1	-3.691255	-7.328449	0.822149
1	-5.021342	-6.512613	-1.129241
6	-3.367839	1.484432	1.167469
7	-4.238795	2.507038	0.988947
6	-5.505072	2.172205	0.311984
1	-5.935239	3.104938	-0.061367
6	-3.852802	3.920678	1.110607
1	-3.232130	4.044004	1.996395
1	-4.767700	4.496736	1.283046
8	-3.672840	0.324902	0.817103
7	-3.525602	-2.224116	-0.596151
1	-3.437189	-1.531605	0.142052
6	-3.368159	-1.776399	-1.910872

8	-3.276724	-2.530764	-2.876750
1	-5.276181	1.549219	-0.557138
6	0.801123	4.732891	-1.487426
1	1.277075	5.713465	-1.591814
1	0.245836	4.531688	-2.407679
1	0.083275	4.779840	-0.667783
6	1.962157	4.617334	1.150013
1	2.531913	4.549697	2.081912
1	1.860382	5.675077	0.889465
1	0.970068	4.203039	1.337390
6	2.696964	3.455117	-2.518305
1	3.388217	2.624376	-2.384227
1	2.039677	3.202231	-3.354966
1	3.249369	4.363757	-2.779558
6	4.082440	4.435353	-0.159848
1	4.004323	5.455778	-0.550518
1	4.620380	4.479564	0.792570
1	4.678184	3.844739	-0.857065
6	5.679665	1.150312	-2.920067
1	5.150266	1.246008	-3.872675
1	5.612281	2.106814	-2.399262
1	6.734511	0.950162	-3.137759
6	6.183079	1.119643	-0.040568
1	5.372424	1.851175	-0.034049
1	6.466199	0.921709	0.998521
1	7.052359	1.544758	-0.551783
6	5.053372	-1.274221	-2.943058
1	4.598454	-2.089327	-2.379790
1	4.431445	-1.105796	-3.826656
1	6.054965	-1.567564	-3.273225
6	6.809909	-1.245396	-0.610509
1	7.660975	-0.968770	-1.242351
1	7.168551	-1.336155	0.419550
1	6.448307	-2.225809	-0.925358
6	4.157271	-4.656921	-0.155072
1	4.526104	-5.543194	-0.680880
1	4.657037	-3.770598	-0.554569
1	4.430806	-4.741806	0.900777
6	1.939661	-5.734671	0.329300
1	2.118378	-6.624947	-0.283176
1	2.331164	-5.929978	1.332734
1	0.861866	-5.580601	0.413427
6	0.677325	-4.436263	-1.959270
1	0.353236	-3.935450	-2.875561
1	0.510336	-5.511280	-2.076569
1	0.044227	-4.076560	-1.144338
6	3.012250	-4.633334	-2.848571
1	2.992042	-5.728068	-2.877685
1	2.620753	-4.261856	-3.800381
1	4.050354	-4.307516	-2.765147
6	-3.114052	4.432387	-0.133146
1	-2.196559	3.842767	-0.252044
1	-3.729993	4.232840	-1.018793
6	-2.763034	5.925972	-0.076489
1	-2.253884	6.185385	-1.011819
1	-3.686778	6.522027	-0.056081
6	-1.884248	6.325310	1.119386
1	-1.015316	5.655476	1.175869
1	-2.445064	6.170927	2.049805
6	-1.402670	7.785246	1.079773
1	-0.954028	8.035052	2.049839

1	-2.272383	8.447654	0.967377
6	-0.383991	8.085178	-0.025381
1	-0.068914	9.134179	0.003426
1	0.512388	7.466034	0.090590
1	-0.789394	7.894097	-1.024432
6	-6.504686	1.444589	1.231223
1	-5.943361	0.842092	1.952135
1	-7.070339	2.186595	1.807556
6	-7.455455	0.522033	0.448194
1	-8.323887	0.288000	1.075286
1	-7.850652	1.056748	-0.428813
6	-6.772566	-0.780400	-0.001930
1	-5.823603	-0.546634	-0.492900
1	-6.503060	-1.362280	0.890905
6	-7.612446	-1.656342	-0.941441
1	-7.001730	-2.514137	-1.251123
1	-7.834538	-1.093657	-1.859132
6	-8.919385	-2.168216	-0.327425
1	-9.445449	-2.840072	-1.014965
1	-8.727672	-2.725284	0.598102
1	-9.604878	-1.349087	-0.083443
7	-3.326160	-0.408265	-1.999756
1	-3.296431	0.092238	-1.117550
6	-2.691656	0.245784	-3.145152
6	-2.951176	1.755607	-3.049478
6	-1.182154	-0.053332	-3.205322
1	-3.164764	-0.147264	-4.052930
6	-2.244044	2.527755	-4.172345
1	-2.570943	2.114431	-2.081926
1	-4.031601	1.946451	-3.059672
6	-0.484263	0.712703	-4.335088
1	-0.728221	0.238908	-2.250469
1	-1.036104	-1.132451	-3.314037
6	-0.739384	2.219871	-4.197928
1	-2.415275	3.603992	-4.044348
1	-2.689649	2.251322	-5.138401
1	0.591183	0.503958	-4.305589
1	-0.854896	0.360185	-5.308855
1	-0.253130	2.772477	-5.011699
1	-0.285219	2.555892	-3.257889

TS2-meta-gaa (Refer to Table S4)

Number of imaginary frequencies : 1
Imaginary frequency : -154.3743 cm(-1)

Electronic energy : HF=-3396.5821186
Zero-point correction= 1.457941 (Hartree/Particle)
Thermal correction to Energy= 1.536964
Thermal correction to Enthalpy= 1.537908
Thermal correction to Gibbs Free Energy= 1.344258
Sum of electronic and zero-point Energies= -3395.124177
Sum of electronic and thermal Energies= -3395.045155
Sum of electronic and thermal Enthalpies= -3395.044210
Sum of electronic and thermal Free Energies= -3395.237860

Cartesian Coordinates

77	1.542351	-0.400335	0.392647
6	1.641065	-1.100255	3.382969

6	0.361039	-1.690415	2.932079
7	2.438466	-0.575870	2.418717
7	0.066706	-1.570760	1.617275
6	2.034099	-1.085665	4.727304
6	3.258843	-0.529894	5.079941
6	4.072551	-0.003304	4.078458
6	3.623060	-0.046396	2.762653
6	-0.503705	-2.392647	3.779114
6	-1.613670	-3.034108	3.249160
6	-1.868974	-2.990135	1.869088
6	-1.001384	-2.193107	1.105747
5	2.003511	-2.338711	-0.285307
8	2.088763	-3.396010	0.617237
8	2.057121	-2.810996	-1.589787
6	2.385720	-4.612612	-0.115378
6	1.888019	-4.253381	-1.560114
5	3.337186	-0.354467	-0.631315
8	3.612985	0.071540	-1.925663
8	4.511616	-0.828537	-0.027260
6	4.963242	-0.323462	-2.274667
6	5.638982	-0.479610	-0.865530
6	0.459843	1.382896	1.255890
6	0.778695	2.004280	2.476970
6	-0.890140	1.387553	0.876940
6	-0.208587	2.559610	3.296720
6	-1.892656	1.914587	1.697271
6	-1.552548	2.503496	2.921696
5	1.851689	1.625269	-0.169705
8	1.189197	2.289620	-1.208028
8	2.955366	2.385651	0.261049
6	1.923163	3.478362	-1.571329
6	2.857724	3.710349	-0.316969
1	0.777756	-0.343580	-0.983859
1	-1.134526	-2.080375	0.038576
1	-2.275422	-3.593261	3.902668
1	-0.302937	-2.464697	4.840978
1	1.387507	-1.495877	5.492826
1	3.570076	-0.509158	6.119733
1	5.036881	0.439486	4.303055
1	4.208279	0.346730	1.943765
1	1.816765	2.057395	2.788487
1	0.068601	3.028057	4.237842
1	-2.324874	2.900157	3.574752
1	-1.173740	0.948437	-0.072846
6	-2.893480	-3.867716	1.246046
6	-3.715192	-3.474700	0.161035
6	-2.981387	-5.195610	1.707081
6	-4.542651	-4.425628	-0.457421
6	-3.817135	-6.126619	1.100028
1	-2.339132	-5.509147	2.524789
6	-4.588387	-5.737378	0.002202
1	-5.141605	-4.115297	-1.301822
1	-3.849308	-7.148519	1.465538
1	-5.236264	-6.454139	-0.494389
6	-3.291593	1.711443	1.205561
7	-4.095467	2.772365	0.947942
6	-5.366892	2.476250	0.262960
1	-5.734396	3.411038	-0.168034
6	-3.618260	4.163384	0.971153
1	-2.982524	4.304044	1.843408
1	-4.491360	4.809250	1.109587

8	-3.676355	0.548641	0.960602
7	-3.721485	-2.140778	-0.275030
1	-3.540846	-1.416757	0.413908
6	-3.646314	-1.759939	-1.619159
8	-3.693872	-2.556555	-2.554390
1	-5.154665	1.797894	-0.567042
6	0.921580	4.605607	-1.821566
1	1.436632	5.548174	-2.036372
1	0.296892	4.360983	-2.685204
1	0.265321	4.752415	-0.963883
6	2.232090	4.626104	0.743203
1	2.858276	4.615271	1.640763
1	2.157971	5.659156	0.391101
1	1.237875	4.278356	1.027773
6	2.688077	3.159678	-2.858936
1	3.337660	2.299209	-2.706364
1	1.969206	2.892341	-3.638441
1	3.273773	4.014606	-3.211867
6	4.261080	4.206991	-0.652407
1	4.220700	5.197379	-1.118464
1	4.854064	4.289811	0.264098
1	4.779586	3.528703	-1.330836
6	5.589121	0.744532	-3.166874
1	5.029211	0.818640	-4.103854
1	5.587995	1.728341	-2.695035
1	6.624098	0.481221	-3.411342
6	6.205229	0.833929	-0.313583
1	5.437416	1.610172	-0.320135
1	6.517006	0.676910	0.724292
1	7.076591	1.178713	-0.878697
6	4.851906	-1.644543	-3.042226
1	4.377383	-2.405959	-2.423190
1	4.210650	-1.491217	-3.914675
1	5.827379	-2.002593	-3.386362
6	6.682237	-1.588141	-0.771550
1	7.522092	-1.391647	-1.446738
1	7.073986	-1.642912	0.248975
1	6.258718	-2.563135	-1.018617
6	3.901745	-4.817206	-0.032316
1	4.219084	-5.745467	-0.517712
1	4.429481	-3.976720	-0.490513
1	4.196992	-4.858300	1.020254
6	1.651635	-5.772885	0.549297
1	1.776116	-6.696073	-0.026912
1	2.058960	-5.942368	1.551131
1	0.584058	-5.567442	0.651021
6	0.392690	-4.523967	-1.769195
1	0.072711	-4.057977	-2.705142
1	0.172164	-5.594230	-1.824103
1	-0.203354	-4.090071	-0.962664
6	2.692592	-4.871506	-2.698983
1	2.608691	-5.963455	-2.683212
1	2.303382	-4.515736	-3.657718
1	3.749684	-4.605649	-2.649463
6	-2.857184	4.543229	-0.305993
1	-2.014394	3.850487	-0.417789
1	-3.509329	4.386687	-1.173834
6	-2.325965	5.983502	-0.301444
1	-1.780568	6.145475	-1.240067
1	-3.163775	6.694645	-0.308796
6	-1.396707	6.297089	0.881571

1	-0.715619	5.451546	1.045291
1	-1.983881	6.390909	1.805004
6	-0.569584	7.572181	0.687068
1	-1.240969	8.416835	0.479090
1	0.059495	7.455872	-0.205936
6	0.308374	7.898534	1.897779
1	0.908913	8.799353	1.730242
1	-0.301370	8.067656	2.793574
1	0.996725	7.074857	2.120189
6	-6.429967	1.855625	1.183934
1	-5.935482	1.176396	1.884336
1	-6.900760	2.648337	1.778296
6	-7.487375	1.071707	0.388838
1	-8.355958	0.880787	1.032773
1	-7.858193	1.691711	-0.441061
6	-6.967598	-0.266360	-0.159525
1	-6.064964	-0.110726	-0.761265
1	-6.652347	-0.899303	0.681333
6	-7.998651	-1.019708	-1.006567
1	-8.293370	-0.393296	-1.860358
1	-8.912543	-1.180840	-0.417086
6	-7.470714	-2.364144	-1.515471
1	-8.217657	-2.887468	-2.123351
1	-6.573351	-2.231019	-2.130245
1	-7.202631	-3.019896	-0.679505
7	-3.512121	-0.405027	-1.772998
1	-3.403435	0.130688	-0.917964
6	-2.929089	0.167289	-2.987260
6	-3.017366	1.696791	-2.885863
6	-1.471247	-0.290809	-3.186215
1	-3.526497	-0.175310	-3.840906
6	-2.339254	2.393527	-4.073217
1	-2.514365	2.012389	-1.960692
1	-4.067561	2.001707	-2.799411
6	-0.802698	0.406122	-4.377241
1	-0.904197	-0.060111	-2.275248
1	-1.454408	-1.378112	-3.307905
6	-0.882714	1.931292	-4.227257
1	-2.386691	3.481234	-3.937261
1	-2.896303	2.168283	-4.993939
1	0.242907	0.085420	-4.446844
1	-1.295709	0.099919	-5.311714
1	-0.415286	2.429772	-5.085872
1	-0.315340	2.218480	-3.333500

TS2-meta-gga (Refer to Table S4)

Number of imaginary frequencies : 1
Imaginary frequency : -179.8395 cm(-1)

Electronic energy : HF=-3396.5836309
Zero-point correction= 1.458211 (Hartree/Particle)
Thermal correction to Energy= 1.537094
Thermal correction to Enthalpy= 1.538038
Thermal correction to Gibbs Free Energy= 1.344466
Sum of electronic and zero-point Energies= -3395.125419
Sum of electronic and thermal Energies= -3395.046537
Sum of electronic and thermal Enthalpies= -3395.045593
Sum of electronic and thermal Free Energies= -3395.239165

Cartesian Coordinates

77	1.574719	-0.132219	0.376819
6	1.638882	-0.769899	3.380176
6	0.506764	-1.580517	2.878680
7	2.387827	-0.135010	2.443612
7	0.250691	-1.504201	1.553084
6	1.950281	-0.664481	4.741482
6	3.046620	0.093387	5.138644
6	3.816237	0.727958	4.164932
6	3.450798	0.587967	2.829603
6	-0.245367	-2.442990	3.684359
6	-1.191499	-3.276642	3.103698
6	-1.392464	-3.262634	1.714121
6	-0.659672	-2.306971	0.993391
5	2.381015	-1.988311	-0.201802
8	2.644664	-2.960472	0.760023
8	2.530414	-2.515898	-1.477190
6	3.167613	-4.140677	0.098626
6	2.625387	-3.961590	-1.364162
5	3.381672	0.178835	-0.575011
8	3.650747	0.633823	-1.860700
8	4.584190	-0.118288	0.085189
6	5.055792	0.427057	-2.148982
6	5.687447	0.375737	-0.710886
6	0.190213	1.489662	1.139968
6	0.342525	2.165313	2.364417
6	-1.123976	1.258828	0.703463
6	-0.760729	2.549498	3.132353
6	-2.238566	1.604685	1.475853
6	-2.057090	2.252828	2.704669
5	1.610339	1.919156	-0.183206
8	0.930227	2.484532	-1.267332
8	2.579967	2.819725	0.299519
6	1.502065	3.769794	-1.588087
6	2.344241	4.118896	-0.294229
1	0.872760	-0.209070	-1.031116
1	-0.764644	-2.208904	-0.078267
1	-1.760935	-3.960334	3.725237
1	-0.075785	-2.490569	4.753141
1	1.337705	-1.159726	5.484692
1	3.294032	0.185405	6.191718
1	4.682671	1.326147	4.425585
1	4.007107	1.056502	2.029359
1	1.341671	2.395617	2.718769
1	-0.610965	3.070203	4.074764
1	-2.911445	2.505914	3.326110
1	-1.283211	0.762170	-0.246771
6	-2.200058	-4.303382	1.028730
6	-3.003898	-4.044181	-0.108190
6	-2.074363	-5.634082	1.471516
6	-3.602621	-5.114733	-0.790980
6	-2.684514	-6.687697	0.799097
1	-1.442114	-5.844077	2.329218
6	-3.438031	-6.422584	-0.347335
1	-4.193152	-4.897396	-1.670830
1	-2.554969	-7.706204	1.152380
1	-3.909452	-7.234955	-0.893002
6	-3.560363	1.123387	0.955201
7	-4.528376	2.003033	0.610603
6	-5.734748	1.472657	-0.043572

1	-6.143037	2.265142	-0.678683
6	-4.417781	3.459989	0.753604
1	-3.875662	3.690659	1.668251
1	-5.433421	3.847968	0.886966
8	-3.714337	-0.103255	0.767307
7	-3.227723	-2.725047	-0.531022
1	-3.230786	-1.997282	0.177121
6	-3.113550	-2.304217	-1.861780
8	-2.913898	-3.071434	-2.800343
1	-5.432078	0.651068	-0.693870
6	0.359447	4.746469	-1.870535
1	0.735423	5.766739	-2.004352
1	-0.159083	4.458457	-2.788969
1	-0.371377	4.743722	-1.060425
6	1.570653	4.950085	0.736470
1	2.161234	5.012325	1.655992
1	1.384002	5.967822	0.381754
1	0.617121	4.483671	0.983417
6	2.355585	3.579289	-2.845306
1	3.119256	2.823034	-2.669478
1	1.714701	3.214833	-3.653112
1	2.822818	4.513889	-3.172737
6	3.687271	4.787562	-0.576909
1	3.540243	5.767933	-1.042721
1	4.231132	4.937717	0.361140
1	4.311823	4.185087	-1.237181
6	5.564291	1.564515	-3.029409
1	5.040068	1.551634	-3.989630
1	5.403934	2.542206	-2.572498
1	6.635362	1.447770	-3.227494
6	6.045100	1.756788	-0.150236
1	5.178450	2.419158	-0.189404
1	6.336570	1.647694	0.899625
1	6.880083	2.219444	-0.685340
6	5.160176	-0.903392	-2.902408
1	4.753865	-1.715865	-2.299394
1	4.555632	-0.843162	-3.812053
1	6.192184	-1.133497	-3.185928
6	6.869476	-0.576000	-0.559934
1	7.709409	-0.255773	-1.186000
1	7.207172	-0.583807	0.481116
1	6.604941	-1.598671	-0.832558
6	4.694022	-4.057388	0.191493
1	5.181915	-4.932725	-0.248327
1	5.058368	-3.156044	-0.306775
1	4.983149	-3.992200	1.244580
6	2.653792	-5.375774	0.831760
1	2.963808	-6.293083	0.319840
1	3.064599	-5.399653	1.846170
1	1.564873	-5.372716	0.910461
6	1.207088	-4.513511	-1.551139
1	0.806734	-4.162990	-2.506439
1	1.191814	-5.607706	-1.549810
1	0.537807	-4.159999	-0.763132
6	3.540281	-4.485761	-2.466091
1	3.660095	-5.571571	-2.385019
1	3.100864	-4.265842	-3.443661
1	4.528945	-4.025047	-2.432184
6	-3.739352	4.132125	-0.444932
1	-2.703051	3.779922	-0.495422
1	-4.224723	3.795755	-1.368736

6	-3.791610	5.668464	-0.373753
1	-3.211002	6.074423	-1.211951
1	-4.828103	5.995497	-0.532327
6	-3.278331	6.279793	0.942306
1	-3.931114	5.975636	1.772251
1	-3.370529	7.372440	0.881567
6	-1.828006	5.917209	1.280904
1	-1.173224	6.278846	0.478576
1	-1.709254	4.827664	1.303700
6	-1.362027	6.487392	2.621962
1	-0.320974	6.217640	2.829043
1	-1.434083	7.581592	2.640214
1	-1.973499	6.101951	3.446916
6	-6.778118	0.993049	0.969638
1	-6.290793	0.280016	1.642125
1	-7.096711	1.842982	1.586942
6	-8.006551	0.344284	0.312400
1	-8.698972	0.040699	1.108544
1	-8.539669	1.097392	-0.284446
6	-7.702051	-0.876085	-0.575687
1	-8.656362	-1.289389	-0.930103
1	-7.162127	-0.561787	-1.479029
6	-6.898589	-1.985181	0.117256
1	-7.386442	-2.248148	1.067007
1	-5.898958	-1.614106	0.372015
6	-6.760791	-3.236546	-0.753277
1	-6.169325	-4.009939	-0.254367
1	-7.741955	-3.665249	-0.992585
1	-6.263956	-3.001200	-1.701019
7	-3.252529	-0.947497	-1.992149
1	-3.310758	-0.424022	-1.125169
6	-2.723912	-0.235343	-3.156604
6	-3.146205	1.237682	-3.051754
6	-1.193283	-0.364927	-3.262605
1	-3.175183	-0.677378	-4.053460
6	-2.565367	2.081263	-4.195452
1	-2.781523	1.638081	-2.094353
1	-4.241049	1.306432	-3.029830
6	-0.626594	0.466570	-4.419426
1	-0.742671	-0.016785	-2.324776
1	-0.931160	-1.421844	-3.370795
6	-1.037995	1.937919	-4.275340
1	-2.846494	3.132973	-4.057698
1	-3.013585	1.758693	-5.146108
1	0.465371	0.375979	-4.432102
1	-0.994069	0.070440	-5.377574
1	-0.645876	2.534363	-5.108954
1	-0.587761	2.327565	-3.354615

TS2-*para-aaa* (Refer to Table S5)

Number of imaginary frequencies : 1
Imaginary frequency : -22.7480 cm(-1)

Electronic energy : HF=-3396.567642
Zero-point correction= 1.456885 (Hartree/Particle)
Thermal correction to Energy= 1.536410
Thermal correction to Enthalpy= 1.537354
Thermal correction to Gibbs Free Energy= 1.340653
Sum of electronic and zero-point Energies= -3395.110757

Sum of electronic and thermal Energies=	-3395.031232
Sum of electronic and thermal Enthalpies=	-3395.030288
Sum of electronic and thermal Free Energies=	-3395.226989

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Cartesian Coordinates

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.....
77      -1.439491   0.290636  -0.088101
 6      -0.064350   2.533254  -1.661840
 6       0.897901   1.413326  -1.716321
 7      -1.211999   2.306529  -0.972666
 7       0.474626   0.233055  -1.213080
 6       0.185898   3.773948  -2.259518
 6      -0.750027   4.795855  -2.132951
 6      -1.917234   4.554766  -1.410394
 6      -2.110513   3.295294  -0.849321
 6       2.203629   1.524508  -2.207319
 6       3.067674   0.441094  -2.122616
 6       2.623780  -0.795298  -1.619415
 6       1.275940  -0.836829  -1.226668
 5      -2.104717  -0.516461  -1.933077
 8      -1.775803   0.122038  -3.123647
 8      -2.649735  -1.765787  -2.184683
 6      -2.280455  -0.667585  -4.231991
 6      -2.417370  -2.090260  -3.582618
 5      -3.519080   0.206862  -0.147393
 8      -4.370705  -0.692899   0.484026
 8      -4.264067   1.113280  -0.911937
 6      -5.704188  -0.536913  -0.070467
 6      -5.668072   0.944566  -0.588287
 6      -0.085967   0.885971   1.578423
 6       0.527124   2.151115   1.571243
 6       0.616265  -0.134650   2.250631
 6       1.845619   2.333602   1.997004
 6       1.932977   0.027174   2.669723
 6       2.598500   1.247505   2.463286
 5      -2.171930   0.699233   1.848798
 8      -2.277771  -0.243880   2.866094
 8      -2.766435   1.907522   2.235611
 6      -3.032872   0.314625   3.962720
 6      -2.952257   1.865065   3.678221
 1      -1.483854  -1.192010   0.443957
 1       0.806026  -1.753634  -0.907146
 1       4.100368   0.563345  -2.430438
 1       2.566983   2.466306  -2.597214
 1       1.097911   3.941441  -2.818534
 1      -0.567906   5.762550  -2.592011
 1      -2.672916   5.321786  -1.280667
 1      -2.999627   3.047624  -0.285924
 1      -0.013054   3.007540   1.181589
 1       2.291528   3.320792   1.932199
 1       0.113337  -1.072469   2.447607
 6       3.524724  -1.972921  -1.525452
 6       3.413627  -2.962204  -0.510441
 6       4.548863  -2.121644  -2.481155
 6       4.295634  -4.051558  -0.501612
 6       5.419821  -3.206024  -2.463494
 1       4.633591  -1.391963  -3.280372
 6       5.285809  -4.179105  -1.470415
 1       4.180495  -4.791137   0.280027
 1       6.188253  -3.296600  -3.225197
 1       5.959621  -5.030199  -1.441517

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7	2.434052	-2.875131	0.503634
1	2.177416	-1.942062	0.801766
6	1.465300	-3.883566	0.689255
8	1.676294	-5.062262	0.423005
6	-2.381624	-0.136546	5.267663
1	-2.877012	0.315377	6.133638
1	-2.466244	-1.223975	5.358064
1	-1.320612	0.117417	5.296554
6	-1.729621	2.533146	4.319580
1	-1.633010	3.550386	3.927736
1	-1.830731	2.593326	5.407585
1	-0.809356	1.995881	4.084001
6	-4.452488	-0.244231	3.855510
1	-4.893292	0.045330	2.903891
1	-4.407638	-1.336804	3.872283
1	-5.092553	0.091608	4.677563
6	-4.209769	2.652875	4.031728
1	-4.400032	2.615390	5.109544
1	-4.078030	3.702314	3.749537
1	-5.091789	2.274951	3.513417
6	-6.742273	-0.820093	1.010953
1	-6.623393	-1.845670	1.372918
1	-6.651088	-0.151331	1.866619
1	-7.753655	-0.719256	0.602660
6	-5.991657	1.975673	0.498033
1	-5.351169	1.824018	1.369007
1	-5.788361	2.978219	0.108624
1	-7.040994	1.937118	0.805631
6	-5.843069	-1.568019	-1.195866
1	-5.088776	-1.404321	-1.965066
1	-5.674000	-2.566355	-0.783221
1	-6.839772	-1.544127	-1.647327
6	-6.498656	1.214307	-1.837547
1	-7.562718	1.047619	-1.638749
1	-6.371875	2.256044	-2.148290
1	-6.198019	0.578300	-2.671206
6	-3.623674	-0.053136	-4.636137
1	-4.063905	-0.559659	-5.500494
1	-4.330321	-0.088938	-3.803879
1	-3.470053	0.999191	-4.892312
6	-1.285583	-0.577718	-5.384603
1	-1.582617	-1.232105	-6.211124
1	-1.250539	0.448744	-5.762554
1	-0.277516	-0.852567	-5.067496
6	-1.118074	-2.904528	-3.628685
1	-1.228074	-3.783400	-2.988381
1	-0.883703	-3.242828	-4.642395
1	-0.273573	-2.319835	-3.252083
6	-3.579651	-2.932538	-4.096005
1	-3.449770	-3.163417	-5.158704
1	-3.619108	-3.877443	-3.545832
1	-4.538727	-2.429198	-3.966011
7	0.293692	-3.403293	1.204032
1	0.101259	-2.415082	1.100533
6	-0.908200	-4.228171	1.363157
6	-1.751252	-3.646416	2.509665
6	-1.708852	-4.286880	0.048390
1	-0.567239	-5.235602	1.623698
6	-3.092004	-4.377613	2.662981
1	-1.951476	-2.587491	2.306568
1	-1.173984	-3.688928	3.441523

6	-3.055786	-5.003107	0.218213
1	-1.895627	-3.264131	-0.297119
1	-1.096310	-4.783955	-0.713217
6	-3.880286	-4.362750	1.344916
1	-3.675025	-3.907783	3.464637
1	-2.915056	-5.418841	2.970637
1	-3.608709	-4.971988	-0.728748
1	-2.886324	-6.064989	0.450103
1	-4.836160	-4.888795	1.465396
1	-4.109365	-3.322122	1.078699
1	2.475887	-0.795054	3.126644
6	4.081998	1.221002	2.709200
8	4.534525	0.612990	3.683632
7	4.924053	1.759289	1.758423
6	4.496186	2.363670	0.496102
1	5.133992	1.970593	-0.304274
1	3.484321	2.036641	0.261243
6	6.331930	1.337114	1.820976
1	6.934366	2.079522	1.286298
1	6.650737	1.331127	2.864362
6	6.491492	-0.058765	1.200534
1	5.867655	-0.752625	1.775426
1	6.083096	-0.045074	0.180813
6	7.928954	-0.579931	1.150001
1	8.564370	0.131168	0.601810
1	8.338755	-0.637942	2.167798
6	8.006881	-1.957936	0.480022
1	7.362077	-2.660150	1.026345
1	7.580251	-1.891299	-0.530976
6	9.423117	-2.535021	0.392185
1	10.070833	-1.832051	-0.150151
1	9.845424	-2.621015	1.402637
6	9.459971	-3.901981	-0.297414
1	8.848994	-4.633885	0.244241
1	9.065935	-3.839418	-1.319262
1	10.479448	-4.298955	-0.357489
6	4.556425	3.897761	0.488950
1	4.108353	4.276187	1.415198
1	5.601659	4.232661	0.497006
6	3.814024	4.483907	-0.716946
1	4.252921	4.090996	-1.646328
1	2.774349	4.127198	-0.695203
6	3.812952	6.015020	-0.764770
1	3.417142	6.405530	0.183356
1	4.845782	6.382699	-0.838877
6	2.982827	6.577391	-1.925262
1	3.365877	6.175718	-2.874334
1	1.950322	6.213157	-1.831737
6	2.981065	8.106948	-1.981370
1	2.574835	8.535910	-1.057803
1	3.996556	8.500148	-2.107883
1	2.375462	8.479075	-2.815135

TS2-*para-gag* (Refer to Table S5)

Number of imaginary frequencies : 1
Imaginary frequency : -109.2556 cm(-1)

Electronic energy : HF=-3396.5644731
Zero-point correction= 1.457583 (Hartree/Particle)

Thermal correction to Energy=	1.536923
Thermal correction to Enthalpy=	1.537867
Thermal correction to Gibbs Free Energy=	1.340575
Sum of electronic and zero-point Energies=	-3395.106890
Sum of electronic and thermal Energies=	-3395.027550
Sum of electronic and thermal Enthalpies=	-3395.026606
Sum of electronic and thermal Free Energies=	-3395.223898

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 Cartesian Coordinates

77	-1.414189	-0.366370	0.280309
6	0.054375	-0.632096	2.960107
6	0.537315	0.649048	2.401055
7	-0.858931	-1.305871	2.214954
7	-0.101031	1.085881	1.295185
6	0.484013	-1.127637	4.195956
6	-0.021248	-2.338420	4.660823
6	-0.949015	-3.025856	3.880997
6	-1.344893	-2.471555	2.666297
6	1.580337	1.411778	2.940158
6	1.958445	2.597137	2.321616
6	1.247854	3.083012	1.207886
6	0.189637	2.276560	0.766632
5	-2.876851	0.806758	1.225595
8	-2.798383	1.046682	2.595410
8	-3.868249	1.589754	0.652888
6	-3.910044	1.895455	2.982401
6	-4.274938	2.590883	1.623948
5	-3.242715	-1.302297	-0.012980
8	-4.068678	-1.284529	-1.132513
8	-3.878409	-1.990348	1.030366
6	-5.389177	-1.749815	-0.747832
6	-5.068063	-2.633877	0.509006
6	0.533225	-1.168562	-0.583106
6	1.341505	-2.010372	0.203384
6	1.203312	-0.373127	-1.539081
6	2.731792	-2.026575	0.084489
6	2.586888	-0.385306	-1.674025
6	3.375530	-1.201141	-0.846403
5	-1.109865	-1.912488	-1.184856
8	-1.169485	-1.689117	-2.565765
8	-1.221221	-3.292780	-0.920793
6	-1.352120	-2.942630	-3.253840
6	-0.936004	-3.997982	-2.157221
1	-1.746129	0.457069	-1.023066
1	-0.465706	2.582902	-0.034097
1	2.808688	3.150426	2.706518
1	2.116471	1.069626	3.815313
1	1.195614	-0.572416	4.793252
1	0.301579	-2.731686	5.619627
1	-1.369882	-3.972285	4.202559
1	-2.078915	-2.942090	2.025738
1	0.869710	-2.698626	0.895514
1	3.312192	-2.716487	0.687867
1	0.617593	0.213999	-2.236713
6	1.568202	4.380494	0.562697
6	1.414199	4.614925	-0.831006
6	2.024911	5.441096	1.367647
6	1.694093	5.884642	-1.355011
6	2.295466	6.698595	0.839086
1	2.122384	5.284629	2.437606

6	2.120232	6.919777	-0.528494
1	1.560644	6.037712	-2.417626
1	2.628083	7.500871	1.490682
1	2.324121	7.896734	-0.956926
7	0.987092	3.591947	-1.708126
1	1.227671	2.645845	-1.442711
6	-0.149599	3.734803	-2.530348
8	-0.516801	4.820326	-2.967609
6	-0.472893	-2.938748	-4.502892
1	-0.522466	-3.903228	-5.019975
1	-0.824491	-2.167155	-5.194821
1	0.569738	-2.721502	-4.263701
6	0.564105	-4.321945	-2.177683
1	0.817634	-4.897241	-1.282167
1	0.831885	-4.918833	-3.054809
1	1.173190	-3.416696	-2.176983
6	-2.826774	-3.032830	-3.648903
1	-3.452732	-2.993618	-2.760704
1	-3.083141	-2.165396	-4.263514
1	-3.045501	-3.940576	-4.220603
6	-1.734261	-5.297883	-2.180241
1	-1.561230	-5.840162	-3.115954
1	-1.416728	-5.941422	-1.353500
1	-2.805923	-5.124787	-2.077914
6	-6.031687	-2.494854	-1.914241
1	-6.142080	-1.818164	-2.766839
1	-5.443416	-3.352049	-2.241862
1	-7.028848	-2.850646	-1.632837
6	-4.669248	-4.069395	0.153205
1	-3.854823	-4.064471	-0.573291
1	-4.306412	-4.573239	1.054608
1	-5.509656	-4.646241	-0.244493
6	-6.220021	-0.506607	-0.413690
1	-5.763468	0.051884	0.402578
1	-6.236862	0.152345	-1.286185
1	-7.250850	-0.765192	-0.151769
6	-6.141548	-2.632381	1.591945
1	-7.073941	-3.067635	1.216615
1	-5.807254	-3.231944	2.444483
1	-6.350863	-1.624325	1.953268
6	-5.013420	0.969626	3.503000
1	-5.883679	1.528998	3.859796
1	-5.331303	0.273868	2.723143
1	-4.617646	0.377370	4.333157
6	-3.443490	2.839666	4.085506
1	-4.227331	3.561160	4.339576
1	-3.206112	2.266657	4.987320
1	-2.546480	3.388930	3.791886
6	-3.431291	3.840853	1.343999
1	-3.581254	4.145927	0.305145
1	-3.710993	4.675781	1.993430
1	-2.365944	3.634255	1.481889
6	-5.754178	2.902677	1.426429
1	-6.100882	3.621487	2.176584
1	-5.908274	3.344436	0.437462
1	-6.373650	2.007102	1.492308
7	-0.767892	2.543176	-2.799130
1	-0.634023	1.779188	-2.146218
6	-2.041630	2.476232	-3.527584
6	-2.127121	1.124337	-4.252528
6	-3.229255	2.680215	-2.567646

1	-2.024394	3.290830	-4.258870
6	-3.486575	0.931731	-4.939468
1	-1.981628	0.318083	-3.524098
1	-1.307474	1.051416	-4.978057
6	-4.582236	2.461004	-3.258221
1	-3.138410	1.971776	-1.737574
1	-3.168354	3.688989	-2.142408
6	-4.636269	1.082124	-3.932341
1	-3.520046	-0.055366	-5.416916
1	-3.606817	1.673023	-5.743458
1	-5.388214	2.559820	-2.520724
1	-4.747207	3.242911	-4.014197
1	-5.603074	0.937627	-4.431718
1	-4.541704	0.303514	-3.164044
1	3.073307	0.208046	-2.442484
6	4.850733	-1.257944	-1.137893
8	5.226386	-1.297850	-2.313888
7	5.752818	-1.283590	-0.102558
6	5.461544	-0.902155	1.281320
1	6.140303	-0.083729	1.560538
1	4.451391	-0.495003	1.328316
6	7.173395	-1.352721	-0.473766
1	7.729559	-1.729207	0.391410
1	7.270812	-2.082883	-1.278323
6	7.736364	0.006403	-0.914407
1	7.183503	0.326944	-1.803614
1	7.534440	0.744585	-0.127100
6	9.243806	-0.013267	-1.209311
1	9.566617	1.016932	-1.401559
1	9.791017	-0.341082	-0.312558
6	9.641959	-0.903619	-2.395883
1	9.356001	-1.941606	-2.185737
1	9.062691	-0.602960	-3.280338
6	11.141409	-0.870173	-2.734380
1	11.720383	-1.164025	-1.847363
1	11.345195	-1.633282	-3.496669
6	11.643611	0.485044	-3.244578
1	11.069366	0.813313	-4.119361
1	11.562761	1.268139	-2.483185
1	12.696902	0.429707	-3.541537
6	5.623863	-2.056646	2.280914
1	4.865066	-2.820111	2.072542
1	6.594585	-2.541021	2.122368
6	5.516854	-1.611101	3.746743
1	5.617270	-2.496915	4.384657
1	6.364619	-0.957300	3.996057
6	4.209848	-0.875083	4.075325
1	4.198963	0.081028	3.539052
1	3.358217	-1.451143	3.685713
6	3.998134	-0.608906	5.574310
1	4.891037	-0.120416	5.987348
1	3.180406	0.114376	5.700628
6	3.674495	-1.866653	6.387196
1	2.786551	-2.372277	5.988882
1	4.496819	-2.589191	6.366754
1	3.478537	-1.623456	7.437055

TS2-*para-gaa* (Refer to Table S5)

Number of imaginary frequencies : 1

Imaginary frequency : -114.8245 cm(-1)

Electronic energy : HF=-3396.5660502
Zero-point correction= 1.456484 (Hartree/Particle)
Thermal correction to Energy= 1.536218
Thermal correction to Enthalpy= 1.537162
Thermal correction to Gibbs Free Energy= 1.339090
Sum of electronic and zero-point Energies= -3395.109566
Sum of electronic and thermal Energies= -3395.029832
Sum of electronic and thermal Enthalpies= -3395.028888
Sum of electronic and thermal Free Energies= -3395.226960

.....
Cartesian Coordinates

.....
77 1.429851 -0.143605 -0.483130
6 -0.130249 1.222852 -2.743999
6 -0.561572 1.930030 -1.518425
7 0.791664 0.239629 -2.579860
7 0.145063 1.658433 -0.401437
6 -0.621884 1.547810 -4.012570
6 -0.179224 0.834967 -5.122573
6 0.759516 -0.178344 -4.940284
6 1.225243 -0.437353 -3.653549
6 -1.636837 2.824119 -1.455325
6 -1.977721 3.405168 -0.240206
6 -1.205416 3.164098 0.911185
6 -0.116206 2.297547 0.741566
5 2.935650 1.312034 -0.623982
8 2.873200 2.295259 -1.608187
8 3.953950 1.590963 0.276139
6 4.018349 3.174452 -1.457549
6 4.397981 2.955431 0.048709
5 3.216700 -1.122106 -0.867781
8 4.054895 -1.798039 0.013679
8 3.804535 -1.082148 -2.140291
6 5.341999 -2.000082 -0.626667
6 4.957032 -1.961699 -2.147407
6 -0.540644 -1.240893 -0.185068
6 -1.376434 -1.480370 -1.291573
6 -1.181593 -1.102581 1.065950
6 -2.765905 -1.524704 -1.174109
6 -2.564591 -1.151897 1.199551
6 -3.378840 -1.343283 0.071981
5 1.082063 -2.238770 -0.149805
8 1.159123 -2.839129 1.112123
8 1.141453 -3.228225 -1.150879
6 1.297085 -4.267269 0.965372
6 0.837992 -4.502736 -0.525882
1 1.826317 -0.240992 1.038968
1 0.578494 2.091943 1.542037
1 -2.853085 4.043823 -0.182335
1 -2.231753 3.033589 -2.333919
1 -1.332778 2.355163 -4.132934
1 -0.556180 1.075075 -6.111863
1 1.137411 -0.759182 -5.774637
1 1.975191 -1.190768 -3.452551
1 -0.927852 -1.677425 -2.258627
1 -3.373655 -1.746926 -2.045066
1 -0.575289 -1.021356 1.960611
6 -1.502121 3.803317 2.216743
6 -1.288395 3.152762 3.462594

6	-2.003463	5.118124	2.230048
6	-1.554839	3.838616	4.656010
6	-2.259936	5.791827	3.419379
1	-2.150196	5.634051	1.285850
6	-2.024729	5.148164	4.636159
1	-1.377892	3.323950	5.590877
1	-2.627824	6.813052	3.396384
1	-2.217217	5.661655	5.573702
7	-0.823841	1.819432	3.523726
1	-1.072139	1.226698	2.742599
6	0.335269	1.457906	4.239016
8	0.710407	2.065511	5.236682
6	0.420341	-4.942311	2.018889
1	0.420017	-6.030366	1.892889
1	0.810447	-4.719089	3.016574
1	-0.609657	-4.583331	1.976305
6	-0.672424	-4.742470	-0.655965
1	-0.951782	-4.696036	-1.712908
1	-0.955091	-5.726447	-0.269552
1	-1.249666	-3.984250	-0.124627
6	2.768309	-4.608171	1.205844
1	3.393248	-4.085448	0.485407
1	3.056468	-4.256333	2.200279
1	2.955526	-5.685612	1.153098
6	1.591061	-5.604072	-1.266565
1	1.401173	-6.579935	-0.807122
1	1.249624	-5.648529	-2.305727
1	2.667980	-5.433231	-1.274452
6	5.951620	-3.314814	-0.149514
1	6.107010	-3.276592	0.932732
1	5.316987	-4.174390	-0.365810
1	6.924468	-3.477836	-0.626009
6	4.471601	-3.312806	-2.681946
1	3.664856	-3.697825	-2.055637
1	4.069518	-3.174204	-3.690558
1	5.277382	-4.051249	-2.735756
6	6.238606	-0.833420	-0.197793
1	5.797902	0.118800	-0.492250
1	6.314403	-0.829329	0.892935
1	7.246839	-0.918572	-0.614881
6	6.019432	-1.373949	-3.069444
1	6.928043	-1.985478	-3.055672
1	5.645112	-1.348843	-4.097741
1	6.283082	-0.354096	-2.785615
6	5.091880	2.675802	-2.429702
1	5.981858	3.312638	-2.421145
1	5.384351	1.651701	-2.188176
1	4.679068	2.671041	-3.442683
6	3.594014	4.594367	-1.816852
1	4.405941	5.304581	-1.627466
1	3.341018	4.647275	-2.880456
1	2.716497	4.907266	-1.247514
6	3.593089	3.842575	1.007203
1	3.746662	3.490069	2.030583
1	3.903344	4.890545	0.952642
1	2.522196	3.784102	0.790506
6	5.885202	3.052973	0.369504
1	6.259852	4.061556	0.164610
1	6.046688	2.841108	1.430679
1	6.475945	2.339272	-0.206764
7	0.970997	0.363461	3.717125

1	0.819950	0.138924	2.739406
6	2.265657	-0.097967	4.234411
6	2.365814	-1.618616	4.041852
6	3.422362	0.641115	3.535743
1	2.276506	0.142893	5.302347
6	3.745891	-2.153876	4.449125
1	2.185249	-1.857628	2.987584
1	1.570879	-2.107290	4.618929
6	4.795397	0.082316	3.933058
1	3.301905	0.543043	2.451714
1	3.352857	1.709056	3.775132
6	4.863444	-1.431248	3.682890
1	3.790966	-3.234399	4.265564
1	3.895490	-2.013755	5.530023
1	5.578861	0.601424	3.367239
1	4.987273	0.284716	4.997227
1	5.845296	-1.824322	3.976673
1	4.739322	-1.622740	2.608903
1	-3.029732	-1.077715	2.178163
6	-4.853364	-1.532084	0.291744
8	-5.236480	-2.238995	1.228814
7	-5.745694	-0.953839	-0.578160
6	-5.458811	0.198268	-1.438047
1	-6.158120	1.001295	-1.164867
1	-4.458754	0.570113	-1.210594
6	-7.166477	-1.252971	-0.350901
1	-7.703764	-1.062776	-1.286688
1	-7.248494	-2.318233	-0.129855
6	-7.783883	-0.427229	0.786766
1	-7.256650	-0.679797	1.712692
1	-7.603182	0.638286	0.593732
6	-9.292745	-0.659048	0.955326
1	-9.673415	0.045285	1.707139
1	-9.809064	-0.408417	0.016645
6	-9.673711	-2.084789	1.377742
1	-9.368277	-2.802054	0.604497
1	-9.109879	-2.356343	2.281187
6	-11.174569	-2.253818	1.643247
1	-11.484454	-1.551205	2.429203
1	-11.736883	-1.970187	0.742543
6	-11.551610	-3.679904	2.053010
1	-11.286930	-4.399876	1.269344
1	-11.025355	-3.981035	2.966517
1	-12.626651	-3.775032	2.242183
6	-5.599976	-0.098130	-2.940727
1	-4.722375	-0.656995	-3.286893
1	-6.463155	-0.755115	-3.097429
6	-5.780089	1.168431	-3.789369
1	-5.899715	0.877492	-4.841163
1	-6.718533	1.663248	-3.500972
6	-4.631524	2.178492	-3.677328
1	-4.544658	2.524174	-2.638289
1	-3.682231	1.675483	-3.913109
6	-4.813492	3.396196	-4.591707
1	-4.868384	3.060066	-5.635938
1	-5.781843	3.865991	-4.372546
6	-3.701906	4.438697	-4.447662
1	-3.635827	4.812255	-3.418557
1	-2.723480	4.022558	-4.715984
1	-3.874214	5.302603	-5.098575

TS2-*para*-gga (Refer to Table S5)

Number of imaginary frequencies : 1
Imaginary frequency : -166.8881 cm(-1)

Electronic energy : HF=-3396.5682288
Zero-point correction= 1.458243 (Hartree/Particle)
Thermal correction to Energy= 1.537278
Thermal correction to Enthalpy= 1.538222
Thermal correction to Gibbs Free Energy= 1.342475
Sum of electronic and zero-point Energies= -3395.109986
Sum of electronic and thermal Energies= -3395.030951
Sum of electronic and thermal Enthalpies= -3395.030007
Sum of electronic and thermal Free Energies= -3395.225754

Cartesian Coordinates

77	1.385524	-0.354561	-0.178807
6	0.236456	-1.733610	-2.663030
6	-0.550982	-0.489452	-2.538545
7	1.122230	-1.983400	-1.664947
7	-0.076387	0.419010	-1.659754
6	0.114927	-2.593524	-3.758439
6	0.900725	-3.740651	-3.814996
6	1.773365	-4.011239	-2.763316
6	1.854801	-3.106506	-1.707820
6	-1.733338	-0.224350	-3.239526
6	-2.408844	0.970822	-3.019014
6	-1.869031	1.951662	-2.166184
6	-0.661298	1.612716	-1.538328
5	2.706109	0.642583	-1.482182
8	2.714066	0.354256	-2.842932
8	3.465774	1.772188	-1.219609
6	3.657177	1.239903	-3.501855
6	3.749197	2.431510	-2.482815
5	3.333943	-0.788977	0.397403
8	4.067041	-0.247076	1.447786
8	4.142244	-1.661840	-0.342775
6	5.470390	-0.559014	1.245847
6	5.391477	-1.857298	0.367651
6	-0.489992	-0.998558	0.904037
6	-1.235179	-2.081636	0.403714
6	-1.219849	-0.004168	1.589841
6	-2.630604	-2.112264	0.469382
6	-2.608519	-0.015456	1.654184
6	-3.338087	-1.050012	1.047348
5	1.274249	-1.358789	1.701973
8	1.268835	-0.710315	2.939022
8	1.520225	-2.732224	1.876998
6	1.556140	-1.661728	3.984055
6	1.277382	-3.043738	3.275320
1	1.546705	0.915767	0.739802
1	-0.133898	2.311259	-0.907574
1	-3.363234	1.141204	-3.506671
1	-2.150916	-0.965072	-3.910869
1	-0.567977	-2.356278	-4.565115
1	0.826650	-4.413306	-4.663505
1	2.392628	-4.901454	-2.755727
1	2.535594	-3.247859	-0.879766
1	-0.713822	-2.917954	-0.048533

1	-3.167367	-2.967214	0.071063
1	-0.679891	0.772864	2.115331
6	-2.516098	3.271215	-1.959159
6	-2.468190	3.976882	-0.725538
6	-3.190487	3.869967	-3.039938
6	-3.066677	5.240743	-0.626641
6	-3.776064	5.126997	-2.933352
1	-3.213275	3.355062	-3.995738
6	-3.704763	5.816324	-1.721135
1	-3.010415	5.757627	0.322229
1	-4.272246	5.568936	-3.792052
1	-4.155384	6.799555	-1.622029
7	-1.833425	3.429747	0.411787
1	-1.844905	2.420814	0.492204
6	-0.793631	4.099521	1.089673
8	-0.723448	5.322585	1.153382
6	0.647878	-1.353532	5.172745
1	0.776642	-2.093064	5.970551
1	0.903716	-0.370015	5.578719
1	-0.404005	-1.329825	4.882131
6	-0.181870	-3.500807	3.401865
1	-0.348666	-4.346631	2.728012
1	-0.414727	-3.824013	4.421125
1	-0.876711	-2.707397	3.121712
6	3.021671	-1.470718	4.377631
1	3.663712	-1.650129	3.518247
1	3.176402	-0.432230	4.683670
1	3.315403	-2.125994	5.203850
6	2.205374	-4.180579	3.691756
1	2.077603	-4.415370	4.753840
1	1.967314	-5.080558	3.115762
1	3.254435	-3.939181	3.516385
6	6.152059	-0.729669	2.600232
1	6.065745	0.200189	3.170029
1	5.710038	-1.528591	3.195172
1	7.216969	-0.949066	2.467203
6	5.236178	-3.140041	1.190946
1	4.393228	-3.054700	1.879039
1	5.027493	-3.974980	0.514798
1	6.142057	-3.378230	1.756699
6	6.092154	0.632551	0.508244
1	5.592778	0.801308	-0.445179
1	5.950772	1.534288	1.109859
1	7.164629	0.492181	0.340919
6	6.515673	-2.018637	-0.649819
1	7.484035	-2.111473	-0.146592
1	6.352733	-2.925429	-1.240625
1	6.561757	-1.174698	-1.339360
6	4.969117	0.464450	-3.645493
1	5.732475	1.044540	-4.173004
1	5.355428	0.176904	-2.665314
1	4.780623	-0.454009	-4.208937
6	3.102652	1.604565	-4.875046
1	3.748688	2.332108	-5.377823
1	3.051652	0.708342	-5.501391
1	2.095922	2.021783	-4.805248
6	2.647535	3.479597	-2.683980
1	2.635213	4.152291	-1.822159
1	2.811726	4.075886	-3.586540
1	1.663558	3.006490	-2.753742
6	5.110176	3.112525	-2.389093

1	5.372682	3.589923	-3.339127
1	5.079127	3.888000	-1.617806
1	5.901515	2.409759	-2.123615
7	0.098945	3.240576	1.669525
1	0.172564	2.301913	1.295143
6	1.305529	3.691428	2.369366
6	1.631359	2.682463	3.483362
6	2.482005	3.848120	1.386693
1	1.069235	4.667154	2.806642
6	2.953421	3.015275	4.188637
1	1.704442	1.678938	3.047149
1	0.801261	2.656695	4.200239
6	3.800130	4.164542	2.106427
1	2.601158	2.916090	0.823094
1	2.234484	4.635599	0.664642
6	4.106400	3.108352	3.178521
1	3.167377	2.251101	4.946012
1	2.859191	3.971311	4.724671
1	4.615009	4.215996	1.373733
1	3.737728	5.155509	2.579772
1	5.047363	3.344440	3.692041
1	4.230797	2.130604	2.694936
1	-3.146529	0.768882	2.178286
6	-4.835493	-0.965631	1.148874
8	-5.346384	-0.602711	2.215284
7	-5.610603	-1.254478	0.053184
6	-7.059622	-1.069302	0.215761
1	-7.571401	-1.688068	-0.527798
1	-7.330296	-1.444074	1.203183
6	-5.125016	-1.463004	-1.312104
1	-5.590139	-0.713021	-1.967029
1	-4.053166	-1.270690	-1.340693
6	-5.438928	-2.871034	-1.847719
1	-5.223783	-3.601486	-1.060455
1	-6.514139	-2.948584	-2.043945
6	-4.660033	-3.217998	-3.127839
1	-5.180879	-4.024553	-3.659476
1	-4.681019	-2.351487	-3.804470
6	-3.202960	-3.652883	-2.891032
1	-2.695551	-3.731754	-3.862083
1	-2.662267	-2.879979	-2.330423
6	-3.065745	-4.995767	-2.159068
1	-3.516884	-4.926497	-1.161728
1	-3.643703	-5.758870	-2.698557
6	-1.614079	-5.458505	-2.016576
1	-1.152849	-5.627286	-2.995459
1	-1.006090	-4.711734	-1.494988
1	-1.547219	-6.394531	-1.451531
6	-7.475864	0.400337	0.070119
1	-6.877645	0.990424	0.770584
1	-7.217955	0.749551	-0.938117
6	-8.972625	0.645119	0.322061
1	-9.169127	1.718048	0.194139
1	-9.562889	0.133384	-0.451202
6	-9.479278	0.207890	1.708633
1	-10.534182	0.501666	1.800300
1	-9.471580	-0.888260	1.781795
6	-8.686770	0.791295	2.886360
1	-7.648004	0.443603	2.841074
1	-8.653807	1.886264	2.792279
6	-9.285630	0.411431	4.243253

1	-10.316255	0.773493	4.344591
1	-9.304682	-0.677348	4.374867
1	-8.702565	0.831876	5.069967

TS2-ortho-aaa (Refer to Table S5)

Number of imaginary frequencies : 1
Imaginary frequency : -167.9762 cm(-1)

Electronic energy : HF=-3396.5558505
Zero-point correction= 1.457415 (Hartree/Particle)
Thermal correction to Energy= 1.536773
Thermal correction to Enthalpy= 1.537717
Thermal correction to Gibbs Free Energy= 1.341449
Sum of electronic and zero-point Energies= -3395.098435
Sum of electronic and thermal Energies= -3395.019078
Sum of electronic and thermal Enthalpies= -3395.018134
Sum of electronic and thermal Free Energies= -3395.214401

Cartesian Coordinates

6	1.596398	0.601975	-1.354932
6	0.250630	0.963358	-1.659625
6	-0.024144	1.186201	-3.024799
6	0.920365	1.005983	-4.036079
6	2.197327	0.549476	-3.714635
6	2.526473	0.352326	-2.373261
77	-1.350422	-0.186421	-0.453506
5	-2.798355	0.581444	0.821635
8	-2.636313	1.158643	2.076515
6	-3.897877	1.144761	2.789408
6	-4.028264	2.418185	3.625259
5	-1.084299	1.957818	-0.595752
8	-0.429240	2.911447	0.199696
6	-1.152388	4.168705	0.102764
6	-0.199209	5.352237	0.222593
6	2.098182	0.410048	0.056260
8	1.974256	-0.676209	0.654235
7	-0.489189	-1.915264	-1.560245
6	-1.012519	-2.160514	-2.782600
6	-0.526045	-3.227995	-3.545918
6	0.437794	-4.070354	-3.011377
6	0.918597	-3.862316	-1.708191
6	0.426608	-2.738169	-1.036161
6	1.803244	-4.861168	-1.060211
6	2.994476	-4.544776	-0.357431
6	3.741655	-5.595661	0.208332
6	3.338288	-6.919286	0.078497
6	2.166189	-7.239345	-0.609146
6	1.415017	-6.210622	-1.163590
7	3.422225	-3.213816	-0.217445
6	4.744762	-2.817283	-0.020767
8	5.713661	-3.554864	-0.193153
6	-2.147760	-1.307489	-3.202582
7	-2.561960	-0.378406	-2.307659
6	-3.638775	0.371104	-2.581885
6	-4.341084	0.257277	-3.778453
6	-3.905004	-0.669023	-4.723963
6	-2.800974	-1.463462	-4.430584
7	4.864384	-1.500375	0.359745

6	6.169558	-1.004200	0.796315
6	6.206543	0.524886	0.709962
6	7.565402	1.082223	1.158267
6	7.928206	0.605604	2.572679
6	7.889527	-0.926799	2.665181
6	6.529793	-1.481561	2.216051
5	-2.418652	-1.789484	0.390767
8	-3.037331	-2.702565	-0.457100
6	-3.624040	-3.769557	0.325542
6	-5.119352	-3.462825	0.437061
8	-2.050207	2.612723	-1.396502
6	-1.851149	4.037658	-1.296395
6	-0.951480	4.468627	-2.462743
6	-3.208125	4.726536	-1.408272
8	-2.434296	-2.255379	1.696722
6	-2.848609	-3.647617	1.691730
6	-1.563543	-4.482298	1.735735
6	-3.687618	-3.914886	2.937794
8	-4.169780	0.437816	0.547616
6	-4.954966	1.004124	1.624444
6	-5.519954	2.336831	1.121253
6	-6.115457	0.059952	1.933209
7	2.712051	1.467749	0.654404
6	2.767905	1.470835	2.127348
6	1.380486	1.732410	2.723414
6	1.353689	1.681636	4.251712
6	-0.047177	1.964196	4.809798
6	-0.134791	1.855772	6.335738
6	-1.538533	2.139963	6.877753
6	3.446761	2.491423	-0.107068
6	2.687868	3.753668	-0.499592
6	3.532863	4.597102	-1.463780
6	2.861468	5.894047	-1.927335
6	3.719811	6.705815	-2.904402
6	3.033177	7.990508	-3.375525
6	-3.409471	-5.084055	-0.420381
6	-3.852660	-0.064573	3.731859
6	-2.140315	4.215937	1.266928
1	-0.463274	-0.194456	0.841494
1	0.736601	-2.478717	-0.032885
1	0.811629	-4.905578	-3.594882
1	-0.906050	-3.416540	-4.542254
1	-2.458594	-2.196786	-5.150183
1	-4.419839	-0.780464	-5.673341
1	-5.206067	0.886726	-3.957864
1	-3.916022	1.076489	-1.811740
1	0.647605	1.195668	-5.071283
1	0.487557	-6.441104	-1.680257
1	4.655284	-5.359969	0.735070
1	1.838397	-8.270046	-0.703162
1	3.940363	-7.702379	0.530706
1	2.730680	-2.472724	-0.192542
1	-0.765922	6.288505	0.169651
1	0.308923	5.324625	1.190847
1	0.553484	5.368375	-0.558784
1	-1.416702	4.158958	-3.403456
1	-0.814879	5.554102	-2.492360
1	0.027871	3.989553	-2.402342
1	-2.821776	3.374585	1.213974
1	-1.589956	4.122286	2.206581
1	-2.707700	5.152065	1.284486

1	-3.118198	5.803737	-1.232279
1	-3.615663	4.582177	-2.414240
1	-3.925201	4.314384	-0.696851
1	-3.195381	2.472428	4.331407
1	-4.017593	3.327635	3.025646
1	-4.959179	2.399622	4.202534
1	-4.722996	3.032743	0.859495
1	-6.111255	2.153093	0.218958
1	-6.166671	2.812674	1.864755
1	-3.692717	-0.986629	3.173723
1	-3.002874	0.055482	4.410597
1	-4.762986	-0.148253	4.334170
1	-6.736822	0.458858	2.742304
1	-6.745483	-0.052970	1.045553
1	-5.766286	-0.929630	2.227656
1	-5.659041	-4.234793	0.994379
1	-5.277250	-2.496480	0.918058
1	-5.544569	-3.403158	-0.569404
1	-3.777586	-5.934169	0.163695
1	-3.958888	-5.061315	-1.366800
1	-2.354873	-5.249030	-0.649616
1	-0.984791	-4.197686	2.619012
1	-1.773616	-5.554740	1.790173
1	-0.942240	-4.294059	0.856889
1	-4.045345	-4.950012	2.950015
1	-3.078034	-3.756710	3.832539
1	-4.551749	-3.250697	2.999137
1	4.041963	-1.073142	0.776210
1	6.906445	-1.420428	0.101280
1	5.419813	0.930930	1.358819
1	5.973455	0.843697	-0.311793
1	5.744662	-1.145406	2.908994
1	6.532619	-2.575941	2.231336
1	7.551327	2.178087	1.114110
1	8.341274	0.749763	0.454335
1	8.111511	-1.255234	3.687452
1	8.677000	-1.346804	2.023754
1	8.918137	0.981482	2.858146
1	7.210857	1.028949	3.290571
1	3.519060	-0.003260	-2.105825
1	2.933651	0.358150	-4.490145
1	3.157818	0.511174	2.483792
1	3.475189	2.248451	2.429959
1	4.319017	2.759792	0.496744
1	3.843761	2.024934	-1.009783
1	-1.023572	1.506145	-3.293334
1	1.016917	2.698701	2.360061
1	0.683364	0.989075	2.324966
1	2.069212	2.405069	4.671531
1	1.686356	0.689592	4.590363
1	-0.361537	2.971204	4.498836
1	-0.762990	1.273752	4.344844
1	0.582156	2.552536	6.792497
1	0.179193	0.849381	6.645754
1	-2.267918	1.424229	6.480963
1	-1.571248	2.074040	7.971325
1	-1.876374	3.144975	6.596815
1	1.740779	3.465680	-0.960181
1	2.436099	4.328944	0.397472
1	4.496841	4.839619	-0.992143
1	3.772656	3.987474	-2.347170

1	1.904134	5.653289	-2.409100
1	2.619229	6.517074	-1.054894
1	4.677389	6.954528	-2.426479
1	3.965898	6.080782	-3.773944
1	2.800214	8.648700	-2.529856
1	3.665284	8.554733	-4.070164
1	2.089842	7.769660	-3.889418

1

Number of imaginary frequencies : 0

Electronic energy : HF=-3396.6174881
 Zero-point correction= 1.460085 (Hartree/Particle)
 Thermal correction to Energy= 1.540490
 Thermal correction to Enthalpy= 1.541434
 Thermal correction to Gibbs Free Energy= 1.341097
 Sum of electronic and zero-point Energies= -3395.157404
 Sum of electronic and thermal Energies= -3395.076998
 Sum of electronic and thermal Enthalpies= -3395.076054
 Sum of electronic and thermal Free Energies= -3395.276391

Cartesian Coordinates

6	0.191139	3.572519	0.704845
6	0.834123	2.349080	0.942841
6	0.203813	1.412391	1.785820
6	-1.009736	1.712608	2.408121
6	-1.605342	2.963903	2.208331
6	-1.008404	3.883409	1.348471
6	2.100481	1.878076	0.286103
7	3.029545	2.722147	-0.240176
6	4.179590	2.098622	-0.918787
6	5.272485	1.640997	0.055567
6	6.493866	1.036649	-0.653300
6	6.211996	-0.292541	-1.366573
6	7.456821	-0.910318	-2.012961
6	7.166425	-2.247122	-2.700081
8	2.295707	0.645846	0.220433
6	3.109094	4.174754	-0.055724
6	2.718718	4.963017	-1.317844
6	2.639168	6.480434	-1.087382
6	1.408482	6.926374	-0.284793
6	1.322345	8.444495	-0.092899
6	0.075335	8.871949	0.685800
7	3.565543	-1.405654	1.754415
6	3.725108	-2.393638	0.821483
7	3.253953	-2.004904	-0.432638
6	3.267745	-2.724200	-1.629941
6	2.578938	-2.175606	-2.745478
6	2.669937	-2.813410	-3.989589
6	3.385449	-3.998580	-4.147488
6	4.019805	-4.555773	-3.035617
6	3.971349	-3.930975	-1.791599
6	1.738538	-0.956533	-2.618273
6	1.952182	0.192048	-3.391300
6	1.103736	1.286022	-3.253143
6	0.049020	1.232099	-2.334350
7	-0.143048	0.129809	-1.572402
6	0.662125	-0.925710	-1.722364

6	-0.940577	2.323298	-2.160617
7	-2.004489	2.045338	-1.366219
6	-2.963149	2.970520	-1.198927
6	-2.904659	4.227101	-1.796909
6	-1.803079	4.535703	-2.594137
6	-0.814079	3.573875	-2.780714
77	-1.904472	0.092913	-0.186692
5	-1.459551	-1.539490	0.937446
8	-1.524359	-2.886218	0.553412
6	-0.840132	-3.696978	1.536733
6	-1.564826	-5.033583	1.654543
6	3.912069	-1.594395	3.156499
6	5.432487	-1.550059	3.393141
6	5.762413	-1.709692	4.884093
6	5.042775	-0.650185	5.732743
6	3.526360	-0.673291	5.484580
6	3.198205	-0.523416	3.993337
8	4.222963	-3.491126	1.076267
5	-3.629748	0.166152	0.900472
8	-3.965811	-0.547884	2.059142
6	-5.383879	-0.425961	2.298359
6	-6.058093	-1.622197	1.614101
5	-2.856249	-1.180790	-1.391723
8	-2.378488	-1.496312	-2.672233
6	-3.069663	-2.684689	-3.125494
6	-3.214535	-2.620900	-4.642433
8	-4.716187	1.003569	0.562630
6	-5.715392	0.942911	1.605280
6	-7.097383	1.029131	0.964280
6	-5.484260	2.145750	2.528947
8	-4.027230	-1.890195	-1.131194
6	-4.420763	-2.602695	-2.323941
6	-5.486290	-1.750523	-3.024263
6	-5.004470	-3.949708	-1.907797
8	-0.905135	-1.461215	2.230696
6	-0.906388	-2.787238	2.811497
6	-2.218480	-2.937095	3.592195
6	0.287470	-2.914642	3.752461
6	-2.201909	-3.882848	-2.719618
6	0.590657	-3.900797	1.027137
6	-5.634507	-0.468819	3.803559
1	-1.485412	0.951848	3.015934
1	0.644684	0.435764	1.930180
1	0.582785	4.277190	-0.010659
1	-1.486472	4.837581	1.149295
1	-2.547500	3.201925	2.691056
1	-3.788246	2.662422	-0.564909
1	-3.704081	4.941790	-1.633033
1	-1.714057	5.508050	-3.069149
1	0.045703	3.797458	-3.400567
1	1.259830	2.164771	-3.867316
1	2.776757	0.223190	-4.097118
1	0.427571	-1.786972	-1.109214
1	2.138702	-2.379577	-4.832534
1	3.431976	-4.485782	-5.116543
1	4.476317	-4.352987	-0.934580
1	4.572726	-5.485977	-3.133958
1	2.886686	-1.059278	-0.478123
1	3.066174	-0.564217	1.484490
1	3.807166	1.258135	-1.504355
1	4.586927	2.835014	-1.618924

1	2.499550	4.460492	0.800143
1	4.144450	4.415706	0.213585
1	-2.226088	-2.670847	-5.110367
1	-3.806068	-3.464396	-5.014736
1	-3.690531	-1.691986	-4.963368
1	-2.634149	-4.832910	-3.050564
1	-1.215379	-3.776425	-3.182470
1	-2.062426	-3.901822	-1.635986
1	-5.888962	-2.244099	-3.914612
1	-6.310641	-1.570950	-2.327614
1	-5.075933	-0.778880	-3.314356
1	-5.931145	-3.793743	-1.346208
1	-5.237368	-4.566974	-2.782459
1	-4.312511	-4.495854	-1.264215
1	-7.888285	0.901154	1.711648
1	-7.230261	2.011340	0.498287
1	-7.223282	0.271936	0.188121
1	-4.506313	2.075013	3.011734
1	-5.507736	3.065837	1.936336
1	-6.250309	2.220401	3.307339
1	-5.643489	-2.544808	2.031806
1	-7.141689	-1.628605	1.771764
1	-5.838127	-1.623071	0.544603
1	-6.691116	-0.291487	4.032801
1	-5.364950	-1.455579	4.192331
1	-5.032346	0.271621	4.334523
1	-1.458551	-5.596215	0.721491
1	-1.142759	-5.640018	2.463486
1	-2.631185	-4.890405	1.840652
1	1.106515	-2.941579	0.953772
1	1.177530	-4.561121	1.671995
1	0.555643	-4.344597	0.027964
1	-2.284666	-3.906596	4.096851
1	-2.269011	-2.149008	4.349357
1	-3.076253	-2.805903	2.930240
1	0.170754	-2.223382	4.593411
1	0.361366	-3.929500	4.158559
1	1.221870	-2.676612	3.244226
1	3.554300	-2.585848	3.466600
1	5.813934	-0.586140	3.026695
1	5.904699	-2.336898	2.797597
1	3.521021	0.468879	3.643611
1	2.116754	-0.581990	3.828759
1	6.846425	-1.652670	5.038888
1	5.452167	-2.710527	5.216377
1	3.031178	0.119873	6.057125
1	3.114028	-1.625530	5.846731
1	5.255172	-0.803352	6.797815
1	5.433207	0.344471	5.473166
1	1.754819	4.594262	-1.691345
1	3.450896	4.747586	-2.104889
1	3.553219	6.823954	-0.582391
1	2.624872	6.985595	-2.061687
1	1.402160	6.443793	0.701553
1	0.501164	6.577725	-0.799735
1	2.222161	8.795124	0.430493
1	1.329506	8.935626	-1.075743
1	0.058116	8.420274	1.684734
1	0.032666	9.959028	0.812666
1	-0.840392	8.561570	0.167978
1	5.586058	2.500073	0.662883

1	4.842788	0.902277	0.739612
1	7.283795	0.875674	0.091857
1	6.899786	1.763096	-1.373132
1	5.786251	-1.002144	-0.647143
1	5.444655	-0.155705	-2.140347
1	8.229395	-1.052368	-1.244584
1	7.878188	-0.202734	-2.741241
1	8.069144	-2.667889	-3.157439
1	6.778380	-2.980616	-1.985763
1	6.413457	-2.135147	-3.488707

TS[1-2]_m

Number of imaginary frequencies : 1
Imaginary frequency : -777.9218 cm(-1)

Electronic energy : HF=-3396.5793117
Zero-point correction= 1.454848 (Hartree/Particle)
Thermal correction to Energy= 1.534808
Thermal correction to Enthalpy= 1.535752
Thermal correction to Gibbs Free Energy= 1.338828
Sum of electronic and zero-point Energies= -3395.124464
Sum of electronic and thermal Energies= -3395.044503
Sum of electronic and thermal Enthalpies= -3395.043559
Sum of electronic and thermal Free Energies= -3395.240484

Cartesian Coordinates

77	-1.383021	0.130096	-0.244277
5	-2.718236	-0.621180	-1.699278
8	-2.608554	-0.268897	-3.044318
8	-3.813286	-1.464333	-1.516137
6	-3.495649	-1.120709	-3.813756
6	-4.576192	-1.512029	-2.746486
5	-1.515660	-1.910171	0.140302
8	-1.045868	-2.839525	-0.789247
8	-1.991203	-2.551403	1.268886
6	-1.115274	-4.172692	-0.215645
6	-2.108513	-3.968587	0.993679
5	-3.084917	0.455795	0.830110
8	-3.309792	0.119206	2.163738
8	-4.197548	1.161227	0.336938
6	-4.708872	0.326715	2.462805
6	-5.098189	1.445343	1.434879
6	-0.335132	2.133494	-2.348798
6	0.721628	1.098538	-2.321282
7	-1.381546	1.965721	-1.501796
7	0.455835	-0.013286	-1.593194
6	-0.282580	3.236236	-3.212350
6	-1.314262	4.167537	-3.207050
6	-2.388432	3.975108	-2.340042
6	-2.384446	2.860636	-1.509048
6	1.949226	1.243033	-2.978847
6	2.909307	0.240883	-2.875623
6	2.636159	-0.907210	-2.123344
6	1.372431	-0.985171	-1.517186
6	-0.083107	1.164917	1.277881
6	-0.577825	1.883208	2.384550
6	1.294349	1.257821	1.043231
6	0.259235	2.676675	3.175706

6	2.134763	2.083740	1.795934
6	1.620306	2.797715	2.882837
1	-0.732022	-0.282358	1.180198
1	1.755047	0.680594	0.254975
1	2.268582	3.416792	3.496390
1	-0.154522	3.204293	4.031585
1	-1.624534	1.786190	2.649686
1	-3.204159	2.644240	-0.834441
1	-3.219825	4.670244	-2.301078
1	-1.282044	5.023132	-3.874317
1	0.547712	3.355425	-3.896908
1	2.175024	2.141459	-3.539936
1	3.874543	0.355944	-3.358870
1	1.083532	-1.858543	-0.947674
6	3.567822	2.065318	1.358758
8	4.177251	0.976172	1.341524
7	4.147545	3.206479	0.902868
6	3.595616	-2.032132	-1.986699
6	4.095546	-2.658619	-3.139011
6	3.972481	-2.525386	-0.714896
6	4.889992	-3.799156	-3.048499
1	3.812319	-2.266547	-4.112001
6	4.752031	-3.688045	-0.632124
6	5.193239	-4.324898	-1.789076
1	5.251685	-4.284208	-3.950047
1	5.008672	-4.071692	0.346851
1	5.798547	-5.222924	-1.704601
7	3.601603	-1.808757	0.435836
6	3.179134	-2.384965	1.632958
8	2.984975	-3.596091	1.759330
7	2.983112	-1.471531	2.628903
1	3.706076	-0.798821	0.418228
1	3.145792	-0.493047	2.409556
6	3.373882	4.430089	0.640645
1	4.079381	5.266442	0.636731
1	2.698917	4.597823	1.477958
6	5.481175	3.071092	0.300972
1	5.988306	4.037519	0.381786
1	6.035220	2.352917	0.906804
6	2.164962	-1.791764	3.794481
6	2.565999	-0.900281	4.977701
6	0.664218	-1.640123	3.488899
1	2.369689	-2.838165	4.045890
6	1.697628	-1.190431	6.212050
1	2.438071	0.152241	4.683870
1	3.629135	-1.041892	5.205204
6	-0.204485	-1.944116	4.714505
1	0.482226	-0.608440	3.170790
1	0.386072	-2.282019	2.648187
6	0.199068	-1.052363	5.898356
1	1.981043	-0.520608	7.033286
1	1.900051	-2.213897	6.558597
1	-1.260163	-1.798885	4.459866
1	-0.087394	-3.000765	4.996851
1	-0.397442	-1.294382	6.786758
1	-0.019718	-0.005395	5.644235
6	2.572215	4.405413	-0.676456
6	1.436947	5.443108	-0.693430
1	2.142939	3.406244	-0.810072
1	3.252456	4.571633	-1.519098
6	0.237919	5.036864	0.174012

1	1.822036	6.421065	-0.369168
1	1.094454	5.579916	-1.727040
6	-0.900626	6.061328	0.174778
1	-0.145003	4.072302	-0.179758
1	0.557428	4.860696	1.207679
1	-0.527141	7.028224	0.540403
1	-1.234245	6.232353	-0.857812
6	5.442676	2.597657	-1.167656
6	6.715543	1.842027	-1.581289
1	5.280879	3.460984	-1.823019
1	4.577658	1.938521	-1.297999
6	6.721721	0.378812	-1.115220
1	6.820162	1.867317	-2.674002
1	7.598701	2.364221	-1.184692
6	8.051264	-0.334716	-1.380952
1	6.477937	0.321668	-0.046875
1	5.912220	-0.159385	-1.628787
1	8.306411	-0.243613	-2.446423
1	8.851363	0.181772	-0.832334
6	-2.089822	5.611579	1.028182
1	-2.906134	6.342469	1.004776
1	-2.484063	4.653629	0.674573
1	-1.795716	5.473114	2.075084
6	8.025481	-1.813383	-0.986608
1	9.000237	-2.288931	-1.144666
1	7.762850	-1.935491	0.070799
1	7.284293	-2.367228	-1.571740
6	-4.845875	0.716705	3.930404
1	-5.885657	0.957265	4.177613
1	-4.531577	-0.118561	4.563741
1	-4.220390	1.576781	4.179133
6	-5.421746	-1.004385	2.191869
1	-4.957417	-1.780874	2.805296
1	-6.487093	-0.956922	2.439723
1	-5.309001	-1.295047	1.143997
6	-6.532143	1.382447	0.919400
1	-7.248126	1.509232	1.738698
1	-6.703107	2.184651	0.194132
1	-6.735504	0.433757	0.420480
6	-4.774587	2.860518	1.932170
1	-4.888877	3.566854	1.104031
1	-5.444580	3.174349	2.738680
1	-3.743408	2.924828	2.290259
6	-5.697758	-0.475444	-2.614737
1	-6.354239	-0.470124	-3.490762
1	-6.300968	-0.717450	-1.735512
1	-5.286241	0.526167	-2.468257
6	-5.164652	-2.909954	-2.907430
1	-5.885157	-3.104003	-2.106960
1	-5.689122	-3.004332	-3.864573
1	-4.393040	-3.680338	-2.857382
6	-2.655924	-2.316242	-4.279658
1	-3.228625	-2.998658	-4.915580
1	-1.801799	-1.945486	-4.854520
1	-2.265450	-2.867208	-3.419554
6	-4.019675	-0.330598	-5.007578
1	-3.192993	-0.088726	-5.683123
1	-4.756951	-0.912846	-5.571076
1	-4.481518	0.608066	-4.694289
6	-1.742120	-4.733241	2.262606
1	-1.784705	-5.814885	2.095220

1	-0.742406	-4.475693	2.616470
1	-2.453192	-4.484133	3.056210
6	-3.575624	-4.217888	0.624280
1	-3.769746	-5.273313	0.407421
1	-4.206906	-3.918776	1.466070
1	-3.860077	-3.610222	-0.237726
6	0.303253	-4.555491	0.206921
1	0.962213	-4.515412	-0.665488
1	0.711946	-3.877982	0.956947
1	0.346528	-5.571765	0.611051
6	-1.611284	-5.126988	-1.299615
1	-0.880047	-5.169688	-2.112819
1	-1.733975	-6.140591	-0.903079
1	-2.563778	-4.799225	-1.719436

2

Number of imaginary frequencies : 0

Electronic energy : HF=-3396.5936784
 Zero-point correction= 1.456560 (Hartree/Particle)
 Thermal correction to Energy= 1.536935
 Thermal correction to Enthalpy= 1.537880
 Thermal correction to Gibbs Free Energy= 1.338645
 Sum of electronic and zero-point Energies= -3395.137119
 Sum of electronic and thermal Energies= -3395.056743
 Sum of electronic and thermal Enthalpies= -3395.055799
 Sum of electronic and thermal Free Energies= -3395.255033

Cartesian Coordinates

77	-1.278262	0.063000	-0.156934
5	-2.642856	-0.778325	-1.598728
8	-2.303529	-0.677602	-2.943312
8	-3.961062	-1.187096	-1.460347
6	-3.396417	-1.197416	-3.742455
6	-4.610149	-1.069512	-2.754645
5	-1.691114	-1.994652	0.026075
8	-0.950736	-2.943051	-0.678107
8	-2.564853	-2.608141	0.908281
6	-1.172884	-4.246554	-0.073197
6	-2.544550	-4.035461	0.677467
5	-2.925930	0.530886	0.955683
8	-3.178915	0.112030	2.256425
8	-3.971944	1.352035	0.512297
6	-4.574701	0.353432	2.547397
6	-4.904966	1.564147	1.602118
6	-0.262453	1.742584	-2.501966
6	0.792713	0.716400	-2.366480
7	-1.296424	1.685228	-1.621795
7	0.539891	-0.278396	-1.484128
6	-0.218833	2.739450	-3.484973
6	-1.242573	3.675412	-3.570671
6	-2.296824	3.601043	-2.662496
6	-2.285023	2.593178	-1.705121
6	2.012367	0.765296	-3.051881
6	2.978081	-0.208623	-2.809649
6	2.718396	-1.229901	-1.888361
6	1.459843	-1.220072	-1.266792
6	-0.058208	1.397497	1.055344

6	-0.529319	2.193135	2.122366
6	1.326901	1.469364	0.841250
6	0.314624	2.997885	2.896612
6	2.187766	2.282894	1.587156
6	1.685763	3.060419	2.633369
1	-0.986962	-0.906480	1.076599
1	1.796470	0.871464	0.073461
1	2.344156	3.683638	3.232146
1	-0.101347	3.576878	3.718079
1	-1.579799	2.159743	2.388563
1	-3.080134	2.477678	-0.978433
1	-3.117947	4.308759	-2.681859
1	-1.215818	4.447048	-4.333652
1	0.601646	2.771199	-4.190782
1	2.229639	1.570925	-3.742452
1	3.937133	-0.165067	-3.316285
1	1.178535	-1.996006	-0.569163
6	3.626767	2.180042	1.185070
8	4.217403	1.088243	1.313830
7	4.229315	3.246596	0.594644
6	3.664175	-2.331584	-1.585683
6	4.175401	-3.116028	-2.631290
6	3.978276	-2.673073	-0.247978
6	4.916626	-4.265546	-2.367765
1	3.937439	-2.842892	-3.655781
6	4.699640	-3.847627	0.009088
6	5.150238	-4.642451	-1.041728
1	5.287190	-4.874574	-3.186790
1	4.903180	-4.117542	1.037510
1	5.710076	-5.547518	-0.823815
7	3.606544	-1.802339	0.789491
6	3.043876	-2.202039	2.002751
8	2.761778	-3.375254	2.253130
7	2.831168	-1.159980	2.859541
1	3.727442	-0.805077	0.639351
1	3.051870	-0.226651	2.524516
6	3.470803	4.437883	0.184638
1	4.183500	5.263090	0.089616
1	2.790411	4.705200	0.991674
6	5.561084	3.021797	0.019745
1	6.080525	3.984433	-0.014870
1	6.103949	2.375748	0.711125
6	1.907986	-1.280296	3.987273
6	2.177616	-0.148421	4.988666
6	0.443152	-1.255345	3.515898
1	2.109539	-2.244568	4.468105
6	1.181208	-0.182645	6.158207
1	2.080362	0.812780	4.464197
1	3.210616	-0.213552	5.351076
6	-0.555550	-1.281501	4.678312
1	0.287323	-0.344371	2.931742
1	0.271543	-2.099332	2.842169
6	-0.272408	-0.136838	5.661665
1	1.381556	0.653402	6.839619
1	1.335746	-1.103691	6.738627
1	-1.572766	-1.203373	4.279018
1	-0.485104	-2.243171	5.207951
1	-0.966070	-0.175877	6.510949
1	-0.446871	0.819434	5.149278
6	2.678671	4.264090	-1.127861
6	1.539036	5.287985	-1.269360

1	2.254016	3.254180	-1.149679
1	3.365652	4.335996	-1.978493
6	0.339895	4.979180	-0.362625
1	1.919075	6.298818	-1.060128
1	1.199271	5.302131	-2.313181
6	-0.800006	5.996371	-0.471230
1	-0.041493	3.981006	-0.605639
1	0.658660	4.917810	0.684125
1	-0.424470	6.998910	-0.222470
1	-1.142416	6.048923	-1.513991
6	5.523735	2.374332	-1.382233
6	6.778104	1.536928	-1.680138
1	5.394534	3.155766	-2.139961
1	4.640981	1.728217	-1.444445
6	6.734207	0.148646	-1.025473
1	6.893049	1.417169	-2.765699
1	7.672259	2.081797	-1.343198
6	8.045578	-0.632070	-1.157901
1	6.463479	0.240540	0.033798
1	5.921268	-0.432253	-1.483646
1	8.333354	-0.684236	-2.217841
1	8.848014	-0.076637	-0.652367
6	-1.980458	5.648710	0.440800
1	-2.794325	6.376988	0.346900
1	-2.382636	4.658689	0.202095
1	-1.672377	5.624813	1.492235
6	7.954959	-2.047965	-0.583454
1	8.914608	-2.572827	-0.654937
1	7.662438	-2.027849	0.472820
1	7.207114	-2.643715	-1.116589
6	-4.722747	0.639200	4.037691
1	-5.754233	0.913434	4.284507
1	-4.464873	-0.255954	4.611865
1	-4.058911	1.444277	4.359935
6	-5.329703	-0.925881	2.163405
1	-4.897732	-1.763179	2.716519
1	-6.396000	-0.858107	2.403406
1	-5.207720	-1.139421	1.098405
6	-6.320540	1.568322	1.032468
1	-7.064266	1.634110	1.833960
1	-6.455653	2.433513	0.375126
1	-6.516436	0.667523	0.448964
6	-4.584539	2.929731	2.220239
1	-4.645630	3.697998	1.443253
1	-5.290080	3.191046	3.015048
1	-3.573141	2.952348	2.632825
6	-5.271939	0.313386	-2.792229
1	-5.843385	0.463304	-3.713602
1	-5.951391	0.405786	-1.941590
1	-4.525794	1.107402	-2.706941
6	-5.668005	-2.160236	-2.877874
1	-6.447244	-2.004673	-2.125294
1	-6.139948	-2.130937	-3.865822
1	-5.249662	-3.155684	-2.722599
6	-3.043896	-2.647697	-4.086035
1	-3.799266	-3.112978	-4.726718
1	-2.084996	-2.665319	-4.612017
1	-2.931293	-3.244106	-3.177753
6	-3.504593	-0.360033	-5.013142
1	-2.613560	-0.511063	-5.630287
1	-4.378972	-0.651984	-5.604743

1	-3.576111	0.705303	-4.784353
6	-2.644769	-4.736309	2.029774
1	-2.557118	-5.822303	1.917591
1	-1.870637	-4.390857	2.717469
1	-3.616814	-4.520956	2.483900
6	-3.769191	-4.365560	-0.182021
1	-3.854811	-5.438985	-0.377124
1	-4.669513	-4.034078	0.342832
1	-3.729759	-3.827237	-1.129562
6	0.008805	-4.512723	0.861867
1	0.941906	-4.479958	0.295041
1	0.084798	-3.759088	1.646486
1	-0.062096	-5.496132	1.336508
6	-1.199273	-5.288448	-1.187553
1	-0.216983	-5.336124	-1.667541
1	-1.427328	-6.281895	-0.787128
1	-1.935984	-5.043879	-1.955046

TS[2-3]_m

Number of imaginary frequencies : 1
Imaginary frequency : -173.0392 cm(-1)

Electronic energy : HF=-3396.5788599
Zero-point correction= 1.456098 (Hartree/Particle)
Thermal correction to Energy= 1.536082
Thermal correction to Enthalpy= 1.537027
Thermal correction to Gibbs Free Energy= 1.336130
Sum of electronic and zero-point Energies= -3395.122762
Sum of electronic and thermal Energies= -3395.042778
Sum of electronic and thermal Enthalpies= -3395.041833
Sum of electronic and thermal Free Energies= -3395.242730

Cartesian Coordinates

77	1.734035	-0.172912	0.531197
6	1.868183	-1.579331	3.254947
6	0.842170	-2.344787	2.512146
7	2.511929	-0.603363	2.565777
7	0.610319	-1.962112	1.235737
6	2.186709	-1.843070	4.592905
6	3.172604	-1.093773	5.225524
6	3.828935	-0.097754	4.504378
6	3.468613	0.112394	3.176854
6	0.154300	-3.442595	3.041972
6	-0.695605	-4.180002	2.229027
6	-0.863402	-3.836828	0.877402
6	-0.204420	-2.673977	0.450304
5	2.817057	-1.693177	-0.438571
8	3.268238	-2.803179	0.270655
8	2.972446	-1.889676	-1.801966
6	3.894710	-3.729517	-0.654156
6	3.278224	-3.290181	-2.033628
5	3.472536	0.648405	-0.225350
8	3.676846	1.378186	-1.392398
8	4.698421	0.449870	0.428063
6	5.101227	1.450676	-1.652669
6	5.705698	1.265639	-0.216152
6	0.084637	0.969590	1.552609
6	0.090543	1.247017	2.932266

6	-1.166033	0.757284	0.950262
6	-1.089232	1.280373	3.679809
6	-2.353661	0.778634	1.686240
6	-2.317287	1.037420	3.063692
5	1.440571	1.938367	0.517043
8	0.749424	2.652638	-0.472102
8	2.180709	2.833807	1.318388
6	1.107220	4.049146	-0.392106
6	1.685529	4.172314	1.068331
1	1.085757	-0.004688	-0.892031
1	-0.292872	-2.318090	-0.566220
1	-1.218243	-5.039119	2.637212
1	0.291259	-3.737134	4.075235
1	1.668537	-2.622019	5.138235
1	3.423650	-1.287745	6.263761
1	4.606446	0.510588	4.953612
1	3.944711	0.863926	2.562603
1	1.035463	1.451463	3.424417
1	-1.052087	1.493023	4.745350
1	-3.237580	1.040527	3.641515
1	-1.208127	0.559058	-0.114743
6	-1.568411	-4.732591	-0.073432
6	-2.353074	-4.264792	-1.156174
6	-1.366563	-6.120422	0.056791
6	-2.861072	-5.183337	-2.088018
6	-1.883882	-7.023803	-0.865067
1	-0.746400	-6.486299	0.869782
6	-2.623685	-6.546401	-1.950003
1	-3.439767	-4.804155	-2.920257
1	-1.694389	-8.086703	-0.749460
1	-3.024997	-7.237005	-2.686209
6	-3.616068	0.404279	0.974188
7	-4.649690	1.280878	0.924445
6	-5.865752	0.852836	0.211435
1	-6.410679	1.753291	-0.085159
6	-4.531468	2.703668	1.275093
1	-3.802261	2.818660	2.076641
1	-5.498322	3.031397	1.672770
8	-3.695613	-0.712009	0.420685
7	-2.644955	-2.898047	-1.291216
1	-2.785542	-2.350015	-0.447442
6	-2.477131	-2.191774	-2.488352
8	-2.135400	-2.725241	-3.542633
1	-5.571946	0.323607	-0.699917
6	-0.145265	4.885401	-0.645890
1	0.053061	5.950557	-0.484829
1	-0.469585	4.758646	-1.682193
1	-0.966472	4.579448	0.003935
6	0.606175	4.480982	2.115982
1	1.031098	4.350572	3.115792
1	0.245987	5.511055	2.029708
1	-0.245309	3.804586	2.025297
6	2.150848	4.316460	-1.478272
1	3.024268	3.688584	-1.316227
1	1.730697	4.042690	-2.449764
1	2.447170	5.369982	-1.512511
6	2.836406	5.162352	1.222831
1	2.501432	6.182719	1.007072
1	3.207710	5.139718	2.252439
1	3.670005	4.928267	0.560114
6	5.430338	2.780664	-2.324980

1	4.898464	2.850984	-3.278471
1	5.141431	3.639279	-1.717726
1	6.504349	2.850450	-2.529408
6	5.785652	2.573002	0.579513
1	4.815373	3.073563	0.583824
1	6.044655	2.340804	1.617447
1	6.545465	3.254348	0.184256
6	5.437606	0.294955	-2.602010
1	5.164330	-0.659897	-2.153118
1	4.845081	0.402731	-3.514800
1	6.497798	0.283628	-2.873946
6	7.039038	0.527913	-0.164653
1	7.810418	1.074946	-0.717485
1	7.371506	0.432475	0.873966
1	6.957187	-0.477399	-0.581232
6	5.406148	-3.498554	-0.561670
1	5.966203	-4.194991	-1.193565
1	5.662333	-2.476464	-0.849978
1	5.724810	-3.639583	0.475447
6	3.550775	-5.151673	-0.220588
1	3.940361	-5.884452	-0.935384
1	4.001265	-5.358552	0.755407
1	2.472030	-5.293396	-0.129247
6	1.949487	-3.987224	-2.352003
1	1.463564	-3.474271	-3.186558
1	2.096303	-5.035509	-2.629445
1	1.264973	-3.952620	-1.501265
6	4.219028	-3.395899	-3.229837
1	4.507533	-4.437901	-3.405192
1	3.711535	-3.029457	-4.127228
1	5.124265	-2.802398	-3.092060
6	-4.118748	3.564803	0.075970
1	-3.170854	3.177709	-0.316414
1	-4.858054	3.455700	-0.728041
6	-3.951818	5.044493	0.434515
1	-4.862242	5.418358	0.924272
1	-3.143653	5.144811	1.172959
6	-3.635950	5.912863	-0.788983
1	-4.491727	5.894068	-1.478599
1	-2.795735	5.469039	-1.337515
6	-3.293151	7.365163	-0.440248
1	-2.451944	7.376020	0.266566
1	-4.140647	7.825165	0.086394
6	-2.934522	8.200646	-1.671801
1	-2.698698	9.236335	-1.403358
1	-2.061729	7.783799	-2.188299
1	-3.762145	8.223346	-2.390844
6	-6.751446	-0.049493	1.075191
1	-6.158271	-0.917381	1.383189
1	-7.032418	0.490326	1.989542
6	-8.008085	-0.517484	0.334056
1	-8.592434	0.355664	0.009206
1	-7.710716	-1.045308	-0.582730
6	-8.895779	-1.435831	1.181450
1	-8.306785	-2.303624	1.510516
1	-9.196638	-0.907355	2.097660
6	-10.148708	-1.924834	0.445232
1	-9.847114	-2.457190	-0.467054
1	-10.735281	-1.057492	0.112148
6	-11.028406	-2.837769	1.303359
1	-11.917632	-3.170408	0.756714

1	-10.480040	-3.732767	1.620560
1	-11.369084	-2.322216	2.209348
7	-2.714396	-0.853930	-2.349347
1	-2.968331	-0.523749	-1.425270
6	-2.210839	0.123759	-3.313304
6	-2.746816	1.506894	-2.918736
6	-0.671791	0.129106	-3.373063
1	-2.598243	-0.145569	-4.304472
6	-2.204651	2.614353	-3.832361
1	-2.429341	1.716081	-1.887334
1	-3.843980	1.495903	-2.921763
6	-0.137848	1.228588	-4.299243
1	-0.281158	0.297747	-2.362016
1	-0.323566	-0.857646	-3.691746
6	-0.668738	2.602420	-3.866894
1	-2.576927	3.588018	-3.489469
1	-2.595465	2.470212	-4.849709
1	0.957883	1.220948	-4.279224
1	-0.442154	1.023029	-5.336312
1	-0.298185	3.390855	-4.534431
1	-0.284108	2.814582	-2.862206

3

Number of imaginary frequencies : 0

Electronic energy : HF=-3396.6054512
 Zero-point correction= 1.456858 (Hartree/Particle)
 Thermal correction to Energy= 1.537735
 Thermal correction to Enthalpy= 1.538679
 Thermal correction to Gibbs Free Energy= 1.336085
 Sum of electronic and zero-point Energies= -3395.148594
 Sum of electronic and thermal Energies= -3395.067717
 Sum of electronic and thermal Enthalpies= -3395.066772
 Sum of electronic and thermal Free Energies= -3395.269366

Cartesian Coordinates

77	0.612515	-1.608886	0.056324
6	-0.606323	-2.049882	2.838589
6	-1.793695	-1.817455	1.982917
7	0.600498	-2.038844	2.213741
7	-1.548785	-1.618500	0.665975
6	-0.701776	-2.303485	4.212516
6	0.448871	-2.567774	4.947990
6	1.677859	-2.578595	4.290720
6	1.708438	-2.307757	2.926372
6	-3.107966	-1.827416	2.464778
6	-4.166287	-1.642737	1.582182
6	-3.915307	-1.464329	0.214563
6	-2.570295	-1.472389	-0.183646
5	0.520094	-3.549195	-0.371252
8	0.015866	-4.475288	0.554510
8	0.895770	-4.202736	-1.545238
6	0.360674	-5.800012	0.087206
6	0.453512	-5.578838	-1.463655
5	2.585420	-1.892967	-0.405007
8	3.358966	-1.394824	-1.471314
8	3.382186	-2.816992	0.317644
6	4.489209	-2.283503	-1.663358

6	4.726703	-2.809991	-0.209878
6	2.112844	1.563338	1.503507
6	2.301822	1.129399	2.826570
6	0.803207	1.797986	1.060015
6	1.218243	0.969539	3.690904
6	-0.281564	1.682745	1.933780
6	-0.073634	1.269162	3.254581
5	3.318708	1.979162	0.615000
8	3.181469	2.819043	-0.462839
8	4.623818	1.683646	0.920130
6	4.506757	2.949645	-1.069869
6	5.447482	2.606890	0.142665
1	0.476402	-1.257340	-1.494873
1	-2.294362	-1.338844	-1.222444
1	-5.187883	-1.628032	1.949338
1	-3.312547	-1.974935	3.518409
1	-1.666755	-2.307647	4.704427
1	0.382846	-2.770417	6.012642
1	2.601972	-2.792598	4.817190
1	2.630082	-2.324630	2.357272
1	3.310447	0.935971	3.179787
1	1.375994	0.621711	4.706995
1	-0.918729	1.182767	3.931638
1	0.638429	2.119782	0.036207
6	-5.016586	-1.281824	-0.766582
6	-5.024436	-0.203100	-1.689352
6	-6.084450	-2.191970	-0.778190
6	-6.066261	-0.105077	-2.626164
6	-7.120782	-2.083891	-1.702912
1	-6.072938	-3.014201	-0.067897
6	-7.096035	-1.042451	-2.634307
1	-6.048775	0.710684	-3.336185
1	-7.928248	-2.809615	-1.705650
1	-7.892173	-0.947805	-3.367433
6	-1.647282	1.997345	1.404512
7	-2.296006	3.100555	1.852866
6	-3.607861	3.386307	1.236263
1	-3.864503	4.421708	1.473867
6	-1.547268	4.208416	2.474778
1	-0.854404	3.795161	3.209984
1	-2.260001	4.831872	3.021684
8	-2.140441	1.248782	0.542647
7	-4.029165	0.775986	-1.587820
1	-3.536222	0.828144	-0.701368
6	-3.447479	1.497791	-2.633182
8	-3.869096	1.508576	-3.786688
1	-3.508473	3.313178	0.147586
6	4.665935	4.366752	-1.607343
1	5.689130	4.527005	-1.962682
1	3.987590	4.526846	-2.448497
1	4.440515	5.115371	-0.845711
6	5.716188	3.811228	1.054119
1	6.179074	3.458513	1.980047
1	6.392348	4.531186	0.584117
1	4.786896	4.326604	1.315336
6	4.564436	1.922955	-2.202278
1	4.359878	0.916868	-1.831133
1	3.792425	2.161833	-2.938302
1	5.533764	1.935215	-2.709113
6	6.754371	1.918220	-0.221035
1	7.365134	2.564610	-0.859630

1	7.324167	1.700610	0.687264
1	6.582000	0.977725	-0.742647
6	5.661109	-1.523466	-2.273031
1	5.379457	-1.129690	-3.254369
1	5.976860	-0.686311	-1.652337
1	6.519230	-2.190892	-2.410610
6	5.549249	-1.841825	0.651436
1	5.150700	-0.825447	0.592625
1	5.496835	-2.165546	1.696339
1	6.604386	-1.825669	0.358400
6	4.031979	-3.383211	-2.632525
1	3.180563	-3.930678	-2.224315
1	3.702298	-2.912629	-3.563861
1	4.840508	-4.083189	-2.869196
6	5.299447	-4.220940	-0.117585
1	6.295612	-4.270570	-0.570874
1	5.390236	-4.517900	0.932389
1	4.655056	-4.947660	-0.615563
6	1.712851	-6.152568	0.720829
1	2.044143	-7.161608	0.454862
1	2.475412	-5.429697	0.419326
1	1.616363	-6.097764	1.809631
6	-0.716175	-6.780244	0.539407
1	-0.534238	-7.779750	0.129537
1	-0.711909	-6.856870	1.631505
1	-1.711012	-6.452686	0.230721
6	-0.910792	-5.654443	-2.159960
1	-0.808841	-5.281637	-3.183274
1	-1.293202	-6.679342	-2.202493
1	-1.644629	-5.026872	-1.645946
6	1.465575	-6.464041	-2.184046
1	1.200621	-7.522273	-2.082877
1	1.480001	-6.218530	-3.250331
1	2.475095	-6.319614	-1.794659
6	-0.773226	5.018846	1.424441
1	-0.258067	4.305899	0.772263
1	-1.476086	5.568053	0.785666
6	0.275663	5.968615	2.009462
1	-0.209416	6.779575	2.570139
1	0.894360	5.417981	2.732412
6	1.185156	6.554896	0.920829
1	0.574232	7.106424	0.191970
1	1.651188	5.728503	0.364940
6	2.282115	7.475009	1.467090
1	2.902889	6.911999	2.178019
1	1.822168	8.290519	2.042197
6	3.169696	8.062117	0.366527
1	3.951932	8.707549	0.780925
1	3.663140	7.270302	-0.209548
1	2.582717	8.662108	-0.338828
6	-4.706459	2.431040	1.721878
1	-4.325404	1.406432	1.668205
1	-4.928095	2.632319	2.777898
6	-5.978582	2.534887	0.872035
1	-6.430343	3.530187	0.989731
1	-5.702833	2.441422	-0.186127
6	-7.012137	1.451969	1.202493
1	-6.538297	0.466711	1.093500
1	-7.318270	1.535191	2.255766
6	-8.250569	1.502776	0.300450
1	-7.928583	1.435619	-0.746565

1	-8.745474	2.477526	0.413217
6	-9.247513	0.378909	0.593347
1	-10.123137	0.438010	-0.062675
1	-8.784318	-0.602177	0.439091
1	-9.605707	0.421519	1.629467
7	-2.363701	2.219827	-2.192640
1	-1.991260	1.943688	-1.289674
6	-1.393155	2.820173	-3.100542
6	-0.863329	4.119319	-2.471728
6	-0.242537	1.841393	-3.405724
1	-1.924564	3.052766	-4.028946
6	0.238856	4.766531	-3.319943
1	-0.450054	3.879837	-1.481019
1	-1.697053	4.811857	-2.306825
6	0.858717	2.494477	-4.251803
1	0.188001	1.495024	-2.455187
1	-0.647981	0.954005	-3.904098
6	1.380697	3.774029	-3.582011
1	0.618184	5.663564	-2.814789
1	-0.186177	5.098274	-4.277900
1	1.675929	1.780504	-4.407149
1	0.459825	2.740680	-5.246433
1	2.156843	4.241140	-4.201554
1	1.846710	3.509947	-2.623903

4

Number of imaginary frequencies : 0

Electronic energy : HF=-2935.6930263
 Zero-point correction= 1.178661 (Hartree/Particle)
 Thermal correction to Energy= 1.245411
 Thermal correction to Enthalpy= 1.246355
 Thermal correction to Gibbs Free Energy= 1.077340
 Sum of electronic and zero-point Energies= -2934.514365
 Sum of electronic and thermal Energies= -2934.447616
 Sum of electronic and thermal Enthalpies= -2934.446672
 Sum of electronic and thermal Free Energies= -2934.615687

Cartesian Coordinates

6	0.753069	2.465514	0.513780
6	-0.820059	2.534920	2.232687
6	-0.123098	3.584650	2.842780
6	1.042480	4.063328	2.258224
6	1.515830	3.505062	1.059285
1	1.013259	1.989040	-0.421692
1	-0.468296	4.014565	3.775510
1	1.602162	4.860482	2.737234
7	-0.361949	1.991518	1.081312
6	-2.060673	1.937134	2.778505
6	-2.744251	2.470768	3.877766
6	-3.628137	0.221872	2.599499
6	-3.900472	1.848757	4.338068
1	-2.385035	3.369817	4.363658
1	-3.916996	-0.672902	2.063452
1	-4.440116	2.257285	5.186725
7	-2.513166	0.821407	2.146581
6	-4.348861	0.699122	3.688595
1	-5.242697	0.176323	4.011613

77	-1.472729	0.194871	0.324896
5	1.262083	-1.174079	-1.115582
8	0.912893	-1.883432	-2.228790
8	1.994703	-0.032330	-1.431831
6	1.920356	0.182979	-2.882920
6	1.468301	-1.240704	-3.410256
5	-2.526625	-1.465178	-0.170736
8	-2.981777	-2.399256	0.793882
8	-2.939852	-1.896726	-1.438014
6	-3.898308	-3.322460	0.154336
6	-3.434559	-3.249417	-1.340962
5	1.069171	-1.723813	0.478824
8	1.500843	-2.930900	0.953185
8	0.447387	-0.968140	1.461720
6	0.649395	-1.641031	2.750850
6	0.970935	-3.115274	2.303654
1	-0.698461	-0.090100	-1.032019
5	-2.799711	1.082871	-0.869756
8	-2.528176	1.546113	-2.162843
8	-4.132760	1.371826	-0.533900
6	-3.649773	2.332798	-2.619292
6	-4.824593	1.773095	-1.739947
6	2.745922	4.034536	0.420284
6	2.864905	5.428588	0.274672
6	3.832583	3.214907	0.024494
6	4.022704	6.016800	-0.222696
1	2.020912	6.052191	0.556103
6	5.002444	3.820388	-0.464954
6	5.099706	5.202822	-0.581268
1	4.084534	7.095752	-0.327380
1	5.838258	3.188585	-0.736688
1	6.014691	5.642638	-0.967737
7	3.746892	1.812214	0.110835
1	2.910552	1.357690	-0.234418
6	4.810059	0.967475	0.427177
8	5.872041	1.355524	0.909840
7	4.526131	-0.351066	0.171199
6	0.377324	-1.205786	-4.476646
1	-0.522414	-0.711614	-4.107060
1	0.725333	-0.691287	-5.378301
1	0.108927	-2.229797	-4.752968
6	0.893269	1.292360	-3.124237
1	-0.088321	1.050972	-2.711327
1	1.243000	2.214976	-2.650016
1	0.786050	1.495631	-4.193738
6	2.632497	-2.127277	-3.863804
1	2.253967	-3.133369	-4.064026
1	3.102584	-1.747276	-4.775579
1	3.396046	-2.210176	-3.084962
6	3.301001	0.640948	-3.346149
1	4.084642	-0.066597	-3.068819
1	3.320440	0.775500	-4.432062
1	3.541789	1.602358	-2.883226
6	-0.276534	-3.989908	2.158842
1	-1.047652	-3.486207	1.573000
1	0.002196	-4.917122	1.649527
1	-0.699072	-4.249248	3.134479
6	-0.616254	-1.493185	3.583375
1	-0.751944	-0.448016	3.871560
1	-1.495438	-1.807054	3.019068
1	-0.541452	-2.089252	4.499005

6	2.029413	-3.823191	3.141549
1	1.679658	-3.955113	4.170622
1	2.225451	-4.813851	2.720863
1	2.972204	-3.273907	3.163897
6	1.832836	-0.924427	3.404808
1	1.589367	0.135653	3.517781
1	2.053899	-1.333893	4.394876
1	2.730525	-0.994670	2.783462
6	-4.542755	-3.446420	-2.371192
1	-4.127132	-3.357701	-3.379812
1	-4.994917	-4.440027	-2.277678
1	-5.327234	-2.694298	-2.267508
6	-2.253820	-4.181174	-1.647018
1	-1.456090	-4.056068	-0.909673
1	-2.554347	-5.233911	-1.667616
1	-1.842989	-3.917250	-2.625154
6	-3.768331	-4.692478	0.812571
1	-4.074437	-4.629596	1.862005
1	-4.414341	-5.425165	0.316655
1	-2.742080	-5.062382	0.786185
6	-5.312037	-2.766101	0.368073
1	-6.081236	-3.426765	-0.044188
1	-5.496197	-2.662483	1.442354
1	-5.412908	-1.779249	-0.091613
6	-5.459741	0.507649	-2.331742
1	-6.137054	0.074484	-1.589025
1	-6.039078	0.721587	-3.235797
1	-4.691731	-0.235324	-2.560594
6	-5.902016	2.789826	-1.376361
1	-6.393281	3.180099	-2.274494
1	-6.666706	2.312740	-0.754930
1	-5.489191	3.628633	-0.812038
6	-3.322845	3.801212	-2.316510
1	-2.374530	4.059429	-2.797494
1	-4.094643	4.481988	-2.689671
1	-3.207523	3.957561	-1.239828
6	-3.810736	2.126467	-4.122510
1	-4.700310	2.643396	-4.498915
1	-2.937945	2.530689	-4.645409
1	-3.887760	1.066562	-4.372628
1	3.761054	-0.541501	-0.465294
6	5.538647	-1.388962	0.336301
6	4.855283	-2.761604	0.358403
6	6.627872	-1.336496	-0.751764
1	6.021810	-1.211508	1.304473
6	5.876587	-3.891461	0.543907
1	4.322108	-2.908920	-0.593175
1	4.090503	-2.788859	1.139023
6	7.654736	-2.462638	-0.562727
1	6.144992	-1.437710	-1.735020
1	7.109435	-0.354376	-0.722405
6	6.975164	-3.840112	-0.529155
1	5.365590	-4.861199	0.524547
1	6.337739	-3.798760	1.537574
1	8.407142	-2.425022	-1.359575
1	8.192523	-2.301851	0.382416
1	7.717084	-4.628277	-0.352764
1	6.526148	-4.044184	-1.511857

TS[4-5]_m

Number of imaginary frequencies : 1
Imaginary frequency : -19.7014 cm(-1)

Electronic energy : HF=-2935.6849253
Zero-point correction= 1.177763 (Hartree/Particle)
Thermal correction to Energy= 1.243569
Thermal correction to Enthalpy= 1.244513
Thermal correction to Gibbs Free Energy= 1.080366
Sum of electronic and zero-point Energies= -2934.507162
Sum of electronic and thermal Energies= -2934.441356
Sum of electronic and thermal Enthalpies= -2934.440412
Sum of electronic and thermal Free Energies= -2934.604559

Cartesian Coordinates

6 0.793792 2.625372 0.189961
6 -0.362321 2.278576 2.178628
6 0.424237 3.242665 2.819321
6 1.451612 3.862263 2.119283
6 1.676941 3.538149 0.774046
1 0.863657 2.357228 -0.856163
1 0.272049 3.478699 3.865485
1 2.105694 4.570382 2.618290
7 -0.169345 1.996184 0.870197
6 -1.404549 1.485614 2.865401
6 -1.827341 1.758207 4.171716
6 -2.873989 -0.318329 2.738166
6 -2.794010 0.954217 4.766109
1 -1.408915 2.593723 4.719146
1 -3.244145 -1.130194 2.126421
1 -3.125534 1.156749 5.779737
7 -1.935169 0.451901 2.161565
6 -3.324696 -0.108297 4.036976
1 -4.077959 -0.766460 4.456209
77 -1.321859 0.253267 0.066762
5 0.468092 -0.726434 -1.008565
8 0.180360 -1.718287 -1.952320
8 1.529160 0.091911 -1.520827
6 1.539484 -0.056976 -2.973798
6 0.931747 -1.502835 -3.162204
5 -2.455133 -1.371226 -0.453765
8 -2.643163 -2.455315 0.418843
8 -3.189564 -1.586617 -1.622045
6 -3.656744 -3.334696 -0.121870
6 -3.635907 -2.963036 -1.647956
5 0.663687 -1.273434 0.694549
8 0.834709 -2.623735 0.891257
8 0.957203 -0.548195 1.829298
6 1.397774 -1.457199 2.881105
6 0.955845 -2.867094 2.324720
1 -1.028453 0.378885 -1.476661
5 -2.994161 1.222045 -0.549164
8 -3.132466 1.903230 -1.753236
8 -4.160325 1.324111 0.212655
6 -4.367759 2.660210 -1.708483
6 -5.201830 1.867336 -0.640587
6 2.831837 4.104229 0.038414
6 3.010119 5.496936 0.006472
6 3.819253 3.269966 -0.540879
6 4.140126 6.070391 -0.568358

1	2.242829	6.128612	0.445879
6	4.961862	3.859524	-1.105063
6	5.122823	5.241345	-1.115561
1	4.255564	7.149933	-0.585130
1	5.727975	3.214378	-1.516889
1	6.015016	5.671840	-1.561394
7	3.681982	1.867122	-0.541010
1	2.787616	1.449178	-0.779067
6	4.709587	0.992035	-0.192004
8	5.791681	1.369021	0.256336
7	4.398096	-0.323664	-0.420130
6	-0.019466	-1.625108	-4.352181
1	-0.885946	-0.972926	-4.231589
1	0.488677	-1.375693	-5.289965
1	-0.381349	-2.653910	-4.427495
6	0.672035	1.066987	-3.557939
1	-0.357679	1.024294	-3.199221
1	1.093530	2.032518	-3.259802
1	0.662152	1.031472	-4.651063
6	1.990004	-2.608540	-3.218869
1	1.485513	-3.578091	-3.176620
1	2.585172	-2.567770	-4.136524
1	2.659452	-2.549626	-2.359022
6	2.969580	0.106207	-3.485024
1	3.664362	-0.593843	-3.021564
1	2.999456	-0.041519	-4.569367
1	3.328330	1.117543	-3.273531
6	-0.432490	-3.310381	2.797161
1	-1.188485	-2.563656	2.552508
1	-0.708185	-4.225624	2.267256
1	-0.446749	-3.513475	3.872452
6	0.719163	-1.041069	4.183095
1	1.057968	-0.041504	4.470640
1	-0.366683	-1.015790	4.084446
1	0.981286	-1.730126	4.992566
6	1.964165	-3.989667	2.547738
1	2.074124	-4.201599	3.616461
1	1.608984	-4.900291	2.056834
1	2.947622	-3.752372	2.141263
6	2.911886	-1.270831	2.993130
1	3.126252	-0.223174	3.223027
1	3.341823	-1.893972	3.783018
1	3.404180	-1.506356	2.049868
6	-4.992037	-3.029325	-2.344775
1	-4.884607	-2.715062	-3.387613
1	-5.384670	-4.052121	-2.339166
1	-5.725845	-2.373379	-1.872915
6	-2.592499	-3.755151	-2.445400
1	-1.605098	-3.666091	-1.986674
1	-2.862444	-4.812505	-2.534538
1	-2.528559	-3.330872	-3.451031
6	-3.268926	-4.774648	0.199930
1	-3.295310	-4.931937	1.282992
1	-3.965948	-5.483279	-0.260694
1	-2.259107	-4.998158	-0.148275
6	-4.977040	-2.970338	0.567949
1	-5.798444	-3.622320	0.254838
1	-4.855884	-3.076612	1.650992
1	-5.250048	-1.933348	0.355417
6	-5.952385	0.671767	-1.239549
1	-6.366961	0.071653	-0.423903

1	-6.779189	0.988294	-1.883115
1	-5.269444	0.039341	-1.811645
6	-6.140323	2.714832	0.211051
1	-6.899948	3.201064	-0.410561
1	-6.656513	2.077504	0.935996
1	-5.599782	3.483460	0.767543
6	-4.005209	4.079302	-1.253522
1	-3.258390	4.491111	-1.938715
1	-4.874237	4.744994	-1.251111
1	-3.570248	4.067224	-0.249691
6	-4.972822	2.690600	-3.108110
1	-5.953939	3.177979	-3.099852
1	-4.320431	3.255889	-3.780992
1	-5.083670	1.684532	-3.516751
1	3.446195	-0.542709	-0.692891
6	5.263165	-1.413867	0.027732
6	4.548710	-2.751612	-0.206417
6	6.629452	-1.431016	-0.681537
1	5.450919	-1.293810	1.106012
6	5.383069	-3.922864	0.327964
1	4.406419	-2.879867	-1.287383
1	3.547536	-2.746305	0.238833
6	7.489123	-2.595713	-0.165808
1	6.457687	-1.538408	-1.761992
1	7.131492	-0.475128	-0.521321
6	6.776058	-3.947500	-0.321697
1	4.857419	-4.867783	0.146858
1	5.489355	-3.825793	1.417954
1	8.451589	-2.610317	-0.690831
1	7.717986	-2.428140	0.896436
1	7.383259	-4.753406	0.108188
1	6.664043	-4.173143	-1.391719

5

Number of imaginary frequencies : 0

Electronic energy : HF=-2935.6929275
 Zero-point correction= 1.178074 (Hartree/Particle)
 Thermal correction to Energy= 1.244535
 Thermal correction to Enthalpy= 1.245479
 Thermal correction to Gibbs Free Energy= 1.078665
 Sum of electronic and zero-point Energies= -2934.514854
 Sum of electronic and thermal Energies= -2934.448392
 Sum of electronic and thermal Enthalpies= -2934.447448
 Sum of electronic and thermal Free Energies= -2934.614263

Cartesian Coordinates

6	0.621350	1.988692	0.698657
6	-0.837187	1.592637	2.480313
6	-0.344869	2.725799	3.139671
6	0.682659	3.466626	2.574890
6	1.207780	3.089815	1.329316
1	0.941085	1.660578	-0.282691
1	-0.734725	3.005022	4.110383
1	1.096215	4.319822	3.103146
7	-0.348678	1.251138	1.259135
6	-1.831912	0.677909	3.073312

6	-2.426339	0.902750	4.322915
6	-2.945453	-1.351830	2.864281
6	-3.303004	-0.043685	4.840731
1	-2.209899	1.802326	4.886347
1	-3.128253	-2.211749	2.235015
1	-3.772150	0.116830	5.806563
7	-2.110804	-0.434460	2.354344
6	-3.561544	-1.197813	4.102771
1	-4.229977	-1.968567	4.471148
77	-1.070333	-0.573732	0.319629
5	-0.021155	-0.539167	-1.444123
8	-0.444383	-1.110891	-2.636801
8	1.197855	0.131407	-1.653352
6	1.373148	0.321379	-3.084245
6	0.517195	-0.858630	-3.679125
5	-2.819009	-1.292893	-0.635466
8	-3.653479	-2.150534	0.091290
8	-3.294574	-1.166445	-1.933960
6	-4.831682	-2.440182	-0.697237
6	-4.312307	-2.174157	-2.154650
5	0.564348	-1.427337	1.429082
8	1.866516	-0.902811	1.576493
8	0.366094	-2.431847	2.365639
6	1.594594	-2.675902	3.096383
6	2.374833	-1.336076	2.878761
1	-1.217124	-2.107220	-0.093412
5	-2.420226	0.919821	-0.512704
8	-1.982719	1.768937	-1.515870
8	-3.562974	1.427314	0.094070
6	-2.715658	3.017889	-1.428983
6	-4.019906	2.582524	-0.667359
6	2.312054	3.837650	0.684950
6	2.224214	5.237459	0.628093
6	3.454952	3.189561	0.137485
6	3.212405	6.009949	0.027331
1	1.339794	5.714690	1.041155
6	4.453364	3.982338	-0.461278
6	4.324129	5.366895	-0.519156
1	3.113130	7.089992	-0.019091
1	5.321126	3.490756	-0.875099
1	5.110764	5.946730	-0.994284
7	3.577241	1.797786	0.246226
1	2.866399	1.315481	0.781443
6	4.452832	0.961736	-0.454013
8	5.359031	1.369517	-1.184154
7	4.213318	-0.362730	-0.237198
6	-0.241530	-0.511347	-4.958689
1	-0.939847	0.311009	-4.793840
1	0.447975	-0.236119	-5.764523
1	-0.820377	-1.379387	-5.289756
6	0.811537	1.710468	-3.413755
1	-0.241356	1.777779	-3.133993
1	1.364058	2.458438	-2.835633
1	0.925321	1.953599	-4.474834
6	1.309727	-2.156021	-3.878844
1	0.609012	-2.962313	-4.116029
1	2.036585	-2.079632	-4.693648
1	1.837707	-2.435511	-2.964172
6	2.854806	0.263475	-3.434071
1	3.312288	-0.664262	-3.093274
1	2.989294	0.335178	-4.519008

1	3.397137	1.093137	-2.974644
6	3.891409	-1.474289	2.832035
1	4.217623	-2.163592	2.054105
1	4.355099	-0.504919	2.632210
1	4.264617	-1.837698	3.795533
6	2.269464	-3.886382	2.444324
1	1.575993	-4.731857	2.467429
1	2.506977	-3.679233	1.398150
1	3.186194	-4.177834	2.966152
6	1.983969	-0.240106	3.878182
1	2.379452	-0.443548	4.877753
1	2.392502	0.715495	3.536662
1	0.898207	-0.138686	3.948018
6	1.243068	-2.982152	4.549140
1	2.147983	-3.082628	5.158090
1	0.613244	-2.202870	4.983152
1	0.692301	-3.926046	4.604089
6	-5.353154	-1.618733	-3.120083
1	-4.882962	-1.407191	-4.085228
1	-6.156210	-2.345139	-3.285575
1	-5.795448	-0.692111	-2.750896
6	-3.601926	-3.383439	-2.775025
1	-2.844755	-3.782823	-2.094470
1	-4.304130	-4.183028	-3.031552
1	-3.091104	-3.061428	-3.686335
6	-5.262718	-3.876628	-0.418620
1	-5.592069	-3.970439	0.621148
1	-6.099521	-4.164494	-1.064026
1	-4.442398	-4.579696	-0.574673
6	-5.916063	-1.457232	-0.245069
1	-6.861250	-1.608898	-0.775656
1	-6.096028	-1.598668	0.825130
1	-5.578515	-0.429491	-0.389620
6	-5.122168	2.096815	-1.612983
1	-5.943252	1.676487	-1.025998
1	-5.524185	2.915520	-2.217141
1	-4.740609	1.318853	-2.277961
6	-4.573406	3.610510	0.313300
1	-4.867336	4.529380	-0.205019
1	-5.459561	3.204163	0.810547
1	-3.842804	3.862569	1.084473
6	-1.845593	3.996802	-0.631385
1	-0.872788	4.090161	-1.121427
1	-2.300523	4.990856	-0.579893
1	-1.676514	3.638621	0.386934
6	-2.930466	3.544930	-2.844717
1	-3.560573	4.440792	-2.841704
1	-1.965829	3.813884	-3.285525
1	-3.392053	2.791562	-3.485663
1	3.335135	-0.641328	0.193409
6	4.987487	-1.370780	-0.956262
6	6.385556	-1.580539	-0.349437
6	4.211662	-2.691587	-0.998092
1	5.130303	-1.013455	-1.984409
6	7.164976	-2.641384	-1.141023
1	6.274296	-1.898665	0.696467
1	6.917834	-0.624909	-0.348035
6	4.978925	-3.752296	-1.798289
1	4.066486	-3.053331	0.027641
1	3.213495	-2.524091	-1.416097
6	6.388689	-3.965027	-1.224214

1	8.149662	-2.803768	-0.686840
1	7.348220	-2.266248	-2.157956
1	4.419397	-4.695035	-1.802660
1	5.056942	-3.427655	-2.845568
1	6.940144	-4.694196	-1.830049
1	6.302108	-4.394376	-0.215601

TS[5-A2]_m

Number of imaginary frequencies : 1
Imaginary frequency : -281.8946 cm(-1)

Electronic energy : HF=-2935.6890098
Zero-point correction= 1.176717 (Hartree/Particle)
Thermal correction to Energy= 1.242793
Thermal correction to Enthalpy= 1.243737
Thermal correction to Gibbs Free Energy= 1.078426
Sum of electronic and zero-point Energies= -2934.512293
Sum of electronic and thermal Energies= -2934.446217
Sum of electronic and thermal Enthalpies= -2934.445273
Sum of electronic and thermal Free Energies= -2934.610584

Cartesian Coordinates

6	0.876394	2.099438	0.453574
6	-0.665601	2.070191	2.208618
6	-0.104418	3.245788	2.724897
6	1.000639	3.815789	2.109518
6	1.533567	3.230661	0.949813
1	1.193523	1.608142	-0.458289
1	-0.501519	3.694375	3.627278
1	1.467886	4.697236	2.537196
7	-0.163008	1.522659	1.072725
6	-1.762589	1.330936	2.867533
6	-2.405575	1.791581	4.024769
6	-3.048840	-0.606133	2.877306
6	-3.398974	1.013796	4.609036
1	-2.137570	2.744619	4.463524
1	-3.263735	-1.538556	2.369780
1	-3.907678	1.359423	5.503671
7	-2.100662	0.148424	2.304334
6	-3.722805	-0.212236	4.029461
1	-4.485045	-0.856833	4.453889
77	-1.030789	-0.377836	0.353049
5	-0.063611	-0.534523	-1.452877
8	-0.582192	-1.054639	-2.629137
8	1.230460	-0.033033	-1.696668
6	1.398014	0.117197	-3.134122
6	0.380462	-0.945330	-3.694194
5	-2.618161	-1.506074	-0.407117
8	-3.266481	-2.451170	0.403262
8	-3.251342	-1.442347	-1.640706
6	-4.514066	-2.821101	-0.238825
6	-4.181129	-2.547230	-1.743561
5	0.468474	-1.197930	1.670784
8	1.829352	-0.854153	1.665578
8	0.157777	-1.871301	2.839614
6	1.374183	-2.132188	3.585342

6	2.340481	-1.034268	3.028923
1	-0.736374	-1.959581	0.468682
5	-2.332984	1.033976	-0.629880
8	-1.976600	1.808625	-1.724964
8	-3.546812	1.468064	-0.104326
6	-2.862836	2.954059	-1.790385
6	-4.129249	2.429193	-1.025986
6	2.728595	3.783010	0.268474
6	2.789017	5.167653	0.044176
6	3.818786	2.966405	-0.147219
6	3.872736	5.760439	-0.594876
1	1.944540	5.777370	0.353785
6	4.914302	3.577872	-0.785608
6	4.931633	4.951052	-1.010268
1	3.886494	6.831369	-0.772135
1	5.737210	2.954154	-1.102732
1	5.789806	5.389990	-1.511733
7	3.800622	1.591638	0.125226
1	3.032223	1.255629	0.689972
6	4.535531	0.584476	-0.517098
8	5.469964	0.801598	-1.290545
7	4.110434	-0.663872	-0.180364
6	-0.359075	-0.515634	-4.960156
1	-0.933799	0.396893	-4.792440
1	0.336338	-0.350875	-5.790632
1	-1.061471	-1.301020	-5.256379
6	1.014141	1.563521	-3.471824
1	-0.012261	1.773390	-3.162299
1	1.680773	2.242772	-2.931310
1	1.121399	1.772078	-4.540842
6	0.989427	-2.338286	-3.895781
1	0.184441	-3.045041	-4.118837
1	1.706407	-2.359869	-4.722444
1	1.490853	-2.682894	-2.988312
6	2.852688	-0.137849	-3.509832
1	3.189715	-1.119147	-3.176611
1	2.978276	-0.083844	-4.597032
1	3.508578	0.611041	-3.059809
6	3.809026	-1.435753	2.986260
1	3.971544	-2.318812	2.368461
1	4.413310	-0.624571	2.573589
1	4.167165	-1.648767	3.998997
6	1.814266	-3.557933	3.236236
1	0.995352	-4.245663	3.465038
1	2.038593	-3.647375	2.169641
1	2.694344	-3.866532	3.808512
6	2.188080	0.320161	3.730391
1	2.588776	0.293674	4.747785
1	2.740219	1.079834	3.169564
1	1.140354	0.625621	3.776198
6	1.064136	-2.018302	5.074053
1	1.976392	-2.116315	5.672078
1	0.588560	-1.064635	5.311843
1	0.378191	-2.817680	5.369980
6	-5.367592	-2.123362	-2.602193
1	-5.032321	-1.924976	-3.624847
1	-6.120567	-2.918073	-2.640436
1	-5.837676	-1.215754	-2.221754
6	-3.426141	-3.702659	-2.412976
1	-2.578693	-4.021007	-1.799565
1	-4.075383	-4.565233	-2.594837

1	-3.030803	-3.355166	-3.371246
6	-4.832558	-4.271111	0.105252
1	-5.037601	-4.364113	1.176709
1	-5.718974	-4.614350	-0.438894
1	-3.997521	-4.932581	-0.133217
6	-5.596050	-1.883228	0.311981
1	-6.585225	-2.117524	-0.093376
1	-5.643008	-1.989145	1.400132
1	-5.353823	-0.841526	0.084695
6	-5.091648	1.651666	-1.929613
1	-5.857556	1.178560	-1.307847
1	-5.593156	2.305459	-2.649819
1	-4.558592	0.864090	-2.466695
6	-4.881056	3.481312	-0.218525
1	-5.274924	4.269081	-0.869937
1	-5.726606	3.015584	0.297518
1	-4.240819	3.941022	0.537318
6	-2.151625	4.101743	-1.061705
1	-1.176704	4.269232	-1.528528
1	-2.722109	5.034505	-1.111229
1	-1.981949	3.850913	-0.010442
6	-3.087953	3.312142	-3.255078
1	-3.826800	4.114820	-3.354354
1	-2.150382	3.659857	-3.699924
1	-3.429049	2.447077	-3.826739
1	3.214056	-0.765567	0.288864
6	4.660326	-1.848293	-0.829877
6	5.985079	-2.306971	-0.197158
6	3.614246	-2.969411	-0.790238
1	4.868712	-1.593146	-1.876507
6	6.510893	-3.570839	-0.894082
1	5.816655	-2.512759	0.868387
1	6.710743	-1.489848	-0.261666
6	4.133091	-4.235372	-1.483646
1	3.378125	-3.198959	0.258193
1	2.684619	-2.614429	-1.246661
6	5.465689	-4.697405	-0.873071
1	7.441975	-3.904062	-0.420317
1	6.760092	-3.329243	-1.937205
1	3.382980	-5.032445	-1.418001
1	4.277480	-4.027426	-2.553160
1	5.842963	-5.578651	-1.405845
1	5.293554	-5.007913	0.167653

A2+HBpin

Number of imaginary frequencies : 0

Electronic energy : HF=-2935.7086639
 Zero-point correction= 1.179005 (Hartree/Particle)
 Thermal correction to Energy= 1.245688
 Thermal correction to Enthalpy= 1.246633
 Thermal correction to Gibbs Free Energy= 1.078693
 Sum of electronic and zero-point Energies= -2934.529659
 Sum of electronic and thermal Energies= -2934.462976
 Sum of electronic and thermal Enthalpies= -2934.462031
 Sum of electronic and thermal Free Energies= -2934.629971

Cartesian Coordinates

6	-1.270335	-2.330963	-0.057730
6	0.195731	-2.790215	1.687892
6	-0.592820	-3.877484	2.083242
6	-1.778549	-4.145928	1.408611
6	-2.161286	-3.342786	0.323905
1	-1.477690	-1.690534	-0.906688
1	-0.320309	-4.471623	2.947732
1	-2.426550	-4.950674	1.742382
7	-0.149659	-2.048305	0.611620
6	1.374221	-2.317517	2.447310
6	2.010154	-3.088279	3.428561
6	2.839707	-0.545839	2.838024
6	3.085909	-2.552339	4.129068
1	1.680409	-4.101325	3.626837
1	3.141427	0.450849	2.534439
1	3.592362	-3.141447	4.887385
7	1.799993	-1.060965	2.159433
6	3.505114	-1.255051	3.834214
1	4.340571	-0.797173	4.352877
77	0.993558	-0.146792	0.241773
5	0.369237	0.212389	-1.672577
8	1.132464	0.270316	-2.837156
8	-0.996094	0.303068	-2.007724
6	-1.133896	0.212374	-3.450764
6	0.283743	0.677103	-3.935236
5	2.041855	1.599228	0.113783
8	3.193631	1.893339	0.862209
8	1.670759	2.734075	-0.619255
6	3.744762	3.145467	0.391578
6	2.472056	3.856128	-0.189687
5	-0.776610	0.754753	1.786163
8	-1.932202	0.031317	2.016344
8	-0.403527	1.515923	2.855206
6	-1.484200	1.469616	3.841372
6	-2.255807	0.153591	3.443893
1	-0.420620	0.979810	0.619274
5	2.570300	-1.095861	-0.656391
8	2.597046	-2.485238	-0.829813
8	3.752810	-0.532627	-1.118538
6	3.937814	-2.866468	-1.226136
6	4.480525	-1.537306	-1.862179
6	-3.439951	-3.529721	-0.401778
6	-3.807730	-4.817334	-0.821553
6	-4.296680	-2.434476	-0.697705
6	-4.968072	-5.039959	-1.556460
1	-3.142951	-5.645772	-0.592281
6	-5.463274	-2.668363	-1.446336
6	-5.784008	-3.952799	-1.876659
1	-5.223486	-6.042286	-1.886195
1	-6.103144	-1.831088	-1.685721
1	-6.690156	-4.103244	-2.456917
7	-3.997809	-1.161645	-0.182875
1	-3.314056	-1.124424	0.563075
6	-4.333098	0.067889	-0.759336
8	-5.014172	0.175498	-1.779338
7	-3.836214	1.132949	-0.058865
6	0.785651	0.006936	-5.211054

1	0.852172	-1.076914	-5.096614
1	0.126719	0.228266	-6.057749
1	1.785693	0.379481	-5.453382
6	-1.428648	-1.256391	-3.780689
1	-0.610178	-1.902399	-3.448505
1	-2.342505	-1.566731	-3.266196
1	-1.580812	-1.409323	-4.853677
6	0.408638	2.201499	-4.052322
1	1.461787	2.456633	-4.200035
1	-0.166101	2.595460	-4.896819
1	0.079160	2.690890	-3.132471
6	-2.298711	1.093090	-3.892180
1	-2.169539	2.124378	-3.558327
1	-2.390432	1.092451	-4.984143
1	-3.233841	0.715240	-3.469167
6	-3.772996	0.216001	3.570191
1	-4.202301	1.010050	2.956904
1	-4.207919	-0.731772	3.238461
1	-4.067882	0.377947	4.611478
6	-2.311229	2.740174	3.634000
1	-1.659625	3.612106	3.735445
1	-2.752633	2.767767	2.634655
1	-3.116025	2.819912	4.370357
6	-1.707738	-1.099809	4.125479
1	-1.952162	-1.108210	5.191349
1	-2.151512	-1.983728	3.661297
1	-0.623004	-1.167705	4.015177
6	-0.858610	1.457176	5.230429
1	-1.628129	1.359535	6.002842
1	-0.140993	0.642482	5.342406
1	-0.327309	2.398313	5.398356
6	2.725721	4.763159	-1.389668
1	1.779228	5.191224	-1.735165
1	3.395290	5.589862	-1.127550
1	3.162482	4.208026	-2.221796
6	1.660279	4.599566	0.879949
1	1.469615	3.950534	1.739591
1	2.163383	5.508820	1.224743
1	0.692916	4.882795	0.454134
6	4.409547	3.861328	1.563137
1	5.268606	3.278603	1.911276
1	4.773508	4.850765	1.265222
1	3.722196	3.981305	2.403305
6	4.783318	2.800603	-0.683382
1	5.279110	3.695381	-1.074057
1	5.542984	2.147757	-0.243801
1	4.318801	2.253091	-1.506601
6	4.093712	-1.375099	-3.337122
1	4.330631	-0.354999	-3.652386
1	4.638642	-2.073134	-3.981111
1	3.019565	-1.515202	-3.472504
6	5.974926	-1.293716	-1.674982
1	6.565859	-2.082271	-2.153970
1	6.252159	-0.338864	-2.132089
1	6.243859	-1.247815	-0.617828
6	4.683259	-3.266218	0.054125
1	4.131069	-4.069467	0.551513
1	5.696495	-3.623948	-0.154643
1	4.744772	-2.421639	0.746601
6	3.848035	-4.052602	-2.180245
1	4.836381	-4.318694	-2.570622

1	3.447628	-4.924445	-1.652720
1	3.186434	-3.837680	-3.021703
1	-3.168537	0.932631	0.674891
6	-3.814776	2.484177	-0.617858
6	-4.790751	3.417915	0.118380
6	-2.385831	3.050027	-0.595245
1	-4.142680	2.394531	-1.658408
6	-4.742792	4.840767	-0.460135
1	-4.519201	3.445607	1.183936
1	-5.804303	3.005371	0.058777
6	-2.341440	4.469218	-1.177090
1	-2.026678	3.083046	0.444397
1	-1.721026	2.374642	-1.138012
6	-3.314208	5.405863	-0.445694
1	-5.421863	5.497569	0.096902
1	-5.109891	4.817390	-1.496049
1	-1.317884	4.858107	-1.126801
1	-2.608716	4.430278	-2.242969
1	-3.296293	6.405856	-0.895899
1	-2.983065	5.522537	0.596638

$\mathbf{1}_o$

Number of imaginary frequencies : 0

Electronic energy : HF=-3396.6214613
 Zero-point correction= 1.460717 (Hartree/Particle)
 Thermal correction to Energy= 1.540610
 Thermal correction to Enthalpy= 1.541554
 Thermal correction to Gibbs Free Energy= 1.344154
 Sum of electronic and zero-point Energies= -3395.160744
 Sum of electronic and thermal Energies= -3395.080851
 Sum of electronic and thermal Enthalpies= -3395.079907
 Sum of electronic and thermal Free Energies= -3395.277307

Cartesian Coordinates

77	-1.416772	-0.336339	-0.095132
5	-2.673343	-1.105245	-1.441221
8	-2.468933	-0.936272	-2.816764
8	-3.855182	-1.806204	-1.212889
6	-3.401779	-1.799762	-3.513488
6	-4.564195	-1.929221	-2.465717
5	-0.685035	-2.224664	0.081554
8	-1.137796	-3.372792	-0.579404
8	0.454334	-2.556482	0.846859
6	-0.179031	-4.437038	-0.394208
6	0.546409	-4.004248	0.924537
5	-2.772839	-0.914616	1.312727
8	-2.706435	-2.013330	2.183210
8	-3.954431	-0.196567	1.587274
6	-3.995710	-2.199487	2.807229
6	-4.598254	-0.749909	2.755755
6	-1.585425	2.342496	-1.707521
6	-0.363022	1.687712	-2.228575
7	-2.149205	1.772987	-0.612250
7	-0.021550	0.512900	-1.645025
6	-2.149684	3.481058	-2.298506
6	-3.295804	4.044966	-1.745860
6	-3.855834	3.461346	-0.609804

6	-3.254104	2.323422	-0.079094
6	0.421411	2.219391	-3.257183
6	1.556413	1.537387	-3.681523
6	1.913992	0.325047	-3.075953
6	1.072222	-0.136385	-2.052990
6	0.668294	0.380615	1.895899
6	1.041974	1.731282	1.887892
6	-0.016766	-0.163182	2.984496
6	0.782337	2.520520	3.017657
6	-0.285375	0.632838	4.099912
6	0.127932	1.968129	4.119838
1	0.957437	-0.260315	1.070241
1	-0.325334	-1.200373	2.940362
1	-0.053700	2.581443	4.997961
1	1.115039	3.551700	3.051377
1	-3.667052	1.791237	0.771187
1	-4.748408	3.867108	-0.145873
1	-3.744054	4.923394	-2.199339
1	-1.712858	3.915408	-3.189698
1	0.164309	3.164905	-3.718893
1	2.177689	1.951268	-4.469573
1	1.278951	-1.069185	-1.543463
6	3.082820	-0.467992	-3.524875
6	3.264602	-0.681322	-4.901275
6	4.004493	-1.041153	-2.611102
6	4.302016	-1.472627	-5.383724
1	2.547691	-0.247988	-5.593061
6	5.048077	-1.842405	-3.107206
6	5.185305	-2.060140	-4.474596
1	4.411302	-1.640142	-6.450826
1	5.737813	-2.288675	-2.404615
1	5.999013	-2.685643	-4.831022
7	3.901534	-0.735711	-1.247702
6	4.294387	-1.560662	-0.191154
8	4.751590	-2.694042	-0.353864
7	4.126487	-0.971858	1.029122
1	3.420974	0.121600	-0.993197
1	3.639171	-0.080156	1.066985
6	1.819864	2.213327	0.700244
8	2.703080	1.471067	0.225217
7	1.577623	3.439755	0.167511
1	-0.799470	0.209835	4.958026
6	0.374613	4.236470	0.445297
1	-0.120298	4.419922	-0.513605
1	-0.316721	3.632694	1.033163
6	2.440461	3.909854	-0.932800
1	2.703632	3.050019	-1.549748
1	1.829131	4.577255	-1.547197
6	3.702818	4.656848	-0.470750
1	4.137239	5.137859	-1.358375
1	3.403446	5.466601	0.204454
6	4.774981	3.787468	0.204862
1	5.536259	4.449995	0.638447
1	4.331034	3.242056	1.044707
6	5.460002	2.795026	-0.742568
1	6.021562	3.353528	-1.506296
1	4.703038	2.210656	-1.276596
6	6.397859	1.820623	-0.022164
1	7.125452	2.384877	0.578415
1	5.808515	1.221983	0.683225
6	7.137403	0.884100	-0.980691

1	7.790456	1.443925	-1.661615
1	7.760477	0.165302	-0.436967
1	6.433178	0.311320	-1.593152
6	0.652959	5.569947	1.153259
1	1.351780	5.394968	1.979367
1	1.160126	6.256073	0.463060
6	-0.627913	6.223877	1.692176
1	-1.108195	5.533967	2.400716
1	-0.353741	7.115092	2.271542
6	-1.640269	6.621145	0.610353
1	-1.936116	5.737831	0.031592
1	-1.160268	7.308741	-0.101503
6	-2.904027	7.276190	1.179878
1	-3.372692	6.587247	1.895944
1	-2.625571	8.170471	1.753752
6	-3.919141	7.655248	0.098676
1	-4.812061	8.122045	0.528400
1	-3.489047	8.361918	-0.621209
1	-4.245308	6.771520	-0.462813
6	4.347447	-1.698300	2.273479
6	5.618214	-1.217686	2.996383
6	3.120614	-1.575806	3.186857
1	4.484645	-2.748160	1.996097
6	5.825435	-1.980227	4.314377
1	5.520623	-0.141798	3.201826
1	6.481950	-1.339663	2.332896
6	3.322396	-2.336062	4.503736
1	2.948814	-0.513101	3.407630
1	2.235304	-1.931697	2.653654
6	4.594774	-1.870509	5.227928
1	6.719287	-1.608406	4.829561
1	6.012105	-3.039666	4.088104
1	2.443428	-2.206065	5.146747
1	3.400415	-3.412120	4.291610
1	4.748558	-2.452251	6.145190
1	4.468178	-0.822489	5.535965
6	-2.677002	-3.127409	-3.764954
1	-3.299252	-3.833803	-4.324110
1	-1.772850	-2.929498	-4.349125
1	-2.373365	-3.577676	-2.816614
6	-3.790503	-1.138379	-4.831075
1	-2.914999	-1.075484	-5.485206
1	-4.559568	-1.720444	-5.350608
1	-4.166711	-0.125097	-4.674671
6	-5.302389	-3.263848	-2.478081
1	-6.086945	-3.259296	-1.714715
1	-5.777091	-3.443148	-3.449065
1	-4.625975	-4.091527	-2.257558
6	-5.562557	-0.765734	-2.529229
1	-6.200932	-0.818044	-3.417101
1	-6.200695	-0.800815	-1.641189
1	-5.040023	0.195452	-2.527188
6	-6.109787	-0.685411	2.554619
1	-6.405522	-1.162734	1.618623
1	-6.640264	-1.171299	3.380902
1	-6.434047	0.359763	2.514989
6	-4.766968	-3.199774	1.936258
1	-4.191928	-4.128865	1.875906
1	-5.753657	-3.432353	2.350364
1	-4.875979	-2.813895	0.919606
6	-4.185045	0.118118	3.951024

1	-4.475573	1.155363	3.755930
1	-4.665295	-0.202516	4.881039
1	-3.100837	0.096696	4.086192
6	-3.786471	-2.763381	4.209268
1	-4.736685	-2.841741	4.748853
1	-3.353863	-3.766515	4.142311
1	-3.102721	-2.144624	4.794583
6	2.008382	-4.430236	1.016461
1	2.090448	-5.519704	0.930307
1	2.632216	-3.973229	0.247477
1	2.420210	-4.146633	1.988869
6	-0.208369	-4.422572	2.193170
1	-0.174931	-5.505444	2.351012
1	0.262644	-3.940211	3.055823
1	-1.247452	-4.087678	2.153380
6	-0.933083	-5.760258	-0.310148
1	-1.412511	-5.975476	-1.270511
1	-0.252698	-6.587412	-0.079586
1	-1.713717	-5.722929	0.452282
6	0.751022	-4.430396	-1.615016
1	0.146096	-4.520830	-2.522236
1	1.313632	-3.494733	-1.678503
1	1.466671	-5.257829	-1.590983

TS[1-2]_o

Number of imaginary frequencies : 1
Imaginary frequency: -712.4880 cm(-1)

Electronic energy : HF=-3396.5803382
Zero-point correction= 1.456352 (Hartree/Particle)
Thermal correction to Energy= 1.535737
Thermal correction to Enthalpy= 1.536681
Thermal correction to Gibbs Free Energy= 1.342038
Sum of electronic and zero-point Energies= -3395.123986
Sum of electronic and thermal Energies= -3395.044601
Sum of electronic and thermal Enthalpies= -3395.043657
Sum of electronic and thermal Free Energies= -3395.238300

Cartesian Coordinates

77	-1.143159	-0.285060	0.069139
5	-2.145213	-1.548506	-1.305983
8	-2.174165	-1.267407	-2.668849
8	-2.833685	-2.730275	-1.046271
6	-2.615100	-2.459545	-3.368302
6	-3.476274	-3.174645	-2.269361
5	-0.410482	-2.191826	0.518010
8	0.197729	-2.971887	-0.465677
8	-0.348563	-2.831648	1.743635
6	0.830401	-4.117599	0.166570
6	0.047247	-4.209815	1.524510
5	-2.815015	-0.715774	1.178119
8	-2.926854	-1.462782	2.346424
8	-4.086003	-0.238829	0.810898
6	-4.326123	-1.710633	2.617180
6	-5.017807	-0.508132	1.885266
6	-1.314631	1.643859	-2.324922
6	-0.057474	0.912352	-2.572332
7	-1.965513	1.368277	-1.162538

7	0.355754	0.091838	-1.578693
6	-1.815692	2.607135	-3.211784
6	-2.980573	3.297856	-2.900018
6	-3.624456	3.020167	-1.694085
6	-3.085223	2.048829	-0.859239
6	0.703798	1.051409	-3.739213
6	1.907340	0.368085	-3.863142
6	2.346329	-0.466797	-2.824590
6	1.504367	-0.574833	-1.710609
6	-0.331433	1.073418	1.732451
6	0.638469	2.086346	1.561363
6	-0.892112	0.976750	3.026043
6	1.005776	2.944239	2.612569
6	-0.539721	1.832241	4.070877
6	0.421507	2.823906	3.870945
1	-0.144748	-0.488060	1.314523
1	-1.598519	0.179849	3.226400
1	0.720821	3.484159	4.679909
1	1.764324	3.703514	2.438769
1	-3.560210	1.761832	0.068616
1	-4.529775	3.539299	-1.399648
1	-3.372237	4.046258	-3.581780
1	-1.294732	2.819033	-4.137165
1	0.372422	1.696997	-4.543239
1	2.515779	0.495220	-4.753197
1	1.755555	-1.235386	-0.896703
6	3.609774	-1.240052	-2.899630
6	3.920350	-1.918831	-4.089757
6	4.500859	-1.347302	-1.797718
6	5.056476	-2.714576	-4.200468
1	3.227070	-1.848859	-4.923210
6	5.647023	-2.151336	-1.919681
6	5.913237	-2.833008	-3.103549
1	5.263792	-3.244577	-5.125205
1	6.309362	-2.235448	-1.069395
1	6.803363	-3.452378	-3.170174
7	4.256825	-0.617931	-0.623869
6	4.439206	-1.108453	0.679138
8	5.089497	-2.121845	0.934551
7	3.803775	-0.339755	1.609961
1	3.636999	0.180660	-0.702453
1	3.205018	0.416247	1.278940
6	1.406497	2.289543	0.285391
8	2.398128	1.580573	0.030936
7	1.048177	3.323565	-0.516077
1	-1.000881	1.705216	5.047199
6	-0.182033	4.097207	-0.296491
1	-0.690616	4.172445	-1.261236
1	-0.831126	3.514102	0.356553
6	1.868983	3.635603	-1.696723
1	2.282232	2.698629	-2.070871
1	1.191572	4.025621	-2.463145
6	2.995021	4.651750	-1.437643
1	3.436866	4.904386	-2.411819
1	2.555426	5.577055	-1.050567
6	4.100865	4.168701	-0.487009
1	4.708435	5.032539	-0.186031
1	3.648051	3.780077	0.431554
6	5.023552	3.101520	-1.089158
1	5.605749	3.551347	-1.906886
1	4.425382	2.300865	-1.538260

6	5.972997	2.479332	-0.059112
1	6.489435	3.278425	0.491743
1	5.377147	1.928058	0.679436
6	7.006790	1.541350	-0.687458
1	7.670244	2.084094	-1.372172
1	7.632493	1.066147	0.076218
1	6.520261	0.742170	-1.255958
6	0.019816	5.492293	0.308599
1	0.650986	5.399193	1.198283
1	0.556584	6.137671	-0.397206
6	-1.315469	6.147183	0.694885
1	-1.842915	5.488930	1.400052
1	-1.109654	7.076863	1.240919
6	-2.234066	6.459659	-0.494522
1	-2.453235	5.539014	-1.049678
1	-1.705513	7.121891	-1.195962
6	-3.559907	7.108588	-0.082077
1	-4.080266	6.445302	0.622613
1	-3.357144	8.037874	0.467575
6	-4.473827	7.406649	-1.273655
1	-5.415888	7.865880	-0.954968
1	-3.992811	8.092776	-1.980946
1	-4.722367	6.490476	-1.823348
6	3.736537	-0.689911	3.022361
6	4.449865	0.366749	3.884639
6	2.270228	-0.841787	3.461333
1	4.254524	-1.648400	3.131909
6	4.335142	0.043610	5.381854
1	3.989207	1.344836	3.683526
1	5.499712	0.438394	3.577198
6	2.152161	-1.167799	4.955468
1	1.749904	0.102083	3.261579
1	1.769157	-1.605264	2.857635
6	2.868149	-0.112367	5.811005
1	4.828240	0.824028	5.974294
1	4.872286	-0.893184	5.589080
1	1.094028	-1.236918	5.233696
1	2.595223	-2.155010	5.151410
1	2.808523	-0.375178	6.874537
1	2.352220	0.850977	5.691340
6	-1.345690	-3.236000	-3.740302
1	-1.570011	-4.140712	-4.314192
1	-0.706082	-2.591312	-4.351332
1	-0.783809	-3.505034	-2.842176
6	-3.376248	-2.040264	-4.620513
1	-2.695977	-1.534954	-5.313444
1	-3.794193	-2.912542	-5.134772
1	-4.189335	-1.350415	-4.385313
6	-3.441214	-4.698294	-2.313413
1	-4.042030	-5.107976	-1.495652
1	-3.855575	-5.070910	-3.256507
1	-2.423624	-5.077944	-2.206630
6	-4.923816	-2.672662	-2.220314
1	-5.497376	-2.996150	-3.094499
1	-5.409495	-3.073183	-1.326162
1	-4.954045	-1.581669	-2.159997
6	-6.383832	-0.812583	1.279065
1	-6.320381	-1.606802	0.533140
1	-7.100122	-1.111455	2.052022
1	-6.776665	0.080841	0.782635
6	-4.665304	-3.068214	1.989931

1	-4.029834	-3.834332	2.441669
1	-5.710923	-3.346199	2.156369
1	-4.454619	-3.055102	0.918069
6	-5.087374	0.759291	2.746831
1	-5.397115	1.601567	2.119756
1	-5.809463	0.662040	3.563558
1	-4.106652	0.995955	3.169444
6	-4.530194	-1.755701	4.128247
1	-5.589700	-1.876387	4.379301
1	-3.984017	-2.606970	4.546022
1	-4.157732	-0.851151	4.613684
6	0.876521	-4.671479	2.717663
1	1.228451	-5.698576	2.573448
1	1.742749	-4.028569	2.882107
1	0.262254	-4.645310	3.622842
6	-1.247689	-5.024857	1.422697
1	-1.048093	-6.092561	1.286834
1	-1.814377	-4.896355	2.348747
1	-1.866981	-4.665624	0.596513
6	0.672397	-5.322458	-0.754540
1	1.234700	-5.157955	-1.678891
1	1.062744	-6.228789	-0.279519
1	-0.373478	-5.489936	-1.018477
6	2.310036	-3.769116	0.341129
1	2.746887	-3.532079	-0.632445
1	2.434849	-2.897962	0.986339
1	2.881704	-4.595673	0.772060

2_o

Number of imaginary frequencies : 0

Electronic energy : HF=-3396.5915298
 Zero-point correction= 1.457584 (Hartree/Particle)
 Thermal correction to Energy= 1.537487
 Thermal correction to Enthalpy= 1.538431
 Thermal correction to Gibbs Free Energy= 1.341990
 Sum of electronic and zero-point Energies= -3395.133946
 Sum of electronic and thermal Energies= -3395.054043
 Sum of electronic and thermal Enthalpies= -3395.053099
 Sum of electronic and thermal Free Energies= -3395.249539

Cartesian Coordinates

77	-1.095238	-0.211992	0.169897
5	-2.315829	-1.288395	-1.244215
8	-2.156647	-1.003720	-2.594801
8	-3.418548	-2.109584	-1.055896
6	-3.082501	-1.811755	-3.362248
6	-4.182424	-2.136605	-2.292511
5	-0.923747	-2.320656	0.277962
8	-0.030960	-3.002481	-0.546178
8	-1.538922	-3.194426	1.157596
6	0.171126	-4.332635	0.002953
6	-1.163579	-4.549703	0.808785
5	-2.776367	-0.325541	1.338529
8	-2.898834	-0.991471	2.551573
8	-3.995194	0.281502	1.007782
6	-4.303239	-1.095162	2.880928
6	-4.903718	0.145249	2.131178

6	-0.978986	1.627066	-2.269164
6	0.181256	0.743034	-2.488288
7	-1.672161	1.454817	-1.109984
7	0.486382	-0.083384	-1.462876
6	-1.354022	2.622526	-3.180914
6	-2.434932	3.450110	-2.901663
6	-3.117292	3.279008	-1.697925
6	-2.704592	2.272768	-0.833010
6	0.955483	0.744107	-3.653731
6	2.065570	-0.089492	-3.740438
6	2.400829	-0.922548	-2.664286
6	1.548470	-0.880957	-1.551920
6	-0.179262	1.255003	1.575247
6	0.963852	2.070730	1.383371
6	-0.737648	1.360136	2.874409
6	1.497337	2.888821	2.398848
6	-0.232151	2.181427	3.884627
6	0.904427	2.955363	3.655000
1	-0.436473	-1.163696	1.278437
1	-1.583901	0.736967	3.131686
1	1.325843	3.586310	4.432576
1	2.393928	3.470043	2.193839
1	-3.224099	2.068416	0.093026
1	-3.960543	3.903936	-1.425760
1	-2.730623	4.222382	-3.604800
1	-0.798986	2.751872	-4.101487
1	0.708109	1.391856	-4.485798
1	2.685140	-0.077389	-4.631886
1	1.715178	-1.525173	-0.704795
6	3.562265	-1.842736	-2.684357
6	3.834283	-2.587456	-3.843985
6	4.396367	-2.017339	-1.548787
6	4.870460	-3.515729	-3.884761
1	3.189924	-2.459480	-4.709302
6	5.433270	-2.962682	-1.595316
6	5.659933	-3.709223	-2.747926
1	5.050586	-4.092068	-4.787274
1	6.048649	-3.094058	-0.715267
1	6.467390	-4.436014	-2.761165
7	4.218722	-1.208047	-0.415585
6	4.197023	-1.684711	0.904301
8	4.582964	-2.811379	1.218100
7	3.703993	-0.756118	1.773080
1	3.757367	-0.316367	-0.560610
1	3.268487	0.076365	1.376549
6	1.802731	2.098109	0.135540
8	2.715313	1.265811	-0.027033
7	1.624086	3.123440	-0.736740
1	-0.717051	2.193889	4.858253
6	0.531941	4.094049	-0.590015
1	0.097382	4.242913	-1.581383
1	-0.240406	3.635279	0.028118
6	2.538374	3.260778	-1.880548
1	2.835027	2.257779	-2.187834
1	1.962066	3.698643	-2.702427
6	3.780989	4.127044	-1.608533
1	4.306419	4.251760	-2.565988
1	3.456768	5.127914	-1.304451
6	4.755383	3.561257	-0.563555
1	5.461559	4.352420	-0.278005
1	4.204440	3.302516	0.347341

6	5.550165	2.340088	-1.043059
1	6.243955	2.653957	-1.837145
1	4.872318	1.606891	-1.494476
6	6.331304	1.652635	0.082843
1	6.916764	2.403433	0.632574
1	5.616576	1.229542	0.800167
6	7.263400	0.547720	-0.420460
1	8.035001	0.951728	-1.087757
1	7.771164	0.044591	0.410037
1	6.707320	-0.215407	-0.974246
6	0.932303	5.443998	0.021033
1	1.539904	5.259598	0.912574
1	1.558318	6.005547	-0.682905
6	-0.294021	6.285253	0.406306
1	-0.883627	5.732614	1.151440
1	0.048064	7.201326	0.905216
6	-1.197219	6.665966	-0.774507
1	-1.589004	5.758926	-1.252409
1	-0.598521	7.181912	-1.539741
6	-2.380781	7.553074	-0.370829
1	-2.963060	7.042102	0.408141
1	-2.004045	8.477806	0.086794
6	-3.294336	7.899171	-1.549501
1	-4.134034	8.530346	-1.238917
1	-2.745961	8.437775	-2.331725
1	-3.712466	6.993719	-2.006742
6	3.479182	-1.023581	3.187654
6	4.239807	-0.001179	4.050584
6	1.975091	-0.990033	3.507761
1	3.873806	-2.025543	3.383776
6	3.963109	-0.204782	5.547727
1	3.918887	1.007433	3.752907
1	5.312634	-0.071784	3.835466
6	1.695777	-1.191839	5.002502
1	1.574606	-0.019419	3.197628
1	1.454389	-1.745044	2.909249
6	2.457419	-0.161971	5.849268
1	4.494231	0.555125	6.134130
1	4.366484	-1.179077	5.859471
1	0.617452	-1.118172	5.186954
1	2.000073	-2.205455	5.301868
1	2.277570	-0.334239	6.917760
1	2.072319	0.840304	5.616709
6	-2.303363	-3.043744	-3.833887
1	-2.912117	-3.697700	-4.465570
1	-1.435533	-2.713320	-4.412057
1	-1.929525	-3.616451	-2.981687
6	-3.560175	-0.993390	-4.557843
1	-2.721270	-0.809026	-5.236237
1	-4.335153	-1.528652	-5.116722
1	-3.957408	-0.024498	-4.248134
6	-4.847449	-3.500638	-2.435874
1	-5.554772	-3.655283	-1.615527
1	-5.402343	-3.561779	-3.378222
1	-4.122163	-4.314630	-2.408187
6	-5.244617	-1.037741	-2.175527
1	-5.898437	-1.011569	-3.052757
1	-5.858598	-1.229905	-1.293039
1	-4.781011	-0.056355	-2.046399
6	-6.319260	-0.045771	1.597910
1	-6.380578	-0.897193	0.918879

1	-7.025690	-0.204817	2.419821
1	-6.634325	0.847519	1.049012
6	-4.790405	-2.434225	2.313066
1	-4.182967	-3.233612	2.743936
1	-5.841198	-2.622593	2.557113
1	-4.653257	-2.463620	1.229305
6	-4.814399	1.445297	2.939794
1	-5.072031	2.287986	2.290033
1	-5.505360	1.448533	3.788355
1	-3.799644	1.607341	3.312999
6	-4.453489	-1.068387	4.397858
1	-5.509812	-1.062605	4.687988
1	-3.988936	-1.960569	4.828686
1	-3.966218	-0.194372	4.835293
6	-1.011030	-5.349616	2.098672
1	-0.640412	-6.358906	1.890331
1	-0.326870	-4.861647	2.794949
1	-1.982935	-5.441461	2.592987
6	-2.295151	-5.129198	-0.044359
1	-2.104861	-6.172509	-0.314770
1	-3.230053	-5.079975	0.520379
1	-2.429402	-4.538351	-0.950125
6	0.404601	-5.293593	-1.157301
1	1.332591	-5.025389	-1.671776
1	0.501364	-6.323206	-0.797390
1	-0.407097	-5.253668	-1.886369
6	1.415673	-4.267669	0.893848
1	2.275408	-3.920881	0.315534
1	1.267973	-3.571492	1.722737
1	1.666905	-5.247693	1.310478

TS[2-3]_o

Number of imaginary frequencies : 1
Imaginary frequency : -177.3066 cm(-1)

Electronic energy : HF=-3396.5666667
Zero-point correction= 1.457478 (Hartree/Particle)
Thermal correction to Energy= 1.536769
Thermal correction to Enthalpy= 1.537714
Thermal correction to Gibbs Free Energy= 1.342496
Sum of electronic and zero-point Energies= -3395.109189
Sum of electronic and thermal Energies= -3395.029897
Sum of electronic and thermal Enthalpies= -3395.028953
Sum of electronic and thermal Free Energies= -3395.224170

Cartesian Coordinates

6	-1.740463	-0.680363	-1.070825
6	-0.483086	-1.171179	-1.519440
6	-0.407747	-1.535958	-2.879205
6	-1.473379	-1.387446	-3.765959
6	-2.670410	-0.830245	-3.315210
6	-2.792701	-0.470850	-1.974277
77	1.345753	-0.194516	-0.581736
5	2.814710	-1.068560	0.593245
8	2.725672	-1.641670	1.857436
6	4.063037	-1.795602	2.403275
6	4.121002	-3.047343	3.276139
5	0.778691	-2.260644	-0.471945

8	0.028625	-2.983123	0.468084
6	0.408047	-4.381237	0.407740
6	-0.812007	-5.267506	0.639333
6	-1.984273	-0.141067	0.319282
8	-1.858142	1.096613	0.483248
7	0.704296	1.589984	-1.810883
6	1.233142	1.661528	-3.053721
6	0.895136	2.723439	-3.900886
6	0.047079	3.721242	-3.447854
6	-0.458645	3.679694	-2.138651
6	-0.092231	2.571881	-1.364716
6	-1.256617	4.823025	-1.622103
6	-2.534391	4.710278	-1.009091
6	-3.211811	5.891544	-0.645913
6	-2.645495	7.142548	-0.861515
6	-1.381756	7.262215	-1.441959
6	-0.708722	6.104976	-1.814922
7	-3.097839	3.450263	-0.767199
6	-4.431801	3.185849	-0.442382
8	-5.361475	3.968682	-0.629743
6	2.194945	0.605595	-3.436457
7	2.466311	-0.331782	-2.495982
6	3.357127	-1.298308	-2.772392
6	4.013720	-1.386114	-3.995304
6	3.735706	-0.434705	-4.974590
6	2.817672	0.570091	-4.691200
7	-4.595480	1.926516	0.084620
6	-5.858269	1.528945	0.700483
6	-5.965966	-0.003149	0.698211
6	-7.244535	-0.488341	1.396769
6	-7.353981	0.071859	2.822651
6	-7.273526	1.605275	2.818187
6	-5.990509	2.090230	2.128772
5	2.573240	1.304575	0.237360
8	3.264100	2.189057	-0.582647
6	3.932658	3.176348	0.242800
6	5.383211	2.712985	0.396516
8	1.526895	-3.168957	-1.256682
6	1.014494	-4.501155	-1.035857
6	-0.045719	-4.787131	-2.108505
6	2.159564	-5.499709	-1.174348
8	2.618680	1.732775	1.559592
6	3.113111	3.098176	1.581809
6	1.879075	4.007686	1.591863
6	3.926844	3.317198	2.853657
8	4.153996	-1.078431	0.168887
6	4.946199	-1.846494	1.104789
6	5.090731	-3.252766	0.513062
6	6.322030	-1.200075	1.234693
7	-2.410528	-0.901767	1.353973
6	-2.310939	-0.279640	2.694253
6	-0.886934	-0.403231	3.253243
6	-0.604620	0.524861	4.437523
6	0.878703	0.505814	4.827116
6	1.233443	1.460594	5.971848
6	2.712328	1.391596	6.364337
6	-2.797004	-2.325641	1.356889
6	-3.459094	-2.873434	0.092389
6	-4.253596	-4.151795	0.391943
6	-4.740029	-4.851221	-0.881510
6	-5.558609	-6.117873	-0.609587

6	-6.023776	-6.814736	-1.890832
6	3.872841	4.523486	-0.470866
6	4.332790	-0.563086	3.273418
6	1.430657	-4.618164	1.517375
1	0.541314	0.006481	0.748639
1	-0.430019	2.447491	-0.346179
1	-0.222930	4.544075	-4.101923
1	1.293035	2.778579	-4.906115
1	2.591579	1.317470	-5.441179
1	4.224620	-0.471036	-5.943194
1	4.724345	-2.187518	-4.166520
1	3.527335	-2.013477	-1.982410
1	-1.362117	-1.686560	-4.805271
1	0.278590	6.178547	-2.262510
1	-4.195674	5.809974	-0.207014
1	-0.928379	8.236016	-1.599572
1	-3.197728	8.029287	-0.562694
1	-2.471158	2.657586	-0.669060
1	-0.539635	-6.320971	0.512830
1	-1.183484	-5.144200	1.660798
1	-1.621603	-5.038741	-0.051594
1	0.400425	-4.644700	-3.097157
1	-0.415538	-5.815296	-2.046246
1	-0.892381	-4.103410	-2.023660
1	2.292080	-3.973937	1.369761
1	0.985154	-4.342158	2.476971
1	1.749569	-5.664082	1.567446
1	1.820341	-6.515923	-0.946648
1	2.532910	-5.492348	-2.203475
1	2.993323	-5.257707	-0.514521
1	3.394073	-2.956455	4.088850
1	3.895867	-3.961053	2.726866
1	5.115594	-3.152458	3.723085
1	4.112104	-3.715067	0.377216
1	5.562084	-3.176709	-0.471734
1	5.708715	-3.904132	1.138591
1	4.240803	0.350316	2.686437
1	3.578376	-0.519773	4.062079
1	5.320887	-0.603547	3.742691
1	6.935688	-1.736654	1.966304
1	6.838358	-1.232561	0.270155
1	6.253625	-0.155962	1.541470
1	5.984525	3.424881	0.970199
1	5.421266	1.737935	0.886763
1	5.829702	2.602390	-0.596002
1	4.295262	5.318007	0.153544
1	4.453907	4.476417	-1.397293
1	2.847625	4.793326	-0.732810
1	1.250703	3.741008	2.446577
1	2.150250	5.064351	1.676559
1	1.283581	3.872659	0.686114
1	4.352837	4.326202	2.869075
1	3.278138	3.213619	3.728124
1	4.741399	2.597709	2.950815
1	-3.755306	1.515130	0.481609
1	-6.659803	1.950381	0.085118
1	-5.088727	-0.415659	1.216198
1	-5.924008	-0.370851	-0.333670
1	-5.115961	1.763218	2.710378
1	-5.958253	3.183803	2.082805
1	-7.266844	-1.584880	1.411045

1	-8.118932	-0.164679	0.814808
1	-7.321906	1.996181	3.841399
1	-8.145671	2.010838	2.286094
1	-8.287484	-0.262020	3.291159
1	-6.532655	-0.331073	3.433187
1	-3.712108	-0.012793	-1.619436
1	-3.502068	-0.673951	-3.996517
1	-2.584147	0.772540	2.605230
1	-3.045259	-0.762507	3.345548
1	-1.924460	-2.926712	1.613802
1	-3.520594	-2.413690	2.174715
1	0.525832	-1.950938	-3.241127
1	-0.683918	-1.446239	3.526924
1	-0.186811	-0.161602	2.448357
1	-1.226487	0.253571	5.303512
1	-0.888817	1.551068	4.162338
1	1.166588	-0.518928	5.104261
1	1.475397	0.762897	3.942822
1	0.611025	1.235297	6.849323
1	0.979893	2.488195	5.674928
1	3.360091	1.624686	5.511596
1	2.951510	2.096666	7.168700
1	2.981445	0.387385	6.713635
1	-4.138473	-2.126927	-0.329285
1	-2.702010	-3.073913	-0.669582
1	-3.640473	-4.849692	0.976677
1	-5.115980	-3.901533	1.026077
1	-5.340663	-4.148024	-1.476273
1	-3.872105	-5.108295	-1.505994
1	-4.956359	-6.814261	-0.009717
1	-6.430991	-5.860905	0.007093
1	-5.170310	-7.112659	-2.511614
1	-6.605829	-7.716743	-1.671870
1	-6.653904	-6.151842	-2.495905

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Number of imaginary frequencies : 0

Electronic energy : HF=-3396.5916628
 Zero-point correction= 1.457513 (Hartree/Particle)
 Thermal correction to Energy= 1.538022
 Thermal correction to Enthalpy= 1.538966
 Thermal correction to Gibbs Free Energy= 1.337951
 Sum of electronic and zero-point Energies= -3395.134150
 Sum of electronic and thermal Energies= -3395.053641
 Sum of electronic and thermal Enthalpies= -3395.052697
 Sum of electronic and thermal Free Energies= -3395.253712

Cartesian Coordinates

6	-2.078983	-0.607269	-0.960620
6	-1.242808	-1.722819	-1.204298
6	-0.832100	-1.944005	-2.535757
6	-1.239955	-1.122247	-3.584113
6	-2.070736	-0.031996	-3.320862
6	-2.468665	0.231993	-2.012285
77	1.829748	-0.294369	-0.469574
5	3.184874	-1.538269	0.402816
8	3.109116	-2.268307	1.601192

6	4.447701	-2.595860	2.041498
6	4.420284	-3.913178	2.811675
5	-0.783125	-2.798281	-0.162999
8	-1.303765	-2.978207	1.088210
6	-0.639072	-4.119469	1.711944
6	-1.711155	-4.948128	2.416203
6	-2.430960	-0.103259	0.412075
8	-1.967959	1.021196	0.711313
7	0.771238	1.369393	-1.585177
6	1.108343	1.476151	-2.890777
6	0.849883	2.649359	-3.605996
6	0.289903	3.736948	-2.948964
6	-0.018620	3.648515	-1.583335
6	0.223591	2.420075	-0.956350
6	-0.476265	4.853528	-0.841192
6	-1.711913	4.928399	-0.154173
6	-2.075413	6.137554	0.464668
6	-1.237909	7.246979	0.409387
6	-0.012301	7.179004	-0.256092
6	0.353079	5.987189	-0.874393
7	-2.548688	3.802988	-0.092301
6	-3.936253	3.829197	0.008542
8	-4.621496	4.844023	-0.100591
6	1.842208	0.331010	-3.471750
7	2.393860	-0.534702	-2.582427
6	3.130728	-1.561794	-3.042914
6	3.322896	-1.798574	-4.400455
6	2.730525	-0.935394	-5.322160
6	1.988454	0.142967	-4.850547
7	-4.465254	2.571873	0.199778
6	-5.884167	2.388083	0.487334
6	-6.300779	0.968292	0.079291
6	-7.774510	0.684568	0.402161
6	-8.083647	0.949377	1.883235
6	-7.691654	2.379702	2.280111
6	-6.214246	2.658259	1.967517
5	3.236436	1.035997	-0.021836
8	3.775955	1.877375	-1.002542
6	4.915693	2.562195	-0.430556
6	6.153228	1.722846	-0.770334
8	0.115769	-3.772881	-0.518743
6	0.045110	-4.834071	0.476363
6	-0.812035	-5.939639	-0.149141
6	1.462415	-5.326814	0.735929
8	3.795311	1.328012	1.223091
6	4.566519	2.547719	1.100294
6	3.646774	3.703347	1.515342
6	5.766981	2.461949	2.037225
8	4.489682	-1.696602	-0.123387
6	5.236685	-2.631003	0.685295
6	5.173278	-3.992560	-0.018282
6	6.684115	-2.154215	0.772346
7	-3.209020	-0.757622	1.301403
6	-3.149481	-0.244000	2.692760
6	-1.759073	-0.460012	3.343747
6	-1.018910	0.827029	3.734757
6	0.455830	0.562392	4.060234
6	1.249895	1.828058	4.400396
6	2.741232	1.545711	4.608095
6	-4.055794	-1.949796	1.113179
6	-4.441201	-2.346109	-0.310844

6	-5.583259	-3.370055	-0.295420
6	-5.981360	-3.828994	-1.702106
6	-7.123846	-4.850838	-1.708691
6	-7.529350	-5.285637	-3.119406
6	5.018370	3.949054	-1.055562
6	4.894472	-1.457000	2.967590
6	0.350113	-3.563085	2.735618
1	1.267360	-0.104403	1.008748
1	0.010170	2.262199	0.092794
1	0.108569	4.665673	-3.481009
1	1.125842	2.731507	-4.650728
1	1.514349	0.825683	-5.545778
1	2.845861	-1.096103	-6.389660
1	3.923198	-2.643945	-4.719320
1	3.580836	-2.184144	-2.279455
1	-0.904830	-1.327241	-4.596403
1	1.303588	5.915180	-1.395699
1	-3.027956	6.196831	0.972839
1	0.648841	8.039487	-0.292863
1	-1.544042	8.166603	0.900214
1	-2.118120	2.883794	-0.080866
1	-1.277401	-5.855756	2.847984
1	-2.144363	-4.363789	3.233401
1	-2.519057	-5.236070	1.740445
1	-0.345776	-6.263413	-1.084039
1	-0.899403	-6.808056	0.510199
1	-1.817643	-5.578034	-0.385093
1	1.092231	-2.910890	2.274407
1	-0.197876	-2.986829	3.484941
1	0.873933	-4.373337	3.252360
1	1.475991	-6.083173	1.527359
1	1.864918	-5.782763	-0.174025
1	2.104399	-4.494289	1.021795
1	3.808444	-3.799146	3.711833
1	4.001736	-4.729848	2.221350
1	5.430434	-4.198163	3.126291
1	4.139336	-4.335122	-0.109428
1	5.586729	-3.891046	-1.026954
1	5.751235	-4.757924	0.509772
1	4.894170	-0.504831	2.433041
1	4.177029	-1.371031	3.788666
1	5.887085	-1.638082	3.393162
1	7.273874	-2.800677	1.431618
1	7.142231	-2.176757	-0.221742
1	6.744457	-1.130553	1.145868
1	7.076888	2.186405	-0.409605
1	6.064097	0.719234	-0.346304
1	6.221858	1.619341	-1.857606
1	5.814031	4.535456	-0.583335
1	5.251373	3.859349	-2.121404
1	4.078454	4.496514	-0.962991
1	3.275229	3.513712	2.525474
1	4.171504	4.663977	1.514389
1	2.782787	3.776162	0.848673
1	6.423606	3.329690	1.912195
1	5.424715	2.441366	3.076041
1	6.349509	1.556142	1.858111
1	-3.829577	1.888770	0.596403
1	-6.425697	3.116123	-0.125379
1	-5.667654	0.255140	0.623014
1	-6.098398	0.820558	-0.987708

1	-5.580008	2.009138	2.589332
1	-5.950642	3.693693	2.206602
1	-8.021826	-0.350603	0.136208
1	-8.411655	1.328765	-0.219985
1	-7.889988	2.551330	3.344700
1	-8.318748	3.092344	1.726198
1	-9.146186	0.771809	2.088007
1	-7.519689	0.236134	2.502310
1	-3.084044	1.099938	-1.794503
1	-2.395416	0.621299	-4.125731
1	-3.406253	0.819631	2.688974
1	-3.932369	-0.764957	3.246735
1	-3.579020	-2.795140	1.616414
1	-4.983751	-1.726823	1.654194
1	-0.184426	-2.790299	-2.740727
1	-1.863644	-1.105586	4.225451
1	-1.143317	-1.015945	2.633777
1	-1.517108	1.306865	4.590290
1	-1.080192	1.528235	2.896665
1	0.533057	-0.151943	4.894276
1	0.922985	0.079803	3.192237
1	0.825975	2.303684	5.296565
1	1.130631	2.551181	3.581704
1	3.184409	1.143486	3.691805
1	3.289071	2.455628	4.882316
1	2.897842	0.816741	5.413498
1	-4.748973	-1.460443	-0.877754
1	-3.587643	-2.775675	-0.838779
1	-5.286718	-4.243389	0.303455
1	-6.460214	-2.938352	0.207235
1	-6.272851	-2.952299	-2.297948
1	-5.104414	-4.259879	-2.205961
1	-6.824557	-5.731757	-1.123935
1	-7.994018	-4.423453	-1.191482
1	-6.683812	-5.735011	-3.653773
1	-8.337361	-6.025060	-3.096333
1	-7.876918	-4.431532	-3.712617

I_p

Number of imaginary frequencies : 0

Electronic energy : HF=-3396.6138386
Zero-point correction= 1.459952 (Hartree/Particle)
Thermal correction to Energy= 1.540078
Thermal correction to Enthalpy= 1.541022
Thermal correction to Gibbs Free Energy= 1.342251
Sum of electronic and zero-point Energies= -3395.153887
Sum of electronic and thermal Energies= -3395.073760
Sum of electronic and thermal Enthalpies= -3395.072816
Sum of electronic and thermal Free Energies= -3395.271587

Cartesian Coordinates

77	1.987191	-0.211085	-0.519984
5	3.223430	1.308620	-0.134669
8	2.985838	2.592157	-0.644656
8	4.374243	1.311966	0.654725
6	3.820748	3.522804	0.086510
6	5.014228	2.603061	0.530979

5	1.630843	-0.152364	1.483661
8	1.563030	1.024803	2.253518
8	1.285829	-1.240286	2.299619
6	1.023206	0.714792	3.561388
6	1.337862	-0.816147	3.680247
5	3.596657	-1.402981	-0.123859
8	3.860779	-2.205056	0.991742
8	4.660703	-1.551023	-1.044920
6	5.232562	-2.650083	0.942483
6	5.538439	-2.606172	-0.595879
6	1.051679	0.481587	-3.411701
6	0.259743	1.386234	-2.546561
7	2.018799	-0.241153	-2.794420
7	0.398940	1.206448	-1.211540
6	0.844294	0.377396	-4.793463
6	1.662254	-0.456949	-5.548429
6	2.681528	-1.162925	-4.908497
6	2.822750	-1.026866	-3.530388
6	-0.529222	2.426116	-3.049520
6	-1.159788	3.296788	-2.167626
6	-1.003804	3.117932	-0.787240
6	-0.216161	2.040631	-0.365960
6	-0.074062	-2.684520	-2.656657
6	0.539493	-2.941924	-1.425663
6	-1.301582	-2.028753	-2.699657
6	-0.063480	-2.512101	-0.237160
6	-1.926904	-1.622209	-1.509874
6	-1.284400	-1.830123	-0.285956
1	-1.775407	-1.821865	-3.654873
1	-1.742838	-1.469141	0.628950
1	0.418408	-2.683522	0.718098
1	3.595711	-1.541438	-2.969105
1	3.354404	-1.811685	-5.459308
1	1.508421	-0.549375	-6.619319
1	0.047368	0.935131	-5.271169
1	-0.625506	2.578215	-4.118052
1	-1.764685	4.116347	-2.541909
1	-0.026888	1.870414	0.687331
6	-3.249423	-0.914303	-1.510839
8	-3.351965	0.193046	-0.943133
7	-4.313405	-1.499952	-2.121383
6	-1.567935	4.060043	0.210279
6	-1.220730	5.415255	0.126177
6	-2.421960	3.623373	1.255654
6	-1.663524	6.338237	1.070849
1	-0.566435	5.731145	-0.681852
6	-2.853298	4.557840	2.214201
6	-2.469958	5.893419	2.119771
1	-1.370918	7.381170	0.997456
1	-3.487547	4.218935	3.020292
1	-2.817766	6.593755	2.874331
7	-2.854997	2.291534	1.249780
6	-3.505280	1.605912	2.275295
8	-3.668745	2.055595	3.410033
7	-3.915423	0.359948	1.885281
1	-2.712526	1.770986	0.390980
1	-3.839831	0.116615	0.902221
6	-5.589586	-0.764828	-2.216896
1	-5.643994	-0.060608	-1.385302
1	-6.393127	-1.492710	-2.085089
6	-4.361020	-2.892084	-2.604799

1	-4.903686	-2.885643	-3.556388
1	-3.354174	-3.240054	-2.818142
6	-4.609029	-0.555139	2.778519
6	-5.913231	-1.056934	2.136240
6	-3.705933	-1.736128	3.174911
1	-4.852188	0.017213	3.679275
6	-6.645458	-2.048779	3.053466
1	-5.670929	-1.553866	1.184530
1	-6.553885	-0.200741	1.894324
6	-4.433760	-2.731722	4.088678
1	-3.377766	-2.249906	2.260458
1	-2.805935	-1.347393	3.661532
6	-5.740702	-3.224724	3.450667
1	-7.554622	-2.414486	2.561032
1	-6.971207	-1.521440	3.961023
1	-3.776154	-3.578439	4.319167
1	-4.661066	-2.240148	5.045189
1	-6.270866	-3.895299	4.137622
1	-5.502999	-3.814794	2.555177
6	-5.738629	-0.037984	-3.567908
6	-5.152603	1.384638	-3.561620
1	-6.804049	0.012356	-3.828564
1	-5.264431	-0.650304	-4.344834
6	-6.120286	2.400030	-2.930675
1	-4.198294	1.378293	-3.023955
1	-4.933299	1.702039	-4.589384
6	-5.487031	3.763775	-2.616069
1	-6.973110	2.527845	-3.611182
1	-6.536254	1.987633	-2.000516
1	-4.890175	4.095470	-3.478100
1	-6.277712	4.514004	-2.487608
6	-5.046445	-3.854694	-1.620119
6	-4.287897	-4.071468	-0.304038
1	-5.172195	-4.815378	-2.136986
1	-6.058303	-3.492148	-1.402718
6	-3.001659	-4.897088	-0.426803
1	-4.052081	-3.097677	0.143479
1	-4.959631	-4.570738	0.405644
6	-2.294402	-5.092575	0.919588
1	-3.241966	-5.878918	-0.859718
1	-2.305082	-4.414014	-1.122450
1	-2.054857	-4.109010	1.343099
1	-2.984411	-5.572248	1.627674
6	-4.616722	3.730459	-1.357271
1	-4.117700	4.687613	-1.178382
1	-5.219999	3.503458	-0.470937
1	-3.847426	2.957673	-1.424812
6	-1.011611	-5.918575	0.805099
1	-0.516463	-6.028365	1.775985
1	-1.219036	-6.924258	0.420006
1	-0.300264	-5.441030	0.121972
6	5.326627	-4.032175	1.582858
1	6.341888	-4.436638	1.502754
1	5.075650	-3.962159	2.645808
1	4.631591	-4.738812	1.124153
6	6.057531	-1.634570	1.744894
1	5.676205	-1.603624	2.769772
1	7.118899	-1.901459	1.781785
1	5.944612	-0.634099	1.320020
6	6.973719	-2.240386	-0.962599
1	7.682453	-2.976918	-0.567939

1	7.084221	-2.215671	-2.051758
1	7.241452	-1.254994	-0.577331
6	5.117040	-3.887839	-1.328402
1	5.167950	-3.715848	-2.408568
1	5.768048	-4.734666	-1.088993
1	4.087401	-4.159033	-1.076113
6	6.096873	2.466458	-0.546404
1	6.674133	3.388632	-0.668204
1	6.784544	1.665529	-0.259949
1	5.652543	2.197621	-1.508906
6	5.641726	2.963215	1.873793
1	6.450864	2.263004	2.104756
1	6.065112	3.973468	1.852422
1	4.908494	2.906062	2.680206
6	2.986909	4.038085	1.267207
1	3.535543	4.773463	1.864797
1	2.083023	4.519341	0.880726
1	2.672894	3.209200	1.906369
6	4.200969	4.672369	-0.841033
1	3.304635	5.240944	-1.108681
1	4.900496	5.357394	-0.349551
1	4.656507	4.311296	-1.765531
6	0.325056	-1.630323	4.477802
1	0.265030	-1.284012	5.515167
1	-0.669651	-1.572189	4.032474
1	0.625207	-2.683165	4.488410
6	2.760979	-1.094580	4.182262
1	2.873437	-0.851205	5.243958
1	2.982450	-2.155534	4.041311
1	3.491373	-0.523589	3.603670
6	-0.477261	1.019620	3.517907
1	-0.627962	2.064594	3.235204
1	-0.981109	0.394253	2.776518
1	-0.959727	0.865237	4.487169
6	1.710793	1.603970	4.593240
1	1.438250	2.649670	4.419150
1	1.399934	1.340047	5.610069
1	2.797711	1.524442	4.528278
1	0.413306	-2.979202	-3.580545
1	1.491082	-3.461510	-1.386951

TS[1-2]_p

Number of imaginary frequencies : 1
Imaginary frequency : -816.3275 cm(-1)

Electronic energy : HF=-3396.5681273
Zero-point correction= 1.454631 (Hartree/Particle)
Thermal correction to Energy= 1.534484
Thermal correction to Enthalpy= 1.535428
Thermal correction to Gibbs Free Energy= 1.337067
Sum of electronic and zero-point Energies= -3395.113496
Sum of electronic and thermal Energies= -3395.033643
Sum of electronic and thermal Enthalpies= -3395.032699
Sum of electronic and thermal Free Energies= -3395.231060

Cartesian Coordinates

77	1.839883	-0.394269	-0.563225
5	3.575285	0.785258	-0.280367

8	3.771926	1.954435	-1.016209
8	4.600799	0.627837	0.646272
6	4.768059	2.754288	-0.327587
6	5.597350	1.656195	0.424806
5	1.637224	-0.096158	1.449022
8	1.764484	1.175146	2.029238
8	1.278466	-1.018652	2.427553
6	1.305642	1.113335	3.404858
6	1.472252	-0.412518	3.727687
5	3.282823	-1.821206	-0.111204
8	3.418299	-2.559239	1.052987
8	4.258557	-2.205165	-1.038621
6	4.669577	-3.282913	1.010168
6	4.943388	-3.379148	-0.535064
6	1.724369	0.847865	-3.415738
6	0.914625	1.756391	-2.573691
7	2.169129	-0.286732	-2.825209
7	0.853438	1.483680	-1.247149
6	2.020804	1.125719	-4.757424
6	2.756007	0.209794	-5.501551
6	3.186322	-0.966277	-4.889158
6	2.877836	-1.168523	-3.547487
6	0.216853	2.847974	-3.102369
6	-0.510567	3.674473	-2.259266
6	-0.548075	3.411768	-0.882572
6	0.147491	2.281675	-0.433659
6	-0.782483	-1.259519	-2.086034
6	-0.203068	-1.210968	-0.804176
6	-2.167440	-1.275323	-2.262143
6	-1.071642	-1.317997	0.297008
6	-3.018177	-1.279676	-1.149386
6	-2.451289	-1.326973	0.128204
1	-2.586604	-1.242471	-3.264953
1	-3.095426	-1.365054	0.995727
1	-0.659335	-1.361358	1.297948
1	3.225396	-2.036816	-3.002635
1	3.761063	-1.711034	-5.429179
1	2.992279	0.415737	-6.540967
1	1.695408	2.051950	-5.214619
1	0.228819	3.047857	-4.166400
1	-1.049275	4.527094	-2.660021
1	0.183912	2.027263	0.616859
6	-4.493857	-1.073897	-1.267154
8	-5.011359	-0.127661	-0.642093
7	-5.228163	-1.881321	-2.082223
6	-1.187872	4.371014	0.054314
6	-0.769822	5.711095	-0.028649
6	-2.171670	4.014545	1.010123
6	-1.269582	6.690357	0.821949
1	-0.009317	5.967828	-0.760923
6	-2.675204	5.015542	1.863809
6	-2.223749	6.327181	1.774296
1	-0.915116	7.713882	0.749101
1	-3.419532	4.747395	2.599334
1	-2.632208	7.071978	2.451654
7	-2.678805	2.706574	1.052933
6	-3.319589	2.122031	2.158029
8	-3.259614	2.602663	3.291267
7	-3.981590	0.968030	1.873460
1	-2.534265	2.123790	0.239175
1	-4.197274	0.700544	0.912640

6	-6.621787	-1.511195	-2.369402
1	-6.971429	-0.868546	-1.561920
1	-7.229535	-2.421193	-2.354912
6	-4.783741	-3.196244	-2.568952
1	-5.214851	-3.337373	-3.565398
1	-3.702647	-3.194601	-2.691827
6	-4.606209	0.206573	2.958070
6	-5.639896	-0.781228	2.398313
6	-3.553656	-0.523913	3.814208
1	-5.125338	0.919311	3.612984
6	-6.298647	-1.584923	3.528826
1	-5.144970	-1.474378	1.706661
1	-6.387532	-0.243140	1.806092
6	-4.211911	-1.331595	4.940697
1	-2.978011	-1.199933	3.167839
1	-2.854725	0.213560	4.217418
6	-5.251353	-2.314999	4.383901
1	-7.014628	-2.300092	3.106455
1	-6.875847	-0.903500	4.169732
1	-3.445940	-1.865574	5.515608
1	-4.705053	-0.641753	5.640272
1	-5.740478	-2.860098	5.200465
1	-4.740874	-3.066418	3.763988
6	-6.764960	-0.813229	-3.734294
6	-5.941788	0.475482	-3.887106
1	-7.830971	-0.598533	-3.889612
1	-6.475649	-1.519616	-4.523543
6	-6.411255	1.642015	-3.007227
1	-4.891487	0.246223	-3.672979
1	-5.972006	0.788254	-4.939820
6	-5.508106	2.884280	-3.089339
1	-7.433121	1.916907	-3.303998
1	-6.456197	1.316649	-1.962855
1	-5.397051	3.191548	-4.139319
1	-6.010375	3.716837	-2.580117
6	-5.207148	-4.355905	-1.649390
6	-4.515749	-4.378648	-0.277552
1	-4.995354	-5.293306	-2.181542
1	-6.294772	-4.320358	-1.510510
6	-3.017242	-4.707456	-0.322691
1	-4.661937	-3.410383	0.219868
1	-5.023718	-5.117384	0.356353
6	-2.361692	-4.721851	1.063334
1	-2.874983	-5.685860	-0.804550
1	-2.491451	-3.975943	-0.946739
1	-2.569976	-3.768726	1.565782
1	-2.826669	-5.503432	1.680418
6	-4.122660	2.692106	-2.458204
1	-3.554443	3.628516	-2.466934
1	-4.216674	2.361533	-1.418936
1	-3.525619	1.941104	-2.986836
6	-0.846554	-4.932444	1.004326
1	-0.402482	-4.946049	2.005507
1	-0.594045	-5.880580	0.513398
1	-0.363120	-4.124376	0.443833
6	4.478088	-4.622907	1.714997
1	5.380259	-5.239483	1.638202
1	4.273500	-4.453688	2.776451
1	3.636017	-5.179441	1.299035
6	5.703409	-2.431848	1.757418
1	5.350926	-2.270420	2.780112

1	6.681011	-2.922545	1.803612
1	5.803600	-1.452013	1.286888
6	6.410700	-3.290131	-0.940659
1	6.990097	-4.112970	-0.508753
1	6.499124	-3.349975	-2.030294
1	6.851078	-2.343976	-0.621523
6	4.278894	-4.595725	-1.191133
1	4.354741	-4.501455	-2.279128
1	4.758452	-5.534352	-0.897233
1	3.217991	-4.647927	-0.929274
6	6.701435	1.035263	-0.439521
1	7.519259	1.738936	-0.623945
1	7.113043	0.164511	0.078913
1	6.300564	0.697003	-1.398949
6	6.157027	2.081010	1.778539
1	6.696494	1.244618	2.234065
1	6.857017	2.916619	1.670220
1	5.360018	2.376608	2.463462
6	4.000177	3.680630	0.624203
1	4.669744	4.350691	1.172609
1	3.306553	4.292301	0.038471
1	3.409410	3.096268	1.334790
6	5.545239	3.565387	-1.357621
1	4.877205	4.287248	-1.838013
1	6.359415	4.124210	-0.883352
1	5.966440	2.927514	-2.137403
6	0.440395	-0.985831	4.693146
1	0.500045	-0.492798	5.669368
1	-0.575549	-0.873833	4.309644
1	0.628030	-2.053938	4.840855
6	2.892477	-0.776697	4.179592
1	3.106177	-0.403773	5.186638
1	2.992002	-1.865225	4.181594
1	3.633913	-0.374092	3.484737
6	-0.154036	1.576102	3.414597
1	-0.219899	2.585556	3.001388
1	-0.776097	0.919139	2.802080
1	-0.573027	1.605919	4.423629
6	2.165579	2.052238	4.244357
1	1.989393	3.088337	3.938536
1	1.912897	1.968492	5.306958
1	3.229113	1.838859	4.119800
1	-0.148609	-1.225455	-2.966172
1	1.267846	-1.901604	-0.411320

2_p

Number of imaginary frequencies : 0

Electronic energy : HF=-3396.5802613
 Zero-point correction= 1.458183 (Hartree/Particle)
 Thermal correction to Energy= 1.537583
 Thermal correction to Enthalpy= 1.538527
 Thermal correction to Gibbs Free Energy= 1.343286
 Sum of electronic and zero-point Energies= -3395.122079
 Sum of electronic and thermal Energies= -3395.042678
 Sum of electronic and thermal Enthalpies= -3395.041734
 Sum of electronic and thermal Free Energies= -3395.236976

Cartesian Coordinates

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.....
77      1.795075 -0.522007 -0.430695
5       3.609222 0.654494 -0.357328
8       3.897095 1.413957 -1.491229
8       4.408616 1.050563 0.699338
6       4.573827 2.618191 -1.047622
6       5.286324 2.122725 0.260365
5       1.550296 0.099553 1.499406
8       1.614629 1.447298 1.858511
8       1.278656 -0.682468 2.614181
6       1.220420 1.580837 3.249355
6       1.477945 0.131801 3.798267
5       3.479868 -1.608224 0.197388
8       3.880876 -1.841812 1.504106
8       4.252704 -2.366656 -0.691403
6       5.048326 -2.692897 1.492766
6       4.932222 -3.386220 0.087983
6       1.895368 0.276761 -3.429384
6       1.093929 1.322522 -2.759338
7       2.183224 -0.818320 -2.689429
7       0.968005 1.247795 -1.410039
6       2.308415 0.380875 -4.763482
6       2.995115 -0.677574 -5.348430
6       3.251731 -1.817972 -4.588889
6       2.835481 -1.840528 -3.260659
6       0.420373 2.316577 -3.476818
6       -0.367779 3.239337 -2.806602
6       -0.482660 3.177165 -1.409743
6       0.207565 2.146498 -0.762037
6       -0.907138 -1.174986 -1.879281
6       -0.278976 -1.102986 -0.618452
6       -2.286887 -1.320839 -2.026698
6       -1.124514 -1.265567 0.497835
6       -3.104136 -1.415211 -0.895235
6       -2.504841 -1.398106 0.368123
1       -2.731962 -1.328483 -3.019358
1       -3.126616 -1.479831 1.252518
1       -0.697355 -1.264219 1.494527
1       3.051514 -2.676282 -2.608988
1       3.775687 -2.671421 -5.005498
1       3.324939 -0.610519 -6.380628
1       2.112615 1.281018 -5.333363
1       0.486005 2.349503 -4.557261
1       -0.901642 4.006601 -3.358114
1       0.187403 2.054539 0.314981
6       -4.592186 -1.362472 -0.991744
8       -5.186954 -0.422916 -0.428410
7       -5.257304 -2.306285 -1.714529
6       -1.193000 4.247843 -0.662987
6       -0.824060 5.571557 -0.968178
6       -2.196870 4.022096 0.313210
6       -1.395739 6.663225 -0.327022
1       -0.044005 5.729480 -1.707623
6       -2.778835 5.138945 0.946378
6       -2.377634 6.432985 0.638634
1       -1.076804 7.671940 -0.570562
1       -3.544569 4.974696 1.690338
1       -2.847600 7.266991 1.152375
7       -2.659117 2.725647 0.594488
6       -3.288780 2.349110 1.795355
8       -3.217300 3.035374 2.816750

```

7	-3.955403	1.164693	1.744464
1	-2.498237	2.004717	-0.096312
1	-4.195885	0.718738	0.859135
6	-6.690964	-2.114057	-1.973194
1	-7.075589	-1.434889	-1.212747
1	-7.196981	-3.076804	-1.845678
6	-4.660727	-3.557464	-2.208189
1	-5.142548	-3.787590	-3.163711
1	-3.605557	-3.400390	-2.422112
6	-4.598836	0.655231	2.959539
6	-5.722869	-0.328925	2.609078
6	-3.579147	0.010060	3.916787
1	-5.039365	1.514708	3.481472
6	-6.408658	-0.849149	3.880384
1	-5.306746	-1.173410	2.046674
1	-6.444115	0.152222	1.940393
6	-4.262767	-0.520599	5.184693
1	-3.074526	-0.815306	3.396577
1	-2.815976	0.751294	4.167432
6	-5.398078	-1.495963	4.839519
1	-7.193967	-1.565892	3.611484
1	-6.908262	-0.013867	4.391739
1	-3.523802	-1.004638	5.834498
1	-4.673811	0.325445	5.753788
1	-5.901984	-1.836676	5.752247
1	-4.971442	-2.390022	4.361987
6	-6.962336	-1.567663	-3.388259
6	-6.240759	-0.251734	-3.717230
1	-8.048213	-1.439386	-3.493252
1	-6.672305	-2.328315	-4.124912
6	-6.748404	0.969777	-2.938883
1	-5.167995	-0.389394	-3.537732
1	-6.342351	-0.054806	-4.793116
6	-5.932008	2.248353	-3.193512
1	-7.797720	1.147903	-3.213030
1	-6.727931	0.754146	-1.865865
1	-5.877544	2.442878	-4.274606
1	-6.468947	3.100813	-2.757708
6	-4.831999	-4.746729	-1.246638
6	-3.981937	-4.681338	0.032130
1	-4.577423	-5.658492	-1.804448
1	-5.892482	-4.836639	-0.979196
6	-2.468439	-4.799698	-0.199280
1	-4.195525	-3.745939	0.564948
1	-4.304782	-5.488614	0.703214
6	-1.655365	-4.774792	1.101472
1	-2.256045	-5.731345	-0.744513
1	-2.122576	-3.979804	-0.838395
1	-1.929427	-3.880608	1.675262
1	-1.931470	-5.638773	1.722422
6	-4.516004	2.212947	-2.602817
1	-4.007124	3.172046	-2.750938
1	-4.550874	2.009394	-1.528092
1	-3.892888	1.437383	-3.061576
6	-0.141984	-4.764685	0.863070
1	0.409541	-4.753354	1.810050
1	0.180298	-5.648176	0.297571
1	0.155345	-3.874276	0.298661
6	4.964422	-3.637395	2.688005
1	5.779454	-4.369090	2.668253
1	5.048195	-3.062538	3.615358

1	4.012542	-4.171161	2.711804
6	6.279162	-1.791299	1.613020
1	6.177843	-1.173256	2.508902
1	7.203217	-2.372995	1.692617
1	6.349232	-1.125593	0.753396
6	6.256724	-3.714670	-0.590805
1	6.841109	-4.416827	0.012979
1	6.070423	-4.180846	-1.563698
1	6.853957	-2.816481	-0.757884
6	4.018723	-4.618802	0.104366
1	3.820532	-4.931299	-0.925497
1	4.478268	-5.459195	0.633163
1	3.058737	-4.392900	0.577627
6	6.666317	1.516068	-0.006952
1	7.386496	2.279779	-0.316328
1	7.039338	1.050236	0.908249
1	6.612842	0.750327	-0.786091
6	5.371503	3.154938	1.380877
1	5.859545	2.710154	2.253630
1	5.962462	4.023018	1.068661
1	4.381963	3.495580	1.688316
6	3.481179	3.661622	-0.775014
1	3.905361	4.630149	-0.493070
1	2.888179	3.799218	-1.684194
1	2.810119	3.325725	0.019931
6	5.499495	3.094763	-2.160408
1	4.904152	3.395598	-3.028272
1	6.087681	3.960462	-1.837853
1	6.183135	2.306029	-2.480303
6	0.503133	-0.329001	4.876759
1	0.564230	0.314972	5.760674
1	-0.527537	-0.326002	4.516231
1	0.749191	-1.350176	5.184389
6	2.927595	-0.091678	4.245624
1	3.157548	0.453845	5.166774
1	3.079712	-1.159214	4.425762
1	3.623180	0.210662	3.459196
6	-0.256448	1.976521	3.255378
1	-0.394453	2.899308	2.687285
1	-0.865273	1.199599	2.788232
1	-0.634354	2.153475	4.265725
6	2.070263	2.675651	3.885406
1	1.833512	3.639244	3.423078
1	1.863197	2.757872	4.957912
1	3.135852	2.485781	3.746515
1	-0.316790	-1.080033	-2.785175
1	1.893961	-1.981650	0.211948

TS[2-3]_p

Number of imaginary frequencies : 1
Imaginary frequency : -22.7480 cm⁻¹)

Electronic energy : HF=-3396.567642
Zero-point correction= 1.456885 (Hartree/Particle)
Thermal correction to Energy= 1.536410
Thermal correction to Enthalpy= 1.537354
Thermal correction to Gibbs Free Energy= 1.340653
Sum of electronic and zero-point Energies= -3395.110757
Sum of electronic and thermal Energies= -3395.031232

Sum of electronic and thermal Enthalpies= -3395.030288
Sum of electronic and thermal Free Energies= -3395.226989

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

77	-1.439491	0.290636	-0.088101
6	-0.064350	2.533254	-1.661840
6	0.897901	1.413326	-1.716321
7	-1.211999	2.306529	-0.972666
7	0.474626	0.233055	-1.213080
6	0.185898	3.773948	-2.259518
6	-0.750027	4.795855	-2.132951
6	-1.917234	4.554766	-1.410394
6	-2.110513	3.295294	-0.849321
6	2.203629	1.524508	-2.207319
6	3.067674	0.441094	-2.122616
6	2.623780	-0.795298	-1.619415
6	1.275940	-0.836829	-1.226668
5	-2.104717	-0.516461	-1.933077
8	-1.775803	0.122038	-3.123647
8	-2.649735	-1.765787	-2.184683
6	-2.280455	-0.667585	-4.231991
6	-2.417370	-2.090260	-3.582618
5	-3.519080	0.206862	-0.147393
8	-4.370705	-0.692899	0.484026
8	-4.264067	1.113280	-0.911937
6	-5.704188	-0.536913	-0.070467
6	-5.668072	0.944566	-0.588287
6	-0.085967	0.885971	1.578423
6	0.527124	2.151115	1.571243
6	0.616265	-0.134650	2.250631
6	1.845619	2.333602	1.997004
6	1.932977	0.027174	2.669723
6	2.598500	1.247505	2.463286
5	-2.171930	0.699233	1.848798
8	-2.277771	-0.243880	2.866094
8	-2.766435	1.907522	2.235611
6	-3.032872	0.314625	3.962720
6	-2.952257	1.865065	3.678221
1	-1.483854	-1.192010	0.443957
1	0.806026	-1.753634	-0.907146
1	4.100368	0.563345	-2.430438
1	2.566983	2.466306	-2.597214
1	1.097911	3.941441	-2.818534
1	-0.567906	5.762550	-2.592011
1	-2.672916	5.321786	-1.280667
1	-2.999627	3.047624	-0.285924
1	-0.013054	3.007540	1.181589
1	2.291528	3.320792	1.932199
1	0.113337	-1.072469	2.447607
6	3.524724	-1.972921	-1.525452
6	3.413627	-2.962204	-0.510441
6	4.548863	-2.121644	-2.481155
6	4.295634	-4.051558	-0.501612
6	5.419821	-3.206024	-2.463494
1	4.633591	-1.391963	-3.280372
6	5.285809	-4.179105	-1.470415
1	4.180495	-4.791137	0.280027
1	6.188253	-3.296600	-3.225197
1	5.959621	-5.030199	-1.441517
7	2.434052	-2.875131	0.503634

1	2.177416	-1.942062	0.801766
6	1.465300	-3.883566	0.689255
8	1.676294	-5.062262	0.423005
6	-2.381624	-0.136546	5.267663
1	-2.877012	0.315377	6.133638
1	-2.466244	-1.223975	5.358064
1	-1.320612	0.117417	5.296554
6	-1.729621	2.533146	4.319580
1	-1.633010	3.550386	3.927736
1	-1.830731	2.593326	5.407585
1	-0.809356	1.995881	4.084001
6	-4.452488	-0.244231	3.855510
1	-4.893292	0.045330	2.903891
1	-4.407638	-1.336804	3.872283
1	-5.092553	0.091608	4.677563
6	-4.209769	2.652875	4.031728
1	-4.400032	2.615390	5.109544
1	-4.078030	3.702314	3.749537
1	-5.091789	2.274951	3.513417
6	-6.742273	-0.820093	1.010953
1	-6.623393	-1.845670	1.372918
1	-6.651088	-0.151331	1.866619
1	-7.753655	-0.719256	0.602660
6	-5.991657	1.975673	0.498033
1	-5.351169	1.824018	1.369007
1	-5.788361	2.978219	0.108624
1	-7.040994	1.937118	0.805631
6	-5.843069	-1.568019	-1.195866
1	-5.088776	-1.404321	-1.965066
1	-5.674000	-2.566355	-0.783221
1	-6.839772	-1.544127	-1.647327
6	-6.498656	1.214307	-1.837547
1	-7.562718	1.047619	-1.638749
1	-6.371875	2.256044	-2.148290
1	-6.198019	0.578300	-2.671206
6	-3.623674	-0.053136	-4.636137
1	-4.063905	-0.559659	-5.500494
1	-4.330321	-0.088938	-3.803879
1	-3.470053	0.999191	-4.892312
6	-1.285583	-0.577718	-5.384603
1	-1.582617	-1.232105	-6.211124
1	-1.250539	0.448744	-5.762554
1	-0.277516	-0.852567	-5.067496
6	-1.118074	-2.904528	-3.628685
1	-1.228074	-3.783400	-2.988381
1	-0.883703	-3.242828	-4.642395
1	-0.273573	-2.319835	-3.252083
6	-3.579651	-2.932538	-4.096005
1	-3.449770	-3.163417	-5.158704
1	-3.619108	-3.877443	-3.545832
1	-4.538727	-2.429198	-3.966011
7	0.293692	-3.403293	1.204032
1	0.101259	-2.415082	1.100533
6	-0.908200	-4.228171	1.363157
6	-1.751252	-3.646416	2.509665
6	-1.708852	-4.286880	0.048390
1	-0.567239	-5.235602	1.623698
6	-3.092004	-4.377613	2.662981
1	-1.951476	-2.587491	2.306568
1	-1.173984	-3.688928	3.441523
6	-3.055786	-5.003107	0.218213

1	-1.895627	-3.264131	-0.297119
1	-1.096310	-4.783955	-0.713217
6	-3.880286	-4.362750	1.344916
1	-3.675025	-3.907783	3.464637
1	-2.915056	-5.418841	2.970637
1	-3.608709	-4.971988	-0.728748
1	-2.886324	-6.064989	0.450103
1	-4.836160	-4.888795	1.465396
1	-4.109365	-3.322122	1.078699
1	2.475887	-0.795054	3.126644
6	4.081998	1.221002	2.709200
8	4.534525	0.612990	3.683632
7	4.924053	1.759289	1.758423
6	4.496186	2.363670	0.496102
1	5.133992	1.970593	-0.304274
1	3.484321	2.036641	0.261243
6	6.331930	1.337114	1.820976
1	6.934366	2.079522	1.286298
1	6.650737	1.331127	2.864362
6	6.491492	-0.058765	1.200534
1	5.867655	-0.752625	1.775426
1	6.083096	-0.045074	0.180813
6	7.928954	-0.579931	1.150001
1	8.564370	0.131168	0.601810
1	8.338755	-0.637942	2.167798
6	8.006881	-1.957936	0.480022
1	7.362077	-2.660150	1.026345
1	7.580251	-1.891299	-0.530976
6	9.423117	-2.535021	0.392185
1	10.070833	-1.832051	-0.150151
1	9.845424	-2.621015	1.402637
6	9.459971	-3.901981	-0.297414
1	8.848994	-4.633885	0.244241
1	9.065935	-3.839418	-1.319262
1	10.479448	-4.298955	-0.357489
6	4.556425	3.897761	0.488950
1	4.108353	4.276187	1.415198
1	5.601659	4.232661	0.497006
6	3.814024	4.483907	-0.716946
1	4.252921	4.090996	-1.646328
1	2.774349	4.127198	-0.695203
6	3.812952	6.015020	-0.764770
1	3.417142	6.405530	0.183356
1	4.845782	6.382699	-0.838877
6	2.982827	6.577391	-1.925262
1	3.365877	6.175718	-2.874334
1	1.950322	6.213157	-1.831737
6	2.981065	8.106948	-1.981370
1	2.574835	8.535910	-1.057803
1	3.996556	8.500148	-2.107883
1	2.375462	8.479075	-2.815135

3_p

Number of imaginary frequencies : 0

Electronic energy : HF=-3396.5935922
Zero-point correction= 1.457917 (Hartree/Particle)
Thermal correction to Energy= 1.538379
Thermal correction to Enthalpy= 1.539323

Thermal correction to Gibbs Free Energy=	1.337076
Sum of electronic and zero-point Energies=	-3395.135675
Sum of electronic and thermal Energies=	-3395.055214
Sum of electronic and thermal Enthalpies=	-3395.054269
Sum of electronic and thermal Free Energies=	-3395.256516

.....
Cartesian Coordinates

.....

77	-1.104346	-0.373162	-0.701363
6	0.582012	1.173065	-2.752278
6	1.598021	0.409375	-1.998400
7	-0.716454	0.878119	-2.471023
7	1.136012	-0.316744	-0.953711
6	0.912341	2.153124	-3.696241
6	-0.100356	2.818020	-4.381480
6	-1.426761	2.475631	-4.119205
6	-1.689820	1.501278	-3.160788
6	2.956225	0.382637	-2.328639
6	3.829679	-0.397338	-1.580702
6	3.353015	-1.183914	-0.518045
6	1.972848	-1.102367	-0.268721
5	-1.039011	-2.159916	-1.578072
8	-0.251110	-2.400014	-2.710023
8	-1.662767	-3.338134	-1.166931
6	-0.570894	-3.723305	-3.205988
6	-1.084684	-4.439530	-1.907174
5	-3.113914	-0.686643	-0.882746
8	-4.109464	-0.941236	0.076390
8	-3.692457	-0.813193	-2.167848
6	-5.233599	-1.580170	-0.581996
6	-5.114336	-1.025233	-2.043433
6	-1.289061	2.180662	1.710839
6	-0.686372	2.556074	0.499570
6	-0.450140	1.739903	2.748317
6	0.699530	2.513652	0.336205
6	0.926227	1.670363	2.581239
6	1.531925	2.066394	1.372564
5	-2.815988	2.333658	1.962293
8	-3.373012	2.082530	3.188770
8	-3.705912	2.821833	1.038359
6	-4.817094	2.221592	3.040018
6	-4.927418	3.148070	1.770402
1	-1.278002	-1.147767	0.669495
1	1.502705	-1.699232	0.496479
1	4.885740	-0.393769	-1.823021
1	3.332967	0.951959	-3.170552
1	1.950375	2.400466	-3.885715
1	0.144001	3.584730	-5.110098
1	-2.249641	2.953249	-4.640016
1	-2.697244	1.181442	-2.922932
1	-1.307014	2.902265	-0.321448
1	1.100772	2.806225	-0.621611
1	-0.889100	1.449482	3.696693
6	4.251267	-2.083382	0.250816
6	4.065111	-2.383797	1.627010
6	5.324332	-2.699113	-0.422125
6	4.917082	-3.299832	2.258278
6	6.168598	-3.602701	0.216214
1	5.468412	-2.501499	-1.479798
6	5.955872	-3.910428	1.561845
1	4.738901	-3.520561	3.302848

1	6.974399	-4.074531	-0.338054
1	6.601825	-4.619532	2.071531
7	3.029736	-1.773942	2.366451
1	2.902742	-0.771377	2.227064
6	2.021916	-2.522178	2.978352
8	2.178256	-3.686873	3.340861
6	-5.378762	2.823390	4.322802
1	-6.452287	3.013758	4.221691
1	-5.236585	2.122448	5.150662
1	-4.880357	3.758370	4.585897
6	-4.842978	4.642119	2.101561
1	-4.718412	5.206050	1.172722
1	-5.749247	4.996204	2.601395
1	-3.984216	4.856737	2.744432
6	-5.368745	0.812972	2.811286
1	-4.930662	0.355137	1.921590
1	-5.110340	0.188105	3.670964
1	-6.458297	0.821822	2.712393
6	-6.126438	2.868535	0.876165
1	-7.061492	3.035217	1.421017
1	-6.113445	3.538886	0.011404
1	-6.113556	1.843011	0.510287
6	-6.530097	-1.222195	0.137781
1	-6.505456	-1.611087	1.159901
1	-6.692458	-0.145543	0.192570
1	-7.387460	-1.672982	-0.374329
6	-5.786960	0.340823	-2.230690
1	-5.449731	1.043338	-1.464257
1	-5.502480	0.744655	-3.207651
1	-6.879460	0.277422	-2.196260
6	-5.000908	-3.094593	-0.495680
1	-4.053530	-3.368825	-0.963621
1	-4.942858	-3.382546	0.557623
1	-5.817504	-3.658196	-0.958892
6	-5.564209	-1.988920	-3.138270
1	-6.626585	-2.235973	-3.034463
1	-5.418726	-1.528751	-4.121042
1	-4.988012	-2.915757	-3.115161
6	-1.667480	-3.545846	-4.262864
1	-1.940909	-4.493878	-4.736748
1	-2.560172	-3.096450	-3.818775
1	-1.303361	-2.865885	-5.039231
6	0.681465	-4.332416	-3.826053
1	0.503271	-5.369733	-4.129566
1	0.968955	-3.764617	-4.716798
1	1.521386	-4.311855	-3.128844
6	0.049431	-5.009068	-1.045756
1	-0.355138	-5.295418	-0.071444
1	0.508931	-5.891647	-1.501794
1	0.826774	-4.259000	-0.874198
6	-2.159563	-5.498116	-2.131549
1	-1.775979	-6.319875	-2.746038
1	-2.474024	-5.913550	-1.169192
1	-3.041952	-5.080018	-2.619888
7	0.840221	-1.835648	3.127528
1	0.687936	-1.031366	2.529745
6	-0.385529	-2.539581	3.531901
6	-1.456924	-1.497215	3.882416
6	-0.882833	-3.505805	2.438127
1	-0.135363	-3.121173	4.427082
6	-2.792826	-2.155314	4.249909

1	-1.616993	-0.853746	3.008020
1	-1.095658	-0.859087	4.698401
6	-2.235069	-4.139631	2.795216
1	-0.990147	-2.947432	1.502261
1	-0.120880	-4.275602	2.282308
6	-3.284063	-3.064113	3.114397
1	-3.532860	-1.376694	4.468840
1	-2.673126	-2.747339	5.169385
1	-2.573004	-4.768774	1.962824
1	-2.117348	-4.802415	3.665805
1	-4.240544	-3.529652	3.386211
1	-3.461332	-2.453845	2.219457
1	1.555699	1.308665	3.385821
6	3.035684	1.907953	1.359025
8	3.523345	1.032733	2.098674
7	3.874906	2.735494	0.671076
6	3.502024	3.656138	-0.408027
1	4.417525	3.862982	-0.970120
1	2.845174	3.143609	-1.114535
6	5.309885	2.619542	0.989477
1	5.775147	3.580048	0.744407
1	5.404924	2.467771	2.067195
6	6.002254	1.470762	0.253270
1	5.449216	0.555048	0.476553
1	5.935264	1.636822	-0.830574
6	7.465630	1.286641	0.665557
1	8.046502	2.187281	0.418618
1	7.518205	1.175173	1.757406
6	8.103848	0.058072	0.006725
1	7.500777	-0.827802	0.246810
1	8.062907	0.166920	-1.087603
6	9.554088	-0.189510	0.436085
1	10.167308	0.685337	0.178864
1	9.594218	-0.280236	1.530102
6	10.153743	-1.445608	-0.200947
1	9.579274	-2.337938	0.074701
1	10.150206	-1.376878	-1.295630
1	11.189580	-1.605816	0.117878
6	2.878984	4.976069	0.059763
1	2.059038	4.765018	0.753370
1	3.627557	5.546624	0.623915
6	2.351903	5.801129	-1.118688
1	3.178831	6.040246	-1.803008
1	1.645140	5.187719	-1.697692
6	1.651749	7.094415	-0.688210
1	0.829997	6.846231	-0.001632
1	2.352504	7.716619	-0.113769
6	1.098602	7.905411	-1.865782
1	1.921552	8.163663	-2.546642
1	0.409242	7.274994	-2.444662
6	0.377113	9.182164	-1.426809
1	-0.473948	8.952003	-0.774937
1	1.048772	9.845182	-0.868650
1	-0.005420	9.744035	-2.285931

TS[1-2]_{m(S1)}

Number of imaginary frequencies : 1
Imaginary frequency : -810.8577 cm(-1)

Electronic energy : HF=-3003.3642828
 Zero-point correction= 1.166978 (Hartree/Particle)
 Thermal correction to Energy= 1.234645
 Thermal correction to Enthalpy= 1.235589
 Thermal correction to Gibbs Free Energy= 1.063999
 Sum of electronic and zero-point Energies= -3002.197305
 Sum of electronic and thermal Energies= -3002.129638
 Sum of electronic and thermal Enthalpies= -3002.128694
 Sum of electronic and thermal Free Energies= -3002.300284

.....
 Cartesian Coordinates

77	-0.947141	-0.199792	0.490241
5	-2.549378	1.173776	0.448495
8	-2.721842	2.116728	1.461755
8	-3.572761	1.288587	-0.489510
6	-3.737365	3.061218	1.033177
6	-4.576525	2.193657	0.032591
5	-0.906921	0.632489	-1.417790
8	-0.666130	1.997365	-1.595428
8	-1.057964	0.007665	-2.642641
6	-0.537815	2.283660	-3.013645
6	-1.207567	1.017744	-3.670911
5	-2.353984	-1.541167	-0.132996
8	-2.237055	-2.459856	-1.175723
8	-3.589047	-1.729635	0.512510
6	-3.536459	-3.040282	-1.428817
6	-4.229047	-2.910162	-0.027055
6	-0.583150	0.606613	3.445890
6	0.459718	1.394697	2.751353
7	-1.326928	-0.232923	2.682005
7	0.475297	1.307915	1.399332
6	-0.813903	0.709572	4.824436
6	-1.805218	-0.062394	5.418266
6	-2.557080	-0.923720	4.620617
6	-2.289266	-0.973085	3.257365
6	1.413547	2.169125	3.422495
6	2.397938	2.833652	2.698475
6	2.421073	2.732323	1.302580
6	1.411275	1.963656	0.705860
6	0.635454	-1.778698	0.756442
6	0.379882	-3.161259	0.652641
6	1.910761	-1.411382	1.209036
6	1.333282	-4.113394	1.025442
6	2.867698	-2.351310	1.611954
6	2.579827	-3.719938	1.514513
1	0.058755	-1.005494	-0.493319
1	2.197230	-0.369829	1.248040
1	3.327618	-4.460904	1.780529
1	1.107510	-5.171260	0.916238
1	-0.563129	-3.491484	0.231018
1	-2.867446	-1.588243	2.578344
1	-3.345608	-1.541551	5.036509
1	-1.991819	0.014481	6.485001
1	-0.234099	1.397549	5.427271
1	1.413533	2.233117	4.503639
1	3.157938	3.414336	3.212227
1	1.347415	1.875833	-0.369742
6	4.208958	-1.810702	1.999764
8	4.704547	-0.878204	1.336152
7	4.884518	-2.356576	3.047625

6	3.412721	3.436949	0.453219
6	3.578693	4.823273	0.597146
6	4.144201	2.754902	-0.549105
6	4.399080	5.543468	-0.267060
1	3.016267	5.339205	1.370606
6	4.953166	3.490923	-1.428134
6	5.068440	4.871731	-1.293632
1	4.499683	6.618720	-0.153713
1	5.483663	2.963958	-2.210637
1	5.699732	5.423078	-1.984849
7	4.085096	1.351830	-0.616366
6	4.009287	0.610816	-1.795641
8	3.922938	1.131884	-2.909497
7	4.019525	-0.738132	-1.583250
1	4.078769	0.832704	0.255453
1	4.065268	-1.063531	-0.622393
6	4.285782	-3.171545	4.099414
1	4.723961	-4.176462	4.117826
1	3.209655	-3.256918	3.963587
6	6.241483	-1.895811	3.322084
1	6.831340	-2.732598	3.708880
1	6.694548	-1.520465	2.405826
6	3.558966	-1.668392	-2.610179
6	4.162526	-3.057817	-2.363653
6	2.022266	-1.745815	-2.651747
1	3.919363	-1.283879	-3.570899
6	3.663145	-4.075640	-3.401588
1	3.869520	-3.394306	-1.358099
1	5.257163	-2.993587	-2.373830
6	1.522951	-2.750268	-3.696266
1	1.669317	-2.056555	-1.662906
1	1.603095	-0.753670	-2.838103
6	2.127753	-4.139038	-3.443755
1	4.082273	-5.065595	-3.183199
1	4.038598	-3.788711	-4.394293
1	0.428442	-2.792028	-3.669978
1	1.805077	-2.407297	-4.702521
1	1.799724	-4.849753	-4.212475
1	1.755996	-4.518252	-2.481157
6	-3.347406	-4.467032	-1.932615
1	-4.312527	-4.966523	-2.070536
1	-2.833781	-4.449042	-2.898635
1	-2.741847	-5.061849	-1.245475
6	-4.205194	-2.177908	-2.507214
1	-3.558063	-2.157767	-3.387933
1	-5.181661	-2.575959	-2.802381
1	-4.327322	-1.149302	-2.158162
6	-5.735172	-2.672983	-0.066246
1	-6.255418	-3.522705	-0.521742
1	-6.117400	-2.548672	0.952039
1	-5.982755	-1.770664	-0.627249
6	-3.900321	-4.073546	0.917532
1	-4.254570	-3.828737	1.924033
1	-4.382279	-5.005285	0.605741
1	-2.820318	-4.239162	0.971107
6	-5.636024	1.332298	0.730099
1	-6.464264	1.937550	1.112513
1	-6.036581	0.610967	0.012849
1	-5.195567	0.767695	1.555708
6	-5.197024	2.960974	-1.129969
1	-5.734165	2.268175	-1.785242

1	-5.912490	3.708091	-0.769356
1	-4.437325	3.467535	-1.728064
6	-2.997726	4.215379	0.346722
1	-3.680109	5.005539	0.017470
1	-2.284625	4.649406	1.054338
1	-2.431357	3.846668	-0.512198
6	-4.495022	3.557471	2.259043
1	-3.819407	4.126179	2.906021
1	-5.319686	4.218035	1.969909
1	-4.900097	2.728685	2.843124
6	-0.527185	0.516881	-4.941484
1	-0.586504	1.267035	-5.737433
1	0.523048	0.274523	-4.770805
1	-1.029217	-0.390144	-5.291911
6	-2.715078	1.180747	-3.901057
1	-2.933949	1.916831	-4.681339
1	-3.130695	0.218189	-4.211623
1	-3.212623	1.473803	-2.973821
6	0.955586	2.423111	-3.312289
1	1.375210	3.217210	-2.687592
1	1.510601	1.509957	-3.095920
1	1.138854	2.688770	-4.358238
6	-1.248241	3.605007	-3.297858
1	-0.738267	4.416416	-2.769447
1	-1.229037	3.836089	-4.368318
1	-2.287314	3.584666	-2.965116
1	6.243080	-1.091948	4.069868
1	4.472301	-2.699808	5.072060

TS[1-2]_{p(S1)}

Number of imaginary frequencies : 1
Imaginary frequency : -790.4841 cm(-1)

Electronic energy : HF=-3003.3523982
Zero-point correction= 1.166842 (Hartree/Particle)
Thermal correction to Energy= 1.234545
Thermal correction to Enthalpy= 1.235489
Thermal correction to Gibbs Free Energy= 1.064459
Sum of electronic and zero-point Energies= -3002.185557
Sum of electronic and thermal Energies= -3002.117853
Sum of electronic and thermal Enthalpies= -3002.116909
Sum of electronic and thermal Free Energies= -3002.287940

Cartesian Coordinates

6	-6.572529	-1.974032	3.700977
6	-7.430916	-1.651187	2.467944
6	-6.566826	-1.198996	1.281157
6	-5.693667	0.001102	1.670744
6	-4.823089	-0.325241	2.899096
6	-5.684959	-0.780686	4.085064
7	-4.880789	0.441463	0.534712
6	-4.411763	1.719628	0.509607
8	-4.655437	2.542108	1.394809
7	-3.597775	2.015855	-0.594110
6	-3.231897	3.303914	-1.015780
6	-2.134517	3.480201	-1.896431
6	-1.851976	4.766953	-2.387318
6	-2.597895	5.877616	-2.010046

6	-3.660732	5.699909	-1.122665
6	-3.980767	4.436288	-0.639017
6	-1.228398	2.385422	-2.328541
6	-0.929696	2.188056	-3.683870
6	0.044103	1.271087	-4.050668
6	0.724901	0.547273	-3.065271
7	0.409225	0.709255	-1.756587
6	-0.531592	1.596794	-1.403609
6	1.795479	-0.421397	-3.389061
7	2.231950	-1.203438	-2.372875
6	3.181811	-2.120727	-2.614035
6	3.749592	-2.304557	-3.870832
6	3.325787	-1.489351	-4.919159
6	2.342046	-0.537670	-4.674896
77	1.418223	-0.649151	-0.306034
6	-0.419356	-1.856977	-0.591982
6	-0.689913	-2.400049	-1.862353
6	-1.992209	-2.699004	-2.266204
6	-3.066461	-2.497167	-1.388892
6	-2.796203	-2.065540	-0.084055
6	-1.495121	-1.774340	0.312610
6	-4.489980	-2.540274	-1.844086
7	-4.931846	-3.606549	-2.570059
6	-4.276783	-4.908449	-2.615044
5	2.895339	0.857641	-0.131329
8	3.658085	1.205055	0.980016
6	4.561862	2.277422	0.613215
6	4.703562	3.216129	1.806791
5	0.742287	0.233147	1.410191
8	0.345500	-0.372303	2.597651
6	0.193870	0.655030	3.606777
6	1.548869	0.777458	4.315834
5	2.891336	-1.575865	0.833218
8	4.108286	-1.983876	0.273707
6	4.812151	-2.807392	1.236471
6	4.516010	-4.267810	0.874036
8	3.149997	1.739737	-1.180848
6	3.844229	2.893279	-0.637947
6	4.771421	3.457513	-1.707897
6	2.763827	3.916330	-0.263278
6	5.912617	1.635831	0.274753
8	0.546425	1.620886	1.504334
6	-0.154200	1.914327	2.740848
6	0.362548	3.241352	3.286940
6	-1.643247	2.021431	2.404302
6	-0.890849	0.221732	4.586757
8	2.841347	-1.932688	2.170806
6	4.157036	-2.359568	2.593194
6	4.842580	-1.139899	3.219897
6	3.998813	-3.468234	3.629410
6	6.306015	-2.524133	1.115046
8	-5.236096	-1.575493	-1.597141
6	-6.285261	-3.574043	-3.111299
1	-2.180144	-3.044003	-3.280191
1	-3.614030	-1.932640	0.613531
1	-1.312499	-1.433020	1.325226
1	3.505277	-2.688756	-1.751650
1	4.513900	-3.061232	-4.011804
1	3.756967	-1.586893	-5.910699
1	2.016084	0.116314	-5.474108
1	0.264151	1.115767	-5.099405

1	-1.458056	2.758278	-4.441538
1	-0.690605	1.712051	-0.339854
1	-1.003035	4.887159	-3.054493
1	-2.345838	6.862999	-2.389566
1	-4.809463	4.310440	0.042071
1	-4.259156	6.550361	-0.807789
1	-3.253061	1.234805	-1.136254
1	-4.852600	-0.154221	-0.293260
1	-6.596787	-2.540747	-3.257457
1	-6.997114	-4.060358	-2.431093
1	-4.021405	-5.182487	-3.645787
1	-3.368545	-4.908921	-2.015688
1	-6.351357	0.834828	1.949151
1	-5.925329	-2.028313	0.958405
1	-7.189584	-0.941642	0.417619
1	-4.114741	-1.121131	2.631877
1	-4.235368	0.559978	3.158633
1	-8.030966	-2.522990	2.180185
1	-8.141324	-0.852112	2.723184
1	-5.045650	-1.035818	4.938782
1	-6.321978	0.054481	4.408946
1	-7.211892	-2.263650	4.543909
1	-5.933552	-2.840557	3.477084
1	4.974027	-3.869710	3.926065
1	3.511570	-3.067036	4.523239
1	3.382055	-4.287376	3.254066
1	4.239626	-0.791305	4.062905
1	5.845193	-1.378985	3.588637
1	4.900730	-0.323744	2.497452
1	6.870684	-3.059276	1.886116
1	6.669770	-2.856618	0.137325
1	6.515917	-1.456690	1.203400
1	4.844565	-4.455466	-0.153244
1	5.041059	-4.968007	1.530962
1	3.443072	-4.474121	0.929246
1	6.667270	2.386637	0.020207
1	6.270261	1.075981	1.143455
1	5.813040	0.936379	-0.559589
1	5.191605	2.691239	2.634056
1	5.315775	4.088131	1.551775
1	3.730257	3.562426	2.159016
1	3.195680	4.842741	0.128679
1	2.182000	4.161215	-1.157564
1	2.077066	3.496514	0.476987
1	4.178075	3.845484	-2.541844
1	5.371941	4.282191	-1.309157
1	5.444593	2.693578	-2.102673
1	-1.092679	1.007554	5.322859
1	-1.823817	-0.019826	4.073117
1	-0.563634	-0.672272	5.126871
1	1.514890	1.499715	5.137802
1	1.823400	-0.200398	4.719684
1	2.325254	1.077626	3.607044
1	-1.798730	2.807128	1.661439
1	-2.017853	1.083836	1.985954
1	-2.245545	2.274908	3.280450
1	0.089770	4.052963	2.605274
1	-0.080986	3.460218	4.264348
1	1.449492	3.236770	3.389617
1	0.117608	-2.530124	-2.575540
1	0.992262	-2.097406	0.274826

1	-6.302659	-4.103696	-4.069192
1	-4.953097	-5.674819	-2.215472

TS[1-2]_m(dtbpy)

Number of imaginary frequencies : 1
Imaginary frequency : -765.5093 cm(-1)

Electronic energy : HF=-3021.2441721
Zero-point correction= 1.401472 (Hartree/Particle)
Thermal correction to Energy= 1.478712
Thermal correction to Enthalpy= 1.479656
Thermal correction to Gibbs Free Energy= 1.287120
Sum of electronic and zero-point Energies= -3019.842700
Sum of electronic and thermal Energies= -3019.765460
Sum of electronic and thermal Enthalpies= -3019.764516
Sum of electronic and thermal Free Energies= -3019.957052

Cartesian Coordinates

77	1.578782	-0.349020	-0.386228
5	2.614824	0.107956	1.401361
8	2.058321	0.972469	2.347701
8	3.867746	-0.318689	1.833824
6	2.872247	0.933640	3.545494
6	4.260919	0.479931	2.976760
5	2.453737	-2.151571	0.149140
8	1.919377	-2.957381	1.161889
8	3.558563	-2.769199	-0.415476
6	2.564725	-4.254244	1.109976
6	3.918155	-3.918816	0.384673
5	3.316625	0.163082	-1.321473
8	3.886774	-0.465496	-2.426547
8	4.081119	1.294730	-0.983821
6	5.222696	0.053345	-2.610192
6	5.099111	1.491165	-1.994400
6	-0.438822	1.803830	0.549423
6	-1.058718	0.547166	1.037132
7	0.713632	1.680002	-0.145186
7	-0.367128	-0.591459	0.801170
6	-0.991937	3.064805	0.806879
6	-0.379320	4.231163	0.346930
6	0.802709	4.062244	-0.390238
6	1.312667	2.791789	-0.602867
6	-2.290083	0.519636	1.698626
6	-2.851305	-0.685186	2.140898
6	-2.109987	-1.842943	1.881527
6	-0.886011	-1.750838	1.225115
6	0.389315	-0.524535	-2.261284
6	0.757021	0.158560	-3.435843
6	-0.881236	-1.118290	-2.239802
6	-0.137317	0.307331	-4.499966
6	-1.793384	-0.957208	-3.288689
6	-1.422586	-0.233798	-4.428169
1	1.529060	-1.471392	-1.545157
1	-1.189739	-1.713087	-1.387262
1	-2.120506	-0.115960	-5.252803
1	0.171768	0.844362	-5.393869
1	1.759941	0.564452	-3.521654
1	2.250746	2.635306	-1.118511

1	1.343721	4.912178	-0.791078
1	-1.900161	3.129207	1.387259
1	-2.820695	1.445231	1.876608
1	-0.275138	-2.625530	1.039031
6	-3.118078	-1.655896	-3.146942
8	-3.158894	-2.887388	-3.067224
7	-4.259696	-0.900126	-3.066763
6	-4.297147	0.562478	-3.001835
1	-5.054118	0.917138	-3.714500
1	-3.337561	0.953393	-3.338473
6	-5.519483	-1.627443	-2.861441
1	-6.339350	-0.938350	-3.092415
1	-5.560655	-2.450820	-3.581434
6	-4.610588	1.122264	-1.607509
6	-4.675369	2.654110	-1.600434
1	-3.851149	0.765612	-0.900559
1	-5.573685	0.728332	-1.261527
6	-5.131832	3.230361	-0.254361
1	-3.693284	3.068716	-1.866784
1	-5.371703	2.986314	-2.383931
6	-5.405825	4.738350	-0.286976
1	-6.044648	2.710849	0.069768
1	-4.373405	3.012127	0.511773
1	-4.493527	5.272426	-0.583765
1	-6.147544	4.950771	-1.068685
6	-5.678081	-2.189775	-1.442171
6	-7.014346	-2.905100	-1.226805
1	-5.582062	-1.373161	-0.718885
1	-4.848827	-2.878737	-1.255819
6	-7.176089	-3.424174	0.206756
1	-7.843684	-2.221302	-1.460969
1	-7.100471	-3.743710	-1.931705
6	-8.499928	-4.154344	0.457519
1	-6.340903	-4.099749	0.440963
1	-7.090439	-2.581647	0.908312
1	-9.335915	-3.480693	0.223626
1	-8.584804	-4.998992	-0.239633
6	-5.911655	5.280258	1.052739
1	-6.080326	6.361889	1.012631
1	-6.859141	4.806238	1.335002
1	-5.196475	5.087125	1.860994
6	-8.636948	-4.661232	1.895704
1	-9.586558	-5.185455	2.050018
1	-7.828341	-5.357513	2.148273
1	-8.593982	-3.833624	2.614287
6	5.566533	0.010203	-4.095263
1	6.540282	0.473827	-4.288157
1	5.614543	-1.030194	-4.431099
1	4.810633	0.519072	-4.697156
6	6.169178	-0.855518	-1.814790
1	6.044912	-1.882801	-2.166058
1	7.217248	-0.565990	-1.943796
1	5.919134	-0.837794	-0.751075
6	6.362589	2.021240	-1.323334
1	7.177494	2.122099	-2.048709
1	6.169242	3.009446	-0.893606
1	6.693688	1.365649	-0.516490
6	4.558116	2.525781	-2.989650
1	4.315906	3.448336	-2.452240
1	5.289681	2.768076	-3.766637
1	3.645960	2.162912	-3.472067

6	5.099942	1.644230	2.436151
1	5.474734	2.285129	3.240700
1	5.955987	1.237662	1.891092
1	4.519751	2.246661	1.733395
6	5.096207	-0.382897	3.916863
1	6.023737	-0.680821	3.418450
1	5.363291	0.171514	4.823313
1	4.566284	-1.291502	4.208762
6	2.236170	-0.105786	4.476922
1	2.750711	-0.164650	5.441335
1	1.193840	0.173377	4.659117
1	2.241494	-1.095576	4.011813
6	2.852578	2.314786	4.191597
1	1.841710	2.543389	4.544463
1	3.528853	2.358449	5.052350
1	3.141466	3.090554	3.479511
6	4.436519	-5.012833	-0.544378
1	4.636618	-5.936281	0.009997
1	3.726283	-5.229970	-1.344427
1	5.372497	-4.687961	-1.008739
6	5.024186	-3.471081	1.347464
1	5.387192	-4.299828	1.963949
1	5.863045	-3.083459	0.761807
1	4.671883	-2.662506	1.989971
6	1.649188	-5.173289	0.291602
1	0.663207	-5.209318	0.765542
1	1.519105	-4.791940	-0.725253
1	2.036555	-6.195349	0.235656
6	2.706022	-4.779400	2.534936
1	1.714898	-4.959343	2.963711
1	3.258370	-5.725134	2.552360
1	3.222428	-4.061127	3.174755
1	-2.458321	-2.823195	2.180927
6	-4.181224	-0.688249	2.907417
6	-0.938912	5.633088	0.616627
6	-2.168442	5.598378	1.540283
1	-1.924950	5.185314	2.525221
1	-2.548234	6.613657	1.690737
1	-2.980693	5.008032	1.110354
6	-1.346494	6.268206	-0.732634
1	-2.114981	5.670545	-1.234168
1	-1.749450	7.274290	-0.571889
1	-0.493596	6.353464	-1.413089
6	0.149816	6.500375	1.288493
1	0.472103	6.060709	2.238285
1	1.034145	6.616253	0.655466
1	-0.243063	7.502231	1.493267
6	-5.249412	0.117825	2.135330
1	-5.422874	-0.304126	1.141824
1	-6.198182	0.097293	2.682524
1	-4.970202	1.167089	2.009519
6	-3.942538	-0.025009	4.284719
1	-4.872528	-0.008249	4.863932
1	-3.191288	-0.573861	4.862227
1	-3.594233	1.007817	4.179342
6	-4.714741	-2.115154	3.127610
1	-5.682474	-2.073171	3.637639
1	-4.862231	-2.644270	2.180984
1	-4.044552	-2.711484	3.755128

TS[1-2]_p(dtbpy)

Number of imaginary frequencies : 1
Imaginary frequency : -782.8664 cm(-1)

Electronic energy : HF=-3021.2464376
Zero-point correction= 1.403234 (Hartree/Particle)
Thermal correction to Energy= 1.479559
Thermal correction to Enthalpy= 1.480503
Thermal correction to Gibbs Free Energy= 1.290310
Sum of electronic and zero-point Energies= -3019.843203
Sum of electronic and thermal Energies= -3019.766879
Sum of electronic and thermal Enthalpies= -3019.765935
Sum of electronic and thermal Free Energies= -3019.956128

Cartesian Coordinates

77	1.400181	0.005890	-0.027690
5	3.115009	1.078620	0.584764
8	3.003779	2.288805	1.273320
8	4.458954	0.739785	0.439911
6	4.292956	2.595087	1.862059
6	5.273480	1.847166	0.894894
5	2.081654	-1.403737	1.278953
8	2.652488	-1.104297	2.527211
8	1.953265	-2.784716	1.147627
6	2.765647	-2.324587	3.299655
6	2.737544	-3.424552	2.178326
5	2.810485	-0.681194	-1.379394
8	3.577650	-1.831375	-1.283577
8	3.049363	-0.046130	-2.604425
6	4.512617	-1.871002	-2.384545
6	3.807584	-0.951652	-3.446675
6	-0.278635	2.588532	-0.498520
6	-0.653900	2.103329	0.851004
7	0.616340	1.832980	-1.177554
7	0.181207	1.198808	1.412204
6	-0.807760	3.757946	-1.044906
6	-0.454430	4.174835	-2.335217
6	0.465776	3.369030	-3.015233
6	0.978492	2.226117	-2.405315
6	-1.829958	2.489024	1.490905
6	-2.173781	1.966764	2.745588
6	-1.228055	1.130145	3.348887
6	-0.077225	0.771679	2.653290
6	-1.481167	-0.475284	-1.321517
6	-0.589813	-0.936270	-0.336713
6	-2.845261	-0.776908	-1.274638
6	-1.117879	-1.769803	0.665269
6	-3.358190	-1.566000	-0.238849
6	-2.479160	-2.048460	0.737952
1	-3.512801	-0.381977	-2.037045
1	-2.872655	-2.652744	1.550591
1	-0.453444	-2.198448	1.406650
1	1.703226	1.586659	-2.897503
1	0.804066	3.612345	-4.014477
1	-1.489022	4.354941	-0.451106
1	-2.515246	3.150649	0.976515
1	0.656586	0.093651	3.071665
6	-4.817352	-1.866400	-0.063927
8	-5.368705	-1.550462	0.999346

7	-5.493697	-2.494894	-1.077860
6	-6.935692	-2.724238	-0.915125
1	-7.161084	-2.676752	0.150123
1	-7.161510	-3.740148	-1.256197
6	-4.879857	-3.095701	-2.272141
1	-5.583027	-2.950581	-3.099210
1	-3.977409	-2.549166	-2.536333
6	-7.794663	-1.719343	-1.701420
6	-7.613753	-0.252192	-1.287535
1	-8.846577	-2.011857	-1.578367
1	-7.573455	-1.822084	-2.771949
6	-8.117580	0.079038	0.122442
1	-6.550908	0.013601	-1.363063
1	-8.137427	0.382586	-2.015656
6	-7.926820	1.554410	0.490899
1	-9.183717	-0.182118	0.199202
1	-7.579249	-0.534983	0.852068
1	-6.857938	1.797784	0.429010
1	-8.432180	2.190722	-0.249655
6	-4.561865	-4.596193	-2.133868
6	-3.347676	-4.935532	-1.254337
1	-4.390370	-4.988316	-3.145927
1	-5.450077	-5.115539	-1.752905
6	-2.003490	-4.472051	-1.832737
1	-3.484369	-4.503434	-0.255363
1	-3.319006	-6.024566	-1.112942
6	-0.787440	-4.918117	-1.011165
1	-1.902729	-4.852689	-2.860494
1	-1.985375	-3.378730	-1.903550
1	-0.885778	-4.536864	0.012418
1	-0.775469	-6.015121	-0.937193
6	-8.444733	1.889373	1.891999
1	-8.268928	2.940256	2.149193
1	-9.523322	1.705913	1.970415
1	-7.952297	1.271355	2.651605
6	0.533699	-4.421622	-1.605177
1	1.390126	-4.701136	-0.985891
1	0.690843	-4.825288	-2.613842
1	0.538692	-3.329661	-1.673291
6	4.691722	-3.325775	-2.811218
1	5.307003	-3.399489	-3.714685
1	5.194513	-3.882521	-2.014666
1	3.730583	-3.809317	-2.998227
6	5.839232	-1.295773	-1.877461
1	6.175889	-1.887867	-1.021558
1	6.617298	-1.327276	-2.646909
1	5.702727	-0.270037	-1.531553
6	4.747951	-0.130993	-4.322987
1	5.393992	-0.782711	-4.920965
1	4.166563	0.490450	-5.012016
1	5.377270	0.530828	-3.724734
6	2.791593	-1.707002	-4.312337
1	2.195919	-0.983495	-4.877622
1	3.281154	-2.379116	-5.023832
1	2.108887	-2.293384	-3.690627
6	5.638929	2.674678	-0.343996
1	6.298066	3.513334	-0.098102
1	6.157389	2.033025	-1.062217
1	4.739218	3.063195	-0.829736
6	6.531532	1.285160	1.548329
1	7.137081	0.766292	0.798434

1	7.140585	2.085489	1.982646
1	6.284505	0.567285	2.332563
6	4.280527	2.005164	3.278417
1	5.205859	2.220166	3.822842
1	3.446202	2.445859	3.833249
1	4.121874	0.924192	3.242114
6	4.462775	4.109406	1.915370
1	3.722962	4.539840	2.597713
1	5.458523	4.379194	2.284196
1	4.318700	4.567168	0.934370
6	2.054688	-4.730882	2.570845
1	2.571020	-5.210307	3.409781
1	1.010749	-4.570837	2.848316
1	2.071400	-5.423525	1.723720
6	4.121504	-3.701933	1.578639
1	4.773498	-4.230016	2.281918
1	3.998942	-4.320159	0.685788
1	4.599998	-2.769696	1.269629
6	1.550474	-2.384261	4.233385
1	1.536351	-1.485630	4.858478
1	0.617655	-2.416726	3.662853
1	1.583405	-3.255924	4.894358
6	4.052377	-2.266878	4.117033
1	3.985177	-1.468039	4.862580
1	4.220965	-3.209884	4.648452
1	4.917613	-2.063954	3.483487
1	-1.112933	0.154202	-2.126429
1	0.964595	-1.275724	-0.899403
1	-1.387001	0.706524	4.332483
6	-3.539932	2.290746	3.360238
6	-3.657557	3.817019	3.575247
1	-2.885671	4.181434	4.261700
1	-3.560885	4.372004	2.636676
1	-4.635746	4.061536	4.003767
6	-4.646198	1.818591	2.384953
1	-4.595974	0.742024	2.191053
1	-5.630559	2.041678	2.808889
1	-4.579945	2.332194	1.420839
6	-3.747078	1.587056	4.712271
1	-4.735958	1.838362	5.108415
1	-3.700239	0.497823	4.613262
1	-3.006189	1.901305	5.455638
6	-1.062393	5.454584	-2.924630
6	-0.647275	6.659634	-2.048964
1	-0.994397	6.554634	-1.016409
1	0.441631	6.773458	-2.026895
1	-1.077040	7.583668	-2.451396
6	-2.603973	5.329885	-2.931791
1	-2.929889	4.477781	-3.537498
1	-3.011339	5.198524	-1.924757
1	-3.052614	6.236170	-3.352942
6	-0.588176	5.710297	-4.366164
1	0.496428	5.850700	-4.420233
1	-0.863455	4.890233	-5.037980
1	-1.055811	6.622004	-4.751392

TS[1-2]_m(bpy)

Number of imaginary frequencies : 1
Imaginary frequency : -797.2314 cm(-1)

Electronic energy : HF=-2706.6802319
 Zero-point correction= 1.177251 (Hartree/Particle)
 Thermal correction to Energy= 1.242640
 Thermal correction to Enthalpy= 1.243584
 Thermal correction to Gibbs Free Energy= 1.077215
 Sum of electronic and zero-point Energies= -2705.502981
 Sum of electronic and thermal Energies= -2705.437592
 Sum of electronic and thermal Enthalpies= -2705.436648
 Sum of electronic and thermal Free Energies= -2705.603017

.....
 Cartesian Coordinates

.....
 77 -0.809265 0.069254 -0.135814
 5 -2.312771 0.530140 1.282340
 8 -2.029816 0.549918 2.648635
 8 -3.660169 0.812572 1.072756
 6 -3.178546 1.089869 3.350589
 6 -4.344728 0.778657 2.350035
 5 -1.813999 1.689438 -0.963604
 8 -1.627689 2.992706 -0.483227
 8 -2.680066 1.700592 -2.043395
 6 -2.219864 3.918738 -1.430757
 6 -3.281095 3.012343 -2.149973
 5 -2.225888 -1.144956 -0.957703
 8 -2.564313 -1.267108 -2.303454
 8 -2.972928 -2.074027 -0.208742
 6 -3.774259 -2.051424 -2.403670
 6 -3.683524 -2.946244 -1.120127
 6 0.969359 -0.862663 2.205423
 6 1.470943 0.504648 1.934442
 7 -0.052390 -1.306625 1.432920
 7 0.758138 1.240641 1.050481
 6 1.481656 -1.656398 3.240098
 6 0.932977 -2.909388 3.487286
 6 -0.126217 -3.345552 2.694111
 6 -0.586807 -2.514804 1.679281
 6 2.611384 1.029655 2.557533
 6 2.989198 2.342989 2.299090
 6 2.212936 3.108764 1.430993
 6 1.110421 2.515254 0.823132
 6 0.833616 -0.634188 -1.508130
 6 0.663529 -1.724491 -2.383918
 6 2.134944 -0.116514 -1.387243
 6 1.745921 -2.298946 -3.055187
 6 3.233433 -0.708423 -2.024275
 6 3.037935 -1.806201 -2.869412
 1 -0.396079 0.445611 -1.652214
 1 2.324372 0.759958 -0.779119
 1 3.880663 -2.253543 -3.389562
 1 1.578835 -3.135563 -3.729643
 1 -0.334483 -2.108079 -2.562841
 1 -1.420857 -2.790528 1.045909
 1 -0.593044 -4.312056 2.847836
 1 1.322832 -3.529014 4.288599
 1 2.289026 -1.290828 3.861103
 1 3.208061 0.420604 3.225356
 1 3.877130 2.758288 2.763598
 1 0.470086 3.053350 0.135176
 6 4.589017 -0.084810 -1.815102
 8 4.787869 1.084456 -2.158357

7	5.562624	-0.856877	-1.229604
6	5.279291	-2.148192	-0.587080
1	6.241592	-2.642020	-0.419653
1	4.726289	-2.782352	-1.280089
6	6.914327	-0.304419	-1.089548
1	7.626276	-1.102810	-1.331351
1	7.023088	0.475834	-1.843394
6	4.512592	-2.059115	0.746117
6	3.919100	-3.418356	1.154249
1	3.701261	-1.330366	0.645595
1	5.182370	-1.679495	1.526354
6	2.678296	-3.794424	0.333149
1	4.685616	-4.201663	1.056559
1	3.645584	-3.392498	2.216449
6	2.108397	-5.177605	0.660641
1	1.904575	-3.035741	0.496392
1	2.903730	-3.748132	-0.738348
1	2.875043	-5.943983	0.479645
1	1.872094	-5.230141	1.732136
6	7.229669	0.250331	0.309423
6	6.358738	1.441586	0.734863
1	8.288414	0.544650	0.321522
1	7.131223	-0.560951	1.041542
6	6.646176	2.729733	-0.045696
1	5.301022	1.176055	0.617306
1	6.513395	1.626429	1.807439
6	5.734577	3.894322	0.354051
1	7.697708	3.017646	0.102621
1	6.507313	2.537503	-1.114017
1	4.694632	3.604414	0.160589
1	5.812741	4.073419	1.436832
6	0.854729	-5.498556	-0.157570
1	0.448375	-6.485823	0.089841
1	0.069882	-4.756133	0.022129
1	1.070867	-5.485210	-1.232125
6	6.050794	5.187353	-0.401633
1	5.377978	6.002077	-0.109914
1	7.077865	5.520066	-0.208758
1	5.947799	5.043337	-1.483405
6	-3.762105	-2.809343	-3.726243
1	-4.628159	-3.475605	-3.805052
1	-3.804510	-2.098523	-4.556982
1	-2.852741	-3.402996	-3.841442
6	-4.949335	-1.065397	-2.360087
1	-4.824712	-0.338563	-3.166539
1	-5.911598	-1.571352	-2.490773
1	-4.957237	-0.515227	-1.415651
6	-5.021105	-3.323355	-0.493244
1	-5.620553	-3.927840	-1.182718
1	-4.853478	-3.912363	0.414293
1	-5.594200	-2.437746	-0.215815
6	-2.817377	-4.197196	-1.318542
1	-2.637974	-4.667052	-0.346235
1	-3.303441	-4.935088	-1.964357
1	-1.848298	-3.936435	-1.752971
6	-4.914451	-0.635955	2.510500
1	-5.483854	-0.743042	3.439355
1	-5.583233	-0.844430	1.671326
1	-4.116862	-1.382545	2.489887
6	-5.474442	1.803251	2.330116
1	-6.218434	1.517177	1.580464

1	-5.976181	1.851723	3.302707
1	-5.110769	2.800993	2.077469
6	-2.922810	2.591625	3.525267
1	-3.715923	3.079563	4.100779
1	-1.976837	2.729582	4.057473
1	-2.835161	3.083844	2.552701
6	-3.286853	0.404157	4.707829
1	-2.420956	0.666184	5.324214
1	-4.189221	0.724851	5.239564
1	-3.308709	-0.682706	4.605696
6	-3.499015	3.329005	-3.626332
1	-3.866670	4.352656	-3.756891
1	-2.579640	3.209883	-4.202681
1	-4.245135	2.646273	-4.044007
6	-4.623982	2.952842	-1.412687
1	-5.169186	3.899493	-1.483288
1	-5.236910	2.166961	-1.863626
1	-4.475856	2.690910	-0.363502
6	-1.092348	4.382681	-2.361112
1	-0.302504	4.846700	-1.762186
1	-0.655138	3.536046	-2.898197
1	-1.440043	5.119060	-3.092101
6	-2.792775	5.104011	-0.661573
1	-1.983276	5.659908	-0.177603
1	-3.317415	5.789660	-1.335699
1	-3.488329	4.779339	0.114447
1	2.460967	4.140751	1.209559

TS[1-2]_{p(bpy)}

Number of imaginary frequencies : 1
Imaginary frequency : -803.0188 cm(-1)

Electronic energy : HF=-2706.6769582
Zero-point correction= 1.176094 (Hartree/Particle)
Thermal correction to Energy= 1.241938
Thermal correction to Enthalpy= 1.242882
Thermal correction to Gibbs Free Energy= 1.071548
Sum of electronic and zero-point Energies= -2705.500864
Sum of electronic and thermal Energies= -2705.435021
Sum of electronic and thermal Enthalpies= -2705.434076
Sum of electronic and thermal Free Energies= -2705.605411

Cartesian Coordinates

77	1.067485	0.394380	-0.172077
5	3.057456	1.117319	-0.139093
8	3.338286	2.465878	0.094748
8	4.246711	0.406687	-0.274760
6	4.745237	2.588188	0.424053
6	5.354632	1.338734	-0.300512
5	1.655064	-0.626195	1.495036
8	2.506003	-0.097841	2.481024
8	1.220354	-1.888310	1.889857
6	2.501587	-0.982221	3.629376
6	2.042727	-2.339627	2.989089
5	2.050619	-1.069415	-1.270162
8	2.583002	-2.259042	-0.801678
8	2.192644	-0.997009	-2.661572
6	3.294425	-2.916146	-1.875115

6	2.606212	-2.301206	-3.146090
6	-0.013225	3.019552	-1.461932
6	-0.000228	3.283310	-0.002438
7	0.481769	1.824181	-1.861065
7	0.530437	2.316007	0.783002
6	-0.480103	3.952953	-2.397671
6	-0.428179	3.650769	-3.753990
6	0.099894	2.423985	-4.151942
6	0.544878	1.541081	-3.172259
6	-0.472746	4.477098	0.557727
6	-0.374795	4.681659	1.929314
6	0.212696	3.694191	2.717165
6	0.653066	2.527728	2.102684
6	-2.012385	0.099790	-1.007276
6	-1.094986	-0.136402	0.033415
6	-3.389318	-0.033424	-0.818210
6	-1.627252	-0.528680	1.276251
6	-3.898685	-0.420795	0.426732
6	-3.001376	-0.638435	1.479067
1	-4.069241	0.166103	-1.642938
1	-3.391310	-0.919726	2.453270
1	-0.954568	-0.774932	2.089724
1	0.975276	0.575593	-3.413659
1	0.169445	2.148138	-5.198754
1	-0.790121	4.366169	-4.485965
1	-0.878976	4.907100	-2.077098
1	-0.912466	5.243614	-0.067469
1	-0.743664	5.601824	2.371443
1	1.139870	1.737554	2.659447
6	-5.367670	-0.553729	0.705984
8	-5.853464	0.047278	1.670784
7	-6.130210	-1.332839	-0.132569
6	-7.586599	-1.333499	0.056499
1	-7.790267	-0.935948	1.050330
1	-7.942485	-2.369301	0.037191
6	-5.608711	-2.327215	-1.082335
1	-6.308151	-2.363757	-1.924135
1	-4.656745	-1.991325	-1.487197
6	-8.324643	-0.519915	-1.021200
6	-7.917355	0.957982	-1.103275
1	-9.401680	-0.598816	-0.818738
1	-8.163757	-0.991744	-1.999737
6	-8.274108	1.791374	0.133626
1	-6.835000	1.020054	-1.278626
1	-8.393882	1.402418	-1.988027
6	-7.861487	3.261852	-0.001836
1	-9.357980	1.731288	0.313623
1	-7.778049	1.367249	1.013259
1	-6.779268	3.311465	-0.185529
1	-8.344017	3.701676	-0.886540
6	-5.452330	-3.737922	-0.485919
6	-4.275593	-3.910622	0.487431
1	-5.328999	-4.438716	-1.323468
1	-6.387558	-4.020570	0.013081
6	-2.893186	-3.820271	-0.174435
1	-4.348172	-3.168505	1.292013
1	-4.372919	-4.891876	0.971563
6	-1.736096	-4.162999	0.771838
1	-2.865743	-4.504508	-1.036206
1	-2.729966	-2.812018	-0.572895
1	-1.728124	-3.449665	1.605019

1	-1.908692	-5.156352	1.211030
6	-8.204008	4.092111	1.237821
1	-7.894922	5.137491	1.123942
1	-9.283093	4.084843	1.434569
1	-7.704150	3.692010	2.127651
6	-0.373000	-4.139178	0.076245
1	0.434789	-4.406967	0.762262
1	-0.352137	-4.843761	-0.765539
1	-0.133133	-3.142052	-0.300569
6	3.121386	-4.423803	-1.715765
1	3.563492	-4.962423	-2.561170
1	3.626121	-4.755765	-0.803522
1	2.069061	-4.700013	-1.633119
6	4.772603	-2.533198	-1.746291
1	5.128744	-2.833039	-0.756477
1	5.388699	-3.031773	-2.501560
1	4.895050	-1.452278	-1.823823
6	3.520686	-2.106647	-4.350642
1	3.921573	-3.065795	-4.695208
1	2.957653	-1.661190	-5.177307
1	4.355114	-1.442904	-4.116444
6	1.329799	-3.045651	-3.557145
1	0.800382	-2.457383	-4.313269
1	1.549530	-4.029909	-3.982134
1	0.662371	-3.175377	-2.700905
6	5.687684	1.603308	-1.774013
1	6.553402	2.263945	-1.884906
1	5.919171	0.653580	-2.264838
1	4.834160	2.049754	-2.292204
6	6.543108	0.692382	0.403934
1	6.880556	-0.178798	-0.166263
1	7.382485	1.391724	0.484506
1	6.272974	0.351365	1.404958
6	4.848253	2.505384	1.952491
1	5.878892	2.627692	2.300818
1	4.242422	3.305916	2.388729
1	4.451343	1.553164	2.313349
6	5.249316	3.938950	-0.071866
1	4.749326	4.742763	0.477822
1	6.327894	4.039297	0.091267
1	5.041488	4.081822	-1.134214
6	1.200825	-3.232162	3.894992
1	1.765097	-3.536434	4.783266
1	0.285504	-2.730969	4.216502
1	0.911362	-4.137207	3.352437
6	3.205310	-3.135425	2.382874
1	3.862848	-3.547246	3.155263
1	2.797486	-3.961586	1.795232
1	3.787099	-2.508517	1.703480
6	1.488186	-0.415655	4.631462
1	1.773651	0.609802	4.887011
1	0.482259	-0.392024	4.202062
1	1.457090	-0.998068	5.557468
6	3.898674	-0.990650	4.241543
1	4.135373	0.000590	4.641448
1	3.961795	-1.710244	5.065127
1	4.657017	-1.243386	3.498321
1	-1.650136	0.387907	-1.989105
1	0.229451	-0.945734	-0.496088
1	0.329044	3.814859	3.788686

TS[1-2]_{m(B1)}

Number of imaginary frequencies : 1
Imaginary frequency : -871.6805 cm(-1)

Electronic energy : HF=-2928.241468
Zero-point correction= 1.179081 (Hartree/Particle)
Thermal correction to Energy= 1.249406
Thermal correction to Enthalpy= 1.250350
Thermal correction to Gibbs Free Energy= 1.070876
Sum of electronic and zero-point Energies= -2927.062387
Sum of electronic and thermal Energies= -2926.992062
Sum of electronic and thermal Enthalpies= -2926.991118
Sum of electronic and thermal Free Energies= -2927.170591

Cartesian Coordinates

77	-2.035410	-0.368393	-0.328012
5	-3.061540	-0.807345	-2.143665
8	-2.983576	0.158402	-3.148518
8	-3.787921	-1.973059	-2.380202
5	-1.789616	-2.426914	-0.607854
8	-0.712107	-2.829965	-1.384520
8	-2.632768	-3.365156	-0.031776
5	-3.766385	-0.853344	0.646493
8	-3.736448	-1.352648	1.942890
8	-5.024373	-0.559001	0.083270
6	-1.546990	2.456203	-1.544725
6	-0.274922	1.761907	-1.850638
7	-2.472208	1.761548	-0.840961
7	-0.216981	0.443163	-1.552588
6	-1.806361	3.767770	-1.967267
6	-3.022649	4.365861	-1.658467
6	-3.966361	3.637277	-0.935364
6	-3.650722	2.337403	-0.553948
6	0.834101	2.416640	-2.399388
6	2.009953	1.709435	-2.622297
6	2.071387	0.343959	-2.317767
6	0.904389	-0.241675	-1.796929
6	-0.986029	0.367137	1.514486
6	-1.655262	0.861709	2.650065
6	0.397648	0.581844	1.462340
6	-0.974178	1.567165	3.648098
6	1.082553	1.336010	2.422521
6	0.393761	1.826129	3.537542
1	-1.364378	-1.072152	0.969892
1	0.974368	0.167371	0.646483
1	0.916096	2.378594	4.313191
1	-1.517987	1.926072	4.518657
1	-2.717565	0.676188	2.760416
1	-4.360342	1.712015	-0.026613
1	-4.931748	4.056402	-0.674059
1	-3.231440	5.380082	-1.983731
1	-1.071438	4.311082	-2.547561
1	0.800628	3.476517	-2.619731
1	2.884388	2.217894	-3.016146
1	0.852730	-1.298679	-1.567454
6	2.537710	1.537075	2.129496
8	3.258220	0.539882	1.912023
7	3.041390	2.793370	1.994627

6	3.280998	-0.472812	-2.584093
6	3.917267	-0.371512	-3.833379
6	3.788868	-1.389171	-1.634575
6	4.988855	-1.194942	-4.167458
1	3.529347	0.333673	-4.563053
6	4.848102	-2.236154	-1.989302
6	5.438394	-2.146083	-3.246666
1	5.455594	-1.110497	-5.144263
1	5.201431	-2.955615	-1.260927
1	6.263235	-2.805785	-3.499940
7	3.276543	-1.393709	-0.321798
6	2.943567	-2.547028	0.384932
8	2.919312	-3.661206	-0.145154
7	2.634681	-2.307716	1.693282
1	3.222444	-0.509367	0.174344
1	2.647876	-1.339180	2.007347
6	2.188771	3.993555	1.957549
1	2.837110	4.856812	2.135866
1	1.490297	3.954399	2.791106
6	4.420503	2.887147	1.483900
1	4.819402	3.866144	1.765326
1	5.005085	2.125237	1.999441
6	1.853781	-3.266225	2.468357
6	2.146826	-3.105245	3.965648
6	0.348113	-3.109027	2.195173
1	2.168022	-4.264481	2.144572
6	1.307789	-4.085216	4.802064
1	1.905801	-2.073283	4.262161
1	3.217409	-3.249454	4.152511
6	-0.491037	-4.096315	3.012740
1	0.055923	-2.083984	2.454793
1	0.163371	-3.228208	1.125640
6	-0.195647	-3.943633	4.512329
1	1.507862	-3.930900	5.869448
1	1.623350	-5.112667	4.570190
1	-1.553959	-3.934791	2.803138
1	-0.256037	-5.123768	2.697397
1	-0.763279	-4.679601	5.095187
1	-0.533500	-2.950478	4.841641
6	1.417959	4.171356	0.638070
6	0.296569	5.218242	0.735047
1	0.985227	3.207106	0.353883
1	2.122347	4.444102	-0.154973
6	-0.934574	4.727068	1.508827
1	0.685291	6.138767	1.195242
1	-0.016412	5.497711	-0.279477
6	-2.049251	5.771904	1.615795
1	-1.328438	3.828433	1.017332
1	-0.647746	4.407344	2.517810
1	-1.659559	6.677480	2.101622
1	-2.359106	6.075471	0.606529
6	4.500440	2.675557	-0.040742
6	5.885669	2.265669	-0.562466
1	4.171373	3.589191	-0.549539
1	3.784181	1.893698	-0.312996
6	6.380825	0.910265	-0.034406
1	5.826163	2.214827	-1.658190
1	6.625310	3.046612	-0.335303
6	7.541894	0.334305	-0.853158
1	6.690911	1.002747	1.014653
1	5.553137	0.191331	-0.037783

1	7.211209	0.199373	-1.891907
1	8.368758	1.058210	-0.881768
6	-3.265021	5.255249	2.389308
1	-4.061573	6.006041	2.441406
1	-3.678621	4.358350	1.914298
1	-2.994139	4.984192	3.416622
6	8.044636	-1.002716	-0.304536
1	8.859848	-1.407892	-0.914517
1	8.416666	-0.898410	0.721756
1	7.238959	-1.744944	-0.289800
6	-0.169041	-4.149772	-1.426599
1	0.920296	-4.072605	-1.371026
1	-0.511421	-4.765973	-0.588593
1	-0.447584	-4.644872	-2.365153
6	-3.146902	-4.492529	-0.715307
1	-2.913614	-5.410880	-0.161169
1	-4.237449	-4.398639	-0.781539
1	-2.757118	-4.594593	-1.733554
6	-4.031614	-2.499651	-3.677220
1	-4.070042	-3.591224	-3.595239
1	-4.991018	-2.158613	-4.085806
1	-3.235989	-2.237098	-4.384503
6	-4.058651	0.474818	-4.021265
1	-3.936021	0.010580	-5.008287
1	-5.029073	0.170822	-3.610328
1	-4.074106	1.562436	-4.158987
6	-6.008008	-1.567166	-0.091150
1	-5.887143	-2.405362	0.605499
1	-7.004548	-1.134863	0.063256
1	-5.944078	-1.963169	-1.111368
6	-4.855198	-1.398258	2.810886
1	-4.526470	-1.099499	3.813716
1	-5.661986	-0.725477	2.495305
1	-5.256368	-2.417813	2.881256

TS[1-2]_{p(B1)}

Number of imaginary frequencies : 1
Imaginary frequency : -806.5739 cm(-1)

Electronic energy : HF=-2928.2392777
Zero-point correction= 1.180364 (Hartree/Particle)
Thermal correction to Energy= 1.249987
Thermal correction to Enthalpy= 1.250931
Thermal correction to Gibbs Free Energy= 1.073311
Sum of electronic and zero-point Energies= -2927.058914
Sum of electronic and thermal Energies= -2926.989291
Sum of electronic and thermal Enthalpies= -2926.988347
Sum of electronic and thermal Free Energies= -2927.165967

Cartesian Coordinates

77	-2.603480	-0.487306	0.032797
5	-4.472688	0.433466	-0.558794
8	-4.745872	1.480209	-1.408380
8	-5.610345	0.015158	0.139247
5	-1.940056	-0.978830	-1.848268
8	-1.541215	0.022800	-2.739338
8	-1.716146	-2.310164	-2.209727
5	-4.001582	-2.011173	-0.279869

8	-4.501081	-2.321946	-1.536100
8	-4.454747	-2.719874	0.838223
6	-2.982981	1.587047	2.375483
6	-1.994025	2.224548	1.475898
7	-3.306014	0.305562	2.090258
7	-1.719009	1.587350	0.310304
6	-3.558869	2.251909	3.466646
6	-4.450134	1.566723	4.287155
6	-4.749769	0.235640	3.999679
6	-4.163824	-0.352142	2.881735
6	-1.333011	3.412534	1.807262
6	-0.417108	3.960339	0.920364
6	-0.159338	3.323538	-0.302904
6	-0.830135	2.115069	-0.541483
6	-0.250081	-0.610826	2.094043
6	-0.622010	-1.109938	0.830024
6	1.086929	-0.455222	2.457430
6	0.413768	-1.621846	0.023518
6	2.108006	-0.849876	1.581513
6	1.750274	-1.473618	0.380064
1	1.336782	0.021909	3.401870
1	2.526053	-1.821499	-0.289427
1	0.170857	-2.101401	-0.917498
1	-4.373794	-1.370232	2.576409
1	-5.434381	-0.336838	4.616377
1	-4.905797	2.068115	5.135541
1	-3.329369	3.292379	3.663875
1	-1.516523	3.895972	2.759164
1	0.103049	4.879344	1.170551
1	-0.687004	1.557256	-1.458307
6	3.525782	-0.422926	1.785040
8	4.111232	0.149238	0.843553
7	4.116318	-0.570334	3.004961
6	0.673673	3.972877	-1.344721
6	0.415876	5.327167	-1.627002
6	1.678763	3.301649	-2.081291
6	1.090859	6.007643	-2.633771
1	-0.361976	5.834321	-1.063529
6	2.347241	3.994143	-3.107501
6	2.051273	5.323568	-3.382949
1	0.858856	7.047400	-2.842533
1	3.103115	3.476391	-3.681465
1	2.587674	5.831177	-4.179648
7	2.058998	1.995474	-1.730852
6	2.708756	1.096757	-2.591735
8	2.632368	1.190332	-3.819525
7	3.395160	0.117397	-1.951103
1	1.965430	1.726021	-0.760090
1	3.571282	0.180758	-0.946566
6	5.334347	0.201533	3.290595
1	5.811947	0.440629	2.340696
1	6.025650	-0.430099	3.855093
6	3.714443	-1.579484	3.994320
1	3.741005	-1.118749	4.988328
1	2.682143	-1.866403	3.804690
6	4.068910	-0.933078	-2.712535
6	5.148975	-1.600254	-1.848912
6	3.074102	-1.974034	-3.259842
1	4.554778	-0.460223	-3.576646
6	5.869259	-2.711122	-2.626721
1	4.682702	-2.029784	-0.952586

1	5.859328	-0.844746	-1.494696
6	3.798564	-3.078960	-4.039651
1	2.521401	-2.417682	-2.421081
1	2.346843	-1.460319	-3.895153
6	4.879307	-3.748771	-3.178199
1	6.610514	-3.195513	-1.980021
1	6.425457	-2.263693	-3.462368
1	3.076441	-3.822832	-4.396748
1	4.267495	-2.642349	-4.933245
1	5.413646	-4.511674	-3.757332
1	4.399057	-4.270132	-2.337862
6	5.026898	1.478130	4.095085
6	4.040852	2.446360	3.421909
1	5.979856	1.989167	4.287499
1	4.629609	1.188061	5.076685
6	4.552306	3.101353	2.132565
1	3.105528	1.911954	3.207363
1	3.776631	3.230973	4.143887
6	3.489697	3.962487	1.438845
1	5.432911	3.719266	2.360652
1	4.878771	2.325805	1.432293
1	2.612565	3.336403	1.221145
1	3.138830	4.744294	2.127988
6	4.613100	-2.832051	3.975680
6	4.688343	-3.539027	2.614322
1	4.226143	-3.521770	4.737641
1	5.625592	-2.560425	4.297446
6	3.375391	-4.185155	2.151963
1	5.024756	-2.816730	1.858467
1	5.470306	-4.308155	2.659552
6	3.452018	-4.734189	0.722116
1	3.100550	-4.993487	2.844583
1	2.559424	-3.455517	2.194606
1	3.786906	-3.930003	0.053147
1	4.223682	-5.514468	0.666082
6	3.992809	4.602526	0.142489
1	3.224424	5.221087	-0.331431
1	4.867183	5.237208	0.331240
1	4.289318	3.835601	-0.581290
6	2.114318	-5.281774	0.219288
1	2.193333	-5.661087	-0.805747
1	1.757723	-6.104302	0.850730
1	1.345614	-4.500450	0.228093
1	-1.012965	-0.265718	2.782572
1	-2.020566	-1.902314	0.570189
6	-1.893166	-2.803842	-3.527134
1	-0.936430	-2.914587	-4.054696
1	-2.355337	-3.794950	-3.460504
1	-2.546904	-2.161642	-4.129323
6	-5.011754	-3.599337	-1.881170
1	-4.797403	-3.774242	-2.940692
1	-4.545814	-4.403816	-1.298892
1	-6.099595	-3.654581	-1.745951
6	-5.816769	-3.110911	0.965215
1	-6.120028	-2.963857	2.009070
1	-6.472964	-2.503473	0.334020
1	-5.958745	-4.170829	0.721206
6	-6.882665	0.594726	-0.122782
1	-7.602973	0.143626	0.568077
1	-6.876317	1.680028	0.033447
1	-7.210897	0.402518	-1.151682

6	-3.800478	2.202651	-2.180940
1	-2.947001	1.588744	-2.467883
1	-4.306539	2.558448	-3.086308
1	-3.449257	3.082802	-1.626481
6	-0.505474	-0.154323	-3.706981
1	0.078658	0.767994	-3.767576
1	0.169320	-0.967952	-3.427491
1	-0.922197	-0.365316	-4.698931

The Optimized Coordinates of all the Stationary Points for the Model System at the B3LYP-D3 Level of Theory

A1_{model}

Number of imaginary frequencies : 0

Electronic energy : HF=-1856.4663767
 Zero-point correction= 0.527910 (Hartree/Particle)
 Thermal correction to Energy= 0.563735
 Thermal correction to Enthalpy= 0.564679
 Thermal correction to Gibbs Free Energy= 0.459291
 Sum of electronic and zero-point Energies= -1855.938467
 Sum of electronic and thermal Energies= -1855.902642
 Sum of electronic and thermal Enthalpies= -1855.901697
 Sum of electronic and thermal Free Energies= -1856.007085

Cartesian Coordinates

77	-1.467659	0.044104	-0.550757
5	-0.551019	-1.569146	-1.355276
8	-0.844966	-2.039306	-2.643398
8	0.500812	-2.330545	-0.810676
6	0.110255	-3.046320	-3.006224
6	0.772091	-3.443124	-1.677453
5	-2.970725	-1.289210	-0.202151
8	-2.861348	-2.667342	0.015872
8	-4.327778	-0.911645	-0.133444
6	-4.170357	-3.237273	0.114670
6	-5.096698	-2.030618	0.332634
5	-0.756078	-0.474035	1.229791
8	0.601171	-0.308820	1.586365
8	-1.482393	-0.920986	2.331110
6	0.727851	-0.515310	3.004785
6	-0.562918	-1.254112	3.382025
6	-1.628020	3.106424	0.076899
6	-0.180631	2.837792	-0.095903
7	-2.441979	2.021697	0.039107
7	0.143748	1.646892	-0.651506
6	-2.142243	4.391151	0.283123
6	-3.512434	4.555384	0.470206
6	-4.337693	3.432444	0.449202
6	-3.762675	2.183027	0.226604
6	0.815634	3.709436	0.354771
6	2.148020	3.325817	0.266191
6	2.491620	2.087617	-0.299607
6	1.432228	1.303737	-0.775812
1	-4.348070	1.269742	0.193398
1	-5.409330	3.514070	0.595284
1	-3.926787	5.546760	0.625409
1	-1.483467	5.251803	0.276770
1	0.553555	4.649933	0.825439

1	2.926472	3.970325	0.662124
1	1.615162	0.340453	-1.237243
6	3.906992	1.652569	-0.392651
6	4.362163	0.370600	0.032533
6	4.837897	2.576149	-0.897122
6	5.735497	0.076702	-0.089800
6	6.188679	2.271014	-1.018537
1	4.473287	3.545253	-1.226800
6	6.625666	1.009897	-0.611206
1	6.083092	-0.889629	0.243607
1	6.882598	2.999531	-1.426134
1	7.676034	0.743148	-0.691704
7	3.455290	-0.551128	0.572335
1	2.503612	-0.239333	0.747468
6	3.697908	-1.888829	0.907694
8	4.812821	-2.405877	0.975015
7	2.544055	-2.570867	1.195360
1	1.690610	-2.248634	0.741658
6	2.621218	-3.997742	1.453455
1	2.945863	-4.573525	0.575979
1	1.630414	-4.346802	1.755040
1	3.328263	-4.198168	2.262066
1	1.632189	-1.095058	3.205057
1	0.804662	0.460329	3.502456
1	-0.416857	-2.342379	3.400420
1	-0.971288	-0.940092	4.347625
1	-6.034702	-2.099693	-0.228170
1	-5.335945	-1.885302	1.394937
1	-4.205034	-3.955538	0.940892
1	-4.405884	-3.771579	-0.816481
1	0.324749	-4.349408	-1.249253
1	1.853241	-3.592464	-1.761817
1	-0.399001	-3.883371	-3.494750
1	0.836762	-2.622987	-3.713515

A2_{model}

Number of imaginary frequencies : 0

Electronic energy : HF=-1856.4536198
 Zero-point correction= 0.526315 (Hartree/Particle)
 Thermal correction to Energy= 0.563049
 Thermal correction to Enthalpy= 0.563993
 Thermal correction to Gibbs Free Energy= 0.453712
 Sum of electronic and zero-point Energies= -1855.927305
 Sum of electronic and thermal Energies= -1855.890571
 Sum of electronic and thermal Enthalpies= -1855.889627
 Sum of electronic and thermal Free Energies= -1855.999908

Cartesian Coordinates

77	1.302763	-0.074834	-0.121108
5	2.065729	-0.030182	1.717433
8	3.256164	-0.592554	2.168412
8	1.414498	0.657333	2.752030
6	3.460306	-0.197360	3.530046
6	2.096472	0.359164	3.977909
5	0.308812	-1.690156	0.591943
8	-0.979457	-2.048997	0.076372
8	0.613318	-2.547226	1.648168

6	-1.551630	-3.071457	0.919603
6	-0.351240	-3.603272	1.709840
5	2.783023	-1.370917	-0.660833
8	2.635060	-2.729071	-0.978533
8	4.116259	-0.982667	-0.892156
6	3.925269	-3.295747	-1.235530
6	4.838287	-2.079506	-1.465115
6	1.249990	2.931508	-0.972562
6	-0.138476	2.644309	-0.538325
7	2.110596	1.882230	-0.954836
7	-0.324257	1.466991	0.103029
6	1.671548	4.206033	-1.364933
6	2.995744	4.399174	-1.749896
6	3.870180	3.314081	-1.732736
6	3.387656	2.071481	-1.327818
6	-1.219126	3.501138	-0.780998
6	-2.500417	3.112424	-0.405935
6	-2.697481	1.888510	0.252411
6	-1.551114	1.135120	0.523954
1	4.015245	1.186825	-1.287523
1	4.910085	3.419607	-2.022283
1	3.337401	5.384321	-2.052066
1	0.978763	5.039062	-1.352723
1	-1.070853	4.439166	-1.303366
1	-3.354224	3.738284	-0.645875
1	-1.611053	0.215190	1.092358
6	-4.051735	1.398144	0.601208
6	-4.514773	0.116109	0.197538
6	-4.928750	2.254561	1.286465
6	-5.841251	-0.247208	0.486355
6	-6.238460	1.881664	1.570593
1	-4.560514	3.226907	1.602486
6	-6.690577	0.625908	1.158737
1	-6.194617	-1.215678	0.159420
1	-6.895935	2.559344	2.106490
1	-7.709794	0.315654	1.371336
7	-3.668975	-0.774294	-0.486611
1	-2.675501	-0.732872	-0.304366
6	-4.046057	-1.614454	-1.538605
8	-5.200120	-1.732577	-1.943548
7	-2.980377	-2.282310	-2.081164
1	-2.087094	-2.248682	-1.599651
6	-3.186391	-3.293814	-3.099353
1	-3.524934	-4.252109	-2.681038
1	-2.246783	-3.458424	-3.632743
1	-3.942328	-2.952086	-3.809379
1	4.240502	-3.884769	-0.363537
1	3.876533	-3.963765	-2.102543
1	5.814022	-2.179409	-0.977635
1	5.005934	-1.887108	-2.534633
1	-0.594846	-3.828037	2.753127
1	0.071865	-4.506025	1.248940
1	-2.039257	-3.831629	0.302077
1	-2.309775	-2.613076	1.567704
1	1.517686	-0.385198	4.541193
1	2.182822	1.264780	4.587816
1	3.784106	-1.059398	4.122570
1	4.249435	0.566346	3.570409

substrate_{model}

Number of imaginary frequencies : 0

Electronic energy : HF=-479.6003344
Zero-point correction= 0.184238 (Hartree/Particle)
Thermal correction to Energy= 0.194682
Thermal correction to Enthalpy= 0.195626
Thermal correction to Gibbs Free Energy= 0.147844
Sum of electronic and zero-point Energies= -479.416096
Sum of electronic and thermal Energies= -479.405653
Sum of electronic and thermal Enthalpies= -479.404709
Sum of electronic and thermal Free Energies= -479.452490

Cartesian Coordinates

6	3.191015	-0.322509	0.011999
6	2.311727	-1.228002	-0.585937
6	0.944386	-0.951460	-0.627107
6	0.447500	0.239389	-0.078670
6	1.339411	1.157359	0.491961
6	2.702014	0.871051	0.550825
1	4.254377	-0.541696	0.050301
1	2.690185	-2.147432	-1.023592
1	0.262304	-1.650910	-1.101358
1	0.950616	2.093534	0.879613
1	3.384555	1.581599	1.008263
6	-1.000297	0.637044	-0.185975
8	-1.293639	1.786491	-0.520255
7	-1.959752	-0.320949	0.040959
6	-3.350640	0.042367	-0.197900
1	-3.906786	-0.848724	-0.506911
1	-3.821858	0.450637	0.707111
1	-3.402313	0.796209	-0.982499
6	-1.774736	-1.502138	0.876387
1	-2.409077	-1.428776	1.769978
1	-2.055280	-2.414007	0.335347
1	-0.741629	-1.594323	1.205583

Ir- π (Refer to Figure S4)

Number of imaginary frequencies : 0

Electronic energy : HF=-2336.0974086
Zero-point correction= 0.714160 (Hartree/Particle)
Thermal correction to Energy= 0.762004
Thermal correction to Enthalpy= 0.762948
Thermal correction to Gibbs Free Energy= 0.630873
Sum of electronic and zero-point Energies= -2335.383249
Sum of electronic and thermal Energies= -2335.335405
Sum of electronic and thermal Enthalpies= -2335.334460
Sum of electronic and thermal Free Energies= -2335.466535

Cartesian Coordinates

77	1.332149	-0.437816	0.159811
5	1.750371	-1.237359	1.948670
8	1.361292	-0.605483	3.141009
8	2.456780	-2.407675	2.227239
6	1.661924	-1.484494	4.233752
6	2.657598	-2.496543	3.641713

5	0.318365	-2.163774	-0.237709
8	-0.395862	-2.892252	0.726525
8	0.021304	-2.668148	-1.516022
6	-1.260536	-3.832917	0.067220
6	-0.738198	-3.880478	-1.374618
5	3.059482	-1.331680	-0.467913
8	3.211071	-2.430480	-1.325275
8	4.340705	-0.835163	-0.130097
6	4.594355	-2.787143	-1.400208
6	5.336213	-1.550260	-0.869958
6	1.195853	2.411260	1.437523
6	-0.199405	1.921123	1.508503
7	2.077855	1.622576	0.772418
7	-0.426808	0.695158	0.974980
6	1.602674	3.626670	2.003862
6	2.924251	4.040187	1.870861
6	3.818869	3.225689	1.177933
6	3.354603	2.023536	0.651489
6	-1.251842	2.648829	2.075866
6	-2.540642	2.121807	2.076920
6	-2.773926	0.857062	1.522751
6	-1.659469	0.183287	1.002917
6	1.315269	-0.113145	-2.752230
6	2.366127	0.678722	-3.243063
6	0.135754	0.498259	-2.316333
6	2.220378	2.060006	-3.323188
6	-0.001544	1.901920	-2.356698
6	1.038691	2.672086	-2.887465
1	1.391074	-1.192888	-2.740135
1	-0.694187	-0.114773	-1.992779
1	0.926737	3.744795	-3.000097
1	3.017053	2.671106	-3.737666
1	3.283966	0.203931	-3.577095
1	4.006317	1.324995	0.138818
1	4.859985	3.503420	1.052742
1	3.248814	4.980452	2.305965
1	0.897240	4.243120	2.547679
1	-1.077644	3.626109	2.509911
1	-3.363069	2.690820	2.499681
1	-1.758403	-0.823510	0.621792
6	-1.321288	2.464975	-1.927184
8	-2.357934	1.791877	-2.105138
7	-1.409883	3.706622	-1.379230
6	-4.095374	0.187036	1.523154
6	-4.850178	0.146070	2.706247
6	-4.578160	-0.489168	0.374728
6	-6.027363	-0.592674	2.785172
1	-4.472609	0.662123	3.584771
6	-5.753090	-1.250090	0.469298
6	-6.461573	-1.308646	1.666086
1	-6.586563	-0.629754	3.715107
1	-6.095941	-1.787188	-0.405706
1	-7.368796	-1.903947	1.718601
7	-3.909976	-0.336027	-0.850873
6	-3.683514	-1.352849	-1.778792
8	-4.018353	-2.524652	-1.591055
7	-3.050135	-0.907285	-2.904698
1	-3.442511	0.549703	-1.023236
1	-2.716806	0.052603	-2.911056
6	-2.495790	-1.832472	-3.874070
1	-3.111811	-2.732842	-3.898967

1	-2.506426	-1.371014	-4.866067
1	-1.465360	-2.115158	-3.624887
1	3.698127	-2.232572	3.877739
1	2.476026	-3.521821	3.981180
1	0.736508	-1.970828	4.570426
1	2.078011	-0.912628	5.070132
1	5.711557	-0.915437	-1.686292
1	6.179850	-1.802171	-0.218207
1	4.862582	-3.037835	-2.432779
1	4.776228	-3.670674	-0.773215
1	-1.550005	-3.901372	-2.105885
1	-0.075445	-4.738477	-1.550556
1	-2.294442	-3.467917	0.102146
1	-1.209040	-4.801685	0.575257
6	-2.740626	4.249103	-1.116329
1	-3.068778	4.003230	-0.098996
1	-2.706456	5.336875	-1.224679
1	-3.457801	3.834472	-1.822884
6	-0.314742	4.488257	-0.816253
1	-0.126629	5.390449	-1.410669
1	-0.587324	4.796890	0.198047
1	0.598201	3.903797	-0.752086

Ir-N (Refer to Figure S4)

Number of imaginary frequencies : 0

Electronic energy : HF=-2336.0947764
 Zero-point correction= 0.713020 (Hartree/Particle)
 Thermal correction to Energy= 0.761487
 Thermal correction to Enthalpy= 0.762432
 Thermal correction to Gibbs Free Energy= 0.626404
 Sum of electronic and zero-point Energies= -2335.381756
 Sum of electronic and thermal Energies= -2335.333289
 Sum of electronic and thermal Enthalpies= -2335.332345
 Sum of electronic and thermal Free Energies= -2335.468372

Cartesian Coordinates

77	-1.736831	-0.007766	0.140372
5	-2.896168	-0.767905	1.570092
8	-2.821225	-0.557563	2.944682
8	-3.933492	-1.665883	1.263354
6	-3.965592	-1.165401	3.553856
6	-4.474199	-2.158930	2.496698
5	-0.830864	1.171659	1.537440
8	-0.841064	2.575799	1.586096
8	0.040041	0.683481	2.527449
6	0.097058	3.031041	2.570225
6	0.473246	1.764885	3.359720
5	-3.178405	1.411749	0.017241
8	-4.031761	1.911737	1.006629
8	-3.530671	1.990418	-1.232147
6	-5.037653	2.729352	0.401011
6	-4.486554	3.036734	-0.998869
6	-1.664638	-2.443036	-1.815463
6	-0.355425	-2.501028	-1.118815
7	-2.476711	-1.412452	-1.475802
7	-0.205259	-1.669410	-0.060882
6	-2.063066	-3.395174	-2.761404

6	-3.307187	-3.272352	-3.373427
6	-4.127054	-2.198545	-3.029282
6	-3.671685	-1.293721	-2.074988
6	0.689215	-3.339124	-1.522239
6	1.891365	-3.321886	-0.823124
6	2.024671	-2.504386	0.305344
6	0.930870	-1.703783	0.648413
1	-4.259991	-0.434250	-1.776449
1	-5.102453	-2.061097	-3.483340
1	-3.630550	-4.006125	-4.105183
1	-1.418632	-4.230765	-3.006329
1	0.581551	-3.977089	-2.391249
1	2.723031	-3.938991	-1.148297
1	0.964480	-1.043656	1.508787
6	3.290717	-2.413185	1.085529
6	4.377361	-1.643173	0.595806
6	3.400115	-3.064282	2.318255
6	5.560067	-1.583173	1.355527
6	4.573319	-2.996310	3.068551
1	2.550452	-3.637059	2.679802
6	5.647577	-2.256469	2.572351
1	6.388686	-1.001796	0.977932
1	4.645432	-3.512717	4.020768
1	6.571792	-2.191516	3.140469
7	4.199783	-0.956831	-0.611250
1	3.243291	-0.877951	-0.945884
6	5.125026	-0.165443	-1.290323
8	6.307085	-0.039909	-0.971941
7	4.575815	0.447385	-2.386503
1	3.564144	0.442652	-2.465036
6	5.309505	1.494101	-3.069858
1	5.320599	2.436466	-2.504335
1	4.847598	1.674624	-4.044283
1	6.343265	1.177820	-3.222842
1	-5.982862	2.170010	0.352855
1	-5.201057	3.629359	1.002931
1	-5.254458	3.022112	-1.779532
1	-3.975512	4.009029	-1.032947
1	1.550076	1.685955	3.544172
1	-0.049549	1.708061	4.323477
1	-0.368674	3.799299	3.196869
1	0.966384	3.471727	2.066179
1	-4.099152	-3.176179	2.677338
1	-5.567031	-2.199505	2.436963
1	-3.676727	-1.647885	4.493493
1	-4.711653	-0.389948	3.775330
7	0.063449	1.782735	-1.978969
6	-0.440629	3.107948	-1.606943
1	-1.529347	3.061570	-1.605902
1	-0.123894	3.368395	-0.600006
1	-0.111598	3.871464	-2.322744
6	-0.676172	1.097231	-3.041642
1	-1.745407	1.206739	-2.852783
1	-0.433345	1.535750	-4.018812
1	-0.407633	0.042823	-3.050662
6	1.243729	1.271464	-1.552662
8	1.640520	0.139306	-1.908206
6	2.126318	2.096545	-0.659450
6	2.620191	3.337964	-1.081925
6	2.590756	1.542422	0.539361
6	3.563627	4.017439	-0.310016

1	2.283093	3.765199	-2.021253
6	3.524776	2.227363	1.314973
1	2.215410	0.582848	0.865137
6	4.015922	3.464475	0.890323
1	3.948867	4.974346	-0.650029
1	3.882315	1.782493	2.238522
1	4.753788	3.991799	1.487794

Ir-O (Refer to Figure S4)

Number of imaginary frequencies : 0

Electronic energy : HF=-2336.0965141
 Zero-point correction= 0.712782 (Hartree/Particle)
 Thermal correction to Energy= 0.761107
 Thermal correction to Enthalpy= 0.762051
 Thermal correction to Gibbs Free Energy= 0.627347
 Sum of electronic and zero-point Energies= -2335.383732
 Sum of electronic and thermal Energies= -2335.335407
 Sum of electronic and thermal Enthalpies= -2335.334463
 Sum of electronic and thermal Free Energies= -2335.469167

Cartesian Coordinates

77	-0.615954	-0.387184	0.113451
5	0.328702	-1.005716	1.768340
8	1.468699	-1.832375	1.862625
8	-0.053280	-0.601298	3.059267
6	1.904040	-1.882504	3.228246
6	0.710451	-1.331702	4.023625
5	0.532555	-1.705731	-0.912419
8	1.919930	-1.502773	-1.154757
8	0.150425	-2.894060	-1.553772
6	2.410340	-2.501377	-2.062165
6	1.306639	-3.569067	-2.062214
5	-1.869191	-1.937082	0.455944
8	-3.219019	-1.901843	0.022683
8	-1.651732	-3.125475	1.167849
6	-3.910801	-3.041446	0.545579
6	-2.789374	-3.977877	1.025133
6	-1.014987	2.407143	1.438126
6	0.317194	2.501472	0.794086
7	-1.682983	1.243746	1.252301
7	0.632524	1.504265	-0.063975
6	-1.565570	3.440450	2.205570
6	-2.811404	3.261837	2.799085
6	-3.487055	2.058661	2.604080
6	-2.886686	1.079968	1.817984
6	1.240411	3.519766	1.064385
6	2.506253	3.469514	0.491328
6	2.833640	2.433556	-0.397001
6	1.819299	1.513214	-0.679375
1	-3.372643	0.134343	1.608631
1	-4.463885	1.879177	3.038818
1	-3.249069	4.054120	3.398673
1	-1.032717	4.375229	2.333876
1	0.997597	4.314254	1.760169
1	3.252728	4.213062	0.752897
1	1.963202	0.721358	-1.402710
6	4.195401	2.292222	-0.963278

6	4.930792	1.076216	-0.878458
6	4.808952	3.421100	-1.531033
6	6.254976	1.055837	-1.352581
6	6.117956	3.385252	-2.000179
1	4.232140	4.339246	-1.604745
6	6.839398	2.194011	-1.899603
1	6.818986	0.137640	-1.264860
1	6.567006	4.271519	-2.438354
1	7.863420	2.142903	-2.259210
7	4.352818	-0.076482	-0.316614
1	3.378381	-0.281906	-0.511739
6	5.029611	-1.074331	0.386273
8	6.238186	-1.060804	0.620440
7	4.203798	-2.098148	0.770614
1	3.195483	-1.953984	0.778560
6	4.723259	-3.162769	1.605913
1	5.671792	-3.525222	1.202666
1	4.002686	-3.984319	1.610976
1	4.900784	-2.845810	2.643049
1	-4.563299	-2.724812	1.372305
1	-4.538616	-3.489953	-0.232862
1	-3.018648	-4.465421	1.979148
1	-2.568490	-4.758910	0.283807
1	1.099139	-3.967177	-3.061462
1	1.552556	-4.409585	-1.399375
1	3.374108	-2.875118	-1.704469
1	2.550912	-2.050735	-3.053584
1	0.093210	-2.139818	4.439462
1	1.012313	-0.670694	4.843346
1	2.159688	-2.911633	3.500393
1	2.801757	-1.259958	3.342841
8	-1.714928	0.361655	-1.912740
6	-2.941172	0.215299	-2.115039
6	-3.909784	1.132671	-1.432167
6	-5.059838	0.654671	-0.789433
6	-3.587200	2.493422	-1.348685
6	-5.895620	1.535543	-0.102978
1	-5.268551	-0.408720	-0.797537
6	-4.428585	3.373800	-0.670584
1	-2.671145	2.845659	-1.811614
6	-5.587191	2.896963	-0.051119
1	-6.781275	1.157325	0.399961
1	-4.175971	4.428673	-0.615925
1	-6.239797	3.582558	0.482139
7	-3.400693	-0.752150	-2.937080
6	-2.477288	-1.783603	-3.400476
1	-1.640545	-1.878578	-2.712070
1	-3.013431	-2.736804	-3.443980
1	-2.099097	-1.548508	-4.403806
6	-4.744828	-0.822551	-3.495244
1	-5.291417	0.103993	-3.328371
1	-4.672114	-0.987411	-4.576369
1	-5.310916	-1.655156	-3.059994

Ir- π -1 Σ_g

Number of imaginary frequencies : 0

Electronic energy : HF=-2336.0986505

Zero-point correction= 0.714063 (Hartree/Particle)

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Thermal correction to Energy=	0.761918
Thermal correction to Enthalpy=	0.762862
Thermal correction to Gibbs Free Energy=	0.630759
Sum of electronic and zero-point Energies=	-2335.384588
Sum of electronic and thermal Energies=	-2335.336733
Sum of electronic and thermal Enthalpies=	-2335.335788
Sum of electronic and thermal Free Energies=	-2335.467892

.....
Cartesian Coordinates

.....
77 -1.369145 -0.435617 -0.210770
5 -1.892278 -1.331641 -1.914306
8 -1.149023 -1.147395 -3.092513
8 -2.995412 -2.149214 -2.156529
6 -1.661651 -2.043157 -4.087348
6 -3.046579 -2.452422 -3.554229
5 -0.451390 -2.187561 0.260467
8 -0.520151 -3.430076 -0.377358
8 0.545916 -2.231550 1.263274
6 0.551449 -4.257690 0.096686
6 1.006252 -3.588992 1.399640
5 -3.060336 -1.193773 0.641477
8 -3.147997 -2.259010 1.553562
8 -4.338621 -0.608003 0.501567
6 -4.522908 -2.501849 1.867593
6 -5.243199 -1.217862 1.427826
6 -1.182539 2.309885 -1.683628
6 0.204405 1.789682 -1.723803
7 -2.061646 1.616459 -0.915674
7 0.417586 0.608822 -1.091628
6 -1.582065 3.463947 -2.369825
6 -2.890213 3.921302 -2.242320
6 -3.778447 3.211453 -1.435501
6 -3.325721 2.059058 -0.798489
6 1.265516 2.461290 -2.340248
6 2.546180 1.918114 -2.297147
6 2.769840 0.707871 -1.627952
6 1.650990 0.096671 -1.041317
6 0.020823 0.604673 2.416155
6 0.157472 2.002917 2.429533
6 -1.113095 0.000658 2.962949
6 -0.821059 2.783322 3.059130
6 -2.100505 0.790284 3.563682
6 -1.944599 2.175509 3.625899
1 0.784758 -0.017575 1.968875
1 -1.220167 -1.075432 2.906319
1 -2.694390 2.787832 4.118818
1 -0.699583 3.859482 3.129177
1 -3.976510 1.434918 -0.195081
1 -4.808221 3.528163 -1.309479
1 -3.209330 4.814364 -2.770820
1 -0.884623 3.996422 -3.005303
1 1.105102 3.407061 -2.843748
1 3.375170 2.438586 -2.766878
1 1.748051 -0.842948 -0.511690
6 4.093992 0.042730 -1.589175
6 4.822415 -0.096017 -2.782198
6 4.615841 -0.515493 -0.396098
6 6.015693 -0.810944 -2.821222
1 4.413562 0.326501 -3.695859
6 5.812962 -1.246773 -0.447259

6	6.497868	-1.399701	-1.648894
1	6.553419	-0.924304	-3.757655
1	6.190426	-1.688370	0.465857
1	7.422190	-1.970321	-1.665645
7	3.962061	-0.281624	0.823097
6	3.805786	-1.221257	1.843053
8	4.187746	-2.389258	1.745920
7	3.194571	-0.703611	2.950366
1	3.476704	0.603798	0.937605
1	2.830996	0.243046	2.884556
6	2.646444	-1.575028	3.970791
1	3.277951	-2.460427	4.060205
1	2.632719	-1.049828	4.930423
1	1.625629	-1.895361	3.726177
1	-3.854429	-1.872220	-4.022390
1	-3.259891	-3.516935	-3.698334
1	-0.988523	-2.906148	-4.177674
1	-1.708155	-1.536975	-5.057797
1	-5.415034	-0.535358	2.273330
1	-6.206145	-1.410616	0.942308
1	-4.633907	-2.709783	2.937786
1	-4.874432	-3.378990	1.307486
1	2.089785	-3.594296	1.540711
1	0.526394	-4.042099	2.278314
1	1.356024	-4.271526	-0.652355
1	0.195628	-5.283374	0.240369
6	1.407669	2.569995	1.833986
8	2.486040	1.957889	1.975768
7	1.374386	3.754614	1.167202
1	-2.982659	0.320868	3.989190
6	0.180716	4.398740	0.626368
1	-0.021238	5.348985	1.134848
1	0.341236	4.605081	-0.436549
1	-0.689937	3.753713	0.713146
6	2.638814	4.330515	0.717265
1	2.557023	5.421322	0.731070
1	3.445141	4.016783	1.378307
1	2.875463	4.005061	-0.303000

Ir- π -TS[1-2]_o (Refer to Figure S6)

Number of imaginary frequencies : 1

Imaginary frequency : -735.8378 cm(-1)

Electronic energy : HF=-2336.0509276

Zero-point correction= 0.708766 (Hartree/Particle)

Thermal correction to Energy= 0.756370

Thermal correction to Enthalpy= 0.757315

Thermal correction to Gibbs Free Energy= 0.626086

Sum of electronic and zero-point Energies= -2335.342162

Sum of electronic and thermal Energies= -2335.294557

Sum of electronic and thermal Enthalpies= -2335.293613

Sum of electronic and thermal Free Energies= -2335.424842

Cartesian Coordinates

77	-1.132190	-0.385657	-0.084755
5	-1.285592	-1.263117	-2.007831
8	-1.044720	-0.540320	-3.175028
8	-1.658827	-2.569817	-2.311058

6	-1.109718	-1.438622	-4.295764
6	-1.797396	-2.694187	-3.734750
5	-0.134453	-2.210636	0.164391
8	1.041481	-2.482811	-0.534725
8	-0.423756	-3.238132	1.049514
6	1.633721	-3.682765	0.000455
6	0.503735	-4.312053	0.831362
5	-2.912873	-1.384538	0.135590
8	-3.228142	-2.457933	0.963884
8	-4.054561	-1.010846	-0.602179
6	-4.538144	-2.936311	0.640104
6	-5.174440	-1.789946	-0.160495
6	-1.019463	2.248164	-1.697911
6	0.394670	1.832479	-1.648189
7	-1.910882	1.467470	-1.029457
7	0.658941	0.742173	-0.892147
6	-1.442150	3.408350	-2.360854
6	-2.780292	3.780913	-2.322370
6	-3.677914	2.986987	-1.610195
6	-3.202620	1.839547	-0.985836
6	1.433835	2.510456	-2.298618
6	2.749306	2.095827	-2.119451
6	3.023881	0.978912	-1.318060
6	1.917461	0.323914	-0.761704
6	-1.332104	0.528771	2.001253
6	-0.696554	1.711945	2.437196
6	-2.302179	-0.001456	2.881038
6	-1.058614	2.348269	3.637700
6	-2.655163	0.618328	4.080822
6	-2.037359	1.808571	4.465480
1	-0.587540	-0.831096	1.361469
1	-2.782847	-0.937825	2.622547
1	-2.300896	2.300655	5.397390
1	-0.554159	3.269483	3.921346
1	-3.860347	1.162569	-0.458054
1	-4.730817	3.237692	-1.542232
1	-3.113215	4.678720	-2.833937
1	-0.726829	4.019857	-2.896381
1	1.226853	3.367098	-2.928529
1	3.559294	2.645846	-2.588602
1	2.037556	-0.588500	-0.203623
6	4.390358	0.456575	-1.075834
6	5.315488	0.415526	-2.132846
6	4.777665	-0.064491	0.186702
6	6.570890	-0.165027	-1.975870
1	5.018758	0.801975	-3.103817
6	6.037847	-0.659270	0.331389
6	6.922693	-0.718101	-0.741947
1	7.261651	-0.201605	-2.813029
1	6.302259	-1.069985	1.297574
1	7.893869	-1.186661	-0.610040
7	3.917061	0.036901	1.301962
6	3.474460	-1.091694	2.011150
8	4.093124	-2.158287	2.019789
7	2.295988	-0.877241	2.660748
1	3.268515	0.817713	1.292693
1	1.819723	0.011891	2.522443
6	1.672567	-1.886764	3.494340
1	2.385048	-2.698697	3.648211
1	1.399818	-1.463284	4.467467
1	0.769437	-2.293269	3.025287

1	-2.865268	-2.726504	-3.987784
1	-1.331285	-3.625110	-4.072645
1	-0.090351	-1.647304	-4.644990
1	-1.669265	-0.971278	-5.112397
1	-5.828461	-1.164407	0.463120
1	-5.749960	-2.136808	-1.025005
1	-5.085454	-3.175419	1.557929
1	-4.447478	-3.852658	0.041982
1	0.849063	-4.697800	1.795649
1	-0.009287	-5.120291	0.294587
1	2.501829	-3.409785	0.610794
1	1.965340	-4.320691	-0.824585
6	0.471171	2.331284	1.726814
8	1.586964	1.784019	1.767699
7	0.286647	3.541527	1.135337
1	-3.408574	0.162075	4.718421
6	-1.001468	4.223523	1.071075
1	-1.089065	4.982907	1.858449
1	-1.092814	4.719450	0.100997
1	-1.818856	3.512607	1.172546
6	1.427179	4.310190	0.656951
1	1.503245	5.252939	1.212848
1	2.338325	3.732546	0.797455
1	1.310554	4.540175	-0.407231

Ir- π -2 σ_g

Number of imaginary frequencies : 0

Electronic energy : HF=-2336.0675871
 Zero-point correction= 0.711929 (Hartree/Particle)
 Thermal correction to Energy= 0.758886
 Thermal correction to Enthalpy= 0.759830
 Thermal correction to Gibbs Free Energy= 0.632233
 Sum of electronic and zero-point Energies= -2335.355658
 Sum of electronic and thermal Energies= -2335.308702
 Sum of electronic and thermal Enthalpies= -2335.307757
 Sum of electronic and thermal Free Energies= -2335.435354

Cartesian Coordinates

77	-1.226053	-0.280919	0.016634
5	-1.479490	-1.567170	-1.684352
8	-1.022021	-1.127157	-2.923855
8	-2.201841	-2.745054	-1.812805
6	-1.300728	-2.146930	-3.897618
6	-2.338335	-3.049172	-3.210856
5	-0.325268	-2.186486	0.129632
8	0.885894	-2.469429	-0.507347
8	-0.780678	-3.294874	0.831351
6	1.285103	-3.811234	-0.176318
6	0.029168	-4.421110	0.474059
5	-2.904526	-1.101913	0.856491
8	-2.986490	-1.692797	2.110823
8	-4.176709	-1.061004	0.259035
6	-4.296619	-2.245259	2.277469
6	-5.143921	-1.539945	1.206801
6	-1.214901	2.073157	-1.914899
6	0.223574	1.829204	-1.686731
7	-2.083368	1.193318	-1.342473

7	0.513348	0.717283	-0.978286
6	-1.688692	3.125071	-2.706987
6	-3.054384	3.269143	-2.923926
6	-3.927457	2.348648	-2.348428
6	-3.402188	1.327305	-1.564140
6	1.261243	2.633401	-2.175155
6	2.582916	2.265539	-1.944147
6	2.880316	1.065595	-1.273907
6	1.777968	0.328293	-0.823787
6	-1.498742	1.394004	1.426582
6	-0.514969	2.215088	2.030237
6	-2.830756	1.758381	1.737397
6	-0.851288	3.259728	2.917246
6	-3.174098	2.793787	2.606613
6	-2.174804	3.547658	3.223279
1	-0.481808	-0.975853	1.255038
1	-3.647699	1.202962	1.285741
1	-2.420417	4.343929	3.920349
1	-0.054991	3.842622	3.374228
1	-4.030672	0.583887	-1.087495
1	-4.999828	2.411405	-2.496837
1	-3.427157	4.082609	-3.538450
1	-0.992177	3.819282	-3.160770
1	1.049101	3.548002	-2.716034
1	3.382976	2.912163	-2.290260
1	1.900597	-0.622908	-0.336223
6	4.261528	0.554262	-1.087381
6	5.211869	0.806847	-2.095675
6	4.658461	-0.239590	0.027459
6	6.497238	0.279863	-2.045453
1	4.913026	1.388072	-2.962949
6	5.957815	-0.771839	0.062350
6	6.863394	-0.524394	-0.963281
1	7.198823	0.479353	-2.849767
1	6.233742	-1.383366	0.911231
1	7.860428	-0.952541	-0.911037
7	3.792965	-0.464750	1.112151
6	3.547368	-1.723325	1.678978
8	4.260817	-2.708542	1.478800
7	2.425506	-1.735640	2.456617
1	3.075835	0.234110	1.302687
1	1.856827	-0.897358	2.513006
6	1.994219	-2.905206	3.193760
1	2.653203	-3.738688	2.946501
1	2.040337	-2.733743	4.276879
1	0.963733	-3.164889	2.928179
1	-3.363707	-2.816244	-3.525959
1	-2.157769	-4.115851	-3.375370
1	-0.371660	-2.685626	-4.124211
1	-1.672154	-1.688336	-4.819341
1	-5.698901	-0.685727	1.618682
1	-5.853124	-2.208176	0.708450
1	-4.653507	-2.059612	3.295704
1	-4.253620	-3.330414	2.114395
1	0.255530	-5.009651	1.368701
1	-0.530505	-5.054458	-0.226550
1	2.147835	-3.772127	0.495166
1	1.582533	-4.330689	-1.092583
6	0.957000	2.007163	1.843927
8	1.505312	0.922199	2.111294
7	1.710396	3.081178	1.463777

1	-4.222337	3.002520	2.809676
6	1.181611	4.300988	0.865807
1	1.262272	5.150636	1.555227
1	1.757425	4.532290	-0.036702
1	0.138302	4.173303	0.585387
6	3.160849	3.051917	1.621245
1	3.494166	4.014396	2.024876
1	3.442427	2.261503	2.315858
1	3.670629	2.883134	0.666937

Ir-N-1 Σ_g^-

Number of imaginary frequencies : 0

Electronic energy : HF=-2336.0975412
 Zero-point correction= 0.713594 (Hartree/Particle)
 Thermal correction to Energy= 0.761777
 Thermal correction to Enthalpy= 0.762721
 Thermal correction to Gibbs Free Energy= 0.628255
 Sum of electronic and zero-point Energies= -2335.383947
 Sum of electronic and thermal Energies= -2335.335764
 Sum of electronic and thermal Enthalpies= -2335.334820
 Sum of electronic and thermal Free Energies= -2335.469287

Cartesian Coordinates

77	1.151309	0.530046	-0.008928
5	0.384078	1.945215	1.168433
8	-0.783633	2.700231	0.984160
8	0.964934	2.259189	2.403934
6	-1.054876	3.429700	2.192306
6	0.274912	3.386301	2.958766
5	-0.022922	1.186106	-1.531361
8	-1.438505	1.214639	-1.488706
8	0.388744	1.563616	-2.819734
6	-1.968121	1.585801	-2.769584
6	-0.735720	2.050860	-3.565250
5	2.446209	2.000428	-0.559666
8	2.187190	3.371786	-0.686426
8	3.817334	1.762257	-0.809111
6	3.348171	4.027329	-1.206174
6	4.487442	3.020969	-0.983146
6	1.635676	-1.394706	2.401247
6	0.208746	-1.589753	2.051664
7	2.306549	-0.477815	1.662494
7	-0.182474	-1.058889	0.871685
6	2.277987	-2.113245	3.415510
6	3.624422	-1.872718	3.674017
6	4.302862	-0.923424	2.911234
6	3.604608	-0.251369	1.911643
6	-0.716340	-2.247990	2.869668
6	-2.049797	-2.320231	2.478819
6	-2.452438	-1.777133	1.249029
6	-1.447868	-1.197946	0.470981
1	4.077254	0.486655	1.272170
1	5.352620	-0.706967	3.077424
1	4.136296	-2.425303	4.455920
1	1.739311	-2.864076	3.981345
1	-0.412327	-2.657870	3.825667
1	-2.784269	-2.778955	3.133372

1	-1.652614	-0.815319	-0.517927
6	-3.860345	-1.811607	0.789890
6	-4.533793	-0.667438	0.274730
6	-4.566942	-3.020890	0.907907
6	-5.889418	-0.788105	-0.081164
6	-5.907423	-3.125004	0.552432
1	-4.035377	-3.893664	1.276751
6	-6.565556	-1.995648	0.062053
1	-6.404804	0.086502	-0.452558
1	-6.427614	-4.072943	0.651082
1	-7.611824	-2.053646	-0.225313
7	-3.866477	0.563125	0.135037
1	-2.897406	0.563484	-0.158483
6	-4.446141	1.830156	0.228444
8	-5.631317	2.033566	0.490192
7	-3.551571	2.835613	-0.030459
1	-2.554963	2.629195	-0.000885
6	-3.951617	4.216024	0.160221
1	-4.925522	4.388070	-0.303816
1	-3.212174	4.864847	-0.316191
1	-4.033304	4.496113	1.219999
1	3.195571	4.240711	-2.273040
1	3.508335	4.976964	-0.684414
1	5.179998	2.962394	-1.829451
1	5.065836	3.248815	-0.076999
1	-0.710851	1.648111	-4.583666
1	-0.677505	3.144973	-3.625988
1	-2.719528	2.369474	-2.635722
1	-2.457028	0.716399	-3.227489
1	0.870134	4.293492	2.788843
1	0.144412	3.251310	4.037191
1	-1.374473	4.447007	1.947615
1	-1.865956	2.929496	2.737922
8	-0.224384	-3.719867	-0.914367
6	0.375438	-3.002797	-1.723117
6	1.860346	-2.804658	-1.556728
6	2.589833	-3.887771	-1.046210
6	2.514541	-1.577189	-1.749130
6	3.947258	-3.756013	-0.760185
1	2.072097	-4.823747	-0.865748
6	3.869878	-1.436867	-1.438030
1	1.967858	-0.710021	-2.118277
6	4.590374	-2.529273	-0.953815
1	4.501932	-4.607224	-0.375018
1	4.332593	-0.461478	-1.541030
1	5.644644	-2.422961	-0.713419
7	-0.280622	-2.359901	-2.740239
6	-1.733604	-2.457130	-2.803886
1	-2.115928	-2.837993	-1.859472
1	-2.160678	-1.468187	-3.001406
1	-2.046794	-3.135650	-3.608450
6	0.346563	-1.767227	-3.919146
1	1.381194	-2.092446	-4.018424
1	-0.194577	-2.099684	-4.812388
1	0.322686	-0.672511	-3.878439

Ir-N-TS[1-2]_o (Refer to Figure S6)

Number of imaginary frequencies : 1
Imaginary frequency : -787.4686 cm(-1)

Electronic energy : HF=-2336.0525315
 Zero-point correction= 0.709061 (Hartree/Particle)
 Thermal correction to Energy= 0.756536
 Thermal correction to Enthalpy= 0.757480
 Thermal correction to Gibbs Free Energy= 0.627590
 Sum of electronic and zero-point Energies= -2335.343470
 Sum of electronic and thermal Energies= -2335.295996
 Sum of electronic and thermal Enthalpies= -2335.295051
 Sum of electronic and thermal Free Energies= -2335.424942

.....
 Cartesian Coordinates

.....
 77 1.244085 0.270092 -0.096862
 5 0.434788 1.838154 1.085800
 8 -0.452337 2.863582 0.715362
 8 0.729718 1.942836 2.442198
 6 -0.820661 3.610597 1.893737
 6 0.213497 3.185313 2.942006
 5 0.015460 1.235609 -1.455613
 8 -1.341348 0.895317 -1.644090
 8 0.353915 2.272114 -2.311904
 6 -1.848657 1.631884 -2.774941
 6 -0.835763 2.768664 -2.940485
 5 2.681286 1.621516 -0.632594
 8 3.232041 2.573746 0.237110
 8 3.341366 1.654309 -1.859514
 6 4.162693 3.383740 -0.499222
 6 4.430905 2.580380 -1.783701
 6 1.412498 -1.292777 2.573377
 6 0.017787 -1.526114 2.143543
 7 2.138374 -0.438954 1.812466
 7 -0.295209 -1.099483 0.901430
 6 1.966799 -1.886285 3.713544
 6 3.267606 -1.569810 4.088688
 6 3.986764 -0.654703 3.322162
 6 3.384153 -0.115770 2.190891
 6 -0.962182 -2.091379 2.969398
 6 -2.278007 -2.158616 2.526348
 6 -2.604397 -1.703253 1.241344
 6 -1.546719 -1.235359 0.459276
 1 3.889645 0.613205 1.570715
 1 4.997320 -0.362332 3.585445
 1 3.709429 -2.027795 4.968147
 1 1.391853 -2.599249 4.291631
 1 -0.715639 -2.424196 3.970434
 1 -3.056213 -2.536803 3.181930
 1 -1.697763 -0.944534 -0.567871
 6 -3.995629 -1.695734 0.732908
 6 -4.585783 -0.539585 0.152235
 6 -4.775297 -2.854161 0.882013
 6 -5.935112 -0.588298 -0.235504
 6 -6.110168 -2.891117 0.491187
 1 -4.308687 -3.738780 1.306287
 6 -6.687504 -1.746587 -0.061881
 1 -6.385207 0.300975 -0.655204
 1 -6.689821 -3.800962 0.614203
 1 -7.728198 -1.754882 -0.373597
 7 -3.833124 0.640178 -0.019255
 1 -2.871467 0.557081 -0.325977
 6 -4.316590 1.941812 0.082789

8	-5.484358	2.234389	0.331747
7	-3.346588	2.886164	-0.158449
1	-2.366543	2.624169	-0.098702
6	-3.663849	4.292878	0.002844
1	-4.578113	4.534274	-0.544295
1	-2.841451	4.885587	-0.404927
1	-3.816779	4.579537	1.051969
1	3.700202	4.356268	-0.711312
1	5.063481	3.551729	0.100260
1	4.451895	3.205971	-2.681854
1	5.376463	2.022853	-1.730997
1	-0.628427	3.012370	-3.986706
1	-1.162275	3.680505	-2.424073
1	-2.860497	1.978599	-2.556822
1	-1.874393	0.969857	-3.649259
1	1.037286	3.905713	3.024431
1	-0.221330	3.034805	3.934751
1	-0.799100	4.681315	1.671722
1	-1.840363	3.331530	2.185689
8	-0.352236	-3.637255	-0.876823
6	0.274186	-2.867002	-1.610661
6	1.757809	-2.676627	-1.421010
6	2.542819	-3.818134	-1.647665
6	2.343163	-1.462415	-1.002983
6	3.927859	-3.769350	-1.518447
1	2.051923	-4.744340	-1.934603
6	3.747301	-1.434774	-0.915269
1	1.438362	-0.173747	-1.629977
6	4.531953	-2.562887	-1.160266
1	4.527061	-4.655987	-1.706274
1	4.242840	-0.507770	-0.648304
1	5.613783	-2.497224	-1.070877
7	-0.331030	-2.184715	-2.635139
6	-1.763555	-2.334723	-2.847305
1	-2.189671	-2.906319	-2.024830
1	-2.239652	-1.349092	-2.896209
1	-1.962348	-2.865555	-3.787671
6	0.375186	-1.477151	-3.692450
1	1.452191	-1.532717	-3.548335
1	0.135436	-1.926146	-4.665452
1	0.082890	-0.421921	-3.722174

Ir-N-2 σ

Number of imaginary frequencies : 0

Electronic energy : HF=-2336.069395
 Zero-point correction= 0.711027 (Hartree/Particle)
 Thermal correction to Energy= 0.758653
 Thermal correction to Enthalpy= 0.759597
 Thermal correction to Gibbs Free Energy= 0.629055
 Sum of electronic and zero-point Energies= -2335.358368
 Sum of electronic and thermal Energies= -2335.310742
 Sum of electronic and thermal Enthalpies= -2335.309798
 Sum of electronic and thermal Free Energies= -2335.440340

Cartesian Coordinates

77	1.247969	0.201545	-0.125824
5	0.445678	2.076814	0.575989

8	-0.818746	2.245903	1.162263
8	1.240006	3.182431	0.809986
6	-0.763130	3.420923	2.000918
6	0.449824	4.190083	1.465876
5	-0.009597	1.276423	-1.409824
8	-1.362856	0.920399	-1.595924
8	0.325742	2.317685	-2.269481
6	-1.842539	1.587198	-2.777913
6	-0.857949	2.747081	-2.959180
5	2.876273	1.077154	-1.013287
8	3.903307	1.735810	-0.330314
8	3.178025	0.993820	-2.370573
6	4.841234	2.250448	-1.287879
6	4.503731	1.494925	-2.584019
6	1.127707	-0.590710	2.825674
6	-0.177011	-1.063887	2.320743
7	1.888421	0.132787	1.961040
7	-0.399473	-0.883870	1.001953
6	1.561637	-0.816744	4.137090
6	2.757656	-0.260577	4.575937
6	3.495856	0.527583	3.695597
6	3.030421	0.696422	2.396490
6	-1.178032	-1.587433	3.148155
6	-2.437169	-1.843620	2.618658
6	-2.680678	-1.609133	1.259569
6	-1.591642	-1.191382	0.490300
1	3.565743	1.285855	1.662529
1	4.424862	0.999777	3.995334
1	3.100886	-0.435722	5.590761
1	0.970431	-1.428730	4.806941
1	-1.000025	-1.740355	4.205410
1	-3.241536	-2.187800	3.261314
1	-1.681587	-1.068362	-0.578014
6	-4.034644	-1.738074	0.670454
6	-4.656403	-0.648326	0.002221
6	-4.755598	-2.927389	0.851999
6	-5.981794	-0.786356	-0.440081
6	-6.067059	-3.056755	0.402534
1	-4.264791	-3.758330	1.351037
6	-6.677841	-1.975195	-0.235274
1	-6.456027	0.056527	-0.924269
1	-6.604884	-3.988507	0.549386
1	-7.702104	-2.057158	-0.588293
7	-3.950310	0.553334	-0.192611
1	-2.951034	0.500688	-0.347097
6	-4.472208	1.840326	-0.131083
8	-5.669424	2.108885	-0.061542
7	-3.487452	2.801819	-0.201728
1	-2.545714	2.530531	0.067501
6	-3.849617	4.198035	-0.042889
1	-4.687487	4.439270	-0.700676
1	-2.993893	4.819161	-0.321598
1	-4.150239	4.450223	0.983715
1	4.689659	3.332852	-1.388118
1	5.863579	2.071243	-0.939537
1	4.521770	2.138336	-3.469629
1	5.183961	0.649611	-2.753063
1	-0.620931	2.952997	-4.006986
1	-1.229666	3.670342	-2.495252
1	-2.872301	1.911560	-2.618229
1	-1.809298	0.885741	-3.621319

1	0.162779	4.952481	0.730053
1	1.038871	4.667558	2.253920
1	-1.703752	3.973089	1.927297
1	-0.625179	3.101807	3.041202
8	-0.388086	-3.573921	-0.601482
6	0.422175	-2.960779	-1.305264
6	1.857942	-2.832545	-0.861444
6	2.617064	-4.010826	-0.931891
6	2.380901	-1.638159	-0.311926
6	3.934736	-4.039858	-0.481822
1	2.162756	-4.910023	-1.341749
6	3.716527	-1.712172	0.135286
1	0.880004	-0.073285	-1.654928
6	4.485271	-2.876376	0.056225
1	4.517859	-4.954530	-0.547651
1	4.185419	-0.823734	0.549909
1	5.513263	-2.870540	0.412512
7	0.060308	-2.396360	-2.500236
6	-1.321975	-2.474225	-2.945655
1	-1.913639	-2.982931	-2.186048
1	-1.722945	-1.465881	-3.106561
1	-1.395178	-3.030889	-3.888868
6	0.994201	-1.835227	-3.464105
1	1.984286	-1.723749	-3.027837
1	1.063163	-2.480607	-4.351027
1	0.653796	-0.845190	-3.790233

Ir-O-1 Σ_g^-

Number of imaginary frequencies : 0

Electronic energy : HF=-2336.0947405
 Zero-point correction= 0.713090 (Hartree/Particle)
 Thermal correction to Energy= 0.761473
 Thermal correction to Enthalpy= 0.762417
 Thermal correction to Gibbs Free Energy= 0.627353
 Sum of electronic and zero-point Energies= -2335.381650
 Sum of electronic and thermal Energies= -2335.333267
 Sum of electronic and thermal Enthalpies= -2335.332323
 Sum of electronic and thermal Free Energies= -2335.467388

Cartesian Coordinates

77	1.295281	0.460002	-0.004505
5	0.586324	1.934855	1.129426
8	-0.450686	2.830662	0.836998
8	1.062910	2.161674	2.428103
6	-0.753374	3.590674	2.016570
6	0.459738	3.361358	2.931496
5	0.197200	1.151246	-1.566969
8	-1.218694	1.174693	-1.577103
8	0.663016	1.490843	-2.839172
6	-1.684252	1.316797	-2.930701
6	-0.444111	1.805118	-3.696500
5	2.699084	1.835937	-0.527099
8	2.545010	3.219059	-0.680905
8	4.056196	1.492746	-0.731094
6	3.761563	3.774355	-1.191480
6	4.819442	2.694871	-0.915771
6	1.590379	-1.445223	2.446001
6	0.149585	-1.496608	2.102090

7	2.353123	-0.634475	1.674004
7	-0.182314	-1.023809	0.877598
6	2.151320	-2.186212	3.491890
6	3.517415	-2.084190	3.742064
6	4.293201	-1.248852	2.939299
6	3.669821	-0.542567	1.913629
6	-0.841780	-1.958485	2.975224
6	-2.177634	-1.886491	2.594806
6	-2.524293	-1.404922	1.321274
6	-1.463126	-1.034124	0.488432
1	4.215773	0.119106	1.248672
1	5.361041	-1.143079	3.097605
1	3.968741	-2.654346	4.548202
1	1.532981	-2.844411	4.091370
1	-0.579859	-2.316267	3.964165
1	-2.956703	-2.181391	3.290611
1	-1.628497	-0.716773	-0.532115
6	-3.936791	-1.307769	0.883095
6	-4.487144	-0.141078	0.278072
6	-4.778670	-2.407429	1.129404
6	-5.859275	-0.133961	-0.038031
6	-6.131335	-2.385631	0.810484
1	-4.345320	-3.299277	1.574086
6	-6.666693	-1.234113	0.229728
1	-6.280158	0.758370	-0.479035
1	-6.755199	-3.251770	1.008881
1	-7.720331	-1.192543	-0.031909
7	-3.686862	0.980977	0.013295
1	-2.723864	0.843674	-0.274525
6	-4.119351	2.310821	-0.024985
8	-5.272108	2.672837	0.210123
7	-3.117521	3.176579	-0.367923
1	-2.152257	2.858932	-0.317215
6	-3.352065	4.605789	-0.302963
1	-4.255265	4.866923	-0.860336
1	-2.498654	5.117945	-0.753792
1	-3.478619	4.970332	0.725966
1	3.646831	3.967477	-2.266816
1	3.980081	4.724416	-0.692149
1	5.525833	2.565076	-1.742430
1	5.391387	2.903172	-0.000731
1	-0.319150	1.300416	-4.659493
1	-0.466495	2.889368	-3.868648
1	-2.514961	2.028374	-2.952327
1	-2.024334	0.338370	-3.287059
1	1.183814	4.184258	2.863120
1	0.183490	3.228420	3.982575
1	-0.897387	4.642993	1.753476
1	-1.683364	3.211480	2.459763
8	-0.513803	-1.894728	-3.204420
6	-0.140479	-2.665577	-2.312489
6	1.329726	-2.771706	-1.997198
6	1.967425	-3.933548	-1.539777
6	2.108625	-1.628048	-2.248421
6	3.336460	-3.924779	-1.259790
1	1.410963	-4.856158	-1.420356
6	3.468710	-1.608740	-1.936246
1	1.633304	-0.754313	-2.680656
6	4.083148	-2.757528	-1.428706
1	3.816948	-4.833879	-0.908733
1	4.032555	-0.691816	-2.072459

1	5.141849	-2.747512	-1.184860
7	-1.043487	-3.432620	-1.616193
6	-2.437044	-3.417620	-2.048560
1	-2.497475	-3.060428	-3.074784
1	-2.846051	-4.432316	-1.987750
1	-3.044897	-2.764123	-1.410125
6	-0.813897	-4.118048	-0.349154
1	0.084281	-3.752054	0.143178
1	-1.660201	-3.919848	0.315699
1	-0.737262	-5.205197	-0.481416

Ir-O-TS[1-2]_o (Refer to Figure S6)

Number of imaginary frequencies : 1

Imaginary frequency : -761.5148 cm(-1)

Electronic energy : HF=-2336.0532798
 Zero-point correction= 0.708816 (Hartree/Particle)
 Thermal correction to Energy= 0.756297
 Thermal correction to Enthalpy= 0.757241
 Thermal correction to Gibbs Free Energy= 0.627329
 Sum of electronic and zero-point Energies= -2335.344463
 Sum of electronic and thermal Energies= -2335.296983
 Sum of electronic and thermal Enthalpies= -2335.296039
 Sum of electronic and thermal Free Energies= -2335.425951

Cartesian Coordinates

77	1.300166	0.301149	-0.145390
5	0.563101	1.906764	1.027808
8	-0.198391	3.016514	0.628099
8	0.782194	1.959899	2.404900
6	-0.573566	3.769294	1.798788
6	0.358088	3.240996	2.894646
5	0.123793	1.257946	-1.550789
8	-1.275372	1.098596	-1.576740
8	0.520675	2.084578	-2.588894
6	-1.749733	1.583854	-2.848122
6	-0.647848	2.555665	-3.277249
5	2.805684	1.578401	-0.654364
8	3.372770	2.518670	0.220751
8	3.506089	1.560142	-1.856987
6	4.357530	3.277051	-0.499485
6	4.629835	2.441622	-1.762682
6	1.379305	-1.287206	2.516277
6	-0.023210	-1.456495	2.077073
7	2.149852	-0.469833	1.759489
7	-0.309401	-1.036174	0.825254
6	1.895304	-1.904791	3.661725
6	3.208097	-1.652792	4.045506
6	3.976831	-0.777352	3.281107
6	3.408238	-0.209982	2.145650
6	-1.034114	-1.957329	2.908355
6	-2.350201	-1.956458	2.462574
6	-2.650571	-1.501118	1.169439
6	-1.567133	-1.110103	0.376308
1	3.953552	0.492833	1.528476
1	4.999220	-0.535061	3.549604
1	3.620403	-2.128765	4.929702
1	1.281667	-2.584577	4.240367

1	-0.809353	-2.283789	3.916518
1	-3.150683	-2.274769	3.123106
1	-1.696276	-0.825122	-0.659166
6	-4.046485	-1.407430	0.680945
6	-4.575765	-0.210575	0.121938
6	-4.893297	-2.516218	0.844737
6	-5.936546	-0.175702	-0.230881
6	-6.236088	-2.470812	0.484157
1	-4.474094	-3.428769	1.260173
6	-6.753002	-1.287715	-0.047938
1	-6.342316	0.742563	-0.632255
1	-6.868191	-3.343600	0.616349
1	-7.798941	-1.229181	-0.335700
7	-3.752881	0.914479	-0.059934
1	-2.794811	0.769311	-0.359094
6	-4.154583	2.249058	0.001577
8	-5.301650	2.619544	0.247422
7	-3.130816	3.121304	-0.263635
1	-2.169939	2.791944	-0.266542
6	-3.352860	4.550733	-0.165520
1	-4.245745	4.833476	-0.728858
1	-2.488173	5.065923	-0.590464
1	-3.489283	4.890790	0.869869
1	3.942098	4.263741	-0.741687
1	5.246555	3.419593	0.123921
1	4.703088	3.050714	-2.669447
1	5.550104	1.847392	-1.673486
1	-0.466551	2.552533	-4.355971
1	-0.865307	3.583657	-2.957444
1	-2.723841	2.059710	-2.713529
1	-1.841501	0.731992	-3.530985
1	1.239514	3.881500	3.028525
1	-0.140550	3.123814	3.861768
1	-0.451898	4.838788	1.604130
1	-1.627900	3.569691	2.026425
8	-0.303949	-1.579577	-2.748519
6	0.087285	-2.474237	-1.990647
6	1.546128	-2.581462	-1.630071
6	2.214339	-3.769807	-1.969184
6	2.250460	-1.473795	-1.111871
6	3.594516	-3.878929	-1.819293
1	1.642377	-4.602870	-2.370794
6	3.646062	-1.602308	-1.002592
1	1.424321	-0.139961	-1.690126
6	4.312207	-2.783430	-1.336035
1	4.104218	-4.798498	-2.092920
1	4.229976	-0.757847	-0.651439
1	5.392798	-2.842564	-1.228636
7	-0.762829	-3.447374	-1.527054
6	-2.131504	-3.492792	-2.021437
1	-2.208251	-2.891195	-2.925727
1	-2.404936	-4.530449	-2.245254
1	-2.840077	-3.104077	-1.279283
6	-0.499157	-4.292215	-0.371804
1	0.504104	-4.122330	0.012997
1	-1.218110	-4.064664	0.426610
1	-0.600703	-5.352979	-0.633092

Ir-O-2 σ

Number of imaginary frequencies : 0

Electronic energy : HF=-2336.0679022
Zero-point correction= 0.711625 (Hartree/Particle)
Thermal correction to Energy= 0.758871
Thermal correction to Enthalpy= 0.759815
Thermal correction to Gibbs Free Energy= 0.630774
Sum of electronic and zero-point Energies= -2335.356278
Sum of electronic and thermal Energies= -2335.309031
Sum of electronic and thermal Enthalpies= -2335.308087
Sum of electronic and thermal Free Energies= -2335.437128

.....
Cartesian Coordinates

.....
77 1.312692 0.234807 -0.210197
5 0.635262 2.126108 0.563383
8 -0.599257 2.325491 1.203067
8 1.474477 3.202282 0.787031
6 -0.470692 3.479141 2.060773
6 0.742053 4.221820 1.489561
5 0.103582 1.401272 -1.451353
8 -1.278182 1.144038 -1.587540
8 0.475380 2.435039 -2.302085
6 -1.729096 1.807291 -2.784245
6 -0.694013 2.919055 -2.979296
5 2.987578 1.054568 -1.056738
8 4.101696 1.490605 -0.327607
8 3.242331 1.139852 -2.418893
6 5.077544 2.016957 -1.239375
6 4.607649 1.521549 -2.618973
6 1.130779 -0.668438 2.721665
6 -0.195228 -1.050495 2.192414
7 1.949853 0.017267 1.880143
7 -0.395666 -0.825366 0.876443
6 1.529749 -0.952742 4.033068
6 2.760820 -0.501719 4.495473
6 3.569602 0.238111 3.636480
6 3.130524 0.473277 2.337975
6 -1.228533 -1.552439 2.994966
6 -2.492372 -1.730932 2.447124
6 -2.712711 -1.445009 1.092389
6 -1.597249 -1.059419 0.341117
1 3.721399 1.030541 1.621382
1 4.532090 0.624916 3.952656
1 3.076874 -0.721801 5.510381
1 0.885345 -1.527011 4.686850
1 -1.070900 -1.746244 4.048687
1 -3.320102 -2.049244 3.073144
1 -1.663566 -0.900998 -0.726937
6 -4.075427 -1.473699 0.509021
6 -4.634676 -0.319629 -0.102074
6 -4.868750 -2.622231 0.654385
6 -5.973653 -0.355170 -0.523709
6 -6.191551 -2.650134 0.221361
1 -4.429213 -3.501248 1.118109
6 -6.741385 -1.504966 -0.359037
1 -6.400847 0.536284 -0.962785
1 -6.785550 -3.551335 0.339083
1 -7.773560 -1.506729 -0.697611
7 -3.860385 0.843606 -0.257601
1 -2.874950 0.745521 -0.477562

6	-4.302508	2.147524	-0.057824
8	-5.475736	2.464154	0.125765
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1	6.073156	1.650116	-0.968337
1	4.668371	2.295008	-3.391693
1	5.178703	0.646877	-2.956623
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1	-2.744137	2.179233	-2.630623
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6	1.670700	-2.770117	-1.157300
6	2.340461	-3.993377	-1.334295
6	2.291726	-1.668716	-0.520679
6	3.648352	-4.166954	-0.888368
1	1.823736	-4.813534	-1.828631
6	3.610779	-1.890239	-0.074159
1	0.932320	0.027807	-1.750853
6	4.283814	-3.102539	-0.249170
1	4.160254	-5.113522	-1.039459
1	4.147492	-1.078319	0.409021
1	5.306589	-3.209588	0.106413
7	-0.661653	-3.548351	-1.288108
6	-1.953167	-3.631261	-1.953104
1	-1.913280	-3.067361	-2.883477
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1	-2.751189	-3.220663	-1.322058
6	-0.554763	-4.318763	-0.059427
1	0.387738	-4.117408	0.444613
1	-1.375782	-4.051099	0.618589
1	-0.619123	-5.395492	-0.264240
