Electronic Supporting Information

for

DFT Study on Ir-Quinoid Catalyzed C-H Functionalization: New Radical Reactivity or Direct Carbene Transfer?

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Computational Details

We modelled the electronic structure and thermochemistry of the mechanistic cycle using Gaussian16 software.[1] We have performed all geometry optimisations using the hybrid functional B3LYP, while using the standard split valence Pople's basis set 6-31G(d,p) for all atoms except Ir, Ru and Br.[2,3] For these heavy elements, we used the LANL2DZ basis with an effective core potential (ECP).[4] To compute the wavefunction for open-shell singlet systems, we used the guess=(read,mix) keyword on a triplet wavefunction generated in a previous calculation.[5] The internal stability of the wavefunctions was verified using the opt=stable keyword. Our choice of functional was based upon previous successful studies on similar

systems. The use of unrestricted B3LYP functional with standard split valence Pople's basis set have been shown to give reliable geometries for stationary point calculations on transition metal carbene systems. We carried out frequency analysis on these stationary points to verify their nature (minima/saddle point) and obtain thermal corrections to the electronic energy. For the transition states, we performed IRC (Intrinsic Reaction Coordinate) calculations to link the TS with its corresponding intermediates, which proved to be really insightful in a few cases where the fate of the product arising from a Transition State was not intuitively obvious.[6] We have performed single point calculations on the optimised structures using the Karlsruhe basis set Def2TZVPP for all systems except for the ones with a Ru centre.[7] In the case of Ru, the wavefunction for the crucial open-shell singlet TS (**^{OSS}TS(B-C)**) generated from Def2TZVPP was converging to a closed shell singlet function, thereby simulating a hydride transfer instead of the desired Hydrogen Atom Transfer. As a result, we had to use the diffuse Pople's basis set 6-31+G(d,p) for all single point calculations on Ru systems. All these single points were computed using both B3LYP-D3BJ and ωB97XD functionals, with an SMD (solvation model density) solvation model to simulate the solvation effects of DCM (dichloromethane).[8] The thermal corrections obtained from the geometry optimisations were added to the single point electronic energies to give the thermochemical values (in this case, the Free Energies) for the transition states. For the two important transition States **^{OSS}TS(B-C)** and **TS(B-D)**, we verified our results across different hybrid and pure functionals. For the Kinetic Isotope effect barrier calculations, we reoptimized the stationary point using the Opt=Tight and Integral=Superfine criteria for more accurate values.

For the Distortion-Interaction (Activation-Strain) analysis,[9] we calculated the electronic energies of the distorted and ground state fragments at the $SMD_{(DCM)}$/B3LYP-D3BJ/Def2TZVPP level of theory. The nature of this interaction energy was analysed using the Energy Decomposition Analysis feature from the ADF (Amsterdam Density Functional) software. The wavefunction was computed at the B3LYP-D3/TZP level of theory.[11]

Table S1. Total Electronic Energies (E) (in a.u) at the $SMD_{(DCM)}$/B3LYP-D3BJ/Def2TZVPP//B3LYP-D3BJ/6-31G(d,p),LANL2DZ(Ir/Ru) for CHD-Quinone Diazide Reactions with Ir(Por)Me and Ru(Por)[a]

	CSS	**OSS**	**Triplet**
Stationary Point	**E**	**E**	**E**

A	-2406.622269	-[b]	-[c]
TS(A-B)	-2406.581318	-[b]	-[c]
B	-2530.601884	-2530.587631	-2530.593961
C	-2530.616451	-2530.618917	-2530.618932
TS(C-P)	-2530.612148	-[b]	-2530.568017
P	-2530.708197	-[b]	-2530.64188
TS(B-D)	-2530.578743	-[b]	-[d]
D	-2530.656614	-[b]	-[d]
TS(B-E)	-[e]	-[b]	-2530.566533
E	-[e]	-[b]	-2530.618894
$^{CSS}\mathbf{B}_{Ru}$	-6248.546341	-	-
$^{OSS}\mathbf{TS(B-C)}_{Ru}$	-	-6248.527782	-
$^{CSS}\mathbf{TS(B-D)}_{Ru}$	-6248.533715	-	-

[a]6-31+G(d,p) was used in place of Def2TZVPP for Ru.
[b]OSS converges to CSS.
[c]Quinone diazide dissociates into a high energy free carbene in its triplet state, without metal involvement
[d]**TS(B-D)** goes to **TS(B-E)** in a triplet state.
[e]**TS(B-E)** goes to a CSS **TS(B-D)** in singlet state.

Table S2. Total Electronic Energies (E) (in a.u) at the $SMD_{(DCM)}$/B3LYP-D3BJ/Def2TZVPP//B3LYP-D3BJ/6-31G(d,p),LANL2DZ(Ir/Ru) for CHD-Quinone Diazide Reactions with Ir(Por)Me and Ru(Por)[a]

	CSS	**OSS**	**Triplet**
Stationary Point			
A	-2405.610157	-[b]	-[c]
TS(A-B)	-2405.56319	-[b]	-[c]
B	-2529.519137	-2529.504970	-2529.519543
TS(B-C)	-2529.450363	-2529.480896	-2529.479208
C	-2529.537387	-2529.543959	-2529.543988
TS(C-P)	-2529.531596	-[b]	-2529.49948
P	-2529.644702	-[b]	-2529.575152
TS(B-D)	-2529.497292	-[b]	-[d]
D	-2529.59259	-[b]	-[d]
TS(B-E)	-[e]	-[d]	-2529.485957
E	-[e]	-[d]	-2529.54384
$^{CSS}\mathbf{B}_{Ru}$	-6247.2651	-	-
$^{OSS}\mathbf{TS(B-C)}_{Ru}$	-	-6247.244361	-
$^{CSS}\mathbf{TS(B-D)}_{Ru}$	-6247.247965	-	-

[a]6-31+G(d,p) was used in place of Def2TZVPP for Ru.
[b]OSS converges to CSS.
[c]Quinone diazide dissociates into a high energy free carbene in its triplet state, without metal involvement
[d]**TS(B-D)** goes to **TS(B-E)** in a triplet state.
[e]**TS(B-E)** goes to a CSS **TS(B-D)** in singlet state.

Table S3. Total Electronic Energies (E) (in a.u) at the $SMD_{(DCM)}$/B3LYP-D3BJ/Def2TZVPP//B3LYP-D3BJ/6-31G(d,p),LANL2DZ(Ir) for S2-DHA System

Stationary Point	E
$\mathbf{B_{DHA\text{-}S2}}$	-2688.727901
$\mathbf{^{CSS}TS(B\text{-}E)_{DHA\text{-}S2}}$	-2688.734178
$\mathbf{^{OSS}TS(B\text{-}C)_{DHA\text{-}S2}}$	-2688.694708
$\mathbf{^{CSS}E_{DHA\text{-}S2}}$	-2688.775424
$\mathbf{P1_{DHA\text{-}S2}}$	-2688.801671
$\mathbf{P2_{DHA\text{-}S2}}$	-2688.828265

Table S4. Total Electronic Energies (E) (in a.u) at the SMD $_{(DCM)}$/ωB97XD/Def2TZVPP/B3LYP-D3BJ/6-31G(d,p), LANL2DZ(Ir) for S2-DHA System

Stationary Point	E
$\mathbf{B_{DHA\text{-}S2}}$	-2687.56082
$\mathbf{^{CSS}TS(B\text{-}E)_{DHA\text{-}S2}}$	-2687.56087
$\mathbf{^{OSS}TS(B\text{-}C)_{DHA\text{-}S2}}$	-2687.50398
$\mathbf{^{CSS}E_{DHA\text{-}S2}}$	-2687.599455
$\mathbf{P2_{DHA\text{-}S2}}$	-2687.660133

Table S5. Total Electronic Energies (E) (in a.u) at the $SMD_{(DCM)}$/B3LYP-D3BJ/Def2TZVPP//B3LYP-D3BJ/6-31G(d,p),LANL2DZ(Ir) for S1-DHA System

Stationary Point	E
$\mathbf{B_{DHA\text{-}S1}}$	-2838.055426
$\mathbf{^{3}TS(B\text{-}E)_{DHA\text{-}S1}}$	-2838.043163
$\mathbf{^{CSS}TS(B\text{-}E)_{DHA\text{-}S1}}$	-2838.052501
$\mathbf{^{3}TS(B\text{-}C)_{DHA\text{-}S1}}$	-2838.04022
$\mathbf{^{OSS}TS(B\text{-}C)_{DHA\text{-}S1}}$	-2838.043379
$\mathbf{^{CSS}E_{DHA\text{-}S1}}$	-2838.072645
$\mathbf{P1_{DHA\text{-}S1}}$	-2838.104226
$\mathbf{P2_{DHA\text{-}S1}}$	-2838.150794

Table S6. Total Electronic Energies (E) (in a.u) at the SMD $_{(DCM)}$/ωB97XD/Def2TZVPP$^{/}$/B3LYP-D3BJ/6-31G(d,p),LANL2DZ (Ir) for S1-DHA System

Stationary Point	E
$\mathbf{B_{DHA\text{-}S1}}$	-2836.827972
$\mathbf{^{3}TS(B\text{-}E)_{DHA\text{-}S1}}$	-2836.819998
$\mathbf{^{CSS}TS(B\text{-}E)_{DHA\text{-}S1}}$	-2836.828031
$\mathbf{^{3}TS(B\text{-}C)_{DHA\text{-}S1}}$	-2836.813502
$\mathbf{^{OSS}TS(B\text{-}C)_{DHA\text{-}S1}}$	-2836.816137
$\mathbf{^{CSS}E_{DHA\text{-}S1}}$	-2836.848995
$\mathbf{P1_{DHA\text{-}S1}}$	-2836.895952
$\mathbf{P2_{DHA\text{-}S1}}$	-2836.929848

Table S7. Total Electronic Energies (E) (in a.u) at the SMD$_{(DCM)}$// B3LYP-D3BJ/Def2TZVPP//B3LYP-D3BJ/6-31G(d,p), LANL2DZ(Ir) for Ir(Por)Cl System

Stationary Point	E
$\mathbf{^{CSS}A_{Cl}}$	-2826.919044
$\mathbf{^{CSS}A'_{Cl}}$[a]	-2826.937853
$\mathbf{^{CSS}TS(A\text{-}B)_{Cl}}$	-2826.931274
$\mathbf{^{CSS}B_{Cl}}$	-2950.960548
$\mathbf{^{CSS}TS(B\text{-}D)_{Cl}}$	-2950.942093
$\mathbf{^{CSS}D_{Cl}}$	-2950.974157

[a] Tetrahedral intermediate formed between the carbene and the Ir catalyst.

Table S8. Total Electronic Energies (E) (in a.u) at the SMD$_{(DCM)}$// ωB97XD/Def2TZVPP$^{/}$/B3LYP-D3BJ/6-31G(d,p),LANL2DZ(Ir) for Ir(Por)Cl System

Stationary Point	E
$\mathbf{^{CSS}A_{Cl}}$	-2825.905486
$\mathbf{^{CSS}A'_{Cl}}$[a]	-2825.923991
$\mathbf{^{CSS}TS(A\text{-}B)_{Cl}}$	-2825.913489
$\mathbf{^{CSS}B_{Cl}}$	-2949.879161
$\mathbf{^{CSS}TS(B\text{-}D)_{Cl}}$	-2949.860731

[a] Tetrahedral intermediate formed between the carbene and the Ir catalyst.

Table S9. Relative Free Energies (ΔG) (in kcal/mol) at the $SMD_{(DCM)}$/B3LYP-D3BJ/Def2TZVPP//B3LYP-D3BJ/6-31G(d,p),LANL2DZ(Ir/Ru) for CHD-Quinone Diazide reactions with Ir(Por)Me and Ru(Por) [a]

	CSS	OSS	Triplet
Stationary Point	**ΔG**	**ΔG**	**ΔG**
A	0	- [b]	- [c]
TS(A-B)	25.3	- [b]	- [c]
B	-4.3	-2.8	-2.7
TS(B-C)	18.7	12.2	12.6
C	-12.3	-15.8	-16.5
TS(C-P)	-8.1	- [b]	18.0
P	-66.8	- [b]	-28.2
TS(B-D)	8.9	- [b]	- [d]
D	-37.7	- [b]	- [d]
TS(B-E)	- [e]	- [e]	13.4
E	- [e]	- [e]	-19.5
$^{CSS}B_{Ru}$	0	-	-
$^{OSS}TS(B\text{-}C)_{Ru}$	-	18.4	-
$^{CSS}TS(B\text{-}D)_{Ru}$	19.9	-	-

[a]6-31+G(d,p) was used in place of Def2TZVPP for Ru
[b]OSS converges to CSS
[c]Quinone diazide dissociates into a high energy free carbene in its triplet state, without metal involvement
[d]**TS(B-D)** goes to **TS(B-E)** in a triplet state
[e]**TS(B-E)** goes to a CSS **TS(B-D)** in singlet state

Table S10. Relative Free Energies (ΔG) (in kcal/mol) at the $SMD_{(DCM)}$/ ωB97XD/Def2TZVPP//B3LYP-D3BJ/6-31G(d,p), LANL2DZ(Ir/Ru) for CHD-Quinone Diazide reactions with Ir(Por)Me and Ru(Por) [a]

	CSS	OSS	Triplet
Stationary Point	**ΔG**	**ΔG**	**ΔG**
A	0	- [b]	- [c]
TS(A-B)	29.1	- [b]	- [c]
B	2.3	3.8	2.6
TS(B-C)	27.7	20.2	20.3
C	-7.9	-14.1	-14.7
TS(C-P)	-2.8	- [b]	15.7
P	-72.3	- [b]	-31.6
TS(B-D)	14.8	- [b]	- [d]
D	-42.8	- [b]	- [d]
TS(B-E)	- [e]	- [e]	18.7
E	- [e]	- [e]	-17.7
$^{CSS}B_{Ru}$	0	-	-
$^{OSS}TS(B\text{-}C)_{Ru}$	-	19.7	-

^{CSS}**TS(B-D)$_{Ru}$**	22.7	-	-

[a]6-31+G(d,p) was used in place of Def2TZVPP for Ru.
[b]OSS converges to CSS.
[c]Quinone diazide dissociates into a high energy free carbene in its triplet state, without metal involvement.
[d]**TS(B-D)** goes to **TS(B-E)** in a triplet state.
[e]**TS(B-E)** goes to a CSS **TS(B-D)** in singlet state.

Table S11. Relative Free Energies (ΔG) (in kcal/mol) at the SMD$_{(DCM)}$/B3LYP-D3BJ/Def2TZVPP[/]/B3LYP-D3BJ/6-31G(d,p), LANL2DZ(Ir) for S2-DHA System

Stationary Point	ΔG
B$_{DHA-S2}$	0
^{CSS}**TS(B-E)$_{DHA-S2}$**	10.1
^{OSS}**TS(B-C)$_{DHA-S2}$**	32.8
^{CSS}**E$_{DHA-S2}$**	-16.9
P1$_{DHA-S2}$	-44.4
P2$_{DHA-S2}$	-65.8

Table S12. Relative Free Energies (ΔG) (in kcal/mol) at the SMD$_{(DCM)}$/ ωB97XD/Def2TZVPP[/]/B3LYP-D3BJ/6-31G(d,p), LANL2DZ(Ir) for S2-DHA System

Stationary Point	ΔG
B$_{DHA-S2}$	0
^{CSS}**TS(B-E)$_{DHA-S2}$**	14.0
^{OSS}**TS(B-C)$_{DHA-S2}$**	47.6
^{CSS}**E$_{DHA-S2}$**	-11.3
P1$_{DHA-S2}$	-50.5
P2$_{DHA-S2}$	-65.1

Table S13. Relative Free Energies (ΔG) (in kcal/mol) at the SMD$_{(DCM)}$/B3LYP-D3BJ/Def2TZVPP[/]/B3LYP-D3BJ/6-31G(d,p), LANL2DZ(Ir) for S1-DHA System

Stationary Point	ΔG
B$_{DHA-S1}$	0
^{3}**TS(B-E)$_{DHA-S1}$**	18.4
^{CSS}**TS(B-E)$_{DHA-S1}$**	15.8
^{3}**TS(B-C)$_{DHA-S1}$**	19.8
^{OSS}**TS(B-C)$_{DHA-S1}$**	18.7
^{CSS}**E$_{DHA-S1}$**	2.0
P1$_{DHA-S1}$	-27.9

Table S14. Relative Free Energies (ΔG) (in kcal/mol) at the SMD $_{(DCM)}$/ ωB97XD/Def2TZVPP$^{/}$/B3LYP-D3BJ/6-31G(d,p),LANL2DZ(Ir) for S1-DHA System

Stationary Point	ΔG
$\mathbf{B_{DHA\text{-}S1}}$	0
$\mathbf{^{3}TS(B\text{-}E)_{DHA\text{-}S1}}$	15.7
$\mathbf{^{CSS}TS(B\text{-}E)_{DHA\text{-}S1}}$	13.1
$\mathbf{^{3}TS(B\text{-}C)_{DHA\text{-}S1}}$	19.3
$\mathbf{^{OSS}TS(B\text{-}C)_{DHA\text{-}S1}}$	18.6
$\mathbf{^{CSS}E_{DHA\text{-}S1}}$	-0.4
$\mathbf{P1_{DHA\text{-}S1}}$	-39.9
$\mathbf{P2_{DHA\text{-}S1}}$	-64.4

Table S15. Relative Free Energies (ΔG) (in kcal/mol) at the SMD$_{(DCM)}$//B3LYP-D3BJ/Def2TZVPP$^{/}$/B3LYP-D3BJ/6-31G(d,p), LANL2DZ(Ir) for Ir(Por)Cl system

Stationary Point	ΔG
$\mathbf{^{CSS}A_{Cl}}$	0
$\mathbf{^{CSS}A'_{Cl}}$[a]	3.7
$\mathbf{^{CSS}TS(A\text{-}B)_{Cl}}$	8.1
$\mathbf{^{CSS}B_{Cl}}$	-28.7
$\mathbf{^{CSS}TS(B\text{-}D)_{Cl}}$	-19.0
$\mathbf{^{CSS}D_{Cl}}$	-35.8

[a] Tetrahedral intermediate formed between the carbene and the Ir catalyst.

Table S16. Relative Free Energies (ΔG) (in kcal/mol) at the SMD$_{(DCM)}$// ωB97XD/Def2TZVPP$^{/}$/B3LYP-D3BJ/6-31G(d,p), LANL2DZ(Ir) for Ir(Por)Cl System

Stationary Point	ΔG
$\mathbf{^{CSS}A_{Cl}}$	0
$\mathbf{^{CSS}A'_{Cl}}$[a]	3.9
$\mathbf{^{CSS}TS(A\text{-}B)_{Cl}}$	10.8
$\mathbf{^{CSS}B_{Cl}}$	-24.4
$\mathbf{^{CSS}TS(B\text{-}D)_{Cl}}$	-14.7
$\mathbf{^{CSS}D_{Cl}}$	-40.4

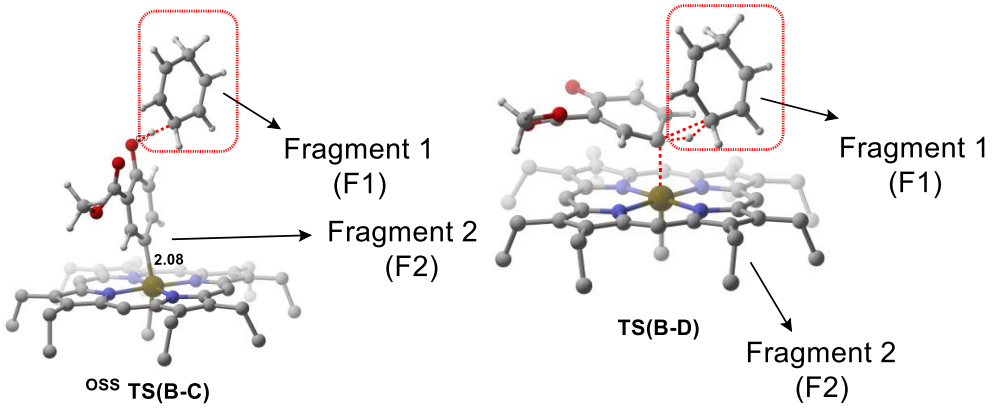
[a] Tetrahedral intermediate formed between the carbene and the Ir catalyst.

Table S17. Relative Free Energies (ΔG) (in kcal/mol) of **TS(B-D)** and **^{OSS}TS(B-C)** using different Hybrid and Pure Functionals[a]

	TS(B-D)	**^{OSS}TS(B-C)**
Stationary Point	**ΔG**	**ΔG**
B3LYP-D3BJ	0	3.3
ωB97XD	0	5.5
M06	0	10.3
BLYP	0	3.1
BP86	0	5.2

[a]All single point energy calculations are done with Def2TZVPP using $SMD_{(DCM)}$.

Table S18. Distortion-Interaction (Activation-Strain) Analysis[a]



Stationary Point	**TS(B-D)**	**^{OSS}TS(B-C)**
Distortion in F1	15.2	18.9
Distortion in F2	17.6	4.3
Total Distortion	32.8	23.2
Interaction Energy	18.3	0.6

[a]Above electronic energies are given in kcal/mol, relative to the separated optimized F1 and F2 fragments.

For the KIE study, we reoptimised the stationary points **TS(B-D)**, **^{3}TS(B-C)**, **^{OSS}TS(B-C)** using the criteria opt=tight and Integral=SuperFine for more accurate thermokinetic values. We performed free energy calculation on these TSs with the standard CHD and its d-8 deuterated analogue. We got the free energy barriers as shown in Table S19.

Table S19. Kinetic Isotope Effect[a,b]

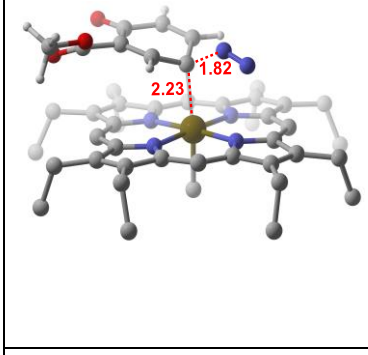
	h-8 1,4 CHD	d-8 1,4 CHD
Stationary Point	**ΔG**	**ΔG**
TS(B-D)	8.24	8.96
^{OSS}TS(B-C)	16.62	17.74
^{3}TS(B-C)	17.12	18.23

[a]Relative free energies are given in kcal/mol.
[b]Barriers are calculated at the B3LYP/6-31G(d,p) level of theory.

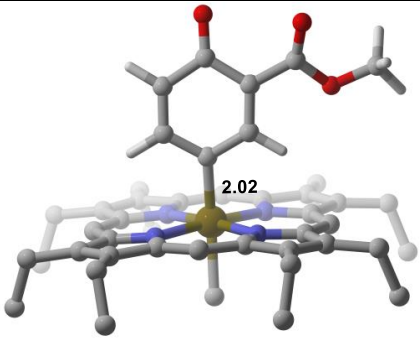
These barriers correspond to the following KIE:

TS(B-D): 3.3
^{OSS}TS(B-C): 6.6
^{3}TS(B-C): 6.5

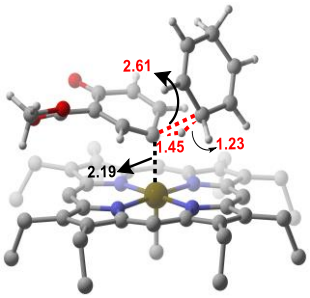
Experimental KIE is 3.2 ± 0.3



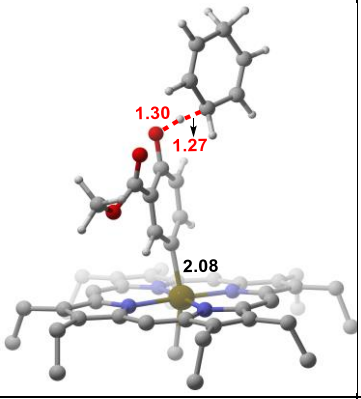
TS(A-B)



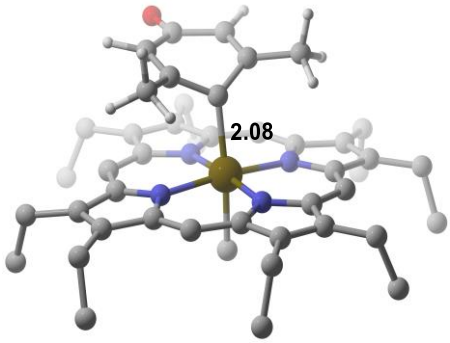
^{CSS}B



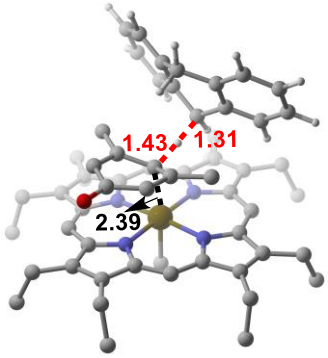
TS(B-D)



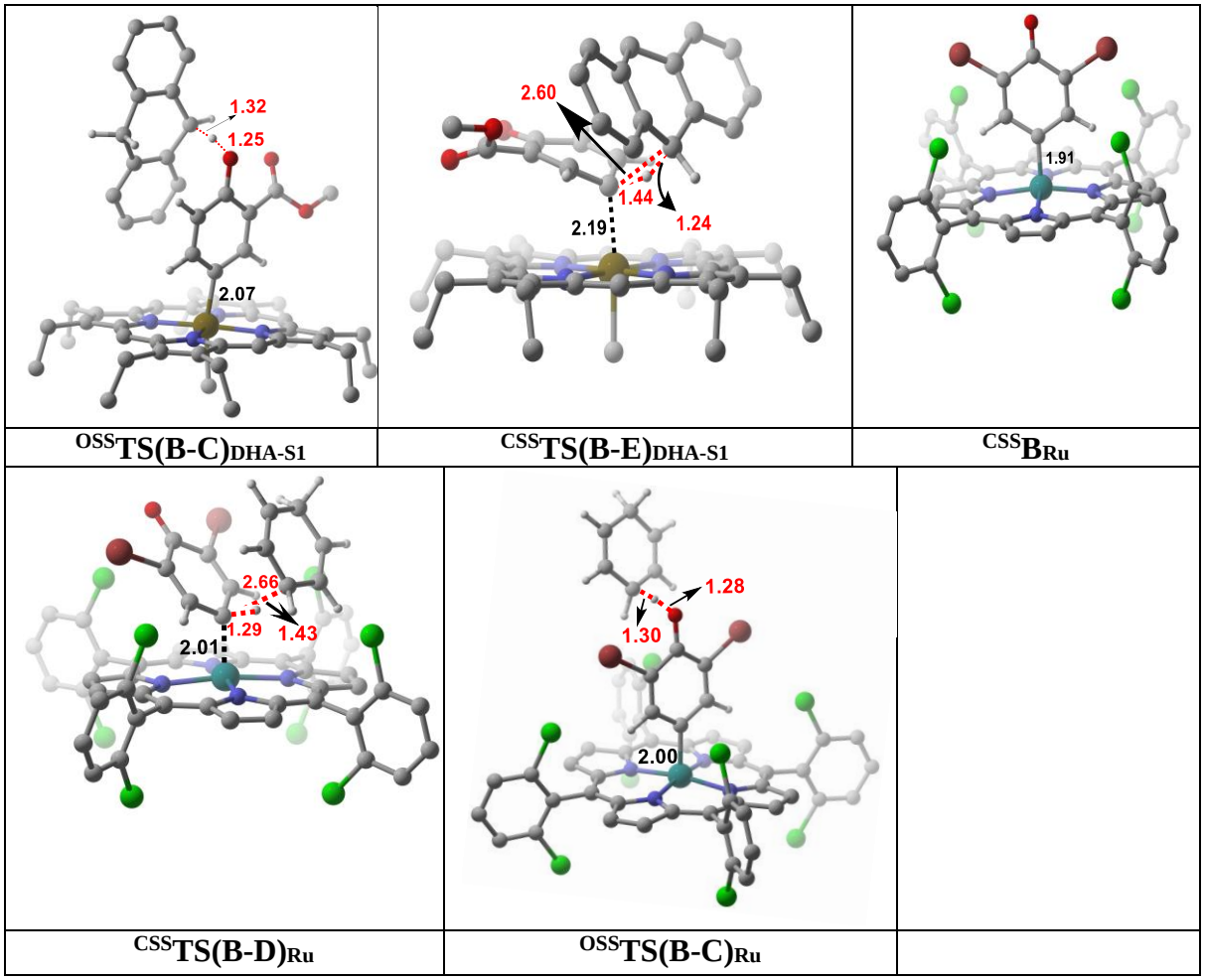
^{OSS}TS(B-C)



B_{DHA-S2}



^{CSS}TS(B-E)$_{DHA-S2}$

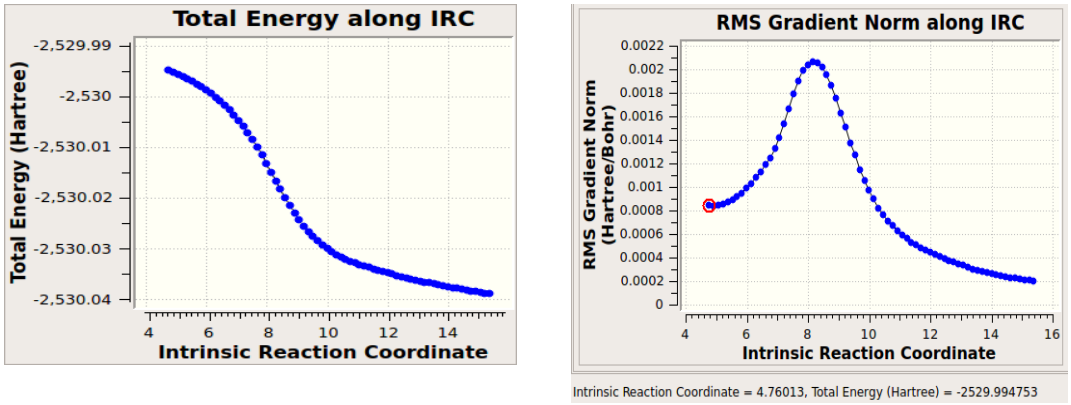


^{OSS}TS(B-C)$_{DHA-S1}$ | ^{CSS}TS(B-E)$_{DHA-S1}$ | ^{CSS}B$_{Ru}$

^{CSS}TS(B-D)$_{Ru}$ | ^{OSS}TS(B-C)$_{Ru}$

Fig. S1. Geometries of important optimised structures. Distances are in Å.

(a)



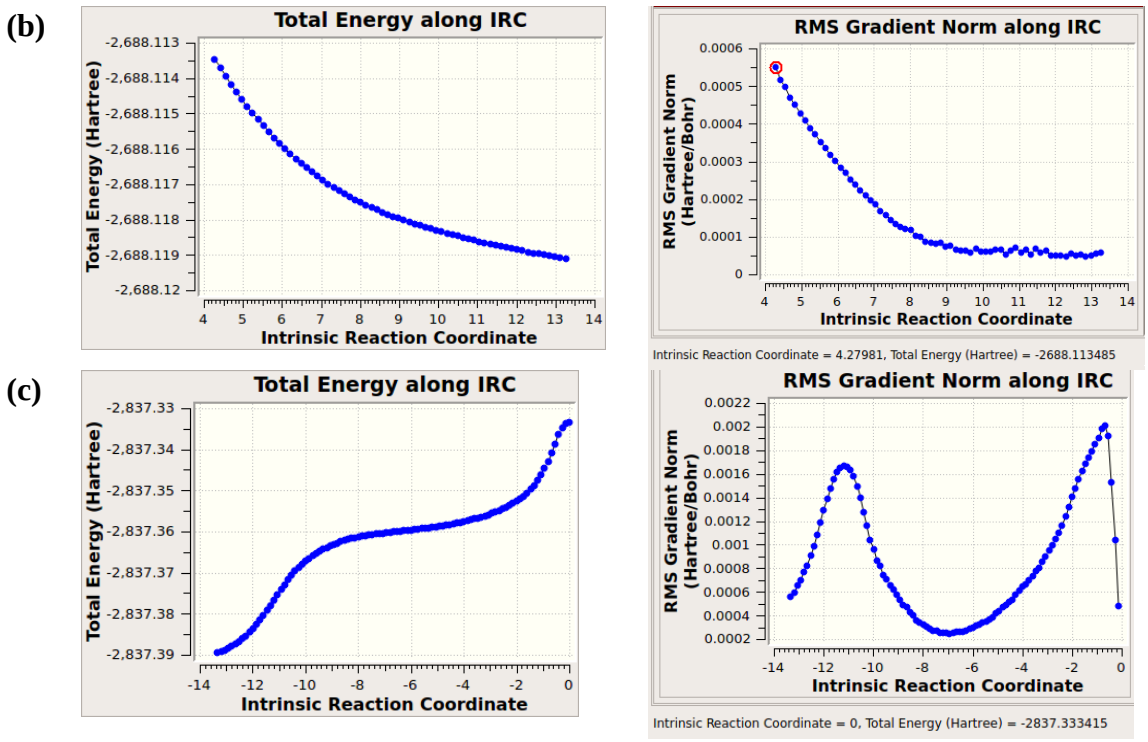
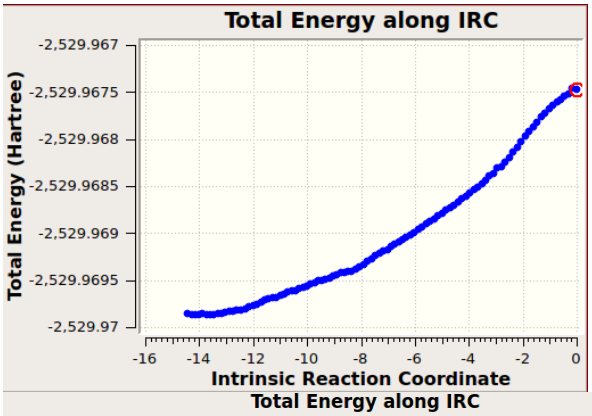


Fig. S2. IRC and gradient plot for (a) **TS(B-D)**, (b) **TS(B-E)$_{\text{DHA-S2}}$** and (c) **TS(B-E)$_{\text{DHA-S1}}$**.

For **TS(B-D)**, the IRC proceeds towards the C-H insertion product, monotonously decreasing in energy throughout the course of its IRC, as can be seen from its gradient plot. For **TS(B-E)$_{\text{DHA-S2}}$** the IRC proceeds towards the ion pair product unlike in the IRC for **TS(B-D)** with the C(carbene) and C(DHA) moving apart while the C(carbene)-H bond is forming. For **TS(B-E)$_{\text{DHA-S1}}$**, the IRC suggests the formation of a 'hidden intermediate', as it passes through a region where its gradient is nearly zero, thereby almost leading to a stationary point corresponding to an ion pair.[10] We stabilised this intermediate from this geometry by optimising it in solvent phase to generate the ion pair.

(a)



(b)

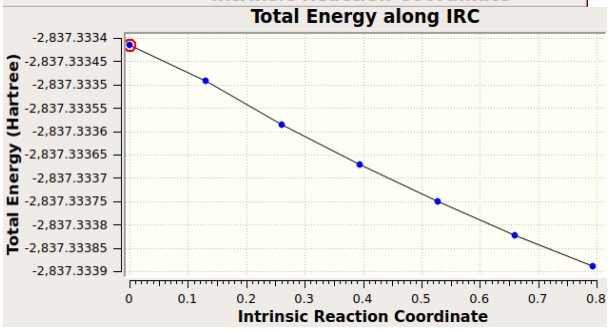
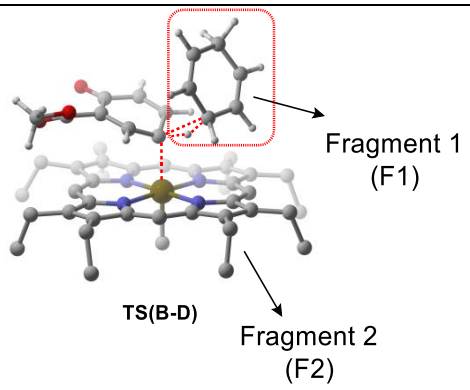


Fig. S3. Reverse IRC plot for C-H insertion (a) **TS(B-D)** and hydride transfer (b) **TS(B-E)**$_{DHA\text{-}S1}$.

(a)



(b)

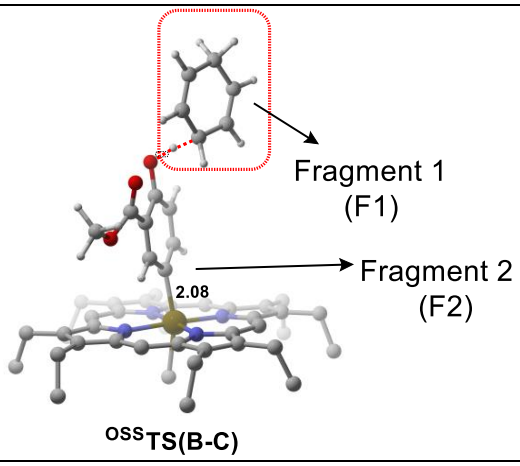


Fig. S4. Energy Decomposition Analysis of (a) **TS(B-D)** and (b) ^{OSS}**TS(B-C)**.

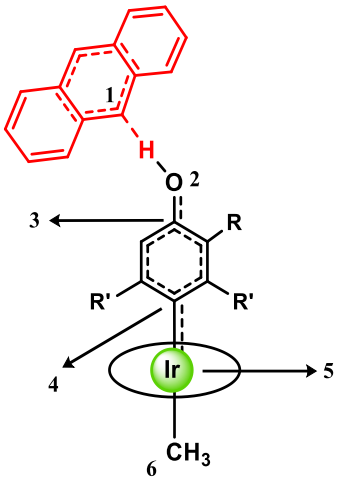
The following fragments from the distortion-interaction study were used for the EDA calculation. The interaction between the two fragments F1 and F2 was computed and decoupled using the ADF software at the B3LYP-D3BJ/TZP level of theory.[11]

The breakdown of the interaction energy is as follows:

Table S20. Energy Decomposition Analysis of **TS(B-D)** and **^{OSS}TS(B-C)**. Energies are in kcal/mol

	TS(B-D)	**^{OSS}TS(B-C)**
Total Pauli Repulsion	82.22	130.18
Total Orbital Interactions	-54.48	-90.81
Electrostatic Interaction	-31.90	-44.8
Dispersion Energy	- 15.06	-5.2
Total Interaction Energy	-19.22	-10.63

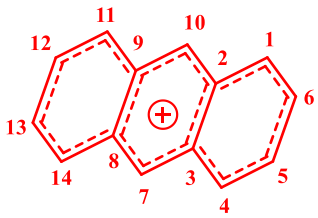
Table S21. Mulliken Spin Populations of select atoms of **^{OSS}TS(B-C)$_{DHA-S1}$** and **^{OSS}TS(B-C)$_{DHA-S2}$**[a]



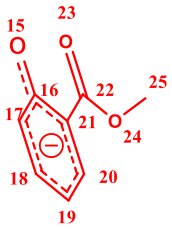
Atom Number	**DHA-S1 spins**	**DHA-S2 spins**
1	0.27	0.25
2	0.20	0.19
3	-0.08	-0.08
4	-0.07	-0.08
5	-0.17	-0.20
6	-0.28	-0.17

[a]S1: R=CO_2Me, R'=H, S2: R=H, R'=Me

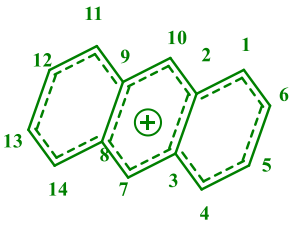
Table S22. Mulliken charges of ion pair fragments DHA-S1 and DHA-S2[a]



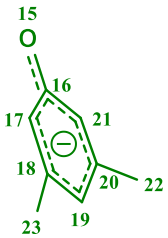
DHA-S1 cation



S1 anion



DHA-S2 cation



S2 anion

Atom Number	DHA-S1 charges	DHA-S2 charges
1	-0.0782757	-0.0112212
2	0.0462462	-0.043596
3	0.203392728	0.3644424
4	-0.004595514	0.3786788
5	0.012626614	-0.1491076
6	0.088016544	0.0643896
7	0.074871412	-0.1747476
8	0.15554030	0.3856752
9	0.03978359	0.3643848
10	0.239967112	-0.2593116
11	-0.05493488	-0.0434844
12	0.114459884	-0.0112104
13	-0.002417954	0.0643536
14	0.030498776	-0.1480644
15	-0.748735	-0.7488297
16	0.038207	0.54742132
17	-0.1420692	-0.38757334
18	0.4217759	0.31128326
19	-0.1583296	-0.38756078
20	0.0026702	0.54740876
21	0.7058922	-0.1129615
22	0.065689	-0.43488686
23	-0.748735	-0.11292696
24	-0.6283394	-
25	0.3475589	-

[a]Condensed Mulliken charges on heavy atoms.

Net Charges:

DHA-S1 cation: 0.868

S1 anion: -0.871

DHA-S2 cation: 0.781

S2 anion: -0.779

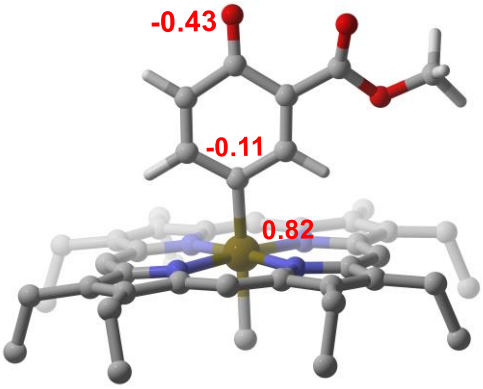
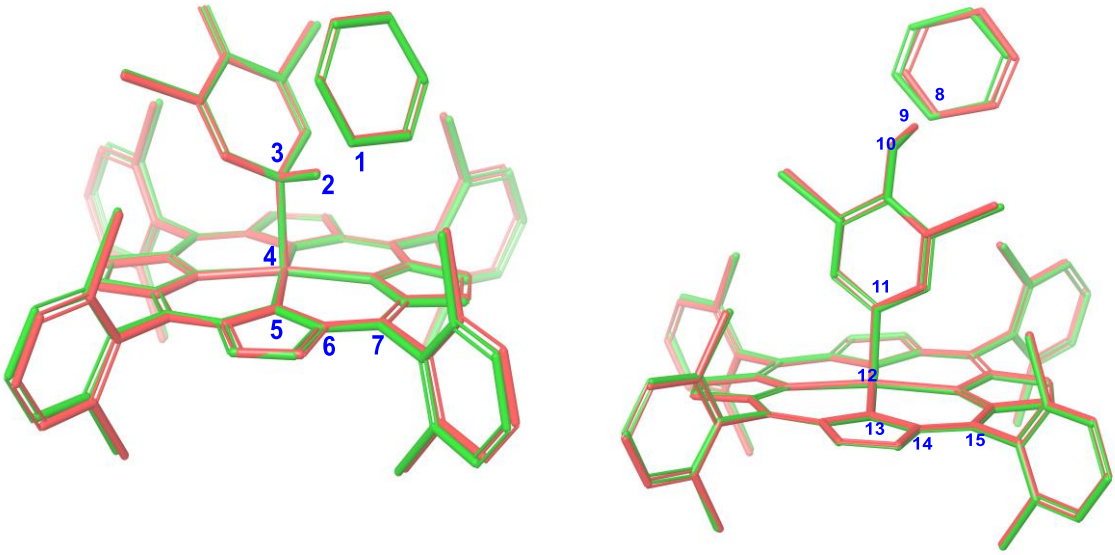


Fig. S5. Mulliken charge populations on the reactive carbene carbon, quinoid oxygen and Ir centres.



^{CSS}**TS(B-D)$_{Ru}$** ^{OSS}**TS(B-C)$_{Ru}$**

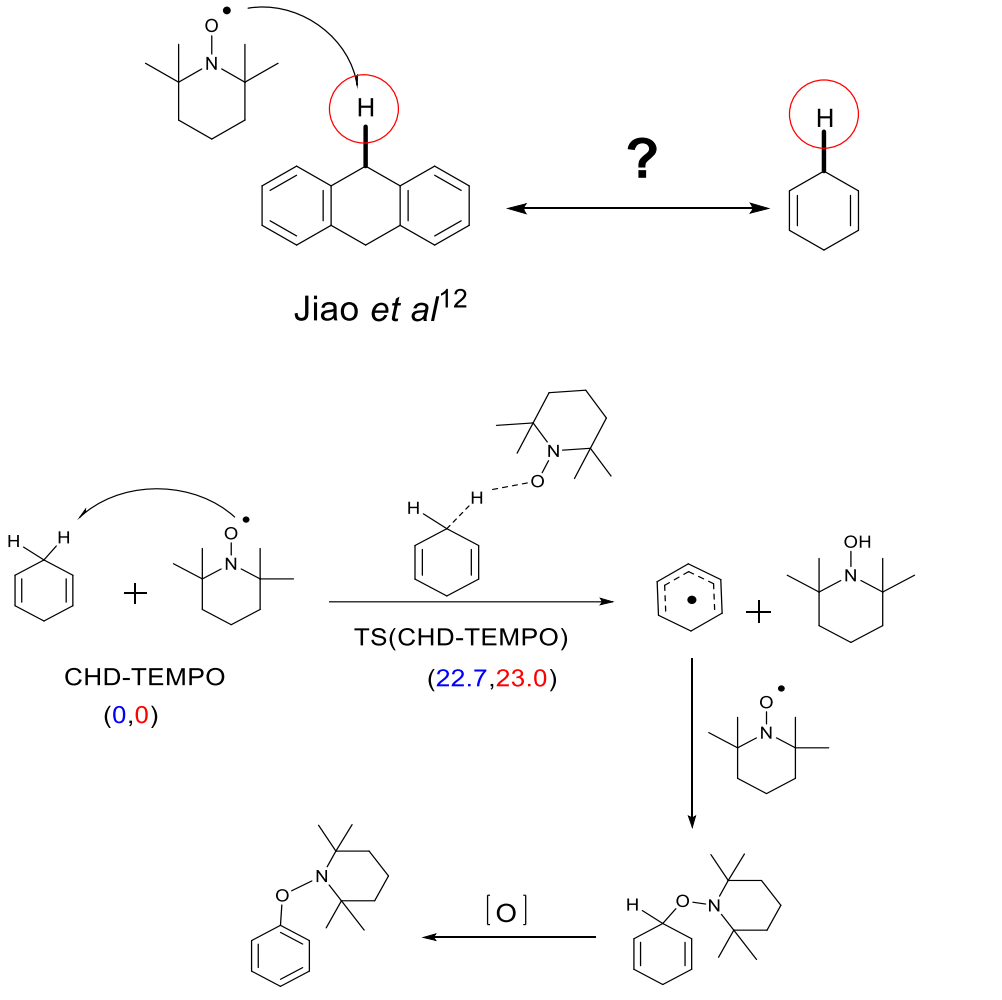
Fig. S6. Overlaid images of (a) ^{CSS}**TS(B-D)$_{Ru}$** and (b) ^{OSS}**TS(B-C)$_{Ru}$** optimised at the 6-31G(d,p) (green) and 6-31+G(d,p) (red) basis sets.

Table S23. Comparison of important geometric parameters for the 6-31G(d,p) and 6-31+G(d,p) basis sets optimised geometries (distances are in Å, angles are in degrees)

Geometric Parameter	6-31G(d,p)	6-31+G(d,p)
1-2	1.43	1.43
2-3	1.29	1.29
1-3	2.66	2.66
3-4	2.01	2.01
1-2-3	155.8	156.3

4-5-6-7	-1.4	-1.5
8-9	1.30	1.30
9-10	1.28	1.28
8-10	2.56	2.57
8-9-10	169.8	169.9
11-12	2.00	2.00
12-13-14-15	-5.3°	-5.7°

Previous works by Jiao *et al*[12] on dehydrogenative C-C couplings on 9,10 dihydroacridine using TEMPO as an aerobic oxidant and quite likely proceeding via a HAT to a TEMPO molecule prompted us to computationally study its analogous reaction with CHD.[12]



Scheme S1. Formation of the TEMPO adduct with CHD.

The computation showed that the competitive HAT to TEMPO pathway had a barrier lower than the catalytic cycle by 2.6 kcal/mol, and the participation of the large excess of TEMPO

could very well be responsible for the generation of the CHD radical which gives the TEMPO adduct. The other plausible reason for the lowering of the arylation yield in the presence of TEMPO which cannot be ruled out is the degradation of the catalyst by the radical additive, a phenomenon which has been observed in several studies involving transition metal catalysts.[13]

References

(1) *Gaussian 16, Revision C.01*, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

(2) (a) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 1988, **37**, 785-789. (b) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652. c) W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257-2261. (d) P. C. Hariharan and J. A. Pople, *Theor. Chim. Acta.*, 1973, **28**, 213-222.

(3) S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456-1465.

(4) P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 299-310.

(5) R. Caballol, O. Castell, F. Illas, I. de P. R. Moreira and J. Malrieu, *J. Phys. Chem. A.*, 1997, **101**, 7860-7866.

(6) (a) K. Fukui, *Acc. Chem. Res.*, 1981, **14**, 363-368. b) H. P. Hratchian and H. B. Schlegel, *Theory and Applications of Computational Chemistry: The First 40 Years*, Eds. C. E. Dykstra, G. Frenking, K. S. Kim, G. Scuseria, Elsevier, Amsterdam, 2005, 195-249. (b) C. Gonzalez and H. B. Schlegel, *J. Chem. Phys.*, 1989, **90**, 2154-2161. (c) C. Gonzalez, H. B. Schlegel, *J. Phys. Chem.*, 1990, **94**, 5523-5527.

(7) F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005,**7**, 3297-3305.

(8) A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B.*, 2009, **113**, 6378-6396.

(9) F. M. Bickelhaupt and K. N. Houk, *Angew. Chem. Int. Ed*., 2017, **56**, 10070-10086.

(10) D. Roca-Lopez, V. Polo, T. Tejero and P. Merino, *J. Org. Chem.*, 2015, **80**, 4076-4083.

(11) G. te Velde, F.M. Bickelhaupt, E. J. Baerends, C. Fonseca Guerra, S. J. A. van Gisbergen, J. G. Snijders and T. Ziegler, *Chemistry with ADF, J. Comput. Chem.* 2001, **22**, 931.

(12) (a) B. Zhang, Y. Cui and N. Jiao, *Chem. Commun.*, 2012, **48**, 4498-4500.

(13) (a) A. C. Albeniz, P. Espinet, R. Lopez-Fernandez and A. Sen, *J. Am. Chem. Soc.*, 2002, **124**, 11278-11279. (b) A. Hernán-Gómez, M. Rodríguez, T. Parella and M. Costas, *Angew. Chem., Int. Ed.*, 2019, **58**, 13904-13911.

Coordinates of optimised stationary points

A

Number of imaginary frequencies : 0 Electronic energy : HF=-2406.0492203
Zero-point correction= 0.902006 (Hartree/Particle)
Thermal correction to Energy= 0.959188
Thermal correction to Enthalpy= 0.960132
Thermal correction to Gibbs Free Energy= 0.808035
Sum of electronic and zero-point Energies= -2405.147215
Sum of electronic and thermal Energies= -2405.090032
Sum of electronic and thermal Enthalpies= -2405.089088
Sum of electronic and thermal Free Energies= -2405.241185

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Cartesian Coordinates

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6	-3.731479	0.827617	0.272833
6	-3.424358	-0.524258	0.195375
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6	-2.283558	-2.409471	-0.027128
6	-3.669468	-2.779775	0.202142
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7	0.596049	-1.702215	-0.545385
6	1.953874	-1.817106	-0.738408
6	2.337369	-3.218859	-0.715078
6	1.185770	-3.939970	-0.544749
77	-0.452434	0.034571	-0.344255
7	1.271282	1.107817	-0.593400

6	2.518842	0.594881	-0.854039
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6	1.400078	2.477513	-0.540460
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6	-5.853479	-1.434446	0.525335
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6	2.436860	-0.388680	2.363601
6	1.325751	0.394432	2.478857
6	3.751904	0.265210	2.131852
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8	3.310068	-2.622805	2.344606
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1	1.913058	4.943372	-2.406826
1	3.462322	4.370108	-3.028277
1	-0.942525	5.766516	0.706818
1	-2.681940	5.968751	0.707941
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1	-5.114810	3.194285	1.242355
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1	-6.043586	-0.636833	1.254345
1	-6.279130	-2.346751	0.957049
1	3.360778	5.954717	-2.235800
1	-5.140935	-4.223873	0.743482
1	-3.499532	-4.834792	0.766029
1	-4.746282	-5.786244	-1.176280
1	-3.436409	-4.745257	-1.766338
1	-5.098910	-4.152868	-1.772737
1	-6.449825	-1.912853	-1.516305
1	-6.189595	-0.189879	-1.237494

1	-7.658212	-0.971461	-0.621008
1	-5.475831	2.830649	-1.241955
1	-4.926950	4.479428	-1.548066
1	-6.421545	4.202533	-0.633025
1	-1.647717	7.172576	-1.232804
1	-2.714456	5.876245	-1.806808
1	-0.964931	5.646595	-1.826850
1	6.210235	0.988371	-3.023973
1	4.764801	1.919105	-3.463972
1	4.621272	0.204391	-3.070992
1	3.810559	-4.719917	-0.412453
1	4.383730	-3.086251	-0.179656
1	5.318454	-4.060533	-2.300139
1	4.249379	-2.706804	-2.703523
1	3.677830	-4.364073	-2.902289
1	0.309691	-5.693737	0.307408
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1	0.418752	-7.112327	-1.746697
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1	5.011710	2.531146	1.255735
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TS(A-B)

Number of imaginary frequencies : 1 Electronic energy : HF=-2406.0163651
Zero-point correction= 0.899021 (Hartree/Particle)
Thermal correction to Energy= 0.955875
Thermal correction to Enthalpy= 0.956819
Thermal correction to Gibbs Free Energy= 0.807451
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.....

Cartesian Coordinates

.....

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6	-3.829078	0.137426	0.401945
6	-3.257851	-1.125689	0.292934
7	-1.932123	-1.370370	0.052113
6	-1.776691	-2.732223	-0.052218
6	-3.060576	-3.382463	0.162073
6	-3.978694	-2.387174	0.376903
6	-0.581260	-3.385917	-0.316867
6	0.661717	-2.803361	-0.540464
7	0.908395	-1.453858	-0.548914
6	2.245265	-1.286047	-0.811942

6	2.886029	-2.584070	-0.931645
6	1.901097	-3.525119	-0.773605
77	-0.455122	0.041628	-0.171752
7	1.015212	1.452445	-0.473548
6	2.330118	1.198210	-0.777167
6	3.055943	2.453732	-0.874542
6	2.149621	3.455590	-0.636214
6	0.866424	2.811899	-0.397508
6	2.023328	-5.017093	-0.828717
6	1.609089	-5.598488	-2.192231
6	4.355277	-2.785867	-1.140596
6	4.796489	-2.572933	-2.599293
6	2.890545	-0.061996	-0.929280
6	-5.459014	-2.512268	0.578455
6	-6.257502	-2.282495	-0.717723
6	-3.292820	-4.861008	0.074805
6	-3.390831	-5.363881	-1.377011
6	-0.336860	3.466875	-0.156370
6	2.366929	4.938180	-0.680920
6	1.940537	5.562532	-2.022045
6	4.505425	2.566334	-1.240593
6	4.748172	2.441086	-2.755588
6	-2.971522	5.090149	0.119358
6	-2.972697	5.620443	-1.325874
6	-5.296416	2.875905	0.476143
6	-6.052065	2.678465	-0.850467
6	0.124130	-0.165436	1.969392
6	-0.118515	-1.497495	2.496259
6	0.925219	-2.348812	2.583499
6	2.320742	-1.917525	2.356545
6	2.520992	-0.448075	2.242266
6	1.449084	0.383555	2.192559
6	3.892203	0.118813	2.112533
8	4.835316	-0.398749	1.552692
8	3.239075	-2.732052	2.322984
6	-0.808499	0.038468	-2.246812
8	3.957845	1.347841	2.684791
6	5.213081	2.024510	2.539701
7	-0.958450	0.939017	2.922351
7	-1.748834	1.716648	2.766909
1	3.954757	-0.099903	-1.120344
1	-0.617949	-4.468626	-0.346841
1	-4.897873	0.173183	0.577130
1	-0.305515	4.550123	-0.143404
1	1.815596	5.420706	0.135692
1	3.425495	5.156240	-0.501924
1	0.882029	5.371353	-2.223243
1	2.514580	5.130858	-2.847428
1	-2.158137	5.566614	0.680470
1	-3.899218	5.392970	0.616547
1	-5.483023	3.887711	0.851517
1	-5.704222	2.192935	1.231623
1	4.897746	3.527590	-0.889856
1	5.078634	1.789881	-0.719676
1	-5.792834	-1.798421	1.341667
1	-5.690595	-3.507502	0.973132
1	2.099797	6.645705	-2.021893
1	-4.214123	-5.117237	0.609005
1	-2.485036	-5.395988	0.589505
1	-3.549053	-6.446635	-1.409195

1	-2.476839	-5.133798	-1.932689
1	-4.222593	-4.879502	-1.897440
1	-5.976884	-3.017354	-1.478240
1	-6.055611	-1.289403	-1.130556
1	-7.334158	-2.367531	-0.538372
1	-5.894887	1.669199	-1.242909
1	-5.694669	3.384266	-1.606449
1	-7.127897	2.832244	-0.718422
1	-3.064099	6.711193	-1.345898
1	-3.807409	5.195585	-1.891648
1	-2.049659	5.343271	-1.844015
1	5.814845	2.513259	-2.990668
1	4.221666	3.231886	-3.298550
1	4.378845	1.481603	-3.129729
1	4.623853	-3.799428	-0.826307
1	4.899486	-2.110287	-0.471706
1	5.876098	-2.718697	-2.707255
1	4.554439	-1.562777	-2.944795
1	4.287987	-3.276439	-3.266527
1	1.412995	-5.468798	-0.037125
1	3.057272	-5.301736	-0.609805
1	1.700570	-6.689496	-2.201167
1	2.239880	-5.194398	-2.989954
1	0.572519	-5.339740	-2.430955
1	1.588013	1.456132	2.133963
1	-1.142275	-1.832784	2.622541
1	0.790063	-3.407365	2.778669
1	6.031857	1.399099	2.902069
1	5.127643	2.932849	3.135919
1	5.395482	2.275177	1.492088
1	0.132601	0.217762	-2.773121
1	-1.521811	0.828900	-2.496805
1	-1.216015	-0.931066	-2.545359

CSS B

Number of imaginary frequencies : 0 Electronic energy : HF=-2529.98407
Zero-point correction= 1.015718 (Hartree/Particle)
Thermal correction to Energy= 1.077568
Thermal correction to Enthalpy= 1.078512
Thermal correction to Gibbs Free Energy= 0.915862
Sum of electronic and zero-point Energies= -2528.968352
Sum of electronic and thermal Energies= -2528.906502
Sum of electronic and thermal Enthalpies= -2528.905558
Sum of electronic and thermal Free Energies= -2529.068208

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Cartesian Coordinates

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6	-4.077968	2.458310	0.667180
6	-2.683914	2.309477	0.285046
7	-2.406444	0.988426	0.075072
6	-3.557504	0.278498	0.303359
6	-4.619552	1.197209	0.680323
6	-1.754183	3.341103	0.179425
6	-0.419208	3.229820	-0.176944
7	0.231854	2.051760	-0.491242
6	1.535899	2.374494	-0.789677
6	1.723608	3.806460	-0.654430
6	0.515036	4.334749	-0.274412

6	2.517788	1.469114	-1.165174
6	2.359203	0.103022	-1.339561
7	1.192039	-0.587907	-1.128223
6	1.439812	-1.910111	-1.429640
6	2.827751	-2.060518	-1.832910
6	3.395492	-0.814756	-1.781082
77	-0.571763	0.192031	-0.460280
7	-1.434238	-1.701076	-0.558316
6	-0.815065	-2.852204	-0.952198
6	-1.751386	-3.960175	-0.863602
6	-2.938616	-3.438764	-0.414151
6	-2.729239	-2.011517	-0.231326
6	4.786055	-0.406601	-2.157088
6	4.868249	0.193187	-3.572280
6	3.453557	-3.351674	-2.266099
6	3.110107	-3.726156	-3.719116
6	0.517344	-2.942852	-1.349297
6	0.158407	5.774654	-0.058344
6	-0.534059	6.405704	-1.279919
6	3.004567	4.524786	-0.949239
6	3.241787	4.728071	-2.456461
6	-3.695255	-1.099821	0.176781
6	-4.245354	-4.143448	-0.207148
6	-5.206242	-3.975528	-1.398296
6	-1.442109	-5.371553	-1.262562
6	-1.483566	-5.582951	-2.786862
6	-6.039043	0.797499	0.949352
6	-6.847625	0.572556	-0.341333
6	-4.758465	3.770208	0.917918
6	-5.133673	4.503881	-0.382424
6	-0.364602	-0.275559	1.494871
6	0.285195	-1.491167	1.857211
6	0.764541	-1.709017	3.123822
6	0.454957	-0.751175	4.209434
6	-0.452649	0.342595	3.832036
6	-0.893525	0.529613	2.558118
8	0.923453	-0.825826	5.348464
6	1.598559	-2.903696	3.398364
8	1.708295	-3.483027	4.455574
6	-1.399535	0.295630	-2.453112
8	2.247594	-3.317712	2.264840
6	3.033959	-4.502434	2.425690
6	3.496777	2.312280	2.091271
6	2.890359	0.942659	2.197901
6	3.807438	-0.145563	1.715784
6	5.063762	0.074261	1.321954
6	5.704856	1.437379	1.303012
6	4.752940	2.535729	1.696850
1	-4.673069	-1.506989	0.405461
1	-2.112419	4.339467	0.401168
1	3.508210	1.870504	-1.335646
1	0.876094	-3.930904	-1.611572
1	-0.841669	-0.394040	-3.090557
1	-2.457565	0.034475	-2.445477
1	-1.269240	1.329301	-2.786522
1	-0.453271	-5.656551	-0.882404
1	-2.156325	-6.049440	-0.783495
1	-0.766969	-4.928655	-3.292901
1	-2.476966	-5.349466	-3.181768
1	3.135099	-4.159950	-1.595842

1	4.540970	-3.280661	-2.158328
1	5.449883	-1.275247	-2.092082
1	5.163852	0.317121	-1.427323
1	-4.060860	-5.209721	-0.038918
1	-4.727405	-3.772591	0.705425
1	3.839252	3.966032	-0.512421
1	2.997134	5.499484	-0.449766
1	-1.245134	-6.619021	-3.047481
1	1.065349	6.341575	0.176173
1	-0.492723	5.869403	0.819220
1	-0.789828	7.452919	-1.090044
1	-1.453835	5.868102	-1.530192
1	0.119346	6.365471	-2.156660
1	2.437726	5.323288	-2.900137
1	3.269023	3.768723	-2.982249
1	4.189993	5.244062	-2.637582
1	4.224479	1.073621	-3.662153
1	4.538647	-0.532830	-4.321829
1	5.893240	0.492944	-3.812656
1	3.573436	-4.676894	-4.001298
1	3.463450	-2.953984	-4.409169
1	2.028218	-3.818484	-3.855439
1	-6.153868	-4.492019	-1.215521
1	-4.763388	-4.383686	-2.311873
1	-5.421618	-2.918323	-1.581518
1	-6.527012	1.571233	1.551441
1	-6.059965	-0.115721	1.556319
1	-7.875610	0.272525	-0.114686
1	-6.390797	-0.207317	-0.958327
1	-6.881164	1.487797	-0.940119
1	-4.111349	4.415373	1.525071
1	-5.662251	3.603439	1.513361
1	-5.620212	5.460821	-0.168542
1	-5.817843	3.897494	-0.983673
1	-4.245870	4.699348	-0.991762
1	0.519350	-2.216853	1.092325
1	-1.532083	1.372456	2.325543
1	-0.704808	1.035557	4.629190
1	3.491188	-4.686362	1.452792
1	2.407420	-5.348216	2.722073
1	3.802117	-4.355034	3.188967
1	2.600162	0.745930	3.241473
1	2.858744	3.152281	2.358013
1	3.402997	-1.153879	1.700940
1	5.134644	3.554465	1.657589
1	5.678625	-0.760717	0.991429
1	6.119250	1.645557	0.301913
1	1.946208	0.907006	1.639399
1	6.585532	1.449240	1.966039

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^{oss}TS(B-C)

Number of imaginary frequencies : 1 Electronic energy : HF=-2529.9477725
Zero-point correction= 1.008364 (Hartree/Particle)
Thermal correction to Energy= 1.069855
Thermal correction to Enthalpy= 1.070799
Thermal correction to Gibbs Free Energy= 0.906165
Sum of electronic and zero-point Energies= -2528.939409
Sum of electronic and thermal Energies= -2528.877917

Sum of electronic and thermal Enthalpies= -2528.876973
Sum of electronic and thermal Free Energies= -2529.041607

Cartesian Coordinates

6	0.794121	-0.035490	4.197367
6	0.128863	-0.649280	3.061834
7	-0.208628	0.319073	2.146045
6	0.219298	1.527868	2.657214
6	0.847122	1.311926	3.948151
6	-0.141756	-2.003734	2.925214
6	-0.823425	-2.612923	1.880523
7	-1.309829	-1.963058	0.771627
6	-1.937517	-2.910686	-0.011667
6	-1.844479	-4.208720	0.631967
6	-1.151345	-4.025473	1.800902
6	-2.547685	-2.667246	-1.233272
6	-2.635090	-1.446685	-1.897830
7	-2.121426	-0.269408	-1.432951
6	-2.377005	0.693706	-2.372928
6	-3.087166	0.097654	-3.494014
6	-3.251760	-1.231210	-3.196818
77	-1.122629	0.017307	0.358023
7	-1.006822	2.046272	-0.035604
6	-1.417114	2.665574	-1.187306
6	-1.124130	4.088235	-1.101065
6	-0.537850	4.298061	0.120504
6	-0.470245	3.003234	0.778096
6	-3.971662	-2.283030	-3.985691
6	-5.393807	-2.551807	-3.461142
6	-3.586706	0.853433	-4.688267
6	-4.898300	1.609372	-4.408099
6	-2.033306	2.036444	-2.262425
6	-0.833064	-5.034867	2.862297
6	-1.820333	-4.988428	4.042778
6	-2.465858	-5.467724	0.106445
6	-3.977890	-5.546416	0.385101
6	0.092680	2.756865	2.027285
6	-0.081513	5.588833	0.730156
6	-1.084951	6.156683	1.750008
6	-1.477753	5.098765	-2.150051
6	-2.956376	5.523611	-2.092395
6	1.381276	2.400834	4.829107
6	0.273431	3.142048	5.599298
6	1.251356	-0.774989	5.418313
6	0.101726	-1.073747	6.397834
6	0.607612	-0.127734	-0.780694
6	1.650596	0.794895	-0.604980
6	2.876498	0.668412	-1.258945
6	3.069627	-0.390118	-2.206877
6	1.987686	-1.288626	-2.409139
6	0.781717	-1.139916	-1.746328
8	4.161298	-0.533885	-2.913760
6	3.965375	1.627297	-0.954884
8	5.160389	1.439986	-1.089217
6	-3.135401	0.547932	1.049768
8	3.476134	2.799049	-0.463077
6	4.469366	3.753974	-0.080926
6	6.000515	-1.523998	-1.421649
6	5.956816	-2.969396	-1.664979

6	6.943306	-3.619595	-2.309401
6	8.189360	-2.929089	-2.785359
6	8.267031	-1.485306	-2.377850
6	7.265789	-0.855846	-1.732999
1	-2.291504	2.668442	-3.104181
1	-2.989820	-3.522197	-1.731410
1	0.193777	-2.649421	3.728116
1	0.495607	3.613718	2.554239
1	-3.004293	1.016588	2.027557
1	-3.601825	1.234645	0.345147
1	-3.694818	-0.387425	1.116730
1	0.890693	5.443809	1.218150
1	0.085327	6.326241	-0.062177
1	-1.260166	5.446772	2.564272
1	-2.049799	6.352673	1.272408
1	1.949633	3.120524	4.226967
1	2.094291	1.974535	5.542693
1	2.021001	-0.189459	5.932334
1	1.732673	-1.715775	5.124422
1	-0.842881	5.983361	-2.031824
1	-1.252685	4.696297	-3.145149
1	0.186277	-4.874191	3.234182
1	-0.840399	-6.038770	2.424578
1	-0.720009	7.093092	2.184236
1	-1.969805	-6.334009	0.556834
1	-2.290754	-5.546760	-0.973619
1	-4.405496	-6.470347	-0.017283
1	-4.503744	-4.699893	-0.066927
1	-4.173401	-5.517834	1.461368
1	-2.839085	-5.196648	3.701947
1	-1.825727	-3.998628	4.509383
1	-1.556202	-5.726631	4.806790
1	-0.678513	-1.670043	5.914990
1	-0.361473	-0.144639	6.743680
1	0.462304	-1.624158	7.272729
1	0.692255	3.936373	6.225450
1	-0.276302	2.450206	6.244707
1	-0.447938	3.592573	4.910763
1	-3.188047	6.253451	-2.874803
1	-3.190826	5.973483	-1.122745
1	-3.616709	4.660604	-2.222268
1	-3.741059	0.158388	-5.520534
1	-2.822069	1.563759	-5.025541
1	-5.233086	2.159976	-5.293106
1	-4.770798	2.322821	-3.588143
1	-5.690430	0.912733	-4.117043
1	-3.397038	-3.217598	-3.971906
1	-4.025379	-1.977423	-5.036015
1	-5.891545	-3.329136	-4.049848
1	-6.000623	-1.642508	-3.509801
1	-5.370666	-2.875373	-2.415919
1	1.534789	1.615644	0.088106
1	-0.019550	-1.843069	-1.944738
1	2.145222	-2.092167	-3.122426
1	3.918760	4.616404	0.296460
1	5.084734	4.038632	-0.938407
1	5.123637	3.347115	0.695325
1	5.152789	-0.995026	-2.209132
1	5.072674	-3.512011	-1.338628
1	7.344876	0.192669	-1.466118

1	6.862408	-4.687178	-2.500341
1	9.181106	-0.949625	-2.623143
1	9.080884	-3.472063	-2.427543
1	5.510471	-1.182315	-0.504739
1	8.259012	-3.008621	-3.885398

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^{oss}C

Number of imaginary frequencies : 0 Electronic energy : HF=-2530.008865
Zero-point correction= 1.014508 (Hartree/Particle)
Thermal correction to Energy= 1.076310
Thermal correction to Enthalpy= 1.077254
Thermal correction to Gibbs Free Energy= 0.914550
Sum of electronic and zero-point Energies= -2528.994357
Sum of electronic and thermal Energies= -2528.932555
Sum of electronic and thermal Enthalpies= -2528.931611
Sum of electronic and thermal Free Energies= -2529.094315

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Cartesian Coordinates

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6	-4.193125	2.277219	0.727851
6	-2.800377	2.196686	0.318265
7	-2.469595	0.894391	0.066600
6	-3.583808	0.131900	0.307495
6	-4.678912	0.994606	0.723195
6	-1.914650	3.268237	0.237882
6	-0.578133	3.218932	-0.127616
7	0.106264	2.077608	-0.502470
6	1.395392	2.459297	-0.797449
6	1.540443	3.887901	-0.590643
6	0.319116	4.358074	-0.177715
6	2.401206	1.607644	-1.227525
6	2.297558	0.241193	-1.434128
7	1.165954	-0.504795	-1.213565
6	1.479681	-1.814739	-1.514569
6	2.867109	-1.895105	-1.938382
6	3.372279	-0.622139	-1.891316
77	-0.626361	0.189440	-0.538847
7	-1.387559	-1.737843	-0.610598
6	-0.715064	-2.863492	-0.992314
6	-1.591106	-4.017965	-0.876575
6	-2.796703	-3.551896	-0.417241
6	-2.655485	-2.113088	-0.255214
6	4.738387	-0.143665	-2.275327
6	4.779037	0.476509	-3.683301
6	3.550485	-3.151851	-2.385870
6	3.200122	-3.540126	-3.833592
6	0.612971	-2.892518	-1.410731
6	-0.081552	5.773295	0.112148
6	-0.800691	6.442906	-1.072980
6	2.800381	4.657825	-0.847071
6	3.031887	4.944927	-2.341561
6	-3.657303	-1.249730	0.174024
6	-4.063023	-4.318785	-0.181993
6	-5.053180	-4.206379	-1.355513
6	-1.214916	-5.417158	-1.260806
6	-1.269150	-5.653756	-2.780990
6	-6.073572	0.526333	1.010800
6	-6.893278	0.279344	-0.268702

6	-4.922819	3.552764	1.023487
6	-5.342410	4.307532	-0.250873
6	-0.272925	-0.252556	1.481817
6	0.485660	-1.362704	1.830739
6	0.899672	-1.588519	3.157233
6	0.485084	-0.702205	4.182983
6	-0.320342	0.392720	3.839054
6	-0.695536	0.603644	2.517838
8	0.835818	-0.863558	5.470813
6	1.795296	-2.692232	3.502700
8	2.164930	-2.960474	4.649124
6	-1.503687	0.268668	-2.545128
8	2.222826	-3.406202	2.442025
6	3.130202	-4.475464	2.741361
6	3.060952	1.019475	1.909817
6	3.819910	-0.119219	1.538381
6	5.143658	-0.019890	1.216982
6	5.878619	1.290595	1.249831
6	4.999025	2.456543	1.603473
6	3.680091	2.295160	1.921755
1	-4.608787	-1.705188	0.423181
1	-2.308721	4.243262	0.499889
1	3.373419	2.052795	-1.396943
1	1.017261	-3.863954	-1.670083
1	-0.923234	-0.406711	-3.175457
1	-2.549912	-0.030057	-2.499413
1	-1.401266	1.310554	-2.857744
1	-0.206283	-5.644796	-0.893718
1	-1.884927	-6.124852	-0.760886
1	-0.596682	-4.969502	-3.307537
1	-2.279776	-5.478676	-3.162308
1	3.285584	-3.977794	-1.713658
1	4.635000	-3.026346	-2.297779
1	5.444875	-0.979235	-2.225795
1	5.086552	0.589767	-1.539988
1	-3.823704	-5.373956	-0.011370
1	-4.546736	-3.965992	0.737068
1	3.654063	4.102954	-0.440472
1	2.764479	5.605919	-0.299538
1	-0.980200	-6.679538	-3.031993
1	0.808032	6.357228	0.371218
1	-0.730948	5.803079	0.995687
1	-1.089622	7.470429	-0.829591
1	-1.703673	5.888604	-1.346735
1	-0.151018	6.468262	-1.953141
1	2.210011	5.538260	-2.754094
1	3.085819	4.014897	-2.915586
1	3.964634	5.496892	-2.495959
1	4.092059	1.325240	-3.755822
1	4.477373	-0.255845	-4.438497
1	5.785897	0.828823	-3.929845
1	3.704929	-4.465937	-4.128062
1	3.501163	-2.749245	-4.527317
1	2.121756	-3.685753	-3.949420
1	-5.971487	-4.766859	-1.152586
1	-4.607497	-4.598478	-2.274813
1	-5.322605	-3.162027	-1.540782
1	-6.586875	1.268977	1.630954
1	-6.042108	-0.394585	1.605926
1	-7.902619	-0.070904	-0.029672

1	-6.411001	-0.470897	-0.902850
1	-6.978819	1.199290	-0.855139
1	-4.294869	4.206592	1.641752
1	-5.812349	3.333413	1.623573
1	-5.864006	5.238242	-0.005236
1	-6.008880	3.691036	-0.861797
1	-4.470052	4.554742	-0.863682
1	0.815134	-2.065086	1.077784
1	-1.304264	1.470367	2.286903
1	-0.630139	1.069114	4.629041
1	3.372203	-4.928264	1.780063
1	2.660806	-5.206408	3.404116
1	4.031832	-4.089981	3.223176
1	1.399092	-1.671870	5.511482
1	3.079271	3.164449	2.176374
1	3.327404	-1.085466	1.494752
1	5.453084	3.443864	1.622573
1	5.705245	-0.904152	0.927646
1	6.380711	1.471008	0.280178
1	2.010142	0.920974	2.143278
1	6.726141	1.230260	1.960465

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^{CSS}TS(C-P)

Number of imaginary frequencies : 1 Electronic energy : HF=-2529.9990475
Zero-point correction= 1.016501 (Hartree/Particle)
Thermal correction to Energy= 1.076758
Thermal correction to Enthalpy= 1.077702
Thermal correction to Gibbs Free Energy= 0.920175
Sum of electronic and zero-point Energies= -2528.982546
Sum of electronic and thermal Energies= -2528.922290
Sum of electronic and thermal Enthalpies= -2528.921345
Sum of electronic and thermal Free Energies= -2529.078873

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Cartesian Coordinates

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6	0.111225	-1.603250	3.753758
6	0.275198	-1.950235	2.373304
6	1.487705	-2.630721	1.974003
6	2.509574	-2.796557	2.840085
6	2.455012	-2.298694	4.248175
6	1.141480	-1.696361	4.627181
6	0.268127	0.233655	1.411185
6	1.662229	0.230362	1.618166
6	2.280819	0.816424	2.721426
6	1.477032	1.472721	3.697958
6	0.083161	1.553491	3.495905
6	-0.490742	0.914060	2.417309
77	-0.545027	0.062557	-0.615373
6	-1.299601	0.004188	-2.602533
6	3.724276	0.725644	2.940463
8	4.398938	0.144685	1.938810
6	5.819875	0.043017	2.113553
8	1.997899	2.023133	4.796937
7	-1.382972	1.914526	-0.333852
6	-0.763027	3.119851	-0.532799
6	-1.681648	4.201216	-0.202886
6	-2.853401	3.615770	0.197345
6	-2.651147	2.175620	0.116515

6	-1.374190	5.659773	-0.360318
6	-1.485825	6.137364	-1.819586
6	0.546135	3.285918	-0.967505
6	1.445039	2.285708	-1.320006
7	1.184886	0.941664	-1.284037
6	2.320134	0.293459	-1.700597
6	3.352591	1.270932	-2.013244
6	2.809801	2.506593	-1.778518
6	-3.586459	1.212837	0.477161
6	-3.425394	-0.168198	0.427927
7	-2.287663	-0.816222	0.020420
6	-2.553556	-2.163999	0.049450
6	-3.909510	-2.382957	0.531137
6	-4.449690	-1.145645	0.766669
6	-4.142023	4.276060	0.585202
6	-5.173413	4.285498	-0.557622
6	2.467945	-1.084855	-1.788119
6	1.512889	-2.048770	-1.480034
7	0.262378	-1.790774	-0.979062
6	-0.377328	-2.995862	-0.831090
6	0.513197	-4.072234	-1.235944
6	1.687952	-3.484304	-1.636172
6	4.712638	0.934297	-2.545883
6	4.702430	0.610404	-4.050745
6	3.428662	3.853792	-1.999797
6	2.989339	4.499700	-3.326402
6	-1.669287	-3.163104	-0.341809
6	0.142082	-5.524523	-1.262254
6	-0.714185	-5.897262	-2.486044
6	2.909229	-4.139311	-2.208675
6	2.957931	-4.068818	-3.745696
6	-4.568019	-3.724858	0.648017
6	-5.079606	-4.257715	-0.702807
6	-5.843309	-0.805769	1.202911
6	-6.758757	-0.420146	0.026614
8	4.293939	1.122883	3.964382
1	-2.026720	-4.183322	-0.260901
1	-4.545374	1.576381	0.828367
1	0.902661	4.306438	-1.047941
1	3.425916	-1.448422	-2.142020
1	3.811824	-3.669404	-1.797339
1	2.943561	-5.188425	-1.894225
1	2.936388	-3.029892	-4.087875
1	2.091584	-4.575658	-4.181396
1	5.125861	0.079472	-1.994605
1	5.394727	1.771866	-2.362020
1	4.520480	3.761484	-1.987787
1	3.171748	4.522840	-1.168956
1	1.051890	-6.135090	-1.258679
1	-0.402701	-5.786794	-0.346394
1	-0.364045	5.870011	0.013135
1	-2.055970	6.246769	0.264890
1	3.865378	-4.541824	-4.135669
1	-3.944334	5.306049	0.901849
1	-4.573692	3.768728	1.457433
1	-6.108487	4.761388	-0.243836
1	-5.399488	3.266776	-0.886847
1	-4.783497	4.830568	-1.422691
1	-2.500839	5.982901	-2.198326
1	-0.805452	5.575306	-2.466417

1	-1.243968	7.201802	-1.907660
1	1.901947	4.615752	-3.361515
1	3.279624	3.872007	-4.174515
1	3.445214	5.486842	-3.456683
1	5.705331	0.354920	-4.409035
1	4.340300	1.468357	-4.625280
1	4.036265	-0.231024	-4.263798
1	-0.981770	-6.959046	-2.473707
1	-0.170740	-5.690073	-3.412893
1	-1.636760	-5.309668	-2.508864
1	-5.406078	-3.660896	1.350942
1	-3.865340	-4.449169	1.079347
1	-5.542361	-5.243830	-0.590082
1	-4.261014	-4.342097	-1.423867
1	-5.822126	-3.576206	-1.128779
1	-5.817007	0.019287	1.925912
1	-6.278915	-1.659735	1.733619
1	-7.764774	-0.164009	0.375257
1	-6.841558	-1.248228	-0.683823
1	-6.353917	0.438688	-0.517022
1	2.293980	-0.283389	0.904390
1	-1.572206	0.938069	2.316457
1	-0.506557	2.089273	4.233123
1	6.190165	-0.421624	1.200621
1	6.058244	-0.572621	2.984520
1	6.261239	1.032796	2.249058
1	2.971687	1.844019	4.771693
1	-0.471985	0.002087	-3.321634
1	-1.897886	-0.901175	-2.759013
1	-1.932881	0.877941	-2.797122
1	-0.842072	-1.203120	4.076072
1	1.558805	-3.003146	0.960589
1	1.011728	-1.385258	5.659796
1	3.411423	-3.314337	2.525695
1	3.270937	-1.581817	4.438111
1	2.678779	-3.128242	4.941462
1	-0.594232	-2.033377	1.739254

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^{CSS}P

Number of imaginary frequencies : 0 Electronic energy : HF=-2530.0981094
Zero-point correction= 1.020602 (Hartree/Particle)
Thermal correction to Energy= 1.080998
Thermal correction to Enthalpy= 1.081943
Thermal correction to Gibbs Free Energy= 0.922560
Sum of electronic and zero-point Energies= -2529.077507
Sum of electronic and thermal Energies= -2529.017111
Sum of electronic and thermal Enthalpies= -2529.016167
Sum of electronic and thermal Free Energies= -2529.175549

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Cartesian Coordinates

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6	-2.073062	-3.719948	-0.859143
6	-0.924848	-2.829819	-0.830079
7	-1.353664	-1.525319	-0.742426
6	-2.729407	-1.552599	-0.735723
6	-3.191130	-2.927872	-0.802942
6	0.404111	-3.230320	-0.878495
6	1.523779	-2.410641	-0.857490

7	1.498396	-1.039128	-0.758364
6	2.803986	-0.609688	-0.761020
6	3.695600	-1.753672	-0.862781
6	2.901562	-2.869469	-0.925985
6	3.208692	0.714298	-0.661342
6	2.388845	1.827624	-0.558123
7	1.013626	1.799649	-0.543781
6	0.586238	3.101000	-0.421094
6	1.736156	3.987765	-0.339674
6	2.852478	3.198301	-0.418880
6	-0.739115	3.501889	-0.340050
6	-1.861047	2.683850	-0.375806
7	-1.834356	1.315024	-0.498563
6	-3.143209	0.886706	-0.518457
6	-4.032502	2.027551	-0.381712
6	-3.237642	3.141316	-0.291488
77	-0.166943	0.141714	-0.662701
6	-0.252904	0.248902	-2.713721
6	-3.655283	4.578119	-0.196621
6	-3.621095	5.299042	-1.556422
6	-5.529468	1.949872	-0.404340
6	-6.097649	1.808600	-1.828136
6	-3.547854	-0.436396	-0.631637
6	4.292839	3.607778	-0.387189
6	4.943298	3.634021	-1.781597
6	1.656170	5.480789	-0.233688
6	1.370806	6.159105	-1.585700
6	3.315717	-4.300354	-1.093903
6	3.191787	-4.789128	-2.548150
6	5.190819	-1.661448	-0.912081
6	5.721995	-1.211051	-2.284480
6	-4.630751	-3.342588	-0.844068
6	-5.264643	-3.163198	-2.235243
6	-1.993543	-5.211021	-0.992710
6	-1.753696	-5.666729	-2.443449
6	-0.430817	0.320240	2.577907
6	0.634550	-0.568558	2.506137
6	1.969002	-0.118417	2.484408
6	2.242737	1.266833	2.548172
6	1.168032	2.167588	2.610710
6	-0.132771	1.700215	2.612925
6	3.093022	-1.053265	2.413129
8	4.280660	-0.708797	2.386599
8	3.493527	1.759778	2.541958
8	2.733334	-2.345008	2.402461
6	3.809149	-3.292923	2.375941
6	-1.880424	-0.146248	2.733880
6	-2.416452	0.279072	4.085300
6	-2.979105	-0.550227	4.964626
6	-3.161388	-2.022029	4.720389
6	-2.622339	-2.455557	3.386433
6	-2.052116	-1.626994	2.510715
1	-4.615987	-0.618844	-0.618636
1	-0.918032	4.565457	-0.231830
1	4.276347	0.894564	-0.638838
1	0.585745	-4.296993	-0.942036
1	-1.191621	-5.599781	-0.352842
1	-2.921000	-5.660698	-0.621871
1	-0.824912	-5.242786	-2.837387
1	-2.568833	-5.331202	-3.091862

1	2.709855	-4.942650	-0.442141
1	4.352308	-4.423078	-0.761231
1	5.623939	-2.637617	-0.665812
1	5.536433	-0.973395	-0.131610
1	-4.716458	-4.391685	-0.541067
1	-5.202143	-2.766696	-0.105542
1	4.845177	2.927579	0.271279
1	4.377307	4.599975	0.068633
1	-1.688480	-6.757678	-2.509951
1	2.596446	5.867610	0.173304
1	0.876353	5.762612	0.485153
1	1.309099	7.246933	-1.477728
1	0.427479	5.802475	-2.010689
1	2.162983	5.929374	-2.304886
1	4.429131	4.346632	-2.434255
1	4.887527	2.651832	-2.261007
1	5.997058	3.924674	-1.719774
1	5.319398	-0.231542	-2.559196
1	5.424211	-1.918706	-3.064546
1	6.814671	-1.143293	-2.281111
1	3.490595	-5.838435	-2.640238
1	3.826955	-4.191232	-3.208802
1	2.162131	-4.692538	-2.905579
1	-6.317470	-3.463682	-2.231762
1	-4.737409	-3.767969	-2.979494
1	-5.207000	-2.119763	-2.559823
1	-5.948332	2.847189	0.063856
1	-5.867228	1.103736	0.206882
1	-7.190483	1.743537	-1.812857
1	-5.707493	0.910896	-2.317376
1	-5.813389	2.667770	-2.443379
1	-3.006368	5.108885	0.511174
1	-4.667413	4.637555	0.218103
1	-3.919199	6.347727	-1.455585
1	-4.300099	4.815599	-2.265424
1	-2.616787	5.267754	-1.989728
1	0.451788	-1.635045	2.489055
1	-0.949015	2.416380	2.631525
1	1.389626	3.228019	2.621367
1	3.331866	-4.270033	2.311557
1	4.407422	-3.215503	3.287277
1	4.447394	-3.120780	1.509493
1	4.097690	0.979923	2.478163
1	0.187139	-0.660528	-3.130276
1	-1.299644	0.333236	-3.016116
1	0.307670	1.126596	-3.044402
1	-2.316100	1.333661	4.331585
1	-1.682578	-2.015512	1.570696
1	-3.334745	-0.161034	5.916740
1	-2.716217	-3.510380	3.135277
1	-2.677477	-2.598100	5.525622
1	-4.228725	-2.285753	4.799042
1	-2.457357	0.381457	1.959184

TS(B-D)

Number of imaginary frequencies : 1 Electronic energy : HF=-2529.9674768
Zero-point correction= 1.011533 (Hartree/Particle)
Thermal correction to Energy= 1.072460

Thermal correction to Enthalpy= 1.073405
Thermal correction to Gibbs Free Energy= 0.913819
Sum of electronic and zero-point Energies= -2528.955944
Sum of electronic and thermal Energies= -2528.895016
Sum of electronic and thermal Enthalpies= -2528.894072
Sum of electronic and thermal Free Energies= -2529.053658

Cartesian Coordinates

6	4.018580	2.197512	-0.291249
6	3.207628	0.991773	-0.379070
7	1.884245	1.336165	-0.463867
6	1.811892	2.706880	-0.448259
6	3.153567	3.260120	-0.333192
6	3.695264	-0.309624	-0.358460
6	2.950761	-1.483069	-0.428872
7	1.584723	-1.549702	-0.560452
6	1.234594	-2.879218	-0.575686
6	2.428156	-3.692180	-0.424521
6	3.492523	-2.826403	-0.337838
6	-0.059699	-3.369482	-0.710886
6	-1.222894	-2.626181	-0.875561
7	-1.283751	-1.256625	-0.886878
6	-2.601475	-0.903817	-1.020160
6	-3.419204	-2.102902	-1.109185
6	-2.565012	-3.172319	-1.015044
77	0.299030	0.040424	-0.638500
7	-0.989556	1.633740	-0.746841
6	-2.358681	1.561332	-0.822370
6	-2.924792	2.894102	-0.697183
6	-1.869061	3.761724	-0.587480
6	-0.657178	2.958315	-0.620261
6	-2.887200	-4.633498	-1.104390
6	-2.612542	-5.217949	-2.501661
6	-4.903952	-2.098362	-1.317166
6	-5.300194	-1.787846	-2.771794
6	-3.092763	0.394643	-0.978809
6	4.951950	-3.154447	-0.235551
6	5.678772	-3.063629	-1.589549
6	2.450305	-5.191278	-0.447547
6	2.380643	-5.764351	-1.874720
6	0.639015	3.448844	-0.505302
6	-1.901078	5.254626	-0.466070
6	-1.638081	5.965485	-1.805748
6	-4.393644	3.185331	-0.655809
6	-5.054397	3.177206	-2.045481
6	3.475288	4.724221	-0.340403
6	3.444801	5.332461	-1.754331
6	5.516673	2.215494	-0.240522
6	6.161241	2.001928	-1.622145
6	-0.041269	0.069064	1.523296
6	-1.295265	-0.546121	1.884443
6	-2.360120	0.241439	2.202417
6	-2.159594	1.688466	2.470055
6	-0.751339	2.127062	2.542827
6	0.271793	1.318197	2.174315
6	-3.728986	-0.337984	2.160803
8	-4.729922	0.210185	1.748511
8	-3.083099	2.473793	2.680567
6	0.505938	0.146584	-2.733684

8	-3.720104	-1.619877	2.611305
6	-4.965836	-2.318627	2.496317
6	1.656826	-1.483025	2.752708
6	0.791394	-1.789863	3.912334
6	0.900245	-1.132633	5.074054
6	1.939128	-0.076251	5.319661
6	2.932046	0.051696	4.200976
6	2.812723	-0.607243	3.039456
1	0.743182	4.525441	-0.436797
1	4.769288	-0.423626	-0.265811
1	-0.171987	-4.447482	-0.695057
1	-4.168249	0.506146	-1.012953
1	0.830251	1.150763	-3.023527
1	1.252290	-0.582291	-3.066214
1	-0.452115	-0.077400	-3.212837
1	-4.876871	2.454327	0.002180
1	-4.551332	4.161705	-0.186495
1	-4.927047	2.209167	-2.540230
1	-4.605681	3.936836	-2.693815
1	-5.365643	-1.362029	-0.648105
1	-5.315451	-3.073771	-1.033503
1	-3.940380	-4.790894	-0.847412
1	-2.306907	-5.190233	-0.357692
1	-2.875813	5.563911	-0.075404
1	-1.160780	5.583708	0.273649
1	1.613515	-5.585474	0.142218
1	3.361766	-5.550806	0.042282
1	-6.127284	3.381607	-1.970496
1	5.071630	-4.164061	0.172037
1	5.435937	-2.479348	0.481318
1	6.743031	-3.297158	-1.482693
1	5.588114	-2.059602	-2.014830
1	5.243636	-3.764920	-2.307904
1	3.233999	-5.423749	-2.468869
1	1.471504	-5.431534	-2.384433
1	2.386492	-6.859057	-1.861058
1	-1.562424	-5.086018	-2.779726
1	-3.218829	-4.708527	-3.256770
1	-2.845948	-6.287136	-2.536570
1	-6.388435	-1.780989	-2.890279
1	-4.883959	-2.535704	-3.453878
1	-4.915954	-0.810832	-3.079427
1	-1.659577	7.053769	-1.687112
1	-2.395535	5.685167	-2.544118
1	-0.662094	5.684510	-2.214106
1	4.465588	4.882774	0.100271
1	2.767729	5.264274	0.301121
1	3.671304	6.403275	-1.728286
1	2.460951	5.200304	-2.214305
1	4.178661	4.841460	-2.400718
1	5.875942	1.441594	0.449789
1	5.856784	3.171053	0.173143
1	7.253984	2.007856	-1.553889
1	5.855686	2.791796	-2.314925
1	5.848733	1.046776	-2.054874
1	-1.438229	-1.604858	1.704383
1	1.300282	1.662960	2.187758
1	-0.595328	3.156634	2.848946
1	-4.825368	-3.260950	3.026122
1	-5.201042	-2.507918	1.446344

1	-5.776520	-1.739832	2.943886
1	0.993673	-0.873969	1.916279
1	3.545139	-0.478859	2.250073
1	0.026329	-2.549982	3.783116
1	3.784483	0.706396	4.366510
1	0.226091	-1.365170	5.894396
1	2.465150	-0.279625	6.265536
1	1.893544	-2.343221	2.118916
1	1.445188	0.895074	5.486355

D

Number of imaginary frequencies : 0 Electronic energy : HF=-2530.0443354
Zero-point correction= 1.017885 (Hartree/Particle)
Thermal correction to Energy= 1.079120
Thermal correction to Enthalpy= 1.080064
Thermal correction to Gibbs Free Energy= 0.917365
Sum of electronic and zero-point Energies= -2529.026451
Sum of electronic and thermal Energies= -2528.965215
Sum of electronic and thermal Enthalpies= -2528.964271
Sum of electronic and thermal Free Energies= -2529.126971

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Cartesian Coordinates

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6	2.405264	0.144294	3.094864
6	0.953679	-0.074952	3.429938
6	0.575413	0.479856	4.776560
6	1.410470	1.184605	5.541553
6	2.835329	1.482081	5.162906
6	3.238969	0.851903	3.858486
6	0.050646	0.542771	2.301688
6	-1.340827	0.017551	2.322624
6	-2.440708	0.792374	2.239253
6	-2.322461	2.278564	2.155734
6	-0.945600	2.811418	2.163774
6	0.138739	2.028852	2.238607
6	-3.786867	0.157669	2.153514
8	-3.798252	-1.042113	2.788591
6	-5.008105	-1.798573	2.653925
8	-3.292711	3.027032	2.112011
8	-4.753418	0.613168	1.579868
77	0.307935	-0.214231	-0.747467
6	0.533211	-0.565563	-2.762074
7	2.105585	0.768603	-0.684460
6	3.343544	0.195943	-0.501820
6	4.366043	1.227655	-0.528020
6	3.720880	2.420848	-0.730220
6	2.302294	2.121638	-0.828176
6	5.838523	0.972618	-0.408125
6	6.463627	0.462207	-1.719033
6	3.573422	-1.157452	-0.288552
6	2.621058	-2.166620	-0.212086
7	1.264397	-1.984253	-0.349135
6	0.673952	-3.218222	-0.205421
6	1.695044	-4.221331	0.043912
6	2.901761	-3.569711	0.039034
6	1.292277	3.059105	-1.003409
6	-0.071653	2.812391	-1.066001
7	-0.652909	1.566073	-1.006738

6	-2.015477	1.756037	-1.061832
6	-2.311075	3.177812	-1.121521
6	-1.106631	3.830890	-1.136973
6	4.316724	3.787304	-0.888605
6	4.426538	4.221396	-2.361452
6	-0.690869	-3.463048	-0.287719
6	-1.693797	-2.533348	-0.528780
7	-1.492486	-1.183727	-0.714480
6	-2.729619	-0.613076	-0.900857
6	-3.756539	-1.640130	-0.848057
6	-3.114657	-2.828966	-0.608678
6	1.429848	-5.688668	0.200305
6	1.214326	-6.401495	-1.147139
6	4.275212	-4.151113	0.191630
6	4.988046	-4.357173	-1.157212
6	-2.965228	0.746827	-1.043846
6	-5.216841	-1.390022	-1.077771
6	-5.552719	-1.151477	-2.560794
6	-3.705603	-4.203735	-0.513670
6	-3.574631	-4.999177	-1.824937
6	-3.695263	3.750639	-1.132120
6	-4.366833	3.680867	-2.514880
6	-0.849291	5.304730	-1.222899
6	-0.478069	5.763114	-2.644621
1	1.599997	4.096238	-1.069473
1	4.606064	-1.456132	-0.149782
1	-1.007430	-4.490008	-0.145970
1	-4.001088	1.056063	-1.085873
1	0.150374	0.299530	-3.308180
1	1.595431	-0.709764	-2.972855
1	-0.031683	-1.463274	-3.023857
1	-4.301690	3.225649	-0.385698
1	-3.654894	4.793530	-0.801624
1	-4.436868	2.647891	-2.869981
1	-3.790494	4.243724	-3.256379
1	-5.537084	-0.531624	-0.477328
1	-5.793939	-2.248659	-0.716033
1	-4.764500	-4.128217	-0.243400
1	-3.224599	-4.761197	0.299850
1	-1.739793	5.846887	-0.888588
1	-0.045795	5.583826	-0.529480
1	0.549541	-5.842631	0.836714
1	2.268682	-6.157277	0.726241
1	-5.378762	4.096854	-2.479937
1	4.209134	-5.110976	0.715151
1	4.886354	-3.500228	0.829325
1	5.990891	-4.772795	-1.014899
1	5.082569	-3.410560	-1.698000
1	4.419118	-5.042867	-1.792480
1	2.100826	-6.302957	-1.781034
1	0.371530	-5.963458	-1.690519
1	1.012436	-7.467769	-1.002253
1	-2.524575	-5.102980	-2.115015
1	-4.091757	-4.483316	-2.639650
1	-4.003990	-6.001366	-1.724804
1	-6.623085	-0.965303	-2.694756
1	-5.276406	-2.020305	-3.166675
1	-5.005025	-0.289286	-2.952770
1	-0.288499	6.841014	-2.675875
1	-1.288225	5.536298	-3.344367

1	0.418782	5.247109	-3.001677
1	5.311662	3.807330	-0.430830
1	3.715269	4.521746	-0.338451
1	4.855530	5.225065	-2.446478
1	3.443083	4.226739	-2.841063
1	5.061708	3.527747	-2.920868
1	6.026398	0.244058	0.390653
1	6.344750	1.894379	-0.101788
1	7.535735	0.275255	-1.599420
1	6.330043	1.195740	-2.519961
1	5.987150	-0.468208	-2.042676
1	-1.452108	-1.061670	2.363461
1	1.138460	2.452417	2.240498
1	-0.872380	3.892201	2.103237
1	-4.928006	-2.614562	3.372295
1	-5.089443	-2.195286	1.639413
1	-5.878737	-1.175738	2.868228
1	0.530244	0.144291	1.378954
1	2.754133	-0.290892	2.161758
1	-0.448865	0.309058	5.100651
1	4.272482	0.983125	3.544368
1	1.064588	1.575565	6.496091
1	3.512557	1.147067	5.964386
1	0.746018	-1.155969	3.403147
1	2.987257	2.572489	5.115164

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^{3}TS(B-C)

Number of imaginary frequencies : 1 Electronic energy : HF=-2529.9512532
Zero-point correction= 1.008107 (Hartree/Particle)
Thermal correction to Energy= 1.069725
Thermal correction to Enthalpy= 1.070669
Thermal correction to Gibbs Free Energy= 0.904526
Sum of electronic and zero-point Energies= -2528.937351
Sum of electronic and thermal Energies= -2528.875734
Sum of electronic and thermal Enthalpies= -2528.874790
Sum of electronic and thermal Free Energies= -2529.040933

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Cartesian Coordinates

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6	0.992793	0.022228	4.116141
6	0.278966	-0.613573	3.020955
7	-0.125104	0.336784	2.118053
6	0.305105	1.557072	2.594025
6	1.005703	1.367071	3.853133
6	0.026435	-1.974293	2.906721
6	-0.693850	-2.603790	1.902141
7	-1.256585	-1.970901	0.814083
6	-1.892840	-2.943584	0.065917
6	-1.729368	-4.232854	0.709122
6	-0.985032	-4.023410	1.842645
6	-2.569755	-2.723050	-1.124161
6	-2.723802	-1.507938	-1.784372
7	-2.216897	-0.315605	-1.346283
6	-2.536864	0.634897	-2.283815
6	-3.288364	0.015320	-3.364713
6	-3.408211	-1.314081	-3.052720
77	-1.140238	0.000374	0.379750

7	-1.063383	2.030210	-0.044059
6	-1.539545	2.632655	-1.176382
6	-1.261045	4.059249	-1.120260
6	-0.616217	4.288612	0.068382
6	-0.498915	3.001505	0.733436
6	-4.139922	-2.387746	-3.800074
6	-5.525500	-2.691634	-3.201971
6	-3.861251	0.751890	-4.537847
6	-5.169940	1.487615	-4.197020
6	-2.205677	1.981816	-2.209195
6	-0.584656	-5.019397	2.888872
6	-1.510121	-4.994662	4.119039
6	-2.336273	-5.513006	0.219072
6	-3.829036	-5.638394	0.574227
6	0.125182	2.776677	1.957782
6	-0.145691	5.591073	0.641388
6	-1.104638	6.159150	1.703059
6	-1.680448	5.054179	-2.159900
6	-3.159034	5.462940	-2.030268
6	1.565908	2.475555	4.692425
6	0.487363	3.207615	5.511374
6	1.529888	-0.698793	5.315410
6	0.441062	-1.014248	6.357139
6	0.600365	-0.098176	-0.785237
6	1.652755	0.801966	-0.598154
6	2.851920	0.703577	-1.310167
6	3.014567	-0.333060	-2.284958
6	1.939618	-1.244640	-2.452799
6	0.756826	-1.119314	-1.740410
8	4.077174	-0.446921	-3.044624
6	3.939352	1.672277	-1.037628
8	5.131090	1.502003	-1.217074
6	-3.058183	0.625185	1.270097
8	3.454563	2.832695	-0.513294
6	4.450721	3.794139	-0.156557
6	5.960004	-1.453238	-1.607356
6	5.911124	-2.898323	-1.864247
6	6.891396	-3.546068	-2.519170
6	8.137728	-2.856591	-2.996119
6	8.222010	-1.415691	-2.579535
6	7.227528	-0.787472	-1.924493
1	-2.516207	2.599130	-3.044201
1	-3.011074	-3.592136	-1.597909
1	0.417027	-2.608784	3.693544
1	0.539972	3.645713	2.454800
1	-2.826952	1.292111	2.100400
1	-3.660509	1.116820	0.508395
1	-3.509489	-0.312274	1.602457
1	0.850858	5.462114	1.082414
1	-0.026246	6.321414	-0.165886
1	-1.231596	5.456505	2.532469
1	-2.093941	6.339323	1.271420
1	2.089425	3.197262	4.053103
1	2.322687	2.070166	5.372341
1	2.313487	-0.093753	5.783786
1	2.014738	-1.631536	5.002069
1	-1.050790	5.947118	-2.083937
1	-1.502356	4.643503	-3.161157
1	0.447885	-4.829607	3.206531
1	-0.587464	-6.024888	2.454903

1	-0.729750	7.104278	2.108996
1	-1.790836	-6.361374	0.645739
1	-2.213558	-5.590470	-0.868262
1	-4.246483	-6.577183	0.196393
1	-4.403986	-4.811098	0.147067
1	-3.970822	-5.611723	1.658931
1	-2.539231	-5.231662	3.832399
1	-1.517906	-4.003588	4.582900
1	-1.186680	-5.722466	4.870060
1	-0.351185	-1.630297	5.920775
1	-0.022633	-0.092391	6.721297
1	0.859370	-1.550509	7.214984
1	0.924548	4.016419	6.105650
1	-0.015844	2.514616	6.192539
1	-0.276816	3.637824	4.856789
1	-3.439386	6.181916	-2.806790
1	-3.348624	5.920154	-1.054260
1	-3.814980	4.591214	-2.117491
1	-4.045512	0.047092	-5.355649
1	-3.127413	1.472220	-4.919497
1	-5.559047	2.024650	-5.068018
1	-5.013532	2.210408	-3.390332
1	-5.933801	0.779914	-3.860533
1	-3.540742	-3.306826	-3.813175
1	-4.255853	-2.088324	-4.847093
1	-6.032047	-3.484321	-3.761960
1	-6.157961	-1.798862	-3.222082
1	-5.440185	-3.010162	-2.158417
1	1.562593	1.600033	0.124513
1	-0.045698	-1.827386	-1.916452
1	2.072800	-2.028769	-3.192188
1	3.905198	4.647059	0.248996
1	5.032560	4.094013	-1.032089
1	5.136448	3.386838	0.591881
1	5.111641	-0.921676	-2.363562
1	5.026464	-3.440244	-1.538065
1	7.311693	0.258971	-1.650900
1	6.805687	-4.611796	-2.718592
1	9.136431	-0.881407	-2.826861
1	9.028815	-3.404736	-2.645329
1	5.493222	-1.127115	-0.672256
1	8.202241	-2.929246	-4.096815

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^{3}C

Number of imaginary frequencies : 0 Electronic energy : HF=-2530.0088853
Zero-point correction= 1.014522 (Hartree/Particle)
Thermal correction to Energy= 1.076316
Thermal correction to Enthalpy= 1.077260
Thermal correction to Gibbs Free Energy= 0.913568
Sum of electronic and zero-point Energies= -2528.994363
Sum of electronic and thermal Energies= -2528.932569
Sum of electronic and thermal Enthalpies= -2528.931625
Sum of electronic and thermal Free Energies= -2529.095317

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Cartesian Coordinates

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6	-4.194471	2.276000	0.730407
6	-2.802170	2.195768	0.319217

7	-2.471075	0.893432	0.068189
6	-3.584711	0.130623	0.310992
6	-4.679700	0.993176	0.727316
6	-1.917028	3.267666	0.236942
6	-0.580835	3.218615	-0.129671
7	0.103674	2.077175	-0.504206
6	1.392694	2.458883	-0.799383
6	1.537589	3.887609	-0.593385
6	0.316178	4.357865	-0.180719
6	2.398749	1.607069	-1.228660
6	2.295194	0.240606	-1.435336
7	1.163600	-0.505366	-1.214937
6	1.477455	-1.815316	-1.515626
6	2.864943	-1.895691	-1.939276
6	3.370103	-0.622715	-1.892126
77	-0.628348	0.188820	-0.538936
7	-1.388920	-1.738841	-0.608669
6	-0.716561	-2.864432	-0.990916
6	-1.592117	-4.019123	-0.873667
6	-2.797256	-3.553258	-0.412917
6	-2.656250	-2.114353	-0.251575
6	4.736482	-0.144193	-2.275136
6	4.778157	0.476560	-3.682816
6	3.548472	-3.152474	-2.386421
6	3.198276	-3.541044	-3.834101
6	0.610988	-2.893226	-1.410840
6	-0.084706	5.773196	0.108311
6	-0.804895	6.441663	-1.076826
6	2.797279	4.657677	-0.850684
6	3.027786	4.944326	-2.345424
6	-3.657835	-1.251098	0.178494
6	-4.063027	-4.320449	-0.175702
6	-5.054806	-4.208768	-1.347921
6	-1.216009	-5.418331	-1.257926
6	-1.271994	-5.655379	-2.777976
6	-6.073804	0.524514	1.016986
6	-6.895017	0.276265	-0.261306
6	-4.924369	3.551455	1.025924
6	-5.345882	4.304994	-0.248530
6	-0.271101	-0.252049	1.481357
6	0.489189	-1.361200	1.829734
6	0.905882	-1.585550	3.155631
6	0.492377	-0.698792	4.181440
6	-0.314753	0.395065	3.838150
6	-0.692580	0.604619	2.517466
8	0.845726	-0.858713	5.468737
6	1.803448	-2.687961	3.500208
8	2.175792	-2.954817	4.646077
6	-1.507574	0.265376	-2.544541
8	2.230003	-3.402031	2.439198
6	3.139664	-4.469633	2.737501
6	3.064473	1.021704	1.901331
6	3.825082	-0.117137	1.533497
6	5.150023	-0.017767	1.217233
6	5.884467	1.293007	1.251198
6	5.003878	2.458714	1.603219
6	3.683746	2.297307	1.916424
1	-4.608842	-1.706764	0.429103
1	-2.311267	4.242736	0.498545
1	3.370999	2.052233	-1.397852

1	1.015249	-3.864662	-1.670272
1	-0.928712	-0.411846	-3.174333
1	-2.554191	-0.031746	-2.497213
1	-1.403925	1.306626	-2.858905
1	-0.206878	-5.645595	-0.891973
1	-1.885236	-6.126053	-0.756999
1	-0.600319	-4.971114	-3.305519
1	-2.283117	-5.480656	-3.158139
1	3.283558	-3.978316	-1.714087
1	4.632963	-3.026857	-2.298224
1	5.442872	-0.979828	-2.225433
1	5.084074	0.588827	-1.539116
1	-3.823149	-5.375486	-0.005035
1	-4.545603	-3.967488	0.743894
1	3.651395	4.103186	-0.444497
1	2.761518	5.605907	-0.303381
1	-0.983094	-6.681164	-3.029026
1	0.804884	6.357587	0.366307
1	-0.733507	5.803474	0.992276
1	-1.093950	7.469292	-0.834036
1	-1.707918	5.886883	-1.349478
1	-0.155887	6.466522	-1.957492
1	2.205507	5.537294	-2.757672
1	3.081578	4.014055	-2.919080
1	3.960308	5.496442	-2.500619
1	4.091318	1.325391	-3.755488
1	4.476948	-0.255456	-4.438523
1	5.785220	0.828881	-3.928520
1	3.703196	-4.466857	-4.128377
1	3.499282	-2.750250	-4.527941
1	2.119931	-3.686806	-3.949976
1	-5.972661	-4.769464	-1.143551
1	-4.610242	-4.601056	-2.267682
1	-5.324814	-3.164568	-1.533202
1	-6.586642	1.267382	1.637255
1	-6.041204	-0.395966	1.612729
1	-7.903912	-0.074223	-0.020749
1	-6.413239	-0.474239	-0.895522
1	-6.981677	1.195749	-0.848303
1	-4.295936	4.206067	1.642866
1	-5.813048	3.332195	1.627303
1	-5.867580	5.235675	-0.003005
1	-6.012840	3.687707	-0.858119
1	-4.474395	4.552084	-0.862626
1	0.817912	-2.063863	1.076720
1	-1.302563	1.470571	2.286940
1	-0.623747	1.071782	4.628175
1	3.380554	-4.922679	1.776038
1	2.672724	-5.200894	3.401641
1	4.041590	-4.082365	3.217328
1	1.409837	-1.666458	5.509021
1	3.082144	3.166457	2.169673
1	3.332919	-1.083515	1.488801
1	5.458028	3.445940	1.624807
1	5.712988	-0.902148	0.930920
1	6.387613	1.473482	0.282014
1	2.012775	0.923094	2.130739
1	6.731159	1.233125	1.962737

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^{3}TS(C-P)

Number of imaginary frequencies : 1 Electronic energy : HF=-2529.9619268
Zero-point correction= 1.014650 (Hartree/Particle)
Thermal correction to Energy= 1.075011
Thermal correction to Enthalpy= 1.075955
Thermal correction to Gibbs Free Energy= 0.917561
Sum of electronic and zero-point Energies= -2528.947277
Sum of electronic and thermal Energies= -2528.886916
Sum of electronic and thermal Enthalpies= -2528.885972
Sum of electronic and thermal Free Energies= -2529.044365

Cartesian Coordinates

6	-0.300234	-0.407195	4.091418
6	-0.761711	-0.920009	2.797913
6	-0.417173	-2.318261	2.547047
6	0.561968	-2.946217	3.224634
6	1.324215	-2.289788	4.342979
6	0.685187	-1.001422	4.787380
6	0.336865	0.238298	1.522299
6	1.670597	-0.305985	1.596610
6	2.758049	0.410598	2.083525
6	2.588092	1.755158	2.517411
6	1.283646	2.307872	2.531293
6	0.222755	1.590608	2.049104
77	-0.585937	0.052670	-0.493933
6	-0.976404	0.394136	-2.588774
6	4.110912	-0.151045	2.062332
8	4.162998	-1.443492	1.698531
6	5.474248	-2.010039	1.585615
8	3.611772	2.524151	2.921913
7	0.154924	1.995459	-0.669177
6	1.451904	2.339135	-0.927447
6	1.584349	3.787214	-0.896186
6	0.334885	4.292628	-0.640675
6	-0.554163	3.152295	-0.492009
6	2.860398	4.530906	-1.149778
6	3.199033	4.647974	-2.646777
6	2.482184	1.442608	-1.191914
6	2.390383	0.058230	-1.285672
7	1.244339	-0.680259	-1.114619
6	1.571855	-1.994223	-1.293823
6	2.989716	-2.110098	-1.585569
6	3.499495	-0.835925	-1.570537
6	-1.897106	3.212507	-0.140420
6	-2.746276	2.143005	0.121977
7	-2.401407	0.808480	0.042565
6	-3.525902	0.082767	0.351496
6	-4.616928	0.982744	0.675382
6	-4.135084	2.259243	0.525441
6	-0.093805	5.726666	-0.563474
6	-0.781804	6.210732	-1.852609
6	0.678166	-3.054460	-1.159288
6	-0.652897	-2.978029	-0.789253
7	-1.329389	-1.813279	-0.456060
6	-2.612518	-2.179355	-0.100723
6	-2.751461	-3.619156	-0.205628
6	-1.543398	-4.110547	-0.634857
6	3.701824	-3.397637	-1.869793

6	3.482636	-3.897297	-3.309103
6	4.909540	-0.392145	-1.818603
6	5.127723	0.156535	-3.240001
6	-3.610168	-1.304164	0.299512
6	-4.021678	-4.370965	0.053762
6	-5.007436	-4.298019	-1.126593
6	-1.178445	-5.529294	-0.952130
6	-1.207926	-5.828282	-2.461903
6	-6.009637	0.546074	1.017406
6	-6.845551	0.188057	-0.225022
6	-4.876998	3.554102	0.670121
6	-5.331397	4.135627	-0.681013
8	5.134704	0.484110	2.337033
1	-4.562262	-1.744261	0.571180
1	-2.322360	4.202868	-0.025378
1	3.464760	1.871541	-1.347646
1	1.071826	-4.047379	-1.343092
1	-0.179722	-5.752293	-0.556690
1	-1.866286	-6.206647	-0.435259
1	-0.517360	-5.174674	-3.003343
1	-2.209307	-5.658274	-2.869040
1	3.370286	-4.168695	-1.162871
1	4.775189	-3.266447	-1.693619
1	5.588980	-1.235420	-1.652763
1	5.190761	0.372613	-1.083401
1	-3.788146	-5.419621	0.265835
1	-4.505397	-3.979795	0.957140
1	3.684854	4.034334	-0.623605
1	2.788671	5.534072	-0.716274
1	-0.927240	-6.867016	-2.663474
1	0.778245	6.356984	-0.359639
1	-0.774165	5.867138	0.285802
1	-1.091505	7.257309	-1.766511
1	-1.668114	5.607586	-2.072608
1	-0.103895	6.121905	-2.707042
1	2.408918	5.185838	-3.179861
1	3.290292	3.659101	-3.106605
1	4.141486	5.184311	-2.797412
1	4.471887	1.010239	-3.435396
1	4.899938	-0.610098	-3.986958
1	6.163549	0.480273	-3.383817
1	4.005662	-4.843068	-3.484340
1	3.850115	-3.161967	-4.031364
1	2.418194	-4.051923	-3.510952
1	-5.929799	-4.843821	-0.903728
1	-4.562183	-4.729997	-2.028024
1	-5.269230	-3.260199	-1.353957
1	-6.514838	1.342584	1.574384
1	-5.973184	-0.318158	1.692144
1	-7.851823	-0.138696	0.056646
1	-6.371758	-0.615559	-0.797157
1	-6.938661	1.052737	-0.889064
1	-4.247687	4.288554	1.187939
1	-5.752568	3.401957	1.310368
1	-5.861279	5.083855	-0.544294
1	-6.001057	3.439205	-1.194751
1	-4.475008	4.313114	-1.338661
1	1.834135	-1.324107	1.275434
1	-0.760751	2.049020	2.048554
1	1.167008	3.323608	2.895059

1	5.318854	-3.031123	1.238655
1	5.983199	-2.003710	2.552456
1	6.073824	-1.447610	0.866326
1	4.430104	1.981501	2.812770
1	-0.050311	0.666613	-3.094628
1	-1.366540	-0.549426	-2.980508
1	-1.715973	1.192488	-2.672583
1	-0.726553	0.524720	4.451890
1	-0.953176	-2.851350	1.773815
1	1.040548	-0.559626	5.715114
1	0.811144	-3.977809	2.986131
1	2.367052	-2.106109	4.030340
1	1.412513	-2.981697	5.196733
1	-1.748908	-0.603014	2.475147

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^{3}P

Number of imaginary frequencies : 0 Electronic energy : HF=-2530.027377
Zero-point correction= 1.016684 (Hartree/Particle)
Thermal correction to Energy= 1.077523
Thermal correction to Enthalpy= 1.078467
Thermal correction to Gibbs Free Energy= 0.917766
Sum of electronic and zero-point Energies= -2529.010693
Sum of electronic and thermal Energies= -2528.949854
Sum of electronic and thermal Enthalpies= -2528.948910
Sum of electronic and thermal Free Energies= -2529.109611

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Cartesian Coordinates

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6	-2.334266	1.251403	4.130940
6	-1.895593	0.754640	2.769105
6	-2.221659	-0.702513	2.575958
6	-2.831137	-1.461388	3.487453
6	-3.271482	-0.958445	4.833568
6	-2.938190	0.492094	5.045584
6	-0.412634	1.061063	2.559621
6	0.562225	0.070749	2.577496
6	1.933083	0.388211	2.495720
6	2.333836	1.739885	2.395351
6	1.348970	2.739458	2.366560
6	0.010658	2.400804	2.440204
77	-0.152272	-0.044042	-0.695931
6	-0.222352	-0.199989	-2.751061
6	2.968093	-0.646522	2.546554
8	2.490244	-1.893455	2.663071
6	3.471150	-2.933124	2.777165
8	3.623835	2.111384	2.322476
7	0.993203	1.668215	-0.745209
6	2.371610	1.731987	-0.758698
6	2.792828	3.129381	-0.793245
6	1.658720	3.887148	-0.804788
6	0.526787	2.965608	-0.766598
6	4.221795	3.575973	-0.815651
6	4.878088	3.420957	-2.198913
6	3.215540	0.653470	-0.702648
6	2.835459	-0.697845	-0.631442
7	1.515093	-1.162029	-0.600395
6	1.587207	-2.559595	-0.553015
6	2.939216	-2.964213	-0.549302

6	3.725418	-1.791868	-0.590712
6	-0.791500	3.335717	-0.690868
6	-1.896735	2.469772	-0.602675
7	-1.823758	1.072058	-0.613217
6	-3.144953	0.606202	-0.582125
6	-4.032048	1.701287	-0.512593
6	-3.245721	2.874842	-0.521977
6	1.529384	5.378335	-0.867719
6	1.172798	5.885589	-2.276588
6	0.481257	-3.427333	-0.530757
6	-0.841504	-3.062182	-0.559644
7	-1.308530	-1.764881	-0.594663
6	-2.687068	-1.829793	-0.635077
6	-3.106989	-3.226836	-0.612553
6	-1.972630	-3.984643	-0.561529
6	3.422360	-4.381906	-0.564541
6	3.430216	-4.991775	-1.978638
6	5.219443	-1.691230	-0.614888
6	5.785642	-1.443972	-2.025272
6	-3.528353	-0.746348	-0.624124
6	-4.533441	-3.679742	-0.683539
6	-5.111521	-3.601774	-2.108153
6	-1.844695	-5.477655	-0.573772
6	-1.521096	-6.032991	-1.972725
6	-5.527007	1.608409	-0.494426
6	-6.131582	1.414080	-1.897844
6	-3.729403	4.292765	-0.524955
6	-3.822588	4.889932	-1.941686
8	4.182224	-0.413436	2.515051
1	-4.592815	-0.944307	-0.616711
1	-1.010351	4.396346	-0.690497
1	4.278690	0.855008	-0.691439
1	0.702325	-4.486963	-0.495620
1	-1.062411	-5.787681	0.130126
1	-2.775400	-5.928075	-0.212228
1	-0.590277	-5.604040	-2.355732
1	-2.316522	-5.779623	-2.680332
1	2.794484	-4.998447	0.090506
1	4.434597	-4.430661	-0.147432
1	5.654600	-2.613095	-0.212376
1	5.538495	-0.889538	0.061168
1	-4.608926	-4.709461	-0.317984
1	-5.147241	-3.070218	-0.008582
1	4.784056	3.007641	-0.066223
1	4.279256	4.624282	-0.504180
1	-1.414768	-7.122466	-1.951053
1	2.467657	5.840258	-0.542977
1	0.762697	5.712624	-0.156991
1	1.068129	6.975342	-2.290003
1	0.232783	5.445518	-2.622859
1	1.951381	5.606307	-2.993145
1	4.352871	4.025236	-2.945402
1	4.843945	2.380472	-2.535721
1	5.925366	3.739183	-2.175864
1	5.385281	-0.517882	-2.448524
1	5.512539	-2.259932	-2.701734
1	6.877658	-1.367871	-2.003714
1	3.783108	-6.028196	-1.961148
1	4.083718	-4.417933	-2.642672
1	2.424922	-4.976808	-2.410463

1	-6.158372	-3.921672	-2.127661
1	-4.543859	-4.242982	-2.789598
1	-5.057079	-2.579800	-2.494960
1	-5.944923	2.515859	-0.044825
1	-5.839015	0.778859	0.151473
1	-7.223289	1.343957	-1.851065
1	-5.747715	0.500555	-2.362062
1	-5.870121	2.251005	-2.552474
1	-3.062429	4.914579	0.084583
1	-4.713461	4.345656	-0.046034
1	-4.171385	5.927422	-1.911082
1	-4.517045	4.313512	-2.560330
1	-2.846195	4.869085	-2.435209
1	0.277961	-0.968078	2.690099
1	-0.736862	3.187677	2.400664
1	1.668913	3.769497	2.264055
1	2.910134	-3.865797	2.736060
1	4.006048	-2.846283	3.726719
1	4.183736	-2.877431	1.954814
1	4.153675	1.277339	2.364137
1	0.424548	0.570613	-3.171533
1	0.119199	-1.201074	-3.015993
1	-1.260800	-0.056490	-3.051194
1	-2.119207	2.294365	4.353349
1	-1.924837	-1.137589	1.630147
1	-3.215378	0.925989	6.004448
1	-3.034437	-2.505813	3.258452
1	-2.813810	-1.567531	5.629744
1	-4.355357	-1.115453	4.958207
1	-2.439840	1.330280	2.003951

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^{CSS}TS(B-C)

Number of imaginary frequencies : 1 Electronic energy : HF=-2529.9387417
Zero-point correction= 1.008871 (Hartree/Particle)
Thermal correction to Energy= 1.070186
Thermal correction to Enthalpy= 1.071131
Thermal correction to Gibbs Free Energy= 0.907151
Sum of electronic and zero-point Energies= -2528.929871
Sum of electronic and thermal Energies= -2528.868555
Sum of electronic and thermal Enthalpies= -2528.867611
Sum of electronic and thermal Free Energies= -2529.031591

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Cartesian Coordinates

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6	0.663742	0.108158	4.234465
6	0.047088	-0.548757	3.095058
7	-0.265711	0.385987	2.137768
6	0.127775	1.614424	2.624793
6	0.710899	1.447427	3.944284
6	-0.205376	-1.909863	2.992313
6	-0.848504	-2.558652	1.946842
7	-1.302821	-1.950284	0.802393
6	-1.902820	-2.925230	0.033912
6	-1.822541	-4.201540	0.722530
6	-1.166334	-3.975638	1.905016
6	-2.479581	-2.725520	-1.212371
6	-2.559696	-1.527345	-1.917028
7	-2.066204	-0.331341	-1.478635

6	-2.313187	0.601133	-2.450719
6	-2.993164	-0.036092	-3.568069
6	-3.149968	-1.357430	-3.234889
77	-1.112113	0.017683	0.327209
7	-1.012303	2.036543	-0.124163
6	-1.405670	2.617836	-1.301125
6	-1.139186	4.047285	-1.244996
6	-0.589343	4.299703	-0.014422
6	-0.517404	3.024276	0.679538
6	-3.843724	-2.439446	-4.006213
6	-5.275053	-2.703961	-3.504962
6	-3.476929	0.678472	-4.793789
6	-4.803510	1.424732	-4.562402
6	-1.989871	1.951330	-2.371851
6	-0.876392	-4.946711	3.009374
6	-1.900950	-4.867463	4.155873
6	-2.422649	-5.480510	0.221118
6	-3.941805	-5.558217	0.458317
6	0.009056	2.822180	1.952145
6	-0.176794	5.615178	0.573407
6	-1.225082	6.192306	1.541653
6	-1.484459	5.024123	-2.328165
6	-2.970875	5.424916	-2.315845
6	1.198010	2.570406	4.809577
6	0.052791	3.318582	5.515759
6	1.082525	-0.586982	5.494599
6	-0.099648	-0.867558	6.440196
6	0.632169	-0.144237	-0.755450
6	1.657063	0.820501	-0.619245
6	2.907589	0.666697	-1.202186
6	3.143509	-0.435996	-2.093186
6	2.067644	-1.341236	-2.314747
6	0.838580	-1.168033	-1.713510
8	4.267001	-0.614722	-2.731891
6	3.991029	1.628887	-0.881858
8	5.187918	1.423774	-0.962972
6	-3.122087	0.518316	0.979136
8	3.493592	2.816979	-0.448689
6	4.478100	3.777562	-0.055073
6	6.098445	-1.550079	-1.214430
6	6.054638	-2.987643	-1.440424
6	7.016325	-3.633735	-2.131605
6	8.225487	-2.929521	-2.675716
6	8.304817	-1.482827	-2.281605
6	7.325521	-0.864106	-1.588367
1	-2.239856	2.556321	-3.235574
1	-2.903023	-3.599183	-1.694034
1	0.107563	-2.526046	3.826956
1	0.381729	3.700125	2.466574
1	-3.042030	1.009741	1.953223
1	-3.598757	1.187831	0.262138
1	-3.692011	-0.411683	1.058619
1	0.780069	5.502126	1.098746
1	0.004517	6.333320	-0.233419
1	-1.416488	5.501415	2.368472
1	-2.175778	6.357483	1.025618
1	1.778154	3.279855	4.206429
1	1.890189	2.176624	5.561433
1	1.826565	0.023207	6.017683
1	1.583894	-1.531277	5.249269

1	-0.867242	5.922326	-2.218701
1	-1.229754	4.599734	-3.306913
1	0.129651	-4.766914	3.407933
1	-0.864120	-5.964816	2.605757
1	-0.891862	7.146702	1.962097
1	-1.936038	-6.328862	0.714072
1	-2.216024	-5.594116	-0.850310
1	-4.353586	-6.496910	0.073878
1	-4.457845	-4.729343	-0.035703
1	-4.168592	-5.495836	1.526974
1	-2.907040	-5.094170	3.790191
1	-1.927229	-3.862447	4.587918
1	-1.656872	-5.577515	4.952595
1	-0.855539	-1.487036	5.947954
1	-0.584498	0.066787	6.738994
1	0.233530	-1.386341	7.344828
1	0.437480	4.138004	6.131464
1	-0.510631	2.638772	6.162107
1	-0.649112	3.736624	4.787786
1	-3.196490	6.129141	-3.123149
1	-3.235130	5.896764	-1.364518
1	-3.613334	4.547293	-2.436492
1	-3.605117	-0.042039	-5.608740
1	-2.714532	1.389116	-5.135535
1	-5.126625	1.945692	-5.469464
1	-4.702021	2.162367	-3.760484
1	-5.592652	0.726222	-4.267837
1	-3.262286	-3.368242	-3.950351
1	-3.876429	-2.167206	-5.066589
1	-5.753157	-3.504070	-4.079307
1	-5.887944	-1.802061	-3.596090
1	-5.272512	-2.993518	-2.449612
1	1.501667	1.679636	0.017635
1	0.045675	-1.877885	-1.921441
1	2.260384	-2.177402	-2.980440
1	3.918628	4.653728	0.273814
1	5.128896	4.032109	-0.895570
1	5.096839	3.389277	0.758677
1	5.171912	-1.006041	-2.060188
1	5.196587	-3.539305	-1.063527
1	7.403127	0.187380	-1.332749
1	6.937869	-4.703009	-2.311935
1	9.195327	-0.934427	-2.578625
1	9.143541	-3.459107	-2.365440
1	5.581292	-1.169813	-0.330797
1	8.239754	-3.015842	-3.778482

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^{CSS}C

Number of imaginary frequencies : 0 Electronic energy : HF=-2529.9990935
Zero-point correction= 1.015320 (Hartree/Particle)
Thermal correction to Energy= 1.076398
Thermal correction to Enthalpy= 1.077342
Thermal correction to Gibbs Free Energy= 0.917738
Sum of electronic and zero-point Energies= -2528.983773
Sum of electronic and thermal Energies= -2528.922695
Sum of electronic and thermal Enthalpies= -2528.921751
Sum of electronic and thermal Free Energies= -2529.081356

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Cartesian Coordinates

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6	-3.079160	-2.293189	4.031655
6	-4.274003	-1.993953	3.452002
6	-4.357528	-1.790233	2.044005
6	-3.234925	-1.863574	1.226621
6	-1.985558	-2.112388	1.782810
6	-1.836734	-2.337804	3.232254
8	-3.907275	1.433547	4.220392
6	-3.382693	1.275531	3.111695
8	-4.077038	1.457043	1.974917
6	-5.449825	1.834519	2.139108
6	-1.994129	0.868969	2.908340
6	-1.459139	0.628750	1.627348
6	-0.131746	0.198915	1.392118
6	0.650287	0.030143	2.560503
6	0.144925	0.202412	3.845232
6	-1.187242	0.631267	4.043158
77	0.649897	0.037880	-0.566121
6	1.521900	0.106478	-2.532279
8	-1.645739	0.750949	5.299651
7	-1.019619	-0.862253	-1.346307
6	-1.210087	-2.210097	-1.518629
6	-2.490201	-2.443754	-2.167874
6	-3.054027	-1.210603	-2.386733
6	-2.117263	-0.223941	-1.873997
6	-0.324855	-3.201834	-1.107542
6	0.920987	-3.017079	-0.519620
7	1.488716	-1.799373	-0.236070
6	2.735623	-2.043601	0.283177
6	2.961104	-3.479724	0.358075
6	1.835765	-4.083401	-0.138313
6	-3.014863	-3.791786	-2.561452
6	-2.366603	-4.330953	-3.849361
6	-4.340224	-0.885906	-3.085893
6	-4.132281	-0.475312	-4.554858
6	-2.302128	1.153062	-1.915785
6	-1.409158	2.128726	-1.487657
7	-0.177805	1.883173	-0.941503
6	0.393872	3.094631	-0.658227
6	-0.519648	4.164731	-1.035867
6	-1.638855	3.565074	-1.550073
6	3.652874	-1.069078	0.658728
6	3.487816	0.309319	0.578833
7	2.358457	0.940686	0.130702
6	2.571399	2.288491	0.240071
6	3.903104	2.529366	0.778582
6	4.472640	1.300918	0.987535
6	4.234720	-4.121194	0.820905
6	5.332383	-4.113607	-0.258696
6	1.578926	-5.545142	-0.351054
6	1.839859	-5.991750	-1.801182
6	1.657091	3.276154	-0.107878
6	4.512318	3.884731	0.975042
6	5.040880	4.494242	-0.336183
6	5.855766	0.982187	1.469519
6	6.819742	0.630253	0.321962
6	-2.856562	4.210101	-2.140034
6	-2.822338	4.255137	-3.678441

6	-0.212038	5.627915	-0.929362
6	0.685118	6.132208	-2.074448
1	1.968121	4.301157	0.058429
1	4.598993	-1.421381	1.053388
1	-0.631512	-4.226960	-1.281318
1	-3.237749	1.503490	-2.336265
1	-3.756792	3.673951	-1.813129
1	-2.954176	5.229827	-1.751446
1	-2.736993	3.247556	-4.096600
1	-1.957568	4.828038	-4.026592
1	-4.859007	-0.077382	-2.555031
1	-5.008486	-1.753458	-3.045110
1	-4.100360	-3.735857	-2.699904
1	-2.849713	-4.507722	-1.746083
1	-1.147278	6.198697	-0.925713
1	0.274649	5.837328	0.031351
1	0.542879	-5.785563	-0.080024
1	2.212130	-6.129875	0.325457
1	-3.728141	4.719834	-4.082157
1	4.034307	-5.154967	1.123828
1	4.605838	-3.609026	1.717549
1	6.254014	-4.575270	0.110875
1	5.562177	-3.091468	-0.574035
1	5.003839	-4.663995	-1.145522
1	2.882666	-5.809412	-2.077578
1	1.212986	-5.430905	-2.500913
1	1.631009	-7.058912	-1.930714
1	-1.281214	-4.407711	-3.736085
1	-2.561675	-3.657120	-4.689077
1	-2.757762	-5.321351	-4.104567
1	-5.084797	-0.230855	-5.036594
1	-3.660580	-1.286690	-5.117334
1	-3.476279	0.397319	-4.625228
1	0.904028	7.199570	-1.965009
1	0.197449	5.978607	-3.041967
1	1.633588	5.587121	-2.095539
1	5.332839	3.815567	1.697666
1	3.774259	4.564441	1.419014
1	5.469329	5.487662	-0.166646
1	4.238267	4.587111	-1.074050
1	5.814978	3.855676	-0.772643
1	5.820051	0.147120	2.180743
1	6.254464	1.836856	2.026967
1	7.818057	0.390042	0.702657
1	6.910056	1.468858	-0.375164
1	6.452163	-0.229692	-0.246130
1	-2.105115	0.824750	0.780036
1	1.686023	-0.279892	2.459483
1	0.751300	0.022901	4.728343
1	-5.841109	1.953583	1.129205
1	-5.529683	2.770494	2.696396
1	-5.999973	1.057475	2.676439
1	-2.587354	1.047775	5.223156
1	-3.324408	-1.717017	0.157254
1	-5.174580	-1.922788	4.053320
1	-1.117169	-2.225958	1.150595
1	-3.004050	-2.459340	5.101511
1	-1.234555	-3.238043	3.434150
1	-5.325640	-1.580375	1.599680
1	-1.150833	-1.538774	3.626762

1	2.349132	-0.609833	-2.612517
1	0.778266	-0.134877	-3.302038
1	1.915076	1.109010	-2.738692

TS(B-E)

Number of imaginary frequencies : 1 Electronic energy : HF=-2529.9503213
Zero-point correction= 1.009273 (Hartree/Particle)
Thermal correction to Energy= 1.070563
Thermal correction to Enthalpy= 1.071508
Thermal correction to Gibbs Free Energy= 0.908740
Sum of electronic and zero-point Energies= -2528.940844
Sum of electronic and thermal Energies= -2528.879554
Sum of electronic and thermal Enthalpies= -2528.878609
Sum of electronic and thermal Free Energies= -2529.041377

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Cartesian Coordinates

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6	0.293262	-1.457748	3.932119
6	1.261183	-1.281104	2.840686
6	2.405198	-0.411622	3.138065
6	2.395253	0.425872	4.191579
6	1.261602	0.478326	5.176202
6	0.263592	-0.628962	4.989298
6	-2.701318	0.492732	2.338135
6	-1.687197	-0.204541	1.724305
6	-0.403633	0.358461	1.480200
6	-0.111667	1.630400	2.056291
6	-1.086777	2.348600	2.689112
6	-2.464454	1.870920	2.811219
77	0.410387	-0.046446	-0.621859
6	0.614331	0.013730	-2.728166
6	-4.024166	-0.144758	2.540244
8	-4.181862	-1.240633	1.728703
6	-5.403342	-1.953799	1.931978
8	-3.350034	2.608319	3.274549
7	-0.072620	-2.028960	-0.645236
6	0.790634	-3.081430	-0.455317
6	0.063061	-4.335220	-0.559975
6	-1.242123	-4.015641	-0.831564
6	-1.318489	-2.565769	-0.894348
6	0.687249	-5.693939	-0.453065
6	1.389979	-6.130378	-1.751546
6	2.153227	-2.957998	-0.217177
6	2.881856	-1.777501	-0.141761
7	2.353441	-0.510614	-0.269997
6	3.402396	0.380654	-0.147069
6	4.632512	-0.350503	0.084250
6	4.310280	-1.686247	0.089147
6	-2.471256	-1.837115	-1.148613
6	-2.593636	-0.452561	-1.203438
7	-1.559997	0.429397	-1.057018
6	-2.087584	1.692281	-1.095960
6	-3.529650	1.610465	-1.271581
6	-3.842214	0.277978	-1.347666
6	-2.394229	-4.940044	-1.086744
6	-2.696767	-5.118010	-2.585601
6	3.294376	1.761307	-0.224263
6	2.138522	2.496206	-0.460961

7	0.896145	1.955091	-0.657511
6	0.016160	2.995524	-0.810584
6	0.733737	4.256787	-0.715913
6	2.052362	3.947198	-0.502076
6	5.986635	0.278690	0.219935
6	6.601930	0.665756	-1.137077
6	5.227339	-2.863309	0.232322
6	5.598699	-3.496820	-1.120803
6	-1.356773	2.868441	-0.983013
6	0.108354	5.608121	-0.886595
6	-0.148044	5.963502	-2.362263
6	3.224081	4.875210	-0.389231
6	4.022645	4.987005	-1.700564
6	-4.444618	2.792277	-1.378212
6	-4.433285	3.432852	-2.777840
6	-5.182051	-0.357303	-1.557278
6	-5.412305	-0.801517	-3.012588
8	-4.886453	0.197672	3.319494
1	-1.922540	3.791181	-1.032410
1	4.208150	2.326465	-0.082357
1	2.708427	-3.879014	-0.083852
1	-3.382929	-2.406557	-1.282122
1	0.046370	-0.818205	-3.149052
1	0.237037	0.965910	-3.101376
1	1.681188	-0.088698	-2.943813
1	-5.284317	-1.219155	-0.888715
1	-5.967146	0.347330	-1.263802
1	-4.649634	-1.520400	-3.328679
1	-5.356997	0.055104	-3.691357
1	-3.290195	-4.564100	-0.577026
1	-2.181394	-5.918099	-0.642258
1	-0.082285	-6.429095	-0.194495
1	1.408881	-5.707882	0.373135
1	-5.464997	2.483082	-1.129496
1	-4.167512	3.541141	-0.626852
1	4.760464	-3.621445	0.873081
1	6.141469	-2.552419	0.749023
1	-6.394438	-1.270404	-3.131585
1	6.659409	-0.412897	0.738060
1	5.920228	1.169903	0.856073
1	7.584093	1.130883	-1.005880
1	5.957398	1.369899	-1.671925
1	6.722526	-0.217440	-1.771701
1	6.110794	-2.770409	-1.759054
1	4.704146	-3.830986	-1.655092
1	6.258945	-4.359084	-0.983821
1	2.175656	-5.421051	-2.029194
1	0.676830	-6.171619	-2.580386
1	1.844833	-7.119853	-1.640203
1	-3.547276	-5.789926	-2.738720
1	-1.830419	-5.536886	-3.106544
1	-2.929932	-4.157410	-3.054746
1	-5.104178	4.296720	-2.820519
1	-4.754251	2.711168	-3.535494
1	-3.427124	3.767791	-3.049137
1	0.757117	6.368405	-0.438918
1	-0.836718	5.652212	-0.331593
1	-0.612293	6.950464	-2.454672
1	-0.808886	5.228795	-2.832361
1	0.789940	5.970682	-2.926027

1	3.890719	4.537929	0.414333
1	2.873898	5.869690	-0.093170
1	4.876332	5.662842	-1.586739
1	3.387919	5.368009	-2.506361
1	4.399499	4.008411	-2.013925
1	-1.881045	-1.215023	1.388063
1	0.891837	2.032380	1.964968
1	-0.894471	3.336849	3.096715
1	-5.366083	-2.805211	1.250434
1	-6.266082	-1.321363	1.705673
1	-5.489868	-2.297162	2.966512
1	0.591352	-0.601572	1.961436
1	3.245979	-0.423493	2.452736
1	-0.455494	-2.238168	3.828909
1	3.238267	1.090109	4.366847
1	-0.500294	-0.744696	5.753680
1	1.654933	0.462450	6.205103
1	1.480248	-2.168215	2.247262
1	0.742895	1.448434	5.095523

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^{3}B

Number of imaginary frequencies : 0 Electronic energy : HF=-2529.976666
Zero-point correction= 1.013757 (Hartree/Particle)
Thermal correction to Energy= 1.076220
Thermal correction to Enthalpy= 1.077164
Thermal correction to Gibbs Free Energy= 0.910434
Sum of electronic and zero-point Energies= -2528.962909
Sum of electronic and thermal Energies= -2528.900446
Sum of electronic and thermal Enthalpies= -2528.899502
Sum of electronic and thermal Free Energies= -2529.066232

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Cartesian Coordinates

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6	5.322697	2.100029	1.279106
6	4.078949	2.001806	1.756389
6	3.402403	0.694478	2.051961
6	4.238099	-0.496046	1.678970
6	5.480673	-0.403496	1.200373
6	6.192056	0.906734	0.981507
6	2.514333	1.251919	-1.232325
6	2.256910	-0.097659	-1.400957
7	1.036570	-0.713358	-1.188780
6	1.209560	-2.052504	-1.461491
6	2.582592	-2.294546	-1.863986
6	3.229240	-1.085848	-1.827747
77	-0.656334	0.171202	-0.510036
6	-1.403276	0.849146	-2.487768
6	0.222747	-3.021484	-1.343038
6	-1.089953	-2.826114	-0.933531
7	-1.626205	-1.614966	-0.567343
6	-2.932450	-1.848896	-0.184933
6	-3.232112	-3.262300	-0.329331
6	-2.092238	-3.867074	-0.792768
6	3.124671	-3.627804	-2.281473
6	2.747083	-3.999943	-3.726739
6	4.644612	-0.774228	-2.204403
6	4.770177	-0.203835	-3.628224
6	-1.879254	-5.306055	-1.153033

6	-1.961678	-5.559805	-2.669211
6	-4.572310	-3.880567	-0.067628
6	-5.563178	-3.664663	-1.225926
6	-3.821038	-0.885927	0.266132
6	-3.586507	0.480334	0.396659
7	-2.398162	1.096696	0.125054
6	-2.568843	2.438463	0.347207
6	-3.933757	2.687386	0.781566
6	-4.565341	1.469766	0.815798
6	-4.507775	4.043566	1.061608
6	-4.881652	4.808203	-0.221222
6	-1.579869	3.406795	0.200329
6	-0.259338	3.213914	-0.190098
7	0.303192	2.003098	-0.510919
6	1.610332	2.233012	-0.837011
6	1.903665	3.652255	-0.717956
6	0.742019	4.261108	-0.315921
6	-5.997709	1.170459	1.141077
6	-6.872058	1.006406	-0.115383
6	3.221277	4.280182	-1.057002
6	3.422509	4.461892	-2.572272
6	0.481863	5.722185	-0.104618
6	-0.208526	6.384088	-1.310913
6	-0.161576	-0.025248	1.488608
6	0.415336	-1.260198	1.873774
6	0.889156	-1.481969	3.151455
6	0.750662	-0.453368	4.184906
6	0.128021	0.788590	3.755702
6	-0.300630	0.988245	2.465067
6	1.629210	-2.736969	3.440028
8	1.097211	-3.792250	2.762321
6	1.827835	-5.016311	2.898135
8	1.110463	-0.620250	5.370808
8	2.617602	-2.834183	4.134837
1	-4.811817	-1.233084	0.534992
1	-1.868635	4.426271	0.428632
1	3.530636	1.577049	-1.414082
1	0.511259	-4.038690	-1.579524
1	-0.574353	0.647607	-3.167536
1	-2.279775	0.234301	-2.692127
1	-1.643428	1.908234	-2.432335
1	-0.902981	-5.640029	-0.780141
1	-2.625069	-5.923432	-0.641633
1	-1.215478	-4.967133	-3.207302
1	-2.946152	-5.277097	-3.054292
1	2.761826	-4.405770	-1.598235
1	4.215028	-3.622693	-2.181918
1	5.251294	-1.681989	-2.120825
1	5.062882	-0.066612	-1.482376
1	-4.449310	-4.954468	0.107416
1	-4.996854	-3.470660	0.856828
1	4.031490	3.667101	-0.648061
1	3.296754	5.255078	-0.563172
1	-1.792630	-6.616052	-2.901434
1	1.429118	6.233915	0.095234
1	-0.134290	5.865898	0.791571
1	-0.392162	7.447243	-1.125877
1	-1.167806	5.903085	-1.525998
1	0.412640	6.293662	-2.207155
1	2.646389	5.108389	-2.993558

1	3.367727	3.500532	-3.092529
1	4.397218	4.911292	-2.787553
1	4.185604	0.715281	-3.734786
1	4.397516	-0.918465	-4.368616
1	5.813300	0.025381	-3.868216
1	3.148640	-4.981324	-3.998441
1	3.141949	-3.260864	-4.430393
1	1.660413	-4.027429	-3.853834
1	-6.534047	-4.118529	-1.003338
1	-5.179958	-4.109538	-2.149338
1	-5.719000	-2.598013	-1.414702
1	-6.405472	1.974841	1.762430
1	-6.058707	0.259235	1.748595
1	-7.909051	0.780409	0.152653
1	-6.498015	0.196792	-0.749744
1	-6.863926	1.922832	-0.713308
1	-3.792902	4.638072	1.643794
1	-5.396869	3.938880	1.692306
1	-5.289771	5.796368	0.013704
1	-5.631016	4.254889	-0.795412
1	-4.007477	4.943016	-0.865730
1	0.529226	-2.051329	1.144618
1	-0.745064	1.937889	2.191610
1	0.018073	1.554050	4.517998
1	1.281500	-5.753501	2.309035
1	1.878229	-5.322924	3.945869
1	2.848302	-4.902853	2.521021
1	3.140043	0.639152	3.119283
1	3.502244	2.903983	1.949632
1	3.791279	-1.473207	1.839978
1	5.757917	3.081832	1.100505
1	6.036631	-1.308012	0.961632
1	6.568528	0.966586	-0.053396
1	2.437694	0.651677	1.532300
1	7.102722	0.944911	1.601570

E

Number of imaginary frequencies : 0 Electronic energy : HF=-2530.0126206
Zero-point correction= 1.013208 (Hartree/Particle)
Thermal correction to Energy= 1.075630
Thermal correction to Enthalpy= 1.076575
Thermal correction to Gibbs Free Energy= 0.908647
Sum of electronic and zero-point Energies= -2528.999412
Sum of electronic and thermal Energies= -2528.936990
Sum of electronic and thermal Enthalpies= -2528.936046
Sum of electronic and thermal Free Energies= -2529.103974

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Cartesian Coordinates

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6	4.082761	2.249813	0.303295
6	3.252280	1.095879	-0.000272
7	1.950231	1.497103	-0.171806
6	1.917974	2.859694	0.004015
6	3.255654	3.344061	0.302873
6	3.703469	-0.215326	-0.103299
6	2.947930	-1.341249	-0.402810
7	1.586796	-1.348551	-0.612981
6	1.227864	-2.644670	-0.891224

6	2.403825	-3.497390	-0.852938
6	3.470671	-2.689390	-0.548342
6	-0.067953	-3.073662	-1.155113
6	-1.210274	-2.289104	-1.207418
7	-1.241001	-0.925444	-1.017759
6	-2.551587	-0.533081	-1.122167
6	-3.389687	-1.688376	-1.398537
6	-2.558412	-2.777159	-1.447845
77	0.352850	0.287469	-0.615165
7	-0.887106	1.906953	-0.537678
6	-2.256295	1.888458	-0.661342
6	-2.789503	3.221086	-0.433524
6	-1.715655	4.042646	-0.213265
6	-0.526457	3.208034	-0.278012
6	-2.910410	-4.205788	-1.733503
6	-2.640707	-4.606849	-3.194781
6	-4.872469	-1.625528	-1.609680
6	-5.259139	-1.077122	-2.994899
6	-3.015626	0.762717	-0.934307
6	4.919546	-3.060440	-0.441910
6	5.713388	-2.733269	-1.719615
6	2.402938	-4.966601	-1.151128
6	2.362673	-5.269518	-2.659853
6	0.772619	3.643633	-0.051046
6	-1.709754	5.519445	0.040216
6	-1.359674	6.338188	-1.215258
6	-4.249519	3.555176	-0.426795
6	-4.847230	3.690491	-1.838134
6	3.617051	4.785673	0.499946
6	3.734827	5.556279	-0.827487
6	5.568820	2.205243	0.496873
6	6.340345	2.139293	-0.833794
6	0.743489	0.575101	-2.616207
6	0.382409	0.290055	2.254645
6	-0.804772	-0.440149	2.045184
6	-2.054828	0.153059	2.174006
6	-2.144311	1.575629	2.518767
6	-0.885399	2.267896	2.773931
6	0.329277	1.644771	2.654710
6	-3.285006	-0.657223	1.963386
8	-4.413838	-0.244352	1.795762
8	-3.221891	2.204274	2.610519
8	-2.989081	-1.984921	1.989913
6	-4.100761	-2.866024	1.820347
6	0.811275	-2.184814	4.738365
6	1.870755	-2.385492	3.693659
6	1.667508	-3.168398	2.593065
6	0.442325	-3.856335	2.392066
6	-0.593816	-3.734499	3.351676
6	-0.448988	-2.951994	4.462172
1	0.901377	4.703397	0.136643
1	4.763635	-0.374706	0.056970
1	-0.200570	-4.135262	-1.329542
1	-4.088293	0.901498	-0.970514
1	0.131340	-0.119689	-3.196651
1	0.494889	1.606692	-2.876899
1	1.804372	0.385928	-2.798361
1	-4.784398	2.785712	0.141418
1	-4.401400	4.490438	0.121536
1	-4.726101	2.765339	-2.410406

1	-4.346943	4.488296	-2.396540
1	-5.324201	-1.005739	-0.825591
1	-5.299068	-2.627985	-1.491442
1	-3.968130	-4.373153	-1.502733
1	-2.346225	-4.867893	-1.064501
1	-2.693172	5.826220	0.410824
1	-0.997348	5.757561	0.840245
1	1.544668	-5.445615	-0.663146
1	3.294128	-5.428450	-0.712864
1	-5.915822	3.923539	-1.791294
1	5.007420	-4.130809	-0.226535
1	5.375139	-2.542123	0.411076
1	6.768406	-3.004227	-1.609725
1	5.655461	-1.665666	-1.952573
1	5.305939	-3.279170	-2.575974
1	3.236895	-4.843452	-3.161487
1	1.472700	-4.832150	-3.122421
1	2.351754	-6.348329	-2.845828
1	-1.586407	-4.463639	-3.450883
1	-3.231776	-3.988843	-3.877474
1	-2.897327	-5.656462	-3.371344
1	-6.346764	-1.036148	-3.111389
1	-4.851618	-1.710927	-3.788754
1	-4.861516	-0.068608	-3.142242
1	-1.355454	7.411566	-0.999330
1	-2.087378	6.150591	-2.010723
1	-0.373032	6.062602	-1.600975
1	4.566169	4.853322	1.042557
1	2.868660	5.274230	1.136528
1	3.990172	6.606503	-0.653140
1	2.793948	5.519782	-1.384868
1	4.509965	5.114819	-1.461319
1	5.838806	1.340296	1.115553
1	5.890895	3.089703	1.057105
1	7.420836	2.096211	-0.662495
1	6.124758	3.018925	-1.447880
1	6.049013	1.256411	-1.411005
1	-0.734549	-1.488859	1.794714
1	1.252748	2.187785	2.825441
1	-0.974388	3.313379	3.047851
1	-3.674879	-3.868915	1.787530
1	-4.632555	-2.649825	0.894047
1	-4.796381	-2.772040	2.659125
1	1.332224	-0.223608	2.178240
1	2.448576	-3.264257	1.846416
1	-1.529965	-4.260088	3.187899
1	2.817813	-1.869778	3.829642
1	-1.263442	-2.856469	5.174390
1	1.205673	-2.446456	5.738064
1	0.298489	-4.457562	1.502314
1	0.578161	-1.106624	4.830323

$^{CSS}B_{Ru}$

Number of imaginary frequencies : 0 Electronic energy : HF=-6014.9231141
Zero-point correction= 0.583384 (Hartree/Particle)
Thermal correction to Energy= 0.639857
Thermal correction to Enthalpy= 0.640801
Thermal correction to Gibbs Free Energy= 0.483109

Sum of electronic and zero-point Energies= -6014.339730
Sum of electronic and thermal Energies= -6014.283258
Sum of electronic and thermal Enthalpies= -6014.282313
Sum of electronic and thermal Free Energies= -6014.440005

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Cartesian Coordinates

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6	-5.482116	-5.493821	-0.671956
6	-4.953875	-5.180155	-1.922154
6	-3.976872	-4.190325	-2.016904
6	-3.502467	-3.497340	-0.892563
6	-4.064714	-3.842037	0.348596
6	-5.043203	-4.827239	0.469906
6	-2.453672	-2.438562	-0.992421
6	-2.905710	-1.111674	-1.022127
7	-2.099236	-0.000125	-0.980803
6	-2.905930	1.111249	-1.022057
6	-4.289678	0.680975	-1.083669
6	-4.289544	-0.681666	-1.083694
6	-2.454149	2.438234	-0.992259
6	-3.503146	3.496799	-0.892365
6	-4.065568	3.841269	0.348775
6	-5.044252	4.826279	0.470103
6	-5.483176	5.492915	-0.671721
6	-4.954761	5.179476	-1.921903
6	-3.977588	4.189818	-2.016672
44	-0.000003	0.000044	-0.773546
7	0.000227	-2.059065	-1.053387
6	1.118077	-2.871705	-1.012514
6	0.683813	-4.245463	-0.964692
6	-0.682935	-4.245595	-0.964730
6	-1.117459	-2.871926	-1.012535
6	2.454217	-2.438116	-0.992346
6	3.503198	-3.496706	-0.892419
6	4.065389	-3.841328	0.348790
6	5.044038	-4.826364	0.470177
6	5.483173	-5.492849	-0.671656
6	4.955000	-5.179245	-1.921898
6	3.977840	-4.189579	-2.016724
17	3.531251	-3.013942	1.797748
17	3.334976	-3.801396	-3.600543
17	-3.531668	3.013727	1.797732
17	-3.334474	3.801833	-3.600445
17	-3.333941	-3.802070	-3.600680
17	-3.530815	-3.014544	1.797581
6	2.906022	-1.111145	-1.022036
7	2.099335	0.000233	-0.980825
6	2.905803	1.111771	-1.021953
6	4.289654	0.681773	-1.083350
6	4.289786	-0.680869	-1.083405
6	2.453745	2.438651	-0.992197
6	3.502521	3.497442	-0.892243
6	4.064578	3.842228	0.348972
6	5.043046	4.827447	0.470352
6	5.482116	5.493952	-0.671493
6	4.954057	5.180196	-1.921747
6	3.977080	4.190348	-2.016568
17	3.530482	3.014805	1.797914
17	3.334356	3.801987	-3.600402
6	1.117526	2.872009	-1.012327

7	-0.000175	2.059165	-1.053214
6	-1.118011	2.871826	-1.012334
6	-0.683729	4.245571	-0.964467
6	0.683019	4.245683	-0.964437
6	-0.000035	-0.000036	1.135099
6	1.241359	-0.000032	1.908639
6	1.232814	-0.000128	3.258713
6	-0.000102	-0.000257	4.083514
6	-1.232985	-0.000214	3.258669
6	-1.241478	-0.000065	1.908599
35	2.918235	-0.000103	4.241784
35	-2.918448	-0.000374	4.241674
8	-0.000118	-0.000415	5.302981
1	2.182085	0.000041	1.379635
1	-2.182195	0.000007	1.379576
1	5.447915	5.062778	1.447351
1	5.291204	5.688935	-2.816901
1	6.243179	6.262823	-0.586554
1	5.448992	-5.061568	1.447171
1	5.292190	-5.687977	-2.817040
1	6.244378	-6.261580	-0.586726
1	-5.449393	5.061344	1.447053
1	-5.291773	5.688321	-2.817048
1	-6.244399	6.261632	-0.586828
1	-5.290893	-5.688960	-2.817319
1	-5.448209	-5.062498	1.446865
1	-6.243199	-6.262678	-0.587077
1	5.141279	-1.343133	-1.137270
1	5.141015	1.344209	-1.137161
1	1.342086	5.100663	-0.933646
1	-1.342939	5.100443	-0.933705
1	-5.141164	1.343241	-1.137600
1	-5.140900	-1.344096	-1.137667
1	1.343034	-5.100325	-0.933943
1	-1.341991	-5.100586	-0.933989

$^{CSS}TS(B\text{-}D)_{Ru}$

Number of imaginary frequencies : 1 Electronic energy : HF=-6248.3637232
Zero-point correction= 0.702127 (Hartree/Particle)
Thermal correction to Energy= 0.764388
Thermal correction to Enthalpy= 0.765332
Thermal correction to Gibbs Free Energy= 0.597374
Sum of electronic and zero-point Energies= -6247.661596
Sum of electronic and thermal Energies= -6247.599335
Sum of electronic and thermal Enthalpies= -6247.598391
Sum of electronic and thermal Free Energies= -6247.766349

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Cartesian Coordinates

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6	-6.686664	-3.712508	-1.602929
6	-6.072827	-3.138643	-2.713704
6	-4.894413	-2.413961	-2.541676
6	-4.296190	-2.240960	-1.282171
6	-4.952004	-2.834750	-0.192717
6	-6.131172	-3.563976	-0.334388
6	-3.032654	-1.458563	-1.119419
6	-3.181031	-0.095395	-0.805140
7	-2.149379	0.803044	-0.627994

6	-2.702918	2.048400	-0.416341
6	-4.145142	1.922627	-0.434488
6	-4.437525	0.607843	-0.663247
6	-1.984549	3.246037	-0.248036
6	-2.792493	4.506658	-0.219913
6	-3.278483	5.094156	0.957134
6	-4.027671	6.270051	0.958642
6	-4.311073	6.894442	-0.252767
6	-3.851827	6.349315	-1.449240
6	-3.105323	5.172957	-1.419744
44	-0.109341	0.364131	-0.731991
7	-0.571002	-1.598379	-1.283031
6	0.343272	-2.594829	-1.534055
6	-0.373778	-3.833741	-1.764890
6	-1.704752	-3.562354	-1.648704
6	-1.831429	-2.151736	-1.341336
6	1.739037	-2.432024	-1.568430
6	2.543296	-3.653987	-1.878597
6	3.030506	-4.499338	-0.868235
6	3.780778	-5.639740	-1.154907
6	4.059573	-5.957206	-2.481681
6	3.595629	-5.145879	-3.514643
6	2.848436	-4.011820	-3.201880
17	2.698891	-4.129348	0.808009
17	2.276857	-3.005421	-4.519266
17	-2.948237	4.337833	2.506130
17	-2.545377	4.514655	-2.942707
17	-4.149726	-1.693834	-3.953874
17	-4.267916	-2.671034	1.414159
6	2.459394	-1.239876	-1.384182
7	1.910694	-0.007694	-1.111767
6	2.938661	0.903694	-1.010418
6	4.193655	0.213450	-1.231994
6	3.900417	-1.098047	-1.459674
6	2.787454	2.271519	-0.726007
6	4.032619	3.098614	-0.729160
6	4.696881	3.453635	0.455703
6	5.856738	4.226792	0.459837
6	6.381609	4.668837	-0.751944
6	5.753612	4.345901	-1.952424
6	4.593991	3.572896	-1.927042
17	4.066904	2.905421	1.997002
17	3.815188	3.199870	-3.451588
6	1.584817	2.958507	-0.480684
7	0.329894	2.389255	-0.447057
6	-0.587900	3.401110	-0.255989
6	0.124761	4.656826	-0.133606
6	1.454504	4.385487	-0.267210
6	0.095671	-0.168524	1.200192
6	1.431971	0.034940	1.799222
6	2.001620	-0.896290	2.581886
6	1.330704	-2.153173	2.995848
6	-0.042599	-2.282413	2.447417
6	-0.620904	-1.380119	1.638351
35	3.818530	-0.653286	3.261869
35	-1.006077	-3.904769	2.964915
8	1.843133	-2.984325	3.725333
1	1.956944	0.951140	1.558992
1	-1.633390	-1.523054	1.285995
1	-0.605672	0.732215	1.801535

1	6.335257	4.470647	1.400755
1	6.148847	4.687722	-2.901510
1	7.285027	5.269969	-0.760707
1	4.136223	-6.262548	-0.342702
1	3.805825	-5.381113	-4.551135
1	4.642686	-6.842825	-2.712855
1	-4.377951	6.681498	1.897649
1	-4.065271	6.823805	-2.399559
1	-4.892918	7.810302	-0.264617
1	-6.496174	-3.245241	-3.705289
1	-6.597341	-4.006649	0.537690
1	-7.603830	-4.279165	-1.726533
1	4.590996	-1.903441	-1.662378
1	5.167997	0.679188	-1.214350
1	2.276861	5.085257	-0.241042
1	-0.339870	5.619653	0.022409
1	-4.839840	2.738805	-0.298062
1	-5.414444	0.155198	-0.750966
1	0.089336	-4.783446	-1.989133
1	-2.531223	-4.248793	-1.760594
6	-1.248572	1.356759	2.916038
6	-2.605144	0.837286	2.821224
6	-3.040648	-0.128798	3.654693
6	-2.192659	-0.696854	4.746687
6	-0.859288	-0.035707	4.883452
6	-0.449805	0.952401	4.059261
1	-3.247757	1.222787	2.038790
1	-4.048532	-0.519064	3.548490
1	-2.731381	-0.644328	5.707447
1	-0.223303	-0.357070	5.703658
1	0.517079	1.421538	4.206966
1	-1.062326	2.339917	2.488392
1	-2.054181	-1.779701	4.583576

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^{OSS}TS(B-C)$_{Ru}$

Number of imaginary frequencies : 1 Electronic energy : HF=-6248.3554578
Zero-point correction= 0.699774 (Hartree/Particle)
Thermal correction to Energy= 0.762845
Thermal correction to Enthalpy= 0.763789
Thermal correction to Gibbs Free Energy= 0.588996
Sum of electronic and zero-point Energies= -6247.655684
Sum of electronic and thermal Energies= -6247.592613
Sum of electronic and thermal Enthalpies= -6247.591669
Sum of electronic and thermal Free Energies= -6247.766462

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Cartesian Coordinates

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6	6.020678	0.670289	-2.556032
6	5.282338	-0.590320	-2.624454
6	5.932799	-1.692646	-3.329816
6	7.057611	-1.511521	-4.050622
6	7.752068	-0.184669	-4.141685
6	7.146068	0.874604	-3.268711
8	3.060779	-0.085709	-3.795958
6	2.162007	-0.052261	-2.863325
6	1.748480	1.158076	-2.229971
6	0.806706	1.211274	-1.229745
6	0.213241	0.014241	-0.739535

6	0.586664	-1.215702	-1.350878
6	1.525942	-1.226411	-2.356166
44	-0.998548	0.044833	0.849104
7	-2.457388	1.263850	0.029171
6	-3.506624	0.838130	-0.758858
6	-4.206952	1.997352	-1.256595
6	-3.577722	3.103960	-0.757791
6	-2.472068	2.645921	0.046761
6	-3.849089	-0.500590	-1.016381
6	-3.227067	-1.643315	-0.492592
7	-2.109556	-1.643161	0.306431
6	-1.839755	-2.947045	0.658655
6	-2.830800	-3.809536	0.045553
6	-3.675322	-3.011948	-0.666574
6	-0.766138	-3.365028	1.458767
6	0.219017	-2.545759	2.037447
7	0.263371	-1.167768	1.967825
6	1.418260	-0.747169	2.593196
6	2.123042	-1.906815	3.084251
6	1.379985	-3.007529	2.758175
6	1.833755	0.588359	2.732331
6	1.125513	1.735393	2.344422
6	1.510778	3.107224	2.614769
6	0.547406	3.911492	2.083059
6	-0.434656	3.048362	1.456568
7	-0.057327	1.738853	1.646817
6	-1.550774	3.468623	0.717211
1	0.540983	2.166082	-0.799871
1	0.154403	-2.146026	-1.008561
1	4.217752	-0.328168	-3.314913
1	5.452531	-2.666156	-3.294975
1	5.609213	1.466515	-1.942860
1	7.499924	-2.343784	-4.592266
1	7.654405	1.834429	-3.224223
1	8.822922	-0.302795	-3.904206
1	4.731211	-0.865960	-1.718247
1	7.755241	0.159334	-5.191889
6	-0.653060	-4.832873	1.718447
6	0.062257	-5.685156	0.861981
6	-1.261255	-5.426699	2.835958
6	0.170613	-7.054877	1.098185
6	-1.168898	-6.793172	3.095076
6	-0.449108	-7.602446	2.218997
1	0.733100	-7.674200	0.409694
1	-1.655652	-7.207402	3.969884
1	-0.370965	-8.667622	2.411374
6	3.195731	0.808402	3.303762
6	4.308389	0.941353	2.454780
6	3.439764	0.892586	4.682302
6	5.596828	1.142688	2.945031
6	4.719067	1.093417	5.199694
6	5.794029	1.216818	4.322542
1	6.425609	1.238358	2.253750
1	4.860943	1.152407	6.272193
1	6.793481	1.373211	4.715324
6	-1.774729	4.942963	0.615424
6	-2.632331	5.617051	1.499512
6	-1.142945	5.721912	-0.367976
6	-2.858739	6.989840	1.415761
6	-1.351608	7.096429	-0.472876

6	-2.213349	7.724104	0.423457
1	-3.529336	7.466959	2.120353
1	-0.843311	7.657266	-1.248135
1	-2.382500	8.793472	0.349042
6	-5.002562	-0.730741	-1.937321
6	-4.802684	-0.911439	-3.315989
6	-6.328019	-0.780631	-1.478947
6	-5.860941	-1.128965	-4.196799
6	-7.404383	-0.996360	-2.338227
6	-7.161388	-1.169715	-3.698918
1	-5.660382	-1.262649	-5.253089
1	-8.411397	-1.027583	-1.939756
1	-7.992087	-1.338369	-4.376549
17	-3.174868	-0.862213	-3.959669
17	-6.654528	-0.569996	0.230277
17	4.075841	0.855912	0.718552
17	2.098825	0.746122	5.801055
17	-0.050036	4.955395	-1.500463
17	-3.451176	4.714521	2.759455
17	0.848493	-5.012652	-0.549611
17	-2.173447	-4.428061	3.950670
35	2.623592	2.817518	-2.813349
35	2.074882	-2.937880	-3.154891
1	-4.536016	-3.311230	-1.246665
1	-2.868612	-4.883318	0.155619
1	-5.073841	1.966657	-1.900312
1	-3.836845	4.139698	-0.920738
1	0.499009	4.990253	2.104055
1	2.395986	3.405483	3.157400
1	3.060367	-1.880371	3.620527
1	1.602237	-4.041895	2.975559

BDHA-S2

Number of imaginary frequencies : 0 Electronic energy : HF=-2147.2668345
Zero-point correction= 0.903962 (Hartree/Particle)
Thermal correction to Energy= 0.957278
Thermal correction to Enthalpy= 0.958222
Thermal correction to Gibbs Free Energy= 0.817652
Sum of electronic and zero-point Energies= -2146.362872
Sum of electronic and thermal Energies= -2146.309557
Sum of electronic and thermal Enthalpies= -2146.308612
Sum of electronic and thermal Free Energies= -2146.449183

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Cartesian Coordinates

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6	0.908508	-4.255192	-0.185206
6	1.316699	-2.866962	-0.035739
7	0.212010	-2.059536	-0.067779
6	-0.883303	-2.863969	-0.253882
6	-0.456563	-4.253678	-0.318816
6	2.624341	-2.426301	0.134439
6	3.056677	-1.108302	0.221987
7	2.247787	-0.000797	0.171672
6	3.057419	1.106154	0.222198
6	4.443114	0.684398	0.339956
6	4.442654	-0.687498	0.339795
6	2.625969	2.424453	0.134804
6	1.318646	2.866012	-0.035493

7	0.213401	2.059347	-0.067685
6	-0.881323	2.864532	-0.254054
6	-0.453611	4.253948	-0.318891
6	0.911445	4.254514	-0.185108
77	0.203639	-0.000085	0.039318
7	-1.833862	0.000619	-0.279079
6	-2.638571	1.107459	-0.374653
6	-4.021266	0.687549	-0.504741
6	-4.021747	-0.684835	-0.504617
6	-2.639348	-1.105691	-0.374387
6	1.854499	5.417749	-0.250810
6	2.522483	5.565666	-1.629906
6	-1.366188	5.416638	-0.569762
6	-1.741471	5.568867	-2.054971
6	-2.194247	2.424862	-0.360952
6	5.618204	-1.617576	0.369306
6	6.017217	-2.119217	-1.030569
6	5.619290	1.613674	0.369730
6	6.018631	2.115483	-1.029991
6	-2.195940	-2.423394	-0.360599
6	-5.189652	-1.614304	-0.629190
6	-5.378047	-2.151406	-2.059129
6	-5.188493	1.617799	-0.629803
6	-5.375737	2.155112	-2.059833
6	-1.370017	-5.415720	-0.569484
6	-1.745578	-5.567834	-2.054631
6	1.850733	-5.419093	-0.251026
6	2.518646	-5.567303	-1.630124
6	-0.302705	-0.000052	2.062134
6	-0.827442	-1.232209	2.643985
6	-2.172750	-1.248417	2.819892
6	-2.956524	0.001357	2.748232
6	-2.171463	1.250391	2.819841
6	-0.826186	1.232685	2.643948
8	-4.188673	0.002010	2.728870
6	0.362541	-0.000191	-2.082127
1	-2.954871	3.190071	-0.460846
1	3.393675	3.188115	0.176846
1	3.391535	-3.190488	0.176297
1	-2.957134	-3.188059	-0.460326
1	-0.116096	-0.891086	-2.499252
1	-0.113274	0.892210	-2.499266
1	1.421971	-0.001892	-2.359846
1	-5.066601	-2.452859	0.066397
1	-6.099175	-1.094265	-0.311979
1	-4.487152	-2.690035	-2.397239
1	-5.549222	-1.329315	-2.760974
1	-2.284798	-5.305720	0.026130
1	-0.891376	-6.337399	-0.221184
1	1.309234	-6.340430	-0.010853
1	2.626226	-5.314272	0.518108
1	-6.098547	1.098333	-0.313174
1	-5.065301	2.456256	0.065884
1	5.396353	-2.477400	1.013333
1	6.473412	-1.109121	0.827571
1	-6.232539	-2.833597	-2.115233
1	6.474160	1.104492	0.827819
1	5.398033	2.473447	1.014030
1	6.871294	2.800008	-0.975106
1	5.186899	2.640778	-1.509133

1	6.293011	1.276608	-1.676674
1	6.292171	-1.280325	-1.676986
1	5.185126	-2.643790	-1.509877
1	6.869410	-2.804344	-0.975898
1	3.078531	-4.664317	-1.891731
1	1.765186	-5.723228	-2.408112
1	3.209290	-6.416674	-1.645097
1	-2.421708	-6.415482	-2.205875
1	-0.850882	-5.728826	-2.663696
1	-2.238244	-4.664496	-2.426635
1	-6.229790	2.837816	-2.116381
1	-5.546987	1.333158	-2.761815
1	-4.484325	2.693230	-2.397387
1	-0.886892	6.337998	-0.221518
1	-2.281123	5.307394	0.025756
1	-2.416934	6.417016	-2.206380
1	-2.234790	4.665866	-2.426930
1	-0.846586	5.729106	-2.663955
1	2.629941	5.312254	0.518283
1	1.313678	6.339445	-0.010481
1	3.213781	6.414508	-1.644769
1	1.769125	5.722291	-2.407850
1	3.081663	4.662286	-1.891659
1	-2.724044	2.164744	3.017603
6	0.066358	-2.417090	2.897454
1	0.123189	-2.591747	3.977976
1	-0.319617	-3.327529	2.431441
1	1.074843	-2.237703	2.527182
6	0.068966	2.416546	2.897528
1	0.125639	2.591244	3.978047
1	1.077354	2.235855	2.527619
1	-0.315745	3.327401	2.431282
1	-2.726315	-2.162178	3.017720

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^{CSS}TS(B-E)$_{DHA-S2}$

Number of imaginary frequencies : 1 Electronic energy : HF=-2688.0873251
Zero-point correction= 1.120237 (Hartree/Particle)
Thermal correction to Energy= 1.183965
Thermal correction to Enthalpy= 1.184909
Thermal correction to Gibbs Free Energy= 1.022387
Sum of electronic and zero-point Energies= -2686.967089
Sum of electronic and thermal Energies= -2686.903360
Sum of electronic and thermal Enthalpies= -2686.902416
Sum of electronic and thermal Free Energies= -2687.064938

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Cartesian Coordinates

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6	4.014867	-3.522939	2.109594
6	3.641191	-2.370892	1.423093
6	3.221014	-1.235663	2.126712
6	3.198880	-1.249411	3.534525
6	3.578115	-2.405699	4.213226
6	3.977825	-3.543098	3.506004
6	2.726205	-0.000086	4.241350
6	3.199658	1.248848	3.534355
6	3.221839	1.234868	2.126546
6	2.802340	-0.000312	1.433983
6	3.642858	2.369701	1.422781

6	4.017281	3.521602	2.109124
6	3.980151	3.542007	3.505526
6	3.579629	2.404986	4.212897
6	0.084959	0.000209	1.544176
6	-0.328687	-1.244553	2.185381
6	-1.510272	-1.233978	2.865344
6	-2.230950	0.000725	3.165152
6	-1.509808	1.235154	2.865308
6	-0.328267	1.245163	2.185251
77	-0.580415	0.000016	-0.755192
6	-1.395467	0.000409	-2.681059
6	0.395227	-2.549909	1.988191
8	-3.362277	0.000943	3.673183
6	0.396051	2.550219	1.987766
7	-2.505573	0.001951	-0.055565
6	-3.269924	1.107192	0.226028
6	-4.556842	0.689022	0.755446
6	-4.557878	-0.680876	0.756429
6	-3.271661	-1.101736	0.227440
6	-5.640989	1.620699	1.201037
6	-6.485704	2.162124	0.034112
6	-2.878452	2.423022	0.016423
6	-1.664613	2.861552	-0.496611
7	-0.609483	2.051955	-0.832426
6	0.400682	2.863805	-1.281357
6	-0.023930	4.253697	-1.216972
6	-1.305940	4.252330	-0.732749
6	-2.882445	-2.418424	0.019087
6	-1.669576	-2.859455	-0.494077
7	-0.613188	-2.051935	-0.830908
6	0.395248	-2.865832	-1.280054
6	-0.031896	-4.254904	-1.214889
6	-1.313539	-4.250995	-0.729688
6	-5.643318	-1.610305	1.203554
6	-6.489683	-2.151391	0.037677
6	1.652105	2.424197	-1.692780
6	2.080742	1.105596	-1.796545
7	1.318277	-0.001925	-1.503757
6	2.078691	-1.111037	-1.795899
6	3.394420	-0.691643	-2.242329
6	3.395701	0.683527	-2.242707
6	0.805777	5.419057	-1.663859
6	0.819980	5.591089	-3.193436
6	-2.227299	5.416600	-0.526890
6	-3.241883	5.581949	-1.672724
6	1.647494	-2.428765	-1.691701
6	4.485859	-1.620272	-2.684061
6	4.292132	-2.125375	-4.125366
6	4.488888	1.609895	-2.684858
6	4.296441	2.114212	-4.126607
6	0.795386	-5.421987	-1.661776
6	0.810043	-5.593527	-3.191407
6	-2.236911	-5.413483	-0.522789
6	-3.251186	-5.578579	-1.668928
1	-3.606079	-3.182151	0.278573
1	-3.600870	3.188225	0.274951
1	2.364911	3.188919	-1.979137
1	2.358856	-3.194965	-1.977694
1	-2.008497	-0.894199	-2.820494
1	-2.013273	0.892125	-2.817874

1	-0.581452	0.003685	-3.412455
1	1.824978	-5.306980	-1.299205
1	0.413266	-6.338180	-1.198908
1	1.201453	-4.696769	-3.681371
1	-0.203578	-5.757948	-3.569425
1	4.543681	-2.480657	-2.005299
1	5.452129	-1.110413	-2.605939
1	5.454247	1.098419	-2.606044
1	4.548009	2.470702	-2.006748
1	-1.649811	-6.332933	-0.423814
1	-2.777195	-5.295517	0.424876
1	1.835295	5.301523	-1.301914
1	0.426059	6.335958	-1.200407
1	1.430143	-6.445751	-3.488111
1	-1.638609	6.335195	-0.429453
1	-2.767281	5.300777	0.421223
1	-3.907866	6.431736	-1.491198
1	-3.855144	4.682565	-1.783244
1	-2.725325	5.746735	-2.623300
1	-0.193395	5.758528	-3.570784
1	1.208534	4.693356	-3.683896
1	1.442338	6.441628	-3.490251
1	3.344402	2.643071	-4.231783
1	4.285771	1.275872	-4.829627
1	5.102425	2.795804	-4.417028
1	5.097050	-2.808306	-4.415599
1	4.282364	-1.287529	-4.828986
1	3.339315	-2.652974	-4.229806
1	-3.918821	-6.426894	-1.486587
1	-2.734444	-5.745608	-2.619011
1	-3.862734	-4.678211	-1.780960
1	-6.291472	-1.088935	1.914932
1	-5.202491	-2.446190	1.759450
1	-7.266843	-2.833970	0.396841
1	-5.867414	-2.691046	-0.683395
1	-6.975954	-1.331115	-0.499541
1	-5.199144	2.456407	1.756411
1	-6.290511	1.101074	1.912444
1	-7.262432	2.845745	0.392229
1	-6.972385	1.342092	-0.503104
1	-5.862208	2.700713	-0.686693
1	-1.984243	2.162179	3.173924
1	3.034534	-0.000109	5.290877
1	3.012305	-0.000441	0.367594
1	1.623558	0.000246	4.238278
1	4.337177	4.401622	1.559550
1	4.272049	4.437902	4.045013
1	4.269143	-4.439110	4.045611
1	4.334117	-4.403268	1.560142
1	3.560868	-2.419543	5.299712
1	3.649909	-2.343993	0.338799
1	3.562354	2.419001	5.299380
1	3.651640	2.342637	0.338489
1	1.497272	0.000130	1.330368
1	-0.320777	-3.370058	1.902859
1	1.019642	-2.546026	1.101151
1	1.040176	-2.757660	2.846633
1	-0.319663	3.370511	1.901238
1	1.040306	2.758414	2.846639
1	1.021236	2.545616	1.101293

1	-1.985026	-2.160788	3.174113

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^{OSS}TS(B-C)$_{DHA-S2}$

Number of imaginary frequencies : 1 Electronic energy : HF=-2688.0479772
Zero-point correction= 1.118152 (Hartree/Particle)
Thermal correction to Energy= 1.182067
Thermal correction to Enthalpy= 1.183011
Thermal correction to Gibbs Free Energy= 1.019059
Sum of electronic and zero-point Energies= -2686.929826
Sum of electronic and thermal Energies= -2686.865910
Sum of electronic and thermal Enthalpies= -2686.864966
Sum of electronic and thermal Free Energies= -2687.028918

Cartesian Coordinates

6	1.365454	4.215228	0.972365
6	0.908220	3.092932	0.169168
7	1.488707	1.937461	0.626927
6	2.363755	2.286983	1.638752
6	2.287802	3.719946	1.860283
6	0.144674	3.189641	-0.990170
6	-0.001061	2.197047	-1.954305
7	0.436526	0.902425	-1.821644
6	0.335116	0.301763	-3.062552
6	-0.255227	1.240338	-3.998673
6	-0.485572	2.405945	-3.308491
6	0.721337	-1.001381	-3.354531
6	1.168809	-1.961635	-2.449650
7	1.352518	-1.743995	-1.112335
6	1.726753	-2.927975	-0.538759
6	1.710484	-3.974446	-1.551632
6	1.395779	-3.367344	-2.742748
77	1.273033	0.079086	-0.167581
7	2.370835	-0.707805	1.384645
6	2.587889	-2.038713	1.617612
6	3.449644	-2.184548	2.782737
6	3.801767	-0.916680	3.175020
6	3.115155	0.004334	2.282792
6	1.326727	-3.977419	-4.110170
6	2.563227	-3.657113	-4.969342
6	2.086888	-5.405624	-1.310850
6	3.606164	-5.643435	-1.383046
6	2.212482	-3.070209	0.759933
6	-1.034971	3.700768	-3.828019
6	0.063099	4.683542	-4.273289
6	-0.492442	0.961093	-5.452320
6	0.789105	1.073541	-6.298211
6	3.138048	1.395593	2.369650
6	4.742479	-0.506482	4.267792
6	6.126933	-0.090333	3.738465
6	3.927309	-3.493175	3.337019
6	5.177662	-4.027800	2.615200
6	3.122354	4.475192	2.850463
6	4.567710	4.694475	2.367610
6	0.961456	5.642173	0.752543
6	1.798613	6.339494	-0.335243
6	-0.554879	-0.604785	0.896868
6	-0.776741	-0.318932	2.296356

6	-1.971397	-0.654315	2.917663
6	-2.982072	-1.392205	2.268382
6	-2.732731	-1.763962	0.932613
6	-1.572195	-1.407953	0.260285
8	-4.113884	-1.684744	2.870507
6	3.232888	0.267875	-1.049937
6	-5.716175	0.162049	2.119952
6	-4.892377	0.596927	0.995774
6	-5.137005	0.067026	-0.294278
6	-6.243963	-0.941420	-0.487294
6	-7.341450	-0.879023	0.548051
6	-7.057113	-0.362229	1.829506
1	2.460399	-4.076903	1.076049
1	0.595524	-1.323981	-4.381508
1	-0.250875	4.168427	-1.234901
1	3.774028	1.822995	3.136037
1	3.755960	1.093815	-0.562411
1	3.786661	-0.661367	-0.909596
1	3.105903	0.469994	-2.116499
1	4.309065	0.323979	4.839318
1	4.859484	-1.333377	4.976391
1	6.043620	0.747529	3.039515
1	6.599844	-0.918361	3.201777
1	3.137631	3.939879	3.808078
1	2.657239	5.445832	3.052956
1	1.057958	6.196908	1.692278
1	-0.100140	5.688986	0.481643
1	4.149558	-3.376648	4.403518
1	3.124044	-4.236809	3.275498
1	-1.657834	4.172093	-3.058296
1	-1.701950	3.499007	-4.673307
1	6.788213	0.210744	4.557377
1	-1.243098	1.658604	-5.839192
1	-0.919161	-0.042402	-5.572175
1	0.586301	0.854048	-7.351318
1	1.554780	0.376867	-5.943892
1	1.207824	2.082270	-6.232352
1	0.660876	4.253869	-5.082676
1	0.743678	4.910309	-3.447129
1	-0.370355	5.623833	-4.628683
1	1.720254	5.808375	-1.288685
1	2.856198	6.358110	-0.055665
1	1.465786	7.371099	-0.488449
1	5.153905	5.239917	3.114090
1	4.580716	5.267291	1.435415
1	5.064721	3.739452	2.172363
1	5.489835	-4.992328	3.028470
1	6.011117	-3.325988	2.714914
1	4.984839	-4.158973	1.546107
1	1.587002	-6.042440	-2.049013
1	1.712894	-5.727677	-0.331784
1	3.851788	-6.691768	-1.184983
1	4.133097	-5.023394	-0.651415
1	3.991173	-5.381816	-2.373273
1	0.425268	-3.626623	-4.628507
1	1.220333	-5.063646	-4.019196
1	2.480659	-4.108233	-5.963445
1	3.472453	-4.037485	-4.493953
1	2.685332	-2.576603	-5.092119
1	-3.512754	-2.312242	0.414332

1	-4.981277	-0.879120	2.544361
1	-6.664260	-0.856741	-1.495951
1	-5.655449	0.797743	3.005622
1	-5.791391	-1.946682	-0.441736
6	0.162125	0.459506	3.179652
1	-0.346696	0.741722	4.104981
1	1.039721	-0.123470	3.457730
1	0.500960	1.369596	2.694494
6	-1.566310	-1.841077	-1.183714
1	-1.214210	-1.049632	-1.834171
1	-0.950658	-2.727850	-1.345440
1	-2.584881	-2.088576	-1.493197
6	-4.299787	0.423033	-1.348635
6	-3.786549	1.447978	1.187469
6	-2.935930	1.759877	0.136244
1	-2.064295	2.382270	0.302504
6	-3.195198	1.249710	-1.139437
1	-2.533264	1.485723	-1.964318
6	-8.620013	-1.364006	0.271572
6	-8.065324	-0.369705	2.808330
6	-9.332867	-0.865709	2.524606
1	-10.101895	-0.860183	3.291242
6	-9.615487	-1.362610	1.249068
1	-10.605213	-1.744048	1.017007
1	-4.493557	0.022417	-2.340605
1	-3.591632	1.837732	2.181601
1	-8.837685	-1.749208	-0.721710
1	-7.842033	0.025740	3.795623
1	-2.163072	-0.341504	3.939832

$^{CSS}E_{DHA\text{-}S2}$

Number of imaginary frequencies : 0 Electronic energy : HF=-2688.1199272
Zero-point correction= 1.122746 (Hartree/Particle)
Thermal correction to Energy= 1.188001
Thermal correction to Enthalpy= 1.188945
Thermal correction to Gibbs Free Energy= 1.020656
Sum of electronic and zero-point Energies= -2686.997181
Sum of electronic and thermal Energies= -2686.931927
Sum of electronic and thermal Enthalpies= -2686.930982
Sum of electronic and thermal Free Energies= -2687.099271

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Cartesian Coordinates

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6	3.785188	-3.648567	2.134803
6	3.806882	-2.457066	1.432845
6	3.478630	-1.236541	2.078378
6	3.090546	-1.259219	3.451348
6	3.093960	-2.467444	4.141602
6	3.444143	-3.655152	3.496952
6	2.542239	0.001070	4.036090
6	3.088179	1.262811	3.452290
6	3.476276	1.241860	2.079307
6	3.571186	0.003004	1.403480
6	3.802166	2.463461	1.434616
6	3.778263	3.654405	2.137432
6	3.437259	3.659364	3.499606
6	3.089315	2.470545	4.143413
6	-0.061432	-0.000768	2.047047

6	-0.685058	-1.241952	2.375075
6	-1.977805	-1.235542	2.838393
6	-2.725122	-0.002746	3.037239
6	-1.979602	1.231135	2.838490
6	-0.686867	1.239474	2.375125
77	-0.542132	-0.000207	-0.820143
6	-0.984148	-0.001028	-2.836084
6	0.083432	-2.532289	2.244873
8	-3.934389	-0.003631	3.362989
6	0.079619	2.530999	2.244876
7	-2.511715	-0.003580	-0.302861
6	-3.298005	1.098314	-0.065281
6	-4.621674	0.676759	0.362717
6	-4.619522	-0.691175	0.362047
6	-3.294530	-1.108173	-0.066275
6	-5.725515	1.605505	0.761467
6	-6.487974	2.188611	-0.440876
6	-2.881767	2.415736	-0.190226
6	-1.616484	2.859697	-0.550437
7	-0.543234	2.045738	-0.818386
6	0.520473	2.865027	-1.115519
6	0.111316	4.255481	-1.010689
6	-1.215267	4.252588	-0.665589
6	-2.874068	-2.424170	-0.192263
6	-1.607249	-2.863791	-0.552340
7	-0.536566	-2.046180	-0.819489
6	0.529858	-2.861798	-1.116831
6	0.125255	-4.253652	-1.012801
6	-1.201435	-4.255297	-0.668123
6	-5.720597	-1.623707	0.759600
6	-6.481602	-2.207041	-0.443569
6	1.789698	2.428602	-1.470818
6	2.218038	1.112250	-1.592930
7	1.451977	0.003209	-1.308473
6	2.221639	-1.103216	-1.593531
6	3.529104	-0.680998	-2.060533
6	3.526872	0.694535	-2.060153
6	1.003316	5.428572	-1.284523
6	1.167937	5.719927	-2.786997
6	-2.133659	5.422449	-0.479003
6	-3.026836	5.680578	-1.705866
6	1.797628	-2.421010	-1.472005
6	4.611476	-1.606550	-2.531171
6	4.379199	-2.112908	-3.966294
6	4.606140	1.623793	-2.530608
6	4.372354	2.129186	-3.965834
6	1.021264	-5.423654	-1.286759
6	1.187355	-5.714002	-2.789262
6	-2.116030	-5.428269	-0.482451
6	-3.007863	-5.688727	-1.709800
1	-3.610067	-3.188890	0.026239
1	-3.620117	3.177927	0.029145
1	2.518131	3.197786	-1.700091
1	2.528549	-3.187694	-1.701725
1	-2.069856	-0.006535	-2.959369
1	-0.559159	0.897238	-3.291627
1	-0.549999	-0.894318	-3.292781
1	2.006978	-5.245749	-0.837982
1	0.620093	-6.313763	-0.790165
1	1.599028	-4.845849	-3.313166

1	0.219453	-5.943167	-3.245303
1	4.690383	-2.469481	-1.857136
1	5.578974	-1.095360	-2.479285
1	5.575390	1.115953	-2.478507
1	4.681952	2.487122	-1.856732
1	-1.522000	-6.323990	-0.270737
1	-2.749916	-5.269507	0.398873
1	1.989781	5.253866	-0.836143
1	0.599315	6.317172	-0.787525
1	1.856026	-6.564715	-2.956952
1	-1.542506	6.320021	-0.267085
1	-2.766663	5.261169	0.402499
1	-3.692341	6.533413	-1.537427
1	-3.642432	4.804666	-1.931682
1	-2.416149	5.890243	-2.589512
1	0.199121	5.945964	-3.242657
1	1.582364	4.853316	-3.311279
1	1.833684	6.572938	-2.954646
1	3.416095	2.655262	-4.041890
1	4.343526	1.291223	-4.668764
1	5.167946	2.813123	-4.278630
1	5.177088	-2.794137	-4.279145
1	4.347385	-1.275121	-4.669306
1	3.424741	-2.642271	-4.042162
1	-3.670642	-6.543818	-1.542054
1	-2.396136	-5.895949	-2.593303
1	-3.626225	-4.814719	-1.935429
1	-6.417789	-1.093059	1.414665
1	-5.305550	-2.436216	1.367328
1	-7.272966	-2.890121	-0.117747
1	-5.808024	-2.758085	-1.108064
1	-6.941228	-1.408007	-1.033965
1	-5.312855	2.418109	1.370680
1	-6.421310	1.071812	1.415537
1	-7.281320	2.868912	-0.114063
1	-6.945263	1.389244	-1.032640
1	-5.815908	2.742650	-1.104411
1	-2.503229	2.157964	3.053421
1	2.558283	0.000672	5.129373
1	3.834554	0.003695	0.352259
1	1.453981	0.000169	3.736796
1	4.031317	4.585261	1.639449
1	3.433722	4.593055	4.053116
1	3.442350	-4.589242	4.049795
1	4.040043	-4.578576	1.636154
1	2.801072	-2.484140	5.187843
1	4.083337	-2.431883	0.385364
1	2.796394	2.485942	5.189664
1	4.078543	2.439503	0.387082
1	0.926831	-0.000031	1.594921
1	-0.570362	-3.355019	1.949530
1	0.886610	-2.455805	1.511687
1	0.541672	-2.798811	3.202403
1	-0.575332	3.352562	1.948842
1	0.536889	2.798637	3.202556
1	0.883301	2.455526	1.512150
1	-2.500094	-2.163140	3.053257

$P1_{DHA\text{-}S2}$

Number of imaginary frequencies : 0 Electronic energy : HF=-925.7255936
Zero-point correction= 0.358328 (Hartree/Particle)
Thermal correction to Energy= 0.377268
Thermal correction to Enthalpy= 0.378212
Thermal correction to Gibbs Free Energy= 0.311736
Sum of electronic and zero-point Energies= -925.367265
Sum of electronic and thermal Energies= -925.348326
Sum of electronic and thermal Enthalpies= -925.347381
Sum of electronic and thermal Free Energies= -925.413857

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Cartesian Coordinates

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6	4.175883	-0.786992	-0.856052
6	2.830751	-0.956336	-1.176567
6	1.844448	-0.155354	-0.591389
6	2.217756	0.840164	0.324368
6	3.570815	1.012270	0.633314
6	4.547602	0.203766	0.054466
6	1.155507	1.677634	0.996471
6	-0.075287	1.864793	0.142448
6	-0.429347	0.887262	-0.799174
6	0.388427	-0.375515	-0.935890
6	-1.547819	1.100078	-1.614147
6	-2.331370	2.242427	-1.475365
6	-1.991839	3.199863	-0.519087
6	-0.861850	3.012837	0.273137
6	-0.233998	-1.617637	-0.117158
6	-0.280020	-1.344480	1.366738
6	-1.412634	-0.877916	1.922887
6	-2.685336	-0.804336	1.179714
6	-2.704143	-1.500051	-0.123456
6	-1.581235	-1.941732	-0.713758
6	0.947098	-1.645834	2.181903
8	-3.693704	-0.287227	1.654878
6	-1.594198	-2.680445	-2.021420
1	-3.683046	-1.646699	-0.571117
1	1.568964	2.651921	1.277583
1	0.346448	-0.698904	-1.981053
1	0.863636	1.191078	1.938230
1	-3.200655	2.384630	-2.109638
1	-2.596572	4.093654	-0.400495
1	5.593456	0.351292	0.306014
1	4.929389	-1.416478	-1.319423
1	3.857679	1.788635	1.337953
1	2.536558	-1.720040	-1.892841
1	-0.580257	3.767053	1.003379
1	-1.807769	0.359161	-2.363311
1	0.459628	-2.445502	-0.310574
1	0.815748	-1.334285	3.221160
1	1.131230	-2.728233	2.174472
1	1.847842	-1.175974	1.781475
1	-2.613319	-2.821754	-2.388651
1	-1.025927	-2.148953	-2.795215
1	-1.125686	-3.666691	-1.914371
1	-1.462976	-0.612892	2.975516

$P2_{DHA-S2}$

Number of imaginary frequencies : 0 Electronic energy : HF=-925.7518749
Zero-point correction= 0.355368 (Hartree/Particle)
Thermal correction to Energy= 0.375915
Thermal correction to Enthalpy= 0.376859
Thermal correction to Gibbs Free Energy= 0.304194
Sum of electronic and zero-point Energies= -925.396507
Sum of electronic and thermal Energies= -925.375960
Sum of electronic and thermal Enthalpies= -925.375015
Sum of electronic and thermal Free Energies= -925.447681

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Cartesian Coordinates

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6	-0.068061	-2.552581	0.362499
6	0.117588	-1.580709	1.353954
6	-0.942113	-0.730782	1.671031
6	-2.166509	-0.850871	1.006307
6	-2.344576	-1.831148	0.031431
6	-1.291618	-2.690634	-0.298414
6	1.438886	-1.468963	2.072261
8	-3.223944	-0.025641	1.277286
6	-1.483835	-3.754836	-1.351959
6	1.061685	2.120274	0.551270
6	-0.224433	2.107361	0.002956
6	-0.519772	1.200762	-1.080945
6	0.479490	0.338083	-1.538588
6	1.761620	0.337522	-0.978606
6	2.065130	1.261069	0.087756
6	-1.837450	1.195755	-1.632432
6	-2.810701	2.021947	-1.141020
6	-2.524259	2.910059	-0.061778
6	-1.270986	2.950458	0.492379
6	3.378391	1.250118	0.649426
6	4.329789	0.373218	0.199902
6	4.025084	-0.549679	-0.843186
6	2.779641	-0.563564	-1.414427
1	-3.301008	-1.892447	-0.478015
1	0.247396	-0.366460	-2.332289
1	1.285886	2.807251	1.363941
1	-2.882308	0.802425	1.641191
1	5.322599	0.372624	0.639388
1	4.789298	-1.242153	-1.182831
1	-3.812235	1.996365	-1.557647
1	-3.308742	3.559480	0.315744
1	-2.054979	0.502731	-2.439513
1	-1.047761	3.632421	1.308807
1	2.541735	-1.266186	-2.208203
1	3.605041	1.949762	1.449409
1	0.760191	-3.204854	0.097148
1	1.526499	-0.516450	2.599955
1	1.554094	-2.273493	2.808990
1	2.275567	-1.541126	1.372133
1	-2.020006	-4.621395	-0.946129
1	-2.071238	-3.380269	-2.196535
1	-0.524526	-4.112924	-1.736306
1	-0.811907	0.042687	2.423581

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^{3}TS(B-E)$_{DHA-S1}$

Number of imaginary frequencies : 1 Electronic energy : HF=-2837.3192727

Zero-point correction= 1.104493 (Hartree/Particle)
Thermal correction to Energy= 1.170757
Thermal correction to Enthalpy= 1.171701
Thermal correction to Gibbs Free Energy= 0.999220
Sum of electronic and zero-point Energies= -2836.214597
Sum of electronic and thermal Energies= -2836.148333
Sum of electronic and thermal Enthalpies= -2836.147389
Sum of electronic and thermal Free Energies= -2836.319870

Cartesian Coordinates

6	-0.785829	-2.325275	2.560843
6	0.560348	-1.914668	2.145277
6	1.461134	-1.366500	3.164998
6	0.921950	-0.805862	4.340038
6	-0.569721	-0.804121	4.578739
6	-1.360015	-1.759545	3.716520
6	-2.414729	1.145584	2.109439
6	-1.670737	0.300167	1.323888
6	-0.266665	0.453665	1.148255
6	0.398607	1.454650	1.920154
6	-0.315366	2.338563	2.680473
6	-1.772850	2.284784	2.787357
77	0.465372	0.132915	-1.012307
6	0.785740	0.455630	-3.076768
6	-3.836588	0.823110	2.371764
8	-4.405450	0.166985	1.315905
6	-5.719900	-0.333826	1.571080
8	-2.405096	3.158660	3.407110
7	-0.501350	-1.629757	-1.357808
6	0.071933	-2.879121	-1.401630
6	-0.943593	-3.870918	-1.713627
6	-2.129024	-3.195037	-1.855022
6	-1.840229	-1.786695	-1.649985
6	-0.679881	-5.336948	-1.882869
6	-0.077467	-5.678917	-3.257604
6	1.412936	-3.147983	-1.160653
6	2.404443	-2.225991	-0.848932
7	2.212649	-0.866022	-0.732711
6	3.438720	-0.308558	-0.428997
6	4.433722	-1.357705	-0.320637
6	3.795007	-2.544757	-0.585385
6	-2.767321	-0.758548	-1.745002
6	-2.525046	0.603519	-1.604322
7	-1.299215	1.158091	-1.360682
6	-1.479373	2.508908	-1.224238
6	-2.888756	2.830277	-1.392907
6	-3.537083	1.647007	-1.631455
6	-3.478795	-3.744312	-2.205784
6	-3.826297	-3.575583	-3.695804
6	3.685325	1.047185	-0.269318
6	2.772631	2.084500	-0.419178
7	1.449562	1.922067	-0.732319
6	0.874143	3.165685	-0.735672
6	1.881396	4.168513	-0.426289
6	3.060686	3.497407	-0.230092
6	5.885711	-1.128436	-0.026102
6	6.683171	-0.674281	-1.262031
6	4.383321	-3.921538	-0.659130
6	4.673996	-4.368170	-2.103459

6	-0.475188	3.426536	-0.942934
6	1.631269	5.645751	-0.392960
6	1.557689	6.269199	-1.798496
6	4.419240	4.058898	0.062606
6	5.308700	4.147570	-1.190638
6	-3.460757	4.214017	-1.337332
6	-3.242793	5.002950	-2.640982
6	-4.992895	1.413804	-1.892757
6	-5.312191	1.230062	-3.386779
8	-4.440810	1.038757	3.400536
1	-0.781894	4.462469	-0.860465
1	4.698935	1.326878	-0.007491
1	1.717245	-4.186580	-1.215868
1	-3.793547	-1.048800	-1.934585
1	0.058202	-0.142137	-3.629764
1	0.661684	1.515185	-3.301587
1	1.807063	0.133566	-3.296277
1	-5.324518	0.532871	-1.331896
1	-5.570787	2.255958	-1.498290
1	-4.759322	0.383124	-3.805609
1	-5.027123	2.120737	-3.955175
1	-4.245330	-3.253129	-1.593634
1	-3.517741	-4.807231	-1.944157
1	-1.614022	-5.892683	-1.749202
1	-0.004165	-5.687239	-1.092588
1	-4.533208	4.153938	-1.125276
1	-3.019041	4.762326	-0.496735
1	3.704394	-4.641096	-0.185208
1	5.310654	-3.952983	-0.077450
1	-6.380950	1.051357	-3.543139
1	6.326364	-2.049704	0.369604
1	5.986782	-0.378763	0.768448
1	7.735080	-0.504707	-1.011264
1	6.274405	0.254004	-1.672427
1	6.636370	-1.431440	-2.050607
1	5.388079	-3.689883	-2.580188
1	3.761092	-4.361398	-2.706761
1	5.092856	-5.379197	-2.126158
1	0.867309	-5.149350	-3.413804
1	-0.758026	-5.380965	-4.060952
1	0.112194	-6.753145	-3.348516
1	-4.821148	-3.975484	-3.916161
1	-3.098942	-4.100353	-4.322680
1	-3.809020	-2.520399	-3.984597
1	-3.663834	6.010596	-2.566309
1	-3.718782	4.493489	-3.484625
1	-2.176704	5.094149	-2.871652
1	2.425723	6.136165	0.179316
1	0.698799	5.851675	0.146693
1	1.365640	7.345355	-1.742246
1	0.759500	5.809369	-2.389260
1	2.497065	6.115533	-2.338568
1	4.920042	3.444987	0.821602
1	4.313961	5.056025	0.502866
1	6.296364	4.551593	-0.946211
1	4.849284	4.795215	-1.943563
1	5.444666	3.161020	-1.644659
1	-2.168317	-0.532313	0.845372
1	1.480700	1.520018	1.881337
1	0.172133	3.133272	3.237004

1	-6.030758	-0.833499	0.652545
1	-6.406993	0.479998	1.816049
1	-5.705679	-1.043267	2.402531
1	0.302272	-0.841572	1.416759
1	-0.775919	-1.004804	5.637078
1	1.031996	-2.546370	1.395187
1	-0.948929	0.212286	4.398201
6	1.785930	-0.215820	5.266269
6	2.846860	-1.310385	2.938310
6	3.692056	-0.710912	3.863724
1	4.761671	-0.674180	3.678615
6	3.159365	-0.160100	5.034423
1	3.812599	0.308986	5.764125
6	-2.693005	-2.045129	4.023897
6	-1.559828	-3.166851	1.743623
6	-3.456433	-2.872104	3.201347
1	-4.492654	-3.075948	3.454138
6	-2.885466	-3.438468	2.056349
1	-3.473525	-4.082899	1.409648
1	1.373332	0.213498	6.175721
1	3.248542	-1.739584	2.026367
1	-3.144390	-1.590042	4.900883
1	-1.115259	-3.584079	0.847739

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^{CSS}TS(B-E)$_{DHA-S1}$

Number of imaginary frequencies : 1 Electronic energy : HF=-2837.3355241
Zero-point correction= 1.106137 (Hartree/Particle)
Thermal correction to Energy= 1.172086
Thermal correction to Enthalpy= 1.173030
Thermal correction to Gibbs Free Energy= 1.003105
Sum of electronic and zero-point Energies= -2836.227278
Sum of electronic and thermal Energies= -2836.161329
Sum of electronic and thermal Enthalpies= -2836.160385
Sum of electronic and thermal Free Energies= -2836.330310

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Cartesian Coordinates

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6	4.403743	1.447623	-0.351976
6	3.329726	0.522739	-0.681764
7	2.133659	1.189648	-0.678272
6	2.394692	2.503747	-0.378404
6	3.824938	2.676807	-0.169560
6	3.488423	-0.831790	-0.949282
6	2.487953	-1.745023	-1.262601
7	1.146793	-1.455021	-1.350626
6	0.489457	-2.625689	-1.647590
6	1.452271	-3.708187	-1.740028
6	2.691527	-3.162342	-1.500455
6	-0.887294	-2.763204	-1.784463
6	-1.844220	-1.763303	-1.661645
7	-1.573904	-0.446328	-1.397303
6	-2.773735	0.214805	-1.331078
6	-3.859955	-0.726930	-1.551261
6	-3.283914	-1.955224	-1.752937
77	0.281204	0.367666	-1.018528
7	-0.586179	2.203971	-0.724682
6	-1.933180	2.472007	-0.721059
6	-2.155063	3.851657	-0.323377

6	-0.917700	4.409071	-0.127724
6	0.060699	3.364268	-0.381115
6	-3.952114	-3.262288	-2.054915
6	-3.917394	-3.621195	-3.551222
6	-5.310831	-0.351085	-1.582040
6	-5.728754	0.300969	-2.912334
6	-2.933906	1.558276	-1.020854
6	4.028539	-3.840154	-1.535169
6	4.773496	-3.617308	-2.863680
6	1.114817	-5.124629	-2.098042
6	0.895728	-5.319322	-3.609226
6	1.437732	3.500912	-0.244910
6	-0.583037	5.814140	0.269390
6	-0.166124	6.687015	-0.927811
6	-3.507094	4.466862	-0.130823
6	-4.186814	4.866727	-1.452100
6	4.491341	3.986402	0.126336
6	4.662167	4.862631	-1.127818
6	5.856112	1.081493	-0.295437
6	6.506232	0.996214	-1.688128
6	0.010504	0.028593	1.132290
6	-1.364347	-0.246386	1.466823
6	-2.137416	0.733600	2.011191
6	-1.509761	1.986127	2.499029
6	-0.033234	1.968983	2.549737
6	0.697137	0.979556	1.978164
6	-3.612598	0.552407	2.029364
8	-4.452688	1.398525	1.802417
8	-2.151656	2.957383	2.899243
6	0.450766	0.857815	-3.061282
8	-3.919722	-0.742487	2.300271
6	-5.307931	-1.081105	2.226111
6	1.064135	-2.243282	1.849148
6	-0.158394	-2.911840	2.347158
6	-0.665173	-2.565185	3.612245
6	0.062600	-1.548926	4.462511
6	1.534553	-1.408527	4.147215
6	2.013732	-1.747807	2.869273
1	1.799409	4.485683	0.026897
1	4.500252	-1.218436	-0.908141
1	-1.254777	-3.761550	-1.992050
1	-3.950454	1.920991	-0.947267
1	1.129933	1.706743	-3.186521
1	0.842260	-0.003093	-3.612925
1	-0.534849	1.119201	-3.458283
1	-4.134948	3.762640	0.426448
1	-3.409308	5.350887	0.507249
1	-4.312580	4.002464	-2.111977
1	-3.584138	5.604522	-1.991767
1	-5.529419	0.336138	-0.755738
1	-5.922712	-1.244187	-1.411223
1	-4.993299	-3.224874	-1.716637
1	-3.474623	-4.063527	-1.476160
1	-1.448994	6.264416	0.764745
1	0.221206	5.807603	1.015373
1	0.213208	-5.443013	-1.559117
1	1.917715	-5.788137	-1.759485
1	-5.175176	5.300368	-1.268770
1	3.897831	-4.914817	-1.368920
1	4.651270	-3.480166	-0.706484

1	5.749483	-4.113184	-2.856807
1	4.930887	-2.550420	-3.048384
1	4.192613	-4.013724	-3.701958
1	1.799582	-5.054711	-4.166264
1	0.086648	-4.678211	-3.971666
1	0.641471	-6.358768	-3.840271
1	-2.887351	-3.679130	-3.916069
1	-4.431690	-2.856408	-4.141034
1	-4.402929	-4.584500	-3.738687
1	-6.788610	0.574659	-2.900823
1	-5.558663	-0.383993	-3.748802
1	-5.143580	1.205578	-3.102584
1	0.079766	7.705046	-0.608398
1	-0.975417	6.743399	-1.662282
1	0.708203	6.266428	-1.434736
1	5.473139	3.802905	0.576135
1	3.911978	4.537752	0.877352
1	5.140910	5.815783	-0.881086
1	3.693614	5.074416	-1.590599
1	5.278251	4.351309	-1.873800
1	5.976205	0.120355	0.220953
1	6.394476	1.818621	0.310038
1	7.561970	0.715350	-1.615287
1	6.441757	1.960241	-2.201670
1	5.996255	0.256892	-2.313150
1	-1.817746	-1.170861	1.132658
1	1.781368	0.997314	1.990376
1	0.430636	2.828542	3.022617
1	-5.371508	-2.117738	2.557318
1	-5.672282	-0.989241	1.199917
1	-5.901265	-0.429775	2.872087
1	0.685611	-1.235428	1.229072
1	-0.074687	-1.779897	5.524614
1	1.538992	-2.756425	1.011321
1	-0.412680	-0.570671	4.304251
6	2.426948	-0.892738	5.089070
6	3.364122	-1.547485	2.551011
6	4.240260	-1.017377	3.493381
1	5.283729	-0.860201	3.237953
6	3.769830	-0.692073	4.768140
1	4.447409	-0.283348	5.511619
6	-1.870505	-3.126191	4.036570
6	-0.860009	-3.815209	1.536817
6	-2.066361	-4.360261	1.966662
1	-2.607432	-5.053015	1.329218
6	-2.574524	-4.011394	3.220032
1	-3.514514	-4.432190	3.564394
1	2.063524	-0.636057	6.080685
1	3.710329	-1.796183	1.553358
1	-2.267976	-2.856738	5.011345
1	-0.457867	-4.065057	0.561874

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^{3}TS(B-C)$_{DHA-S1}$

Number of imaginary frequencies : 1 Electronic energy : HF=-2837.3162758
Zero-point correction= 1.104064 (Hartree/Particle)
Thermal correction to Energy= 1.170189
Thermal correction to Enthalpy= 1.171133
Thermal correction to Gibbs Free Energy= 0.998480

Sum of electronic and zero-point Energies= -2836.212212
Sum of electronic and thermal Energies= -2836.146087
Sum of electronic and thermal Enthalpies= -2836.145142
Sum of electronic and thermal Free Energies= -2836.317796

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Cartesian Coordinates

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6	3.092285	-0.969970	1.707247
6	4.319887	-0.359066	1.447767
6	4.990726	-0.570356	0.242901
6	4.410879	-1.422821	-0.724208
6	3.190690	-2.062917	-0.435772
6	2.530067	-1.835009	0.763531
6	5.023523	-1.537814	-2.049946
6	6.455250	-1.226999	-2.172340
6	7.089409	-0.439064	-1.189682
6	6.281779	0.150293	-0.060807
6	8.454890	-0.172426	-1.305160
6	9.193737	-0.655633	-2.384408
6	8.563696	-1.423602	-3.368649
6	7.207503	-1.705743	-3.258798
8	3.441696	0.045638	-3.296879
6	2.374452	0.097102	-2.533998
6	2.246887	0.959967	-1.397577
6	1.083477	0.907212	-0.622816
6	0.022072	0.050009	-0.924798
6	0.128632	-0.771858	-2.059267
6	1.278857	-0.758129	-2.830226
77	-1.650688	-0.003847	0.349801
6	-3.663395	0.292396	1.193932
7	-0.659933	-0.095540	2.113847
6	-0.345217	-1.237484	2.817402
6	0.364748	-0.881471	4.031703
6	0.474993	0.486845	4.043692
6	-0.170585	0.973662	2.839886
6	0.828984	-1.863185	5.064949
6	-0.306342	-2.340637	5.988328
6	-0.650654	-2.530692	2.417638
6	-1.345946	-2.904903	1.275575
7	-1.843816	-2.033023	0.338372
6	-2.499997	-2.790191	-0.609544
6	-2.399213	-4.197448	-0.261776
6	-1.682083	-4.268908	0.904147
6	-0.275301	2.306597	2.473177
6	-0.896027	2.813397	1.336385
7	-1.515842	2.052976	0.383853
6	-1.963821	2.905829	-0.593059
6	-1.616766	4.274212	-0.238767
6	-0.953473	4.216410	0.959050
6	1.084984	1.361311	5.097195
6	0.037313	1.975137	6.043425
6	-3.156671	-2.288597	-1.724195
6	-3.268455	-0.953345	-2.102577
7	-2.729316	0.098609	-1.416975
6	-3.015182	1.238352	-2.118338
6	-3.777352	0.896410	-3.309354
6	-3.938538	-0.465619	-3.297400
6	-3.037261	-5.314411	-1.031662
6	-4.540891	-5.460099	-0.734844
6	-1.343624	-5.481149	1.718215

6	-2.305688	-5.692599	2.901457
6	-2.643990	2.524748	-1.742595
6	-4.319535	1.890487	-4.291483
6	-5.607653	2.573541	-3.797202
6	-4.697144	-1.325556	-4.262715
6	-6.097235	-1.706199	-3.748225
6	-1.991852	5.485033	-1.038527
6	-3.452129	5.917521	-0.813527
6	-0.412582	5.343343	1.785671
6	-1.334152	5.721259	2.959263
1	-2.925637	3.322500	-2.420019
1	-3.622320	-3.016645	-2.378171
1	-0.317915	-3.330665	3.068334
1	0.184704	3.028492	3.137447
1	-3.494286	0.383203	2.268945
1	-4.093888	1.199807	0.774467
1	-4.247768	-0.591760	0.938611
1	0.578596	5.074527	2.172457
1	-0.259791	6.220879	1.148661
1	-1.494062	4.866254	3.623508
1	-2.314642	6.039269	2.591876
1	1.662597	2.164001	4.622492
1	1.803228	0.778028	5.683085
1	1.619473	-1.407430	5.670419
1	1.288056	-2.728784	4.571604
1	-1.325279	6.313919	-0.777754
1	-1.829230	5.291187	-2.105699
1	-0.316280	-5.400786	2.094189
1	-1.361446	-6.367827	1.075647
1	-0.907109	6.538415	3.549504
1	-2.529674	-6.255535	-0.794935
1	-2.892683	-5.155189	-2.107339
1	-4.980556	-6.275284	-1.318341
1	-5.078932	-4.537938	-0.974919
1	-4.705856	-5.669885	0.326341
1	-3.331652	-5.825807	2.545131
1	-2.300261	-4.826763	3.570688
1	-2.026495	-6.577044	3.482916
1	-1.106569	-2.815487	5.412546
1	-0.745812	-1.495738	6.527296
1	0.062057	-3.062909	6.723650
1	0.511487	2.615381	6.794081
1	-0.518616	1.189581	6.564258
1	-0.687287	2.577563	5.487150
1	-3.700083	6.797536	-1.415562
1	-3.623917	6.162022	0.239230
1	-4.144412	5.113260	-1.081237
1	-4.519215	1.388931	-5.244373
1	-3.561454	2.653860	-4.505012
1	-5.975284	3.299212	-4.529750
1	-5.434536	3.097984	-2.852389
1	-6.394312	1.833121	-3.622674
1	-4.127614	-2.238943	-4.475106
1	-4.793476	-0.801168	-5.219305
1	-6.623587	-2.340515	-4.468677
1	-6.700724	-0.810074	-3.574447
1	-6.031768	-2.247180	-2.799085
1	4.357318	-0.625876	-2.710662
1	6.893828	0.224934	0.846241
1	4.706911	-2.416975	-2.616448

1	6.023537	1.179430	-0.350766
1	9.131760	-1.803559	-4.212518
1	10.254765	-0.436343	-2.457697
1	1.574974	-2.308240	0.958333
1	2.571704	-0.769942	2.636914
1	8.943609	0.425640	-0.539774
1	6.711550	-2.308063	-4.015319
1	4.760296	0.303100	2.189724
1	2.753496	-2.718979	-1.181377
1	-0.681297	-1.440255	-2.328302
1	1.028992	1.552546	0.240231
6	3.324442	1.902643	-1.022816
8	4.392695	2.055176	-1.585625
8	2.987428	2.639596	0.077045
6	3.986950	3.554730	0.522966
1	4.851214	3.018632	0.927477
1	4.325886	4.196506	-0.293740
1	3.515884	4.147465	1.308470
1	1.386404	-1.405060	-3.695856

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^{OSS}TS(B-C)$_{DHA-S1}$

Number of imaginary frequencies : 1 Electronic energy : HF=-2837.3185652
Zero-point correction= 1.104139 (Hartree/Particle)
Thermal correction to Energy= 1.170232
Thermal correction to Enthalpy= 1.171176
Thermal correction to Gibbs Free Energy= 0.999984
Sum of electronic and zero-point Energies= -2836.214426
Sum of electronic and thermal Energies= -2836.148333
Sum of electronic and thermal Enthalpies= -2836.147389
Sum of electronic and thermal Free Energies= -2836.318581

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Cartesian Coordinates

.....

6	-9.265949	-0.006527	-1.906784
6	-8.240551	0.902838	-1.643439
6	-6.993640	0.466489	-1.196127
6	-6.773210	-0.911436	-0.987911
6	-7.809332	-1.819502	-1.263117
6	-9.045190	-1.374015	-1.719470
6	-5.466983	-1.369662	-0.497855
6	-4.647322	-0.413019	0.243849
6	-4.820642	0.972656	0.017558
6	-5.854593	1.434467	-0.981751
6	-3.976100	1.879621	0.653564
6	-2.937697	1.438013	1.475194
6	-2.752752	0.068767	1.690511
6	-3.605417	-0.845497	1.086515
8	-3.795398	-1.511265	-2.427566
6	-2.661710	-1.135881	-1.891097
6	-1.777642	-2.056980	-1.237313
6	-0.559124	-1.615811	-0.736609
6	-0.211710	-0.251788	-0.720112
6	-1.057494	0.646034	-1.408601
6	-2.248846	0.220220	-1.963945
77	1.520145	0.361860	0.243206
6	3.604750	0.871150	0.666761
7	1.377497	-0.914548	1.826124
6	0.846048	-0.625852	3.059622

6	0.898797	-1.807441	3.903698
6	1.481307	-2.800927	3.160065
6	1.784167	-2.231343	1.858223
6	0.450575	-1.853507	5.333327
6	1.489071	-1.260148	6.302722
6	0.355351	0.614417	3.444118
6	0.322913	1.769120	2.674200
7	0.739929	1.861064	1.366844
6	0.541986	3.168021	0.968058
6	-0.028831	3.926987	2.065110
6	-0.161827	3.062080	3.122830
6	2.382098	-2.914455	0.808688
6	2.673853	-2.415259	-0.457267
7	2.409210	-1.141389	-0.873376
6	2.807541	-1.041216	-2.179824
6	3.350921	-2.318224	-2.618219
6	3.269638	-3.170834	-1.547655
6	1.822827	-4.199138	3.579112
6	3.303314	-4.360655	3.969115
6	0.849184	3.681354	-0.283472
6	1.419234	2.996021	-1.351989
7	1.757527	1.671780	-1.336114
6	2.256624	1.357874	-2.573008
6	2.236443	2.543113	-3.417117
6	1.718758	3.561104	-2.658175
6	-0.334511	5.393881	2.020427
6	0.915771	6.269241	2.221646
6	-0.655703	3.352274	4.508052
6	0.486874	3.543109	5.521847
6	2.722738	0.106314	-2.959311
6	2.761006	2.601688	-4.820057
6	4.294826	2.721504	-4.877144
6	1.538096	5.002925	-3.026041
6	2.664711	5.901313	-2.484228
6	3.937618	-2.577035	-3.972959
6	5.378192	-2.050848	-4.107345
6	3.735414	-4.591656	-1.445695
6	5.094048	-4.725663	-0.734530
1	3.072781	0.019256	-3.981276
1	0.621526	4.728455	-0.445414
1	-0.031038	0.693108	4.453341
1	2.633502	-3.952894	0.988841
1	4.170500	0.919543	-0.263163
1	3.588007	1.845465	1.161686
1	4.000661	0.093935	1.323893
1	2.984988	-5.189779	-0.913649
1	3.808523	-5.023136	-2.449576
1	5.047664	-4.316589	0.279481
1	5.868256	-4.173438	-1.275910
1	1.581639	-4.898750	2.769214
1	1.192366	-4.488896	4.426452
1	0.243349	-2.890892	5.616746
1	-0.498725	-1.314827	5.442436
1	3.925496	-3.653333	-4.175254
1	3.308266	-2.117512	-4.744761
1	-1.310656	2.539204	4.844700
1	-1.278034	4.253182	4.490980
1	5.403033	-5.773804	-0.667508
1	-1.072819	5.635415	2.792433
1	-0.805166	5.646080	1.062247

1	0.663732	7.333397	2.173292
1	1.667721	6.059405	1.454882
1	1.373791	6.068863	3.194997
1	1.125060	4.382750	5.230096
1	1.119277	2.651535	5.571868
1	0.094396	3.742110	6.524111
1	1.707477	-0.217454	6.052576
1	2.430265	-1.815384	6.246482
1	1.129609	-1.296986	7.336039
1	3.523959	-5.392751	4.259759
1	3.554164	-3.706412	4.809560
1	3.959589	-4.091331	3.135944
1	5.777060	-2.244067	-5.108356
1	6.034726	-2.533484	-3.376915
1	5.419442	-0.972743	-3.923953
1	2.312339	3.454146	-5.341164
1	2.444774	1.708823	-5.373064
1	4.649700	2.752034	-5.912297
1	4.772256	1.874005	-4.375773
1	4.629539	3.632855	-4.372303
1	0.572802	5.365015	-2.650610
1	1.492599	5.097717	-4.116157
1	2.501508	6.948365	-2.759102
1	3.633587	5.587956	-2.884770
1	2.724768	5.838527	-1.393284
1	-4.698578	-1.522516	-1.562020
1	-6.236994	2.424372	-0.708235
1	-5.433750	-2.394157	-0.128049
1	-5.343102	1.570585	-1.949840
1	-1.934081	-0.275879	2.311698
1	-2.272635	2.156828	1.939417
1	-9.837965	-2.087679	-1.923124
1	-10.231076	0.349334	-2.254640
1	-4.113411	2.944799	0.482520
1	-3.467690	-1.911608	1.233157
1	-8.409762	1.966907	-1.790286
1	-7.632330	-2.880109	-1.107148
1	-0.800396	1.697294	-1.461685
1	0.091707	-2.346574	-0.277545
6	-2.198349	-3.457467	-0.992094
8	-3.330572	-3.832012	-0.749435
8	-1.140865	-4.310320	-1.008727
6	-1.454355	-5.665563	-0.669828
1	-1.879454	-5.725759	0.336001
1	-2.174553	-6.084866	-1.376885
1	-0.509761	-6.207891	-0.719388
1	-2.921359	0.915976	-2.455463

$^{CSS}E_{DHA\text{-}S1}$

Number of imaginary frequencies : 1 Electronic energy : HF=-2837.4326677
Zero-point correction= 1.108332 (Hartree/Particle)
Thermal correction to Energy= 1.174282
Thermal correction to Enthalpy= 1.175227
Thermal correction to Gibbs Free Energy= 1.005033
Sum of electronic and zero-point Energies= -2836.324336
Sum of electronic and thermal Energies= -2836.258385
Sum of electronic and thermal Enthalpies= -2836.257441
Sum of electronic and thermal Free Energies= -2836.427635

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Cartesian Coordinates

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6	3.610267	-0.054649	4.283916
6	2.835908	-1.017851	3.636248
6	3.289581	-1.539315	2.388217
6	4.516725	-1.085061	1.834317
6	5.267989	-0.136631	2.498146
6	4.809641	0.380397	3.724460
6	2.517655	-2.512873	1.720974
6	1.339206	-3.062877	2.256527
6	0.855901	-2.596843	3.517380
6	1.500971	-1.419462	4.159229
6	-0.293581	-3.175501	4.051536
6	-0.960691	-4.184845	3.361635
6	-0.496540	-4.643382	2.114087
6	0.640454	-4.090550	1.563980
6	-0.012339	0.680024	2.266772
6	-1.067089	-0.215902	2.086383
6	-2.399266	0.123120	2.363957
6	-2.735240	1.478043	2.816318
6	-1.587351	2.353914	3.026863
6	-0.296540	1.979302	2.756550
6	-3.453345	-0.883037	2.185844
8	-4.662818	-0.716182	2.248331
8	-3.898780	1.895898	3.035503
8	-2.933805	-2.132722	1.951269
6	-3.892515	-3.180236	1.815587
77	0.003113	0.462143	-0.954462
6	0.037692	0.813226	-2.975645
7	1.281930	-1.125358	-1.272940
6	2.655788	-1.059991	-1.365326
6	3.181807	-2.366987	-1.721934
6	2.102496	-3.212139	-1.837044
6	0.915519	-2.418426	-1.566169
6	4.628977	-2.671674	-1.974638
6	5.090076	-2.252534	-3.381143
6	3.415893	0.078541	-1.127284
6	2.946103	1.343784	-0.793057
7	1.618766	1.694587	-0.691075
6	1.576971	3.035132	-0.383980
6	2.931960	3.549317	-0.255750
6	3.780619	2.500836	-0.510204
6	-0.395543	-2.884375	-1.611550
6	-1.554906	-2.141740	-1.429203
7	-1.598565	-0.790638	-1.163228
6	-2.923639	-0.440391	-1.065666
6	-3.757818	-1.612601	-1.282008
6	-2.909936	-2.667798	-1.501416
6	2.096313	-4.661591	-2.223871
6	1.769038	-4.886666	-3.709867
6	0.414679	3.780734	-0.223232
6	-0.892907	3.322454	-0.321534
7	-1.257848	2.025702	-0.599468
6	-2.630817	1.972277	-0.549782
6	-3.160437	3.284211	-0.208554
6	-2.084082	4.123546	-0.078253
6	3.280894	4.977102	0.043520
6	3.215475	5.882614	-1.198502
6	5.280274	2.505290	-0.549032

6	5.846677	2.608113	-1.975566
6	-3.393009	0.833469	-0.769357
6	-4.616448	3.586150	-0.016998
6	-5.393181	3.727773	-1.336561
6	-2.073855	5.587609	0.245444
6	-1.870725	6.476498	-0.993519
6	-5.257174	-1.599429	-1.272912
6	-5.865363	-1.014250	-2.558888
6	-3.255644	-4.097649	-1.793250
6	-3.206421	-4.436715	-3.292794
1	-4.466319	0.945071	-0.679950
1	0.542182	4.828976	0.021336
1	4.490483	-0.031910	-1.208227
1	-0.526897	-3.937795	-1.830877
1	-0.582169	1.685113	-3.210425
1	1.065707	1.005281	-3.300862
1	-0.351898	-0.058672	-3.511664
1	-2.569430	-4.760328	-1.251334
1	-4.258037	-4.313255	-1.408673
1	-2.211882	-4.243436	-3.707465
1	-3.923000	-3.826234	-3.851886
1	1.367969	-5.205885	-1.609823
1	3.074666	-5.100785	-2.000635
1	4.802916	-3.745127	-1.843864
1	5.255592	-2.165227	-1.230185
1	-5.626727	-2.621610	-1.136840
1	-5.607578	-1.027255	-0.406069
1	5.664674	1.595122	-0.072889
1	5.654719	3.344454	0.047013
1	-3.448711	-5.491124	-3.465261
1	4.289658	5.022604	0.468018
1	2.604477	5.370607	0.811818
1	3.463772	6.918097	-0.941317
1	2.213963	5.872311	-1.640217
1	3.919960	5.542643	-1.964673
1	5.519979	3.535586	-2.456915
1	5.504536	1.774193	-2.596685
1	6.942106	2.597261	-1.963626
1	4.941892	-1.179510	-3.538693
1	4.520130	-2.783018	-4.150718
1	6.152408	-2.475999	-3.527603
1	1.758926	-5.955180	-3.950795
1	2.512830	-4.399563	-4.348691
1	0.789337	-4.469996	-3.963707
1	-6.959536	-1.013009	-2.507274
1	-5.565654	-1.600644	-3.433951
1	-5.532463	0.015891	-2.720188
1	-4.716525	4.512572	0.558127
1	-5.061340	2.796754	0.599257
1	-6.451467	3.936629	-1.145566
1	-5.332173	2.813177	-1.935015
1	-4.988672	4.546447	-1.941546
1	-1.281338	5.798081	0.974163
1	-3.017379	5.857174	0.731082
1	-1.855961	7.536520	-0.717246
1	-2.678258	6.324077	-1.717251
1	-0.926730	6.242944	-1.496427
1	-1.817671	3.353723	3.386037
1	1.486159	-1.482319	5.251700
1	2.861826	-2.874421	0.756537

1	0.822809	-0.560491	3.912753
1	6.206663	0.211636	2.080615
1	5.400426	1.128729	4.243780
1	-1.856874	-4.620669	3.791123
1	-1.034648	-5.426374	1.590414
1	-0.679274	-2.820700	5.002228
1	1.021882	-4.425822	0.606452
1	3.268532	0.358505	5.228140
1	4.848443	-1.504549	0.891837
1	0.996599	0.408491	1.981289
1	-4.382367	-3.386905	2.773677
1	-4.658229	-2.930593	1.080674
1	-3.334398	-4.058447	1.490887
1	0.518699	2.684643	2.900620
1	-0.858599	-1.214483	1.724765

$P1_{DHA-S1}$

Number of imaginary frequencies : 0 Electronic energy : HF=-1074.9551918
Zero-point correction= 0.345405 (Hartree/Particle)
Thermal correction to Energy= 0.365798
Thermal correction to Enthalpy= 0.366742
Thermal correction to Gibbs Free Energy= 0.295126
Sum of electronic and zero-point Energies= -1074.609787
Sum of electronic and thermal Energies= -1074.589394
Sum of electronic and thermal Enthalpies= -1074.588450
Sum of electronic and thermal Free Energies= -1074.660066

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Cartesian Coordinates

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6	-4.385576	0.946206	-1.222142
6	-3.361999	0.043619	-1.498861
6	-2.321240	-0.167048	-0.587078
6	-2.311618	0.535468	0.627445
6	-3.347376	1.436359	0.900047
6	-4.376021	1.648075	-0.014971
6	-1.190440	0.328996	1.619290
6	-0.534290	-1.027093	1.509081
6	-0.554336	-1.729799	0.295507
6	-1.197945	-1.121144	-0.929657
6	0.044544	-2.992866	0.223964
6	0.679654	-3.549936	1.330320
6	0.713385	-2.842986	2.533385
6	0.101327	-1.595244	2.618153
6	-0.124470	-0.389861	-1.861550
6	0.498801	0.751717	-1.134612
6	1.793637	0.788483	-0.768711
6	2.718472	-0.331435	-1.119919
6	2.164698	-1.346830	-2.042961
6	0.871548	-1.369738	-2.390167
8	3.853380	-0.425253	-0.674807
1	2.872256	-2.092079	-2.392550
1	-1.569287	0.473520	2.637133
1	-1.603339	-1.926984	-1.552612
1	-0.426822	1.106033	1.471295
1	1.142912	-4.528754	1.255564
1	1.205167	-3.266863	3.403563
1	-5.171719	2.349903	0.215731
1	-5.188187	1.095815	-1.937713

1	-3.344409	1.973343	1.845177
1	-3.368421	-0.512727	-2.433470
1	0.111197	-1.049464	3.558099
1	0.013678	-3.542075	-0.712434
1	-0.718760	0.010975	-2.695413
6	2.341626	1.970140	-0.042284
8	3.463907	2.406778	-0.144831
8	1.393914	2.540510	0.753932
6	1.822462	3.725149	1.442156
1	2.670775	3.502366	2.093546
1	2.121283	4.497676	0.729371
1	0.963040	4.052646	2.026759
1	-0.157568	1.571459	-0.862221
1	0.489536	-2.152457	-3.042799

$P2_{DHA\text{-}S1}$

Number of imaginary frequencies : 0 Electronic energy : HF=-1075.0068239
Zero-point correction= 0.344284 (Hartree/Particle)
Thermal correction to Energy= 0.365170
Thermal correction to Enthalpy= 0.366114
Thermal correction to Gibbs Free Energy= 0.293244
Sum of electronic and zero-point Energies= -1074.662540
Sum of electronic and thermal Energies= -1074.641654
Sum of electronic and thermal Enthalpies= -1074.640709
Sum of electronic and thermal Free Energies= -1074.713580

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Cartesian Coordinates

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6	-2.217952	0.338107	2.218815
6	-1.748373	-0.748791	1.501837
6	-0.368994	-1.007092	1.407036
6	0.550894	-0.139542	2.047000
6	0.062717	0.960891	2.770591
6	-1.301700	1.190241	2.854305
8	1.878264	-0.314899	1.985376
6	0.246360	-0.257290	-1.836356
6	1.431127	0.333131	-1.382212
6	1.364205	1.594201	-0.684353
6	0.115407	2.188162	-0.471183
6	-1.070197	1.589119	-0.909060
6	-1.003181	0.328815	-1.608687
6	2.576090	2.180313	-0.209403
6	3.780262	1.558542	-0.402169
6	3.845279	0.307528	-1.081477
6	2.706070	-0.285516	-1.556937
6	-2.222443	-0.295560	-2.010207
6	-3.432843	0.291974	-1.750520
6	-3.498219	1.545865	-1.076478
6	-2.351057	2.171860	-0.667225
1	0.783169	1.616130	3.247407
1	0.063499	3.130903	0.067140
1	0.297329	-1.207424	-2.362171
1	2.039718	-1.111763	1.425835
1	-4.352614	-0.195790	-2.059388
1	-4.466400	1.997545	-0.882543
1	4.693967	2.010353	-0.028519
1	4.807675	-0.177209	-1.214671
1	2.519577	3.127372	0.320009

1	2.750014	-1.245984	-2.061643
1	-2.395033	3.120902	-0.140359
1	-2.169478	-1.253440	-2.519920
1	-3.282161	0.537107	2.273738
6	0.155283	-2.134788	0.634982
8	1.351871	-2.421951	0.545906
8	-0.790405	-2.860828	0.010307
6	-0.305429	-3.960906	-0.770674
1	0.354298	-3.604283	-1.565765
1	0.248035	-4.665323	-0.145535
1	-1.192395	-4.433597	-1.191503
1	-2.434268	-1.407423	0.984217
1	-1.662612	2.047789	3.415213

A_{Cl}

Number of imaginary frequencies : 0 Electronic energy : HF=-2826.3381847
Zero-point correction= 0.866159 (Hartree/Particle)
Thermal correction to Energy= 0.922681
Thermal correction to Enthalpy= 0.923626
Thermal correction to Gibbs Free Energy= 0.773636
Sum of electronic and zero-point Energies= -2825.472026
Sum of electronic and thermal Energies= -2825.415503
Sum of electronic and thermal Enthalpies= -2825.414559
Sum of electronic and thermal Free Energies= -2825.564549

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Cartesian Coordinates

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6	1.513408	-3.787492	-0.594100
6	0.356542	-2.925681	-0.404726
7	0.752329	-1.613183	-0.451882
6	2.099897	-1.601878	-0.712585
6	2.596020	-2.966853	-0.771201
6	-0.941914	-3.360938	-0.175007
6	-2.058582	-2.569184	0.060990
7	-2.056813	-1.197926	0.139966
6	-3.351774	-0.794742	0.350276
6	-4.212096	-1.962826	0.443764
6	-3.410836	-3.061788	0.264788
6	-3.776145	0.525159	0.441027
6	-2.991768	1.665691	0.320486
7	-1.630248	1.673351	0.119533
6	-1.230533	2.987366	0.061990
6	-2.382669	3.850491	0.255414
6	-3.473308	3.032320	0.409519
77	-0.437410	0.028115	-0.160729
7	1.179508	1.257120	-0.480797
6	1.181728	2.628744	-0.431518
6	2.521816	3.119313	-0.712123
6	3.306461	2.018091	-0.947484
6	2.451256	0.853404	-0.797258
6	-4.912725	3.419620	0.568339
6	-5.701472	3.326189	-0.750503
6	-2.343760	5.348171	0.200573
6	-2.320709	5.888306	-1.240969
6	0.071379	3.419807	-0.160185
6	-3.811940	-4.504639	0.194156
6	-3.953996	-5.010241	-1.253105
6	-5.700605	-1.914126	0.616067

6	-6.440483	-1.610549	-0.699647
6	2.873746	-0.465309	-0.889534
6	4.749462	1.959003	-1.350852
6	4.934613	1.683091	-2.853979
6	2.899533	4.567351	-0.801215
6	2.514280	5.199103	-2.151170
6	4.036248	-3.331585	-0.961043
6	4.494455	-3.248344	-2.427691
6	1.468802	-5.285051	-0.612279
6	1.004159	-5.848317	-1.967431
6	0.100364	-0.132010	2.228148
6	1.447394	0.426884	2.262490
6	2.528999	-0.386185	2.302291
6	2.381234	-1.858246	2.456758
6	0.997366	-2.341496	2.639588
6	-0.082438	-1.542875	2.572111
7	-0.863561	0.717089	2.698316
7	-1.675253	1.456887	2.941908
8	3.331065	-2.633913	2.478595
6	3.879771	0.218987	2.119859
8	4.827164	-0.305041	1.576271
17	-0.913793	0.076174	-2.468321
8	3.908848	1.479837	2.620352
6	5.122726	2.208328	2.388736
1	3.927000	-0.624645	-1.077278
1	-1.100806	-4.432871	-0.180903
1	-4.834132	0.682741	0.613857
1	0.231892	4.491612	-0.152749
1	2.422917	5.128415	0.012383
1	3.979288	4.672076	-0.648522
1	1.437380	5.118223	-2.326974
1	3.019976	4.685146	-2.973966
1	-1.463744	5.718500	0.741162
1	-3.214417	5.755378	0.725884
1	-4.974606	4.442342	0.955541
1	-5.389230	2.780918	1.322586
1	5.237609	2.907449	-1.098748
1	5.261891	1.183774	-0.768634
1	-5.965173	-1.156451	1.364239
1	-6.052991	-2.870854	1.016614
1	2.790383	6.258023	-2.184611
1	-4.761430	-4.645673	0.721923
1	-3.076091	-5.122855	0.723456
1	-4.234728	-6.068167	-1.274828
1	-3.015273	-4.891265	-1.802099
1	-4.719990	-4.439815	-1.786773
1	-6.232254	-2.383176	-1.445628
1	-6.114653	-0.654260	-1.119480
1	-7.522994	-1.567157	-0.541907
1	-5.666427	2.310569	-1.155782
1	-5.272666	3.993740	-1.503779
1	-6.750458	3.602512	-0.602732
1	-2.278663	6.982247	-1.251383
1	-3.216384	5.573284	-1.784495
1	-1.454248	5.504749	-1.787883
1	5.996350	1.634681	-3.115777
1	4.467236	2.471162	-3.452141
1	4.467564	0.735425	-3.137248
1	4.200252	-4.347697	-0.587908
1	4.650552	-2.677914	-0.331380

1	5.553476	-3.508775	-2.522436
1	4.354286	-2.240584	-2.830882
1	3.915356	-3.933700	-3.054721
1	0.803503	-5.648421	0.181000
1	2.462959	-5.678396	-0.376459
1	0.971679	-6.942557	-1.949879
1	1.684342	-5.536903	-2.765863
1	0.006573	-5.478944	-2.224712
1	1.558720	1.499193	2.168027
1	-1.093560	-1.918397	2.672500
1	0.894016	-3.407980	2.803635
1	5.990460	1.609265	2.671096
1	5.051209	3.103535	3.006215
1	5.201306	2.481867	1.334397

TS(A-B)$_{CI}$

Number of imaginary frequencies : 1 Electronic energy : HF=-2826.3335068
Zero-point correction= 0.864644 (Hartree/Particle)
Thermal correction to Energy= 0.920574
Thermal correction to Enthalpy= 0.921518
Thermal correction to Gibbs Free Energy= 0.774056
Sum of electronic and zero-point Energies= -2825.468863
Sum of electronic and thermal Energies= -2825.412933
Sum of electronic and thermal Enthalpies= -2825.411989
Sum of electronic and thermal Free Energies= -2825.559451

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Cartesian Coordinates

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6	1.493661	0.385052	2.166550
6	0.138092	-0.151778	1.955528
6	-0.087343	-1.506192	2.494464
6	0.954477	-2.338996	2.647286
6	2.356175	-1.911214	2.440904
6	2.554242	-0.444183	2.273921
77	-0.433197	0.039809	-0.073960
17	-0.922462	0.083415	-2.446007
8	3.277501	-2.717267	2.471959
6	3.929628	0.118223	2.143488
8	3.994670	1.358370	2.686122
6	5.246696	2.037345	2.512216
7	-1.768784	1.542600	0.226894
6	-3.134608	1.399761	0.401039
6	-3.751708	2.707391	0.440167
6	-2.749212	3.632986	0.276211
6	-1.510783	2.899267	0.129844
6	-5.225969	2.948945	0.563810
6	-5.971950	2.754254	-0.768881
6	-3.802069	0.189321	0.518781
6	-3.252539	-1.081711	0.398441
7	-1.931641	-1.349559	0.160300
6	-1.803395	-2.710259	0.022947
6	-3.100736	-3.338053	0.219850
6	-3.999051	-2.329188	0.453916
6	-0.262522	3.462510	-0.091409
6	0.924345	2.786876	-0.354300
7	1.054970	1.425954	-0.414677
6	2.356498	1.149041	-0.750592
6	3.095005	2.393313	-0.884528

6	2.208214	3.410311	-0.636554
6	-2.871446	5.123749	0.176846
6	-2.882068	5.621107	-1.280202
6	-0.623200	-3.383486	-0.257523
6	0.627437	-2.821298	-0.484849
7	0.901733	-1.479393	-0.477887
6	2.234374	-1.331503	-0.761930
6	2.850156	-2.639900	-0.902068
6	1.850052	-3.564229	-0.742452
6	-3.364421	-4.808094	0.090809
6	-3.470924	-5.265395	-1.375527
6	-5.483316	-2.427244	0.640283
6	-6.263632	-2.158708	-0.659649
6	2.897477	-0.119176	-0.897011
6	4.310416	-2.865082	-1.147304
6	4.716488	-2.661827	-2.617745
6	1.939871	-5.056772	-0.833948
6	1.499076	-5.593881	-2.207485
6	4.534013	2.482274	-1.295302
6	4.728575	2.326124	-2.814502
6	2.440600	4.889046	-0.715674
6	1.987274	5.490074	-2.058729
8	4.867317	-0.417841	1.594222
7	-0.833061	0.842787	2.819789
7	-1.613075	1.648293	2.743728
1	3.956176	-0.174005	-1.112599
1	-0.682759	-4.464187	-0.308848
1	-4.870955	0.241903	0.687528
1	-0.216082	4.545057	-0.098297
1	1.915285	5.393881	0.104652
1	3.505661	5.098160	-0.567210
1	0.922947	5.304197	-2.231204
1	2.536819	5.036069	-2.888513
1	-2.045803	5.601431	0.718622
1	-3.789685	5.448456	0.677718
1	-5.399182	3.966007	0.931249
1	-5.650469	2.277221	1.320132
1	4.946543	3.445508	-0.974490
1	5.114401	1.709443	-0.776564
1	-5.809748	-1.720218	1.413057
1	-5.738244	-3.424269	1.015518
1	2.156712	6.571360	-2.083754
1	-4.291830	-5.058971	0.616905
1	-2.569180	-5.374868	0.590872
1	-3.651127	-6.343289	-1.438883
1	-2.552669	-5.036432	-1.924192
1	-4.291722	-4.748735	-1.881641
1	-5.991978	-2.887085	-1.429255
1	-6.034843	-1.164710	-1.055409
1	-7.343420	-2.222525	-0.490879
1	-5.823956	1.741540	-1.155279
1	-5.598210	3.450531	-1.525381
1	-7.046472	2.923518	-0.646143
1	-2.957730	6.712346	-1.322470
1	-3.729236	5.196142	-1.826491
1	-1.970389	5.317599	-1.803167
1	5.788532	2.380655	-3.082224
1	4.195196	3.113407	-3.355432
1	4.335175	1.365709	-3.160003
1	4.571289	-3.882239	-0.837652

1	4.883742	-2.196304	-0.495607
1	5.790905	-2.822439	-2.752568
1	4.477669	-1.650006	-2.959874
1	4.181150	-3.360182	-3.268779
1	1.327988	-5.515483	-0.047508
1	2.970032	-5.368475	-0.633994
1	1.566298	-6.686020	-2.243988
1	2.130655	-5.183341	-3.000989
1	0.466879	-5.305263	-2.429144
1	1.639072	1.453337	2.073418
1	-1.111001	-1.841404	2.612251
1	0.818056	-3.385329	2.898118
1	6.071056	1.423578	2.881208
1	5.162734	2.959089	3.087337
1	5.415138	2.262616	1.456631

B_{Cl}

Number of imaginary frequencies : 0 Electronic energy : HF=-2950.3150711
Zero-point correction= 0.981005 (Hartree/Particle)
Thermal correction to Energy= 1.042430
Thermal correction to Enthalpy= 1.043374
Thermal correction to Gibbs Free Energy= 0.881245
Sum of electronic and zero-point Energies= -2949.334066
Sum of electronic and thermal Energies= -2949.272641
Sum of electronic and thermal Enthalpies= -2949.271697
Sum of electronic and thermal Free Energies= -2949.433826

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Cartesian Coordinates

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6	4.982888	2.469949	1.519654
6	3.738802	2.256561	1.955828
6	3.133293	0.890325	2.095117
6	4.032280	-0.208903	1.606406
6	5.276398	0.002278	1.171276
6	5.918469	1.363028	1.113954
6	2.311784	0.120531	-1.331977
7	1.172010	-0.595910	-1.073127
6	1.419613	-1.904909	-1.416878
6	2.786897	-2.026360	-1.889974
6	3.338029	-0.772015	-1.841977
6	2.458324	1.487535	-1.151496
6	1.483378	2.377858	-0.724374
7	0.201170	2.042414	-0.367552
6	-0.458454	3.208239	-0.047914
6	0.454302	4.327316	-0.185111
6	1.656570	3.813796	-0.604450
6	-1.788642	3.302418	0.334706
6	-2.699682	2.257266	0.452480
6	-4.092291	2.389840	0.840261
6	-4.621125	1.122986	0.854075
6	-3.552164	0.216034	0.470835
7	-2.409996	0.936921	0.242487
6	-4.788446	3.694384	1.086294
6	-5.178591	4.413246	-0.218074
77	-0.588734	0.160038	-0.347309
17	-1.396991	0.464917	-2.664950
6	-3.680407	-1.160522	0.329513
6	-2.715790	-2.053041	-0.121015

7	-1.429291	-1.728772	-0.462562
6	-0.811387	-2.868603	-0.897289
6	-1.742429	-3.979941	-0.822428
6	-2.923758	-3.474750	-0.338836
6	-6.037278	0.709686	1.118976
6	-6.842087	0.491182	-0.175411
6	2.912975	4.549550	-0.957799
6	3.075157	4.756063	-2.474713
6	0.079591	5.763781	0.022975
6	-0.659472	6.365250	-1.186423
6	0.509790	-2.948169	-1.326445
6	3.405977	-3.296135	-2.390792
6	2.997624	-3.629496	-3.837171
6	4.699235	-0.333811	-2.285384
6	4.695820	0.278049	-3.697805
6	-1.441109	-5.376760	-1.275255
6	-1.523483	-5.535673	-2.804357
6	-4.226530	-4.187933	-0.137256
6	-5.199909	-3.987011	-1.313276
6	-0.178710	-0.197228	1.507760
6	0.490543	-1.423184	1.888038
6	0.947826	-1.658608	3.146501
6	0.715317	-0.660597	4.224453
6	-0.083027	0.520995	3.841927
6	-0.515031	0.723034	2.574963
6	1.671868	-2.923373	3.458433
8	2.387996	-3.345356	2.383446
6	3.072016	-4.593962	2.565513
8	1.176326	-0.772100	5.356952
8	1.622573	-3.525277	4.506258
1	-4.651775	-1.579638	0.563123
1	-2.159784	4.296145	0.554819
1	3.431873	1.905145	-1.372075
1	0.863742	-3.926964	-1.626512
1	-0.441622	-5.671912	-0.932064
1	-2.141113	-6.072119	-0.799942
1	-0.824671	-4.859824	-3.306296
1	-2.527811	-5.292430	-3.163405
1	3.128210	-4.128981	-1.732450
1	4.496628	-3.214855	-2.331744
1	5.382837	-1.189303	-2.260940
1	5.098383	0.392568	-1.569744
1	-4.038228	-5.258314	-0.001622
1	-4.699770	-3.844073	0.790539
1	3.776383	4.002429	-0.563318
1	2.915241	5.524252	-0.457887
1	-1.288691	-6.561328	-3.106508
1	0.983207	6.349283	0.223141
1	-0.547655	5.859674	0.917850
1	-0.930404	7.409671	-1.001782
1	-1.573813	5.805473	-1.404706
1	-0.030656	6.325898	-2.080733
1	2.242895	5.340600	-2.878043
1	3.087007	3.797366	-3.001717
1	4.007184	5.283949	-2.700606
1	4.027773	1.143131	-3.747306
1	4.343960	-0.449485	-4.435277
1	5.700560	0.602391	-3.987204
1	3.456134	-4.566260	-4.169813
1	3.310168	-2.832596	-4.518357

1	1.911490	-3.727314	-3.925123
1	-6.145538	-4.508508	-1.134037
1	-4.766681	-4.369413	-2.242195
1	-5.415189	-2.925227	-1.465791
1	-6.531626	1.473800	1.728341
1	-6.051589	-0.209961	1.716600
1	-7.867050	0.177919	0.047353
1	-6.375381	-0.275273	-0.801253
1	-6.883954	1.412562	-0.763702
1	-4.146892	4.352184	1.685933
1	-5.687241	3.519631	1.687200
1	-5.674434	5.366470	-0.008659
1	-5.858629	3.794274	-0.810662
1	-4.296614	4.611491	-0.834405
1	0.685615	-2.159268	1.120827
1	-1.072877	1.617434	2.327441
1	-0.269912	1.234662	4.638393
1	3.594993	-4.779775	1.627814
1	2.359038	-5.394924	2.776405
1	3.779136	-4.524616	3.395381
1	2.858734	0.709971	3.147070
1	3.108752	3.100959	2.226545
1	3.624980	-1.216399	1.619078
1	5.364625	3.486804	1.450629
1	5.878573	-0.838052	0.831840
1	6.302960	1.554454	0.098466
1	2.179229	0.856284	1.553495
1	6.818430	1.381506	1.750269

$TS(B\text{-}D)_{CI}$

Number of imaginary frequencies : 1 Electronic energy : HF=-2950.2896246
Zero-point correction= 0.976374 (Hartree/Particle)
Thermal correction to Energy= 1.036678
Thermal correction to Enthalpy= 1.037622
Thermal correction to Gibbs Free Energy= 0.878352
Sum of electronic and zero-point Energies= -2949.318168
Sum of electronic and thermal Energies= -2949.257864
Sum of electronic and thermal Enthalpies= -2949.256920
Sum of electronic and thermal Free Energies= -2949.416190

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Cartesian Coordinates

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6	0.481266	-1.685523	3.932224
6	1.443991	-1.498937	2.844053
6	2.616087	-0.670405	3.133784
6	2.688780	0.069817	4.253822
6	1.619782	0.061169	5.303314
6	0.535840	-0.941997	5.049841
6	-2.400055	0.237642	2.244415
6	-1.368655	-0.529403	1.819326
6	-0.077335	0.064651	1.473451
6	0.232705	1.321324	2.154516
6	-0.759159	2.088128	2.649762
6	-2.173021	1.653777	2.634737
77	0.313953	0.028959	-0.539577
6	-3.780471	-0.315423	2.183518
8	-3.793495	-1.625276	2.539109
6	-5.040397	-2.302411	2.329229

8	-3.073217	2.406855	2.993147
7	-1.421761	-1.036889	-0.874022
6	-1.540641	-2.401749	-0.903600
6	-2.937898	-2.760844	-1.093183
6	-3.642538	-1.585632	-1.164992
6	-2.676993	-0.508412	-1.016899
6	-3.443727	-4.163486	-1.245472
6	-3.193024	-4.733019	-2.653343
6	-0.496336	-3.296286	-0.705610
6	0.843268	-2.986626	-0.497729
7	1.367995	-1.717655	-0.436286
6	2.727133	-1.836630	-0.273466
6	3.079605	-3.241055	-0.195383
6	1.911004	-3.954173	-0.330065
6	-2.994240	0.840399	-0.930997
6	-2.109719	1.895906	-0.758993
7	-0.746090	1.786796	-0.680181
6	-0.236984	3.051127	-0.557008
6	-1.328233	4.013145	-0.543662
6	-2.491058	3.294829	-0.650330
6	-5.109226	-1.378634	-1.395847
6	-5.427679	-0.920934	-2.830499
6	3.622427	-0.776358	-0.183887
6	3.316346	0.578325	-0.220482
7	2.053347	1.099165	-0.316053
6	2.169249	2.466787	-0.334403
6	3.572808	2.832624	-0.221581
6	4.283856	1.662492	-0.151565
6	4.479031	-3.765486	-0.074011
6	5.232783	-3.761320	-1.416524
6	1.734741	-5.441677	-0.395318
6	1.647232	-5.964621	-1.840848
6	1.111136	3.361802	-0.421231
6	4.092874	4.237692	-0.268348
6	4.150150	4.800332	-1.700296
6	5.770480	1.476074	-0.102535
6	6.373801	1.155561	-1.482261
6	-1.156445	5.499586	-0.463998
6	-0.781361	6.125804	-1.819379
6	-3.905933	3.787532	-0.663412
6	-4.502517	3.870391	-2.079771
8	-4.764435	0.285759	1.809463
1	1.361900	4.414705	-0.368209
1	4.669749	-1.035034	-0.079462
1	-0.750729	-4.349610	-0.724534
1	-4.045746	1.092872	-0.967788
1	-4.518818	3.131154	-0.034388
1	-3.946939	4.776764	-0.195585
1	-4.487559	2.893523	-2.572596
1	-3.924636	4.559567	-2.703442
1	-5.490788	-0.643876	-0.676710
1	-5.644718	-2.312816	-1.191599
1	-4.517436	-4.189312	-1.030020
1	-2.969615	-4.814447	-0.499806
1	-2.084525	5.952092	-0.099374
1	-0.386602	5.747285	0.277541
1	0.829936	-5.734261	0.151703
1	2.570221	-5.931259	0.116884
1	-5.538816	4.221724	-2.048482
1	4.453331	-4.785789	0.323775

1	5.038416	-3.169002	0.657585
1	6.254278	-4.136070	-1.295491
1	5.282872	-2.751194	-1.833463
1	4.719504	-4.391768	-2.148472
1	2.561994	-5.728035	-2.392133
1	0.813783	-5.498692	-2.374616
1	1.505454	-7.050020	-1.858677
1	-2.125092	-4.728215	-2.891200
1	-3.699155	-4.124771	-3.408773
1	-3.560415	-5.761193	-2.734917
1	-6.503432	-0.768086	-2.963335
1	-5.092602	-1.666924	-3.557590
1	-4.916090	0.017093	-3.064603
1	-0.652690	7.209520	-1.731134
1	-1.561441	5.930913	-2.561351
1	0.149845	5.698943	-2.204365
1	5.094151	4.271294	0.174878
1	3.464410	4.888953	0.352152
1	4.520054	5.830755	-1.703976
1	3.159674	4.787127	-2.164272
1	4.812215	4.194236	-2.325713
1	6.023579	0.670783	0.599125
1	6.239048	2.382464	0.296083
1	7.457039	1.011215	-1.415078
1	6.177626	1.969831	-2.185888
1	5.929538	0.247957	-1.901346
1	-1.538534	-1.569437	1.572307
1	1.256294	1.676368	2.127358
1	-0.581296	3.086638	3.036612
1	-4.929167	-3.279131	2.800161
1	-5.228408	-2.417940	1.259082
1	-5.863800	-1.745195	2.780250
1	0.804781	-0.792284	1.904671
1	3.400931	-0.633440	2.387446
1	-0.314821	-2.409823	3.792809
1	3.557498	0.698289	4.432506
1	-0.213383	-1.072136	5.825991
1	2.068894	-0.116721	6.293459
1	1.610063	-2.352538	2.185930
1	1.176852	1.066772	5.385288
17	0.661607	0.099204	-2.963537

D_{Cl}

Number of imaginary frequencies : 0 Electronic energy : HF=-2950.3323129
Zero-point correction= 0.981880 (Hartree/Particle)
Thermal correction to Energy= 1.042403
Thermal correction to Enthalpy= 1.043348
Thermal correction to Gibbs Free Energy= 0.883558
Sum of electronic and zero-point Energies= -2949.350433
Sum of electronic and thermal Energies= -2949.289910
Sum of electronic and thermal Enthalpies= -2949.288965
Sum of electronic and thermal Free Energies= -2949.448755

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Cartesian Coordinates

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6	2.201260	-0.061304	3.098402
6	0.747616	-0.342111	3.369527
6	0.319134	0.076886	4.751042

6	1.110769	0.743141	5.592894
6	2.530047	1.124527	5.275106
6	2.990472	0.606769	3.940723
6	-0.150224	0.366695	2.294370
6	-1.539745	-0.161445	2.263187
6	-2.634282	0.620942	2.216300
6	-2.513447	2.109062	2.228385
6	-1.136876	2.639393	2.298552
6	-0.054595	1.851687	2.334423
6	-3.977807	-0.004170	2.051426
8	-4.028604	-1.210192	2.668031
6	-5.227842	-1.965859	2.448571
8	-3.483891	2.857056	2.212139
8	-4.903087	0.466102	1.424553
77	0.356881	-0.136820	-0.652855
17	0.675661	-0.430158	-2.938572
7	2.105568	0.923026	-0.498953
6	3.365244	0.395097	-0.345870
6	4.342914	1.469196	-0.340323
6	3.647123	2.640546	-0.498692
6	2.242502	2.285128	-0.604638
6	5.825680	1.272090	-0.241732
6	6.456974	0.839382	-1.577483
6	3.652413	-0.953735	-0.181756
6	2.742830	-2.003513	-0.137095
7	1.380766	-1.874230	-0.263329
6	0.839320	-3.133029	-0.163789
6	1.899630	-4.099727	0.061654
6	3.079599	-3.400129	0.074244
6	1.194624	3.182684	-0.764242
6	-0.154440	2.877826	-0.874112
7	-0.680211	1.607544	-0.872987
6	-2.044637	1.733438	-0.995531
6	-2.404049	3.140750	-1.022280
6	-1.232183	3.849016	-0.958033
6	4.184371	4.034856	-0.618210
6	4.278157	4.511352	-2.079148
6	-0.511943	-3.433267	-0.279132
6	-1.546489	-2.545592	-0.543008
7	-1.403098	-1.185758	-0.692695
6	-2.651050	-0.669127	-0.942505
6	-3.628871	-1.743253	-0.961046
6	-2.945651	-2.904678	-0.699652
6	1.694282	-5.580561	0.173744
6	1.526165	-6.262213	-1.196470
6	4.475573	-3.929873	0.207926
6	5.191864	-4.066054	-1.148026
6	-2.943577	0.681224	-1.066197
6	-5.082677	-1.559078	-1.277762
6	-5.335291	-1.312447	-2.776103
6	-3.475218	-4.306724	-0.658289
6	-3.251923	-5.064046	-1.979726
6	-3.811781	3.649491	-1.083893
6	-4.406986	3.604967	-2.502357
6	-1.041687	5.335086	-0.990251
6	-0.651395	5.853585	-2.386106
1	1.457389	4.233556	-0.795650
1	4.697151	-1.214108	-0.058804
1	-0.786058	-4.476127	-0.170084
1	-3.988574	0.942804	-1.163884

1	-4.430659	3.066967	-0.392231
1	-3.837789	4.678920	-0.712284
1	-4.408090	2.585482	-2.900310
1	-3.820828	4.223309	-3.189667
1	-5.482332	-0.726362	-0.688620
1	-5.638367	-2.450458	-0.964979
1	-4.546820	-4.285484	-0.431750
1	-3.003330	-4.859766	0.163469
1	-1.966076	5.824607	-0.666767
1	-0.272713	5.628520	-0.264503
1	0.813462	-5.788857	0.793731
1	2.545462	-6.028103	0.698192
1	-5.438139	3.972170	-2.504964
1	4.448942	-4.906708	0.702686
1	5.061272	-3.274130	0.864283
1	6.211124	-4.444276	-1.019082
1	5.245210	-3.101276	-1.661319
1	4.649562	-4.755011	-1.802414
1	2.416182	-6.109838	-1.814243
1	0.674534	-5.842455	-1.740213
1	1.365821	-7.339331	-1.083817
1	-2.187271	-5.110770	-2.227798
1	-3.758639	-4.554052	-2.804374
1	-3.636790	-6.087169	-1.918573
1	-6.402917	-1.174817	-2.974659
1	-4.979576	-2.156962	-3.374411
1	-4.805322	-0.419870	-3.121134
1	-0.510837	6.939320	-2.378727
1	-1.429748	5.612306	-3.116205
1	0.277476	5.389348	-2.731765
1	5.176563	4.084487	-0.156774
1	3.551131	4.727979	-0.050364
1	4.661991	5.535060	-2.135789
1	3.297065	4.484296	-2.562544
1	4.944859	3.861603	-2.653998
1	6.051644	0.521991	0.526655
1	6.295523	2.202070	0.096060
1	7.536861	0.692080	-1.473983
1	6.285256	1.597584	-2.347317
1	6.014557	-0.095492	-1.934374
1	-1.649340	-1.240758	2.230569
1	0.946379	2.268672	2.379594
1	-1.061300	3.721433	2.315491
1	-5.197454	-2.784081	3.167942
1	-5.238900	-2.358819	1.429330
1	-6.110261	-1.342535	2.604430
1	0.347374	0.022318	1.340470
1	2.591638	-0.416706	2.149753
1	-0.703204	-0.161609	5.035377
1	4.029186	0.786326	3.671278
1	0.731079	1.033465	6.570143
1	3.200639	0.759605	6.068691
1	0.563037	-1.418369	3.231916
1	2.636946	2.220733	5.309706

CHD-TEMPO

Number of imaginary frequencies : 0 Electronic energy : HF=-717.2626838

Zero-point correction= 0.386820 (Hartree/Particle)
Thermal correction to Energy= 0.405889
Thermal correction to Enthalpy= 0.406833
Thermal correction to Gibbs Free Energy= 0.338892
Sum of electronic and zero-point Energies= -716.875864
Sum of electronic and thermal Energies= -716.856795
Sum of electronic and thermal Enthalpies= -716.855851
Sum of electronic and thermal Free Energies= -716.923791
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Cartesian Coordinates
.....

6	0.938000	1.357471	-0.357763
6	1.996962	-1.022035	0.081518
6	1.890558	-0.710085	1.584357
6	1.998057	0.780278	1.902837
6	0.889494	1.533650	1.169798
1	0.921639	-1.074423	1.946192
1	2.663775	-1.283935	2.107148
1	1.904940	0.937172	2.982938
1	2.984113	1.166603	1.620078
1	-0.080134	1.165810	1.525055
1	0.929315	2.606287	1.389621
6	-0.389732	1.817649	-0.969486
1	-0.559496	2.866807	-0.708430
1	-0.371457	1.719699	-2.054942
1	-1.220332	1.224836	-0.586002
6	2.089844	2.159562	-0.993954
1	2.186017	1.882498	-2.046427
1	1.870957	3.230001	-0.933107
1	3.047477	1.985313	-0.499661
6	1.513785	-2.452559	-0.187279
1	1.605279	-2.699092	-1.244932
1	2.115503	-3.153170	0.399231
1	0.467221	-2.568507	0.101955
6	3.443785	-0.882651	-0.431154
1	4.059558	-1.691801	-0.026557
1	3.449101	-0.951025	-1.521497
1	3.901786	0.064254	-0.139943
7	1.106072	-0.095189	-0.687628
8	0.864036	-0.430478	-1.905204
1	-1.355411	-1.298218	-1.240048
6	-2.293454	-1.428057	-0.678935
6	-2.039404	-1.241592	0.791568
6	-3.333941	-0.480571	-1.209899
6	-2.625089	-0.298286	1.533077
1	-1.339216	-1.928537	1.261313
6	-3.923119	0.462538	-0.472263
1	-3.594157	-0.581324	-2.261266
6	-3.620766	0.688252	0.985043
1	-2.392096	-0.223785	2.593560
1	-4.660619	1.120759	-0.926606
1	-4.550930	0.645350	1.573620
1	-2.598891	-2.468066	-0.874745
1	-3.248610	1.715255	1.133679

TS(CHD-TEMPO)

Number of imaginary frequencies : 1 Electronic energy : HF=-717.2373741
Zero-point correction= 0.380689 (Hartree/Particle)

Thermal correction to Energy= 0.398903
Thermal correction to Enthalpy= 0.399847
Thermal correction to Gibbs Free Energy= 0.334697
Sum of electronic and zero-point Energies= -716.842655
Sum of electronic and thermal Energies= -716.824441
Sum of electronic and thermal Enthalpies= -716.823497
Sum of electronic and thermal Free Energies= -716.888647
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Cartesian Coordinates
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6	-0.969177	-1.342860	0.170867
6	-1.962050	1.071112	0.036911
6	-3.262685	0.441240	-0.499738
6	-3.034246	-0.861900	-1.263084
6	-2.321615	-1.862358	-0.354628
1	-3.922089	0.236802	0.352740
1	-3.770107	1.183056	-1.126122
1	-3.993629	-1.273478	-1.595321
1	-2.447119	-0.679698	-2.170506
1	-2.966505	-2.080065	0.505729
1	-2.146382	-2.811312	-0.873003
6	-0.492086	-2.241841	1.321178
1	-0.456650	-3.280896	0.979511
1	0.503065	-1.950249	1.658657
1	-1.179512	-2.173054	2.168266
6	0.098117	-1.366410	-0.944027
1	1.017460	-0.895207	-0.601105
1	0.325893	-2.405263	-1.204186
1	-0.228856	-0.858866	-1.852530
6	-2.319538	2.135016	1.086013
1	-1.425659	2.642274	1.450646
1	-2.991607	2.875882	0.642136
1	-2.820724	1.671586	1.939817
6	-1.161266	1.744068	-1.096593
1	-1.700245	2.626794	-1.454964
1	-0.187320	2.068494	-0.727965
1	-0.997793	1.081430	-1.947629
7	-1.184573	0.014082	0.727876
8	-0.181888	0.474789	1.500974
1	0.822884	0.775444	0.949262
6	2.185990	1.181938	0.749122
6	2.906797	0.027670	1.285489
6	2.449444	1.492965	-0.651391
6	3.604334	-0.819675	0.503942
1	2.832004	-0.163030	2.353173
6	3.146750	0.669648	-1.461277
1	2.055575	2.423595	-1.052846
6	3.762109	-0.615554	-0.978806
1	4.093498	-1.686405	0.941355
1	3.299730	0.934022	-2.504620
1	4.830765	-0.644717	-1.251939
1	2.088352	2.038651	1.419912
1	3.326823	-1.471021	-1.525250