

Electronic Supplementary Information

**Mechanistic Insights on Rhodium-Catalyzed Enantioselective Allylic Alkylation for
Quaternary Stereogenic Centers**

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PART-B

Optimized Cartesian Coordinates of All Stationary Points (Page No. S16-S169)

(I) AIM Analysis on A3 and A4

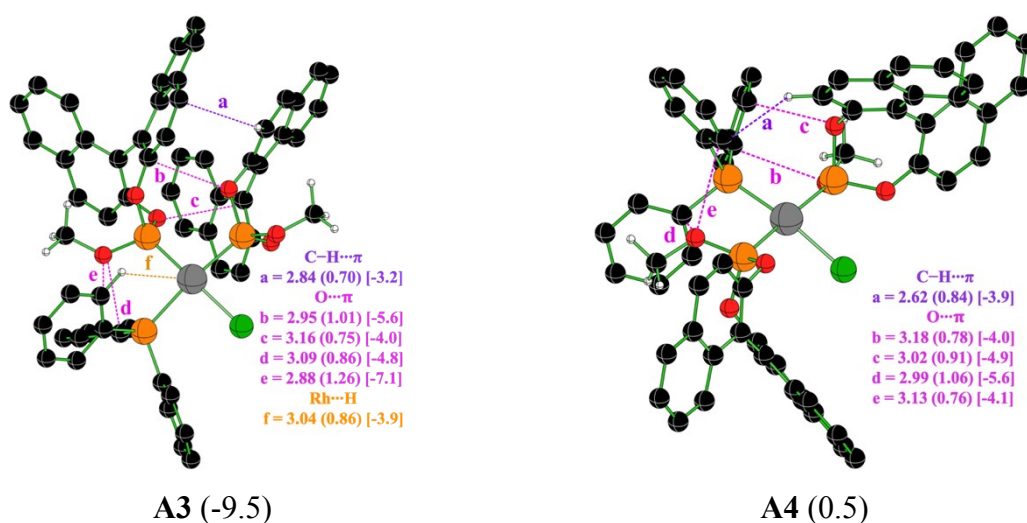


Fig. S1 The optimized geometries and the key noncovalent interactions as identified through the topological analysis of the electron density by using the AIM formalism on the possible active catalysts **A3** and **A4**. Important interatomic distances (in Å) and the corresponding electron densities ($\rho \times 10^{-2}$ a.u.) at the bond critical points are provided in parentheses and the strength (in kcal/mol) of respective noncovalent interactions obtained using the Espinosa formulation (ref. 44) is given in square brackets.

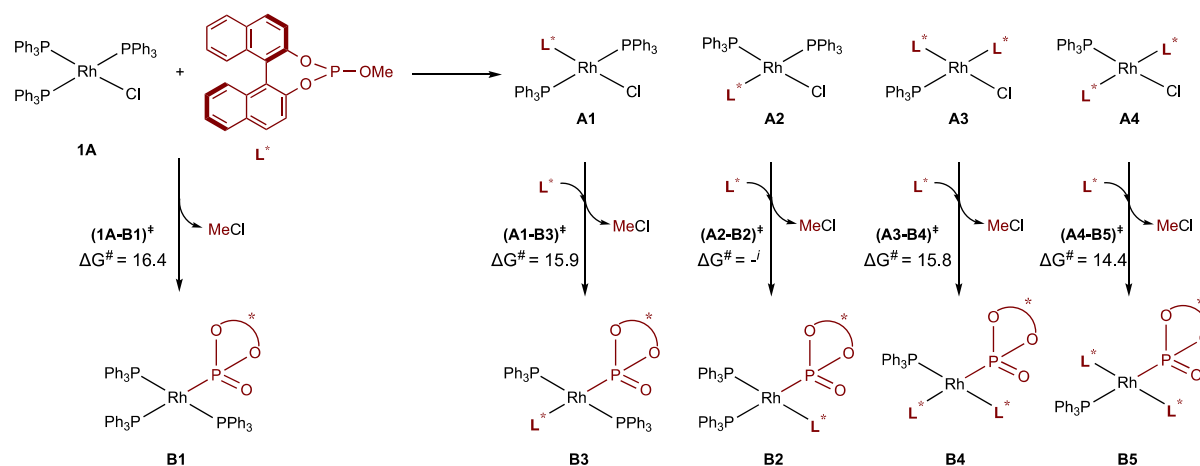
Table S1 Estimated Strengths of Important Noncovalent Interactions in the Possible Active Catalysts **A3** and **A4**. The Topological Quantities are Derived from the *Atoms-in-Molecules* (AIM) Analysisⁱ

A3						
NCI	bond path ⁱⁱ	ρ	$\nabla^2\rho$	G	$V=1/4\nabla^2\rho - 2G$	$E=1/2(V)$ (kcal/mol)
C-H... π	a	0.007	-0.006	0.004	-0.010	-3.2
O... π	b	0.010	-0.009	0.008	-0.018	-5.6
	c	0.008	-0.006	0.006	-0.013	-4.0
	d	0.009	-0.008	0.007	-0.015	-4.8
	e	0.013	-0.011	0.010	-0.023	-7.1
Rh...H	f	0.009	-0.007	0.005	-0.013	-3.9
total strength						-28.6
A4						
NCI	bond path ⁱⁱ	ρ	$\nabla^2\rho$	G	$V=1/4\nabla^2\rho - 2G$	$E=1/2(V)$ (kcal/mol)
C-H... π	a	0.008	-0.007	0.005	-0.012	-3.9
O... π	b	0.008	-0.006	0.006	-0.013	-4.0
	c	0.009	-0.008	0.007	-0.016	-4.9
	d	0.011	-0.009	0.008	-0.018	-5.6

	e	0.008	-0.007	0.006	-0.013	-4.1
total strength						-22.5

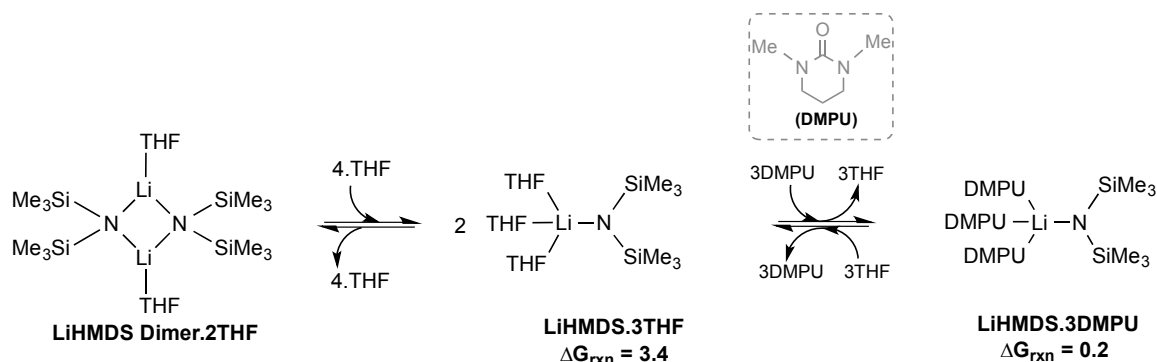
ⁱ ρ = electron density, $\nabla^2\rho$ = Laplacian of the electron density; G, V, and H are respectively the kinetic, potential, and total electron energy densities at the bond critical points. ⁱⁱ See Fig. S1 for details of bond paths.

(II) Rh-Catalyzed Arbuzov Rearrangement



Scheme S1 The generation of potential active catalysts through an *in situ* Rh-catalyzed Arbuzov rearrangement reaction and the corresponding elementary step barriers (in kcal/mol) computed with respect to the respective preceding intermediates. ⁱGeometry failed to converge even after repeated attempts.

(III) LiHMDS in the Presence of THF and DMPU



Scheme S2 The possible structure of LiHMDS in the presence of solvent THF and DMPU additive at the SMD_(THF)/B3LYP-D3/6-31G^{**},SDD(Rh) level of theory. Relative Gibbs free energies are in kcal/mol.

(IV) C–O Bond Oxidative Addition

Table S2 The Relative Gibbs Free Energies (ΔG in kcal/mol) of the C–O Bond Oxidative Addition Transition State $(3-4)_{A1}^\ddagger$ with Respect to the Separated Reactants Obtained at the $SMD_{(THF)}/B3LYP-D3/6-31G^{**},SDD(Rh)$ Level of Theory

$(3-4)_{A1}^\ddagger$	ΔG
without LiHMDS	24.5
LiHMDS.1THF	28.0
LiHMDS.2THF	30.3
LiHMDS.2THF (3-membered TS)	35.5
LiHMDS.2THF (OBz as a leaving group)	33.7
LiHMDS.1THF.1DMPU	26.5
LiHMDS.1DMPU	20.7
Coordination to Chloride	
LiHMDS.2THF	32.1
LiHMDS.1THF.1DMPU	27.5

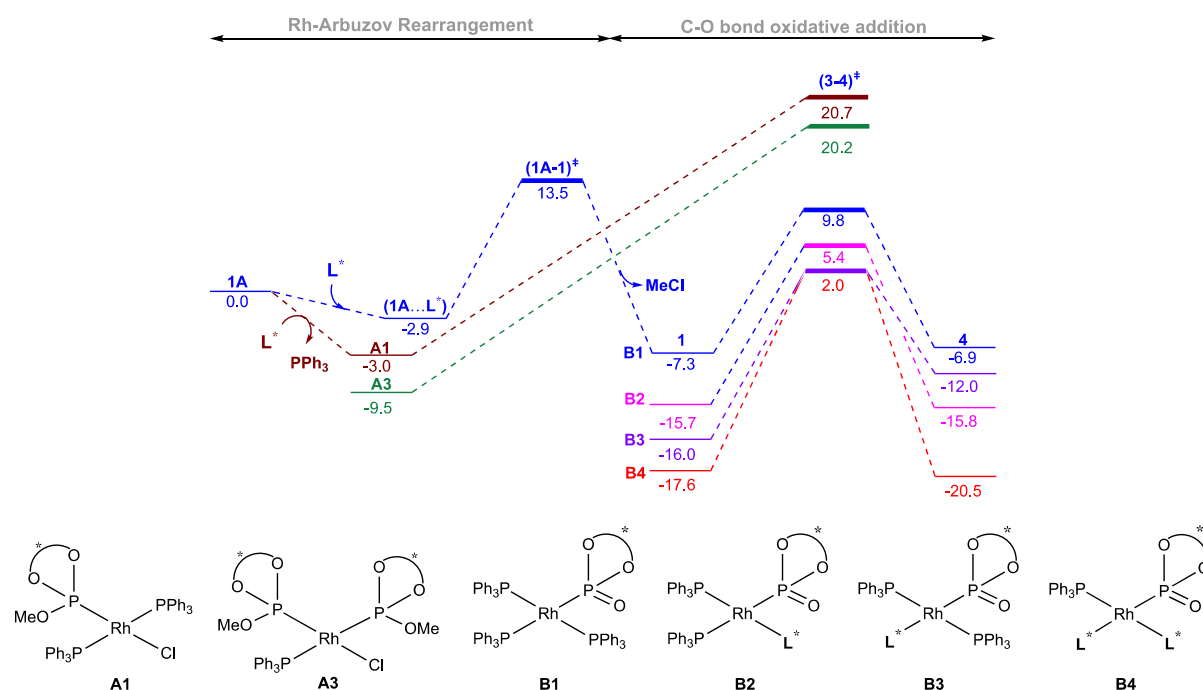


Fig. S2 Gibbs free energy (kcal/mol) profile obtained at the $SMD_{(THF)}/B3LYP-D3/6-31G^{**},SDD(Rh)$ level of theory for the C–O bond oxidative addition considering different possible active catalyst combinations obtained through the Rh-catalyzed Arbuzov rearrangement.

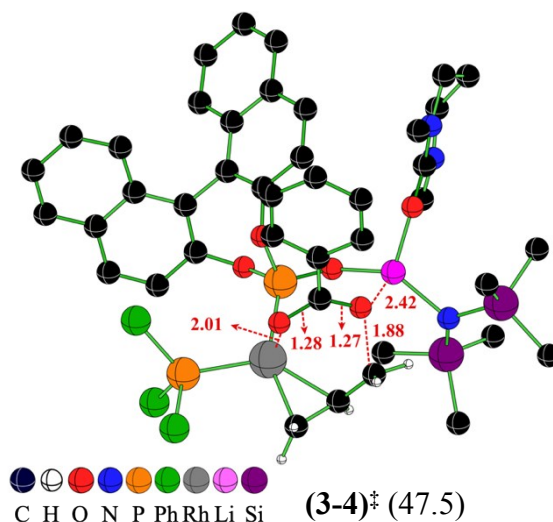
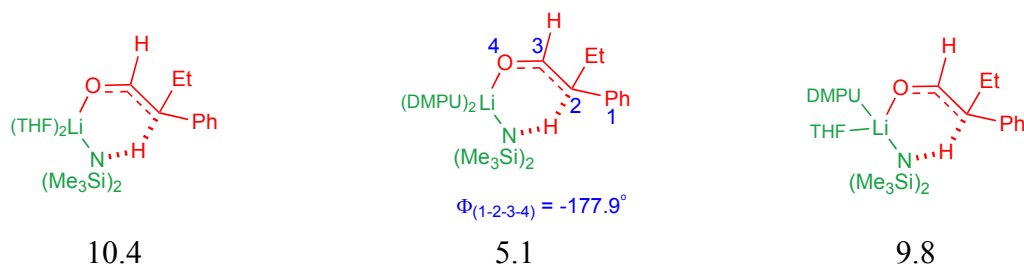


Fig. S3 Optimized geometry of the the C–O bond oxidative addition transition state **(3-4)[‡]** in the dissociative pathway wherein one of the PPh₃ ligands is removed from **B1**. Relative Gibbs free energy (in kcal/mol) given in parentheses is computed with respect to the separated reactants. Distances are in Å.

(V) Enolate Formation

(V.1) Different Possibilities for LiHMDS Promoted Deprotonation

E-Enolate



Z-Enolate

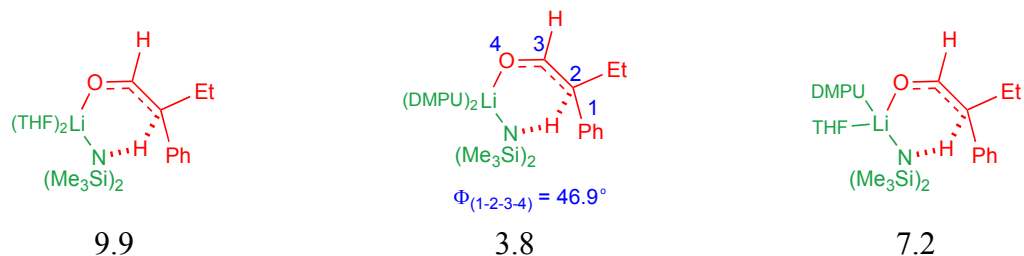
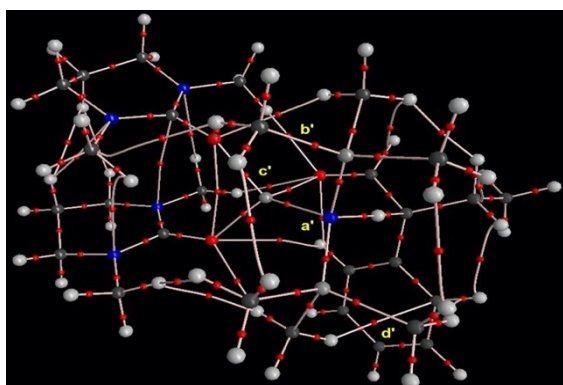
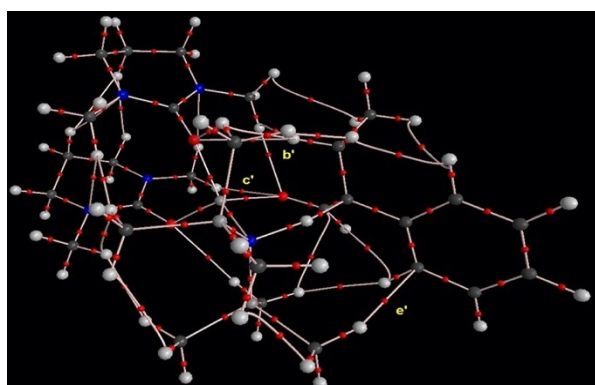
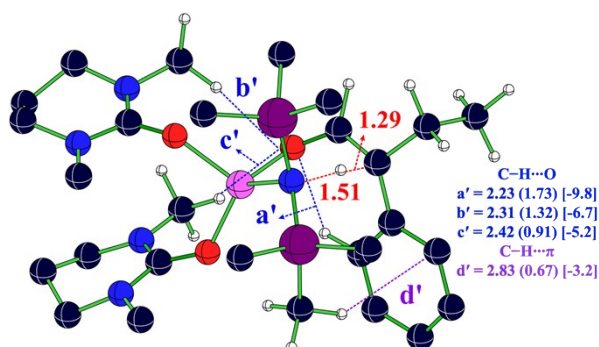


Fig. S4 The LiHMDS promoted deprotonation transition states **(5-6)[‡]** and the corresponding relative Gibbs free energies (in kcal/mol).

(V.2) AIM Analysis



(5-6)_Z[‡] (3.8)



(5-6)_E[‡] (5.1)

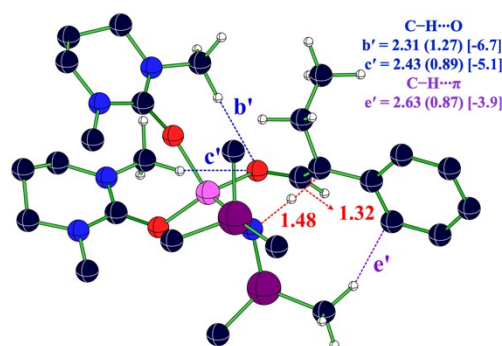


Fig. S5 Topological analysis on LiHMDS promoted deprotonation transition states using AIM Analysis.

Table S3 Estimated Strengths of the Important Noncovalent Interactions in the Deprotonation Transition States. The Topological Quantities are Derived from the *Atoms-in-Molecules* (AIM) Analysisⁱ

(5-6) _Z [‡]						
NCI	bond path ⁱⁱ	ρ	$\nabla^2\rho$	G	$V=1/4\nabla^2\rho - 2G$	$E=1/2(V)$ (kcal/mol)
C-H...O	a'	0.017	-0.015	0.014	-0.031	-9.8
	b'	0.013	-0.010	0.009	-0.021	-6.7
	c'	0.009	-0.008	0.007	-0.017	-5.2
C-H...π	d'	0.007	-0.006	0.005	-0.010	-3.3
total strength						-25.1
(5-6) _E [‡]						
NCI	bond path ⁱⁱ	ρ	$\nabla^2\rho$	G	$V=1/4\nabla^2\rho - 2G$	$E=1/2(V)$ (kcal/mol)
C-H...O	b'	0.013	-0.010	0.009	-0.021	-6.7
	c'	0.009	-0.008	0.007	-0.016	-5.1
C-H...π	e'	0.009	-0.007	0.005	-0.012	-3.9
total strength						-15.7

$i\rho$ = electron density, $\nabla^2\rho$ = Laplacian of the electron density; G, V, and H are respectively the kinetic, potential, and total electron energy densities at the bond critical points. ⁱⁱ See Fig. S5 for details of bond paths.

(VI) Enantioselective C–C Bond Formation

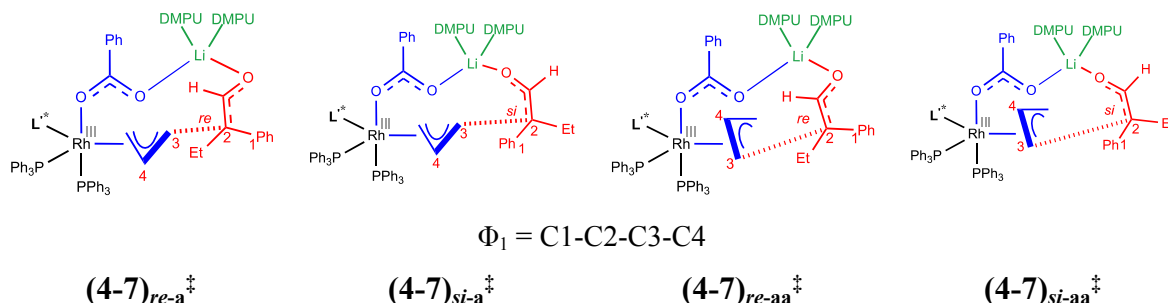


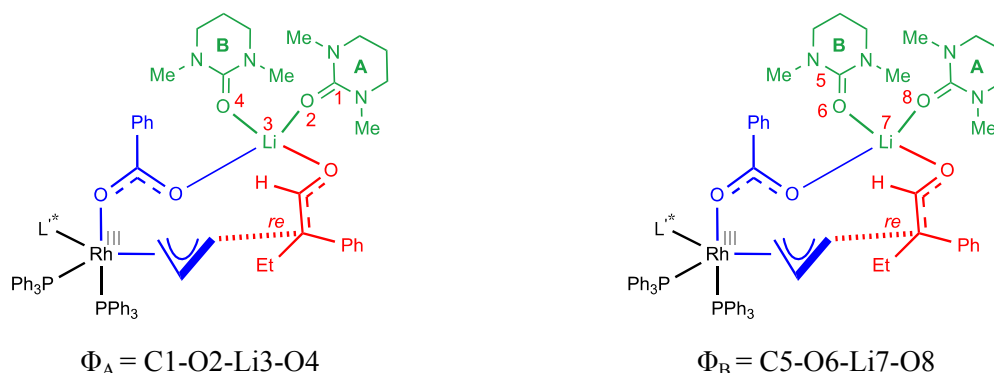
Fig. S6 Different possibilities for the enantiocontrolling C–C bond formation between the Li-Z-enolate and Rh- π -allyl. Subscripts **a** and **aa** denote the different orientations of the allyl moiety. When the C4-H is *anti* to the -OBz group, subscript **a** is used while the corresponding *syn* disposition is denoted as **aa**.

Table S4 The Relative Gibbs Free Energies (in kcal/mol)ⁱ of Various Conformers of the C–C Bond Formation Transition States (4-7)[‡] Arising due to the Possible Rotations (Φ_1) Around the Incipient C–C Bond along the Reaction Coordinate ⁱⁱ

(4-7) _{re-a} [‡]		(4-7) _{si-a} [‡]		(4-7) _{re-aa} [‡]		(4-7) _{si-aa} [‡]	
Φ_1	ΔG	Φ_1	ΔG	Φ_1	ΔG	Φ_1	ΔG
- ^{iv}	- ^{iv}	-20.8	-15.6	-65.8	-12.1	-36.7	-6.7
- ^{iv}	- ^{iv}	58.9	-0.2	50.0	-17.1	70.5	-9.9
153.1	-14.7	174.6	-8.0	70.4	-15.9	71.3	-10.2
-174.8	-23.0	167.5	-1.8	165.1	-14.9	-167.7	-13.5
-82.8	-15.1	-42.8	-21.7	-66.2	-12.3	-69.1	-21.2
-159.6	-8.5	-44.4	-20.9	-179.8	-16.6	- ^{iv}	- ^{iv}

ⁱ Computed with respect to the separated reactants, ⁱⁱ Corresponds to the optimized values of Φ_1 in each conformer (as qualitatively shown in Fig. S4). ⁱⁱⁱ Highlighted entries represent the lowest energy transition state (4-7)[‡], which were further examined with different conformers of DMPU (as shown Table S4). ^{iv} Geometry optimization failed to converge even after repeated attempts.

Table S5 The Relative Gibbs Free Energies (in kcal/mol)ⁱ of Additional Conformers of the C–C Bond Formation Transition States **(4-7)**[‡] Arising due to Various Orientations of the Li-Bound DMPUⁱⁱ



(4-7)_{re-a} [‡]	Φ_A	Φ_B	ΔG	(4-7)_{si-a} [‡]	Φ_A	Φ_B	ΔG
<i>re_1</i>	-166.1	-82.6	-22.3	<i>si_1</i>	-9.0	-114.2	-20.1
<i>re_2</i>	-28.0	169.1	-25.8	<i>si_2</i>	89.6	-178.4	-19.5
<i>re_3</i>	-29.7	-104.5	-24.2	<i>si_3</i>	21.5	-129.6	-23.4
				<i>si_4</i>	-101.6	-178.1	-21.6

ⁱ Computed with respect to the separated reactants, ⁱⁱ Corresponds to the optimized values of Φ_A and Φ_B in each conformer.

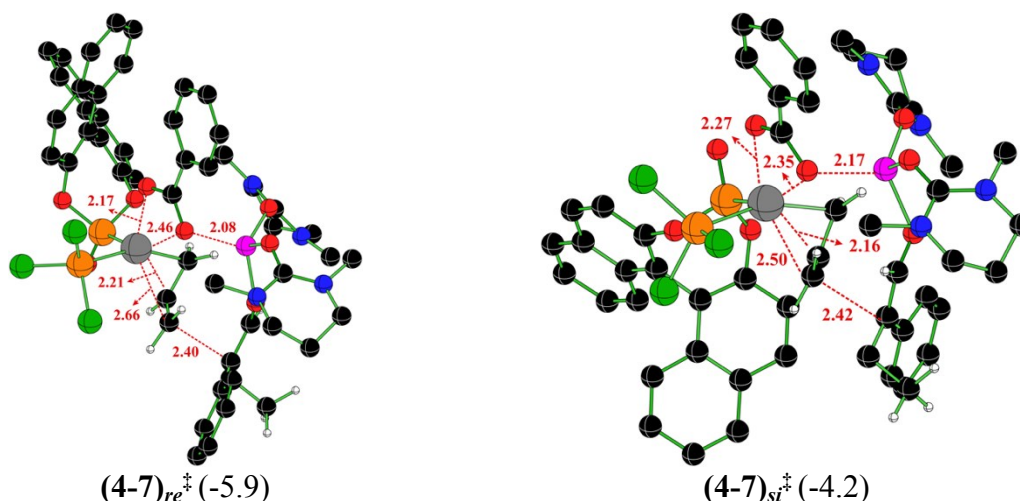


Fig. S7 Optimized geometry of the enantiocontrolling C–C bond formation transition state **(4-7)**[‡] in the dissociative pathway wherein one of the PPh₃ ligands is removed from **B1**. Relative Gibbs free energy (in kcal/mol) given in parentheses is with respect to the separated reactants. Distances are in Å.

(VII) AIM Analysis for Enantioselective C–C Bond Formation

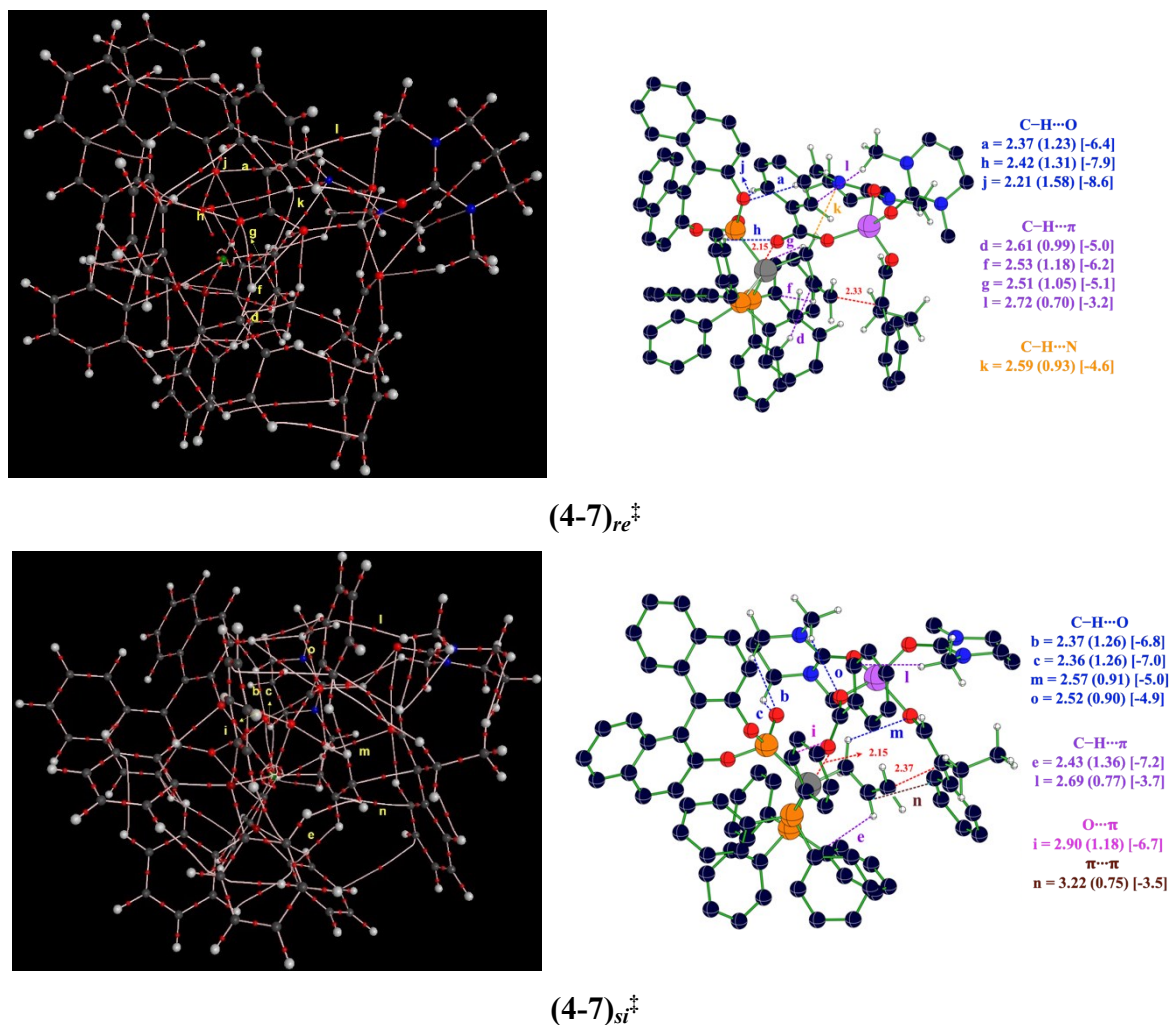
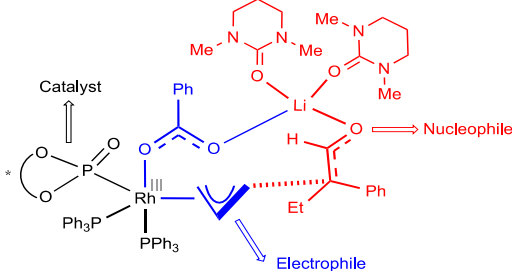


Fig. S8 Topological analysis for the enantiocontrolling C–C bond formation transition states performed using AIM Analysis.

Table S6 Estimated Strengths of the Important Noncovalent Interactions in the Enantiocontrolling C–C Bond Formation Transition States. The Topological Quantities are Derived from the *Atoms-in-Molecules* (AIM) Analysisⁱ

						
(4-7)_{re}[‡]						
NCI	bond path ⁱⁱ	ρ	$\nabla^2\rho$	G	$V=1/4\nabla^2\rho - 2G$	$E=1/2(V)$ (kcal/mol)

C-H $\cdots$ O	a	0.012	-0.009	0.009	-0.020	-6.4
	h	0.013	-0.013	0.011	-0.025	-7.9
	j	0.016	-0.012	0.012	-0.027	-8.6
C-H $\cdots\pi$	d	0.010	-0.008	0.007	-0.016	-5.0
	f	0.012	-0.011	0.009	-0.020	-6.2
	g	0.011	-0.009	0.007	-0.016	-5.1
	l	0.007	-0.005	0.004	-0.010	-3.2
C-H $\cdots$ N	k	0.009	-0.007	0.006	-0.015	-4.6
total strength						-46.9
(4-7) $_{st}^\ddagger$						
NCI	bond path ⁱⁱ	ρ	$\nabla^2\rho$	G	$V=1/4\nabla^2\rho-2G$	$E=1/2(V)$ (kcal/mol)
C-H $\cdots$ O	b	0.013	-0.010	0.010	-0.022	-6.8
	c	0.013	-0.011	0.010	-0.022	-7.0
	m	0.009	-0.008	0.007	-0.016	-5.0
	o	0.009	-0.008	0.007	-0.016	-4.9
C-H $\cdots\pi$	e	0.014	-0.012	0.010	-0.023	-7.2
	l	0.008	-0.006	0.005	-0.012	-3.7
O $\cdots\pi$	i	0.012	-0.011	0.009	-0.021	-6.7
$\pi\cdots\pi$	n	0.007	-0.006	0.005	-0.011	-3.5
Total Strength						-44.8

ⁱ ρ = electron density, $\nabla^2\rho$ = Laplacian of the electron density; G, V, and H are respectively the kinetic, potential, and total electron energy densities at the bond critical points. ⁱⁱ See Fig. S8 for details of bond paths.

(VIII) NCI-Plots for Enantiocontrolling C-C Bond Formation

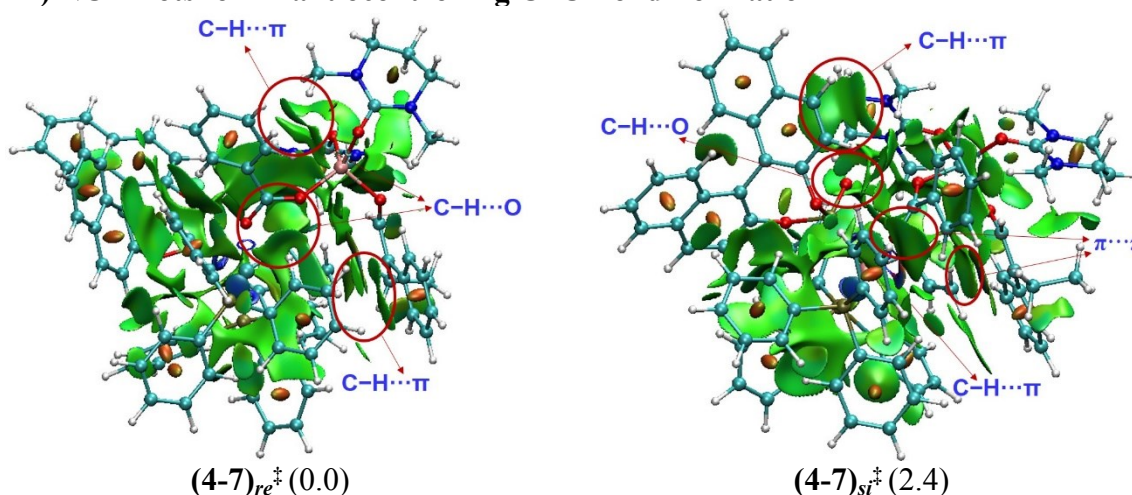


Fig. S9 The noncovalent interaction (NCI) plots of the enantiocontrolling C-C bond formation transition states. The blue and green color regions respectively represent strong and weak interactions while the red color denotes a repulsive interaction. The relative Gibbs free energies (in kcal/mol) with respect to the lowest energy transition state are provided in parentheses.

(IX) Distortion-Interaction/Activation-Strain Analysis of the Enantiocontrolling C–C Bond Formation

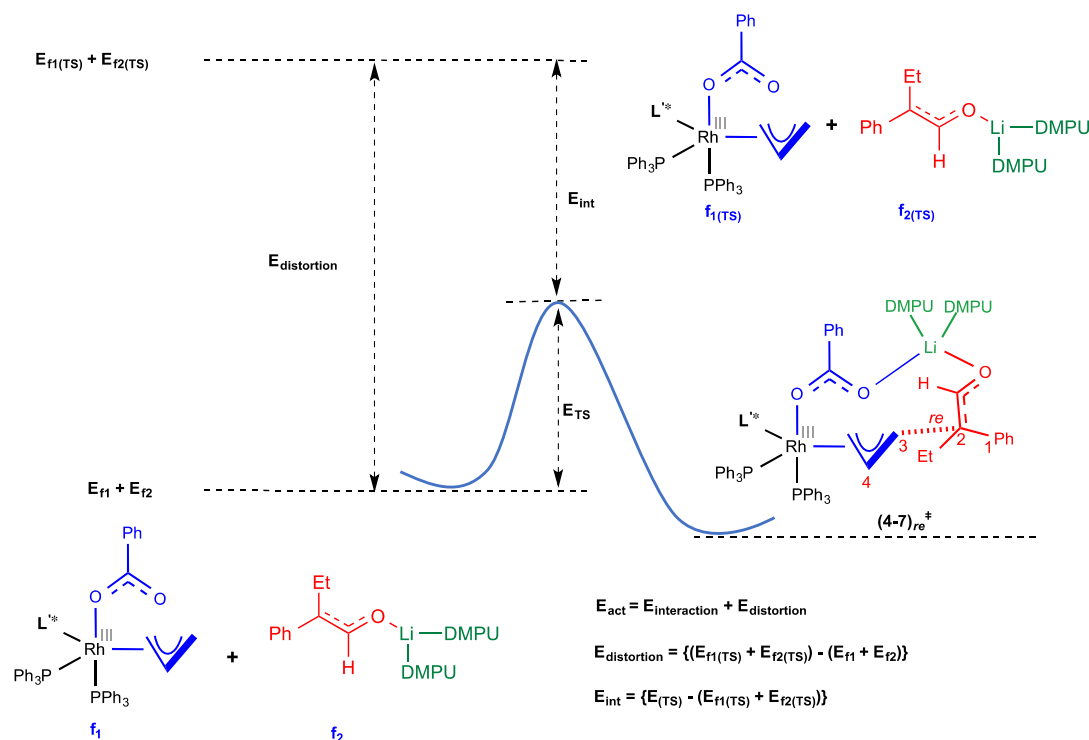


Fig. S10 A general representation of the fragments used in calculating the distortion and interaction energies in the enantiocontrolling C–C bond formation transition states in the Distortion-Interaction/Activation Strain Analysis.

Table S7 Relative Distortion ($\Delta\Delta E_d^\ddagger$) and Interaction Energies ($\Delta\Delta E_i^\ddagger$) (in kcal/mol) in the Enantiocontrolling C–C Bond Formation Transition States with Respect to the Lower Energy Transition State $(4-7)_{re}^\ddagger$

TS	$\Delta\Delta E_d^\ddagger (f_1)$	$\Delta\Delta E_d^\ddagger (f_2)$	$\Delta\Delta E_d^\ddagger$ [$\Delta\Delta E_d^\ddagger (f_1) + \Delta\Delta E_d^\ddagger (f_2)$]	$\Delta\Delta E_i^\ddagger$	$\Delta\Delta E^\ddagger$ ($\Delta\Delta E_d^\ddagger + \Delta\Delta E_i^\ddagger$)
$(4-7)_{re}^\ddagger$	0	0	0	0	0
$(4-7)_{si}^\ddagger$	4.2	0.7	4.9	-2.2	2.7

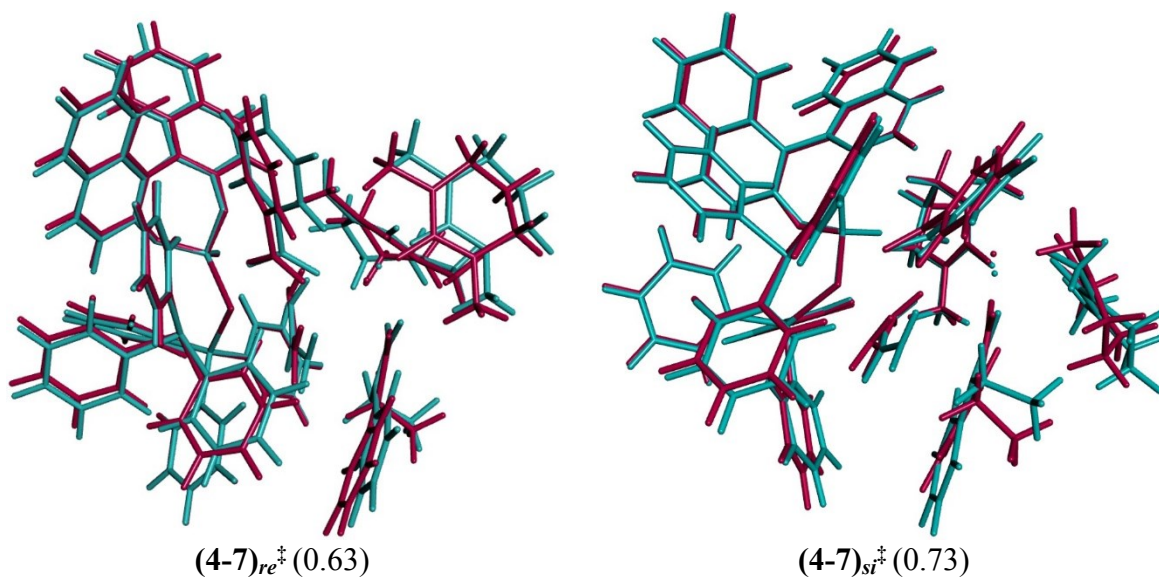


Fig. S11 Overlaid images of the enantiocontrolling C–C bond formation transition states (red) and the corresponding pre-reacting complex (cyan). The total geometric deviation is expressed in terms of the root mean square deviation (RMSD in Å) is given in parentheses. More geometric deviation, with respect to the pre-reacting complex can be noted in the higher energy C–C bond formation transition state $(4-7)_{si}^{\ddagger}$ as compared to the lower energy transition state $(4-7)_{re}^{\ddagger}$ similar to the DIAS analysis presented in Table S6.

(X) Energetic Span Calculations

Table S8 The Calculation of the Energetic Span (δE in kcal/mol) by using Different Likely Combinations of TDI and TDTS (the highlighted combination give the maximum δE)^a

TDI	TDTS	δE
0.0	13.5	13.5
	9.8	9.8
	-25.8	-25.8
-2.9	13.5	16.4
	9.8	12.7
	-25.8	-22.9
-7.3	13.5	-19.7
	9.8	17.1
	-25.8	-18.5
-6.5	13.5	-20.5
	9.8	16.3
	-25.8	-19.3
-6.9	13.5	-20.1
	9.8	-23.8
	-25.8	-18.9
-28.5	13.5	1.5
	9.8	-2.2
	-25.8	2.7
-37.9	13.5	10.9
	9.8	7.2
	-25.8	-28.4

^a The energetic span calculation corresponding to the Gibbs free energy profile shown in Fig. 4 in the main text. The Gibbs free energy of the overall reaction, **2** + **5** + LiHMDS.3DMPU $\rightarrow$ **8** + Li-OBz.3DMPU + H-N(SiMe₃)₂ can be calculated using $\Delta G_r = ((G_p) - (G_R)) = ((G_8 + G_{(Li-OBz.3DMPU)} + G_{(H-N(SiMe_3)_2)}) - (G_2 + G_5 + G_{(LiHMDS.3DMPU)})) = -40.5$ kcal/mol.

(XI) Hammett Studies on the Enantiocontrolling C–C Bond Formation Transition States

Table S9 The Gibbs Free Energies (in kcal/mol) of the Enantiocontrolling C–C Bond Formation Transition States for the *para*-Substituted (G_X) and Unsubstituted (G_H) Substrates and the Corresponding Substituent Constants

<i>p</i> -substituent	substituent constant	$(\Delta G_X - \Delta G_H)$		$\log(k_X/k_H)$	
(X)	σ	(4-7)_{re} [‡]	(4-7)_{si} [‡]	(4-7)_{re} [‡]	(4-7)_{si} [‡]
NH ₂	-0.66	0.8	0.5	-0.6	-0.3

OH	-0.38	-2.1	0.3	1.5	-0.2
OMe	-0.27	-2.2	0.2	1.6	-0.1
Me	-0.14	0.4	1.3	-0.3	-0.9
H	0.0	0.0	0.0	0.0	0.0
F	0.15	-2.7	-0.2	2.0	0.1
Br	0.26	-0.7	-1.6	0.5	1.2
COCH ₃	0.47	-2.2	-3.2	1.6	2.4
CF ₃	0.53	-4.8	-3.5	3.5	2.6
CN	0.70	-4.9	-4.2	3.6	3.1

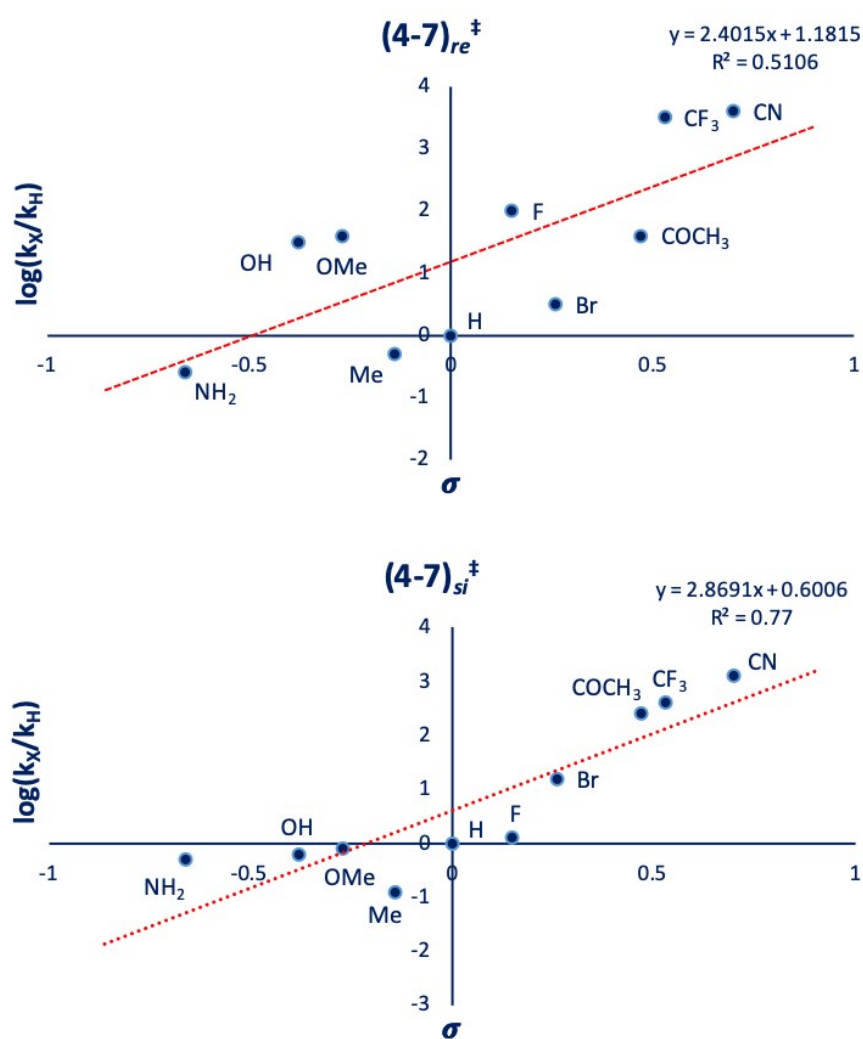


Fig. S12 Hammett plots for the enantiocontrolling C–C bond formation transition state for different substituent at *para*-position in the substrate.

PART-B

The optimized Cartesian coordinates of all the stationary points obtained at the SMD_(THF)/B3LYP-D3/6-31G**,SDD(Rh) level of theory

```
-----
1A [Rh(Cl)(PPh3)3]
-----
Number of imaginary frequencies : 0
Electronic energy : HF=-3680.0564377
Zero-point correction= 0.830887 (Hartree/Particle)
Thermal correction to Energy= 0.884215
Thermal correction to Enthalpy= 0.885159
Thermal correction to Gibbs Free Energy= 0.740557
Sum of electronic and zero-point Energies= -3679.225551
Sum of electronic and thermal Energies= -3679.172223
Sum of electronic and thermal Enthalpies= -3679.171279
Sum of electronic and thermal Free Energies= -3679.315881
Standard State and RRHO Corrected G = -3679.299845
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Cartesian Coordinates

```
-----
45 -0.027885 0.478442 -0.444386
15 2.274651 0.905852 -0.087207
15 -0.025019 -1.764399 -0.095025
15 -2.296313 0.890668 -0.018427
6 3.172103 -0.051759 1.219108
6 3.734392 -1.303967 0.919711
6 3.224889 0.408310 2.545273
6 4.309841 -2.084560 1.922535
1 3.737961 -1.667156 -0.100142
6 3.803471 -0.373758 3.547040
1 2.809206 1.376285 2.804161
6 4.340389 -1.626301 3.241519
1 4.732863 -3.052282 1.667980
1 3.833659 -0.000726 4.567145
1 4.784870 -2.236390 4.022756
6 3.483998 0.909914 -1.491033
6 4.863209 0.718246 -1.306529
6 2.999511 1.118544 -2.792162
6 5.733289 0.718901 -2.399077
1 5.265274 0.559584 -0.311668
6 3.871108 1.123800 -3.882137
1 1.938434 1.282235 -2.945178
6 5.239849 0.918129 -3.690102
1 6.796523 0.563194 -2.238095
1 3.477910 1.284203 -4.882346
1 5.916926 0.914563 -4.539876
6 2.388480 2.626349 0.589887
6 1.294980 3.141598 1.303335
6 3.546316 3.406848 0.465154
6 1.358570 4.407850 1.885575
1 0.384079 2.556395 1.382012
6 3.606142 4.678222 1.041290
1 4.403635 3.032839 -0.084825
6 2.515039 5.180702 1.754055
1 0.496298 4.791428 2.422756
1 4.507231 5.275322 0.930401
1 2.563777 6.170993 2.198646
6 0.047769 -2.547400 1.577581
6 -0.345752 -3.872626 1.829255
6 0.559523 -1.783936 2.635141
6 -0.239606 -4.410788 3.113032
1 -0.740847 -4.487342 1.027253
6 0.676732 -2.324100 3.916217
1 0.857875 -0.758621 2.452169
6 0.271725 -3.638576 4.159585
1 -0.555343 -5.434493 3.293773
1 1.081900 -1.716283 4.719843
1 0.353975 -4.059751 5.157689
6 1.384305 -2.584669 -0.988710
6 1.858709 -1.978874 -2.162644
6 2.002545 -3.762606 -0.542872
6 2.938597 -2.518302 -2.862906
1 1.394881 -1.063087 -2.512795
6 3.081774 -4.304285 -1.244112
1 1.670759 -4.249189 0.366628
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```

```
6 3.558551 -3.680916 -2.400402
1 3.304240 -2.015066 -3.753163
1 3.558562 -5.208792 -0.876430
1 4.408472 -4.096776 -2.934218
6 -1.471715 -2.594136 -0.916937
6 -2.625131 -2.960940 -0.206634
6 -1.456098 -2.782732 -2.310246
6 -3.731365 -3.495373 -0.871587
1 -2.670341 -2.834829 0.867550
6 -2.561731 -3.315517 -2.972281
1 -0.580526 -2.511250 -2.889655
6 -3.706851 -3.671776 -2.255144
1 -4.613978 -3.766370 -0.299371
1 -2.526966 -3.450352 -4.049814
1 -4.569501 -4.084490 -2.770552
6 -3.190030 -0.150886 1.221629
6 -4.505789 -0.608781 1.060199
6 -2.479383 -0.537817 2.368418
6 -5.087215 -1.440483 2.019812
1 -5.074833 -0.347732 0.175857
6 -3.058504 -1.368353 3.327735
1 -1.454942 -0.210138 2.495593
6 -4.365981 -1.827872 3.152017
1 -6.103348 -1.796360 1.873362
1 -2.478313 -1.671086 4.194574
1 -4.817922 -2.486062 3.888764
6 -2.449196 2.582615 0.736290
6 -2.613796 3.713076 -0.081487
6 -2.318505 2.771798 2.121486
6 -2.654772 4.992797 0.472853
1 -2.701878 3.596172 -1.154121
6 -2.355332 4.054161 2.674168
1 -2.195537 1.924013 2.785071
6 -2.523728 5.170089 1.852075
1 -2.785533 5.852542 -0.178443
1 -2.256823 4.175922 3.749441
1 -2.554356 6.167561 2.281521
6 -3.437545 0.955104 -1.459799
6 -4.689457 1.592481 -1.418548
6 -3.037563 0.314873 -2.640145
6 -5.526482 1.574643 -2.534755
1 -5.008400 2.106609 -0.516949
6 -3.878752 0.291209 -3.754436
1 -2.063804 -0.159801 -2.682316
6 -5.123950 0.920439 -3.703352
1 -6.491524 2.071891 -2.492553
1 -3.557044 -0.214176 -4.660670
1 -5.777584 0.907329 -4.571192
17 -0.078494 2.519187 -1.857468
-----
```

L* [(R)-BINOL-P(OMe)]

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-----
Number of imaginary frequencies : 0
Electronic energy : HF=-1376.4186682
Zero-point correction= 0.307007 (Hartree/Particle)
Thermal correction to Energy= 0.326300
Thermal correction to Enthalpy= 0.327244
Thermal correction to Gibbs Free Energy= 0.259608
Sum of electronic and zero-point Energies= -1376.111661
Sum of electronic and thermal Energies= -1376.092368
Sum of electronic and thermal Enthalpies= -1376.091424
Sum of electronic and thermal Free Energies= -1376.159060
Standard State and RRHO Corrected G= -1376.153601
-----
```

Cartesian Coordinates

```
-----
6 -3.812518 1.052215 1.233746
6 -2.479145 0.828717 0.967730
6 -2.058195 -0.306415 0.218389
6 -3.063111 -1.235428 -0.217309
6 -4.431154 -0.967039 0.062341
6 -4.803329 0.154856 0.767470
-----
```


1	-4.105815	1.923684	1.812306
1	-1.735483	1.521715	1.342750
6	-0.676580	-0.571136	-0.082387
6	-2.673769	-2.419805	-0.898892
1	-5.178723	-1.675602	-0.285117
1	-5.851122	0.347693	0.978906
6	-1.346297	-2.698806	-1.112759
6	-0.360785	-1.777052	-0.693404
1	-3.441153	-3.114893	-1.228245
1	-1.025195	-3.610189	-1.606413
6	0.419382	0.374192	0.272102
6	0.443492	1.737850	-0.189154
6	1.483012	-0.067748	1.046526
6	-0.508335	2.250864	-1.115102
6	1.484112	2.617840	0.262570
6	2.505103	0.797503	1.499700
6	-0.456371	3.561481	-1.538017
1	-1.279304	1.594324	-1.500568
6	1.500438	3.967838	-0.182477
6	2.493490	2.119304	1.130087
1	3.282666	0.388138	2.136270
6	0.548911	4.435966	-1.060284
1	-1.191824	3.925623	-2.249838
1	2.289822	4.622215	0.178607
1	3.270050	2.794377	1.479004
1	0.573544	5.468203	-1.397271
8	0.965816	-2.099487	-0.934047
8	1.563571	-1.394505	1.447995
15	1.867953	-2.656406	0.383136
8	3.339445	-2.395936	-0.247745
6	3.757122	-1.242661	-1.019748
1	4.193404	-0.495871	-0.352067
1	4.515217	-1.593608	-1.723480
1	2.921107	-0.805512	-1.568278

PPh₃

Number of imaginary frequencies : 0
 Electronic energy : HF=-1036.3534076
 Zero-point correction= 0.273872 (Hartree/Particle)
 Thermal correction to Energy= 0.289819
 Thermal correction to Enthalpy= 0.290764
 Thermal correction to Gibbs Free Energy= 0.226723
 Sum of electronic and zero-point Energies= -1036.079536
 Sum of electronic and thermal Energies= -1036.063588
 Sum of electronic and thermal Enthalpies= -1036.062644
 Sum of electronic and thermal Free Energies= -1036.126685
 Standard State and RRHO Corrected G= -1036.119225

Cartesian Coordinates

15	-0.000147	0.000219	-1.244537
6	-1.558330	0.579793	-0.431313
6	-2.222743	1.667886	-1.023036
6	-2.106425	0.001763	0.724613
6	-3.396537	2.176074	-0.464773
1	-1.818687	2.120974	-1.925443
6	-3.287633	0.503871	1.276470
1	-1.611024	-0.840243	1.197804
6	-3.933586	1.592687	0.686058
1	-3.895359	3.020595	-0.932335
1	-3.700794	0.044963	2.170738
1	-4.851855	1.981704	1.117196
6	0.277109	-1.639275	-0.431726
6	1.054265	-1.825577	0.722383
6	-0.335636	-2.758219	-1.021779
6	1.209800	-3.099645	1.274208
1	1.537828	-0.976008	1.194302
6	-0.189096	-4.028845	-0.463498
1	-0.931993	-2.634491	-1.922858
6	0.587090	-4.202869	0.685609
1	1.815760	-3.228477	2.167082
1	-0.673175	-4.882647	-0.929704
1	0.709041	-5.192649	1.116764
6	1.281224	1.059797	-0.431779
6	2.556239	1.089403	-1.022562
6	1.054428	1.825021	0.723061
6	3.583487	1.851478	-0.464256
1	2.746836	0.511699	-1.924125
6	2.080112	2.596602	1.274907

1	0.077121	1.818506	1.195442
6	3.346554	2.609709	0.685579
1	4.564715	1.859719	-0.930920
1	1.889022	3.185064	2.168333
1	4.142829	3.210076	1.116794

THF

Number of imaginary frequencies : 0
 Electronic energy : HF=-232.4694296
 Zero-point correction= 0.116780 (Hartree/Particle)
 Thermal correction to Energy= 0.121679
 Thermal correction to Enthalpy= 0.122623
 Thermal correction to Gibbs Free Energy= 0.088545
 Sum of electronic and zero-point Energies= -232.352649
 Sum of electronic and thermal Energies= -232.347750
 Sum of electronic and thermal Enthalpies= -232.346806
 Sum of electronic and thermal Free Energies= -232.380884
 Standard State and RRHO Corrected G= -232.377437

Cartesian Coordinates

6	-1.165807	-0.426572	-0.134709
8	-0.000120	-1.255572	-0.000294
6	1.165602	-0.426839	0.135128
6	0.731290	0.994574	-0.233929
6	-0.730945	0.994880	0.233705
1	-1.528790	-0.469065	-1.173741
1	-1.957486	-0.818017	0.515781
1	1.527661	-0.469114	1.174509
1	1.957744	-0.818662	-0.514552
1	1.346715	1.761287	0.245047
1	0.782362	1.139736	-1.319349
1	-0.781927	1.140583	1.319056
1	-1.346158	1.761569	-0.245579

DMPU

Number of imaginary frequencies : 0
 Electronic energy : HF=-420.6499904
 Zero-point correction= 0.184966 (Hartree/Particle)
 Thermal correction to Energy= 0.194455
 Thermal correction to Enthalpy= 0.195399
 Thermal correction to Gibbs Free Energy= 0.150243
 Sum of electronic and zero-point Energies= -420.465024
 Sum of electronic and thermal Energies= -420.455535
 Sum of electronic and thermal Enthalpies= -420.454591
 Sum of electronic and thermal Free Energies= -420.499747
 Standard State and RRHO Corrected G= -420.496128

Cartesian Coordinates

6	0.000284	-0.836290	-0.076511
6	-1.239968	1.319153	0.198846
6	1.238903	1.319656	0.199848
6	-0.000458	2.016526	-0.341208
1	-2.143921	1.721775	-0.271431
1	2.143145	1.723393	-0.268888
1	0.000053	1.970083	-1.436061
6	-2.430884	-0.839223	0.081585
1	-3.211513	-0.370036	-0.527270
1	-2.295684	-1.870855	-0.238320
1	-2.765982	-0.836718	1.129908
6	2.431291	-0.838077	0.081350
1	2.763825	-0.839710	1.130499
1	2.297943	-1.868527	-0.243148
1	3.212923	-0.365633	-0.523628
8	0.000773	-2.073623	-0.117208
1	-1.335456	1.493188	1.283245
1	-0.000846	3.069742	-0.044854
1	1.332813	1.492795	1.284540
7	-1.181624	-0.113321	-0.085417
7	1.181839	-0.112534	-0.086067

5 (2-phenylbutanal)

Number of imaginary frequencies : 0
 Electronic energy : HF=-463.5475123
 Zero-point correction= 0.194877 (Hartree/Particle)
 Thermal correction to Energy= 0.205412

Thermal correction to Enthalpy= 0.206356
 Thermal correction to Gibbs Free Energy= 0.157849
 Sum of electronic and zero-point Energies= -463.352635
 Sum of electronic and thermal Energies= -463.342100
 Sum of electronic and thermal Enthalpies= -463.341156
 Sum of electronic and thermal Free Energies= -463.389663
 Standard State and RRHO Corrected G= -463.385324

Cartesian Coordinates

```

6 -2.776482 -0.940537 0.523021
6 -1.405674 -1.079650 0.752527
6 -0.490835 -0.188246 0.176974
6 -0.977807 0.855966 -0.624791
6 -2.347298 0.997085 -0.854605
6 -3.251137 0.098190 -0.281600
1 -3.472590 -1.642952 0.973340
1 -1.040850 -1.889990 1.378686
1 -2.708421 1.810512 -1.477940
1 -4.317271 0.207791 -0.459539
1 -0.280254 1.561706 -1.068340
6 1.009667 -0.343645 0.404154
1 1.152517 -1.129925 1.159134
6 1.777095 -0.714016 -0.877604
1 1.248102 -1.540304 -1.365929
1 1.741913 0.136830 -1.566965
6 3.232069 -1.112338 -0.614764
1 3.289294 -1.974143 0.061026
1 3.735541 -1.387305 -1.547940
1 3.790581 -0.288283 -0.161771
6 1.504647 0.945442 1.041668
8 2.267300 1.734719 0.519800
1 1.077565 1.148807 2.047959

```

2 (allyl benzoate)

Number of imaginary frequencies : 0
 Electronic energy : HF=-537.5543661
 Zero-point correction= 0.176705 (Hartree/Particle)
 Thermal correction to Energy= 0.187616
 Thermal correction to Enthalpy= 0.188560
 Thermal correction to Gibbs Free Energy= 0.138047
 Sum of electronic and zero-point Energies= -537.377661
 Sum of electronic and thermal Energies= -537.366750
 Sum of electronic and thermal Enthalpies= -537.365806
 Sum of electronic and thermal Free Energies= -537.416319
 Standard State and RRHO Corrected G= -537.411386

Cartesian Coordinates

```

6 3.735684 0.385573 -0.000188
1 4.756271 0.004166 -0.000332
6 3.508350 1.698528 -0.000379
6 2.698328 -0.693114 0.000243
1 2.809678 -1.340167 0.880151
8 1.383605 -0.107397 0.000315
6 0.348074 -0.973472 0.000141
8 0.493561 -2.183354 -0.000089
1 2.501688 2.105442 -0.000250
1 4.330504 2.408760 -0.000686
1 2.809402 -1.340632 -0.879350
6 -0.972238 -0.283038 0.000072
6 -1.088040 1.115401 0.000205
6 -2.127879 -1.078394 -0.000138
6 -2.350441 1.707720 0.000131
1 -0.195752 1.731013 0.000367
6 -3.387019 -0.482397 -0.000210
1 -2.021283 -2.158098 -0.000241
6 -3.499579 0.911538 -0.000076
1 -2.438349 2.790232 0.000233
1 -4.279490 -1.101310 -0.000369
1 -4.481442 1.376533 -0.000133

```

LiHMDS-Dimer.2THF

Number of imaginary frequencies : 0
 Electronic energy : HF=-2226.9832229
 Zero-point correction= 0.699019 (Hartree/Particle)
 Thermal correction to Energy= 0.747364
 Thermal correction to Enthalpy= 0.748308

Thermal correction to Gibbs Free Energy= 0.617304
 Sum of electronic and zero-point Energies= -2226.284204
 Sum of electronic and thermal Energies= -2226.235859
 Sum of electronic and thermal Enthalpies= -2226.234915
 Sum of electronic and thermal Free Energies= -2226.365919
 Standard State and RRHO Corrected G= -2226.353764

Cartesian Coordinates

```

3 1.178532 -0.207932 0.241506
3 -1.175426 0.154201 0.128253
7 0.244483 1.560944 0.149045
7 -0.241696 -1.617411 0.136139
14 0.053519 2.450510 1.610772
14 0.722732 2.320670 -1.318835
14 -0.196636 -2.448924 1.637825
14 -0.597974 -2.300422 -1.396719
6 -1.053797 1.521814 2.848870
1 -2.059754 1.363148 2.443364
1 -0.653201 0.545624 3.138847
1 -1.156856 2.115026 3.766894
6 1.712705 2.752193 2.491996
1 2.388123 3.355274 1.873478
1 1.583706 3.274043 3.449238
1 2.217500 1.800020 2.700277
6 -0.797983 4.142864 1.405499
1 -0.891602 4.648454 2.375659
1 -0.256265 4.819835 0.735938
1 -1.811171 4.022082 1.002416
6 -0.742937 3.062920 -2.279767
1 -1.220111 3.869314 -1.709512
1 -0.425965 3.483074 -3.243335
1 -1.509247 2.306035 -2.487428
6 1.564998 1.078994 -2.492298
1 2.416445 0.581926 -2.013193
1 0.886347 0.301742 -2.855590
1 1.953181 1.607313 -3.372842
6 1.994011 3.729207 -1.132461
1 1.639161 4.542164 -0.489714
1 2.941724 3.370824 -0.713275
1 2.218851 4.165215 -2.114815
6 1.139905 -1.704810 2.778736
1 0.988780 -2.048547 3.810315
1 2.139600 -2.028869 2.466475
1 1.146611 -0.609257 2.804691
6 -1.852233 -2.345612 2.570650
1 -2.644802 -2.852082 2.005735
1 -1.795646 -2.821398 3.558526
1 -2.165654 -1.306033 2.719916
6 0.240324 -4.300196 1.552096
1 -0.586156 -4.906015 1.165608
1 1.114593 -4.484042 0.915089
1 0.481090 -4.677918 2.554686
6 -1.677947 -3.868660 -1.381898
1 -2.055277 -4.075260 -2.392286
1 -1.123883 -4.754440 -1.053502
1 -2.548857 -3.758189 -0.723594
6 0.964348 -2.761391 -2.380429
1 0.720560 -3.096396 -3.397201
1 1.654520 -1.914807 -2.467386
1 1.503194 -3.580364 -1.887242
6 -1.596752 -1.068529 -2.463519
1 -2.659887 -1.106840 -2.200989
1 -1.270257 -0.027105 -2.375526
1 -1.517378 -1.335059 -3.525318
6 4.085466 0.496773 0.359764
6 4.645746 -1.355990 -1.129976
1 5.048329 0.102702 -0.780399
1 4.588260 0.480528 1.335525
1 3.603789 1.465819 0.228121
1 5.502827 -2.031292 -1.192600
1 4.114735 -1.389410 -2.085776
1 6.087471 0.172574 -0.448715
1 4.927111 0.761370 -1.644119
6 -4.066738 -0.565411 0.224469
6 -4.532992 1.271766 -1.312440
6 -5.086526 -0.091839 -0.837852
1 -4.526558 -0.667069 1.214297
1 -3.569609 -1.503478 -0.028097
1 -5.318808 2.000918 -1.525706

```

1	-3.920905	1.147452	-2.211183
1	-6.076786	0.022897	-0.388309
1	-5.173584	-0.804356	-1.661993
1	2.915535	-2.455362	-0.281400
1	4.236181	-2.131763	0.875909
1	-4.226631	2.129893	0.675136
1	-2.834973	2.376107	-0.416390
8	3.047876	-0.506131	0.356540
8	-3.043749	0.457314	0.288028
6	3.692808	-1.744988	0.002128
6	-3.643220	1.694530	-0.148805

LiHMDS.3THF

Number of imaginary frequencies : 0
Electronic energy : HF=-1578.453863
Zero-point correction= 0.584970 (Hartree/Particle)
Thermal correction to Energy= 0.621579
Thermal correction to Enthalpy= 0.622523
Thermal correction to Gibbs Free Energy= 0.512864
Sum of electronic and zero-point Energies= -1577.868893
Sum of electronic and thermal Energies= -1577.832284
Sum of electronic and thermal Enthalpies= -1577.831340
Sum of electronic and thermal Free Energies= -1577.940999
Standard State and RRHO Corrected G= -1577.929052

Cartesian Coordinates

3	-0.375426	0.140328	0.091375
7	1.448287	-0.566476	0.171617
14	2.519006	0.419875	1.051210
14	1.922747	-1.793861	-0.901638
6	1.696829	2.038511	1.632216
1	0.794220	1.848635	2.222092
1	2.389899	2.628870	2.246204
1	1.402390	2.654211	0.774868
6	3.193234	-0.406228	2.636003
1	3.872739	0.254052	3.191936
1	2.374512	-0.682028	3.313320
1	3.743981	-1.325885	2.401783
6	4.063209	1.000070	0.081274
1	3.777197	1.582304	-0.804368
1	4.708093	1.640385	0.698555
1	4.675948	0.159170	-0.266148
6	0.512182	-3.026492	-1.242672
1	0.827209	-3.814500	-1.939278
1	0.174316	-3.515928	-0.320517
1	-0.349554	-2.515507	-1.682438
6	3.389310	-2.867617	-0.308353
1	4.298330	-2.273922	-0.151158
1	3.156004	-3.364625	0.642050
1	3.634389	-3.652037	-1.037266
6	2.431570	-1.139774	-2.624657
1	1.607341	-0.582535	-3.089285
1	3.286436	-0.455627	-2.554156
1	2.711767	-1.948095	-3.313900
6	0.417759	2.199147	-1.958573
6	-1.024755	4.051369	-1.578573
6	0.428395	3.726416	-1.956736
1	0.081559	1.802172	-2.926166
1	1.376176	1.742169	-1.703980
1	-1.677237	3.946206	-2.452862
1	-1.155269	5.056777	-1.169670
1	0.730916	4.141370	-2.921834
1	1.114457	4.100784	-1.188817
6	-0.866113	-0.423877	2.962014
6	-3.174736	0.075096	3.215024
6	-2.175441	-1.083625	3.378703
1	-0.442412	0.177150	3.779403
1	-0.101634	-1.110587	2.593338
1	-3.181030	0.695711	4.117091
1	-4.198025	-0.263184	3.031684
1	-2.141268	-1.480372	4.396932
1	-2.414485	-1.903151	2.693436
6	-2.356247	-0.442947	-2.130754
6	-3.359247	-2.508125	-1.502529
6	-3.608756	-1.279533	-2.390257
1	-1.534418	-0.733792	-2.798135
1	-2.512274	0.634684	-2.219839
1	-2.660227	-3.195984	-1.990536

1	-4.270042	-3.059012	-1.253178
1	-3.732154	-1.524290	-3.448523
1	-4.502859	-0.742215	-2.053523
6	-1.333329	2.961963	-0.550341
6	-2.604236	0.867975	2.023886
6	-2.707545	-1.877221	-0.273006
8	-0.541312	1.819921	-0.943736
8	-1.231124	0.439279	1.864269
8	-1.972065	-0.733438	-0.765585
1	-2.386401	2.664102	-0.530870
1	-1.034147	3.265901	0.460532
1	-3.121440	0.653498	1.084316
1	-2.624569	1.949805	2.196509
1	-3.462345	-1.530749	0.444585
1	-2.008848	-2.540516	0.242778

LiHMDS.3DMPU

Number of imaginary frequencies : 0
Electronic energy : HF=-2143.0033687
Zero-point correction= 0.790085 (Hartree/Particle)
Thermal correction to Energy= 0.840098
Thermal correction to Enthalpy= 0.841042
Thermal correction to Gibbs Free Energy= 0.705256
Sum of electronic and zero-point Energies= -2142.213284
Sum of electronic and thermal Energies= -2142.163271
Sum of electronic and thermal Enthalpies= -2142.162326
Sum of electronic and thermal Free Energies= -2142.298113
Standard State and RRHO Corrected G= -2142.28483

Cartesian Coordinates

3	0.204862	-0.163752	-0.698319
6	-1.724347	0.016775	1.741247
6	-3.268151	1.828594	2.494709
6	-2.303112	0.266658	4.153541
6	-3.579997	0.956454	3.700019
1	-2.649146	2.689304	2.790452
1	-2.514787	-0.458806	4.945696
1	-3.988354	1.567816	4.509970
6	2.651695	-1.967338	-0.575919
6	5.083757	-1.496415	-0.670490
6	4.217840	-3.132090	0.980819
6	5.299977	-2.871746	-0.055683
1	5.786568	-1.327886	-1.491626
1	4.250267	-4.173149	1.321110
1	5.253100	-3.633598	-0.841899
6	-2.546044	1.692445	0.149867
1	-2.051245	2.669970	0.205081
1	-2.007297	1.072044	-0.558594
1	-3.571912	1.841411	-0.205562
6	-0.719225	-1.471180	3.395109
1	-1.170659	-2.170174	4.107428
1	-0.413239	-2.013394	2.504654
1	0.171271	-1.027475	3.860501
6	3.454562	-0.337297	-2.173379
1	4.371973	-0.133160	-2.730641
1	2.678354	-0.653561	-2.873168
1	3.107188	0.572104	-1.674194
6	1.781752	-3.374927	1.222569
1	1.881022	-3.035488	2.262004
1	0.846676	-2.998849	0.817367
1	1.767060	-4.471897	1.217806
7	-2.577225	1.057439	1.459931
7	-1.695113	-0.453850	3.035150
8	-1.034803	-0.525847	0.853063
8	1.483916	-1.688709	-0.933189
7	1.117329	1.663324	-0.405548
14	1.779875	1.836029	1.147139
14	1.053329	2.934320	-1.527769
6	0.599832	2.633075	2.427409
1	0.234765	3.608083	2.081585
1	-0.275282	1.998429	2.600365
1	1.090163	2.788402	3.398398
6	2.292245	0.166139	1.905749
1	2.503712	0.259272	2.979355
1	1.503859	-0.578130	1.774387
1	3.199994	-0.214393	1.423728
6	3.377275	2.890985	1.240486
1	3.217413	3.927980	0.920144

1	3.774048	2.924104	2.264698	6	-5.775207	-2.217982	0.764544
1	4.162755	2.469263	0.599919	6	-4.539196	-3.783555	-0.655448
6	2.707622	3.318255	-2.414179	6	-2.256956	-3.327419	-1.335536
1	2.622285	4.211887	-3.047923	6	-6.831505	-3.101785	0.818477
1	3.522541	3.496986	-1.702058	1	-5.831215	-1.286399	1.314409
1	3.017637	2.489621	-3.063435	6	-5.652972	-4.664549	-0.593914
6	0.494405	4.623445	-0.814503	6	-3.353655	-4.151237	-1.348295
1	-0.492348	4.547128	-0.339519	1	-1.325698	-3.599948	-1.819440
1	1.191129	5.002944	-0.056564	6	-6.780885	-4.332512	0.122023
1	0.421137	5.387793	-1.600506	1	-7.709908	-2.852269	1.406938
6	-0.176869	2.578218	-2.932480	1	-5.589261	-5.615358	-1.116942
1	-0.034751	1.570378	-3.338453	1	-3.318093	-5.106092	-1.865509
1	-1.207755	2.644125	-2.568616	1	-7.624192	-5.015609	0.166208
1	-0.069851	3.296371	-3.756365	8	-1.507364	-0.632677	1.747702
1	-1.592223	1.001083	4.562462	8	-1.167020	-1.317657	-0.688422
1	-4.328795	0.203159	3.429945	15	-0.271260	-0.975486	0.669492
1	-4.189773	2.226132	2.056353	8	0.143324	-2.398176	1.328026
1	5.256885	-0.707666	0.077866	6	-0.747515	-3.444812	1.767778
1	6.286787	-2.926609	0.413235	1	-0.914146	-4.150197	0.950480
1	4.370417	-2.494286	1.865362	1	-0.242520	-3.949683	2.594145
7	3.726394	-1.402327	-1.209056	1	-1.701036	-3.041124	2.112514
7	2.890025	-2.880526	0.422582	15	0.426972	2.366675	-0.042706
8	-1.204252	-0.757066	-2.126372	17	3.355402	1.592838	1.474126
6	-2.361467	-1.196479	-1.933328	15	2.881797	-1.467561	0.117228
6	-4.834417	-0.853980	-2.038382	6	2.223213	-2.725990	-1.074961
6	-3.915574	-2.825563	-0.860519	6	1.728699	-3.971992	-0.659289
6	-4.980201	-2.354096	-1.837659	6	2.123960	-2.381142	-2.432917
1	-5.117139	-0.313396	-1.121688	6	1.168665	-4.857736	-1.582374
1	-3.903123	-3.919017	-0.802966	1	1.773049	-4.254477	0.385227
1	-5.977045	-2.591121	-1.454063	6	1.556113	-3.263717	-3.352705
7	-2.587433	-2.384113	-1.284247	1	2.494610	-1.422191	-2.780731
7	-3.460989	-0.520931	-2.413828	6	1.080143	-4.508186	-2.932020
1	-4.128331	-2.449924	0.152821	1	0.797911	-5.820687	-1.242000
1	-4.852668	-2.866724	-2.797742	1	1.492124	-2.979424	-4.399365
1	-5.496887	-0.505351	-2.836946	1	0.643604	-5.198071	-3.648688
6	-3.285010	0.707117	-3.170304	6	4.366899	-0.834544	-0.786920
1	-3.572645	1.589010	-2.582916	6	5.633008	-1.427854	-0.690553
1	-2.244279	0.808571	-3.462787	6	4.200439	0.277952	-1.628676
1	-3.913156	0.675941	-4.068535	6	6.706698	-0.923676	-1.429255
6	-1.477941	-3.127636	-0.709296	1	5.797789	-2.273885	-0.033149
1	-1.560693	-4.183040	-0.997965	6	5.270708	0.773344	-2.372656
1	-0.533078	-2.725247	-1.063897	1	3.237180	0.774247	-1.685002
1	-1.493454	-3.057231	0.384399	6	6.528519	0.173101	-2.274618
-----				1	7.684042	-1.389679	-1.338217
A1				1	5.119948	1.639270	-3.010556
-----				1	7.366479	0.563610	-2.845482
Number of imaginary frequencies : 0				6	3.527909	-2.439686	1.535512
Electronic energy : HF=-4020.1247844				6	4.194619	-3.668712	1.394764
Zero-point correction= 0.863205 (Hartree/Particle)				6	3.337929	-1.908924	2.820519
Thermal correction to Energy= 0.920197				6	4.663982	-4.349137	2.519586
Thermal correction to Enthalpy= 0.921141				1	4.338109	-4.102779	0.410308
Thermal correction to Gibbs Free Energy= 0.769402				6	3.809764	-2.590916	3.943549
Sum of electronic and zero-point Energies= -4019.261579				1	2.823920	-0.959088	2.931158
Sum of electronic and thermal Energies= -4019.204587				6	4.472565	-3.811460	3.795247
Sum of electronic and thermal Enthalpies= -4019.203643				1	5.176231	-5.299505	2.398491
Sum of electronic and thermal Free Energies= -4019.355383				1	3.657120	-2.168773	4.932866
Standard State and RRHO Corrected G= -4019.338977				1	4.836525	-4.343730	4.669700
-----				6	1.640087	3.209079	-1.170384
Cartesian Coordinates				6	2.608039	4.078543	-0.641212
-----				6	1.675799	2.918416	-2.543477
45	1.449638	0.337497	0.543310	6	3.578062	4.647729	-1.466528
6	-6.464726	1.369921	-1.235283	1	2.613122	4.304956	0.417720
6	-5.488420	0.453182	-0.911274	6	2.650989	3.486007	-3.366953
6	-4.568794	0.698408	0.146671	1	0.941863	2.254193	-2.984964
6	-4.666695	1.948358	0.844782	6	3.605940	4.352876	-2.831740
6	-5.695605	2.865220	0.497274	1	4.316445	5.319572	-1.037809
6	-6.581802	2.584594	-0.518068	1	2.657918	3.251155	-4.427798
1	-7.146087	1.161492	-2.055304	1	4.363396	4.796052	-3.472194
1	-5.404345	-0.462302	-1.484294	6	-1.094348	2.337584	-1.092913
6	-3.533878	-0.236940	0.505401	6	-2.109002	3.303748	-1.033279
6	-3.712322	2.264757	1.846945	6	-1.188797	1.319438	-2.057209
1	-5.757243	3.803617	1.042482	6	-3.176041	3.266344	-1.933388
1	-7.360103	3.295541	-0.779891	1	-2.085100	4.081544	-0.280023
6	-2.671333	1.410461	2.108786	6	-2.256093	1.283007	-2.954392
6	-2.573844	0.184770	1.415070	1	-0.430319	0.546529	-2.098737
1	-3.794224	3.207246	2.380988	6	-3.251370	2.260962	-2.898354
1	-1.914667	1.647358	2.845302	1	-3.959854	4.013979	-1.863485
6	-3.480947	-1.610763	-0.067651	1	-2.312139	0.483959	-3.688418
6	-4.603711	-2.513661	0.011826	1	-4.088859	2.230307	-3.588920
6	-2.324687	-2.083047	-0.669365	6	0.138401	3.619153	1.269979

6	-0.108137	4.974675	0.993545
6	0.202999	3.196650	2.605424
6	-0.328970	5.877438	2.034431
1	-0.115236	5.328087	-0.032903
6	-0.016822	4.100867	3.646605
1	0.440549	2.159648	2.822025
6	-0.291059	5.440312	3.361920
1	-0.523359	6.922271	1.809265
1	0.034083	3.759633	4.676646
1	-0.461218	6.145265	4.170894

A2

Number of imaginary frequencies : 0
 Electronic energy : HF=-4020.1208192
 Zero-point correction= 0.863614 (Hartree/Particle)
 Thermal correction to Energy= 0.920448
 Thermal correction to Enthalpy= 0.921392
 Thermal correction to Gibbs Free Energy= 0.769882
 Sum of electronic and zero-point Energies= -4019.257205
 Sum of electronic and thermal Energies= -4019.200372
 Sum of electronic and thermal Enthalpies= -4019.199427
 Sum of electronic and thermal Free Energies= -4019.350937
 Standard State and RRHO Corrected G= -4019.334535

Cartesian Coordinates

45	0.485739	0.049699	0.690491
15	1.506067	1.688757	-0.544846
6	-3.737501	-0.457033	-0.503508
6	-3.960929	-1.772493	-1.043589
6	-2.704684	0.292566	-1.042687
6	-4.877437	-2.693178	-0.463290
6	-3.196711	-2.206582	-2.179728
6	-1.963353	-0.118756	-2.170392
6	-5.050336	-3.954353	-0.991463
1	-5.434518	-2.399510	0.418607
6	-3.412793	-3.507814	-2.710085
6	-2.220600	-1.340010	-2.742019
1	-1.201427	0.546257	-2.553790
6	-4.321283	-4.366119	-2.132654
1	-5.748483	-4.641872	-0.522564
1	-2.835924	-3.814740	-3.578904
1	-1.655613	-1.669661	-3.609556
1	-4.472201	-5.361067	-2.541369
8	-2.343645	1.491765	-0.429829
6	-4.537853	0.110585	0.616159
6	-5.970585	0.243433	0.529841
6	-3.911469	0.587204	1.760763
6	-6.699034	-0.061278	-0.654980
6	-6.707913	0.732273	1.660140
6	-4.637664	1.066811	2.876943
6	-8.070306	0.069968	-0.704514
1	-6.163818	-0.392979	-1.536607
6	-8.122492	0.843512	1.580842
6	-6.007242	1.120031	2.833957
1	-4.080746	1.379273	3.754217
6	-8.795950	0.514300	0.426121
1	-8.598610	-0.165564	-1.624173
1	-8.662142	1.204905	2.452624
1	-6.570029	1.476994	3.692052
1	-9.877020	0.606204	0.375230
8	-2.541077	0.542259	1.921430
15	-1.402195	1.226418	0.931462
8	-1.284888	2.743444	1.477703
6	-2.393736	3.672603	1.487007
1	-2.790251	3.809072	0.479172
1	-3.183797	3.322768	2.156663
1	-1.994861	4.617570	1.858196
17	-0.579055	-1.851498	1.825424
15	2.395752	-1.444552	0.630560
6	4.122887	-0.871920	0.258869
6	4.635161	-0.859373	-1.048021
6	4.933254	-0.382350	1.297512
6	5.917626	-0.372704	-1.307047
1	4.038890	-1.229249	-1.872840
6	6.210162	0.113898	1.035794
1	4.572882	-0.385778	2.319750
6	6.708562	0.120470	-0.268613
1	6.289132	-0.373059	-2.327658

1	6.813887	0.494262	1.854912
1	7.704435	0.503930	-0.472490
6	2.664568	-2.216546	2.290038
6	3.200291	-3.500860	2.449366
6	2.386128	-1.448370	3.431674
6	3.456938	-4.005233	3.726910
1	3.411180	-4.120296	1.584680
6	2.657638	-1.946979	4.705813
1	1.936299	-0.466830	3.320206
6	3.192756	-3.229052	4.856949
1	3.863638	-5.006930	3.835593
1	2.436020	-1.340170	5.579441
1	3.394931	-3.622834	5.849142
6	2.142724	-2.845785	-0.548498
6	3.192701	-3.685493	-0.958318
6	0.856762	-3.071678	-1.067115
6	2.960843	-4.721528	-1.865169
1	4.198874	-3.525288	-0.585496
6	0.626822	-4.108754	-1.972314
1	0.034379	-2.436823	-0.759452
6	1.678162	-4.935139	-2.375728
1	3.785003	-5.358976	-2.172957
1	-0.377174	-4.266783	-2.356387
1	1.500604	-5.740339	-3.083358
6	0.525199	3.087135	-1.275840
6	0.255305	4.234122	-0.512407
6	0.015087	3.012582	-2.580650
6	-0.514638	5.272163	-1.037103
1	0.643487	4.317563	0.496071
6	-0.761476	4.049015	-3.102993
1	0.233305	2.153113	-3.204830
6	-1.031590	5.180800	-2.332297
1	-0.709779	6.153496	-0.432550
1	-1.146874	3.971625	-4.115862
1	-1.632414	5.989318	-2.739207
6	2.818740	2.623289	0.358432
6	3.473269	3.741343	-0.188652
6	3.122960	2.240123	1.671741
6	4.441463	4.424334	0.546954
1	3.208504	4.100051	-1.177727
6	4.083679	2.931424	2.413032
1	2.593491	1.400793	2.111217
6	4.752782	4.017591	1.848219
1	4.943226	5.282409	0.108608
1	4.307998	2.616996	3.428455
1	5.503670	4.554634	2.421028
6	2.262623	1.000039	-2.090489
6	3.357845	1.567869	-2.756377
6	1.643485	-0.128535	-2.649664
6	3.825550	1.011131	-3.947704
1	3.873566	2.424712	-2.340869
6	2.111688	-0.687190	-3.840345
1	0.803095	-0.581762	-2.138047
6	3.207293	-0.118038	-4.492588
1	4.683894	1.454802	-4.444383
1	1.628192	-1.572756	-4.243060
1	3.581031	-0.552426	-5.415524

A3

Number of imaginary frequencies : 0
 Electronic energy : HF=-4360.1991555
 Zero-point correction= 0.895640 (Hartree/Particle)
 Thermal correction to Energy= 0.956382
 Thermal correction to Enthalpy= 0.957326
 Thermal correction to Gibbs Free Energy= 0.798326
 Sum of electronic and zero-point Energies= -4359.303515
 Sum of electronic and thermal Energies= -4359.242773
 Sum of electronic and thermal Enthalpies= -4359.241829
 Sum of electronic and thermal Free Energies= -4359.400830
 Standard State and RRHO Corrected G= -4359.38376

Cartesian Coordinates

45	-1.989243	-1.298382	0.582632
6	6.042744	1.245393	1.060539
6	4.719693	1.561136	0.836760
6	3.703469	1.173595	1.755428
6	4.098273	0.432342	2.916584
6	5.472872	0.146003	3.132267

6	6.430152	0.541151	2.224983
1	6.794082	1.535514	0.331586
1	4.441489	2.091003	-0.065760
6	2.308311	1.463723	1.530952
6	3.098898	-0.053800	3.801918
1	5.750766	-0.415119	4.020897
1	7.476603	0.302511	2.391209
6	1.770510	0.111353	3.507473
6	1.382848	0.840350	2.359416
1	3.400373	-0.603556	4.689191
1	0.990160	-0.307798	4.133640
6	1.881874	2.389712	0.444593
6	2.392307	3.733512	0.334512
6	0.942449	1.987403	-0.488065
6	3.234361	4.321446	1.320160
6	2.011193	4.540785	-0.790997
6	0.547266	2.778513	-1.587224
6	3.706597	5.608610	1.180165
1	3.499507	3.748995	2.200748
6	2.530879	5.858354	-0.913522
6	1.097028	4.024873	-1.749839
1	-0.182910	2.373405	-2.277608
6	3.366690	6.383601	0.045811
1	4.342834	6.033747	1.951282
1	2.242661	6.449142	-1.779273
1	0.818897	4.641334	-2.600111
1	3.753673	7.393343	-0.056390
8	0.018315	0.959618	2.172497
8	0.329298	0.745847	-0.359036
15	-0.841197	0.565667	0.794177
8	-1.751811	1.894573	0.727486
6	-1.478758	3.227932	1.197793
1	-1.260791	3.866883	0.339706
1	-2.385469	3.571408	1.701298
1	-0.641701	3.244059	1.896830
6	2.003914	-1.641259	-1.588911
6	2.315117	-0.539351	-2.458174
6	0.758207	-2.234724	-1.722544
6	3.472767	0.268147	-2.281421
6	1.401845	-0.190858	-3.508404
6	-0.146270	-1.899697	-2.752133
6	3.729090	1.337139	-3.112392
1	4.148764	0.050356	-1.464062
6	1.710607	0.900545	-4.365601
6	0.188021	-0.915947	-3.650008
1	-1.089824	-2.431860	-2.803978
6	2.849579	1.650622	-4.176029
1	4.611087	1.948655	-2.944194
1	1.014829	1.144497	-5.164446
1	-0.488515	-0.659735	-4.459670
1	3.066839	2.492044	-4.827578
8	0.357541	-3.207863	-0.807727
6	2.938913	-2.131227	-0.539708
6	4.277089	-2.567742	-0.848313
6	2.514799	-2.235071	0.776555
6	4.777013	-2.634581	-2.179568
6	5.147141	-2.983872	0.215030
6	3.355454	-2.680940	1.819520
6	6.070471	-3.034535	-2.437379
1	4.126405	-2.372118	-3.004877
6	6.479913	-3.377207	-0.083423
6	4.654699	-3.024781	1.546624
1	2.953168	-2.715130	2.824505
6	6.939827	-3.395616	-1.380610
1	6.424171	-3.077659	-3.463634
1	7.127196	-3.673365	0.738136
1	5.317391	-3.344773	2.345519
1	7.959734	-3.699763	-1.597628
8	1.233299	-1.837914	1.143241
15	-0.151483	-2.610788	0.665002
8	-0.203640	-3.980611	1.504302
6	0.781448	-5.040880	1.430271
1	1.176941	-5.145402	0.418361
1	1.595735	-4.837857	2.129941
1	0.264460	-5.957327	1.720419
17	-3.262245	-3.356204	0.348299
15	-3.954814	-0.024341	0.064486
6	-3.635069	1.157446	-1.319593
6	-4.063915	2.491279	-1.322294
6	-2.872981	0.683623	-2.399293

6	-3.741807	3.333359	-2.388322
1	-4.626873	2.889134	-0.485889
6	-2.567275	1.523327	-3.472469
1	-2.500872	-0.336195	-2.390960
6	-2.997495	2.852222	-3.468095
1	-4.071271	4.368550	-2.371367
1	-1.979779	1.142186	-4.301956
1	-2.748182	3.509679	-4.296225
6	-5.435713	-0.960686	-0.513559
6	-6.209585	-1.643575	0.439726
6	-5.797495	-1.038516	-1.864750
6	-7.327496	-2.377698	0.048766
1	-5.940269	-1.599228	1.490323
6	-6.915801	-1.781200	-2.254807
1	-5.219352	-0.517415	-2.620004
6	-7.683866	-2.450117	-1.301339
1	-7.917344	-2.897910	0.798276
1	-7.186623	-1.828314	-3.306003
1	-8.554592	-3.024166	-1.605738
6	-4.667565	0.954829	1.452328
6	-5.907513	1.604356	1.324623
6	-3.987118	1.023720	2.676727
6	-6.434623	2.337184	2.388540
1	-6.465354	1.533086	0.395774
6	-4.519069	1.752360	3.742722
1	-3.046105	0.497963	2.800049
6	-5.739113	2.416276	3.598336
1	-7.390796	2.839880	2.274060
1	-3.981094	1.794907	4.685537
1	-6.152366	2.983760	4.427437

A3-LIHMDS

Number of imaginary frequencies : 0
 Electronic energy : HF=-5661.890187
 Zero-point correction= 1.313316 (Hartree/Particle)
 Thermal correction to Energy= 1.404097
 Thermal correction to Enthalpy= 1.405041
 Thermal correction to Gibbs Free Energy= 1.181127
 Sum of electronic and zero-point Energies= -5660.576871
 Sum of electronic and thermal Energies= -5660.486090
 Sum of electronic and thermal Enthalpies= -5660.485146
 Sum of electronic and thermal Free Energies= -5660.709060
 Standard State and RRHO Corrected G= -5660.684005

Cartesian Coordinates

45	-1.142416	0.945719	-0.669635
6	6.164958	-2.658680	1.487372
6	5.384876	-1.522149	1.502571
6	4.016286	-1.570577	1.891271
6	3.474500	-2.843161	2.268197
6	4.308717	-3.992896	2.259027
6	5.627955	-3.908957	1.874608
1	7.200617	-2.593357	1.165866
1	5.810793	-0.579857	1.183426
6	3.162625	-0.407170	1.873334
6	2.096692	-2.940402	2.599626
1	3.875229	-4.947964	2.544762
1	6.253133	-4.796933	1.857074
6	1.273938	-1.850857	2.485448
6	1.804275	-0.604731	2.084544
1	1.693312	-3.902731	2.901413
1	0.211442	-1.912194	2.684713
6	3.710157	0.953304	1.612804
6	4.778266	1.518499	2.398256
6	3.173647	1.739102	0.607469
6	5.297095	0.882697	3.561301
6	5.324066	2.795103	2.030484
6	3.694686	2.999510	0.246008
6	6.320845	1.450456	4.288567
1	4.871845	-0.060064	3.883896
6	6.391377	3.344081	2.792273
6	4.771054	3.505112	0.930185
1	3.223586	3.536182	-0.568792
6	6.887113	2.686489	3.895309
1	6.693531	0.945830	5.175472
1	6.800673	4.304882	2.490537
1	5.195063	4.466577	0.654605
1	7.699616	3.118315	4.472455

8	0.888077	0.430247	1.995279
8	2.058920	1.298092	-0.101337
15	0.580803	1.352916	0.636799
8	0.488531	2.785120	1.373576
6	1.141919	3.247440	2.572006
1	1.965045	3.908866	2.294733
1	0.390227	3.802227	3.138323
1	1.516505	2.416373	3.170808
6	2.853030	-0.732719	-2.434100
6	4.030528	0.088945	-2.348973
6	1.704682	-0.150967	-2.950737
6	5.206963	-0.332603	-1.670895
6	4.014486	1.409227	-2.912103
6	1.682020	1.141667	-3.515058
6	6.308220	0.490126	-1.573345
1	5.224892	-1.307428	-1.201228
6	5.176468	2.222225	-2.817320
6	2.827390	1.897924	-3.520003
1	0.748600	1.504900	-3.931305
6	6.302032	1.777087	-2.161710
1	7.186318	0.148661	-1.032431
1	5.148616	3.216888	-3.255003
1	2.829638	2.889914	-3.962125
1	7.178067	2.414001	-2.080996
8	0.507573	-0.857697	-2.940951
6	2.814264	-2.145832	-1.958730
6	3.720146	-3.151944	-2.452227
6	1.843432	-2.550308	-1.054644
6	4.669009	-2.894377	-3.481566
6	3.654803	-4.484196	-1.919032
6	1.749498	-3.866565	-0.552740
6	5.533138	-3.875153	-3.918175
1	4.706900	-1.911035	-3.934194
6	4.570334	-5.468213	-2.381382
6	2.657419	-4.810514	-0.960658
1	0.966128	-4.086324	0.163296
6	5.497692	-5.172788	-3.354668
1	6.245064	-3.650532	-4.707357
1	4.514096	-6.466755	-1.955466
1	2.613229	-5.822692	-0.568732
1	6.190232	-5.933766	-3.702581
8	0.922243	-1.636157	-0.556615
15	-0.283793	-0.989400	-1.476645
8	-1.265680	-2.205761	-1.884242
6	-0.993874	-3.176369	-2.927104
1	-1.812461	-3.894105	-2.882678
1	-0.984011	-2.687826	-3.903196
1	-0.043328	-3.685437	-2.755203
17	-3.153315	0.385859	-1.940162
15	-1.936932	3.184249	-0.388706
6	-0.615756	4.434318	-0.710794
6	-0.485761	5.623478	0.017852
6	0.314934	4.146101	-1.720917
6	0.559413	6.507581	-0.259145
1	-1.182162	5.858563	0.815176
6	1.349895	5.038521	-2.006057
1	0.242703	3.210011	-2.265607
6	1.477987	6.220089	-1.271535
1	0.655645	7.421621	0.320342
1	2.063211	4.800427	-2.789587
1	2.290620	6.909351	-1.483111
6	-3.272532	3.682495	-1.558185
6	-4.598508	3.316043	-1.274611
6	-2.993407	4.356695	-2.754778
6	-5.624793	3.632895	-2.162730
1	-4.829775	2.782457	-0.359534
6	-4.023581	4.665578	-3.647256
1	-1.977908	4.652611	-2.995583
6	-5.340202	4.307030	-3.353762
1	-6.645244	3.344296	-1.926974
1	-3.793325	5.193849	-4.568404
1	-6.140141	4.550718	-4.047306
6	-2.666391	3.614132	1.247710
6	-3.462933	4.758881	1.423244
6	-2.454106	2.763447	2.341335
6	-4.020758	5.047424	2.669512
1	-3.658295	5.419936	0.584784
6	-3.016923	3.049193	3.586216
1	-1.851529	1.874009	2.218252
6	-3.800498	4.192795	3.753224

1	-4.633757	5.935957	2.790844
1	-2.848724	2.372777	4.419399
1	-4.243303	4.414704	4.720102
3	-3.615603	-1.533643	-0.492411
8	-2.357154	-1.956096	0.844989
6	-2.181119	-2.667410	1.859083
6	-2.022437	-4.905218	2.913025
6	-2.109246	-2.876392	4.345200
6	-1.422743	-4.217116	4.130352
1	-3.063386	-5.202962	3.108958
1	-1.580979	-2.289839	5.103904
1	-1.547948	-4.845741	5.016581
7	-2.119325	-2.097357	3.105488
7	-1.966226	-4.017223	1.749127
1	-1.462807	-5.813047	2.668014
1	-0.349862	-4.062603	3.974106
1	-3.140878	-3.019946	4.698523
6	-2.397683	-0.674413	3.243207
1	-2.282059	-0.196384	2.275033
1	-3.417296	-0.501400	3.609229
1	-1.687921	-0.235846	3.951898
6	-2.156622	-4.651985	0.449584
1	-1.931753	-3.939374	-0.339888
1	-1.476301	-5.505436	0.369179
1	-3.186403	-5.011854	0.326012
7	-5.435862	-2.113263	-0.248641
14	-6.124002	-1.371708	1.111557
14	-6.028144	-3.357956	-1.230207
6	-5.418410	0.386443	1.342571
1	-5.670484	0.817264	2.320483
1	-4.328642	0.416916	1.238336
1	-5.835418	1.045917	0.571856
6	-5.795355	-2.324040	2.736590
1	-6.180646	-1.800834	3.622291
1	-6.269484	-3.314012	2.705438
1	-4.721998	-2.485495	2.883359
6	-8.019382	-1.147444	1.046989
1	-8.320964	-0.570973	0.163552
1	-8.540167	-2.112603	1.003056
1	-8.393563	-0.615187	1.932267
6	-4.687464	-3.917385	-2.465758
1	-5.076671	-4.645089	-3.189937
1	-4.290487	-3.066200	-3.033764
1	-3.849276	-4.392541	-1.942636
6	-7.545841	-2.881789	-2.284358
1	-8.401260	-2.611872	-1.652459
1	-7.324223	-2.013557	-2.918622
1	-7.866819	-3.700605	-2.942642
6	-6.546174	-4.933355	-0.278445
1	-5.723444	-5.306484	0.345662
1	-7.394228	-4.733344	0.389586
1	-6.846650	-5.747771	-0.951828

A4

Number of imaginary frequencies : 0
 Electronic energy : HF=-4360.1815486
 Zero-point correction= 0.895297 (Hartree/Particle)
 Thermal correction to Energy= 0.956220
 Thermal correction to Enthalpy= 0.957165
 Thermal correction to Gibbs Free Energy= 0.795740
 Sum of electronic and zero-point Energies= -4359.286252
 Sum of electronic and thermal Energies= -4359.225328
 Sum of electronic and thermal Enthalpies= -4359.224384
 Sum of electronic and thermal Free Energies= -4359.385808
 Standard State and RRHO Corrected G= -4359.367741

Cartesian Coordinates

6	4.229288	-3.809504	4.562090
6	4.754712	-4.320749	3.351055
6	4.746367	-3.558683	2.203071
6	4.211389	-2.239702	2.200027
6	3.640661	-1.740643	3.420436
6	3.679446	-2.548054	4.589998
6	3.025260	-0.459996	3.434754
6	2.940193	0.286784	2.285792
6	3.507492	-0.207008	1.092630
6	4.184826	-1.414513	1.021329
6	4.805967	-1.823080	-0.268398

6	6.199982	-2.164225	-0.383144
6	6.711814	-2.628303	-1.641609
6	5.843016	-2.707882	-2.763744
6	4.535226	-2.303513	-2.663924
6	4.038697	-1.840828	-1.424380
6	8.084915	-2.979303	-1.751062
6	8.935974	-2.854496	-0.676199
6	8.443963	-2.359765	0.555258
6	7.114877	-2.024430	0.698337
8	2.704548	-1.456855	-1.396010
15	2.231362	0.110051	-1.158665
8	2.740412	0.947419	-2.436923
6	4.121014	1.218757	-2.784673
8	3.386858	0.578227	-0.049861
45	0.043739	0.371711	-0.600336
15	0.308306	2.610121	-0.140885
6	-1.068390	3.589951	-0.905345
6	-1.606309	4.750977	-0.333536
6	-2.633273	5.444289	-0.977361
6	-3.134114	4.990462	-2.200095
6	-2.605010	3.833494	-2.776304
6	-1.581634	3.135819	-2.131487
15	-2.138314	0.459874	0.084213
8	-2.607183	1.770074	0.904181
6	-3.894675	2.422242	0.815005
17	-0.450988	-1.907065	-1.290231
8	-3.352119	0.429433	-1.051572
6	-3.811714	-0.770896	-1.579134
6	-4.554438	-1.637791	-0.791878
6	-4.940389	-2.899516	-1.365220
6	-4.659704	-3.158705	-2.749122
6	-3.970189	-2.182819	-3.518684
6	-3.532302	-1.018641	-2.939532
6	-5.057725	-4.397418	-3.321578
6	-5.683223	-5.360670	-2.562620
6	-5.927151	-5.123843	-1.188638
6	-5.566965	-3.927938	-0.606329
6	-4.896532	-1.258819	0.608695
6	-6.253718	-1.206552	1.085988
6	-6.504877	-0.885146	2.463318
6	-5.414312	-0.586152	3.324279
6	-4.129477	-0.563968	2.840995
6	-3.891286	-0.885953	1.487491
6	-7.844610	-0.844738	2.937961
6	-8.903554	-1.080950	2.091058
6	-8.661908	-1.358025	0.723983
6	-7.375123	-1.419674	0.235172
8	-2.570947	-0.815210	1.045212
6	1.795378	3.500581	-0.796947
6	2.976008	3.574641	-0.041485
6	4.109365	4.206754	-0.554715
6	4.082637	4.769670	-1.832477
6	2.915396	4.691909	-2.595750
6	1.780689	4.061065	-2.083215
6	0.329910	3.075132	1.646514
6	0.693516	4.362973	2.077961
6	0.699124	4.680685	3.436952
6	0.352040	3.714637	4.385120
6	0.004593	2.427931	3.968296
6	-0.004695	2.110606	2.608830
1	-6.397016	-5.895175	-0.584900
1	-5.750944	-3.770008	0.449856
1	-4.844861	-4.573412	-4.372919
1	-5.977295	-6.305926	-3.009684
1	-3.766352	-2.385313	-4.566390
1	-2.963795	-0.279671	-3.493385
1	-7.211106	-1.623497	-0.816144
1	-3.283729	-0.302979	3.468152
1	-9.499807	-1.519156	0.051632
1	-8.015603	-0.611884	3.985851
1	-5.613540	-0.349664	4.365751
1	-9.923068	-1.043143	2.463705
1	-4.043683	2.822699	-0.189322
1	-4.705080	1.737035	1.070090
1	-3.860416	3.239162	1.537049
1	3.016133	3.144264	0.951956
1	0.883527	4.014043	-2.690920
1	5.012304	4.258254	0.047252
1	2.883054	5.126203	-3.591100
1	4.964547	5.263436	-2.230799

1	0.988075	5.117141	1.355309
1	-0.247555	1.101878	2.293712
1	0.981512	5.680745	3.753526
1	-0.251093	1.665348	4.698532
1	0.362432	3.961471	5.443048
1	-1.246059	5.112357	0.622492
1	-1.184229	2.226117	-2.573818
1	-3.046243	6.337704	-0.517228
1	-2.991331	3.466466	-3.722997
1	-3.935344	5.530647	-2.696382
1	6.759334	-1.638699	1.646459
1	3.860287	-2.328344	-3.513064
1	9.121913	-2.238536	1.395411
1	8.452008	-3.340297	-2.708383
1	6.233629	-3.074124	-3.709056
1	9.984282	-3.121982	-0.772333
1	5.141912	-3.972109	1.282999
1	2.442586	1.247732	2.266436
1	5.162571	-5.327218	3.324374
1	3.252257	-2.150711	5.507149
1	2.597464	-0.087633	4.361575
1	4.248089	-4.419674	5.460484
1	4.709516	1.446448	-1.895217
1	4.548737	0.361587	-3.309790
1	4.099002	2.087337	-3.442941

(1A...L*)

Number of imaginary frequencies : 0
 Electronic energy : HF=-5056.5079199
 Zero-point correction= 1.140848 (Hartree/Particle)
 Thermal correction to Energy= 1.214581
 Thermal correction to Enthalpy= 1.215525
 Thermal correction to Gibbs Free Energy= 1.030612
 Sum of electronic and zero-point Energies= -5055.367072
 Sum of electronic and thermal Energies= -5055.293339
 Sum of electronic and thermal Enthalpies= -5055.292395
 Sum of electronic and thermal Free Energies= -5055.477308
 Standard State and RRHO Corrected G= -5055.458033

Cartesian Coordinates

45	-0.704618	-0.042234	-0.421809
6	4.372553	0.077156	-0.972562
6	5.252609	1.200798	-0.787390
6	3.254550	0.255270	-1.778179
6	6.333172	1.187220	0.140501
6	4.999085	2.419174	-1.504730
6	3.002258	1.451415	-2.486335
6	7.124349	2.299786	0.331529
1	6.522148	0.293140	0.722180
6	5.844217	3.542214	-1.294975
6	3.871940	2.505754	-2.365021
1	2.100447	1.505232	-3.084814
6	6.886987	3.489362	-0.397964
1	7.934220	2.264630	1.054864
1	5.635344	4.455045	-1.846962
1	3.683258	3.434491	-2.896402
1	7.519091	4.358115	-0.238557
8	2.356254	-0.779828	-1.937684
6	4.582425	-1.224562	-0.275035
6	5.797263	-1.986242	-0.401060
6	3.568074	-1.756271	0.510377
6	6.837001	-1.624650	-1.303839
6	5.965602	-3.182474	0.376190
6	3.729455	-2.928079	1.283711
6	7.987347	-2.376714	-1.404379
1	6.713193	-0.747793	-1.928528
6	7.171239	-3.926678	0.258671
6	4.916634	-3.615270	1.232859
1	2.897164	-3.259259	1.896278
6	8.166002	-3.533250	-0.607916
1	8.762568	-2.081707	-2.105896
1	7.286734	-4.823276	0.862430
1	5.057342	-4.514349	1.826651
1	9.080852	-4.112653	-0.692270
8	2.333095	-1.129391	0.580817
15	1.259821	-1.159865	-0.722196
8	1.134404	-2.732430	-1.130033
15	-1.004536	-0.824775	1.752528

6	-0.345047	-2.522218	2.104270
6	-0.474676	-3.517758	1.128687
6	0.247968	-2.855222	3.333346
6	-0.020090	-4.815577	1.363359
1	-0.896622	-3.264635	0.168440
6	0.708866	-4.152599	3.567695
1	0.356013	-2.108366	4.111365
6	0.577149	-5.136627	2.583960
1	-0.122519	-5.568055	0.586406
1	1.172106	-4.391804	4.520872
1	0.940467	-6.144008	2.767293
6	-0.252135	0.119245	3.158527
6	1.083934	0.528300	3.056373
6	-0.950573	0.382471	4.348888
6	1.697719	1.224757	4.098039
1	1.645622	0.298062	2.162980
6	-0.332926	1.072319	5.393598
1	-1.978909	0.064250	4.467014
6	0.988656	1.507053	5.267239
1	2.725170	1.557108	3.984739
1	-0.890858	1.275535	6.303483
1	1.463304	2.056072	6.075698
6	-2.751971	-0.942829	2.341904
6	-3.251236	-2.072906	3.003719
6	-3.560219	0.198818	2.242177
6	-4.530671	-2.051611	3.564970
1	-2.647700	-2.969109	3.090956
6	-4.832764	0.222041	2.811928
1	-3.186576	1.078418	1.736696
6	-5.320229	-0.903356	3.480493
1	-4.908185	-2.937777	4.066973
1	-5.435768	1.121717	2.732514
1	-6.311994	-0.889610	3.923664
15	-0.611210	2.419732	0.124117
6	-1.897845	3.132066	1.270391
6	-1.679863	3.098831	2.659920
6	-3.141857	3.592175	0.809480
6	-2.677547	3.485257	3.554355
1	-0.725004	2.773745	3.051489
6	-4.141231	3.978989	1.705882
1	-3.346661	3.652113	-0.250575
6	-3.918207	3.920306	3.083222
1	-2.480271	3.439569	4.621699
1	-5.094358	4.331949	1.320839
1	-4.697583	4.217443	3.779244
6	0.921735	3.135558	0.900709
6	0.904697	4.398862	1.522212
6	2.139414	2.454470	0.815811
6	2.064317	4.940892	2.074083
1	-0.018307	4.965892	1.576407
6	3.302864	2.992166	1.374834
1	2.178872	1.489368	0.328725
6	3.267942	4.232823	2.009519
1	2.026637	5.915678	2.552802
1	4.232215	2.438117	1.316654
1	4.172929	4.648120	2.444429
6	-0.754274	3.519829	-1.368085
6	0.243060	4.440755	-1.724257
6	-1.869567	3.387683	-2.211735
6	0.108231	5.231591	-2.869335
1	1.135987	4.546374	-1.120305
6	-2.016930	4.195254	-3.338039
1	-2.612725	2.630036	-2.007300
6	-1.026923	5.122315	-3.673200
1	0.894798	5.936452	-3.125918
1	-2.895832	4.076402	-3.964802
1	-1.133609	5.742823	-4.558913
15	-2.808072	-1.003542	-1.343840
6	-4.005494	-2.152634	-0.473708
6	-5.291650	-1.805313	-0.040031
6	-3.590587	-3.486232	-0.298968
6	-6.124428	-2.752591	0.563196
1	-5.669600	-0.801052	-0.177616
6	-4.414427	-4.428056	0.313582
1	-2.628384	-3.807041	-0.679869
6	-5.690088	-4.063910	0.751519
1	-7.117386	-2.454406	0.888493
1	-4.062078	-5.448792	0.435164
1	-6.338993	-4.795472	1.224787
6	-3.906791	0.340638	-1.995773

6	-4.587547	1.174137	-1.091052
6	-3.994645	0.638512	-3.365671
6	-5.377299	2.232730	-1.541399
1	-4.487638	1.013862	-0.025253
6	-4.766347	1.713061	-3.814377
1	-3.450089	0.043374	-4.088057
6	-5.470740	2.507795	-2.907476
1	-5.899459	2.853780	-0.818982
1	-4.811998	1.928252	-4.878417
1	-6.074316	3.339396	-3.259876
6	-2.600192	-2.097404	-2.839934
6	-3.736992	-2.539145	-3.541452
6	-1.344978	-2.572828	-3.230876
6	-3.615246	-3.416843	-4.617640
1	-4.723871	-2.197597	-3.243397
6	-1.222519	-3.462474	-4.303216
1	-0.463082	-2.255180	-2.696702
6	-2.353858	-3.882746	-5.002630
1	-4.504673	-3.741270	-5.151043
1	-0.237257	-3.819065	-4.591879
1	-2.257847	-4.570413	-5.838569
6	2.145188	-3.626936	-1.638320
1	2.994657	-3.084816	-2.055251
1	2.480909	-4.281429	-0.830677
1	1.670598	-4.223520	-2.421903
17	-0.466947	0.604785	-2.815120

(1A...1)

Number of imaginary frequencies : 0
 Electronic energy : HF=-5056.505948
 Zero-point correction= 1.141396 (Hartree/Particle)
 Thermal correction to Energy= 1.215309
 Thermal correction to Enthalpy= 1.216253
 Thermal correction to Gibbs Free Energy= 1.028879
 Sum of electronic and zero-point Energies= -5055.364552
 Sum of electronic and thermal Energies= -5055.290639
 Sum of electronic and thermal Enthalpies= -5055.289695
 Sum of electronic and thermal Free Energies= -5055.477069
 Standard State and RRHO Corrected G = -5055.456503

Cartesian Coordinates

45	-0.940071	0.018711	0.138815
6	4.254293	-0.737533	0.127142
6	5.071459	-1.920060	0.057856
6	3.372028	-0.623991	1.194248
6	5.867712	-2.232115	-1.080779
6	5.048115	-2.862625	1.139402
6	3.368763	-1.533984	2.273921
6	6.608662	-3.392850	-1.136423
1	5.875450	-1.552559	-1.924697
6	5.838935	-4.040420	1.058729
6	4.203674	-2.622258	2.255492
1	2.694534	-1.343020	3.099766
6	6.605730	-4.304789	-0.053435
1	7.197917	-3.611901	-2.022395
1	5.810970	-4.739535	1.890543
1	4.206050	-3.326608	3.082695
1	7.199135	-5.212819	-0.108117
8	2.485674	0.433871	1.287455
6	4.308745	0.318831	-0.921907
6	5.525197	1.009947	-1.262122
6	3.149714	0.699477	-1.576542
6	6.745780	0.808042	-0.558989
6	5.509924	1.976826	-2.324047
6	3.122137	1.654215	-2.614633
6	7.889827	1.490695	-0.910329
1	6.769293	0.116685	0.274732
6	6.711819	2.652744	-2.669609
6	4.290840	2.265686	-2.995311
1	2.171808	1.887129	-3.083136
6	7.880591	2.413263	-1.983652
1	8.806562	1.325325	-0.351607
1	6.683979	3.376300	-3.480145
1	4.291525	3.000397	-3.795495
1	8.791183	2.941425	-2.250923
8	1.928793	0.135598	-1.199419
15	1.228742	0.696742	0.211477
8	1.362189	2.296309	0.094864

15	-2.558838	-0.270729	-1.535595
6	-2.631144	1.136562	-2.741979
6	-3.700055	2.044168	-2.780259
6	-1.561580	1.322211	-3.635173
6	-3.705423	3.101598	-3.692754
1	-4.546997	1.920716	-2.116870
6	-1.572763	2.372823	-4.551397
1	-0.715895	0.643517	-3.626318
6	-2.645597	3.267136	-4.584470
1	-4.543345	3.792652	-3.703774
1	-0.738955	2.493869	-5.237211
1	-2.651695	4.088633	-5.294819
6	-2.006596	-1.633244	-2.665971
6	-2.893286	-2.467862	-3.360265
6	-0.625039	-1.822059	-2.834898
6	-2.406400	-3.474682	-4.196422
1	-3.963981	-2.364409	-3.233284
6	-0.139996	-2.829309	-3.669753
1	0.073108	-1.189096	-2.297787
6	-1.030857	-3.662661	-4.350345
1	-3.106883	-4.121586	-4.717122
1	0.931892	-2.969783	-3.773716
1	-0.656214	-4.454294	-4.992940
6	-4.316438	-0.644970	-1.150057
6	-5.346747	-0.614598	-2.108222
6	-4.629525	-0.995546	0.169013
6	-6.654006	-0.939955	-1.747478
1	-5.131819	-0.329479	-3.132965
6	-5.935087	-1.333407	0.526924
1	-3.848455	-0.992991	0.919408
6	-6.949706	-1.304713	-0.429908
1	-7.441288	-0.910174	-2.495336
1	-6.156900	-1.603164	1.554768
1	-7.968767	-1.558845	-0.152325
15	-0.723927	-2.299542	0.772253
6	-2.169917	-3.443433	0.541811
6	-2.267124	-4.154014	-0.666765
6	-3.164114	-3.632508	1.513454
6	-3.345281	-5.005255	-0.906511
1	-1.494692	-4.056777	-1.420620
6	-4.239920	-4.489544	1.272507
1	-3.109454	-3.122915	2.467487
6	-4.339900	-5.172151	0.059483
1	-3.402706	-5.537048	-1.851700
1	-4.998567	-4.621848	2.038797
1	-5.179534	-5.835293	-0.128237
6	0.640270	-3.449956	0.311024
6	0.646521	-4.766325	0.810329
6	1.646796	-3.055890	-0.577284
6	1.650214	-5.658103	0.438100
1	-0.135114	-5.093607	1.488998
6	2.641300	-3.958863	-0.964523
1	1.663113	-2.050126	-0.971325
6	2.647920	-5.256838	-0.456479
1	1.648658	-6.667844	0.838723
1	3.418103	-3.637886	-1.650314
1	3.429232	-5.951410	-0.750567
6	-0.618058	-2.131662	2.609372
6	0.404025	-2.708352	3.376193
6	-1.591848	-1.352074	3.260260
6	0.453907	-2.502365	4.757681
1	1.171132	-3.308552	2.902786
6	-1.549387	-1.160884	4.640904
1	-2.383249	-0.881901	2.687010
6	-0.520478	-1.731403	5.394500
1	1.258788	-2.949177	5.334445
1	-2.311678	-0.555531	5.122474
1	-0.478478	-1.575099	6.468413
6	2.418990	3.149168	0.623736
1	2.126207	4.166116	0.374471
1	2.481393	3.042471	1.704865
1	3.377385	2.911020	0.161884
15	-1.633553	2.150306	0.838733
6	-1.747719	3.623003	-0.253444
6	-2.591180	4.706991	0.047576
6	-0.896852	3.708793	-1.363565
6	-2.580589	5.850956	-0.750982
1	-3.248733	4.667140	0.909387
6	-0.880378	4.859171	-2.152042
1	-0.245065	2.881257	-1.605929

6	-1.721969	5.931040	-1.849968
1	-3.236236	6.681934	-0.506975
1	-0.217024	4.910040	-3.009821
1	-1.710393	6.824367	-2.467923
6	-3.314818	1.993231	1.590342
6	-4.467900	2.245902	0.830287
6	-3.464228	1.551929	2.915408
6	-5.736633	2.064136	1.379276
1	-4.377013	2.603053	-0.186996
6	-4.735453	1.354904	3.457839
1	-2.592830	1.371768	3.533994
6	-5.875669	1.609947	2.692255
1	-6.615319	2.266947	0.774090
1	-4.831894	1.014721	4.485147
1	-6.864014	1.461778	3.117603
6	-0.596620	2.743976	2.257985
6	-0.317385	4.102711	2.463295
6	-0.046003	1.799819	3.139526
6	0.495255	4.502589	3.525995
1	-0.703891	4.855276	1.786346
6	0.756916	2.202829	4.207017
1	-0.230137	0.743102	2.989869
6	1.034260	3.557369	4.400619
1	0.729071	5.555192	3.651641
1	1.172985	1.453022	4.873961
1	1.678447	3.874465	5.215293
17	4.111703	5.795205	1.990238

(1A-1)*

Number of imaginary frequencies : 1
 Electronic energy : HF=-5056.4782075
 Zero-point correction= 1.138102 (Hartree/Particle)
 Thermal correction to Energy= 1.212054
 Thermal correction to Enthalpy= 1.212998
 Thermal correction to Gibbs Free Energy= 1.025208
 Sum of electronic and zero-point Energies= -5055.340106
 Sum of electronic and thermal Energies= -5055.266154
 Sum of electronic and thermal Enthalpies= -5055.265210
 Sum of electronic and thermal Free Energies= -5055.452999
 Standard State and RRHO Corrected G= -5055.431945

Cartesian Coordinates

45	-0.967636	0.042578	0.128726
6	4.232048	-0.726849	0.119830
6	5.068567	-1.893582	0.020863
6	3.323235	-0.662568	1.171335
6	5.892944	-2.148797	-1.112432
6	5.040562	-2.879684	1.062768
6	3.321719	-1.618922	2.214043
6	6.653458	-3.295124	-1.199912
1	5.906593	-1.435841	-1.928293
6	5.850200	-4.041636	0.950518
6	4.171623	-2.694011	2.170741
1	2.630343	-1.470313	3.034454
6	6.643260	-4.250578	-0.155318
1	7.263592	-3.468773	-2.081960
1	5.816177	-4.774245	1.753025
1	4.168524	-3.429884	2.970361
1	7.251108	-5.147305	-0.234327
8	2.428206	0.370052	1.298954
6	4.288595	0.362023	-0.894810
6	5.496711	1.088390	-1.184465
6	3.134039	0.726713	-1.568584
6	6.700862	0.899280	-0.450109
6	5.489327	2.078615	-2.224186
6	3.118987	1.703027	-2.589271
6	7.837370	1.618662	-0.748927
1	6.715629	0.187233	0.366510
6	6.683377	2.792423	-2.516313
6	4.282418	2.350548	-2.925067
1	2.176553	1.924716	-3.078853
6	7.836767	2.566677	-1.799888
1	8.740769	1.462581	-0.166113
1	6.661898	3.534020	-3.310834
1	4.287804	3.101312	-3.710581
1	8.741051	3.124109	-2.026499
8	1.925998	0.138469	-1.219793
15	1.203611	0.769089	0.184467

8	1.365780	2.301188	0.099337
15	-2.624495	-0.201490	-1.517736
6	-2.730612	1.259399	-2.658430
6	-3.812528	2.152285	-2.648544
6	-1.668703	1.505123	-3.546422
6	-3.839087	3.251864	-3.509589
1	-4.653071	1.986018	-1.985655
6	-1.701538	2.596609	-4.413031
1	-0.811390	0.841447	-3.571846
6	-2.788116	3.474584	-4.399363
1	-4.686905	3.930439	-3.482934
1	-0.872897	2.762992	-5.095712
1	-2.811009	4.328038	-5.070707
6	-2.058562	-1.496936	-2.721626
6	-2.933777	-2.306057	-3.459117
6	-0.674266	-1.662460	-2.896345
6	-2.434411	-3.267044	-4.340891
1	-4.005922	-2.220646	-3.330322
6	-0.176618	-2.623006	-3.777814
1	0.016599	-1.050736	-2.325277
6	-1.056547	-3.432797	-4.499948
1	-3.126697	-3.895584	-4.894231
1	0.897113	-2.746321	-3.885478
1	-0.671771	-4.188766	-5.178609
6	-4.376342	-0.626150	-1.147543
6	-5.417165	-0.564844	-2.092718
6	-4.671472	-1.045723	0.155653
6	-6.716046	-0.927106	-1.736337
1	-5.217486	-0.224984	-3.103873
6	-5.968613	-1.420022	0.509299
1	-3.882114	-1.068991	0.897378
6	-6.993300	-1.360004	-0.435361
1	-7.511319	-0.872424	-2.474391
1	-6.175946	-1.743772	1.524633
1	-8.005815	-1.642598	-0.161066
15	-0.716166	-2.282148	0.677725
6	-2.160166	-3.426941	0.418922
6	-2.274804	-4.083710	-0.818202
6	-3.133563	-3.671479	1.399229
6	-3.350181	-4.932860	-1.077177
1	-1.517053	-3.945799	-1.580477
6	-4.206138	-4.527522	1.139845
1	-3.066024	-3.202445	2.373367
6	-4.324430	-5.154212	-0.101254
1	-3.421371	-5.420944	-2.044858
1	-4.948581	-4.702064	1.913625
1	-5.161959	-5.815817	-0.303553
6	0.640377	-3.429666	0.176852
6	0.637565	-4.763887	0.626704
6	1.651952	-3.009299	-0.693244
6	1.639642	-5.646456	0.228703
1	-0.149580	-5.112924	1.288065
6	2.645765	-3.902301	-1.105798
1	1.675801	-1.988467	-1.047063
6	2.645455	-5.217314	-0.643609
1	1.631094	-6.670077	0.592623
1	3.428728	-3.559552	-1.774188
1	3.426978	-5.903773	-0.956137
6	-0.611966	-2.195459	2.523057
6	0.376451	-2.844493	3.275648
6	-1.567525	-1.413752	3.198196
6	0.414245	-2.704742	4.666109
1	1.129498	-3.448703	2.785066
6	-1.538283	-1.288765	4.586647
1	-2.334189	-0.890721	2.636017
6	-0.540901	-1.929662	5.326173
1	1.195204	-3.206047	5.231043
1	-2.287461	-0.680804	5.085230
1	-0.509029	-1.825368	6.406833
6	2.887127	3.369223	0.745435
1	2.194421	4.166565	0.949664
1	3.131734	2.662362	1.518357
1	3.378014	3.310186	-0.210857
15	-1.627732	2.138257	0.944315
6	-1.809268	3.657635	-0.079090
6	-2.694360	4.692804	0.269342
6	-0.969530	3.823783	-1.189046
6	-2.739490	5.866644	-0.484005
1	-3.342606	4.592578	1.133240
6	-1.010687	5.003056	-1.933337

1	-0.273993	3.039751	-1.454183
6	-1.895971	6.025128	-1.586175
1	-3.428175	6.658691	-0.203545
1	-0.356444	5.115848	-2.792494
1	-1.929298	6.940216	-2.170859
6	-3.281867	1.941269	1.751710
6	-4.458504	2.138647	1.011274
6	-3.391983	1.522044	3.087618
6	-5.709968	1.925601	1.587719
1	-4.398826	2.476760	-0.014991
6	-4.645495	1.292986	3.658902
1	-2.503716	1.380521	3.691942
6	-5.808622	1.493178	2.911865
1	-6.606152	2.084799	0.995151
1	-4.710277	0.969898	4.694276
1	-6.782977	1.319918	3.359649
6	-0.550780	2.705113	2.346270
6	-0.261328	4.058830	2.569036
6	0.020407	1.744096	3.194570
6	0.591113	4.436814	3.609001
1	-0.674572	4.824347	1.922517
6	0.859869	2.124350	4.241915
1	-0.172244	0.691033	3.029659
6	1.155661	3.473225	4.447432
1	0.823144	5.488100	3.753985
1	1.292218	1.360880	4.882714
1	1.826323	3.771615	5.248007
17	4.658020	4.774295	1.529506

(1...MeCl)

Number of imaginary frequencies : 0

Electronic energy : HF=-5056.5037225

Zero-point correction= 1.138135 (Hartree/Particle)

Thermal correction to Energy= 1.213051

Thermal correction to Enthalpy= 1.213995

Thermal correction to Gibbs Free Energy= 1.023019

Sum of electronic and zero-point Energies= -5055.365588

Sum of electronic and thermal Energies= -5055.290672

Sum of electronic and thermal Enthalpies= -5055.289728

Sum of electronic and thermal Free Energies= -5055.480703

Standard State and RRHO Corrected G= -5055.458685

Cartesian Coordinates

45	-1.000642	0.066127	0.108203
6	4.169871	-0.673330	0.146074
6	4.979128	-1.862244	0.151818
6	3.246483	-0.499368	1.175373
6	5.820706	-2.220541	-0.940650
6	4.907702	-2.767307	1.263475
6	3.207909	-1.376520	2.286459
6	6.556315	-3.386138	-0.925854
1	5.866425	-1.571282	-1.807079
6	5.689662	-3.953400	1.254465
6	4.025873	-2.475832	2.337930
1	2.509110	-1.149774	3.082381
6	6.500747	-4.261764	0.185321
1	7.180660	-3.638035	-1.778715
1	5.621222	-4.623963	2.107537
1	3.989331	-3.149915	3.189879
1	7.087889	-5.175679	0.185882
8	2.390826	0.564635	1.211148
6	4.258938	0.332621	-0.947829
6	5.482789	1.015881	-1.273633
6	3.111612	0.675403	-1.648713
6	6.679305	0.851661	-0.519617
6	5.500548	1.945859	-2.367884
6	3.125852	1.592628	-2.724456
6	7.829477	1.535908	-0.848099
1	6.676867	0.187762	0.336695
6	6.708179	2.623381	-2.689471
6	4.302211	2.198354	-3.090642
1	2.190459	1.803669	-3.231687
6	7.852522	2.422766	-1.951015
1	8.725464	1.399259	-0.249000
1	6.704742	3.317839	-3.526009
1	4.325284	2.902511	-3.918137
1	8.767187	2.952685	-2.201158
8	1.898726	0.125095	-1.281443

15	1.143842	0.892169	0.062110
8	1.270359	2.381641	-0.155537
15	-2.645133	-0.194494	-1.551063
6	-2.788647	1.316134	-2.620257
6	-3.890616	2.182885	-2.555684
6	-1.737848	1.634780	-3.497429
6	-3.953750	3.318767	-3.365244
1	-4.719393	1.967205	-1.891347
6	-1.804818	2.766326	-4.309867
1	-0.863562	0.996087	-3.557932
6	-2.915954	3.610458	-4.251198
1	-4.816585	3.975170	-3.298296
1	-0.983988	2.988844	-4.986019
1	-2.966868	4.493394	-4.881690
6	-2.009428	-1.422387	-2.794388
6	-2.840850	-2.254166	-3.557801
6	-0.617349	-1.528799	-2.955559
6	-2.292271	-3.179803	-4.448405
1	-3.917140	-2.214984	-3.442648
6	-0.070803	-2.452928	-3.847065
1	0.043886	-0.901606	-2.367192
6	-0.907159	-3.287253	-4.592581
1	-2.952012	-3.826176	-5.020817
1	1.008447	-2.528136	-3.944770
1	-0.483541	-4.016140	-5.277808
6	-4.393716	-0.708296	-1.272897
6	-5.401927	-0.621517	-2.250507
6	-4.716353	-1.234377	-0.016083
6	-6.695339	-1.063841	-1.973017
1	-5.179203	-0.202467	-3.226599
6	-6.007106	-1.690202	0.258186
1	-3.953631	-1.278688	0.751936
6	-6.999205	-1.604456	-0.719036
1	-7.465077	-0.988759	-2.736032
1	-6.235112	-2.099625	1.237713
1	-8.006557	-1.951432	-0.506382
15	-0.683105	-2.232861	0.664433
6	-2.090464	-3.419019	0.384005
6	-2.198473	-4.022701	-0.880526
6	-3.034156	-3.751894	1.367316
6	-3.243933	-4.900387	-1.164675
1	-1.457434	-3.819976	-1.644817
6	-4.076020	-4.638256	1.083071
1	-2.967955	-3.326554	2.361768
6	-4.192129	-5.207144	-0.185814
1	-3.312276	-5.344222	-2.153709
1	-4.796111	-4.881914	1.859435
1	-5.006904	-5.890608	-0.407502
6	0.695816	-3.375089	0.206922
6	0.719212	-4.692144	0.705016
6	1.677950	-2.976738	-0.705142
6	1.720420	-5.578268	0.313739
1	-0.049387	-5.025251	1.395988
6	2.668303	-3.876010	-1.113676
1	1.681245	-1.967104	-1.091120
6	2.696634	-5.172223	-0.603021
1	1.733432	-6.587841	0.715159
1	3.427762	-3.550992	-1.816955
1	3.476113	-5.862528	-0.912186
6	-0.630692	-2.121894	2.511662
6	0.365860	-2.719526	3.295266
6	-1.632639	-1.370623	3.155199
6	0.368400	-2.560094	4.684178
1	1.155195	-3.295535	2.829058
6	-1.637121	-1.225693	4.542026
1	-2.409686	-0.888287	2.570626
6	-0.631233	-1.815641	5.312207
1	1.156816	-3.021721	5.272307
1	-2.421134	-0.641855	5.014268
1	-0.627693	-1.695230	6.391762
6	3.766635	3.557233	0.711228
1	2.963331	4.196091	1.070680
1	3.705630	2.575254	1.170264
1	3.746233	3.476821	-0.372125
15	-1.688782	2.117079	1.015345
6	-2.053902	3.653822	0.060352
6	-3.100430	4.524590	0.406606
6	-1.193924	4.003866	-0.992001
6	-3.289138	5.716735	-0.295398
1	-3.766406	4.285153	1.228080

6	-1.379891	5.202452	-1.681218
1	-0.365770	3.350819	-1.238451
6	-2.428813	6.059443	-1.340548
1	-4.104488	6.379247	-0.017904
1	-0.708186	5.460112	-2.494945
1	-2.574624	6.988539	-1.884778
6	-3.260033	1.819663	1.950150
6	-4.468200	1.720971	1.241439
6	-3.284550	1.644837	3.342908
6	-5.667152	1.455331	1.901628
1	-4.475059	1.866055	0.168740
6	-4.483573	1.364581	4.002519
1	-2.371401	1.723171	3.920515
6	-5.678256	1.267703	3.285764
1	-6.587689	1.382945	1.330191
1	-4.481381	1.231367	5.080870
1	-6.610212	1.054117	3.801496
6	-0.542776	2.729772	2.337358
6	-0.290467	4.094249	2.535593
6	0.099446	1.793824	3.163063
6	0.599220	4.509842	3.528914
1	-0.769432	4.837480	1.908054
6	0.976287	2.211506	4.164229
1	-0.073473	0.734187	3.016167
6	1.235762	3.571576	4.345125
1	0.796794	5.570163	3.660901
1	1.465101	1.469808	4.789885
1	1.931143	3.898645	5.113109
17	5.358991	4.324047	1.195265

(A1...B3)

Number of imaginary frequencies : 0
 Electronic energy : HF=-5396.5768775
 Zero-point correction= 1.173122 (Hartree/Particle)
 Thermal correction to Energy= 1.250853
 Thermal correction to Enthalpy= 1.251797
 Thermal correction to Gibbs Free Energy= 1.057355
 Sum of electronic and zero-point Energies= -5395.403756
 Sum of electronic and thermal Energies= -5395.326024
 Sum of electronic and thermal Enthalpies= -5395.325080
 Sum of electronic and thermal Free Energies= -5395.519522
 Standard State and RRHO Corrected G= -5395.498501

Cartesian Coordinates

45	0.007114	-0.182890	0.234836
6	-5.114658	-0.698960	-0.490472
6	-6.224101	-0.549645	0.413969
6	-4.092236	-1.563329	-0.125883
6	-7.241688	0.428160	0.225895
6	-6.286708	-1.365761	1.592805
6	-4.158754	-2.381043	1.023674
6	-8.268295	0.572602	1.134194
1	-7.195830	1.085007	-0.634097
6	-7.367915	-1.202754	2.500638
6	-5.244471	-2.293194	1.858618
1	-3.351254	-3.080864	1.203678
6	-8.341847	-0.255336	2.280188
1	-9.024682	1.335219	0.972353
1	-7.399488	-1.833193	3.385605
1	-5.307282	-2.918902	2.744538
1	-9.158377	-0.132524	2.985675
8	-2.973889	-1.701935	-0.932387
6	-5.011038	0.087916	-1.750355
6	-6.030355	0.065142	-2.766683
6	-3.888809	0.866111	-1.985715
6	-7.140382	-0.823915	-2.716521
6	-5.914234	0.937736	-3.901025
6	-3.771694	1.738601	-3.089684
6	-8.095098	-0.826305	-3.710247
1	-7.226559	-1.516798	-1.887749
6	-6.926218	0.921929	-4.899121
6	-4.780875	1.788271	-4.019174
1	-2.882206	2.353637	-3.168532
6	-7.997722	0.062478	-4.807573
1	-8.928784	-1.520363	-3.652824
1	-6.829974	1.597665	-5.744967
1	-4.711547	2.460697	-4.869560
1	-8.762139	0.055215	-5.579129

8	-2.813040	0.831368	-1.101133
15	-1.817781	-0.494914	-1.027915
8	-1.326718	-0.785650	-2.544379
15	0.634516	-2.465976	0.251602
6	-0.551664	-3.742807	-0.346274
6	-0.741264	-3.832525	-1.734547
6	-1.231789	-4.630286	0.497672
6	-1.615587	-4.777036	-2.267470
1	-0.213009	-3.154678	-2.397419
6	-2.112540	-5.572959	-0.040678
1	-1.082116	-4.595063	1.571215
6	-2.311264	-5.644746	-1.420193
1	-1.757960	-4.832070	-3.342902
1	-2.639991	-6.252367	0.622981
1	-2.999176	-6.376249	-1.834335
6	2.208871	-3.251207	-0.271819
6	2.665063	-4.433434	0.338910
6	2.874510	-2.758362	-1.400797
6	3.797079	-5.081635	-0.151268
1	2.136283	-4.849945	1.190732
6	3.997082	-3.424308	-1.899629
1	2.522391	-1.856303	-1.883925
6	4.466045	-4.577569	-1.271355
1	4.153788	-5.984144	0.336754
1	4.512115	-3.028649	-2.769123
1	5.351054	-5.080670	-1.648112
6	0.566579	-2.507733	2.089002
6	1.720257	-2.622844	2.880779
6	-0.667687	-2.249328	2.719542
6	1.640541	-2.494229	4.268431
1	2.682361	-2.801763	2.419029
6	-0.743253	-2.135110	4.108049
1	-1.567971	-2.132207	2.128082
6	0.410623	-2.253027	4.886389
1	2.543650	-2.583405	4.865577
1	-1.702947	-1.935082	4.573654
1	0.352653	-2.153209	5.966262
6	2.737329	3.537352	-0.225144
1	2.166898	4.432528	0.029649
1	3.468058	3.333165	0.557465
1	3.241212	3.661927	-1.186158
15	-0.780949	1.739295	1.325268
6	-1.210583	3.247283	0.380566
6	-1.790804	4.351021	1.025683
6	-0.972302	3.304251	-0.999034
6	-2.113182	5.498808	0.301722
1	-1.986484	4.318896	2.093124
6	-1.302738	4.450497	-1.721381
1	-0.527832	2.455627	-1.503133
6	-1.871280	5.549372	-1.072586
1	-2.547125	6.352664	0.813060
1	-1.111897	4.485934	-2.790338
1	-2.121238	6.444292	-1.635286
6	-2.289424	1.430593	2.353416
6	-3.564966	1.690503	1.822412
6	-2.192039	0.933567	3.662678
6	-4.708458	1.467375	2.588621
1	-3.666593	2.078379	0.816798
6	-3.341140	0.694576	4.419062
1	-1.226056	0.740845	4.110311
6	-4.602336	0.961802	3.885904
1	-5.684541	1.679598	2.166115
1	-3.243072	0.312376	5.431404
1	-5.497940	0.779958	4.472566
6	0.512919	2.206803	2.550080
6	0.998118	3.514092	2.675236
6	1.089438	1.181508	3.323590
6	2.032033	3.792942	3.572833
1	0.621770	4.329153	2.067005
6	2.102910	1.470447	4.235622
1	0.759311	0.154118	3.206879
6	2.579251	2.779309	4.360798
1	2.402605	4.812344	3.624212
1	2.527183	0.669311	4.834360
1	3.381459	3.002434	5.058861
17	1.691561	6.790283	1.408819
6	5.160562	-0.204620	-0.245361
6	6.073580	-1.315889	-0.221493
6	4.320499	-0.034064	0.846598
6	6.864178	-1.683118	-1.346753

6	6.165918	-2.127931	0.958517
6	4.430593	-0.807969	2.021477
6	7.711255	-2.768841	-1.299540
1	6.784977	-1.106610	-2.260566
6	7.056016	-3.235609	0.977278
6	5.348227	-1.827255	2.080396
1	3.776561	-0.571484	2.852455
6	7.817758	-3.551523	-0.124915
1	8.297021	-3.031459	-2.175876
1	7.113797	-3.836872	1.880940
1	5.441516	-2.430890	2.979052
1	8.490933	-4.403544	-0.100964
8	3.364916	0.966015	0.845360
6	5.070828	0.730524	-1.401391
6	6.208247	1.471317	-1.883421
6	3.852102	0.949749	-2.023933
6	7.470132	1.452958	-1.225458
6	6.068158	2.299068	-3.048319
6	3.705460	1.761311	-3.169848
6	8.537153	2.176866	-1.711578
1	7.587568	0.869990	-0.319930
6	7.193387	3.020677	-3.532007
6	4.801844	2.406722	-3.685137
1	2.719776	1.859975	-3.612282
6	8.405910	2.959419	-2.883524
1	9.486978	2.151982	-1.185096
1	7.071363	3.634922	-4.420355
1	4.707008	3.030628	-4.569328
1	9.257205	3.520316	-3.258084
8	2.696132	0.338624	-1.539563
15	2.005251	0.876851	-0.124662
8	1.772962	2.453804	-0.323747
6	-2.122543	-1.329719	-3.628649
1	-2.645553	-0.522028	-4.144429
1	-1.414965	-1.804558	-4.310828
1	-2.837127	-2.066712	-3.261965

(A1-B3)*

Number of imaginary frequencies : 1
 Electronic energy : HF=-5396.5469902
 Zero-point correction= 1.169958 (Hartree/Particle)
 Thermal correction to Energy= 1.247886
 Thermal correction to Enthalpy= 1.248830
 Thermal correction to Gibbs Free Energy= 1.050407
 Sum of electronic and zero-point Energies= -5395.377032
 Sum of electronic and thermal Energies= -5395.299105
 Sum of electronic and thermal Enthalpies= -5395.298160
 Sum of electronic and thermal Free Energies= -5395.496583
 Standard State and RRHO Corrected G= -5395.473193

Cartesian Coordinates

45	0.070647	0.197094	0.166021
6	5.238840	0.442874	-0.479883
6	6.319552	0.325201	0.463134
6	4.250298	1.382238	-0.220432
6	7.292898	-0.711478	0.390548
6	6.394378	1.239539	1.567031
6	4.328453	2.292707	0.856857
6	8.290473	-0.821026	1.335408
1	7.234776	-1.440214	-0.408660
6	7.445796	1.109162	2.514295
6	5.390114	2.231440	1.724259
1	3.547437	3.037247	0.956568
6	8.378069	0.102322	2.404985
1	9.012726	-1.629104	1.261858
1	7.487274	1.814275	3.340599
1	5.461755	2.928524	2.554532
1	9.171800	0.006117	3.140068
8	3.161065	1.498780	-1.065230
6	5.122352	-0.449947	-1.666264
6	6.163627	-0.571138	-2.653257
6	3.966080	-1.190416	-1.859260
6	7.318469	0.260595	-2.653348
6	6.027559	-1.536545	-3.707405
6	3.828952	-2.151728	-2.884962
6	8.295576	0.121823	-3.615204
1	7.422795	1.021526	-1.888852
6	7.061607	-1.664273	-4.674451

6	4.853660	-2.335554	-3.779663
1	2.910164	-2.725644	-2.932614
6	8.175979	-0.857170	-4.630510
1	9.164089	0.774077	-3.596906
1	6.947619	-2.408229	-5.458730
1	4.767770	-3.077328	-4.568809
1	8.957561	-0.960381	-5.377622
8	2.877638	-1.029335	-1.008330
15	1.939911	0.345442	-1.064933
8	1.493454	0.520880	-2.615051
15	-0.472248	2.486589	0.031649
6	0.770100	3.660173	-0.664086
6	0.970372	3.627038	-2.053507
6	1.482865	4.586906	0.107834
6	1.883981	4.489216	-2.656138
1	0.419996	2.916823	-2.662664
6	2.403369	5.446299	-0.499429
1	1.329280	4.645089	1.179842
6	2.610331	5.396317	-1.878680
1	2.032974	4.449109	-3.731426
1	2.955577	6.156331	0.109969
1	3.328529	6.063356	-2.346864
6	-2.006582	3.327391	-0.529953
6	-2.339762	4.607762	-0.051158
6	-2.768175	2.756615	-1.555716
6	-3.443277	5.282932	-0.568102
1	-1.736754	5.077402	0.720241
6	-3.861596	3.448025	-2.085428
1	-2.517061	1.772521	-1.929623
6	-4.206853	4.703599	-1.587476
1	-3.703794	6.264299	-0.181716
1	-4.452698	2.992630	-2.873213
1	-5.068959	5.228790	-1.987129
6	-0.382431	2.682611	1.859506
6	-1.515970	2.954101	2.641490
6	0.838893	2.403434	2.506059
6	-1.431819	2.947801	4.035221
1	-2.466958	3.160319	2.167527
6	0.920513	2.414543	3.898610
1	1.724293	2.175803	1.923720
6	-0.215251	2.679840	4.667728
1	-2.320194	3.156241	4.624861
1	1.870088	2.197700	4.377037
1	-0.152472	2.677835	5.752068
6	-3.224697	-3.703316	0.361041
1	-2.434993	-4.415756	0.521155
1	-3.566313	-3.086898	1.172788
1	-3.711938	-3.649726	-0.597782
15	0.758390	-1.654981	1.441402
6	1.174902	-3.252135	0.643437
6	1.784278	-4.286456	1.371995
6	0.905870	-3.437689	-0.719170
6	2.108825	-5.491920	0.747361
1	2.010220	-4.151754	2.425431
6	1.234190	-4.642321	-1.341519
1	0.431643	-2.644744	-1.282421
6	1.835137	-5.670767	-0.610777
1	2.576590	-6.286817	1.321099
1	1.020276	-4.776905	-2.398180
1	2.090321	-6.607630	-1.098191
6	2.250545	-1.309328	2.487306
6	3.535964	-1.624065	2.011769
6	2.128650	-0.725174	3.757760
6	4.661892	-1.375471	2.796155
1	3.658734	-2.074669	1.035116
6	3.260644	-0.458871	4.531129
1	1.154865	-0.481091	4.161563
6	4.530404	-0.785266	4.054890
1	5.644834	-1.633459	2.417377
1	3.141574	-0.006906	5.512037
1	5.412750	-0.583360	4.655094
6	-0.557216	-2.003543	2.688271
6	-1.029210	-3.293936	2.959949
6	-1.150594	-0.907593	3.339875
6	-2.071829	-3.484714	3.869808
1	-0.608432	-4.151904	2.448596
6	-2.172762	-1.104074	4.267136
1	-0.829339	0.104098	3.110427
6	-2.641107	-2.393724	4.529887
1	-2.446795	-4.487975	4.049314

1	-2.613937	-0.246234	4.766645
1	-3.453169	-2.546977	5.234844
17	-4.791962	-5.378074	1.043098
6	-5.103358	0.347826	-0.286444
6	-5.995618	1.469474	-0.395698
6	-4.237860	0.303858	0.801097
6	-6.798496	1.698970	-1.549115
6	-6.053554	2.435173	0.664769
6	-4.320182	1.234533	1.861998
6	-7.622996	2.799606	-1.638355
1	-6.745655	1.001341	-2.376658
6	-6.923348	3.552398	0.546728
6	-5.218446	2.270519	1.802160
1	-3.655834	1.097436	2.706907
6	-7.696015	3.734978	-0.578164
1	-8.217631	2.954332	-2.534361
1	-6.955365	4.271020	1.361826
1	-5.284024	2.989786	2.614229
1	-8.352486	4.596536	-0.659658
8	-3.308387	-0.698942	0.926598
6	-5.050744	-0.731774	-1.310665
6	-6.199887	-1.525888	-1.657654
6	-3.842405	-1.034239	-1.920632
6	-7.450881	-1.400113	-0.990465
6	-6.082629	-2.521839	-2.685321
6	-3.720965	-2.017238	-2.928165
6	-8.528901	-2.182057	-1.344075
1	-7.549803	-0.685725	-0.181955
6	-7.218416	-3.301860	-3.035133
6	-4.826625	-2.732647	-3.316829
1	-2.744049	-2.186728	-3.368166
6	-8.420066	-3.134877	-2.385033
1	-9.469913	-2.071524	-0.812553
1	-7.112861	-4.046209	-3.820301
1	-4.747907	-3.488798	-4.093185
1	-9.279244	-3.741888	-2.655542
8	-2.690606	-0.360343	-1.540331
15	-1.965860	-0.867096	-0.100419
8	-1.842253	-2.402412	-0.171166
6	2.330759	0.938467	-3.721920
1	2.848568	0.074427	-4.143699
1	1.654126	1.360762	-4.467335
1	3.053463	1.691701	-3.407802

(B3...MeCl)

Number of imaginary frequencies : 0
 Electronic energy : HF=-5396.5724827
 Zero-point correction= 1.170153 (Hartree/Particle)
 Thermal correction to Energy= 1.248832
 Thermal correction to Enthalpy= 1.249776
 Thermal correction to Gibbs Free Energy= 1.050306
 Sum of electronic and zero-point Energies= -5395.402330
 Sum of electronic and thermal Energies= -5395.323651
 Sum of electronic and thermal Enthalpies= -5395.322707
 Sum of electronic and thermal Free Energies= -5395.522177
 Standard State and RRHO Corrected G= -5395.498837

Cartesian Coordinates

45	0.105559	0.168420	0.118451
6	5.295329	0.398718	-0.452599
6	6.354649	0.282052	0.514032
6	4.310370	1.350703	-0.225718
6	7.315363	-0.768218	0.477024
6	6.417738	1.211060	1.606543
6	4.377179	2.274907	0.841088
6	8.290395	-0.877751	1.445205
1	7.264326	-1.507128	-0.313404
6	7.447057	1.080727	2.577706
6	5.421341	2.215754	1.729616
1	3.599934	3.026280	0.917000
6	8.367490	0.059865	2.503163
1	9.002638	-1.696706	1.399224
1	7.480162	1.796702	3.394981
1	5.483718	2.923149	2.551927
1	9.143560	-0.036480	3.256876
8	3.238516	1.461498	-1.090509
6	5.194549	-0.505535	-1.631770
6	6.253686	-0.643656	-2.597242

6	4.035079	-1.237137	-1.840456
6	7.416963	0.176167	-2.580028
6	6.128649	-1.614491	-3.647798
6	3.909162	-2.203545	-2.863279
6	8.411154	0.021628	-3.521826
1	7.514095	0.941093	-1.818568
6	7.179776	-1.758438	-4.593884
6	4.948400	-2.402313	-3.737664
1	2.986164	-2.769329	-2.924644
6	8.301285	-0.962299	-4.533439
1	9.285714	0.665288	-3.490576
1	7.073424	-2.506059	-5.375801
1	4.870167	-3.148004	-4.523968
1	9.095945	-1.077864	-5.264803
8	2.935977	-1.065304	-1.008372
15	2.002258	0.316302	-1.076865
8	1.569718	0.477238	-2.634891
15	-0.437925	2.455644	-0.004624
6	0.811660	3.618715	-0.710917
6	1.013501	3.571514	-2.099683
6	1.525068	4.553198	0.051145
6	1.927300	4.427732	-2.710901
1	0.464366	2.853914	-2.701365
6	2.446301	5.406243	-0.564081
1	1.371473	4.621805	1.122636
6	2.653503	5.342857	-1.942788
1	2.076766	4.376417	-3.785712
1	2.998888	6.121869	0.038523
1	3.371969	6.005036	-2.417527
6	-1.960433	3.339422	-0.542084
6	-2.236693	4.635005	-0.067221
6	-2.769842	2.786419	-1.540090
6	-3.330219	5.344024	-0.559184
1	-1.596512	5.089725	0.682922
6	-3.852104	3.512284	-2.047330
1	-2.566712	1.788169	-1.906496
6	-4.140873	4.783082	-1.552273
1	-3.545546	6.337217	-0.174927
1	-4.480199	3.070593	-2.813961
1	-4.994784	5.334565	-1.934113
6	-0.328384	2.665869	1.822773
6	-1.447717	2.968222	2.613542
6	0.894033	2.374027	2.461001
6	-1.350179	2.974308	4.006692
1	-2.399161	3.188667	2.147212
6	0.990126	2.397345	3.852303
1	1.769938	2.125952	1.872689
6	-0.133010	2.689976	4.630306
1	-2.228933	3.205341	4.602469
1	1.940719	2.169152	4.323125
1	-0.059275	2.697723	5.714019
6	-4.256472	-3.813669	0.496816
1	-3.415782	-4.454696	0.750348
1	-4.192380	-2.867062	1.024031
1	-4.312796	-3.654049	-0.576556
15	0.746016	-1.664476	1.438709
6	1.222613	-3.264619	0.675216
6	1.860297	-4.264883	1.426669
6	0.975995	-3.481273	-0.686907
6	2.241508	-5.465070	0.824046
1	2.066035	-4.107168	2.481070
6	1.361375	-4.680387	-1.287346
1	0.468425	-2.719383	-1.263238
6	1.995278	-5.673006	-0.535279
1	2.732834	-6.232564	1.415412
1	1.165962	-4.838566	-2.344440
1	2.296591	-6.604610	-1.006433
6	2.197730	-1.301838	2.540008
6	3.504423	-1.540486	2.076694
6	2.029885	-0.793373	3.837157
6	4.604716	-1.293446	2.896941
1	3.663136	-1.934316	1.080925
6	3.135908	-0.527980	4.648490
1	1.039863	-0.607402	4.232589
6	4.426317	-0.779181	4.183170
1	5.603496	-1.498316	2.527595
1	2.980217	-0.134823	5.649454
1	5.288209	-0.579387	4.813353
6	-0.603476	-2.035325	2.641986
6	-1.079449	-3.331525	2.875255

6	-1.217966	-0.953272	3.295812
6	-2.147372	-3.541400	3.750685
1	-0.638978	-4.177574	2.360135
6	-2.266715	-1.168986	4.188778
1	-0.892592	0.063156	3.092611
6	-2.739529	-2.463966	4.413570
1	-2.519266	-4.549803	3.909243
1	-2.725707	-0.321960	4.690717
1	-3.570310	-2.631914	5.093129
17	-5.793176	-4.664654	1.018789
6	-5.051527	0.365419	-0.307672
6	-5.945528	1.487418	-0.391275
6	-4.162121	0.307908	0.762079
6	-6.775594	1.722739	-1.524625
6	-5.980977	2.448244	0.674583
6	-4.225284	1.237585	1.827814
6	-7.603516	2.822626	-1.589723
1	-6.740749	1.029526	-2.356894
6	-6.853225	3.565706	0.581286
6	-5.120985	2.276478	1.792235
1	-3.544671	1.095504	2.658643
6	-7.652788	3.753329	-0.524011
1	-8.219036	2.980538	-2.471067
1	-6.866359	4.280799	1.400202
1	-5.167048	2.992189	2.609039
1	-8.311264	4.615045	-0.586163
8	-3.245291	-0.697819	0.872991
6	-5.017495	-0.702208	-1.343909
6	-6.171017	-1.497835	-1.669887
6	-3.817593	-0.996149	-1.977343
6	-7.404033	-1.387449	-0.966406
6	-6.075300	-2.486661	-2.706840
6	-3.721506	-1.970566	-2.997517
6	-8.484185	-2.179094	-1.291026
1	-7.485040	-0.678690	-0.150896
6	-7.214038	-3.274601	-3.028177
6	-4.833280	-2.685074	-3.369798
1	-2.754097	-2.135319	-3.459699
6	-8.397344	-3.124487	-2.340833
1	-9.409655	-2.081496	-0.730344
1	-7.125305	-4.012456	-3.821760
1	-4.769415	-3.433928	-4.154841
1	-9.258221	-3.738529	-2.589548
8	-2.663649	-0.332713	-1.605679
15	-1.910435	-0.926630	-0.188345
8	-1.815870	-2.426991	-0.306367
6	2.416173	0.881117	-3.738207
1	2.945469	0.014519	-4.140527
1	1.745697	1.286098	-4.498865
1	3.130503	1.644672	-3.429545

(A2-B2)*

Number of imaginary frequencies : 1
 Electronic energy : HF=-5396.5581529
 Zero-point correction= 1.169794 (Hartree/Particle)
 Thermal correction to Energy= 1.247445
 Thermal correction to Enthalpy= 1.248389
 Thermal correction to Gibbs Free Energy= 1.053520
 Sum of electronic and zero-point Energies= -5395.388359
 Sum of electronic and thermal Energies= -5395.310708
 Sum of electronic and thermal Enthalpies= -5395.309764
 Sum of electronic and thermal Free Energies= -5395.504633
 Standard State and RRHO Corrected G= -5395.483045

Cartesian Coordinates

45	1.540361	-0.173179	-0.255319
6	-2.519413	-2.399265	1.019505
6	-3.282159	-1.850631	2.106980
6	-1.187353	-2.702924	1.256098
6	-4.592000	-1.323465	1.929212
6	-2.691929	-1.770667	3.413020
6	-0.601427	-2.634878	2.536404
6	-5.289694	-0.781242	2.985900
1	-5.033438	-1.331878	0.940358
6	-3.450514	-1.229715	4.487528
6	-1.350558	-2.198756	3.601986
1	0.437446	-2.921462	2.644777
6	-4.722975	-0.746861	4.283089

1	-6.280078	-0.367083	2.820284
1	-2.994525	-1.186677	5.473376
1	-0.909861	-2.140960	4.593225
1	-5.287322	-0.322023	5.108116
8	-0.371276	-3.088795	0.193251
6	-3.092416	-2.621734	-0.335348
6	-4.258567	-3.443425	-0.543254
6	-2.477199	-2.081975	-1.454550
6	-4.891267	-4.162182	0.510006
6	-4.802119	-3.578162	-1.864688
6	-2.998286	-2.228546	-2.759280
6	-6.017310	-4.923340	0.280186
1	-4.476238	-4.114642	1.509394
6	-5.971816	-4.359555	-2.065882
6	-4.150515	-2.944865	-2.956665
1	-2.479227	-1.740050	-3.575316
6	-6.576153	-5.014466	-1.016625
1	-6.477724	-5.462071	1.103598
1	-6.375553	-4.435077	-3.072336
1	-4.572712	-3.041988	-3.952435
1	-7.469344	-5.610037	-1.181853
8	-1.337829	-1.297953	-1.340816
15	0.127918	-1.829964	-0.789515
8	0.745812	-2.690162	-2.013330
15	3.230609	-1.568203	0.772722
6	5.053369	-1.281188	0.572439
6	5.641526	-0.196467	1.245108
6	5.862275	-2.074937	-0.253866
6	6.997607	0.089959	1.092456
1	5.047225	0.424571	1.902675
6	7.221355	-1.789210	-0.401329
1	5.448292	-2.925698	-0.781155
6	7.794429	-0.706490	0.267466
1	7.426200	0.936390	1.621769
1	7.830128	-2.417250	-1.045493
1	8.851323	-0.486173	0.147270
6	3.020718	-1.292356	2.586337
6	3.950977	-1.791156	3.515068
6	1.922866	-0.555589	3.053123
6	3.778081	-1.559626	4.879525
1	4.812619	-2.355566	3.172115
6	1.755485	-0.316300	4.419019
1	1.200243	-0.169869	2.340442
6	2.681759	-0.818941	5.334059
1	4.502155	-1.952496	5.587564
1	0.901247	0.260617	4.761154
1	2.554004	-0.633861	6.396930
6	3.063523	-3.389838	0.542193
6	2.807970	-4.277926	1.597043
6	3.143140	-3.895162	-0.766989
6	2.642261	-5.642447	1.347971
1	2.731891	-3.914262	2.615469
6	3.000649	-5.261162	-1.009504
1	3.297880	-3.217577	-1.599791
6	2.744191	-6.138693	0.047382
1	2.436699	-6.316265	2.174974
1	3.075071	-5.636975	-2.025851
1	2.619591	-7.200828	-0.143416
6	-0.371181	4.288929	1.121045
1	0.576757	4.667942	1.461592
1	-0.621126	4.316398	0.075272
1	-1.104051	3.961816	1.839142
15	3.009922	1.512036	-0.995928
6	3.866988	2.615843	0.190350
6	4.719969	3.653694	-0.221932
6	3.594164	2.456962	1.555942
6	5.330045	4.479131	0.723016
1	4.894057	3.831114	-1.278667
6	4.199379	3.288387	2.499779
1	2.899936	1.690175	1.876763
6	5.076012	4.293435	2.085397
1	5.993794	5.273886	0.394950
1	3.980427	3.151426	3.554957
1	5.547902	4.941166	2.818844
6	4.269742	0.671653	-2.052234
6	5.610374	1.063156	-2.153441
6	3.823932	-0.433313	-2.802243
6	6.481970	0.376499	-3.002325
1	5.992019	1.883525	-1.558341
6	4.695657	-1.112001	-3.653846

1	2.793695	-0.767697	-2.705197
6	6.028201	-0.705254	-3.758555
1	7.521868	0.684532	-3.060896
1	4.334546	-1.961185	-4.227519
1	6.711351	-1.236148	-4.415455
6	2.219288	2.715087	-2.156522
6	1.740801	3.940505	-1.667772
6	1.986123	2.379252	-3.498858
6	1.040340	4.810775	-2.502815
1	1.898825	4.211009	-0.631049
6	1.292621	3.257060	-4.334459
1	2.345748	1.437820	-3.901007
6	0.812637	4.471893	-3.837982
1	0.667590	5.749529	-2.102750
1	1.126437	2.988239	-5.374089
1	0.265851	5.149152	-4.487837
17	-1.240961	6.524027	1.309309
6	-3.212467	1.573705	-1.091110
6	-4.317328	1.018544	-1.827853
6	-2.009042	1.746985	-1.763793
6	-5.528608	0.611733	-1.199563
6	-4.199330	0.824633	-3.244630
6	-1.882281	1.535116	-3.155576
6	-6.566784	0.074286	-1.929174
1	-5.623928	0.712881	-0.125436
6	-5.300112	0.297421	-3.972451
6	-2.965458	1.116010	-3.886501
1	-0.920153	1.735633	-3.614005
6	-6.462232	-0.071756	-3.333369
1	-7.472246	-0.244249	-1.420440
1	-5.195220	0.168203	-5.046931
1	-2.882486	0.972483	-4.960636
1	-7.291588	-0.488103	-3.897891
8	-0.894329	2.224231	-1.110396
6	-3.324582	1.941111	0.347876
6	-4.331991	2.848410	0.834853
6	-2.412970	1.437391	1.264112
6	-5.219135	3.550021	-0.029419
6	-4.433628	3.098250	2.245185
6	-2.500204	1.691629	2.650173
6	-6.174752	4.407352	0.471148
1	-5.130352	3.416468	-1.100748
6	-5.441070	3.975830	2.729826
6	-3.509275	2.485586	3.133885
1	-1.769014	1.229617	3.303245
6	-6.300916	4.614470	1.865453
1	-6.832699	4.935964	-0.212955
1	-5.507666	4.144388	3.801717
1	-3.599627	2.671940	4.200292
1	-7.062156	5.289068	2.246649
8	-1.370399	0.631802	0.835235
15	-0.071600	1.372053	0.081200
8	0.445938	2.509653	0.989272
6	0.188242	-3.932721	-2.504489
1	-0.770527	-3.754212	-2.997252
1	0.906132	-4.317552	-3.230113
1	0.064057	-4.649587	-1.691356

(B2...MeCl)

Number of imaginary frequencies : 0
 Electronic energy : HF=-5396.5861526
 Zero-point correction= 1.171032 (Hartree/Particle)
 Thermal correction to Energy= 1.249202
 Thermal correction to Enthalpy= 1.250146
 Thermal correction to Gibbs Free Energy= 1.053738
 Sum of electronic and zero-point Energies= -5395.415121
 Sum of electronic and thermal Energies= -5395.336950
 Sum of electronic and thermal Enthalpies= -5395.336006
 Sum of electronic and thermal Free Energies= -5395.532414
 Standard State and RRHO Corrected G= -5395.510428

Cartesian Coordinates

45	1.571965	-0.104024	-0.123015
6	-2.480892	-2.506197	1.008537
6	-3.319204	-2.027239	2.073256
6	-1.145384	-2.744374	1.296574
6	-4.645014	-1.561010	1.848418
6	-2.794390	-1.953663	3.407160

6	-0.624452	-2.683790	2.605794
6	-5.416570	-1.082344	2.884292
1	-5.039758	-1.562919	0.839919
6	-3.628036	-1.482478	4.458543
6	-1.442146	-2.317804	3.646897
1	0.421873	-2.919692	2.757336
6	-4.912712	-1.057138	4.207377
1	-6.417734	-0.712437	2.682395
1	-3.219861	-1.444632	5.465421
1	-1.051184	-2.270254	4.659549
1	-5.534976	-0.684338	5.015830
8	-0.264961	-3.063813	0.268806
6	-2.983659	-2.721138	-0.375173
6	-4.096866	-3.594099	-0.653672
6	-2.351220	-2.119790	-1.452872
6	-4.732165	-4.375489	0.352430
6	-4.580517	-3.717069	-1.999409
6	-2.815849	-2.251200	-2.781063
6	-5.806435	-5.186985	0.055984
1	-4.359692	-4.336022	1.368839
6	-5.698381	-4.551580	-2.269567
6	-3.921189	-3.017500	-3.045747
1	-2.290078	-1.713288	-3.560885
6	-6.308080	-5.268341	-1.264583
1	-6.269537	-5.773241	0.844757
1	-6.057914	-4.617624	-3.293382
1	-4.299582	-3.103773	-4.059947
1	-7.161172	-5.904320	-1.482871
8	-1.255875	-1.290734	-1.273133
15	0.218979	-1.781356	-0.703542
8	0.862073	-2.638839	-1.917438
15	3.373166	-1.541421	0.634438
6	5.173751	-1.094292	0.503075
6	5.639475	-0.037255	1.303616
6	6.079885	-1.726409	-0.359903
6	6.964021	0.390329	1.230082
1	4.969874	0.452787	1.998158
6	7.410029	-1.303556	-0.425661
1	5.767563	-2.557306	-0.979737
6	7.856906	-0.241683	0.361543
1	7.292616	1.216493	1.854543
1	8.094855	-1.807924	-1.101550
1	8.890355	0.087653	0.301701
6	3.190205	-1.574762	2.472537
6	4.114430	-2.252702	3.286596
6	2.142986	-0.865628	3.077119
6	3.978399	-2.232989	4.674164
1	4.941352	-2.792432	2.834763
6	2.013607	-0.836943	4.468270
1	1.427557	-0.337659	2.451853
6	2.928395	-1.523311	5.267814
1	4.695122	-2.765285	5.293106
1	1.196179	-0.281368	4.918681
1	2.828913	-1.504554	6.349507
6	3.334048	-3.308552	0.110043
6	3.018157	-4.358840	0.983284
6	3.561480	-3.601109	-1.246546
6	2.959291	-5.674854	0.516325
1	2.813325	-4.160444	2.029250
6	3.530826	-4.917651	-1.703668
1	3.750697	-2.797202	-1.950340
6	3.227386	-5.960016	-0.823087
1	2.708943	-6.476267	1.205817
1	3.726162	-5.126711	-2.751710
1	3.190736	-6.984726	-1.181828
6	-1.471061	4.820201	1.084601
1	-0.509828	5.169259	1.455833
1	-1.354337	4.278629	0.151463
1	-1.972049	4.204110	1.827719
15	2.928768	1.704213	-0.805653
6	3.752445	2.767698	0.446704
6	4.538029	3.877522	0.092290
6	3.530114	2.496392	1.803477
6	5.138503	4.660512	1.078661
1	4.669689	4.140505	-0.952748
6	4.125582	3.284302	2.790311
1	2.880599	1.676754	2.086099
6	4.939740	4.360020	2.429688
1	5.752269	5.510056	0.792798
1	3.947227	3.058801	3.837978

1	5.405044	4.972721	3.196845
6	4.230477	1.020715	-1.925972
6	5.550994	1.482406	-1.990122
6	3.837345	-0.033280	-2.771767
6	6.454442	0.912414	-2.890653
1	5.893966	2.266355	-1.326357
6	4.739611	-0.594873	-3.675622
1	2.822835	-0.418962	-2.709129
6	6.052575	-0.120807	-3.738415
1	7.478901	1.272306	-2.917670
1	4.417614	-1.406392	-4.322486
1	6.759987	-0.561494	-4.435172
6	2.104322	2.975242	-1.870659
6	1.478837	4.074599	-1.260636
6	2.019032	2.829796	-3.262836
6	0.788655	5.010642	-2.028888
1	1.498443	4.176938	-0.181808
6	1.325943	3.770216	-4.029540
1	2.494389	1.990134	-3.758703
6	0.709355	4.862689	-3.415686
1	0.302074	5.849987	-1.539665
1	1.272657	3.647317	-5.107905
1	0.168556	5.591288	-4.013177
17	-2.518604	6.287764	0.772193
6	-3.178702	1.472558	-1.037100
6	-4.208929	0.908710	-1.867160
6	-1.941068	1.729364	-1.617681
6	-5.438256	0.423547	-1.336684
6	-3.995274	0.788702	-3.281119
6	-1.721919	1.589667	-3.009005
6	-6.405967	-0.118499	-2.154446
1	-5.602396	0.468238	-0.266777
6	-5.025964	0.254470	-4.100607
6	-2.736969	1.161480	-3.827336
1	-0.743577	1.855129	-3.395794
6	-6.208866	-0.191129	-3.554543
1	-7.326440	-0.497973	-1.719662
1	-4.849899	0.182010	-5.171237
1	-2.581010	1.075649	-4.899707
1	-6.983361	-0.611646	-4.189682
8	-0.901663	2.226674	-0.877121
6	-3.395225	1.772081	0.404799
6	-4.461065	2.627624	0.859268
6	-2.511809	1.273335	1.353356
6	-5.321297	3.328023	-0.033691
6	-4.647203	2.836947	2.267846
6	-2.686445	1.489649	2.738766
6	-6.327469	4.144803	0.434813
1	-5.169444	3.227931	-1.101509
6	-5.706351	3.671039	2.718278
6	-3.748301	2.233003	3.188484
1	-1.973431	1.038742	3.418998
6	-6.536347	4.309555	1.824848
1	-6.961743	4.673794	-0.271131
1	-5.837373	3.806983	3.789071
1	-3.901059	2.387225	4.253145
1	-7.337464	4.951101	2.180823
8	-1.422976	0.524691	0.958421
15	-0.091531	1.369037	0.346906
8	0.333183	2.436026	1.328025
6	0.347393	-3.900749	-2.400616
1	-0.604591	-3.755510	-2.916758
1	1.091316	-4.279697	-3.101880
1	0.222513	-4.609686	-1.580404

(A3...B4)

Number of imaginary frequencies : 0
Electronic energy : HF=-5736.6459667
Zero-point correction= 1.205194 (Hartree/Particle)
Thermal correction to Energy= 1.286620
Thermal correction to Enthalpy= 1.287564
Thermal correction to Gibbs Free Energy= 1.086595
Sum of electronic and zero-point Energies= -5735.440773
Sum of electronic and thermal Energies= -5735.359347
Sum of electronic and thermal Enthalpies= -5735.358403
Sum of electronic and thermal Free Energies= -5735.559372
Standard State and RRHO Corrected G= -5735.538335

Cartesian Coordinates

15	1.125780	-1.806723	0.413241
8	0.497104	-2.757418	1.556142
6	0.289161	2.886114	-3.241217
1	0.184729	2.880103	-4.327236
1	-0.617376	3.285033	-2.784254
1	1.161902	3.477943	-2.956474
6	1.243798	-3.663750	2.404242
1	1.849432	-3.106630	3.122024
1	0.495745	-4.253376	2.936416
1	1.878924	-4.317287	1.804105

(B4...MeCl)

Number of imaginary frequencies : 0
 Electronic energy : HF=-5736.6467296
 Zero-point correction= 1.202979 (Hartree/Particle)
 Thermal correction to Energy= 1.285125
 Thermal correction to Enthalpy= 1.286069
 Thermal correction to Gibbs Free Energy= 1.081234
 Sum of electronic and zero-point Energies= -5735.443750
 Sum of electronic and thermal Energies= -5735.361605
 Sum of electronic and thermal Enthalpies= -5735.360661
 Sum of electronic and thermal Free Energies= -5735.565496
 Standard State and RRHO Corrected G= -5735.542702

Cartesian Coordinates

45	-0.490954	-0.803162	-0.778381
6	2.702843	2.647415	0.646650
6	3.351264	2.647753	1.928078
6	1.322990	2.507342	0.620002
6	4.766965	2.598814	2.068474
6	2.552301	2.648945	3.120639
6	0.532056	2.455207	1.786604
6	5.358003	2.600289	3.312761
1	5.383292	2.542658	1.178942
6	3.195604	2.683534	4.388260
6	1.138045	2.561217	3.015293
1	-0.537502	2.320550	1.677624
6	4.568250	2.664964	4.486734
1	6.439774	2.545882	3.394458
1	2.577208	2.701169	5.282178
1	0.541862	2.544488	3.923712
1	5.048482	2.678534	5.460869
8	0.667563	2.429018	-0.608036
6	3.447816	2.741814	-0.639155
6	4.321023	3.840643	-0.955040
6	3.253377	1.770082	-1.609668
6	4.502280	4.954947	-0.087679
6	5.018663	3.845337	-2.210517
6	3.913995	1.783081	-2.855201
6	5.354975	5.985426	-0.419397
1	3.953668	4.995006	0.845619
6	5.901040	4.917584	-2.515310
6	4.798826	2.792866	-3.139198
1	3.721084	0.975251	-3.550228
6	6.074331	5.964384	-1.638475
1	5.472224	6.824974	0.260021
1	6.430744	4.897540	-3.464366
1	5.333157	2.803532	-4.084713
1	6.748629	6.779911	-1.883514
8	2.388517	0.707888	-1.360181
15	0.754806	0.972411	-1.410251
8	0.523971	1.453044	-2.928379
15	-1.678937	-2.844186	-0.813110
6	-0.566237	-4.284172	-1.137574
6	-0.146099	-5.161894	-0.129159
6	-0.044362	-4.436818	-2.433362
6	0.771990	-6.175706	-0.411894
1	-0.528099	-5.056298	0.878524
6	0.872090	-5.450583	-2.712609
1	-0.353566	-3.765367	-3.228902
6	1.285225	-6.322670	-1.701284
1	1.084802	-6.849666	0.380808
1	1.263070	-5.557821	-3.720558
1	2.000080	-7.111099	-1.918662
6	-2.598356	-3.249690	0.720760
6	-3.140579	-4.515334	0.996348
6	-2.742084	-2.223912	1.669657
6	-3.833994	-4.740146	2.187276

1	-3.006728	-5.334224	0.297063
6	-3.429111	-2.453137	2.860937
1	-2.326208	-1.242006	1.467204
6	-3.980672	-3.709922	3.119524
1	-4.253523	-5.722027	2.387345
1	-3.549579	-1.645323	3.576116
1	-4.526433	-3.884055	4.042381
6	-2.830836	-2.981508	-2.250032
6	-3.813633	-3.979696	-2.337411
6	-2.663369	-2.096044	-3.324198
6	-4.629282	-4.068893	-3.465973
1	-3.965239	-4.677380	-1.522176
6	-3.473993	-2.192596	-4.456997
1	-1.902206	-1.323108	-3.272455
6	-4.463003	-3.174629	-4.527532
1	-5.396086	-4.836917	-3.514462
1	-3.335413	-1.493516	-5.276760
1	-5.101725	-3.244205	-5.403422
6	-4.902774	3.026385	-2.621445
1	-4.356700	2.940065	-3.557977
1	-5.151813	2.043953	-2.230101
1	-4.332177	3.595806	-1.893596
17	-6.459744	3.927317	-2.954883
6	-5.110071	0.577389	0.875710
6	-5.880936	0.058663	1.976183
6	-4.777005	-0.297119	-0.157306
6	-6.078796	0.794203	3.179693
6	-6.445163	-1.257465	1.896304
6	-5.372754	-1.580467	-0.249984
6	-6.802267	0.268199	4.228732
1	-5.636034	1.779241	3.274426
6	-7.201242	-1.763851	2.987129
6	-6.206649	-2.039760	0.735062
1	-5.146371	-2.178639	-1.122531
6	-7.380481	-1.020490	4.132524
1	-6.925555	0.846725	5.140132
1	-7.621935	-2.762967	2.904184
1	-6.657389	-3.025257	0.657211
1	-7.952636	-1.421540	4.964317
8	-3.955463	0.058634	-1.195786
6	-4.693498	2.005329	0.822725
6	-5.645163	3.084944	0.890741
6	-3.361118	2.323727	0.619825
6	-7.052036	2.872890	0.940707
6	-5.172826	4.440932	0.852185
6	-2.894126	3.656904	0.560145
6	-7.932738	3.931528	0.991609
1	-7.436120	1.860364	0.922366
6	-6.107780	5.509580	0.921777
6	-3.781907	4.694818	0.701635
1	-1.836775	3.826677	0.391499
6	-7.460342	5.265332	0.995235
1	-9.001695	3.739367	1.019155
1	-5.730530	6.528898	0.898643
1	-3.435447	5.724155	0.665163
1	-8.165613	6.090304	1.039405
8	-2.439973	1.304717	0.462403
15	-2.342843	0.631561	-1.098265
8	-2.306439	1.716284	-2.142328
6	4.380502	-1.521858	-0.226300
6	5.368701	-0.905585	-1.069761
6	3.393291	-2.277762	-0.839935
6	6.300923	0.053020	-0.581181
6	5.396477	-1.221256	-2.469584
6	3.393931	-2.569624	-2.220036
6	7.236463	0.624831	-1.415012
1	6.256845	0.349366	0.459987
6	6.396441	-0.637883	-3.295361
6	4.399941	-2.075395	-3.014335
1	2.600629	-3.195534	-2.613764
6	7.302779	0.261381	-2.782018
1	7.925024	1.366974	-1.021412
1	6.414872	-0.900538	-4.350058
1	4.427601	-2.309442	-4.075038
1	8.053642	0.711145	-3.425161
8	2.358220	-2.806821	-0.077384
6	4.372499	-1.347627	1.251907
6	5.519753	-1.669618	2.064336
6	3.232525	-0.899979	1.902141
6	6.688852	-2.284546	1.534118

6	5.487788	-1.397116	3.473176	6	-4.674402	3.827426	-1.200877
6	3.191831	-0.641223	3.290011	6	-6.103893	3.173518	1.107347
6	7.773732	-2.567479	2.336083	1	-4.197537	2.810250	2.014492
1	6.722225	-2.542988	0.482734	6	-6.070827	3.887048	-1.198750
6	6.628868	-1.686321	4.269406	1	-4.138013	4.105748	-2.100391
6	4.307205	-0.862513	4.055959	6	-6.788983	3.555007	-0.049552
1	2.274006	-0.248910	3.711356	1	-6.651941	2.926918	2.012068
6	7.754465	-2.253455	3.715645	1	-6.593104	4.199888	-2.098394
1	8.650782	-3.041257	1.904202	1	-7.874195	3.600651	-0.051302
1	6.588931	-1.458658	5.331598	6	-1.674361	4.167475	1.514255
1	4.294511	-0.643678	5.119493	6	-2.379794	5.315602	1.910035
1	8.619816	-2.473877	4.334006	6	-0.560403	3.755659	2.262832
8	2.068712	-0.618937	1.197351	6	-1.975788	6.032346	3.036849
15	1.158067	-1.766540	0.432916	1	-3.242734	5.649671	1.342847
8	0.531604	-2.688576	1.603378	6	-0.160296	4.473560	3.390947
6	0.317291	2.823492	-3.345613	1	-0.004772	2.873989	1.957053
1	0.304496	2.799700	-4.436787	6	-0.868232	5.612415	3.779874
1	-0.644799	3.170380	-2.966788	1	-2.528231	6.918608	3.335370
1	1.132467	3.463733	-3.001035	1	0.702001	4.139807	3.960842
6	1.278408	-3.569977	2.475010	1	-0.560484	6.171405	4.658928
1	1.870499	-2.993180	3.188741	6	-1.508371	4.232282	-1.388662
1	0.532106	-4.158517	3.011214	6	-0.759791	5.398491	-1.169419
1	1.927870	-4.227977	1.895220	6	-1.724922	3.797356	-2.707269
-----				6	-0.239915	6.115456	-2.249334
(A4...B5)				1	-0.576785	5.751855	-0.160826
-----				6	-1.220871	4.527735	-3.782787
Number of imaginary frequencies : 0				1	-2.265455	2.876921	-2.892521
Electronic energy : HF=-5736.6485897				6	-0.471803	5.685506	-3.556687
Zero-point correction= 1.206335 (Hartree/Particle)				1	0.342856	7.013255	-2.064382
Thermal correction to Energy= 1.287344				1	-1.404825	4.186280	-4.797266
Thermal correction to Enthalpy= 1.288288				1	-0.070227	6.247140	-4.395213
Thermal correction to Gibbs Free Energy= 1.088990				6	-1.096848	-0.874151	4.093012
Sum of electronic and zero-point Energies= -5735.442254				1	-0.907958	-1.932875	3.922073
Sum of electronic and thermal Energies= -5735.361245				1	-0.899991	-0.622801	5.134596
Sum of electronic and thermal Enthalpies= -5735.360301				1	-2.128598	-0.630382	3.848506
Sum of electronic and thermal Free Energies= -5735.559599				17	-3.632674	-2.651774	5.481082
Standard State and RRHO Corrected G= -5735.53895				6	2.388272	-2.464045	0.811794
-----				6	3.143678	-3.051541	-0.262253
Cartesian Coordinates				6	1.005245	-2.528957	0.727401
-----				6	4.549702	-2.875397	-0.395153
45	-1.161506	1.083590	0.433929	6	2.460953	-3.811149	-1.270853
6	-3.442216	-1.873116	-1.472927	6	0.321314	-3.234920	-0.283070
6	-2.743339	-2.222481	-2.681554	6	5.244262	-3.452770	-1.435320
6	-3.778918	-0.538810	-1.297459	1	5.074515	-2.261931	0.327065
6	-2.176730	-3.511063	-2.888848	6	3.212758	-4.422863	-2.310866
6	-2.552487	-1.227516	-3.699049	6	1.043095	-3.895564	-1.246111
6	-3.646815	0.431404	-2.311494	1	-0.762885	-3.244189	-0.266995
6	-1.464541	-3.799161	-4.033308	6	4.576011	-4.253797	-2.392995
1	-2.293251	-4.269058	-2.123149	1	6.314060	-3.287213	-1.524408
6	-1.824683	-1.562449	-4.873226	1	2.681537	-5.007995	-3.057344
6	-3.066652	0.081906	-3.504739	1	0.532637	-4.456404	-2.022608
1	-3.995473	1.437095	-2.110203	1	5.138699	-4.714206	-3.199910
6	-1.286565	-2.819179	-5.039530	8	0.228729	-1.915228	1.703880
1	-1.031662	-4.787109	-4.161890	6	3.034681	-1.795832	1.977238
1	-1.691370	-0.798703	-5.634958	6	4.018954	-2.465053	2.791350
1	-2.945955	0.818319	-4.293751	6	2.670370	-0.510560	2.349833
1	-0.724627	-3.061088	-5.936978	6	4.364328	-3.834373	2.611954
8	-4.256146	-0.102166	-0.057445	6	4.662717	-1.746270	3.854687
6	-3.806649	-2.869909	-0.427023	6	3.278143	0.192563	3.408741
6	-4.618911	-4.022207	-0.729131	6	5.321993	-4.438177	3.397662
6	-3.438027	-2.676710	0.896060	1	3.856625	-4.414945	1.851623
6	-5.176280	-4.257192	-2.017837	6	5.658278	-2.394018	4.635832
6	-4.915201	-4.965739	0.312150	6	4.278613	-0.406894	4.130241
6	-3.741294	-3.585995	1.931877	1	2.953213	1.206749	3.608019
6	-5.939360	-5.376577	-2.272313	6	5.990707	-3.710311	4.410475
1	-5.005992	-3.538995	-2.810772	1	5.560633	-5.486400	3.241539
6	-5.695893	-6.115297	0.012589	1	6.143341	-1.827897	5.426906
6	-4.452280	-4.721086	1.633553	1	4.775054	0.131214	4.932271
1	-3.428282	-3.354541	2.948209	1	6.749509	-4.196791	5.016545
6	-6.193603	-6.325219	-1.253591	8	1.689231	0.181939	1.634744
1	-6.355075	-5.527877	-3.264591	15	0.118237	-0.269759	1.740367
1	-5.900283	-6.822479	0.812363	8	-0.170801	-0.057769	3.311419
1	-4.690652	-5.434019	2.418028	6	3.557587	1.706967	-0.627107
1	-6.791199	-7.206062	-1.469909	6	4.546041	1.756125	0.414917
8	-2.659342	-1.583586	1.260027	6	2.488306	2.585422	-0.541826
15	-3.060449	0.005354	1.095113	6	5.583140	0.788095	0.529228
8	-3.930318	0.383397	2.386080	6	4.466775	2.784844	1.413323
15	-2.148671	3.220497	0.007227	6	2.399948	3.598412	0.434937
6	-3.982021	3.422528	-0.050861	6	6.508616	0.855716	1.547051
6	-4.711942	3.107661	1.108170	1	5.629137	-0.022819	-0.187485

6	5.454681	2.840841	2.434665	6	-4.342038	-4.768383	1.750528
6	3.388021	3.709242	1.383250	1	-3.269445	-3.394013	3.013391
1	1.549499	4.269846	0.409259	6	-6.169273	-6.397270	-1.068625
6	6.457732	1.901121	2.501020	1	-6.389956	-5.617533	-3.080740
1	7.279714	0.094677	1.623929	1	-5.814197	-6.876996	0.991800
1	5.389193	3.633775	3.175328	1	-4.547325	-5.480117	2.545314
1	3.338992	4.490590	2.136613	1	-6.772114	-7.280321	-1.259804
1	7.199644	1.946352	3.292929	8	-2.578854	-1.622941	1.301099
8	1.442719	2.487097	-1.459572	15	-2.984500	-0.028810	1.128644
6	3.626333	0.742792	-1.759666	8	-3.874437	0.322543	2.426535
6	4.760540	0.680089	-2.646223	15	-2.195511	3.217919	-0.015149
6	2.555078	-0.094127	-2.028098	6	-4.034422	3.366116	-0.069694
6	5.857151	1.582853	-2.557446	6	-4.747978	3.022973	1.091443
6	4.785920	-0.306435	-3.688784	6	-4.745349	3.753163	-1.214138
6	2.566330	-1.055951	-3.060512	6	-6.141055	3.045211	1.098892
6	6.931402	1.486718	-3.415774	1	-4.218177	2.734924	1.992188
1	5.842664	2.364033	-1.807010	6	-6.143256	3.768441	-1.204524
6	5.915558	-0.388501	-4.547122	1	-4.221911	4.050579	-2.115347
6	3.672583	-1.172179	-3.862421	6	-6.844369	3.409841	-0.052862
1	1.698260	-1.693433	-3.180418	1	-6.676492	2.777017	2.005152
6	6.972241	0.483728	-4.413207	1	-6.680158	4.067514	-2.100336
1	7.753311	2.191579	-3.327579	1	-7.930556	3.421255	-0.048773
1	5.922602	-1.152015	-5.320790	6	-1.745395	4.231846	1.455979
1	3.704319	-1.922709	-4.646349	6	-2.488257	5.364866	1.825384
1	7.829248	0.414276	-5.076854	6	-0.606172	3.887081	2.200576
8	1.411194	-0.054960	-1.234037	6	-2.095363	6.134146	2.921195
15	0.376607	1.228821	-1.222031	1	-3.371120	5.646952	1.260409
8	-0.348110	1.224265	-2.652776	6	-0.216722	4.657470	3.297535
6	-5.085775	-0.387326	2.840542	1	-0.021967	3.015757	1.918502
1	-5.734389	0.322762	3.355814	6	-0.961058	5.782068	3.659257
1	-5.618378	-0.823154	1.993097	1	-2.676272	7.009023	3.198875
1	-4.742025	-1.158176	3.537083	1	0.665814	4.375157	3.864345
6	0.296267	1.362677	-3.939745	1	-0.660890	6.382513	4.513325
1	0.603298	0.379369	-4.299477	6	-1.591083	4.209245	-1.443357
1	-0.452083	1.785785	-4.610718	6	-0.859673	5.393061	-1.263723
1	1.156123	2.032170	-3.882335	6	-1.807056	3.733111	-2.747873
-----				6	-0.356063	6.085806	-2.367188
(A4-B5)*				1	-0.676476	5.778886	-0.267047
-----				6	-1.319720	4.438769	-3.847369
Number of imaginary frequencies : 1				1	-2.332813	2.798782	-2.902548
Electronic energy : HF=-5736.6224127				6	-0.587466	5.614137	-3.660141
Zero-point correction= 1.203331 (Hartree/Particle)				1	0.213652	6.997599	-2.211939
Thermal correction to Energy= 1.284373				1	-1.502869	4.064055	-4.850282
Thermal correction to Enthalpy= 1.285317				1	-0.198375	6.156493	-4.517119
Thermal correction to Gibbs Free Energy= 1.085090				6	-1.431039	-1.036267	4.310252
Sum of electronic and zero-point Energies= -5735.419081				1	-1.336419	-1.854558	3.618405
Sum of electronic and thermal Energies= -5735.338040				1	-0.799065	-1.002128	5.181723
Sum of electronic and thermal Enthalpies= -5735.337096				1	-2.220310	-0.315217	4.191816
Sum of electronic and thermal Free Energies= -5735.537323				17	-3.007380	-2.396918	5.543378
Standard State and RRHO Corrected G= -5735.515959				6	2.407039	-2.403222	0.864914
-----				6	3.120756	-3.030641	-0.214702
Cartesian Coordinates				6	1.019068	-2.445468	0.829647
-----				6	4.524259	-2.877331	-0.397358
45	-1.136773	1.129512	0.485940	6	2.398752	-3.810688	-1.179224
6	-3.419007	-1.954635	-1.413573	6	0.299923	-3.174685	-0.142642
6	-2.752202	-2.330356	-2.631818	6	5.179493	-3.495040	-1.440091
6	-3.746642	-0.616329	-1.252584	1	5.078748	-2.248362	0.288790
6	-2.188773	-3.622410	-2.825317	6	3.110078	-4.463581	-2.222524
6	-2.593177	-1.359002	-3.676813	6	0.981468	-3.874001	-1.107193
6	-3.641247	0.330965	-2.291359	1	-0.783041	-3.171851	-0.094454
6	-1.508606	-3.935968	-3.982476	6	4.472339	-4.315872	-2.352059
1	-2.280018	-4.361728	-2.038124	1	6.247998	-3.345932	-1.567035
6	-1.900559	-1.720772	-4.864356	1	2.548093	-5.063381	-2.934278
6	-3.101198	-0.045419	-3.494877	1	0.439389	-4.450143	-1.850611
1	-3.980049	1.342004	-2.100180	1	5.003898	-4.807910	-3.161548
6	-1.363887	-2.979943	-5.016703	8	0.285534	-1.809802	1.811800
1	-1.074784	-4.925016	-4.099362	6	3.098204	-1.712889	1.990040
1	-1.791146	-0.974800	-5.647295	6	4.098032	-2.370462	2.793870
1	-3.003700	0.674436	-4.302221	6	2.751959	-0.412570	2.332790
1	-0.827215	-3.241466	-5.924076	6	4.426679	-3.747630	2.641824
8	-4.196873	-0.160645	-0.012466	6	4.776770	-1.632005	3.821677
6	-3.762718	-2.932080	-0.343536	6	3.398310	0.307280	3.359973
6	-4.581945	-4.088376	-0.610368	6	5.398987	-4.341367	3.417328
6	-3.360860	-2.719038	0.966706	1	3.893846	-4.341963	1.909744
6	-5.175854	-4.335587	-1.880279	6	5.786158	-2.269956	4.593123
6	-4.846960	-5.023344	0.446623	6	4.411012	-0.282470	4.072290
6	-3.628168	-3.627270	2.015127	1	3.089157	1.329882	3.541172
6	-5.945497	-5.457380	-2.102424	6	6.100830	-3.594967	4.393730
1	-5.028845	-3.624292	-2.683944	1	5.623768	-5.395596	3.281520
6	-5.634612	-6.176191	0.180505	1	6.297057	-1.688632	5.356659

1	4.932732	0.271367	4.847483	1	-1.935738	-0.894917	-5.665041
1	6.870738	-4.073287	4.992398	1	-3.166939	0.712179	-4.277465
8	1.765041	0.260851	1.626824	1	-0.890069	-3.120769	-5.967968
15	0.168825	-0.144663	1.862659	8	-4.176516	-0.169874	0.051135
8	-0.170634	0.117636	3.347624	6	-3.718497	-2.932753	-0.333097
6	3.520025	1.720499	-0.735141	6	-4.515570	-4.099239	-0.628561
6	4.530333	1.812560	0.282013	6	-3.318555	-2.742620	0.981300
6	2.443488	2.590909	-0.655970	6	-5.116454	-4.319758	-1.900219
6	5.579850	0.858896	0.404273	6	-4.750476	-5.074225	0.398429
6	4.462504	2.872304	1.248345	6	-3.550307	-3.700026	1.995832
6	2.364049	3.630919	0.293546	6	-5.863030	-5.451054	-2.151669
6	6.530173	0.971536	1.394833	1	-4.994811	-3.580170	-2.682059
1	5.615505	0.023160	-0.284167	6	-5.513863	-6.235953	0.102978
6	5.474941	2.973548	2.241800	6	-4.236141	-4.850735	1.703994
6	3.371189	3.781884	1.215812	1	-3.175100	-3.500450	2.992492
1	1.504111	4.290596	0.267839	6	-6.055528	-6.429170	-1.147747
6	6.491602	2.048824	2.313277	1	-6.313499	-5.588960	-3.130613
1	7.311068	0.221228	1.478514	1	-5.669241	-6.966303	0.892955
1	5.418073	3.789772	2.957545	1	-4.408611	-5.595686	2.475725
1	3.328917	4.584319	1.947292	1	-6.639897	-7.319217	-1.362324
1	7.252934	2.129538	3.083714	8	-2.559460	-1.646743	1.354628
8	1.383865	2.451531	-1.547208	15	-2.951889	-0.042477	1.189227
6	3.571089	0.721059	-1.837478	8	-3.865228	0.285225	2.486955
6	4.687237	0.638186	-2.745347	15	-2.195185	3.221194	-0.035621
6	2.498862	-0.130163	-2.057087	6	-4.032504	3.388681	-0.071030
6	5.778994	1.550688	-2.707782	6	-4.737933	2.998123	1.080044
6	4.699922	-0.380357	-3.756784	6	-4.751088	3.836676	-1.188002
6	2.498072	-1.121735	-3.062033	6	-6.130260	3.036531	1.105429
6	6.837905	1.433799	-3.582527	1	-4.201171	2.658994	1.958781
1	5.772781	2.355963	-1.983176	6	-6.148949	3.866695	-1.161835
6	5.813804	-0.482979	-4.633245	1	-4.232596	4.167086	-2.080916
6	3.588559	-1.256866	-3.881918	6	-6.841847	3.463174	-0.020085
1	1.632134	-1.767800	-3.145113	1	-6.658288	2.729371	2.003829
6	6.867468	0.398982	-4.547306	1	-6.692164	4.212071	-2.037003
1	7.656341	2.146490	-3.532597	1	-7.927772	3.486017	-0.003544
1	5.811261	-1.271253	-5.381841	6	-1.709706	4.275935	1.397872
1	3.609247	-2.031163	-4.642865	6	-2.481074	5.373458	1.811182
1	7.712618	0.312855	-5.224156	6	-0.505185	3.996252	2.064933
8	1.373677	-0.081495	-1.242489	6	-2.054880	6.170247	2.875039
15	0.326780	1.195566	-1.217369	1	-3.412138	5.608170	1.305261
8	-0.444644	1.150224	-2.627534	6	-0.082327	4.794189	3.128852
6	-5.023107	-0.458746	2.859084	1	0.101779	3.151952	1.751496
1	-5.652769	0.221222	3.435222	6	-0.857013	5.882522	3.535939
1	-5.581597	-0.840224	2.002037	1	-2.659452	7.017252	3.186907
1	-4.678921	-1.275198	3.498409	1	0.849661	4.560536	3.635544
6	0.167098	1.223864	-3.933210	1	-0.530557	6.504349	4.364754
1	0.422563	0.218224	-4.271775	6	-1.602416	4.175984	-1.494032
1	-0.580933	1.657956	-4.598071	6	-0.863249	5.359960	-1.349794
1	1.055715	1.857480	-3.922278	6	-1.836760	3.673242	-2.785000
				6	-0.367815	6.024766	-2.473955
(B5...MeCl)				1	-0.667012	5.766652	-0.363878
				6	-1.357773	4.350912	-3.905637
Number of imaginary frequencies : 0				1	-2.373357	2.741180	-2.912493
Electronic energy : HF=-5736.650562				6	-0.616109	5.525477	-3.753389
Zero-point correction= 1.203184 (Hartree/Particle)				1	0.208400	6.936734	-2.345693
Thermal correction to Energy= 1.285330				1	-1.554666	3.954943	-4.897791
Thermal correction to Enthalpy= 1.286274				1	-0.233298	6.045922	-4.626669
Thermal correction to Gibbs Free Energy= 1.080795				6	-1.922711	-1.383849	4.724006
Sum of electronic and zero-point Energies= -5735.447378				1	-1.541635	-1.927180	3.863196
Sum of electronic and thermal Energies= -5735.365232				1	-1.126644	-1.179055	5.435764
Sum of electronic and thermal Enthalpies= -5735.364288				1	-2.414304	-0.467798	4.411998
Sum of electronic and thermal Free Energies= -5735.569767				17	-3.169429	-2.431831	5.565719
Standard State and RRHO Corrected G= -5735.546401				6	2.404080	-2.335085	1.042665
				6	3.057294	-3.037340	-0.029383
Cartesian Coordinates				6	1.013939	-2.355521	1.082691
				6	4.453194	-2.919771	-0.285641
45	-1.133005	1.157553	0.556514	6	2.281798	-3.859699	-0.913730
6	-3.398508	-1.930653	-1.385705	6	0.246146	-3.130968	0.183829
6	-2.749404	-2.280180	-2.620977	6	5.051016	-3.608108	-1.318856
6	-3.750819	-0.601481	-1.201841	1	5.048269	-2.262548	0.336745
6	-2.141561	-3.549492	-2.829641	6	2.934071	-4.583398	-1.948704
6	-2.658325	-1.304305	-3.669029	6	0.869339	-3.894002	-0.771339
6	-3.710814	0.349327	-2.242499	1	-0.831289	-3.108778	0.279764
6	-1.481154	-3.837347	-4.004793	6	4.290979	-4.467864	-2.148773
1	-2.183221	-4.290275	-2.039600	1	6.114831	-3.485209	-1.501763
6	-1.991875	-1.642450	-4.878122	1	2.330224	-5.212848	-2.598059
6	-3.206640	-0.009831	-3.467002	1	0.284001	-4.502844	-1.453984
1	-4.076468	1.348586	-2.039265	1	4.777192	-5.014422	-2.951869
6	-1.409213	-2.879260	-5.044966	8	0.334587	-1.659968	2.058303
1	-1.008484	-4.807091	-4.132604	6	3.157862	-1.572569	2.075008

6	4.194953	-2.171922	2.875186
6	2.830461	-0.245183	2.324003
6	4.513405	-3.558665	2.813744
6	4.927889	-1.359677	3.805593
6	3.533730	0.546886	3.259152
6	5.524177	-4.096470	3.581091
1	3.942742	-4.203538	2.156435
6	5.974789	-1.941992	4.570830
6	4.578440	0.008313	3.965512
1	3.238188	1.583187	3.373320
6	6.276745	-3.280563	4.459385
1	5.741004	-5.159118	3.514972
1	6.526921	-1.306033	5.258546
1	5.140982	0.618166	4.666827
1	7.076510	-3.715095	5.052419
8	1.817656	0.366870	1.615850
15	0.216575	0.022408	2.017640
8	-0.072692	0.440210	3.437000
6	3.535871	1.622265	-0.871541
6	4.614002	1.745638	0.070283
6	2.481287	2.516875	-0.765841
6	5.648729	0.774208	0.177399
6	4.636113	2.859461	0.975777
6	2.490348	3.609847	0.126749
6	6.666274	0.916639	1.094779
1	5.618838	-0.098870	-0.463140
6	5.716665	2.991042	1.890701
6	3.563178	3.791179	0.965628
1	1.643555	4.287101	0.122395
6	6.714646	2.045165	1.949103
1	7.433653	0.151582	1.169812
1	5.726442	3.847507	2.560209
1	3.588583	4.635287	1.649469
1	7.527942	2.149313	2.661489
8	1.366347	2.362121	-1.577405
6	3.502552	0.572051	-1.926761
6	4.562382	0.427164	-2.893288
6	2.405233	-0.267837	-2.045665
6	5.666590	1.322705	-2.964747
6	4.502187	-0.638305	-3.853511
6	2.333978	-1.307349	-2.999164
6	6.670238	1.147808	-3.893392
1	5.714028	2.161845	-2.281387
6	5.560502	-0.799756	-4.788112
6	3.373741	-1.501874	-3.870893
1	1.454559	-1.940519	-3.001776
6	6.629054	0.068222	-4.807204
1	7.499186	1.849322	-3.926095
1	5.502838	-1.622314	-5.496612
1	3.339486	-2.312570	-4.592633
1	7.431119	-0.063384	-5.527820
8	1.326763	-0.159606	-1.179337
15	0.297253	1.132851	-1.166605
8	-0.501051	1.058804	-2.564910
6	-5.077039	-0.434919	2.822107
1	-5.485850	0.055446	3.706765
1	-5.794406	-0.381706	2.000088
1	-4.850888	-1.477427	3.056891
6	0.085019	1.114887	-3.882207
1	0.339264	0.106163	-4.212024
1	-0.677126	1.534879	-4.540036
1	0.970329	1.752835	-3.898439

MeCl			
Number of imaginary frequencies : 0			
Electronic energy : HF=-500.1140005			
Zero-point correction= 0.037797 (Hartree/Particle)			
Thermal correction to Energy= 0.040830			
Thermal correction to Enthalpy= 0.041774			
Thermal correction to Gibbs Free Energy= 0.015141			
Sum of electronic and zero-point Energies= -500.076203			
Sum of electronic and thermal Energies= -500.073171			
Sum of electronic and thermal Enthalpies= -500.072227			
Sum of electronic and thermal Free Energies= -500.098860			
Standard State and RRHO Corrected G= -500.095841			
Cartesian Coordinates			
6	0.000000	-0.000000	-1.148582

1	0.000000	1.035940	-1.489059
1	-0.897150	-0.517970	-1.489059
1	0.897150	-0.517970	-1.489059
17	-0.000000	0.000000	0.668157

B1 [Rh(BINOL-P=O)(PPh3)3 or 1]			
Number of imaginary frequencies : 0			
Electronic energy : HF=-4556.3815476			
Zero-point correction= 1.099702 (Hartree/Particle)			
Thermal correction to Energy= 1.169337			
Thermal correction to Enthalpy= 1.170281			
Thermal correction to Gibbs Free Energy= 0.993335			
Sum of electronic and zero-point Energies= -4555.281846			
Sum of electronic and thermal Energies= -4555.212210			
Sum of electronic and thermal Enthalpies= -4555.211266			
Sum of electronic and thermal Free Energies= -4555.388212			
Standard State and RRHO Corrected G= -4555.369161			
Cartesian Coordinates			
45	-0.743742	0.096659	-0.268824
15	-1.247044	2.422735	-0.208444
6	4.126685	0.686733	0.676584
6	4.821805	0.333389	1.885261
6	2.949262	1.421970	0.784358
6	5.940430	-0.547903	1.900330
6	4.355025	0.840562	3.144696
6	2.475635	1.894992	2.032587
6	6.581605	-0.872667	3.075728
1	6.279446	-0.985914	0.969578
6	5.046140	0.496537	4.338530
6	3.177473	1.634002	3.182772
1	1.564096	2.479976	2.041292
6	6.140691	-0.338248	4.310766
1	7.427314	-1.554551	3.055702
1	4.681122	0.897713	5.280996
1	2.826019	2.011254	4.139854
1	6.657886	-0.597862	5.230172
8	2.245746	1.775131	-0.335184
6	4.584706	0.245314	-0.669063
6	5.904911	0.513318	-1.174616
6	3.691783	-0.426433	-1.497542
6	6.840599	1.336734	-0.485413
6	6.299256	-0.030178	-2.444444
6	4.078772	-0.959211	-2.749855
6	8.099215	1.571443	-0.995487
1	6.549090	1.794761	0.452474
6	7.610333	0.218688	-2.934595
6	5.362848	-0.785411	-3.201951
1	3.334998	-1.501843	-3.323426
6	8.498262	0.996979	-2.226308
1	8.789614	2.209310	-0.450377
1	7.894099	-0.210803	-3.892395
1	5.671432	-1.199861	-4.158212
1	9.495663	1.183976	-2.614102
8	2.395334	-0.630935	-1.094556
15	1.281448	0.653620	-1.184567
8	1.233574	1.180350	-2.598645
15	-3.067534	-0.487921	0.141382
6	-4.482910	0.712056	0.008586
6	-4.912730	1.439025	1.129337
6	-5.140890	0.916570	-1.215029
6	-5.969132	2.345723	1.027765
1	-4.425584	1.303743	2.088250
6	-6.187942	1.832284	-1.318552
1	-4.838066	0.363134	-2.095724
6	-6.607470	2.550119	-0.196279
1	-6.281699	2.898908	1.908682
1	-6.674625	1.981478	-2.278185
1	-7.426095	3.260111	-0.275319
6	-3.598414	-1.708927	-1.148414
6	-4.687827	-2.580836	-1.010032
6	-2.891402	-1.702914	-2.360005
6	-5.043533	-3.439138	-2.050688
1	-5.249389	-2.620187	-0.085574
6	-3.248578	-2.557769	-3.404868
1	-2.035495	-1.045742	-2.469129
6	-4.324855	-3.433062	-3.250137
1	-5.880032	-4.120142	-1.920849

1	-2.672640	-2.548995	-4.325698
1	-4.601840	-4.107367	-4.055573
6	-3.423438	-1.194495	1.814254
6	-4.710907	-1.563908	2.244112
6	-2.371596	-1.254106	2.736302
6	-4.922175	-2.017552	3.545636
1	-5.561623	-1.462887	1.579229
6	-2.583423	-1.687813	4.046229
1	-1.380398	-0.955978	2.419159
6	-3.858616	-2.080175	4.451727
1	-5.922151	-2.305609	3.857542
1	-1.748939	-1.726120	4.740961
1	-4.028454	-2.423397	5.468418
6	0.017272	3.781712	-0.303539
6	0.594122	4.088546	-1.546928
6	0.402339	4.521695	0.822470
6	1.538037	5.107126	-1.655364
1	0.330980	3.508354	-2.423514
6	1.354848	5.538830	0.711884
1	-0.037447	4.317055	1.792261
6	1.925339	5.834773	-0.525914
1	1.977853	5.328255	-2.624050
1	1.643230	6.100287	1.596453
1	2.664194	6.626749	-0.612594
6	-2.332294	2.973801	-1.599093
6	-2.794796	4.294524	-1.731585
6	-2.589323	2.065779	-2.634000
6	-3.551052	4.671198	-2.841067
1	-2.537139	5.043176	-0.990424
6	-3.323420	2.448322	-3.758265
1	-2.204588	1.055891	-2.553414
6	-3.820266	3.748022	-3.856636
1	-3.912874	5.692326	-2.922475
1	-3.510429	1.726737	-4.548665
1	-4.399600	4.048002	-4.725395
6	-2.035772	2.828209	1.413632
6	-2.966111	3.853618	1.631020
6	-1.588903	2.077428	2.152694
6	-3.448407	4.109009	2.915594
1	-3.348121	4.437670	0.803923
6	-2.072641	2.330421	3.797461
1	-0.864835	1.284514	2.349420
6	-3.008431	3.346970	4.001132
1	-4.180342	4.897858	3.064631
1	-1.725627	1.728120	4.632180
1	-3.393042	3.543831	4.997880
15	-0.026805	-2.195257	-0.158983
6	-1.095563	-3.558030	0.544696
6	-1.992089	-4.263066	-0.275639
6	-1.027891	-3.908982	1.902657
6	-2.803937	-5.269787	0.248015
1	-2.057550	-4.039154	-1.332755
6	-1.844018	-4.911637	2.427934
1	-0.337546	-3.401593	2.564963
6	-2.739364	-5.594722	1.603823
1	-3.490535	-5.793684	-0.410627
1	-1.776780	-5.154730	3.484623
1	-3.374702	-6.375850	2.012089
6	0.442164	-2.973814	-1.776501
6	0.722394	-4.348466	-1.873277
6	0.485375	-2.200210	-2.945585
6	1.057753	-4.925727	-3.098990
1	0.663988	-4.979902	-0.993215
6	0.811178	-2.779267	-4.173953
1	0.280309	-1.137116	-2.906517
6	1.102543	-4.142553	-4.254611
1	1.275917	-5.988822	-3.149262
1	0.839004	-2.158657	-5.065329
1	1.356968	-4.592607	-5.210215
6	1.434675	-2.374757	0.966106
6	2.462188	-3.306076	0.767989
6	1.442422	-1.601151	2.136389
6	3.453766	-3.481343	1.735124
1	2.506803	-3.889441	-0.143953
6	2.414146	-1.801383	3.117845
1	0.688430	-0.833038	2.276315
6	3.421739	-2.747025	2.922256
1	4.252217	-4.197005	1.558929
1	2.399943	-1.198651	4.019632
1	4.192021	-2.885449	3.674391

B1 (O-Coordination)			
Number of imaginary frequencies : 0			
Electronic energy : HF=-4556.3633038			
Zero-point correction= 1.098219 (Hartree/Particle)			
Thermal correction to Energy= 1.168360			
Thermal correction to Enthalpy= 1.169305			
Thermal correction to Gibbs Free Energy= 0.990280			
Sum of electronic and zero-point Energies= -4555.265085			
Sum of electronic and thermal Energies= -4555.194943			
Sum of electronic and thermal Enthalpies= -4555.193999			
Sum of electronic and thermal Free Energies= -4555.373023			
Standard State and RRHO Corrected G= -4555.353183			
Cartesian Coordinates			
45	-1.124077	0.059731	0.143828
15	-0.439341	2.237789	-0.364403
6	5.191181	0.123505	0.816633
6	6.549185	0.185268	1.279368
6	4.254899	0.989366	1.379747
6	7.546339	-0.744194	0.864205
6	6.931767	1.201482	2.220462
6	4.637845	1.987857	2.310965
6	8.843517	-0.653485	1.320304
1	7.271692	-1.541321	0.182955
6	8.281085	1.273587	2.662374
6	5.947516	2.104242	2.706102
1	3.869288	2.656984	2.685210
6	9.223067	0.371480	2.220824
1	9.581500	-1.379368	0.989743
1	8.553170	2.055470	3.367464
1	6.243934	2.877121	3.410710
1	10.250294	0.434981	2.568553
8	2.945640	0.931848	1.006283
6	4.735724	-0.844531	-0.220442
6	5.299892	-0.884980	-1.541775
6	3.670776	-1.691102	0.068170
6	6.280961	0.046587	-1.987967
6	4.819190	-1.854639	-2.486239
6	3.205488	-2.651908	-0.860097
6	6.774664	0.006087	-3.274150
1	6.627450	0.813599	-1.306027
6	5.359986	-1.878518	-3.801277
6	3.780135	-2.744698	-2.103134
1	2.381852	-3.290154	-0.563301
6	6.319282	-0.971316	-4.192306
1	7.515230	0.736274	-3.588920
1	4.987507	-2.624303	-4.499614
1	3.417654	-3.475054	-2.821119
1	6.718822	-0.994826	-5.202236
8	3.043527	-1.619164	1.289745
15	1.909791	-0.359443	1.563390
8	0.949061	-0.437724	0.341366
15	-3.357372	0.465162	0.140077
6	-4.053346	2.171689	0.435262
6	-4.284109	2.639711	1.739192
6	-4.359735	3.022242	-0.640540
6	-4.812640	3.912856	1.960127
1	-4.059739	2.014413	2.595316
6	-4.876765	4.299583	-0.418716
1	-4.204606	2.692031	-1.659542
6	-5.108218	4.750185	0.883196
1	-4.986061	4.248749	2.978509
1	-5.099865	4.937902	-1.268795
1	-5.517143	5.741852	1.055289
6	-4.290094	-0.028201	-1.380449
6	-5.657393	0.247206	-1.555819
6	-3.594705	-0.662561	-2.419951
6	-6.313144	-0.131105	-2.728128
1	-6.210560	0.773442	-0.784649
6	-4.246885	-1.032867	-3.597838
1	-2.536027	-0.870680	-2.301285
6	-5.610087	-0.773256	-3.751638
1	-7.371451	0.084439	-2.845234
1	-3.688233	-1.524430	-4.389402
1	-6.121458	-1.060489	-4.666130
6	-4.156312	-0.421028	1.561334
6	-5.430346	-1.000891	1.525696

6	-3.439606	-0.434498	2.770441
6	-5.978310	-1.571455	2.677084
1	-5.995669	-1.034648	0.602421
6	-3.989821	-1.000141	3.921041
1	-2.447341	0.007744	2.803557
6	-5.264965	-1.568759	3.877242
1	-6.961803	-2.030225	2.629046
1	-3.420049	-0.999876	4.846157
1	-5.695033	-2.016096	4.768944
6	1.279053	2.397265	-1.032487
6	1.757572	1.404259	-1.896885
6	2.074865	3.523641	-0.784133
6	3.014189	1.523465	-2.487988
1	1.159888	0.522025	-2.083745
6	3.338236	3.637269	-1.367497
1	1.723133	4.310905	-0.125571
6	3.812638	2.636846	-2.218139
1	3.381390	0.734096	-3.136613
1	3.950973	4.509164	-1.154275
1	4.800507	2.716406	-2.662273
6	-1.310408	3.114041	-1.737447
6	-1.355642	4.509680	-1.868312
6	-1.843181	2.318848	-2.762114
6	-1.979340	5.092692	-2.972744
1	-0.911482	5.147017	-1.111122
6	-2.455734	2.901183	-3.872754
1	-1.791807	1.239673	-2.678066
6	-2.539008	4.291902	-3.972867
1	-2.024413	6.175239	-3.053458
1	-2.877557	2.266796	-4.647387
1	-3.026566	4.750446	-4.828569
6	-0.447833	3.353911	1.101257
6	-1.480109	4.263535	1.368222
6	0.563435	3.172770	2.065367
6	-1.493608	4.988358	2.563366
1	-2.282517	4.409074	0.656588
6	0.543286	3.895255	3.257252
1	1.377374	2.481449	1.874405
6	-0.485764	4.808396	3.510642
1	-2.303177	5.688117	2.749695
1	1.334099	3.746083	3.987494
1	-0.499925	5.372560	4.439013
15	-1.351850	-2.328877	0.236158
6	-2.930928	-3.277081	0.469811
6	-3.826333	-3.424021	-0.602985
6	-3.273733	-3.841387	1.707986
6	-5.031792	-4.106619	-0.441555
1	-3.579340	-3.020303	-1.576146
6	-4.478821	-4.528480	1.867072
1	-2.606423	-3.748785	2.556830
6	-5.363599	-4.662451	0.795978
1	-5.707075	-4.204773	-1.287109
1	-4.724927	-4.954955	2.835373
1	-6.301426	-5.195707	0.923916
6	-0.729146	-3.038520	-1.355951
6	-0.975620	-4.368538	-1.739757
6	0.020823	-2.218016	-2.211164
6	-0.484766	-4.858307	-2.951162
1	-1.557033	-5.022535	-1.098234
6	0.506462	-2.706272	-3.425623
1	0.231526	-1.200419	-1.908669
6	0.253421	-4.027516	-3.799569
1	-0.683110	-5.888527	-3.233348
1	1.090354	-2.054819	-4.069488
1	0.629210	-4.409801	-4.744602
6	-0.285949	-3.093559	1.538036
6	0.484231	-4.244244	1.321793
6	-0.287987	-2.508997	2.814097
6	1.233361	-4.799545	2.361143
1	0.509825	-4.712148	0.343954
6	0.449981	-3.072993	3.855927
1	-0.862562	-1.606254	2.990258
6	1.214686	-4.219625	3.631177
1	1.833129	-5.686152	2.174817
1	0.437391	-2.606827	4.837120
1	1.798671	-4.653272	4.438060

B2

Number of imaginary frequencies : 0

Electronic energy : HF=-4896.4584935
Zero-point correction= 1.131930 (Hartree/Particle)
Thermal correction to Energy= 1.205252
Thermal correction to Enthalpy= 1.206196
Thermal correction to Gibbs Free Energy= 1.021790
Sum of electronic and zero-point Energies= -4895.326564
Sum of electronic and thermal Energies= -4895.253242
Sum of electronic and thermal Enthalpies= -4895.252298
Sum of electronic and thermal Free Energies= -4895.436703
Standard State and RRHO Corrected G= -4895.417018

Cartesian Coordinates

45	1.466193	0.118455	0.269571
15	3.138976	1.788672	-0.196011
6	-3.438266	-1.480910	1.256979
6	-4.627230	-0.863750	1.789172
6	-2.283980	-1.419503	2.026231
6	-5.804489	-0.676643	1.010968
6	-4.631847	-0.378405	3.138302
6	-2.284295	-0.939354	3.355286
6	-6.919026	-0.060984	1.538705
1	-5.812169	-1.004288	-0.021115
6	-5.805418	0.228325	3.660756
6	-3.443054	-0.462985	3.911882
1	-1.350343	-0.958968	3.906333
6	-6.928866	0.387277	2.880874
1	-7.795971	0.087247	0.914912
1	-5.788713	0.587563	4.686608
1	-3.452356	-0.100781	4.936138
1	-7.815014	0.867727	3.285350
8	-1.075827	-1.905851	1.566451
6	-3.436519	-2.156236	-0.070761
6	-4.364359	-3.211635	-0.393169
6	-2.497954	-1.816473	-1.031606
6	-5.263314	-3.765451	0.562113
6	-4.367288	-3.769617	-1.716746
6	-2.483769	-2.372297	-2.328464
6	-6.141126	-4.770795	0.218788
1	-5.248431	-3.395617	1.580024
6	-5.298148	-4.793554	-2.042901
6	-3.421567	-3.311504	-2.673542
1	-1.733726	-2.022557	-3.027654
6	-6.173802	-5.282685	-1.100346
1	-6.811624	-5.177652	0.970540
1	-5.294615	-5.191999	-3.054316
1	-3.437425	-3.731337	-3.675340
1	-6.877340	-6.068547	-1.359680
8	-1.503301	-0.889320	-0.742274
15	-0.247996	-1.355248	0.225178
8	0.188262	-2.803935	-0.365456
15	3.028695	-1.743414	0.328953
6	4.768844	-1.457041	0.909297
6	5.813652	-1.229579	-0.000052
6	5.058139	-1.416331	2.283523
6	7.108017	-0.968151	0.452583
1	5.627060	-1.259970	-1.066360
6	6.351123	-1.150155	2.734025
1	4.276311	-1.591058	3.013859
6	7.382238	-0.923714	1.820034
1	7.898127	-0.792847	-0.271777
1	6.549351	-1.118993	3.801657
1	8.389474	-0.717031	2.170705
6	2.461161	-2.965154	1.604334
6	2.647246	-4.349565	1.487592
6	1.841149	-2.459973	2.758804
6	2.220125	-5.208213	2.502648
1	3.108927	-4.769576	0.601394
6	1.422966	-3.318643	3.776840
1	1.669657	-1.390889	2.852253
6	1.609276	-4.696691	3.650281
1	2.362267	-6.279761	2.392363
1	0.942561	-2.909652	4.661206
1	1.276260	-5.367631	4.437096
6	3.266621	-2.725584	-1.217004
6	4.302845	-3.663637	-1.360987
6	2.391298	-2.519483	-2.294255
6	4.454586	-4.379124	-2.550364
1	5.004701	-3.829489	-0.550221
6	2.541929	-3.234777	-3.482395

1	1.592511	-1.793597	-2.202440
6	3.574633	-4.166638	-3.613970
1	5.262649	-5.099065	-2.644542
1	1.855851	-3.058055	-4.306146
1	3.695823	-4.720180	-4.540921
6	2.652663	3.422686	-0.932340
6	2.261102	4.487528	-0.105961
6	2.633797	3.604276	-2.323701
6	1.861160	5.702402	-0.661638
1	2.235383	4.356359	0.968209
6	2.222734	4.818850	-2.876977
1	2.941523	2.804282	-2.988059
6	1.835831	5.872696	-2.047807
1	1.560383	6.515320	-0.006397
1	2.211865	4.938788	-3.956846
1	1.518443	6.818838	-2.477440
6	4.086999	2.289433	1.296940
6	4.982078	3.373330	1.304669
6	3.866868	1.581994	2.486486
6	5.665520	3.715104	2.471532
1	5.129897	3.965165	0.406998
6	4.545802	1.929166	3.655635
1	3.152891	0.764354	2.491935
6	5.450798	2.991538	3.648554
1	6.356959	4.552970	2.464197
1	4.364856	1.369971	4.569219
1	5.979772	3.263281	4.557820
6	4.363497	1.229843	-1.459359
6	5.712179	1.611614	-1.470915
6	3.879412	0.414179	-2.492501
6	6.559292	1.170453	-2.488467
1	6.117772	2.225467	-0.675790
6	4.727407	-0.031405	-3.508005
1	2.836100	0.118124	-2.490246
6	6.072564	0.343894	-3.505350
1	7.605521	1.462923	-2.478324
1	4.338551	-0.682658	-4.285221
1	6.738663	-0.007027	-4.288491
6	-2.539409	1.974639	-1.279770
6	-3.273881	1.247443	-2.277539
6	-1.183728	2.195159	-1.494121
6	-4.614437	0.812881	-2.076075
6	-2.629194	0.884223	-3.507777
6	-0.543297	1.821420	-2.698697
6	-5.290835	0.104354	-3.045174
1	-5.101127	1.030246	-1.133695
6	-3.364463	0.177758	-4.498857
6	-1.257407	1.203021	-3.695648
1	0.508818	2.056445	-2.808605
6	-4.668789	-0.204020	-4.279018
1	-6.308779	-0.225969	-2.857417
1	-2.864489	-0.075439	-5.430826
1	-0.775349	0.930645	-4.631375
1	-5.215261	-0.755583	-5.038781
8	-0.425180	2.812408	-0.526831
6	-3.146204	2.446465	-0.006182
6	-4.296482	3.310805	0.029895
6	-2.548922	2.099467	1.201480
6	-4.904359	3.836067	-1.146416
6	-4.851389	3.697464	1.296611
6	-3.067594	2.525215	2.445882
6	-6.020294	4.641874	-1.077876
1	-4.474680	3.601534	-2.112925
6	-6.012300	4.517004	1.332440
6	-4.210240	3.282472	2.493941
1	-2.552412	2.210435	3.345091
6	-6.594490	4.975644	0.172313
1	-6.460204	5.029160	-1.992849
1	-6.426003	4.784361	2.301765
1	-4.628410	3.587671	3.449211
1	-7.479820	5.604004	0.212340
8	-1.443262	1.278562	1.226328
15	0.085632	1.869926	0.795407
8	0.562857	2.843318	1.841618
6	-0.368216	-4.091509	-0.028167
1	-1.384357	-4.194714	-0.413817
1	0.282553	-4.824930	-0.507031
1	-0.361386	-4.242755	1.052135

B3

Number of imaginary frequencies : 0
Electronic energy : HF=-4896.4581932
Zero-point correction= 1.131640 (Hartree/Particle)
Thermal correction to Energy= 1.205263
Thermal correction to Enthalpy= 1.206207
Thermal correction to Gibbs Free Energy= 1.019957
Sum of electronic and zero-point Energies= -4895.326553
Sum of electronic and thermal Energies= -4895.252930
Sum of electronic and thermal Enthalpies= -4895.251986
Sum of electronic and thermal Free Energies= -4895.438236
Standard State and RRHO Corrected G= -4895.417513

Cartesian Coordinates

45	0.081966	0.919739	0.612603
15	-0.617629	-0.240115	2.567857
6	-3.994041	-1.116955	-1.364662
6	-4.168728	-2.515010	-1.659549
6	-2.830234	-0.505844	-1.806507
6	-5.240248	-3.285640	-1.127243
6	-3.197324	-3.188580	-2.475351
6	-1.861745	-1.167141	-2.591472
6	-5.366489	-4.627074	-1.415338
1	-5.955913	-2.813099	-0.466018
6	-3.364547	-4.570782	-2.764159
6	-2.055279	-2.481238	-2.937748
1	-0.979743	-0.619613	-2.901174
6	-4.427826	-5.278616	-2.251256
1	-6.189342	-5.192630	-0.987456
1	-2.622807	-5.061366	-3.389295
1	-1.320353	-3.000269	-3.547057
1	-4.542033	-6.335679	-2.473268
8	-2.603109	0.830817	-1.509618
6	-4.972184	-0.339197	-0.553353
6	-6.367293	-0.245506	-0.897847
6	-4.543193	0.348697	0.573380
6	-6.888987	-0.754221	-2.120487
6	-7.273678	0.418116	-0.003512
6	-5.430368	0.992277	1.465308
6	-8.229349	-0.647495	-2.422674
1	-6.215726	-1.223427	-2.828185
6	-8.652956	0.496215	-0.338226
6	-6.775033	1.006039	1.191115
1	-5.015612	1.466278	2.349082
6	-9.126405	-0.028599	-1.519624
1	-8.599922	-1.037973	-3.366221
1	-9.326580	0.991512	0.356366
1	-7.470259	1.489599	1.871647
1	-10.181626	0.041564	-1.767164
8	-3.198068	0.396127	0.907648
15	-2.074093	1.233020	0.018376
8	-2.545414	2.777028	0.046413
15	0.788138	2.155574	-1.309584
6	-0.434643	3.216987	-2.230986
6	-1.191192	2.692893	-3.290924
6	-0.636862	4.556789	-1.864121
6	-2.111580	3.489343	-3.973959
1	-1.064058	1.661066	-3.594443
6	-1.555643	5.353832	-2.549152
1	-0.072020	4.992231	-1.047618
6	-2.295021	4.824370	-3.609070
1	-2.681731	3.062616	-4.794529
1	-1.687977	6.391128	-2.254033
1	-3.007499	5.445707	-4.144451
6	2.066631	3.432052	-0.915326
6	3.091724	3.800434	-1.796147
6	1.956431	4.090808	0.318437
6	3.984800	4.816345	-1.451443
1	3.217148	3.286608	-2.741816
6	2.846646	5.111193	0.658561
1	1.184083	3.791182	1.020505
6	3.863487	5.477175	-0.225835
1	4.782085	5.084531	-2.139100
1	2.751330	5.608259	1.619787
1	4.561643	6.265673	0.040713
6	1.444705	1.095166	-2.667704
6	1.717951	1.606227	-3.949039
6	1.615162	-0.277952	-2.435918
6	2.168550	0.764949	-4.966842

1	1.557412	2.657831	-4.162769
6	2.047542	-1.121971	-3.461610
1	1.403755	-0.684160	-1.452581
6	2.331189	-0.601604	-4.725247
1	2.380760	1.176573	-5.949564
1	2.168152	-2.182375	-3.270392
1	2.675244	-1.259718	-5.518252
6	0.570067	-0.990080	3.772126
6	1.396109	-0.131891	4.515173
6	0.655606	-2.372500	3.986278
6	2.299122	-0.650001	5.440928
1	1.357050	0.938143	4.348732
6	1.566943	-2.889251	4.911392
1	0.013867	-3.054271	3.439325
6	2.392016	-2.030836	5.638648
1	2.937464	0.026264	6.002702
1	1.625066	-3.963619	5.063122
1	3.101005	-2.432998	6.357076
6	-1.601586	0.810776	3.730470
6	-1.989998	0.328361	4.992826
6	-1.934393	2.127652	3.381936
6	-2.742091	1.124886	5.856609
1	-1.693511	-0.666219	5.310496
6	-2.680570	2.927970	4.250483
1	-1.599542	2.537172	2.435586
6	-3.096738	2.424636	5.484382
1	-3.042014	0.732930	6.824393
1	-2.928284	3.945713	3.961921
1	-3.678664	3.045535	6.159745
6	-1.658246	-1.701358	2.124950
6	-2.726679	-2.173468	2.898462
6	-1.288750	-2.410726	0.971716
6	-3.391368	-3.348085	2.539400
1	-3.055546	-1.627916	3.775066
6	-1.933438	-3.600119	0.631898
1	-0.497512	-2.025382	0.337019
6	-2.986042	-4.074126	1.417295
1	-4.225311	-3.696818	3.142360
1	-1.631997	-4.139729	-0.259537
1	-3.501192	-4.988959	1.141400
6	4.101493	-1.715255	-0.194791
6	4.148575	-2.682800	-1.256980
6	3.039081	-1.774776	0.704965
6	5.070110	-2.584996	-2.338321
6	3.189609	-3.751530	-1.288943
6	2.116549	-2.848341	0.687220
6	5.061227	-3.497393	-3.370925
1	5.773777	-1.761270	-2.358034
6	3.220250	-4.688221	-2.358092
6	2.197872	-3.823908	-0.274736
1	1.358104	-2.874270	1.457492
6	4.135308	-4.568624	-3.380499
1	5.766623	-3.388633	-4.190034
1	2.491643	-5.495289	-2.359985
1	1.487808	-4.646910	-0.284323
1	4.142564	-5.284239	-4.197761
8	2.877389	-0.821791	1.676411
6	5.100499	-0.620835	-0.065796
6	6.512713	-0.857968	0.062623
6	4.645512	0.689575	-0.009127
6	7.071940	-2.164915	0.145787
6	7.407752	0.262642	0.147939
6	5.522968	1.793647	0.094976
6	8.431976	-2.354051	0.263866
1	6.411761	-3.024048	0.124301
6	8.806337	0.031642	0.257216
6	6.878391	1.582286	0.149940
1	5.094144	2.788611	0.122813
6	9.313779	-1.247339	0.308073
1	8.830670	-3.362676	0.329837
1	9.469778	0.891435	0.310874
1	7.563481	2.423299	0.219444
1	10.384229	-1.410466	0.395657
8	3.296891	0.939023	-0.094285
15	2.320620	0.750476	1.283090
8	2.804425	1.623956	2.407157
6	-3.738581	3.322423	-0.567257
1	-4.586707	3.213348	0.112251
1	-3.531140	4.378195	-0.740726
1	-3.950719	2.829669	-1.516455

B4			
Number of imaginary frequencies : 0			
Electronic energy : HF=-5236.5237304			
Zero-point correction= 1.163501 (Hartree/Particle)			
Thermal correction to Energy= 1.241036			
Thermal correction to Enthalpy= 1.241980			
Thermal correction to Gibbs Free Energy= 1.047860			
Sum of electronic and zero-point Energies= -5235.360230			
Sum of electronic and thermal Energies= -5235.282694			
Sum of electronic and thermal Enthalpies= -5235.281750			
Sum of electronic and thermal Free Energies= -5235.475870			
Standard State and RRHO Corrected G= -5235.454477			
Cartesian Coordinates			
45	-0.773512	1.289285	-0.165274
15	-1.543349	3.519639	-0.351920
6	2.890464	-0.205767	2.220112
6	2.917060	-1.589373	2.604765
6	1.706930	0.493019	2.405281
6	3.999754	-2.453418	2.277431
6	1.791464	-2.146345	3.299152
6	0.583421	-0.052882	3.061028
6	3.993264	-3.777397	2.659329
1	4.831026	-2.062255	1.702046
6	1.831605	-3.508436	3.705816
6	0.642844	-1.342519	3.529690
1	-0.310492	0.553601	3.160149
6	2.909605	-4.308395	3.400032
1	4.823925	-4.420937	2.383983
1	0.978949	-3.912279	4.246093
1	-0.208909	-1.777134	4.045066
1	2.922403	-5.350859	3.704852
8	1.608315	1.798959	1.930517
6	4.058557	0.487087	1.612018
6	5.341240	0.551213	2.264455
6	3.913463	1.159169	0.408141
6	5.571522	0.016768	3.563692
6	6.435538	1.208492	1.606647
6	4.978131	1.832773	-0.228543
6	6.815338	0.084270	4.153595
1	4.751366	-0.444437	4.100286
6	7.709036	1.248199	2.236856
6	6.222182	1.835343	0.349407
1	4.785876	2.314176	-1.179476
6	7.902168	0.692602	3.481453
1	6.960830	-0.329399	5.147555
1	8.527891	1.738972	1.716787
1	7.054921	2.328714	-0.143572
1	8.878925	0.731900	3.954953
8	2.694706	1.152548	-0.261151
15	1.361368	1.975041	0.278608
8	1.718320	3.550042	0.176566
6	-3.294197	3.733469	-0.894793
6	-4.312313	3.614711	0.065512
6	-3.641249	3.960962	-2.235080
6	-5.649773	3.725141	-0.310311
1	-4.060145	3.410038	1.100881
6	-4.984179	4.064497	-2.607471
1	-2.873080	4.063751	-2.993501
6	-5.990827	3.947028	-1.647247
1	-6.426375	3.624749	0.442530
1	-5.238890	4.241710	-3.648679
1	-7.034476	4.026784	-1.938198
6	-1.427518	4.658285	1.080427
6	-2.005527	5.938614	1.039132
6	-0.764325	4.241438	2.242467
6	-1.891244	6.797599	2.132323
1	-2.548207	6.262858	0.156086
6	-0.653946	5.103041	3.335733
1	-0.350498	3.243276	2.303780
6	-1.211283	6.382168	3.281069
1	-2.337546	7.787027	2.089105
1	-0.139992	4.767987	4.232303
1	-1.126686	7.050320	4.133579
6	-0.566545	4.281185	-1.717911
6	-0.036341	5.576045	-1.668123
6	-0.309577	3.479335	-2.843395

6	0.734932	6.061005	-2.726925
1	-0.203963	6.205128	-0.801183
6	0.452333	3.969845	-3.904268
1	-0.700917	2.465574	-2.881881
6	0.980419	5.262343	-3.846034
1	1.146659	7.065025	-2.673366
1	0.638886	3.340771	-4.770148
1	1.581265	5.643306	-4.667017
6	-4.560910	-1.612257	-0.315323
6	-4.678052	-2.544213	-1.401951
6	-4.357373	-0.272948	-0.622097
6	-4.716322	-3.953786	-1.203922
6	-4.688588	-2.055363	-2.752934
6	-4.373184	0.212349	-1.950263
6	-4.791110	-4.824565	-2.269380
1	-4.666382	-4.345684	-0.194878
6	-4.785843	-2.980188	-3.828748
6	-4.556657	-0.660935	-2.994075
1	-4.247239	1.277812	-2.107931
6	-4.837836	-4.336937	-3.597768
1	-4.807429	-5.895763	-2.088437
1	-4.801491	-2.592320	-4.844374
1	-4.579256	-0.298350	-4.018533
1	-4.902460	-5.033276	-4.429015
8	-4.148151	0.632072	0.390866
6	-4.576395	-2.026743	1.114495
6	-5.679502	-2.743272	1.697967
6	-3.516528	-1.667033	1.942353
6	-6.875009	-3.031663	0.978991
6	-5.606530	-3.162722	3.069730
6	-3.453772	-2.069332	3.297795
6	-7.911324	-3.727166	1.563342
1	-6.971817	-2.687965	-0.044090
6	-6.688157	-3.889348	3.638363
6	-4.465218	-2.819313	3.843618
1	-2.588379	-1.767638	3.878329
6	-7.816727	-4.174395	2.903232
1	-8.813025	-3.928480	0.991499
1	-6.609150	-4.206724	4.675300
1	-4.416068	-3.139135	4.881156
1	-8.638616	-4.726490	3.350118
8	-2.449978	-0.951078	1.453529
15	-2.596532	0.697888	1.076772
8	-2.763290	1.512848	2.335222
6	2.594861	4.291417	1.056172
1	3.614111	3.900420	1.019519
1	2.580921	5.318772	0.688130
1	2.219262	4.261430	2.080755
6	2.764743	-1.462607	-2.086179
6	4.136411	-1.058192	-2.242285
6	1.785789	-0.605624	-2.570109
6	5.207998	-1.731025	-1.590059
6	4.450380	0.088015	-3.046054
6	2.087549	0.541885	-3.334326
6	6.513587	-1.326680	-1.763840
1	4.985489	-2.561414	-0.930077
6	5.810798	0.454734	-3.235799
6	3.395356	0.861962	-3.598612
1	1.266653	1.147573	-3.699901
6	6.824656	-0.237956	-2.613922
1	7.311290	-1.845567	-1.240120
1	6.032273	1.314359	-3.863405
1	3.636397	1.733372	-4.201438
1	7.859566	0.060637	-2.753778
8	0.442139	-0.878417	-2.368668
6	2.392993	-2.743381	-1.421962
6	2.912411	-4.014205	-1.862774
6	1.484224	-2.753842	-0.376001
6	3.729531	-4.153393	-3.020250
6	2.570265	-5.205952	-1.137201
6	1.128386	-3.922539	0.329185
6	4.215389	-5.383377	-3.408192
1	3.964944	-3.277281	-3.612031
6	3.101327	-6.456587	-1.555382
6	1.684506	-5.123853	-0.029042
1	0.434586	-3.832272	1.156229
6	3.913450	-6.547956	-2.662924
1	4.832623	-5.459444	-4.298936
1	2.841178	-7.344856	-0.985313
1	1.437939	-6.028536	0.519423

1	4.310059	-7.509622	-2.975434
8	0.893408	-1.570233	0.049354
15	-0.254576	-0.796052	-0.847079
8	-1.449410	-1.828980	-1.129172
6	-1.351408	-3.071279	-1.870571
1	-1.475654	-3.897089	-1.168090
1	-2.164088	-3.075824	-2.596544
1	-0.396625	-3.161790	-2.388595

B5

Number of imaginary frequencies : 0
Electronic energy : HF=-5236.5292498
Zero-point correction= 1.163513 (Hartree/Particle)
Thermal correction to Energy= 1.241081
Thermal correction to Enthalpy= 1.242026
Thermal correction to Gibbs Free Energy= 1.047874
Sum of electronic and zero-point Energies= -5235.365737
Sum of electronic and thermal Energies= -5235.288168
Sum of electronic and thermal Enthalpies= -5235.287224
Sum of electronic and thermal Free Energies= -5235.481376
Standard State and RRHO Corrected G= -5235.460081

Cartesian Coordinates

45	0.797800	0.118962	0.741190
15	1.951377	2.210791	0.775822
6	4.599660	-1.543840	-1.279691
6	4.889906	-1.127169	-2.625375
6	3.304564	-1.944947	-0.992859
6	6.153975	-0.603223	-3.014701
6	3.852531	-1.191863	-3.617506
6	2.277649	-2.003468	-1.958240
6	6.393054	-0.206768	-4.312541
1	6.935403	-0.499771	-2.272085
6	4.133094	-0.773763	-4.947268
6	2.554666	-1.643888	-3.254136
1	1.291531	-2.322309	-1.641962
6	5.377477	-0.297378	-5.294040
1	7.367248	0.191741	-4.581423
1	3.338139	-0.834092	-5.686292
1	1.777239	-1.680547	-4.012399
1	5.579314	0.018488	-6.313503
8	2.984730	-2.301271	0.314344
6	5.591583	-1.489143	-0.168477
6	6.849697	-2.184093	-0.206242
6	5.278353	-0.782839	0.986792
6	7.207165	-3.063223	-1.267672
6	7.775504	-2.028562	0.880938
6	6.180953	-0.631215	2.061466
6	8.421493	-3.714054	-1.275067
1	6.505357	-3.227680	-2.076878
6	9.025928	-2.703835	0.834286
6	7.416887	-1.226462	1.997747
1	5.868979	-0.039837	2.915978
6	9.348860	-3.525195	-0.221965
1	8.667308	-4.383525	-2.094516
1	9.719515	-2.566182	1.659912
1	8.125461	-1.110638	2.813231
1	10.305002	-4.039987	-0.244199
8	4.048021	-0.150648	1.114556
15	2.647926	-1.025339	1.320159
8	2.822201	-1.741405	2.753717
6	0.910611	3.718055	0.538931
6	-0.283228	3.784234	1.272127
6	1.250758	4.773555	-0.314256
6	-1.125586	4.888541	1.153506
1	-0.565757	2.960864	1.920002
6	0.398012	5.874452	-0.441531
1	2.169118	4.738829	-0.890874
6	-0.790235	5.935624	0.288930
1	-2.047815	4.924792	1.726930
1	0.666891	6.685553	-1.112767
1	-1.450854	6.791944	0.186717
6	2.663562	2.605616	2.433974
6	3.314046	3.832572	2.652989
6	2.491769	1.727969	3.513445
6	3.817285	4.151583	3.913680
1	3.425734	4.540698	1.837167
6	2.988455	2.052520	4.778647

1	1.959915	0.792852	3.374791
6	3.659462	3.259550	4.979124
1	4.326642	5.098979	4.065861
1	2.846641	1.359883	5.603430
1	4.048998	3.510771	5.961622
6	3.314822	2.399038	-0.444765
6	4.648715	2.641561	-0.090795
6	2.987487	2.231894	-1.801777
6	5.631037	2.747231	-1.077869
1	4.933002	2.732437	0.950843
6	3.969616	2.349159	-2.784541
1	1.965689	2.004871	-2.084324
6	5.293536	2.614170	-2.425490
1	6.662372	2.929131	-0.788604
1	3.705700	2.209839	-3.828493
1	6.059201	2.692061	-3.190813
6	-3.355205	-0.560692	2.296721
6	-4.257605	0.551659	2.181049
6	-2.087802	-0.326413	2.820013
6	-5.491655	0.463112	1.476385
6	-3.893676	1.821172	2.741961
6	-1.726321	0.927721	3.367100
6	-6.334259	1.548858	1.372616
1	-5.758359	-0.471317	0.997253
6	-4.797174	2.914403	2.639971
6	-2.621703	1.969648	3.357629
1	-0.733195	1.033844	3.792093
6	-5.995782	2.784821	1.974198
1	-7.262619	1.457444	0.815716
1	-4.513625	3.863870	3.088033
1	-2.352691	2.929283	3.791214
1	-6.672575	3.630523	1.892374
8	-1.145955	-1.332233	2.852803
6	-3.708863	-1.930776	1.838450
6	-4.859027	-2.641269	2.331989
6	-2.867977	-2.585003	0.947914
6	-5.721507	-2.114777	3.335540
6	-5.148950	-3.952322	1.822244
6	-3.126568	-3.894528	0.484934
6	-6.828377	-2.813575	3.766900
1	-5.497854	-1.148482	3.771470
6	-6.305856	-4.640641	2.278660
6	-4.257961	-4.554085	0.893596
1	-2.425503	-4.336906	-0.211985
6	-7.136986	-4.084188	3.224600
1	-7.467258	-2.386683	4.535162
1	-6.515589	-5.625812	1.869266
1	-4.478518	-5.550770	0.521597
1	-8.017136	-4.621048	3.567066
8	-1.758777	-1.935642	0.447576
15	-0.371348	-1.767032	1.392434
8	0.258005	-3.105846	1.656922
6	3.242292	-3.114746	2.947866
1	4.200503	-3.305362	2.459178
1	3.346641	-3.242714	4.026758
1	2.467591	-3.778599	2.560431
6	-3.463707	-0.614864	-2.159041
6	-4.461270	-1.655050	-2.196243
6	-2.135265	-0.999351	-2.281941
6	-5.816863	-1.423055	-1.829199
6	-4.085309	-2.986436	-2.570337
6	-1.759298	-2.312359	-2.644983
6	-6.746219	-2.440601	-1.854380
1	-6.112594	-0.434451	-1.499110
6	-5.073903	-4.005378	-2.618686
6	-2.717999	-3.274893	-2.828532
1	-0.704102	-2.527232	-2.771573
6	-6.379428	-3.743065	-2.268916
1	-7.768901	-2.241428	-1.547005
1	-4.770104	-5.007311	-2.911314
1	-2.436071	-4.282268	-3.122042
1	-7.123539	-4.533958	-2.291568
8	-1.096959	-0.095679	-2.143677
6	-3.849210	0.815347	-1.999756
6	-4.801107	1.449840	-2.879246
6	-3.278543	1.597974	-1.011473
6	-5.330759	0.807153	-4.033669
6	-5.215024	2.799752	-2.615636
6	-3.671259	2.927860	-0.751773
6	-6.243463	1.440932	-4.849166

1	-5.001755	-0.194734	-4.280682
6	-6.171216	3.417965	-3.466634
6	-4.643789	3.508822	-1.524408
1	-3.192597	3.453479	0.064475
6	-6.683084	2.754218	-4.558497
1	-6.625549	0.927579	-5.727034
1	-6.481188	4.435400	-3.241830
1	-4.970431	4.525429	-1.324491
1	-7.410057	3.238045	-5.204415
8	-2.279232	1.079153	-0.196088
15	-0.762391	0.804751	-0.777019
8	-0.289297	2.141434	-1.552915
6	-0.840987	2.739657	-2.744456
1	-1.567108	3.503997	-2.461964
1	-0.003304	3.203422	-3.270207
1	-1.311587	1.992396	-3.385470

B6

Number of imaginary frequencies : 0
Electronic energy : HF=-5576.591529
Zero-point correction= 1.195945 (Hartree/Particle)
Thermal correction to Energy= 1.277195
Thermal correction to Enthalpy= 1.278139
Thermal correction to Gibbs Free Energy= 1.076610
Sum of electronic and zero-point Energies= -5575.395584
Sum of electronic and thermal Energies= -5575.314334
Sum of electronic and thermal Enthalpies= -5575.313390
Sum of electronic and thermal Free Energies= -5575.514919
Standard State and RRHO Corrected G= -5575.49304

Cartesian Coordinates

45	-0.001024	-0.166477	-0.146884
6	4.244818	-2.040697	-1.188019
6	5.034210	-1.418413	-2.214527
6	2.934140	-2.367442	-1.496185
6	6.332591	-0.888824	-1.969141
6	4.483628	-1.279307	-3.533352
6	2.365141	-2.199533	-2.775150
6	7.067257	-0.310001	-2.980568
1	6.739093	-0.932218	-0.965729
6	5.279517	-0.698462	-4.559197
6	3.144959	-1.688112	-3.784926
1	1.324005	-2.478110	-2.907920
6	6.547059	-0.231337	-4.295249
1	8.050890	0.097533	-2.765466
1	4.856800	-0.615697	-5.557305
1	2.737621	-1.567298	-4.785129
1	7.141325	0.217875	-5.085718
8	2.118342	-2.889267	-0.491036
6	4.756526	-2.307093	0.184412
6	5.938811	-3.095029	0.424606
6	4.060773	-1.839038	1.290220
6	6.649216	-3.751661	-0.619620
6	6.414504	-3.265332	1.768146
6	4.514393	-2.019658	2.614605
6	7.785390	-4.486673	-0.357808
1	6.284119	-3.678819	-1.636876
6	7.598098	-4.016455	2.002453
6	5.682255	-2.700530	2.846476
1	3.931126	-1.589182	3.419838
6	8.277582	-4.610863	0.963260
1	8.304881	-4.980292	-1.174260
1	7.950227	-4.120232	3.025625
1	6.053044	-2.823976	3.859541
1	9.179257	-5.185639	1.154131
8	2.886564	-1.105693	1.140573
15	1.489639	-1.751920	0.532276
8	0.898705	-2.714855	1.678944
6	-4.148748	-2.043466	1.145269
6	-4.924392	-1.368058	2.148919
6	-2.817052	-2.323674	1.428003
6	-6.236651	-0.874944	1.900010
6	-4.351302	-1.127021	3.442708
6	-2.241039	-2.061721	2.692383
6	-6.956307	-0.228833	2.881538
1	-6.666307	-0.998886	0.913931
6	-5.131166	-0.482332	4.441970
6	-3.002640	-1.500395	3.688176

1	-1.197741	-2.318528	2.836051
6	-6.408494	-0.044741	4.174115
1	-7.950734	0.148109	2.658987
1	-4.686393	-0.322222	5.421240
1	-2.574033	-1.312452	4.669402
1	-6.989248	0.457996	4.942241
8	-2.014496	-2.902301	0.466177
6	-4.693729	-2.402400	-0.192094
6	-5.867103	-3.219606	-0.356981
6	-4.021382	-1.986759	-1.335849
6	-6.554795	-3.812405	0.740345
6	-6.362651	-3.486467	-1.678088
6	-4.487712	-2.284565	-2.636494
6	-7.689098	-4.571511	0.549055
1	-6.172921	-3.667860	1.743885
6	-7.543466	-4.261038	-1.840083
6	-5.648568	-2.995998	-2.803869
1	-3.917813	-1.912386	-3.479555
6	-8.202245	-4.788274	-0.752307
1	-8.190749	-5.012836	1.405909
1	-7.910532	-4.437908	-2.848145
1	-6.026831	-3.205833	-3.800536
1	-9.102217	-5.381180	-0.888912
8	-2.883433	-1.213904	-1.235095
15	-1.416819	-1.901830	-0.757392
8	-0.876203	-2.813037	-1.825404
6	1.463431	-3.994474	2.062845
1	2.441204	-3.861859	2.531979
1	0.762796	-4.422332	2.781160
1	1.549838	-4.648915	1.193611
6	-4.730653	1.727880	-1.144332
6	-5.866021	1.160997	-1.823975
6	-3.521257	1.753775	-1.823707
6	-7.101867	0.904737	-1.165537
6	-5.752256	0.796825	-3.206414
6	-3.398654	1.383220	-3.179794
6	-8.164431	0.341668	-1.838293
1	-7.196531	1.136559	-0.112019
6	-6.876009	0.243899	-3.878101
6	-4.502712	0.944347	-3.866474
1	-2.422971	1.455744	-3.648594
6	-8.059529	0.018671	-3.212467
1	-9.089473	0.138122	-1.306422
1	-6.772198	-0.021807	-4.927043
1	-4.423122	0.666899	-4.913852
1	-8.906506	-0.420517	-3.731465
8	-2.369674	2.219715	-1.203337
6	-4.821747	2.252348	0.246609
6	-5.768442	3.269698	0.625854
6	-3.949696	1.794385	1.221171
6	-6.609593	3.927701	-0.315622
6	-5.852334	3.677081	2.000562
6	-4.014090	2.201016	2.570001
6	-7.508465	4.893089	0.083137
1	-6.533738	3.669910	-1.365028
6	-6.802201	4.664329	2.380614
6	-4.968538	3.107574	2.956489
1	-3.314039	1.765851	3.272987
6	-7.620033	5.258052	1.446224
1	-8.134691	5.382070	-0.657745
1	-6.860818	4.949105	3.428081
1	-5.046025	3.413799	3.995803
1	-8.339234	6.014133	1.747564
8	-2.951977	0.878257	0.891846
15	-1.640031	1.400583	0.046875
8	-1.073433	2.674328	0.875528
6	-1.518989	4.044334	0.745987
1	-2.550150	4.159237	1.086190
1	-0.855143	4.629386	1.384539
1	-1.431009	4.379520	-0.289098
6	4.468030	1.889733	1.124619
6	5.466468	1.338509	2.000909
6	3.185243	2.044913	1.630167
6	6.751111	0.938079	1.537536
6	5.157193	1.140918	3.388025
6	2.861550	1.814779	2.984216
6	7.688546	0.418071	2.402752
1	6.983014	1.028022	0.482929
6	6.159733	0.636279	4.260407
6	3.841502	1.405439	3.854965

1	1.838897	1.981643	3.306099
6	7.402130	0.285839	3.783138
1	8.654969	0.101524	2.021198
1	5.914847	0.508909	5.311838
1	3.612534	1.248632	4.905432
1	8.155954	-0.112569	4.455968
8	2.161034	2.501036	0.809509
6	4.769280	2.278725	-0.281155
6	5.820606	3.206683	-0.613897
6	3.996045	1.788286	-1.321469
6	6.583975	3.892641	0.372553
6	6.097778	3.492093	-1.993875
6	4.250096	2.078089	-2.678398
6	7.588482	4.766884	0.017461
1	6.364118	3.731436	1.420817
6	7.151485	4.386652	-2.325830
6	5.299913	2.897116	-3.008161
1	3.616927	1.622285	-3.430110
6	7.889352	5.008326	-1.344195
1	8.151765	5.279621	0.792024
1	7.354662	4.578268	-3.376374
1	5.523429	3.109975	-4.049472
1	8.690044	5.692641	-1.609286
8	2.924082	0.940120	-1.057789
15	1.536851	1.512823	-0.373800
8	0.976259	2.656083	-1.371329
6	1.453819	4.021397	-1.453638
1	2.478168	4.056888	-1.830514
1	0.787275	4.523728	-2.156290
1	1.400161	4.505293	-0.476848

(3...4)_{A1}

Number of imaginary frequencies : 0

Electronic energy : HF=-3521.2930037

Zero-point correction= 0.765475 (Hartree/Particle)

Thermal correction to Energy= 0.816849

Thermal correction to Enthalpy= 0.817794

Thermal correction to Gibbs Free Energy= 0.676620

Sum of electronic and zero-point Energies= -3520.527529

Sum of electronic and thermal Energies= -3520.476154

Sum of electronic and thermal Enthalpies= -3520.475210

Sum of electronic and thermal Free Energies= -3520.616384

Standard State and RRHO Corrected G= -3520.600518

Cartesian Coordinates

6	2.241755	-3.678626	3.861409
6	1.349445	-2.601710	3.871356
6	0.448960	-2.433398	2.823476
6	0.434804	-3.348541	1.758674
6	1.318190	-4.440708	1.759878
6	2.222745	-4.597717	2.807792
6	-0.487440	-3.119871	0.628829
8	-0.433678	-4.022817	-0.327459
6	-1.633023	-4.265056	-1.179728
6	-2.232108	-3.110182	-1.943474
6	-3.402178	-2.459939	-1.425711
45	-1.725691	-1.174653	-1.240521
8	-1.235567	-2.118890	0.604577
15	0.532715	-0.875040	-1.741766
8	1.067813	-1.890321	-2.886028
6	2.376856	-1.879023	-3.505357
15	-2.561804	0.679740	0.127555
6	-3.494271	2.102117	-0.582231
6	-4.608766	2.678613	0.050992
6	-5.231790	3.801629	-0.496753
6	-4.750225	4.365585	-1.680988
6	-3.646250	3.796590	-2.319598
6	-3.025866	2.669831	-1.777071
17	-2.312668	-0.255472	-3.382769
8	1.278312	0.506812	-2.333454
6	1.490940	1.566037	-1.465542
6	2.525408	1.506943	-0.542130
6	2.661390	2.602077	0.382116
6	1.799248	3.743499	0.254722
6	0.805590	3.762838	-0.759203
6	0.645834	2.688007	-1.596968
6	1.931192	4.825640	1.166322
6	2.855482	4.786548	2.185200

6	3.678990	3.645894	2.340439
6	3.584425	2.585003	1.465887
6	3.413923	0.310478	-0.499771
6	4.847620	0.411767	-0.598222
6	5.653837	-0.765127	-0.434816
6	5.023628	-2.020084	-0.214632
6	3.655136	-2.120625	-0.212776
6	2.866803	-0.960293	-0.385183
6	7.069045	-0.660011	-0.516894
6	7.675972	0.547488	-0.779033
6	6.883150	1.702597	-0.980199
6	5.509431	1.637531	-0.891114
8	1.491620	-1.144982	-0.390210
6	-3.782376	-0.089167	1.284997
6	-5.018518	-0.520618	0.770959
6	-5.933685	-1.186559	1.584742
6	-5.621829	-1.451528	2.922660
6	-4.393639	-1.036445	3.438738
6	-3.480652	-0.354781	2.627871
6	-1.409223	1.502256	1.319799
6	-1.728857	2.700185	1.980162
6	-0.885103	3.208543	2.968600
6	0.280010	2.522195	3.323558
6	0.609689	1.337597	2.665283
6	-0.223148	0.838700	1.660851
1	4.388742	3.602519	3.161841
1	4.213642	1.715503	1.612493
1	1.271942	5.681758	1.049535
1	2.943438	5.617264	2.879395
1	0.155479	4.628531	-0.847941
1	-0.115122	2.670187	-2.367172
1	4.919139	2.530838	-1.057373
1	3.148057	-3.069498	-0.075406
1	7.361940	2.649685	-1.212417
1	7.663283	-1.559874	-0.379435
1	5.640005	-2.903447	-0.072468
1	8.758003	0.615029	-0.845029
1	3.067975	-2.487747	-2.917167
1	2.251032	-2.318336	-4.497118
1	2.765440	-0.863808	-3.599523
1	-5.264581	-0.331567	-0.269905
1	-2.535348	-0.029954	3.049411
1	-6.888187	-1.503217	1.173219
1	-4.143169	-1.234661	4.477472
1	-6.332351	-1.975988	3.555461
1	-2.637226	3.237966	1.728710
1	0.050880	-0.072136	1.147703
1	-1.140311	4.140661	3.465359
1	1.522204	0.805442	2.915848
1	0.935235	2.920291	4.092287
1	-4.990984	2.255965	0.974273
1	-2.192779	2.211362	-2.293044
1	-6.091702	4.236904	0.004981
1	-3.271669	4.221601	-3.246780
1	-5.236600	5.239374	-2.105806
1	-2.088857	-3.161246	-3.019856
1	-2.360602	-4.704095	-0.489910
1	-1.266545	-5.040254	-1.852154
1	-0.242073	-1.599996	2.819423
1	1.298730	-5.149961	0.940372
1	1.358677	-1.891619	4.692775
1	2.912062	-5.436576	2.803593
1	2.949603	-3.803560	4.675794
1	-3.801991	-2.777761	-0.463433
1	-4.138949	-2.049145	-2.111228
(3-4) _{AI} [‡]			
Number of imaginary frequencies : 1			
Electronic energy : HF=-3521.2792082			
Zero-point correction= 0.763744 (Hartree/Particle)			
Thermal correction to Energy= 0.814727			
Thermal correction to Enthalpy= 0.815671			
Thermal correction to Gibbs Free Energy= 0.677449			
Sum of electronic and zero-point Energies= -3520.515464			
Sum of electronic and thermal Energies= -3520.464481			
Sum of electronic and thermal Enthalpies= -3520.463537			
Sum of electronic and thermal Free Energies= -3520.601759			
Standard State and RRHO Corrected G= -3520.58738			

Cartesian Coordinates			
6	1.253277	-4.166336	4.001147
6	0.324728	-3.121150	3.980193
6	-0.318037	-2.780964	2.791018
6	-0.037267	-3.490521	1.614025
6	0.883144	-4.548633	1.641588
6	1.529918	-4.880457	2.831165
6	-0.683459	-3.100984	0.324163
8	-0.454577	-3.810882	-0.702422
6	-1.979753	-3.935694	-1.921334
6	-2.541168	-2.742772	-2.437224
6	-3.558934	-2.000922	-1.723231
45	-1.775162	-0.943074	-1.391077
8	-1.423018	-2.059941	0.342097
15	0.553566	-0.747990	-1.796171
8	1.028576	-1.734152	-2.985814
6	2.360805	-1.821746	-3.548175
15	-2.500178	0.717437	0.149326
6	-3.326697	2.249372	-0.446762
6	-4.499363	2.763423	0.129723
6	-5.026692	3.980013	-0.310051
6	-4.387028	4.701046	-1.320516
6	-3.216288	4.198873	-1.894337
6	-2.693154	2.980018	-1.463776
17	-2.227130	0.307395	-3.406086
8	1.396502	0.607376	-2.303004
6	1.683707	1.607474	-1.386635
6	2.677930	1.418368	-0.437209
6	2.874264	2.455481	0.541379
6	2.125649	3.676155	0.436159
6	1.185441	3.833388	-0.616726
6	0.959080	2.812324	-1.504961
6	2.317699	4.700283	1.402636
6	3.194302	4.531233	2.450333
6	3.906724	3.315005	2.579135
6	3.750810	2.306490	1.652958
6	3.472336	0.157045	-0.430539
6	4.911916	0.153088	-0.488527
6	5.620778	-1.089813	-0.367371
6	4.891294	-2.302043	-0.228164
6	3.519536	-2.297280	-0.264134
6	2.829216	-1.071380	-0.394652
6	7.041619	-1.090913	-0.410070
6	7.746049	0.077398	-0.594221
6	7.049799	1.299252	-0.753610
6	5.673170	1.336870	-0.700874
8	1.443835	-1.144822	-0.441756
6	-3.746034	-0.058628	1.267516
6	-4.995014	-0.424580	0.735529
6	-5.942602	-1.070413	1.528333
6	-5.651207	-1.377523	2.861440
6	-4.412722	-1.021423	3.396399
6	-3.467027	-0.359844	2.607597
6	-1.259549	1.378494	1.348894
6	-1.430396	2.625164	1.973642
6	-0.543410	3.042245	2.967064
6	0.516476	2.219764	3.357079
6	0.698643	0.985512	2.732334
6	-0.178413	0.569806	1.728863
1	4.578127	3.171307	3.421006
1	4.292906	1.377236	1.779912
1	1.745288	5.618768	1.302549
1	3.329640	5.319030	3.185707
1	0.629295	4.763121	-0.695954
1	0.241953	2.901409	-2.312209
1	5.158183	2.280680	-0.834999
1	2.937426	-3.209449	-0.189863
1	7.605614	2.216795	-0.924791
1	7.561415	-2.039835	-0.305357
1	5.435169	-3.236059	-0.117801
1	8.831513	0.063782	-0.630636
1	2.940883	-2.565226	-2.996416
1	2.236979	-2.143540	-4.584150
1	2.870457	-0.857274	-3.521311
1	-5.228556	-0.197154	-0.299849
1	-2.515225	-0.079320	3.044610
1	-6.906439	-1.337202	1.103818
1	-4.178450	-1.251638	4.432075
1	-6.386585	-1.887907	3.476984

1	-2.256345	3.270232	1.693155
1	-0.027988	-0.388229	1.253877
1	-0.681864	4.011804	3.437268
1	1.528408	0.344164	3.014323
1	1.207523	2.549433	4.126572
1	-5.000212	2.227566	0.928165
1	-1.798517	2.583705	-1.922860
1	-5.934865	4.365456	0.144966
1	-2.713122	4.750405	-2.683682
1	-4.798521	5.647868	-1.659024
1	-2.335355	-2.520706	-3.480252
1	-2.505331	-4.460661	-1.130065
1	-1.393888	-4.562299	-2.583850
1	-1.037980	-1.972382	2.763420
1	1.086739	-5.095949	0.727691
1	0.103626	-2.569297	4.889307
1	2.248240	-5.695046	2.846883
1	1.758816	-4.425353	4.927274
1	-3.961223	-2.443496	-0.812868
1	-4.280189	-1.431836	-2.305129

4_{A1}

Number of imaginary frequencies : 0
 Electronic energy : HF=-3521.3102852
 Zero-point correction= 0.764894 (Hartree/Particle)
 Thermal correction to Energy= 0.816568
 Thermal correction to Enthalpy= 0.817512
 Thermal correction to Gibbs Free Energy= 0.677105
 Sum of electronic and zero-point Energies= -3520.545391
 Sum of electronic and thermal Energies= -3520.493717
 Sum of electronic and thermal Enthalpies= -3520.492773
 Sum of electronic and thermal Free Energies= -3520.633181
 Standard State and RRHO Corrected G= -3520.618466

Cartesian Coordinates

6	-3.221810	-5.195494	2.915938
6	-3.808113	-3.967158	2.597143
6	-3.306079	-3.203707	1.542873
6	-2.211498	-3.665758	0.797870
6	-1.630164	-4.900312	1.118073
6	-2.131766	-5.661375	2.173553
6	-1.628948	-2.857276	-0.335842
8	-0.715463	-3.308547	-1.032803
6	-2.014242	-1.632457	-3.446849
6	-3.004228	-0.638140	-3.498672
6	-3.814969	-0.317060	-2.392200
45	-1.649455	-0.165105	-1.764952
8	-2.187980	-1.684082	-0.462181
15	0.614052	-0.691442	-1.770116
8	0.990676	-1.719289	-2.946478
6	2.324759	-2.123105	-3.337828
15	-2.039274	1.161682	0.248368
6	-2.369922	2.958230	0.030296
6	-3.575935	3.566891	0.409962
6	-3.767277	4.937009	0.213550
6	-2.756971	5.717513	-0.350519
6	-1.548690	5.121017	-0.720111
6	-1.360373	3.751829	-0.539666
17	-1.151049	1.772378	-3.136369
8	1.783302	0.441035	-2.117963
6	2.285690	1.299963	-1.154409
6	3.112267	0.825353	-0.144244
6	3.545477	1.764215	0.858708
6	3.216348	3.153983	0.714751
6	2.450802	3.580730	-0.402623
6	1.978661	2.668239	-1.312664
6	3.637188	4.080037	1.708062
6	4.339734	3.661504	2.815415
6	4.641051	2.287870	2.976193
6	4.254225	1.366884	2.027270
6	3.490541	-0.615415	-0.097222
6	4.859621	-1.060480	-0.030581
6	5.139252	-2.461099	0.123242
6	4.065936	-3.393353	0.165956
6	2.770095	-2.970050	0.007846
6	2.508335	-1.591723	-0.148068
6	6.489647	-2.897993	0.204320
6	7.531517	-2.003572	0.106284

6	7.260467	-0.628290	-0.088557
6	5.962571	-0.169464	-0.153875
8	1.177040	-1.237644	-0.327730
6	-3.488663	0.559619	1.233348
6	-4.748184	0.462311	0.618273
6	-5.858930	0.005780	1.327280
6	-5.733350	-0.360620	2.670007
6	-4.493559	-0.244466	3.298410
6	-3.380662	0.214830	2.589197
6	-0.680194	1.087032	1.490856
6	-0.129089	2.222205	2.103229
6	0.842138	2.084010	3.097001
6	1.266880	0.816047	3.495873
6	0.720737	-0.319535	2.892770
6	-0.243525	-0.185852	1.895701
1	5.173228	1.953956	3.862432
1	4.473406	0.317932	2.183339
1	3.382094	5.128678	1.578083
1	4.653338	4.377185	3.569824
1	2.220045	4.636639	-0.513113
1	1.362933	2.953190	-2.158272
1	5.775487	0.885773	-0.313028
1	1.926402	-3.651648	-0.013822
1	8.083560	0.072865	-0.193291
1	6.682517	-3.960005	0.332938
1	4.288637	-4.448767	0.295645
1	8.559231	-2.350192	0.163806
1	2.613709	-3.013039	-2.774803
1	2.269642	-2.359500	-4.402312
1	3.050169	-1.324399	-3.175551
1	-4.872059	0.766518	-0.411748
1	-2.431578	0.292057	3.104192
1	-6.821563	-0.062068	0.828615
1	-4.383024	-0.514543	4.344698
1	-6.595847	-0.724475	3.221030
1	-0.452365	3.215778	1.815854
1	-0.669306	-1.069817	1.439939
1	1.274155	2.970848	3.550044
1	1.048190	-1.311459	3.190720
1	2.026561	0.714565	4.264647
1	-4.368574	2.986297	0.866748
1	-0.422583	3.298258	-0.826400
1	-4.707250	5.392594	0.512118
1	-0.752810	5.718464	-1.156012
1	-2.908164	6.783177	-0.498017
1	-2.937539	0.093050	-4.299540
1	-2.127520	-2.531605	-2.853941
1	-1.290567	-1.689253	-4.252968
1	-3.751543	-2.248863	1.293678
1	-0.787021	-5.247100	0.529758
1	-4.654463	-3.599482	3.170619
1	-1.674190	-6.615995	2.418557
1	-3.612066	-5.788171	3.738949
1	-4.139988	-1.082654	-1.695724
1	-4.433059	0.573023	-2.465037

(3...4)_{A1-LiHMDS,1THF}

Number of imaginary frequencies : 0
 Electronic energy : HF=-4634.7843357
 Zero-point correction= 1.116537 (Hartree/Particle)
 Thermal correction to Energy= 1.192570
 Thermal correction to Enthalpy= 1.193514
 Thermal correction to Gibbs Free Energy= 1.001705
 Sum of electronic and zero-point Energies= -4633.667799
 Sum of electronic and thermal Energies= -4633.591766
 Sum of electronic and thermal Enthalpies= -4633.590821
 Sum of electronic and thermal Free Energies= -4633.782631
 Standard State and RRHO Corrected G= -4633.762014

Cartesian Coordinates

3	3.539826	-1.867256	-0.121594
6	0.934074	-3.131231	-0.203295
6	-0.374422	-3.238995	-0.930859
45	-1.718444	-1.585563	-0.746312
17	-2.984430	-2.410294	-2.619043
6	-1.531006	-3.601488	-0.158308
8	-0.488241	-1.003277	0.897594
6	0.748656	-0.920941	0.814812

8	1.490328	-1.753744	0.082146
6	1.493434	0.102330	1.573441
6	0.976810	0.532547	2.805980
6	1.664438	1.491081	3.545147
6	2.850923	2.042399	3.049016
6	3.351760	1.633458	1.811197
6	2.681780	0.656932	1.078061
15	-0.956040	0.271258	-1.990284
8	0.555208	0.642212	-1.376292
6	1.278733	1.779005	-1.705974
6	0.849539	3.030050	-1.295618
6	1.643011	4.169506	-1.686135
6	2.899940	3.960579	-2.349206
6	3.313262	2.639005	-2.666855
6	2.503258	1.570174	-2.377265
6	3.701134	5.080226	-2.703064
6	3.276001	6.364233	-2.448579
6	2.016821	6.577051	-1.838835
6	1.223911	5.512396	-1.468306
6	-0.414265	3.180702	-0.522797
6	-1.599862	2.643818	-1.011686
6	-2.858440	2.973985	-0.461864
6	-2.930462	3.757743	0.661989
6	-1.746738	4.200040	1.309239
6	-0.471539	3.903469	0.721494
6	-1.800670	4.906017	2.541686
6	-0.647310	5.287943	3.189858
6	0.612602	4.972861	2.626389
6	0.698442	4.305087	1.424141
8	-1.591254	1.818207	-2.125380
15	-3.760868	-0.928162	0.399979
6	-3.529121	-0.200743	2.079223
6	-4.334190	-0.534838	3.181483
6	-4.147992	0.098124	4.412334
6	-3.162882	1.078244	4.556833
6	-2.361225	1.420415	3.465723
6	-2.537096	0.780555	2.237203
8	-0.762957	0.178362	-3.601780
6	-0.337132	-1.034216	-4.254011
6	-4.918516	0.271887	-0.394840
6	-5.796767	1.063927	0.362380
6	-6.631292	1.990745	-0.264285
6	-6.609828	2.128964	-1.655167
6	-5.751129	1.332854	-2.416445
6	-4.905581	0.413690	-1.791014
6	-4.827953	-2.401740	0.692077
6	-6.032903	-2.599406	0.003898
6	-6.766924	-3.775225	0.186047
6	-6.311889	-4.761702	1.061775
6	-5.112644	-4.570782	1.756068
6	-4.372420	-3.405008	1.566141
1	1.521698	5.251080	3.151754
1	1.670570	4.051469	1.019711
1	-2.775413	5.122512	2.970982
1	-0.699751	5.819105	4.135848
1	-3.896339	4.008676	1.090466
1	-3.746760	2.597208	-0.948625
1	0.258898	5.700975	-1.014293
1	2.790608	0.557474	-2.629186
1	1.667549	7.591110	-1.666158
1	4.654719	4.899139	-3.192426
1	4.270586	2.484732	-3.156605
1	3.893786	7.212953	-2.727313
1	-1.028797	-1.229470	-5.075755
1	0.669280	-0.872528	-4.650409
1	-0.343674	-1.888733	-3.576140
1	-6.403165	-1.839983	-0.676798
1	-3.441247	-3.266915	2.107012
1	-7.697884	-3.914422	-0.356619
1	-4.751528	-5.331527	2.442664
1	-6.885589	-5.673094	1.204599
1	-5.113375	-1.282852	3.081614
1	-1.900581	1.045609	1.402352
1	-4.778744	-0.171248	5.255033
1	-1.595764	2.183286	3.564795
1	-3.021528	1.573025	5.513788
1	-5.820467	0.973707	1.443408
1	-4.230404	-0.189445	-2.386319
1	-7.296475	2.606328	0.334988
1	-5.725812	1.434845	-3.497776

1	-7.256776	2.854143	-2.140831
1	-0.300338	-3.571384	-1.962541
1	0.882923	-3.589563	0.785342
1	1.752589	-3.578481	-0.764929
1	0.051427	0.107262	3.175015
1	3.057125	0.375607	0.103423
1	1.271422	1.814629	4.503784
1	4.262303	2.069797	1.413923
1	3.379953	2.796231	3.624208
1	-1.415742	-3.731518	0.917226
1	-2.319091	-4.202527	-0.602463
7	4.991751	-1.868076	1.054191
14	4.770525	-2.553033	2.594753
14	6.333885	-0.997574	0.473325
6	7.146177	0.165073	1.747983
1	7.603407	-0.393993	2.573882
1	7.936376	0.774594	1.289513
1	6.408337	0.848858	2.184763
6	5.840093	0.115840	-0.997465
1	5.332781	-0.459170	-1.781930
1	5.169686	0.927664	-0.690724
1	6.725805	0.581021	-1.449823
6	7.727185	-2.121167	-0.183428
1	8.084102	-2.803541	0.598466
1	7.369308	-2.741232	-1.015908
1	8.591929	-1.548999	-0.545412
6	4.673016	-1.294657	4.022704
1	5.607419	-0.732567	4.135951
1	3.873156	-0.565662	3.847799
1	4.467953	-1.790248	4.981353
6	6.127393	-3.799798	3.087901
1	6.219727	-4.602850	2.345283
1	7.107413	-3.310550	3.160498
1	5.923812	-4.268322	4.060125
6	3.116534	-3.500762	2.667114
1	3.005395	-4.030652	3.621873
1	2.266315	-2.812402	2.580996
1	3.033209	-4.248125	1.867646
6	4.462782	-3.439442	-2.415796
6	2.634920	-2.141592	-2.996082
6	3.493726	-4.426488	-3.066488
1	5.004343	-3.828169	-1.551437
1	5.180872	-3.031771	-3.140177
6	2.393631	-3.511572	-3.666606
1	3.052028	-1.419245	-3.708239
1	1.755630	-1.705628	-2.522265
1	3.984751	-5.049259	-3.818116
1	3.070891	-5.086176	-2.302453
1	2.487133	-3.425985	-4.751958
1	1.394170	-3.895407	-3.448875
8	3.604239	-2.374345	-1.950944

(3-4)_{AI-LHMDS.I.THF}[‡]

Number of imaginary frequencies : 1
 Electronic energy : HF=-4634.7760608
 Zero-point correction= 1.114288 (Hartree/Particle)
 Thermal correction to Energy= 1.190255
 Thermal correction to Enthalpy= 1.191199
 Thermal correction to Gibbs Free Energy= 0.999811
 Sum of electronic and zero-point Energies= -4633.661773
 Sum of electronic and thermal Energies= -4633.585806
 Sum of electronic and thermal Enthalpies= -4633.584862
 Sum of electronic and thermal Free Energies= -4633.776250
 Standard State and RRHO Corrected G= -4633.755916

Cartesian Coordinates

3	3.467939	-1.826023	-0.121736
6	0.811403	-3.373797	-0.271832
6	-0.478069	-3.452601	-0.872253
45	-1.716801	-1.595262	-0.726157
17	-3.018600	-2.426955	-2.579169
6	-1.654019	-3.568326	-0.039104
8	-0.493848	-0.979668	0.875103
6	0.764135	-0.912256	0.810501
8	1.504720	-1.672006	0.074536
6	1.454361	0.098376	1.659725
6	0.943566	0.405753	2.928063
6	1.598185	1.338540	3.731113

6	2.748029	1.983398	3.264534
6	3.245003	1.694256	1.991173
6	2.605007	0.747936	1.193002
15	-0.955233	0.291788	-2.000578
8	0.555668	0.654547	-1.407527
6	1.283468	1.788275	-1.740274
6	0.864101	3.038043	-1.318251
6	1.661441	4.175752	-1.706433
6	2.912108	3.963125	-2.380125
6	3.315316	2.641207	-2.709114
6	2.501799	1.574683	-2.420284
6	3.718430	5.079932	-2.731455
6	3.304224	6.364832	-2.463978
6	2.051027	6.581646	-1.843492
6	1.253278	5.519755	-1.475395
6	-0.391783	3.190873	-0.533547
6	-1.587422	2.665277	-1.009373
6	-2.837352	3.019271	-0.455164
6	-2.891187	3.809200	0.665255
6	-1.697259	4.231035	1.307029
6	-0.430979	3.911668	0.712994
6	-1.732250	4.937587	2.539721
6	-0.568716	5.294841	3.183686
6	0.682320	4.954566	2.615159
6	0.749798	4.288780	1.410748
8	-1.602988	1.829080	-2.118331
15	-3.699912	-0.918693	0.406105
6	-3.453902	-0.167128	2.070429
6	-4.265856	-0.477561	3.175170
6	-4.080519	0.175807	4.395066
6	-3.089383	1.151581	4.526049
6	-2.284150	1.471986	3.431426
6	-2.460603	0.814917	2.212418
8	-0.794414	0.187518	-3.613672
6	-0.376613	-1.036080	-4.253461
6	-4.827644	0.290834	-0.416070
6	-5.714823	1.075371	0.339716
6	-6.549946	2.000199	-0.287926
6	-6.518895	2.146252	-1.677932
6	-5.650605	1.358917	-2.436738
6	-4.805604	0.439387	-1.810707
6	-4.794277	-2.369405	0.700992
6	-5.953344	-2.578964	-0.059367
6	-6.717673	-3.734725	0.121527
6	-6.338435	-4.689930	1.065640
6	-5.184704	-4.487888	1.829550
6	-4.413861	-3.341328	1.643203
1	1.598935	5.211707	3.138046
1	1.714661	4.016575	1.001345
1	-2.700651	5.172580	2.973608
1	-0.606495	5.825218	4.130816
1	-3.850924	4.080162	1.095331
1	-3.734106	2.659019	-0.937924
1	0.293131	5.711896	-1.012728
1	2.781800	0.561580	-2.678308
1	1.710330	7.596736	-1.660074
1	4.667363	4.895926	-3.228676
1	4.268751	2.484669	-3.205594
1	3.926095	7.211349	-2.740286
1	-1.078682	-1.243214	-5.063122
1	0.625267	-0.880905	-4.662942
1	-0.374111	-1.880833	-3.562107
1	-6.263820	-1.844796	-0.795003
1	-3.519105	-3.195628	2.240106
1	-7.612609	-3.883123	-0.476283
1	-4.882276	-5.224336	2.568742
1	-6.936128	-5.585918	1.207171
1	-5.051008	-1.220138	3.086772
1	-1.820228	1.064329	1.376595
1	-4.716258	-0.075529	5.239483
1	-1.512161	2.228840	3.520656
1	-2.946522	1.660433	5.475355
1	-5.746465	0.980499	1.419878
1	-4.130207	-0.161205	-2.406748
1	-7.222540	2.608626	0.310166
1	-5.617537	1.466436	-3.517214
1	-7.166131	2.870524	-2.164419
1	-0.516741	-3.729485	-1.921101
1	0.893566	-3.636992	0.777670
1	1.675976	-3.639925	-0.868274

1	0.045454	-0.090113	3.276112
1	2.980114	0.545265	0.197920
1	1.207726	1.565801	4.718468
1	4.128797	2.201867	1.617530
1	3.252214	2.713693	3.890424
1	-1.495273	-3.643381	1.036192
1	-2.503849	-4.137668	-0.404967
7	4.957998	-1.883825	1.027998
14	4.766702	-2.601178	2.556757
14	6.289649	-1.016270	0.424901
6	7.126134	0.145725	1.685340
1	7.599821	-0.413386	2.501947
1	7.906024	0.758856	1.214049
1	6.393816	0.826349	2.136796
6	5.765121	0.100784	-1.032325
1	5.244588	-0.474397	-1.807995
1	5.096548	0.906918	-0.706917
1	6.638324	0.573383	-1.501131
6	7.671984	-2.136295	-0.262689
1	8.045952	-2.820483	0.509632
1	7.298113	-2.754778	-1.089294
1	8.528509	-1.561965	-0.640642
6	4.722209	-1.373686	4.014681
1	5.673314	-0.839325	4.125260
1	3.940540	-0.619204	3.866581
1	4.518038	-1.883524	4.966064
6	6.119269	-3.876140	2.989810
1	6.186105	-4.660781	2.225075
1	7.106798	-3.401116	3.054603
1	5.929933	-4.367502	3.953704
6	3.105310	-3.534343	2.647766
1	2.995968	-4.062074	3.604018
1	2.262206	-2.837585	2.562568
1	3.012173	-4.281626	1.849158
6	4.386930	-3.468616	-2.443381
6	2.580214	-2.136955	-2.987870
6	3.412014	-4.428148	-3.131564
1	4.921943	-3.891021	-1.590908
1	5.112226	-3.046389	-3.152478
6	2.290577	-3.494052	-3.663537
1	3.022626	-1.428714	-3.699997
1	1.719915	-1.672860	-2.506799
1	3.896732	-5.003174	-3.924263
1	3.008520	-5.134755	-2.399973
1	2.322039	-3.396644	-4.751387
1	1.300909	-3.870501	-3.392976
8	3.539777	-2.411896	-1.947401

4Al-LHMDS.1THF

Number of imaginary frequencies : 0
 Electronic energy : HF=-4634.8144134
 Zero-point correction= 1.114833 (Hartree/Particle)
 Thermal correction to Energy= 1.191694
 Thermal correction to Enthalpy= 1.192638
 Thermal correction to Gibbs Free Energy= 0.998447
 Sum of electronic and zero-point Energies= -4633.699581
 Sum of electronic and thermal Energies= -4633.622720
 Sum of electronic and thermal Enthalpies= -4633.621776
 Sum of electronic and thermal Free Energies= -4633.815967
 Standard State and RRHO Corrected G= -4633.795004

Cartesian Coordinates

3	3.982401	0.849725	-0.399651
6	1.505342	-1.105228	-2.805805
6	1.097756	-2.441880	-2.984462
45	-0.362941	-1.426828	-1.585948
17	-1.825583	-1.675327	-3.494249
6	0.893558	-3.301377	-1.895225
8	0.694920	-1.169198	0.205954
6	1.516749	-0.240664	0.562765
8	2.143840	0.501535	-0.224772
6	1.704190	-0.093468	2.046623
6	1.115023	-0.985771	2.954041
6	1.328861	-0.839241	4.324250
6	2.122359	0.206716	4.803241
6	2.695704	1.112447	3.906037
6	2.487987	0.961963	2.536058
15	-0.924366	0.799547	-1.673642

8	-0.524341	1.614040	-0.317604
6	-0.749988	2.993788	-0.259361
6	-2.043419	3.463428	-0.117313
6	-2.235052	4.889471	-0.143966
6	-1.087118	5.750882	-0.207547
6	0.216086	5.186178	-0.280313
6	0.385879	3.824448	-0.328425
6	-1.274885	7.160078	-0.218693
6	-2.538074	7.706687	-0.195304
6	-3.671647	6.859346	-0.169448
6	-3.525105	5.489402	-0.143798
6	-3.167662	2.495838	0.040375
6	-3.353236	1.475664	-0.885109
6	-4.425677	0.563196	-0.818784
6	-5.313349	0.640666	0.225798
6	-5.130563	1.593388	1.261827
6	-4.042415	2.526480	1.182439
6	-5.981887	1.606895	2.400403
6	-5.761970	2.482910	3.438431
6	-4.671619	3.384030	3.378288
6	-3.837623	3.408339	2.281713
8	-2.469997	1.331628	-1.951789
15	-1.858037	-2.624218	-0.055181
6	-2.123202	-1.867930	1.603316
6	-2.420695	-2.681189	2.711563
6	-2.661256	-2.108924	3.960790
6	-2.608744	-0.721006	4.120305
6	-2.312973	0.090675	3.025222
6	-2.069580	-0.480849	1.775175
8	-0.177441	1.681047	-2.804699
6	-0.538642	1.613235	-4.203411
6	-3.547019	-3.047640	-0.636407
6	-4.690620	-2.677767	0.086871
6	-5.962098	-3.011187	-0.384735
6	-6.106152	-3.722674	-1.577130
6	-4.971493	-4.103409	-2.298653
6	-3.700012	-3.764042	-1.836457
6	-1.124845	-4.256759	0.423675
6	-1.776884	-5.481900	0.231129
6	-1.169764	-6.676009	0.634849
6	0.085337	-6.660151	1.242953
6	0.737267	-5.439959	1.448123
6	0.139517	-4.249645	1.040834
1	-4.485740	4.059398	4.208477
1	-3.000386	4.095406	2.263003
1	-6.803181	0.896006	2.439962
1	-6.412568	2.478058	4.308055
1	-6.140501	-0.059408	0.289557
1	-4.513678	-0.193393	-1.589820
1	-4.403946	4.855402	-0.131976
1	1.361205	3.359020	-0.417266
1	-4.667547	7.293078	-0.174403
1	-0.396263	7.798869	-0.256155
1	1.076245	5.848527	-0.321245
1	-2.669180	8.784752	-0.208276
1	-1.576591	1.926513	-4.341226
1	0.126996	2.307422	-4.717422
1	-0.403166	0.601310	-4.591984
1	-2.759859	-5.519175	-0.223760
1	0.660238	-3.311229	1.187997
1	-1.688533	-7.617421	0.476818
1	1.714273	-5.412707	1.922471
1	0.552352	-7.589020	1.557688
1	-2.466507	-3.759740	2.602212
1	-1.818354	0.160999	0.946498
1	-2.889983	-2.748556	4.808544
1	-2.268155	1.168799	3.137296
1	-2.793727	-0.276215	5.093903
1	-4.596575	-2.123815	1.013076
1	-2.827330	-4.058418	-2.407377
1	-6.838599	-2.716521	0.185538
1	-5.074097	-4.660795	-3.225280
1	-7.096067	-3.982214	-1.941611
1	0.654348	-2.715473	-3.937837
1	2.177309	-0.818773	-2.008384
1	1.466668	-0.436816	-3.658665
1	0.482427	-1.782803	2.588540
1	2.933093	1.662519	1.840344
1	0.868379	-1.538061	5.016407
1	3.306528	1.932841	4.271174

1	2.289026	0.319445	5.870905
1	1.505302	-3.223854	-1.005221
1	0.402952	-4.255766	-2.059065
7	5.460614	0.094894	0.537229
14	5.480248	-1.577226	0.827031
14	6.464043	1.296018	1.194814
6	6.790239	1.130134	3.067629
1	7.384135	0.236336	3.297024
1	7.336473	1.995935	3.465774
1	5.846698	1.045792	3.620961
6	5.675798	3.018199	0.952490
1	5.451013	3.204801	-0.105341
1	4.738193	3.119076	1.515732
1	6.347065	3.816520	1.295278
6	8.178961	1.401896	0.365482
1	8.721430	0.452183	0.456276
1	8.080430	1.616950	-0.706822
1	8.809118	2.187550	0.803795
6	4.983937	-2.084830	2.598787
1	5.699819	-1.710747	3.340746
1	3.999873	-1.680449	2.864266
1	4.936201	-3.177017	2.709815
6	7.173247	-2.402612	0.512339
1	7.528749	-2.205219	-0.507214
1	7.936649	-2.019748	1.202056
1	7.131932	-3.492311	0.644093
6	4.233166	-2.467648	-0.307549
1	4.287742	-3.557605	-0.186303
1	3.209928	-2.164871	-0.064711
1	4.403998	-2.244144	-1.368462
6	5.255088	1.443030	-2.896792
6	3.043440	2.271590	-2.798772
6	4.509391	0.842622	-4.082116
1	5.878433	0.739262	-2.340552
1	5.865416	2.305914	-3.198366
6	3.338434	1.828090	-4.244187
1	2.906946	3.355537	-2.715678
1	2.176963	1.772384	-2.367366
1	5.131683	0.761800	-4.977275
1	4.141579	-0.155824	-3.819438
1	3.648191	2.683782	-4.852900
1	2.464466	1.376368	-4.720271
8	4.202205	1.881345	-2.007868

(3-4)_{Al-LiHMDS.2THF}[‡]

Number of imaginary frequencies : 1
 Electronic energy : HF=-4867.2660442
 Zero-point correction= 1.235096 (Hartree/Particle)
 Thermal correction to Energy= 1.316599
 Thermal correction to Enthalpy= 1.317544
 Thermal correction to Gibbs Free Energy= 1.116274
 Sum of electronic and zero-point Energies= -4866.030948
 Sum of electronic and thermal Energies= -4865.949445
 Sum of electronic and thermal Enthalpies= -4865.948501
 Sum of electronic and thermal Free Energies= -4866.149770
 Standard State and RRHO Corrected G= -4866.129719

Cartesian Coordinates

3	3.743497	-1.106338	-0.159733
6	1.327650	-2.969357	-0.333897
6	0.087049	-3.351527	-0.906882
45	-1.547085	-1.822970	-0.750305
17	-2.635325	-2.964573	-2.583594
6	-1.023381	-3.722914	-0.058949
8	-0.490568	-0.952567	0.849475
6	0.719797	-0.577963	0.789187
8	1.628094	-1.136774	0.072402
6	1.105327	0.600984	1.616217
6	0.433094	0.858223	2.819188
6	0.743652	1.996076	3.560930
6	1.708326	2.894809	3.092639
6	2.377771	2.639176	1.894019
6	2.092502	1.485222	1.164792
15	-1.279079	0.216113	-1.997140
8	0.009306	0.992698	-1.299880
6	0.421226	2.285232	-1.590472
6	-0.367531	3.365916	-1.237452
6	0.104468	4.682458	-1.591676

6	1.417483	4.832499	-2.153323
6	2.210106	3.679022	-2.396381
6	1.712437	2.425960	-2.143769
6	1.900156	6.131074	-2.471397
6	1.115791	7.245611	-2.278808
6	-0.196367	7.098623	-1.769923
6	-0.687479	5.854941	-1.435433
6	-1.671935	3.164917	-0.550869
6	-2.635864	2.323326	-1.092401
6	-3.975461	2.331685	-0.642854
6	-4.334068	3.102441	0.433943
6	-3.355965	3.845804	1.144999
6	-2.004516	3.862124	0.665205
6	-3.681300	4.542087	2.340289
6	-2.710488	5.199984	3.061948
6	-1.367535	5.182198	2.613679
6	-1.025101	4.538976	1.443787
8	-2.338885	1.501578	-2.170422
15	-3.621572	-1.636803	0.402483
6	-3.570543	-0.749893	2.015912
6	-4.277922	-1.187109	3.149759
6	-4.276141	-0.426581	4.320341
6	-3.575647	0.781338	4.372334
6	-2.873642	1.223272	3.250017
6	-2.865915	0.461371	2.080124
8	-0.967085	0.194676	-3.591754
6	-0.522638	-0.980171	-4.300867
6	-5.057573	-0.835163	-0.442395
6	-6.134808	-0.331690	0.306238
6	-7.213327	0.282272	-0.330868
6	-7.237668	0.392618	-1.724302
6	-6.177105	-0.116758	-2.475726
6	-5.089977	-0.721672	-1.839745
6	-4.270543	-3.310376	0.809569
6	-5.325176	-3.881519	0.083572
6	-5.737992	-5.189941	0.349105
6	-5.109201	-5.938925	1.344819
6	-4.058208	-5.375555	2.075405
6	-3.636130	-4.074795	1.804738
1	-0.597151	5.673557	3.201048
1	0.009797	4.517772	1.124587
1	-4.711567	4.523376	2.685913
1	-2.967252	5.718690	3.981142
1	-5.364160	3.112274	0.777831
1	-4.699505	1.730970	-1.174077
1	-1.699106	5.767031	-1.058792
1	2.307253	1.537368	-2.308545
1	-0.826690	7.974747	-1.646143
1	2.902618	6.223266	-2.881495
1	3.215666	3.797893	-2.789359
1	1.493028	8.232950	-2.529048
1	-1.337620	-1.332406	-4.936278
1	0.326783	-0.681574	-4.918998
1	-0.230428	-1.784671	-3.624902
1	-5.826745	-3.310784	-0.690561
1	-2.817016	-3.647671	2.374914
1	-6.555745	-5.619448	-0.222829
1	-3.564475	-5.949642	2.854488
1	-5.434465	-6.954437	1.552270
1	-4.840456	-2.113669	3.121535
1	-2.302351	0.807158	1.223086
1	-4.828132	-0.777062	5.188046
1	-2.321279	2.155833	3.279660
1	-3.576621	1.374571	5.282594
1	-6.130914	-0.401780	1.388683
1	-4.267824	-1.103652	-2.430494
1	-8.033666	0.676167	0.262590
1	-6.183989	-0.032992	-3.558821
1	-8.076667	0.874135	-2.218641
1	0.092776	-3.616771	-1.959886
1	1.501297	-3.207775	0.710281
1	2.209911	-2.993801	-0.960597
1	-0.328933	0.169198	3.160830
1	2.618439	1.280953	0.244461
1	0.224711	2.188244	4.495203
1	3.129815	3.331118	1.528351
1	1.938520	3.790210	3.662986
1	-0.837218	-3.750981	1.014060
1	-1.725090	-4.474559	-0.409446
7	4.904068	-0.183377	1.083053

6	6.111677	-3.002565	-0.466800
6	4.360911	-4.525675	-0.145033
6	6.704132	-4.292513	0.132609
1	6.340868	-2.107135	0.110964
1	6.435142	-2.858607	-1.503402
6	5.487795	-4.977614	0.775263
1	4.344922	-5.110827	-1.076992
1	3.372354	-4.575150	0.314931
1	7.121737	-4.926032	-0.656708
1	7.500767	-4.080335	0.850381
1	5.580424	-6.065907	0.826604
1	5.314388	-4.591759	1.785155
8	4.661827	-3.146323	-0.436644
14	4.829602	-0.869467	2.635922
14	5.938849	1.056252	0.559784
6	6.466191	2.310292	1.900958
1	7.064652	1.841675	2.692247
1	7.073502	3.116571	1.467684
1	5.594488	2.772625	2.379141
6	5.161899	2.121254	-0.818415
1	4.737093	1.503562	-1.615771
1	4.355013	2.752905	-0.430666
1	5.909834	2.787794	-1.268621
6	7.586083	0.416747	-0.174774
1	8.120472	-0.216631	0.545151
1	7.426188	-0.183549	-1.079400
1	8.256781	1.242922	-0.447576
6	4.423101	0.324342	4.067352
1	5.190105	1.095254	4.201754
1	3.469220	0.834554	3.895634
1	4.339162	-0.224013	5.015918
6	6.440719	-1.749647	3.172150
1	6.723940	-2.540207	2.467329
1	7.278997	-1.041913	3.217794
1	6.349789	-2.210003	4.165390
6	3.457352	-2.192267	2.747055
1	3.523572	-2.738147	3.697249
1	2.463740	-1.732246	2.702002
1	3.530109	-2.926057	1.939138
6	4.739159	-0.941497	-2.962544
6	2.459865	-0.996401	-2.967048
6	4.413617	-2.264366	-3.667884
1	5.620419	-0.966868	-2.322208
1	4.850972	-0.118715	-3.682959
6	2.860586	-2.267838	-3.735252
1	2.291209	-0.161767	-3.659792
1	1.594556	-1.094642	-2.316926
1	4.881917	-2.321927	-4.653765
1	4.768032	-3.103105	-3.065184
1	2.485176	-2.239408	-4.761299
1	2.450936	-3.162106	-3.257304
8	3.590959	-0.679373	-2.130798

(3-4)_{Al-LHMDS.2THF}⁺ (3-membered TS)

Number of imaginary frequencies : 1
 Electronic energy : HF=-4867.2531632
 Zero-point correction= 1.232089 (Hartree/Particle)
 Thermal correction to Energy= 1.314611
 Thermal correction to Enthalpy= 1.315556
 Thermal correction to Gibbs Free Energy= 1.109121
 Sum of electronic and zero-point Energies= -4866.021074
 Sum of electronic and thermal Energies= -4865.938552
 Sum of electronic and thermal Enthalpies= -4865.937608
 Sum of electronic and thermal Free Energies= -4866.144042
 Standard State and RRHO Corrected G= -4866.121457

Cartesian Coordinates

6	6.130680	2.251723	1.405176
8	4.840927	1.612427	1.557305
6	4.389638	1.712817	2.927966
6	5.339799	2.702624	3.602361
6	6.645570	2.469122	2.827135
3	4.173000	0.156750	0.411577
8	2.228479	0.245401	0.694627
6	1.273443	-0.476956	0.981173
8	0.910702	-1.516608	0.241008
6	2.147334	-1.933370	-1.209350
6	1.242845	-2.292177	-2.259960

6	0.344097	-3.380223	-2.040864
45	-0.614727	-1.549434	-1.373447
6	0.521159	-0.262893	2.252067
6	0.501701	1.023212	2.812834
6	-0.126228	1.242152	4.036069
6	-0.712392	0.173175	4.723247
6	-0.681539	-1.110516	4.175493
6	-0.080402	-1.326430	2.935734
15	-0.698749	0.786358	-1.546322
8	-0.579839	1.639334	-0.117029
6	-0.733377	3.022033	-0.065679
6	-1.977743	3.598798	-0.276690
6	-2.050825	5.036065	-0.310296
6	-0.880411	5.810492	-0.006201
6	0.341412	5.146539	0.287649
6	0.420926	3.776963	0.239319
6	-0.957206	7.229827	-0.027297
6	-2.129051	7.870812	-0.360240
6	-3.274742	7.110727	-0.697178
6	-3.237579	5.733395	-0.672666
6	-3.170383	2.729289	-0.483458
6	-3.139551	1.741892	-1.459043
6	-4.229169	0.886679	-1.726554
6	-5.376885	1.009554	-0.982976
6	-5.454837	1.947599	0.080583
6	-4.340731	2.813032	0.348332
6	-6.601492	2.005948	0.918981
6	-6.650380	2.861654	1.995692
6	-5.543652	3.697910	2.278796
6	-4.422642	3.676838	1.477597
8	-1.996383	1.580652	-2.227304
15	-2.419053	-2.554803	-0.126353
6	-1.939476	-4.220425	0.535327
6	-2.843179	-5.292250	0.614235
6	-2.450250	-6.514019	1.167362
6	-1.152905	-6.683421	1.654510
6	-0.245096	-5.624053	1.579776
6	-0.633748	-4.406593	1.019764
8	0.442596	1.353517	-2.537805
6	0.449568	2.648707	-3.191182
6	-3.063642	-1.720990	1.391884
6	-3.704075	-2.444779	2.412645
6	-4.257128	-1.781416	3.508057
6	-4.176496	-0.388894	3.599949
6	-3.532155	0.334781	2.596689
6	-2.978739	-0.327492	1.499325
6	-3.952735	-2.935771	-1.067348
6	-5.197923	-2.387915	-0.731334
6	-6.330599	-2.690229	-1.492664
6	-6.232250	-3.547747	-2.589403
6	-4.993501	-4.101852	-2.927490
6	-3.859920	-3.791806	-2.178088
7	4.879242	0.033164	-1.415743
14	6.021972	-1.172163	-1.771380
6	7.719853	-0.842863	-0.956187
14	4.629673	1.462060	-2.304876
6	6.219246	2.468773	-2.647521
6	3.816666	1.183091	-4.009869
6	3.454099	2.629920	-1.373202
6	5.443468	-2.890602	-1.178407
6	6.415731	-1.417926	-3.625022
8	4.553996	-1.349567	1.722033
6	5.879878	-1.526363	2.274875
6	5.672978	-2.209724	3.624709
6	4.433996	-3.073450	3.346605
6	3.600520	-2.145429	2.464923
1	-5.575122	4.358403	3.140728
1	-3.580023	4.312309	1.721779
1	-7.435765	1.344692	0.699273
1	-7.528106	2.890005	2.634793
1	-6.222998	0.357422	-1.175491
1	-4.117329	0.137259	-2.502364
1	-4.121902	5.168466	-0.943252
1	1.352437	3.250365	0.408496
1	-4.191425	7.618337	-0.983737
1	-0.063774	7.799729	0.214928
1	1.221508	5.738225	0.523744
1	-2.174904	8.955836	-0.378144
1	0.630502	3.444865	-2.467491
1	1.268021	2.611615	-3.909515

1	-0.495777	2.820381	-3.708668
1	-5.290462	-1.725071	0.121127
1	-2.899611	-4.215371	-2.453266
1	-7.289985	-2.258746	-1.220279
1	-4.908401	-4.769864	-3.780029
1	-7.114191	-3.785239	-3.177742
1	-3.857677	-5.179310	0.247534
1	0.086934	-3.601237	0.942803
1	-3.163452	-7.332074	1.218314
1	0.769863	-5.745752	1.948364
1	-0.850266	-7.634012	2.084430
1	-3.779461	-3.525434	2.354043
1	-2.472814	0.243867	0.733813
1	-4.752749	-2.353001	4.288013
1	-3.457091	1.414069	2.663562
1	-4.608251	0.128114	4.452352
1	1.334591	-1.777153	-3.211745
1	-0.201489	-3.805513	-2.877924
1	0.560531	-4.077638	-1.235989
1	2.558898	-2.710876	-0.574923
1	2.762375	-1.040417	-1.301197
1	0.968190	1.839430	2.275453
1	-0.065015	-2.319646	2.509625
1	-0.155955	2.243291	4.456287
1	-1.143444	-1.940580	4.700506
1	-1.197148	0.343469	5.680329
1	2.502306	2.120377	-1.200774
1	3.861663	2.914453	-0.396805
1	3.254159	3.546636	-1.942211
1	6.005302	3.405889	-3.179606
1	6.728033	2.730394	-1.710763
1	6.933649	1.902700	-3.258851
1	2.843840	0.690254	-3.889747
1	3.649975	2.127979	-4.544782
1	4.432672	0.546055	-4.655840
1	5.516391	-1.692917	-4.190044
1	6.829006	-0.511896	-4.085235
1	7.151224	-2.221227	-3.768998
1	8.166964	0.069742	-1.371893
1	7.627891	-0.692939	0.125863
1	8.434513	-1.661425	-1.117888
1	5.056177	-2.847965	-0.155589
1	4.640274	-3.267141	-1.825553
1	6.256203	-3.628461	-1.207753
1	6.353875	-0.543956	2.343380
1	6.464923	-2.154920	1.593231
1	2.960895	-2.676005	1.753719
1	2.975710	-1.476305	3.067662
1	6.547414	-2.787267	3.935612
1	5.453495	-1.467506	4.400796
1	4.717056	-3.975149	2.792171
1	3.898421	-3.375649	4.250372
1	4.445911	0.718027	3.386874
1	3.344802	2.034183	2.925264
1	5.992348	3.204387	0.877948
1	6.764043	1.603684	0.794104
1	4.989290	3.730137	3.453089
1	5.432175	2.522971	4.676815
1	7.347349	3.304754	2.891761
1	7.149061	1.566960	3.193325
17	-1.802029	-1.576381	-3.435684

(3-4)_{Al-LHMDS,2THF}[‡] (OBz as a leaving group)

Number of imaginary frequencies : 1
 Electronic energy : HF=-4867.2532082
 Zero-point correction= 1.231646 (Hartree/Particle)
 Thermal correction to Energy= 1.315148
 Thermal correction to Enthalpy= 1.316092
 Thermal correction to Gibbs Free Energy= 1.104294
 Sum of electronic and zero-point Energies= -4866.021563
 Sum of electronic and thermal Energies= -4865.938060
 Sum of electronic and thermal Enthalpies= -4865.937116
 Sum of electronic and thermal Free Energies= -4866.148914
 Standard State and RRHO Corrected G= -4866.12433

Cartesian Coordinates

6	4.374848	-1.539964	-3.208828
8	3.940027	-1.814882	-1.846694

6	2.904545	-2.817419	-1.858814
6	2.309338	-2.754121	-3.261895
6	3.556684	-2.470241	-4.112272
3	5.015963	-0.692144	-0.500415
8	4.460560	1.780524	-2.735622
6	3.998796	1.927387	-1.598087
6	3.354953	3.239329	-1.221219
6	3.128354	3.583518	0.117959
6	2.478948	4.777255	0.437818
6	2.037434	5.630045	-0.578471
6	2.265836	5.294509	-1.917337
6	2.929716	4.109733	-2.234494
8	4.002095	1.003210	-0.675396
7	6.997924	-0.726561	-0.450290
14	7.764574	0.783842	-0.315050
6	6.854192	1.925548	0.914380
14	7.749497	-2.229778	-0.666570
6	8.788040	-2.366423	-2.267125
6	8.935373	-2.754822	0.741930
6	6.486895	-3.654592	-0.759482
6	9.569181	0.738587	0.325445
6	7.859776	1.734814	-1.963979
8	4.299140	-1.394070	1.299026
6	5.224952	-1.164221	2.387561
6	5.355539	-2.509815	3.094454
6	3.941208	-3.090239	2.940398
6	3.532217	-2.598114	1.548042
6	2.125090	0.370384	-0.249680
6	1.241972	0.692556	-1.298942
45	-0.752539	0.181294	-0.261083
17	-0.266588	-2.132820	0.506617
6	0.351444	1.797738	-1.205152
15	-2.648644	0.635486	-1.221251
8	-2.614151	1.822549	-2.301005
6	-3.645726	2.109193	-3.287417
15	-1.510842	0.928495	1.722503
6	0.067274	1.226811	2.597596
6	0.788205	0.115527	3.073381
6	2.036377	0.295964	3.664132
6	2.582836	1.577775	3.776938
6	1.869952	2.682811	3.306520
6	0.617327	2.513240	2.714226
8	-3.930095	0.889696	-0.222200
6	-5.245380	0.904384	-0.691489
6	-5.834259	-0.275592	-1.112481
6	-7.161822	-0.196290	-1.661206
6	-7.855110	1.061295	-1.642956
6	-7.211633	2.212532	-1.111545
6	-5.917208	2.144066	-0.658068
6	-9.171878	1.137328	-2.173191
6	-9.778348	0.030664	-2.723147
6	-9.084107	-1.201985	-2.772455
6	-7.811781	-1.313719	-2.255322
6	-5.084530	-1.557397	-0.996657
6	-3.819763	-1.681955	-1.552770
6	-3.074687	-2.877674	-1.520763
6	-3.591270	-3.973496	-0.875538
6	-4.838736	-3.894408	-0.201294
6	-5.594204	-2.674264	-0.245596
6	-6.791948	-2.599849	0.519647
6	-7.230648	-3.675870	1.259949
6	-6.500833	-4.888877	1.274627
6	-5.329078	-4.991108	0.559476
8	-3.229101	-0.581649	-2.184362
6	-2.453579	2.504292	1.740043
6	-2.105455	3.523138	0.837589
6	-2.834433	4.711441	0.801859
6	-3.924546	4.891528	1.657717
6	-4.277251	3.879584	2.553230
6	-3.547543	2.690285	2.597541
6	-2.443195	-0.250039	2.763263
6	-3.206910	-1.267095	2.174451
6	-3.950207	-2.135321	2.974923
6	-3.926681	-1.999489	4.364713
6	-3.155791	-0.995843	4.957967
6	-2.412638	-0.123018	4.162788
1	-8.142002	-3.589637	1.844552
1	-7.356501	-1.675474	0.534767
1	-4.747434	-5.908883	0.577585
1	-6.860937	-5.730074	1.859624

1	-3.027150	-4.900661	-0.836198
1	-2.096125	-2.894919	-1.984672
1	-7.291505	-2.262968	-2.307956
1	-5.392296	3.010218	-0.268850
1	-9.557501	-2.067673	-3.226645
1	-9.687841	2.093411	-2.143417
1	-7.752479	3.154263	-1.087197
1	-10.783295	0.101624	-3.128782
1	-4.322110	2.864714	-2.883899
1	-3.125933	2.500076	-4.163516
1	-4.200057	1.208583	-3.554368
1	0.381845	-0.883444	2.960044
1	0.076313	3.380330	2.352395
1	2.586902	-0.564362	4.028467
1	2.289107	3.679583	3.400072
1	3.560787	1.714299	4.228874
1	-1.281088	3.384789	0.149277
1	-3.847508	1.909926	3.287103
1	-2.554056	5.490937	0.099522
1	-5.127144	4.009260	3.216786
1	-4.497662	5.813520	1.624081
1	-3.207050	-1.394916	1.100705
1	-1.814744	0.653502	4.629950
1	-4.536984	-2.921091	2.510391
1	-3.129453	-0.892093	6.038728
1	-4.502770	-2.679351	4.986062
1	1.289900	0.100468	-2.210701
1	0.561841	2.553278	-0.452629
1	-0.136254	2.172624	-2.099509
1	2.091636	0.935505	0.672201
1	2.537182	-0.620647	-0.184163
1	3.454224	2.907728	0.900192
1	3.118493	3.833744	-3.266835
1	2.312144	5.041566	1.477877
1	1.928118	5.956729	-2.709915
1	1.523714	6.554542	-0.328569
1	5.785148	1.969653	0.682558
1	6.956994	1.559592	1.944497
1	7.249802	2.949949	0.889265
1	10.229362	0.165706	-0.338060
1	9.982185	1.754412	0.395503
1	9.636181	0.288706	1.323758
1	6.856785	1.887700	-2.378058
1	8.339342	2.717761	-1.856974
1	8.438018	1.163617	-2.703009
1	8.172004	-2.160616	-3.152507
1	9.609592	-1.638140	-2.270421
1	9.232739	-3.362816	-2.396808
1	9.835350	-2.130253	0.779838
1	8.443370	-2.676027	1.720400
1	9.264166	-3.796516	0.622836
1	5.939628	-3.756290	0.184842
1	5.747180	-3.487273	-1.547939
1	6.987882	-4.611781	-0.956096
1	2.185063	-2.589560	-1.068006
1	3.345266	-3.805253	-1.660657
1	5.452474	-1.723827	-3.272830
1	4.192932	-0.479581	-3.401402
1	1.792278	-3.677105	-3.539079
1	1.596859	-1.923710	-3.331015
1	4.101277	-3.402473	-4.299498
1	3.329483	-2.009263	-5.077386
1	3.787126	-3.332168	0.776812
1	2.465898	-2.363802	1.467795
1	4.809490	-0.396625	3.054106
1	6.154113	-0.804193	1.943194
1	3.274041	-2.681369	3.706958
1	3.909448	-4.180854	3.013713
1	5.672226	-2.406459	4.136222
1	6.085650	-3.137747	2.572126

(3-4)_{Al-LiHMDS,1THF,1DMPU}[‡]

Number of imaginary frequencies : 1
Electronic energy : HF=-5055.4528336
Zero-point correction= 1.302254 (Hartree/Particle)
Thermal correction to Energy= 1.388766
Thermal correction to Enthalpy= 1.389710
Thermal correction to Gibbs Free Energy= 1.176246
Sum of electronic and zero-point Energies= -5054.150579

Sum of electronic and thermal Energies=	-5054.064068	1	-0.146340	-1.061301	-3.952727		
Sum of electronic and thermal Enthalpies=	-5054.063123	1	-5.642898	-3.587710	-1.406763		
Sum of electronic and thermal Free Energies=	-5054.276588	1	-2.688394	-4.160408	1.678989		
Standard State and RRHO Corrected G=	-5054.254147	1	-6.135997	-6.002566	-1.376483		
.....		1	-3.204522	-6.571687	1.723358		
Cartesian Coordinates		1	-4.926629	-7.511734	0.189312		
.....		1	-4.803917	-2.984222	2.626961		
3	3.839598	-1.166906	0.244295	1	-2.587742	0.463321	1.291854
6	1.357397	-2.747091	-0.860594	1	-4.930591	-2.022838	4.888174
6	0.156691	-3.075218	-1.523262	1	-2.755807	1.439262	3.541947
45	-1.558546	-1.698056	-1.075246	1	-3.919472	0.203185	5.363596
17	-2.473178	-2.438010	-3.195620	1	-6.231772	-1.043030	1.221347
6	-0.941619	-3.677351	-0.801713	1	-4.394806	-1.043084	-2.674616
8	-0.608727	-1.098316	0.700420	1	-8.236480	0.020934	0.276586
6	0.579362	-0.637009	0.743666	1	-6.414615	0.011341	-3.623007
8	1.541423	-0.988536	-0.012583	1	-8.346485	0.562861	-2.150779
6	0.848436	0.420513	1.765975	1	0.179583	-3.087963	-2.608447
6	0.118544	0.449379	2.960309	1	1.532415	-3.171041	0.121026
6	0.317724	1.482618	3.874518	1	2.242191	-2.535770	-1.442037
6	1.229806	2.503416	3.589036	1	-0.601627	-0.333159	3.161216
6	1.960566	2.473907	2.398116	1	2.345521	1.395832	0.569010
6	1.787518	1.424246	1.496665	1	-0.247360	1.497503	4.801682
15	-1.408122	0.540072	-1.866664	1	2.669102	3.264356	2.173396
8	-0.249623	1.321100	-0.975104	1	1.370555	3.319001	4.292668
6	0.013667	2.675781	-1.121999	1	-0.765434	-3.929029	0.243169
6	-0.889885	3.602096	-0.634695	1	-1.598038	-4.368306	-1.323337
6	-0.587851	4.999627	-0.813842	7	4.684842	-0.886438	1.985709
6	0.667214	5.373251	-1.402676	6	5.853201	-2.918557	-0.833532
6	1.563677	4.363277	-1.843078	6	4.110778	-4.435490	-0.331441
6	1.238663	3.034603	-1.721929	6	6.275425	-4.292722	-1.336777
6	0.985007	6.749423	-1.563594	1	6.371987	-2.652453	0.095058
6	0.096086	7.730198	-1.186885	1	5.978941	-2.107948	-1.553575
6	-1.160038	7.366378	-0.646016	6	5.428638	-5.210476	-0.443478
6	-1.493743	6.041320	-0.465987	1	3.390146	-4.745674	-1.098355
6	-2.172973	3.148273	-0.034394	1	3.641783	-4.540231	0.650716
6	-3.022493	2.316307	-0.755268	1	5.997983	-4.414675	-2.390377
6	-4.364654	2.106412	-0.369855	1	7.351033	-4.462167	-1.237756
6	-4.830703	2.635147	0.808314	1	5.283400	-6.212802	-0.854903
6	-3.958797	3.341526	1.677707	1	5.896297	-5.308480	0.542274
6	-2.608019	3.586880	1.263709	8	4.435417	-3.040626	-0.559499
6	-4.383322	3.777991	2.961816	14	4.048150	-1.740475	3.312575
6	-3.505884	4.398114	3.823086	14	6.006808	0.180763	2.096366
6	-2.160668	4.606153	3.431351	6	7.307701	-0.245428	3.434259
6	-1.725198	4.220402	2.182059	1	7.733938	-1.244092	3.278391
8	-2.596093	1.717217	-1.936631	1	8.138317	0.473168	3.404667
15	-3.650343	-1.921692	0.044422	1	6.892001	-0.218985	4.449082
6	-3.683751	-1.329379	1.788419	6	5.518067	1.984300	2.501065
6	-4.340634	-2.023111	2.819990	1	4.887956	2.430418	1.724885
6	-4.419711	-1.474758	4.101413	1	4.950867	2.027927	3.439075
6	-3.854187	-0.225020	4.367182	1	6.402399	2.626138	2.616302
6	-3.204364	0.471444	3.347189	6	7.022478	0.249462	0.482259
6	-3.112882	-0.078767	2.067523	1	7.670709	-0.632164	0.397771
8	-0.959608	0.795959	-3.413106	1	6.376912	0.272818	-0.399546
6	0.124643	-0.002852	-3.936914	1	7.672792	1.134268	0.457847
6	-5.163675	-1.125832	-0.661978	6	3.557647	-0.643616	4.796388
6	-6.262501	-0.823020	0.159897	1	4.425136	-0.118193	5.215809
6	-7.399642	-0.216533	-0.374336	1	2.831013	0.117436	4.487721
6	-7.461597	0.087143	-1.737419	1	3.103772	-1.227546	5.608780
6	-6.379097	-0.222494	-2.562686	6	5.214161	-3.084662	4.014866
6	-5.234249	-0.819899	-2.028913	1	5.531571	-3.774610	3.221295
6	-4.132355	-3.696469	0.136503	1	6.121986	-2.658413	4.456141
6	-5.102594	-4.232871	-0.722078	1	4.720063	-3.683076	4.792468
6	-5.382320	-5.601976	-0.704301	6	2.465037	-2.717547	2.887723
6	-4.704175	-6.448567	0.173857	1	2.173229	-3.339409	3.744410
6	-3.736469	-5.921234	1.034702	1	1.618178	-2.064789	2.660900
6	-3.445706	-4.558071	1.010457	1	2.615486	-3.391919	2.037954
1	-1.463123	5.067138	4.124807	8	4.174005	-0.226594	-1.371712
1	-0.689177	4.369165	1.900484	6	4.149469	0.430408	-2.436139
1	-5.411442	3.588983	3.259412	6	3.757833	0.570194	-4.885051
1	-3.836828	4.714989	4.807931	6	4.440448	2.604311	-3.645275
1	-5.862732	2.473827	1.105383	6	4.713363	1.754591	-4.876842
1	-5.004735	1.532435	-1.024261	1	3.990124	-0.109459	-5.709959
1	-2.466228	5.789029	-0.062100	1	3.489353	3.142368	-3.757060
1	1.903366	2.249032	-2.061317	1	5.746103	1.388934	-4.858301
1	-1.872671	8.140061	-0.374608	7	4.396548	1.777445	-2.435507
1	1.945323	7.010528	-2.001042	7	3.888324	-0.179944	-3.635153
1	2.504704	4.660844	-2.295397	6	4.686105	2.459548	-1.180649
1	0.347518	8.778904	-1.316072	1	4.081397	3.367475	-1.103062
1	0.288374	0.346866	-4.957490	1	4.449950	1.805080	-0.347703
1	1.036853	0.145241	-3.351234	1	5.745465	2.737173	-1.122539

6	3.557846	-1.597405	-3.672842
1	3.872652	-2.075337	-2.747072
1	2.479056	-1.753476	-3.809180
1	4.079313	-2.069293	-4.512329
1	4.580494	2.355887	-5.780671
1	5.227485	3.353928	-3.511913
1	2.721433	0.910709	-5.021761

(3-4)_{Al-LiHMSD,1DMPU*}

Number of imaginary frequencies : 1
 Electronic energy : HF=-4822.9719922
 Zero-point correction= 1.183064 (Hartree/Particle)
 Thermal correction to Energy= 1.262901
 Thermal correction to Enthalpy= 1.263845
 Thermal correction to Gibbs Free Energy= 1.065310
 Sum of electronic and zero-point Energies= -4821.788928
 Sum of electronic and thermal Energies= -4821.709091
 Sum of electronic and thermal Enthalpies= -4821.708147
 Sum of electronic and thermal Free Energies= -4821.906682
 Standard State and RRHO Corrected G= -4821.886026

Cartesian Coordinates

6	1.860868	-0.904298	5.560135
6	0.640985	-0.485182	5.017618
6	0.289352	-0.857571	3.721953
6	1.174251	-1.635391	2.957561
6	2.397427	-2.053468	3.499901
6	2.732625	-1.694992	4.804820
6	0.796067	-2.010306	1.571419
8	1.727378	-2.334806	0.746104
6	1.266881	-3.703811	-0.465638
6	0.127555	-3.484781	-1.297252
6	-1.186179	-3.925200	-0.898399
45	-1.210206	-1.832277	-0.630115
8	-0.435131	-1.989109	1.290461
15	-0.259497	0.312930	-0.730386
8	1.380724	0.350666	-0.788183
6	2.172433	1.484157	-1.255487
17	-2.065107	-1.595916	-2.874739
8	-0.540628	1.364304	-1.976930
6	-1.571920	2.290839	-1.966924
6	-1.523055	3.386976	-1.117237
6	-2.632521	4.305147	-1.151321
6	-3.672367	4.118407	-2.123233
6	-3.623472	3.000878	-2.998539
6	-2.604924	2.086936	-2.906721
6	-4.774307	5.015493	-2.150841
6	-4.877393	6.041893	-1.239523
6	-3.874215	6.207010	-0.254643
6	-2.782465	5.366459	-0.213719
6	-0.394905	3.555494	-0.155488
6	0.394292	4.757802	-0.086477
6	1.377506	4.899896	0.950859
6	1.575746	3.842693	1.880055
6	0.885019	2.664190	1.749804
6	-0.061656	2.525683	0.712502
6	2.156460	6.087757	1.016624
6	2.002381	7.088174	0.083614
6	1.059015	6.936099	-0.960878
6	0.274722	5.805884	-1.041982
8	-0.656093	1.272930	0.580713
1	-3.967809	7.001168	0.480722
1	-2.035278	5.503911	0.558264
1	-5.548352	4.858948	-2.897605
1	-5.729460	6.714985	-1.263757
1	-4.424162	2.859780	-3.718872
1	-2.563281	1.195582	-3.522152
1	-0.436047	5.702744	-1.853534
1	1.053356	1.821051	2.410146
1	0.955320	7.716417	-1.709394
1	2.887073	6.183678	1.815663
1	2.307879	3.965232	2.671854
1	2.608015	7.988014	0.138740
1	1.647645	2.022795	-2.042484
1	2.392023	2.149653	-0.422506
1	3.091010	1.062917	-1.652230
1	0.329833	-3.245204	-2.336846
1	1.166517	-4.409727	0.354678

1	2.252875	-3.630956	-0.918157
1	-0.660309	-0.557673	3.293715
1	3.072721	-2.649444	2.898018
1	-0.039669	0.122005	5.606893
1	3.676376	-2.024449	5.229010
1	2.129862	-0.617887	6.572995
1	-1.275365	-4.482475	0.034642
1	-1.884589	-4.235827	-1.669580
15	-3.381945	-1.672842	0.364604
3	3.053353	-1.173219	-0.256235
8	4.045686	0.061080	0.791159
6	4.591803	1.182255	0.932353
6	6.034517	3.027191	0.064581
6	5.172265	3.109379	2.383693
6	5.368872	3.911227	1.106824
1	7.086629	2.842708	0.327968
1	4.608546	3.686555	3.123107
1	5.990022	4.790417	1.300701
7	4.412014	1.894871	2.091086
7	5.332908	1.747675	-0.069196
1	6.026950	3.515735	-0.915733
1	4.396673	4.256292	0.739508
1	6.142453	2.856378	2.837940
6	3.760208	1.248357	3.221113
1	3.066685	0.491969	2.865817
1	4.490067	0.767160	3.886330
1	3.211645	1.999671	3.796698
6	5.674684	0.987476	-1.266399
1	5.178823	0.017422	-1.269583
1	5.376653	1.549116	-2.160052
1	6.759193	0.828538	-1.312934
7	4.010013	-2.239880	-1.600646
14	5.280871	-3.117965	-0.881615
14	3.642396	-2.234209	-3.263221
6	4.989018	-3.314933	0.989962
1	5.834132	-3.820386	1.475603
1	4.867833	-2.332851	1.461245
1	4.085101	-3.901064	1.192865
6	7.008354	-2.312440	-1.023516
1	7.796991	-3.004316	-0.697760
1	7.235473	-2.013957	-2.054387
1	7.082276	-1.415793	-0.397193
6	5.517549	-4.892972	-1.550240
1	4.581874	-5.464908	-1.519896
1	5.869306	-4.896100	-2.589325
1	6.259985	-5.441341	-0.954682
6	2.229222	-1.032081	-3.687781
1	1.883841	-1.204018	-4.715838
1	1.368291	-1.165459	-3.025208
1	2.538477	0.017022	-3.622415
6	3.056398	-3.920341	-3.947378
1	3.848698	-4.676877	-3.914253
1	2.208134	-4.312383	-3.372272
1	2.729248	-3.832374	-4.992226
6	5.107397	-1.721301	-4.377996
1	5.500994	-0.738866	-4.085858
1	5.935994	-2.437677	-4.307727
1	4.817074	-1.659952	-5.435595
6	-4.522168	-3.072403	-0.032702
6	-5.408317	-3.592345	0.925588
6	-4.554348	-3.588321	-1.337974
6	-6.291071	-4.620088	0.588894
1	-5.414779	-3.197548	1.935882
6	-5.443630	-4.611662	-1.672506
1	-3.890411	-3.181046	-2.091894
6	-6.309869	-5.134442	-0.709795
1	-6.966525	-5.015143	1.342697
1	-5.455109	-5.000329	-2.687042
1	-6.996851	-5.934978	-0.969714
6	-3.258525	-1.790439	2.204772
6	-3.665948	-0.783736	3.089548
6	-2.681879	-2.960758	2.731381
6	-3.491484	-0.939276	4.469242
1	-4.130654	0.121876	2.717707
6	-2.518589	-3.118242	4.105162
1	-2.356584	-3.748634	2.059851
6	-2.917044	-2.102616	4.980584
1	-3.814643	-0.148156	5.140227
1	-2.069917	-4.028540	4.492764
1	-2.779883	-2.220534	6.051705

6	-4.441989	-0.197756	0.057353	6	-1.790453	-3.136859	-0.551212
6	-5.723365	-0.306207	-0.504055	6	-2.878307	-3.227264	0.327044
6	-3.965478	1.073096	0.425416	6	-4.053503	-3.866923	-0.071457
6	-6.518131	0.830162	-0.675584	6	-4.157904	-4.418378	-1.349054
1	-6.110301	-1.273377	-0.804262	6	-3.077610	-4.328757	-2.232801
6	-4.779734	2.196812	0.292703	6	-1.903760	-3.687437	-1.839944
1	-2.966228	1.182624	0.830604	1	8.224398	-1.534740	0.165646
6	-6.055969	2.080201	-0.263912	1	6.594449	0.294612	0.029067
1	-7.504775	0.730221	-1.119496	1	5.634889	-3.697925	2.836461
1	-4.410711	3.167264	0.605463	1	7.773845	-3.530337	1.593719
1	-6.676715	2.963041	-0.385340	1	3.434711	-2.770050	3.437612
				1	1.684347	-1.045285	3.088658
(3-4)_{Al}-LiHMDS.2THF[‡] (THF coordination to chloride)				1	6.178259	1.292760	2.832881
				1	3.305691	3.828446	-1.739308
Number of imaginary frequencies : 1				1	8.036819	2.704083	3.568801
Electronic energy : HF=-4867.2598816				1	7.173105	5.545349	0.457448
Zero-point correction= 1.233286 (Hartree/Particle)				1	5.272964	5.198717	-1.034577
Thermal correction to Energy= 1.315549				1	8.573563	4.826484	2.372247
Thermal correction to Enthalpy= 1.316493				1	-0.499981	4.332536	-0.113619
Thermal correction to Gibbs Free Energy= 1.111089				1	0.789689	3.935312	-1.279539
Sum of electronic and zero-point Energies= -4866.026596				1	-0.664766	2.898097	-1.162298
Sum of electronic and thermal Energies= -4865.944333				1	-2.818725	-2.797285	1.319413
Sum of electronic and thermal Enthalpies= -4865.943388				1	-1.069665	-3.623678	-2.531607
Sum of electronic and thermal Free Energies= -4866.148793				1	-4.887049	-3.927267	0.621266
Standard State and RRHO Corrected G= -4866.126771				1	-3.149707	-4.755706	-3.229182
				1	-5.075942	-4.909862	-1.657513
Cartesian Coordinates				1	-0.109981	-5.189798	-0.657589
				1	2.609240	-1.895604	-0.081382
6	0.040745	1.003855	-4.128262	1	1.800084	-6.730617	-0.843606
6	-0.946362	0.660827	-3.188824	1	4.514187	-3.447884	-0.221751
45	-0.107498	-0.186923	-1.257841	1	4.127938	-5.876247	-0.613424
17	-2.134843	0.621624	-0.209164	1	0.320248	-4.221917	2.036257
6	-1.287933	-0.714814	-2.901312	1	-1.072629	-0.155207	1.850882
8	1.613728	-0.818804	-2.258176	1	0.133408	-4.172696	4.489721
6	2.340767	-0.009291	-2.938110	1	-1.282742	-0.111015	4.308793
8	1.944780	1.026410	-3.542423	1	-0.670686	-2.121886	5.648347
6	3.803824	-0.329440	-3.001014	1	-1.576021	1.462630	-2.816917
6	4.259457	-1.637842	-2.799854	1	0.358582	0.264384	-4.855334
6	5.627033	-1.910313	-2.804091	1	0.136714	2.037397	-4.440869
6	6.547123	-0.875105	-2.993395	1	3.540060	-2.429353	-2.634235
6	6.094919	0.432355	-3.196564	1	4.366121	1.715032	-3.362029
6	4.727197	0.704012	-3.212390	1	5.973999	-2.927609	-2.647632
15	1.245336	1.275976	0.090970	1	6.807129	1.240324	-3.337956
8	2.629535	1.542305	-0.771016	1	7.612848	-1.085803	-2.980286
6	3.700852	2.281140	-0.296838	1	-0.823615	-1.478213	-3.524980
6	4.497802	1.761781	0.706129	1	-2.306706	-0.941489	-2.599054
6	5.591570	2.571229	1.179539	3	-4.640054	1.387124	0.251507
6	5.874851	3.818427	0.525237	7	-6.014137	0.034973	0.494730
6	5.046379	4.256407	-0.543642	14	-6.722432	-0.486786	-0.954376
6	3.962971	3.511096	-0.936872	14	-6.263755	-0.401332	2.115138
6	6.967959	4.609981	0.971914	6	-7.619973	-1.708426	2.435383
6	7.742760	4.212031	2.037693	1	-7.725699	-1.898160	3.512400
6	7.441807	3.004141	2.710845	1	-8.599505	-1.381048	2.064358
6	6.397088	2.207146	2.295096	1	-7.389676	-2.666828	1.955831
6	4.180245	0.433074	1.297752	6	-6.765992	1.091073	3.193281
6	2.917730	0.175884	1.821570	1	-6.890823	0.820866	4.250499
6	2.658054	-0.953427	2.629322	1	-6.005483	1.876461	3.131172
6	3.633712	-1.899843	2.818989	1	-7.714730	1.522421	2.847023
6	4.886991	-1.785329	2.162094	6	-4.688380	-1.123812	2.921781
6	5.162597	-0.615587	1.379146	1	-4.705891	-1.060525	4.018288
6	5.858456	-2.820178	2.235733	1	-4.575902	-2.183150	2.659742
6	7.043416	-2.728146	1.540358	1	-3.787624	-0.610697	2.570657
6	7.302576	-1.590772	0.737468	6	-7.389421	-2.276360	-1.005640
6	6.391806	-0.559287	0.664565	1	-6.632303	-3.004451	-0.698515
8	1.870266	1.072035	1.629808	1	-8.263554	-2.408402	-0.357814
15	-0.262549	-2.229998	-0.081964	1	-7.698053	-2.536207	-2.027782
6	1.109963	-3.425815	-0.354764	6	-5.460548	-0.399488	-2.383548
6	0.897141	-4.796999	-0.575331	1	-5.925461	-0.586872	-3.360728
6	1.980451	-5.672851	-0.673390	1	-4.955159	0.572202	-2.427207
6	3.285804	-5.193413	-0.542219	1	-4.687472	-1.163063	-2.229133
6	3.504697	-3.832442	-0.319427	6	-8.247546	0.550089	-1.464792
6	2.425270	-2.951653	-0.233861	1	-9.079554	0.348977	-0.775911
8	0.679229	2.764969	0.448374	1	-8.054119	1.627701	-1.423089
6	0.037301	3.518087	-0.601690	1	-8.599688	0.311872	-2.478021
6	-0.367881	-2.185764	1.763099	6	-5.807466	3.367269	-1.820361
6	-0.032442	-3.319034	2.523408	6	-3.483848	3.573589	-1.398055
6	-0.136959	-3.291697	3.914389	6	-5.265420	4.571823	-2.597913
6	-0.588040	-2.139246	4.565354	1	-6.535474	3.663647	-1.056320
6	-0.930202	-1.012549	3.815940	1	-6.261978	2.611029	-2.464879
6	-0.813346	-1.033530	2.424400	6	-4.008257	4.947400	-1.798688

1	-2.908917	3.115202	-2.212567	6	2.579959	-3.117287	-0.617787
1	-2.879074	3.557350	-0.491908	8	0.502898	2.327383	0.964768
1	-4.988344	4.274054	-3.615152	6	-0.289230	3.139557	0.067243
1	-5.997534	5.380501	-2.665889	6	-0.138449	-2.723197	1.504153
1	-3.279144	5.518645	-2.379809	6	0.316348	-3.916721	2.092183
1	-4.275120	5.529552	-0.909312	6	0.307117	-4.070167	3.478542
6	-3.041624	2.254948	2.768474	6	-0.163462	-3.038964	4.297614
6	-4.366450	3.915568	1.914902	6	-0.628707	-1.856888	3.720149
6	-2.112216	3.474992	2.728313	6	-0.614057	-1.697248	2.332447
1	-2.554412	1.317916	2.507922	6	-1.634321	-3.436249	-0.859629
1	-3.536097	2.149006	3.744771	6	-2.641914	-3.786078	0.050366
6	-3.030306	4.620881	2.216683	6	-3.797435	-4.434395	-0.392171
1	-5.072105	4.029062	2.749846	6	-3.960893	-4.738661	-1.744220
1	-4.855571	4.238668	0.995318	6	-2.960210	-4.394261	-2.657993
1	-1.682251	3.685860	3.711144	6	-1.807712	-3.743255	-2.220586
1	-1.289561	3.292776	2.032156	1	8.487950	-0.923408	-0.002622
1	-3.164009	5.412735	2.958449	1	6.652424	0.691513	0.187463
1	-2.617453	5.078810	1.313153	1	6.175247	-3.865631	2.121435
8	-4.664896	2.778815	-1.147284	1	8.275168	-3.207110	0.978669
8	-4.035474	2.524383	1.764529	1	3.894614	-3.331137	2.874109
				1	1.956085	-1.780380	2.861281
(3-4)_{Al}-LHMDS,ITHF,1DMPU[‡] (THF and DMPU coordination to chloride)				1	6.128871	1.131243	3.072580
				1	2.880918	4.003975	-1.023023
Number of imaginary frequencies : 1				1	7.791112	2.633088	4.059867
Electronic energy : HF=-5055.4514491				1	6.516080	5.822130	1.470404
Zero-point correction= 1.302017 (Hartree/Particle)				1	4.660349	5.483652	-0.078813
Thermal correction to Energy= 1.388551				1	8.022492	4.981566	3.250377
Thermal correction to Enthalpy= 1.389495				1	-0.523129	4.051724	0.616061
Thermal correction to Gibbs Free Energy= 1.177014				1	0.284051	3.398495	-0.828157
Sum of electronic and zero-point Energies= -5054.149432				1	-1.208941	2.624063	-0.207077
Sum of electronic and thermal Energies= -5054.062899				1	-2.533671	-3.555285	1.104020
Sum of electronic and thermal Enthalpies= -5054.061954				1	-1.034705	-3.483145	-2.936425
Sum of electronic and thermal Free Energies= -5054.274435				1	-4.568441	-4.698209	0.325107
Standard State and RRHO Corrected G= -5054.252633				1	-3.077324	-4.630442	-3.711912
				1	-4.861830	-5.240311	-2.085538
Cartesian Coordinates				1	0.123394	-5.349694	-1.394037
				1	2.724330	-2.092340	-0.300793
6	0.049971	1.303273	-3.864317	1	2.089102	-6.768508	-1.828791
6	-0.913827	0.770989	-2.994423	1	4.685693	-3.532811	-0.676125
45	-0.064219	-0.339183	-1.215352	1	4.384263	-5.880647	-1.454954
17	-2.164908	0.108950	-0.107690	1	0.689663	-4.725058	1.472571
6	-1.192099	-0.649468	-2.948172	1	-0.985123	-0.779610	1.897128
8	1.706032	-0.713891	-2.263046	1	0.669657	-4.994920	3.918497
6	2.400645	0.212742	-2.814935	1	-1.002447	-1.051065	4.344810
8	1.968952	1.303352	-3.279450	1	-0.167127	-3.158861	5.377277
6	3.876324	-0.037494	-2.906640	1	-1.578037	1.473092	-2.501638
6	4.378884	-1.343706	-2.937196	1	0.399339	0.704250	-4.698465
6	5.755331	-1.562138	-2.988898	1	0.110797	2.375781	-4.004064
6	6.636844	-0.477638	-2.993972	1	3.688392	-2.177195	-2.915887
6	6.137691	0.828180	-2.960513	1	4.363452	2.057769	-2.895746
6	4.761272	1.049639	-2.927639	1	6.138993	-2.578013	-3.014991
15	1.188274	0.977673	0.359229	1	6.820622	1.673044	-2.956438
8	2.522203	1.517726	-0.457481	1	7.709232	-0.649093	-3.019930
6	3.500299	2.299515	0.135588	1	-0.684173	-1.272366	-3.684679
6	4.372386	1.729006	1.044447	1	-2.202071	-0.972399	-2.709836
6	5.355545	2.584021	1.657706	3	-4.529430	1.409389	0.636104
6	5.461523	3.950867	1.228189	7	-5.989142	0.099574	0.880689
6	4.568411	4.449436	0.241076	14	-6.817848	-0.236522	-0.567446
6	3.588199	3.644058	-0.283417	14	-5.868614	-0.899635	2.252952
6	6.444198	4.793812	1.815436	6	-6.481684	-2.700839	2.047454
6	7.277860	4.327303	2.806339	1	-6.138777	-3.318928	2.888557
6	7.150230	2.992667	3.259787	1	-7.574802	-2.772042	2.014904
6	6.216749	2.145541	2.702697	1	-6.091677	-3.151851	1.127847
6	4.235207	0.288980	1.397688	6	-6.862686	-0.241765	3.746608
6	3.020586	-0.207679	1.857898	1	-6.732783	-0.873019	4.636563
6	2.905075	-1.491741	2.433926	1	-6.572925	0.779177	4.021392
6	3.983824	-2.339818	2.439388	1	-7.935759	-0.219765	3.513743
6	5.206101	-1.955952	1.827558	6	-4.070709	-1.093224	2.844050
6	5.337416	-0.630400	1.294104	1	-4.001790	-1.678504	3.770604
6	6.291227	-2.866504	1.709444	1	-3.480786	-1.602052	2.075463
6	7.455485	-2.500467	1.071613	1	-3.597675	-0.123839	3.016651
6	7.578563	-1.201420	0.522287	6	-8.427047	-1.262180	-0.420997
6	6.551395	-0.290031	0.634587	1	-8.238570	-2.315651	-0.188008
8	1.874028	0.580423	1.833355	1	-9.091841	-0.864017	0.356660
15	-0.123875	-2.527626	-0.333959	1	-8.981672	-1.232400	-1.369294
6	1.281830	-3.615405	-0.810757	6	-5.743692	-1.219278	-1.809215
6	1.116504	-4.938735	-1.250751	1	-6.148352	-1.224989	-2.830795
6	2.231149	-5.746383	-1.489014	1	-4.718112	-0.834413	-1.849460
6	3.518830	-5.248191	-1.277408	1	-5.664190	-2.263491	-1.480938
6	3.690196	-3.933382	-0.838137	6	-7.398505	1.368198	-1.417459

1	-8.233357	1.804273	-0.851573	6	1.983277	5.030740	0.433014
1	-6.601076	2.115100	-1.458318	6	2.590803	3.840369	0.095181
1	-7.756534	1.186413	-2.439871	6	3.930772	1.263295	-0.701133
6	-4.538277	2.864782	3.296057	6	5.139066	2.037029	-0.833772
6	-2.364869	2.384369	2.722594	6	6.336043	1.600655	-0.171814
6	-3.931520	2.324108	4.595455	6	6.321952	0.390665	0.574238
1	-5.570663	2.561593	3.113085	6	5.191061	-0.384766	0.622518
1	-4.474570	3.962797	3.252076	6	4.019419	0.045063	-0.041355
6	-2.432171	2.125961	4.241645	6	7.521600	2.376057	-0.288178
1	-1.979078	3.391012	2.512379	6	7.546232	3.524035	-1.047710
1	-1.778158	1.658588	2.161674	6	6.379174	3.936565	-1.733780
1	-4.085073	3.012460	5.430748	6	5.209465	3.215073	-1.629569
1	-4.393793	1.367819	4.853091	8	2.919734	-0.793527	0.061646
1	-1.783243	2.820215	4.782271	1	2.418985	5.654852	1.208112
1	-2.107010	1.110363	4.481989	1	3.493047	3.535696	0.611834
8	-4.417848	2.744569	-0.721033	1	-0.701904	4.931341	-1.662366
8	-3.724834	2.300088	2.253315	1	0.328731	6.387271	0.057995
6	-3.676929	3.395933	-1.492349	1	-0.765939	2.834190	-2.905554
6	-2.756496	3.788093	-3.775847	1	0.194871	0.568458	-3.361167
6	-2.326739	5.429022	-1.962730	1	4.329432	3.541841	-2.170867
6	-1.697174	4.649558	-3.107094	1	5.159307	-1.323712	1.165063
1	-2.296147	3.099580	-4.491871	1	6.406256	4.828338	-2.353586
1	-3.027092	6.185504	-2.348212	1	8.415063	2.035711	0.229072
1	-0.896796	4.012446	-2.717025	1	7.225512	0.077102	1.089713
7	-3.018580	4.516323	-1.050783	1	8.459222	4.106165	-1.132946
7	-3.467523	2.981905	-2.782294	1	4.513123	-1.489898	-2.930517
6	-3.354320	5.050987	0.263259	1	5.192105	-2.262585	-1.466176
1	-4.165716	5.790130	0.200795	1	4.779150	-3.255810	-2.892016
1	-3.659635	4.241752	0.922047	1	-0.198842	-4.760771	-1.484277
1	-2.472086	5.544667	0.681086	1	0.091669	-5.143531	1.537476
6	-4.262800	1.882916	-3.315724	1	1.169442	-5.820198	0.215899
1	-4.617264	1.255994	-2.504846	1	1.655647	-0.373137	2.634089
1	-5.126822	2.256643	-3.881625	1	3.524757	-4.180567	3.280876
1	-3.639153	1.281867	-3.983617	1	3.137100	0.654202	4.361248
1	-1.559121	5.957275	-1.388638	1	5.008522	-3.169476	5.009360
1	-1.258679	5.337246	-3.835786	1	4.815020	-0.749660	5.540782
1	-3.470630	4.413104	-4.332568	1	-1.797205	-3.600790	0.940065
				1	-2.326204	-3.593129	-0.811637
(3-4) _{A3} [‡]				6	-4.348849	0.236000	-0.427156
				6	-5.620968	-0.258503	-0.888634
Number of imaginary frequencies : 1				6	-3.290606	0.229336	-1.323970
Electronic energy : HF=-3861.3381386				6	-6.731660	-0.452899	-0.019699
Zero-point correction= 0.795764 (Hartree/Particle)				6	-5.780082	-0.607813	-2.272069
Thermal correction to Energy= 0.850530				6	-3.440006	-0.113891	-2.684579
Thermal correction to Enthalpy= 0.851474				6	-7.935464	-0.925072	-0.496414
Thermal correction to Gibbs Free Energy= 0.704483				1	-6.623706	-0.237236	1.036541
Sum of electronic and zero-point Energies= -3860.542374				6	-7.039820	-1.077710	-2.733674
Sum of electronic and thermal Energies= -3860.487609				6	-4.670016	-0.501889	-3.153116
Sum of electronic and thermal Enthalpies= -3860.486664				1	-2.565467	-0.078460	-3.321756
Sum of electronic and thermal Free Energies= -3860.633656				6	-8.099986	-1.229213	-1.868824
Standard State and RRHO Corrected G= -3860.617967				1	-8.764543	-1.070730	0.190279
				1	-7.144132	-1.327793	-3.786367
Cartesian Coordinates				1	-4.800757	-0.761352	-4.199987
				1	-9.056440	-1.594097	-2.231877
6	4.161582	-1.195431	4.795930	8	-2.023729	0.632200	-0.912089
6	3.215037	-0.405370	4.134985	6	-4.142868	0.705101	0.971255
6	2.377993	-0.972972	3.176444	6	-4.942530	1.746570	1.563610
6	2.490471	-2.338824	2.873797	6	-3.136633	0.148480	1.745216
6	3.442335	-3.128561	3.532712	6	-5.884257	2.508455	0.816565
6	4.273010	-2.556760	4.496148	6	-4.767009	2.066761	2.952103
6	1.641481	-2.922213	1.794141	6	-2.968048	0.447102	3.115870
8	1.981300	-4.031704	1.285591	6	-6.630985	3.501122	1.413591
6	0.471416	-5.051053	0.525053	1	-6.006251	2.309939	-0.241639
6	-0.347647	-4.443074	-0.456002	6	-5.564732	3.085579	3.540314
6	-1.499722	-3.641294	-0.106686	6	-3.784572	1.375098	3.712237
45	-0.002807	-2.236021	-0.550809	1	-2.183984	-0.065525	3.663654
8	0.624866	-2.233549	1.438271	6	-6.482339	3.787533	2.791618
15	2.157436	-1.521465	-1.220207	1	-7.337878	4.072527	0.818716
8	3.162154	-2.645931	-1.800520	1	-5.426103	3.306626	4.595531
6	4.497854	-2.382208	-2.301652	1	-3.671060	1.610102	4.766836
17	-0.705626	-2.241692	-2.856198	1	-7.083113	4.567393	3.250482
8	2.390069	-0.369999	-2.399534	8	-2.262455	-0.783010	1.195842
6	1.907502	0.902014	-2.111346	15	-1.113503	-0.343822	0.072875
6	2.627988	1.725285	-1.259389	8	-0.183317	0.772285	0.766107
6	2.040205	2.989933	-0.905399	6	-0.603843	2.080578	1.232247
6	0.812754	3.395354	-1.531768	1	-1.361039	2.506884	0.573671
6	0.170896	2.524785	-2.451946	1	-0.992162	1.999498	2.249035
6	0.694361	1.284948	-2.719063	1	0.288689	2.704555	1.224652
6	0.224069	4.638979	-1.173864				
6	0.793999	5.444402	-0.214397	(3-4) _{A3-LiHMDs, IDMPU} [‡]			

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Number of imaginary frequencies : 1
Electronic energy : HF=-5163.0343074
Zero-point correction= 1.214346 (Hartree/Particle)
Thermal correction to Energy= 1.298545
Thermal correction to Enthalpy= 1.299490
Thermal correction to Gibbs Free Energy= 1.091886
Sum of electronic and zero-point Energies= -5161.819962
Sum of electronic and thermal Energies= -5161.735762
Sum of electronic and thermal Enthalpies= -5161.734818
Sum of electronic and thermal Free Energies= -5161.942422
Standard State and RRHO Corrected G= -5161.921169

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Cartesian Coordinates

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6 -1.651698 2.780810 -4.696228
6 -1.285623 1.549118 -5.249303
6 -1.342586 0.390389 -4.475196
6 -1.797583 0.460452 -3.151837
6 -2.186703 1.687725 -2.601572
6 -2.097478 2.847654 -3.373876
6 -1.800868 -0.763114 -2.298236
8 -2.879900 -1.058031 -1.661265
6 -3.163019 -2.883942 -1.477985
6 -2.175687 -3.623151 -0.749625
6 -1.057059 -4.261790 -1.404342
45 -0.295696 -2.533947 -0.487582
8 -0.733460 -1.434992 -2.242439
15 -0.358154 -0.476936 0.736073
8 -1.785943 0.327381 0.806919
6 -2.029646 1.466354 1.691223
17 0.114964 -3.844220 1.481565
8 0.078734 -0.281028 2.322331
6 1.423879 -0.299258 2.687532
6 2.243661 0.778064 2.384472
6 3.636329 0.672230 2.738213
6 4.090751 -0.461890 3.490868
6 3.170896 -1.488715 3.832785
6 1.864913 -1.422313 3.417449
6 5.463635 -0.560962 3.846050
6 6.369897 0.396077 3.450695
6 5.932603 1.497900 2.677553
6 4.604156 1.635680 2.338504
6 1.692483 1.974990 1.685914
6 1.839101 3.309821 2.209444
6 1.374625 4.428184 1.437078
6 0.729879 4.200920 0.191409
6 0.510670 2.922925 -0.255401
6 0.978468 1.829889 0.505529
6 1.545110 5.746011 1.941739
6 2.117495 5.964857 3.174292
6 2.531466 4.863196 3.960562
6 2.396540 3.574068 3.492349
8 0.699788 0.565557 -0.001293
1 6.651217 2.240600 2.342374
1 4.292697 2.478697 1.736281
1 5.786847 -1.425033 4.420931
1 7.419082 0.302075 3.715430
1 3.522282 -2.344740 4.402218
1 1.155752 -2.218126 3.609296
1 2.711284 2.744244 4.113582
1 -0.002122 2.717520 -1.187716
1 2.955900 5.034480 4.945765
1 1.201560 6.579955 1.334863
1 0.394410 5.052825 -0.393324
1 2.238912 6.976086 3.551709
1 -2.528741 1.103833 2.590704
1 -1.105257 1.967233 1.967751
1 -2.684108 2.138448 1.141145
1 -2.461925 -3.929905 0.251284
1 -3.206521 -3.016161 -2.555802
1 -4.107981 -2.706569 -0.970568
1 -1.043773 -0.565690 -4.893496
1 -2.554429 1.733395 -1.583334
1 -0.947091 1.491873 -6.279469
1 -2.384844 3.801473 -2.941172
1 -1.593386 3.683901 -5.296867
1 -1.004141 -4.219858 -2.492484
1 -0.646726 -5.168287 -0.967181
6 3.775170 0.102165 -1.739004

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6 3.865369 1.540073 -1.781238
6 2.724851 -0.492439 -2.421690
6 4.800312 2.273851 -0.998503
6 2.955640 2.282254 -2.607208
6 1.830192 0.231550 -3.233830
6 4.844754 3.650524 -1.041593
1 5.470778 1.739905 -0.338355
6 3.042658 3.700356 -2.645653
6 1.954259 1.592631 -3.341022
1 1.045523 -0.315244 -3.736418
6 3.965922 4.375967 -1.880934
1 5.558220 4.183384 -0.419203
1 2.345244 4.242382 -3.279403
1 1.262964 2.156574 -3.960747
1 4.013784 5.460746 -1.907535
8 2.540694 -1.871203 -2.368834
6 4.731733 -0.734753 -0.962075
6 6.157588 -0.662231 -1.158200
6 4.260870 -1.641346 -0.024111
6 6.749872 0.096805 -2.206438
6 7.028863 -1.407418 -0.294193
6 5.111832 -2.380841 0.825861
6 8.118187 0.152416 -2.362226
1 6.110869 0.632146 -2.898585
6 8.436022 -1.314291 -0.470977
6 6.471620 -2.245008 0.709464
1 4.658363 -3.031321 1.565146
6 8.974791 -0.546549 -1.478699
1 8.542854 0.735104 -3.174820
1 9.079565 -1.874772 0.202391
1 7.137130 -2.792061 1.371040
1 10.051632 -0.486776 -1.607574
8 2.894317 -1.833192 0.154328
15 1.947635 -2.576295 -0.981744
8 2.528735 -4.063570 -1.206368
6 3.858899 -4.398628 -1.677162
1 4.261251 -3.619048 -2.326237
1 4.519609 -4.549895 -0.821093
1 3.759461 -5.330279 -2.237611
3 -3.878112 -0.290139 -0.022900
8 -4.485137 1.484683 -0.293883
6 -5.412675 2.317304 -0.118447
6 -6.899191 3.607600 1.425596
6 -7.128317 3.860243 -1.025879
6 -7.021852 4.612297 0.291677
1 -7.856693 3.093302 1.592195
1 -7.125392 4.554823 -1.871388
1 -7.904188 5.239874 0.445051
7 -5.981080 2.965000 -1.180636
7 -5.862848 2.611839 1.137211
1 -6.630555 4.110960 2.360778
1 -6.140752 5.263584 0.269198
1 -8.065847 3.286792 -1.073236
6 -5.655459 2.580319 -2.546829
1 -4.823885 1.882522 -2.549015
1 -6.520168 2.104787 -3.026696
1 -5.378898 3.466299 -3.129737
6 -5.433907 1.813351 2.280512
1 -5.052108 0.849284 1.949498
1 -4.672595 2.337558 2.870442
1 -6.301865 1.629766 2.921235
7 -5.151796 -1.557096 0.754891
14 -6.669938 -1.511480 -0.018424
14 -4.833788 -2.380456 2.212544
6 -6.465816 -1.056616 -1.857554
1 -7.435095 -0.858522 -2.333989
1 -5.847661 -0.161121 -1.971831
1 -5.982042 -1.865773 -2.419101
6 -7.903584 -0.241265 0.698393
1 -8.881186 -0.310968 0.202300
1 -8.066138 -0.406904 1.770527
1 -7.544436 0.785453 0.575924
6 -7.634311 -3.161081 -0.010848
1 -7.028341 -3.986046 -0.405251
1 -7.954276 -3.443585 0.999799
1 -8.538889 -3.089708 -0.629992
6 -3.076967 -2.036795 2.848046
1 -2.895397 -2.579568 3.785313
1 -2.314724 -2.365529 2.135073
1 -2.909660 -0.973674 3.051075

```

6	-4.955439	-4.283741	2.097276
1	-5.987944	-4.619131	1.945048
1	-4.360750	-4.675468	1.262790
1	-4.586357	-4.760878	3.015177
6	-6.003121	-1.899939	3.646906
1	-5.960251	-0.822676	3.852207
1	-7.047148	-2.146064	3.414533
1	-5.743452	-2.423883	4.576751
3_{B1}			
Number of imaginary frequencies : 0			
Electronic energy : HF=-4057.5629777			
Zero-point correction= 1.002851 (Hartree/Particle)			
Thermal correction to Energy= 1.066728			
Thermal correction to Enthalpy= 1.067673			
Thermal correction to Gibbs Free Energy= 0.902955			
Sum of electronic and zero-point Energies= -4056.560127			
Sum of electronic and thermal Energies= -4056.496249			
Sum of electronic and thermal Enthalpies= -4056.495305			
Sum of electronic and thermal Free Energies= -4056.660023			
Standard State and RRHO Corrected G= -4056.642336			
Cartesian Coordinates			
6	-2.157728	6.922891	-0.220232
6	-1.959683	5.862851	0.669963
6	-1.169234	4.778327	0.298082
6	-0.572200	4.752294	-0.973030
6	-0.771152	5.816797	-1.865539
6	-1.562912	6.898824	-1.485657
6	0.240306	3.570521	-1.342202
8	0.834678	3.664359	-2.517416
6	1.371982	2.515592	-3.249868
6	2.222531	1.539204	-2.481530
6	3.015776	1.871493	-1.340211
45	1.271104	0.707300	-0.760142
8	0.334568	2.622087	-0.552302
15	-0.966082	0.259110	-1.471217
8	-1.335680	1.089339	-2.679820
8	-1.698149	-1.264607	-1.818852
6	-2.248808	-2.094132	-0.885245
6	-3.385758	-1.736934	-0.159278
6	-3.837562	-2.627727	0.876756
6	-3.205918	-3.906385	1.042974
6	-2.137823	-4.268295	0.179182
6	-1.661335	-3.377463	-0.748032
6	-3.637246	-4.772181	2.084301
6	-4.639027	-4.397279	2.951532
6	-5.251256	-3.128978	2.806787
6	-4.865472	-2.272238	1.797868
6	-4.076670	-0.447398	-0.440733
6	-5.473339	-0.373415	-0.779459
6	-6.084951	0.913028	-0.966425
6	-5.291855	2.087964	-0.853709
6	-3.945087	1.999854	-0.604421
6	-3.346002	0.732486	-0.412695
6	-7.468579	0.988965	-1.283860
6	-8.225972	-0.150349	-1.439901
6	-7.618696	-1.420794	-1.294837
6	-6.282508	-1.528870	-0.974456
8	-1.994198	0.688369	-0.165945
1	-6.028583	-2.823900	3.501891
1	-5.334871	-1.299219	1.715029
1	-3.147079	-5.736981	2.190187
1	-4.954084	-5.064001	3.749141
1	-1.677198	-5.246393	0.288903
1	-0.819421	-3.616982	-1.387998
1	-5.832930	-2.510279	-0.878950
1	-3.313173	2.879768	-0.544099
1	-8.210043	-2.320136	-1.443679
1	-7.916252	1.971495	-1.412251
1	-5.764221	3.056891	-0.993095
1	-9.281498	-0.078735	-1.686651
1	2.616823	0.795039	-3.173614
1	1.959185	3.001885	-4.036240
1	0.509326	2.010746	-3.690198
1	-0.999685	3.954119	0.980704
1	-0.313279	5.789448	-2.847770
1	-2.416065	5.882131	1.654928

1	-1.719084	7.721430	-2.177082
1	-2.775444	7.767734	0.071228
1	2.953774	2.880150	-0.938306
1	3.981856	1.399276	-1.199631
15	2.199536	-1.327078	-1.226417
15	1.470572	0.766245	1.746725
6	1.208179	2.502759	2.364358
6	1.882271	3.574459	1.751987
6	0.297050	2.798543	3.391261
6	1.690585	4.887027	2.180325
1	2.546408	3.387337	0.919046
6	0.091135	4.117128	3.809100
1	-0.259941	2.005454	3.875562
6	0.792847	5.165260	3.213918
1	2.227776	5.694105	1.690009
1	-0.619980	4.317926	4.605798
1	0.632144	6.189029	3.539469
6	0.435094	-0.180835	2.957936
6	-0.852625	-0.579364	2.572057
6	0.860698	-0.449644	4.270493
6	-1.683824	-1.261023	3.464850
1	-1.209913	-0.357543	1.572922
6	0.034090	-1.139319	5.158330
1	1.839726	-0.123593	4.605240
6	-1.238767	-1.552785	4.755416
1	-2.674432	-1.568043	3.146638
1	0.383781	-1.348089	6.165782
1	-1.881944	-2.093397	5.444470
6	3.198280	0.351189	2.296517
6	4.243216	1.286521	2.209654
6	3.518501	-0.964214	2.679030
6	5.559874	0.921381	2.497785
1	4.043045	2.310190	1.920015
6	4.834981	-1.327145	2.969566
1	2.743272	-1.716201	2.752292
6	5.863877	-0.387905	2.878080
1	6.347849	1.665892	2.424189
1	5.050532	-2.351937	3.258122
1	6.888729	-0.671303	3.100233
6	1.470288	-2.240669	-2.659417
1	1.604414	-3.635503	-2.756763
6	0.832865	-1.546021	-3.696672
6	1.099072	-4.318923	-3.863780
1	2.095751	-4.195139	-1.967893
6	0.336134	-2.230598	-4.806927
1	0.692230	-0.474292	-3.629014
6	0.464237	-3.617871	-4.892325
1	1.200501	-5.399122	-3.919776
1	-0.165413	-1.677418	-5.595874
1	0.067693	-4.151056	-5.751771
6	3.981216	-1.231377	-1.703464
6	4.406507	-1.409366	-3.027465
6	4.930858	-0.899582	-0.722133
6	5.756414	-1.261875	-3.361123
1	3.692534	-1.665721	-3.802773
6	6.277209	-0.764397	-1.055297
1	4.616702	-0.747802	0.302243
6	6.694086	-0.942551	-2.378187
1	6.071122	-1.401996	-4.391448
1	6.995628	-0.514910	-0.279834
1	7.742807	-0.832691	-2.639591
6	2.174460	-2.588628	0.114466
6	3.243809	-3.461143	0.375337
6	1.010118	-2.692768	0.884095
6	3.149605	-4.397856	1.405707
1	4.153164	-3.408429	-0.212365
6	0.915395	-3.628502	1.914501
1	0.178907	-2.031692	0.685786
6	1.989660	-4.478620	2.182804
1	3.986628	-5.061182	1.604562
1	0.007892	-3.676110	2.508067
1	1.925151	-5.201436	2.991289
(3-4)_{B1}⁺			
Number of imaginary frequencies : 1			
Electronic energy : HF=-4057.5333619			
Zero-point correction= 1.000551 (Hartree/Particle)			
Thermal correction to Energy= 1.064369			
Thermal correction to Enthalpy= 1.065313			

Thermal correction to Gibbs Free Energy= 0.900233
Sum of electronic and zero-point Energies= -4056.532811
Sum of electronic and thermal Energies= -4056.468993
Sum of electronic and thermal Enthalpies= -4056.468049
Sum of electronic and thermal Free Energies= -4056.633129
Standard State and RRHO Corrected G= -4056.61532

Cartesian Coordinates

```

6 -1.538120 0.837082 -3.993365
6 -2.428112 0.697163 -2.904525
45 -1.313604 0.103544 -0.993084
6 -2.826128 -0.569578 -2.353366
8 -0.009676 -1.012363 -2.273105
6 0.704284 -0.416370 -3.147092
8 0.412533 0.693676 -3.689394
6 1.960818 -1.103160 -3.581419
6 2.209932 -2.430734 -3.206467
6 3.399634 -3.052844 -3.582730
6 4.351202 -2.351210 -4.328691
6 4.102783 -1.029531 -4.711798
6 2.908434 -0.409600 -4.347675
15 0.573912 1.340370 -0.186235
8 1.938003 0.716391 -0.991845
6 3.088986 1.462839 -0.857297
6 3.840723 1.346478 0.300112
6 4.966150 2.231125 0.461956
6 5.339711 3.100672 -0.618979
6 4.566532 3.107971 -1.812527
6 3.444968 2.324461 -1.919252
6 6.463332 3.958628 -0.468689
6 7.181155 3.991078 0.705820
6 6.790695 3.167166 1.788532
6 5.716304 2.312100 1.669459
6 3.464269 0.334601 1.326122
6 2.171949 0.263627 1.850187
6 1.883339 -0.587656 2.951978
6 2.834581 -1.422836 3.472429
6 4.121535 -1.502599 2.877679
6 4.431212 -0.636542 1.778220
6 5.077545 -2.456230 3.317291
6 6.290948 -2.591658 2.679741
6 6.587313 -1.770983 1.565629
6 5.688193 -0.819508 1.132201
8 1.130264 1.039371 1.429767
15 -1.346905 -1.927055 0.277859
6 0.261247 -2.762888 0.663604
6 0.268754 -3.871862 1.529133
6 1.448175 -4.576171 1.765895
6 2.635289 -4.189997 1.135389
6 2.635765 -3.087947 0.282106
6 1.457932 -2.371000 0.053719
8 0.567067 2.845685 -0.272000
6 -2.126768 -1.932258 1.943241
6 -3.033355 -2.901427 2.401127
6 -3.512706 -2.848545 3.712234
6 -3.078307 -1.845785 4.583197
6 -2.164254 -0.888505 4.137492
6 -1.701460 -0.925611 2.822440
6 -2.205664 -3.245605 -0.683727
6 -3.605894 -3.238931 -0.805123
6 -4.254936 -4.169210 -1.615668
6 -3.515051 -5.109824 -2.338264
6 -2.122745 -5.114287 -2.237655
6 -1.471010 -4.193129 -1.413529
1 7.530870 -1.895076 1.041192
1 5.932163 -0.213047 0.268191
1 4.819778 -3.095514 4.158239
1 7.010902 -3.331957 3.016994
1 2.598647 -2.065670 4.316154
1 0.885200 -0.556043 3.369403
1 5.426835 1.696021 2.512507
1 2.808854 2.338422 -2.797090
1 7.340183 3.212569 2.724809
1 6.737927 4.601329 -1.301657
1 4.859714 3.766180 -2.626154
1 8.034728 4.655000 0.809630
1 -4.192382 -2.499708 -0.273212
1 -0.389268 -4.217548 -1.341195
1 -5.339006 -4.152227 -1.687447

```

```

1 -1.537319 -5.839317 -2.796326
1 -4.019997 -5.830755 -2.974950
1 -0.645978 -4.191842 2.017869
1 1.478688 -1.516366 -0.603874
1 1.438998 -5.428026 2.440444
1 3.554009 -2.766754 -0.198689
1 3.556361 -4.734182 1.323063
1 -3.363957 -3.699327 1.745787
1 -1.012259 -0.166277 2.472198
1 -4.219002 -3.599718 4.054742
1 -1.826002 -0.098329 4.799822
1 -3.450893 -1.811104 5.603027
1 -2.987297 1.591911 -2.655738
1 -1.408822 0.003619 -4.675018
1 -1.408192 1.820744 -4.429996
1 1.471228 -2.961854 -2.619265
1 2.703168 0.613529 -4.641448
1 3.586484 -4.081561 -3.287972
1 4.840268 -0.482824 -5.292457
1 5.282628 -2.833299 -4.612491
1 -2.472615 -1.470016 -2.850571
1 -3.821378 -0.660767 -1.932874
15 -2.794504 1.543589 0.145839
6 -2.870170 3.258709 -0.556330
6 -3.816394 4.154820 -0.027164
6 -2.005741 3.699161 -1.565913
6 -3.912383 5.455360 -0.518936
1 -4.482515 3.836293 0.769136
6 -2.101684 5.005161 -2.053554
1 -1.241163 3.039464 -1.950916
6 -3.054720 5.883268 -1.537039
1 -4.652321 6.134138 -0.104388
1 -1.420169 5.334672 -2.832868
1 -3.125928 6.898183 -1.918253
6 -2.667200 1.991659 1.940256
6 -3.744785 1.875253 2.831097
6 -1.476500 2.585973 2.391507
6 -3.620533 2.306758 4.153581
1 -4.688990 1.454601 2.510039
6 -1.353198 3.002718 3.716475
1 -0.649920 2.746517 1.710946
6 -2.421967 2.859630 4.605390
1 -4.465431 2.204697 4.828797
1 -0.420072 3.449385 4.047949
1 -2.324578 3.188018 5.636381
6 -4.523616 0.927694 -0.045343
6 -5.406213 1.469511 -0.991399
6 -4.930531 -0.196640 0.693637
6 -6.667473 0.900581 -1.189915
1 -5.117563 2.333401 -1.579753
6 -6.195093 -0.752671 0.504204
1 -4.261570 -0.639849 1.421688
6 -7.066960 -0.208540 -0.443281
1 -7.336611 1.330717 -1.929623
1 -6.492085 -1.616054 1.092955
1 -8.049368 -0.645787 -0.596494

```

4_{B1} (O-Coordination)

Number of imaginary frequencies : 0
Electronic energy : HF=-4057.562228
Zero-point correction= 1.002537 (Hartree/Particle)
Thermal correction to Energy= 1.066752
Thermal correction to Enthalpy= 1.067696
Thermal correction to Gibbs Free Energy= 0.904267
Sum of electronic and zero-point Energies= -4056.559691
Sum of electronic and thermal Energies= -4056.495476
Sum of electronic and thermal Enthalpies= -4056.494532
Sum of electronic and thermal Free Energies= -4056.657961
Standard State and RRHO Corrected G= -4056.6417

Cartesian Coordinates

```

6 -2.633232 6.379209 -0.322061
6 -2.645811 5.074315 0.178623
6 -1.717846 4.138592 -0.281305
6 -0.776219 4.499772 -1.254703
6 -0.771448 5.807094 -1.757335
6 -1.693816 6.744278 -1.292227
6 0.261141 3.513489 -1.743819

```

8	1.059269	3.839381	-2.635946
6	1.560480	0.824796	-3.349208
6	2.852296	0.827954	-2.774655
6	3.197877	1.717529	-1.753888
45	1.261827	0.548487	-1.154149
8	0.208193	2.381916	-1.120458
15	-0.983833	-0.068763	-1.644631
8	-1.386666	0.275165	-3.050048
8	-1.558385	-1.666318	-1.436073
6	-2.179952	-2.201167	-0.340801
6	-3.346162	-1.666037	0.206514
6	-3.834403	-2.231052	1.438241
6	-3.229437	-3.418533	1.969388
6	-2.150197	-4.016074	1.265652
6	-1.627453	-3.410563	0.152754
6	-3.700608	-3.958273	3.196608
6	-4.714946	-3.345992	3.898382
6	-5.300239	-2.160740	3.391929
6	-4.877470	-1.622946	2.194847
6	-4.057419	-0.549115	-0.471640
6	-5.446347	-0.637410	-0.847193
6	-6.082373	0.498085	-1.454410
6	-5.319727	1.667042	-1.724204
6	-3.978642	1.708441	-1.437197
6	-3.362683	0.599202	-0.814747
6	-7.457663	0.424351	-1.806811
6	-8.182251	-0.728418	-1.603214
6	-7.547889	-1.865175	-1.048121
6	-6.219837	-1.821323	-0.681601
8	-2.009750	0.681701	-0.530308
1	-6.087334	-1.666116	3.954202
1	-5.329499	-0.707928	1.830438
1	-3.230920	-4.861704	3.577975
1	-5.060735	-3.761861	4.840373
1	-1.715034	-4.936924	1.644107
1	-0.774039	-3.825349	-0.370287
1	-5.751771	-2.707399	-0.270268
1	-3.370830	2.574114	-1.669396
1	-8.111156	-2.784700	-0.915105
1	-7.923746	1.298315	-2.255050
1	-5.808054	2.518972	-2.189727
1	-9.231423	-0.774191	-1.880997
1	3.497968	-0.022305	-2.965623
1	1.014625	1.749843	-3.474083
1	1.311998	0.030091	-4.042208
1	-1.710107	1.323777	0.097243
1	-0.032533	6.071701	-2.506590
1	-3.376092	4.785451	0.929815
1	-1.681537	7.758112	-1.683461
1	-3.352501	7.108892	0.040518
1	2.756084	2.705172	-1.763429
1	4.127454	1.573759	-1.213906
15	2.137537	-1.654999	-0.976129
15	1.597650	1.267102	1.265447
6	1.383925	3.107087	1.464047
6	2.096873	4.013601	0.661667
6	0.479580	3.630280	2.402276
6	1.926197	5.389657	0.800311
1	2.771836	3.655567	-0.101162
6	0.304223	5.010309	2.536408
1	-0.107640	2.972658	3.029962
6	1.025475	5.896592	1.739017
1	2.483782	6.062461	0.155298
1	-0.410912	5.385689	3.262832
1	0.877816	6.968192	1.835304
6	0.522063	0.664522	2.643815
6	-0.800017	0.295096	2.362944
6	0.952889	0.676555	3.981616
6	-1.661308	-0.097223	3.389939
1	-1.164408	0.309417	1.343911
6	0.094134	0.274758	5.005226
1	1.956097	1.001016	4.233861
6	-1.213444	-0.121029	4.711846
1	-2.678084	-0.390980	3.152223
1	0.447700	0.278071	6.032450
1	-1.881081	-0.438079	5.508113
6	3.313263	0.946129	1.901277
6	4.377000	1.814752	1.601618
6	3.601456	-0.236137	2.605218
6	5.684211	1.503924	1.980595

1	4.201810	2.743001	1.074647
6	4.908602	-0.543412	2.985952
1	2.809763	-0.924637	2.865736
6	5.957769	0.320433	2.670102
1	6.487687	2.192821	1.735951
1	5.099629	-1.467339	3.523769
1	6.975765	0.078160	2.961132
6	1.376331	-2.970105	-2.028267
1	1.572588	-4.322815	-1.696217
6	0.652265	-2.656679	-3.184610
6	1.051258	-5.332737	-2.504533
1	2.128101	-4.595034	-0.805657
6	0.134952	-3.669279	-3.994546
1	0.445704	-1.627626	-3.442164
6	0.331365	-5.008507	-3.657711
1	1.206331	-6.372236	-2.230060
1	-0.436088	-3.403874	-4.879417
1	-0.078752	-5.795576	-4.284035
6	3.927377	-1.780949	-1.420609
6	4.381617	-2.568794	-2.488552
6	4.858187	-1.035482	-0.677849
6	5.742422	-2.606302	-2.805572
1	3.683511	-3.151113	-3.079119
6	6.215132	-1.082095	-0.992521
1	4.524401	-0.421699	0.147381
6	6.661467	-1.865879	-2.060353
1	6.080132	-3.218944	-3.636575
1	6.918790	-0.503323	-0.401507
1	7.718325	-1.898887	-2.309033
6	2.098696	-2.423358	0.694512
6	3.158548	-3.201850	1.192590
6	0.945448	-2.271847	1.469097
6	3.059359	-3.795998	2.450565
1	4.062077	-3.339593	0.610254
6	0.848186	-2.860567	2.730524
1	0.123023	-1.682504	1.094274
6	1.908292	-3.620078	3.226223
1	3.886139	-4.390892	2.827867
1	-0.051617	-2.710960	3.318332
1	1.840912	-4.073669	4.210929

4_{B1} (P-Coordination)

Number of imaginary frequencies : 0
 Electronic energy : HF=-4057.5530243
 Zero-point correction= 1.001240 (Hartree/Particle)
 Thermal correction to Energy= 1.065671
 Thermal correction to Enthalpy= 1.066615
 Thermal correction to Gibbs Free Energy= 0.901290
 Sum of electronic and zero-point Energies= -4056.551784
 Sum of electronic and thermal Energies= -4056.487353
 Sum of electronic and thermal Enthalpies= -4056.486409
 Sum of electronic and thermal Free Energies= -4056.651735
 Standard State and RRHO Corrected G= -4056.634456

Cartesian Coordinates

6	0.549815	6.839147	1.157333
6	0.637301	5.645459	1.879569
6	0.519647	4.420343	1.222390
6	0.305338	4.375926	-0.161653
6	0.213852	5.575797	-0.878494
6	0.338295	6.801873	-0.224317
6	0.194725	3.064164	-0.909911
8	-0.041790	3.078029	-2.127831
6	-1.163963	-0.004595	-1.815176
6	-0.082610	-0.432021	-2.598011
6	1.104435	0.345586	-2.685939
45	0.722811	-0.033233	-0.568710
8	0.365242	2.018411	-0.167089
15	-1.685345	-0.579298	2.018228
8	-0.315747	-0.351441	1.325546
8	-2.568354	-1.399555	0.786062
6	-3.926875	-1.499467	0.969643
6	-4.746778	-0.438849	0.605525
6	-6.162012	-0.553171	0.837986
6	-6.693762	-1.784272	1.353552
6	-5.805983	-2.846633	1.673857
6	-4.451121	-2.699392	1.507661
6	-8.094326	-1.907617	1.565209

6	-8.946619	-0.856927	1.310034
6	-8.422705	0.372340	0.842100
6	-7.071525	0.520279	0.614542
6	-4.119440	0.798756	0.070818
6	-4.498704	1.371916	-1.192386
6	-3.956436	2.640971	-1.587199
6	-3.040478	3.300164	-0.724079
6	-2.617412	2.696042	0.431792
6	-3.116183	1.426522	0.806046
6	-4.326102	3.200673	-2.839945
6	-5.179324	2.534604	-3.691648
6	-5.694682	1.269283	-3.319643
6	-5.366057	0.705913	-2.105110
8	-2.617992	0.877116	1.960939
1	-9.091918	1.210107	0.666260
1	-6.689645	1.472847	0.267404
1	-8.478607	-2.850965	1.945761
1	-10.014526	-0.962002	1.479506
1	-6.214155	-3.771472	2.073393
1	-3.755488	-3.488504	1.764829
1	-5.761292	-0.268449	-1.840447
1	-1.882151	3.160073	1.075807
1	-6.351079	0.734259	-4.000654
1	-3.906986	4.164516	-3.118491
1	-2.640429	4.267285	-1.012738
1	-5.448570	2.969189	-4.650221
1	-0.040798	-1.463113	-2.939712
1	-1.383048	1.050172	-1.701199
1	-1.954470	-0.698505	-1.556472
1	0.601375	3.490790	1.771759
1	0.052644	5.525680	-1.950032
1	0.803791	5.668619	2.953211
1	0.271531	7.727351	-0.790016
1	0.646199	7.793548	1.668079
1	0.996388	1.422169	-2.746319
1	1.965652	-0.097423	-3.177345
15	1.087849	-2.360411	-0.475881
15	2.912357	0.715162	0.291321
6	3.292080	2.447553	-0.250862
6	3.205102	2.801591	-1.606888
6	3.677753	3.430322	0.673061
6	3.490411	4.099951	-2.026732
1	2.899063	2.070017	-2.341404
6	3.959013	4.731718	0.251334
1	3.744177	3.197545	1.728655
6	3.862757	5.073284	-1.097214
1	3.403284	4.351866	-3.079643
1	4.236731	5.481190	0.986679
1	4.067080	6.089707	-1.420796
6	2.999536	0.867010	2.124433
6	1.816108	1.195164	2.804662
6	4.198536	0.763916	2.847834
6	1.827578	1.383994	4.187344
1	0.889294	1.276304	2.252863
6	4.203679	0.948003	4.231701
1	5.131739	0.546451	2.340552
6	3.018355	1.252575	4.905862
1	0.902132	1.628804	4.701273
1	5.136936	0.858045	4.780449
1	3.024999	1.393603	5.983086
6	4.453373	-0.193477	-0.190870
6	5.172704	0.170750	-1.343183
6	4.875885	-1.324660	0.527069
6	6.261971	-0.587699	-1.774969
1	4.893093	1.046678	-1.914573
6	5.967658	-2.078742	0.095190
1	4.364291	-1.618910	1.432467
6	6.659948	-1.720537	-1.062081
1	6.800524	-0.286471	-2.669047
1	6.268241	-2.950763	0.668291
1	7.505358	-2.312385	-1.400851
6	-0.431910	-3.399390	-0.316857
6	-0.620448	-4.221118	0.804042
6	-1.380888	-3.447517	-1.351706
6	-1.716716	-5.083208	0.877415
1	0.089262	-4.206962	1.622116
6	-2.477491	-4.303360	-1.273724
1	-1.265127	-2.843767	-2.242271
6	-2.646031	-5.130947	-0.161394
1	-1.838470	-5.717547	1.750836

1	-3.196831	-4.326312	-2.087146
1	-3.498996	-5.800835	-0.103372
6	1.952728	-3.106307	-1.922715
6	1.582721	-4.344840	-2.471839
6	3.067722	-2.436536	-2.449073
6	2.308809	-4.888532	-3.533973
1	0.736719	-4.892861	-2.073967
6	3.794808	-2.985068	-3.504903
1	3.377056	-1.491290	-2.026782
6	3.413993	-4.211559	-4.054054
1	2.009715	-5.846291	-3.950149
1	4.658355	-2.451970	-3.891498
1	3.976379	-4.639274	-4.879127
6	2.090463	-2.914796	0.963106
6	2.978675	-3.995781	0.849213
6	1.930056	-2.280738	2.205118
6	3.711718	-4.419395	1.958372
1	3.113198	-4.500337	-0.101047
6	2.669448	-2.706964	3.309944
1	1.232435	-1.458778	2.298746
6	3.565616	-3.771648	3.188444
1	4.403182	-5.251113	1.857927
1	2.549410	-2.195070	4.260141
1	4.145875	-4.097191	4.047212

(3...4)BI-LiHMDS.IDMPU

Number of imaginary frequencies : 0
 Electronic energy : HF=-5359.2673996
 Zero-point correction= 1.422238 (Hartree/Particle)
 Thermal correction to Energy= 1.515288
 Thermal correction to Enthalpy= 1.516232
 Thermal correction to Gibbs Free Energy= 1.291383
 Sum of electronic and zero-point Energies= -5357.845161
 Sum of electronic and thermal Energies= -5357.752112
 Sum of electronic and thermal Enthalpies= -5357.751168
 Sum of electronic and thermal Free Energies= -5357.976016
 Standard State and RRHO Corrected G= -5357.952738

Cartesian Coordinates

6	3.544906	-1.614104	5.030682
6	2.418051	-0.795353	4.895276
6	1.492782	-1.045429	3.886152
6	1.691903	-2.123714	3.007292
6	2.820970	-2.943851	3.143481
6	3.744516	-2.685172	4.155500
6	0.713042	-2.329148	1.917143
8	0.911413	-3.415023	1.195087
6	0.335807	-3.639304	-0.134442
6	-1.107102	-3.270927	-0.359942
6	-2.128916	-3.349187	0.635087
45	-1.637261	-1.280926	0.209087
8	-0.211504	-1.517484	1.770136
15	0.239576	0.043092	-0.545044
8	1.496310	-0.818900	-0.584107
8	0.502822	1.016778	-1.927226
6	-0.089569	2.244994	-2.076104
6	0.319378	3.333967	-1.309866
6	-0.412252	4.568781	-1.449385
6	-1.440119	4.676564	-2.446610
6	-1.720705	3.561515	-3.280602
6	-1.070789	2.369634	-3.089296
6	-2.177035	5.886157	-2.568790
6	-1.933180	6.954731	-1.735557
6	-0.935153	6.848892	-0.737925
6	-0.195740	5.693277	-0.601244
6	1.450164	3.200109	-0.348792
6	2.574798	4.100339	-0.358839
6	3.529432	4.050110	0.711872
6	3.392122	3.059839	1.722493
6	2.392943	2.123724	1.647735
6	1.438921	2.189404	0.604379
6	4.610516	4.972822	0.726385
6	4.783443	5.882870	-0.293696
6	3.877418	5.896405	-1.380803
6	2.801697	5.034102	-1.409147
8	0.423040	1.264658	0.627833
1	-0.753657	7.683681	-0.066696
1	0.550660	5.630442	0.181040

1	-2.948891	5.945068	-3.332157
1	-2.507195	7.871560	-1.834204
1	-2.480775	3.654394	-4.051537
1	-1.291162	1.500268	-3.694543
1	2.118051	5.057368	-2.250067
1	2.304658	1.321176	2.370525
1	4.030619	6.592204	-2.200979
1	5.308641	4.937344	1.558950
1	4.116307	3.027333	2.531183
1	5.618201	6.577685	-0.274039
1	-1.374536	-3.515555	-1.388288
1	0.482261	-4.716123	-0.267333
1	0.982846	-3.102573	-0.826040
1	0.615071	-0.421458	3.770372
1	2.981550	-3.759539	2.448844
1	2.259545	0.035246	5.576395
1	4.627731	-3.308852	4.247574
1	4.269434	-1.414305	5.815141
1	-1.843844	-3.608400	1.652212
1	-3.128535	-3.668907	0.362828
15	-3.087329	-1.096747	-1.556768
8	4.182768	-0.184311	0.608965
7	4.251907	-2.967647	-1.194371
6	5.090097	0.662633	0.450623
6	7.006785	1.961066	1.344744
6	6.349398	2.229685	-1.036996
6	7.517069	1.996189	-0.088953
1	6.632537	2.950536	1.646862
1	6.661056	2.055048	-2.072982
1	8.257033	2.792926	-0.208390
7	5.245091	1.316416	-0.739371
7	5.953339	0.958760	1.472967
1	8.001565	1.042206	-0.323515
1	7.813077	1.690457	2.034294
1	5.994816	3.266811	-0.967691
6	5.702053	0.442579	2.809247
1	5.575083	1.272944	3.516368
1	4.795689	-0.156941	2.805603
1	6.539425	-0.177453	3.151273
6	4.254529	1.145192	-1.794983
1	4.592905	0.421846	-2.548707
1	3.302998	0.815059	-1.380729
14	5.826781	-3.155992	-0.561615
14	3.816831	-3.609265	-2.709549
3	3.250839	-1.458546	-0.418427
6	6.654915	-4.846482	-0.911953
1	6.064548	-5.672415	-0.495397
1	6.785183	-5.043207	-1.982803
1	7.650903	-4.892041	-0.449916
6	5.863230	-3.016015	1.333367
1	5.319098	-2.131271	1.668992
1	5.395292	-3.895959	1.791719
1	6.891424	-2.953787	1.714617
6	7.060754	-1.862528	-1.239419
1	8.020881	-1.877787	-0.705672
1	7.270486	-2.045552	-2.300918
1	6.646022	-0.852171	-1.162098
6	5.092223	-3.298603	-4.103220
1	4.756464	-3.724003	-5.058797
1	5.245804	-2.222651	-4.258754
1	6.071887	-3.736557	-3.877679
6	2.203559	-2.864653	-3.388118
1	2.174820	-1.776796	-3.266881
1	2.114749	-3.094014	-4.457894
6	3.511507	-5.495592	-2.709946
1	2.759790	-5.765876	-1.956424
1	3.145263	-5.849737	-3.683480
1	4.422959	-6.058303	-2.475512
1	1.316355	-3.276490	-2.895868
1	4.094603	2.111001	-2.284929
15	-2.982516	-0.067618	1.981048
6	-2.290173	-0.460344	3.665483
6	-2.022542	-1.793827	4.022702
6	-1.961936	0.546287	4.588212
6	-1.492375	-2.114664	5.271311
1	-2.206016	-2.589536	3.313666
6	-1.415660	0.225959	5.835120
1	-2.128714	1.588807	4.345898
6	-1.187687	-1.104212	6.186649
1	-1.299240	-3.154604	5.519408

1	-1.171787	1.024955	6.529970
1	-0.762941	-1.351834	7.155211
6	-3.227576	1.762535	2.145246
6	-2.285050	2.624352	1.569354
6	-4.278700	2.316733	2.897451
6	-2.405055	4.008929	1.713200
1	-1.455131	2.213271	1.008092
6	-4.403467	3.699507	3.032927
1	-5.004041	1.671166	3.381056
6	-3.469234	4.550484	2.435469
1	-1.673082	4.660503	1.248242
1	-5.227614	4.110412	3.609683
1	-3.568250	5.627834	2.536808
6	-4.731631	-0.693714	2.067542
6	-5.048143	-1.921610	2.672578
6	-5.759582	0.004598	1.408852
6	-6.347954	-2.429797	2.627369
1	-4.287824	-2.494400	3.187903
6	-7.059181	-0.503848	1.366137
1	-5.554199	0.950531	0.923643
6	-7.360811	-1.724208	1.973552
1	-6.565617	-3.380522	3.106148
1	-7.830998	0.056543	0.846365
1	-8.371385	-2.120931	1.937831
6	-2.353938	-0.917666	-3.243135
6	-3.141435	-0.412236	-4.293106
6	-1.037189	-1.310120	-3.509189
6	-2.612198	-0.282384	-5.575893
1	-4.165330	-0.104886	-4.111220
6	-0.509225	-1.179607	-4.796600
1	-0.412968	-1.698452	-2.714014
6	-1.290705	-0.661557	-5.829167
1	-3.229624	0.120087	-6.373973
1	0.517123	-1.473678	-4.982420
1	-0.873185	-0.551905	-6.826076
6	-4.160998	-2.581881	-1.776395
6	-3.894181	-3.530080	-2.774733
6	-5.204581	-2.825887	-0.867732
6	-4.660786	-4.695620	-2.864803
1	-3.093096	-3.365215	-3.487372
6	-5.975147	-3.982953	-0.967539
1	-5.412799	-2.112909	-0.081594
6	-5.703425	-4.923779	-1.965594
1	-4.441607	-5.421148	-3.643021
1	-6.782210	-4.148144	-0.259705
1	-6.300177	-5.828447	-2.040069
6	-4.255179	0.327443	-1.517682
6	-5.603103	0.235790	-1.900811
6	-3.736760	1.574848	-1.146168
6	-6.416661	1.369746	-1.883464
1	-6.025103	-0.714813	-2.206016
6	-4.551200	2.707570	-1.126520
1	-2.695544	1.660313	-0.866045
6	-5.895769	2.605649	-1.488806
1	-7.460045	1.284424	-2.173650
1	-4.131996	3.660410	-0.819280
1	-6.534497	3.484154	-1.467136

(3-4)_{B1-LiHMDs.IDMPU*}

Number of imaginary frequencies : 1
 Electronic energy : HF=-5359.2387566
 Zero-point correction= 1.419085 (Hartree/Particle)
 Thermal correction to Energy= 1.512092
 Thermal correction to Enthalpy= 1.513036
 Thermal correction to Gibbs Free Energy= 1.289450
 Sum of electronic and zero-point Energies= -5357.819671
 Sum of electronic and thermal Energies= -5357.726664
 Sum of electronic and thermal Enthalpies= -5357.725720
 Sum of electronic and thermal Free Energies= -5357.949306
 Standard State and RRHO Corrected G= -5357.926775

Cartesian Coordinates

6	3.193455	-0.489551	5.533655
6	2.167707	0.321507	5.036570
6	1.476304	-0.053305	3.885441
6	1.826039	-1.233403	3.214954
6	2.858283	-2.041440	3.708466
6	3.533036	-1.674172	4.872666

6	1.074188	-1.647808	1.990506	1	6.393724	-5.478200	-1.719848
8	1.633922	-2.456809	1.189133	1	7.216916	-5.325744	-0.163674
6	0.393363	-3.786917	0.280264	6	5.541763	-3.211590	1.459544
6	-0.876932	-3.372061	-0.162396	1	5.108561	-2.244246	1.722997
6	-1.977041	-3.217785	0.758475	1	4.956119	-3.994500	1.958841
45	-1.468093	-1.196427	0.271528	1	6.561526	-3.255274	1.865478
8	-0.094588	-1.170683	1.874346	6	6.878878	-2.322206	-1.148263
15	0.252473	0.254260	-0.672885	1	7.825227	-2.393420	-0.594277
8	1.524469	-0.519652	-0.962609	1	7.089355	-2.584912	-2.192984
8	0.189751	1.276974	-2.040513	1	6.556905	-1.276633	-1.135825
6	-0.395747	2.513991	-2.053861	6	4.772831	-3.632243	-4.021727
6	0.149375	3.578554	-1.340462	1	4.403672	-4.051139	-4.967977
6	-0.572410	4.825492	-1.329576	1	4.970306	-2.565183	-4.187813
6	-1.739782	4.977818	-2.151627	1	5.736522	-4.111004	-3.807063
6	-2.165210	3.891252	-2.961552	6	1.900242	-3.119035	-3.222762
6	-1.518708	2.683463	-2.900407	1	1.948030	-2.026876	-3.175517
6	-2.466336	6.199169	-2.120456	1	1.693647	-3.417178	-4.258643
6	-2.082050	7.234023	-1.297645	6	3.180953	-5.766099	-2.559511
6	-0.946021	7.081923	-0.467124	1	2.448483	-6.015411	-1.779851
6	-0.210692	5.915801	-0.486117	1	2.775606	-6.122452	-3.516866
6	1.418772	3.407840	-0.581422	1	4.086871	-6.346810	-2.349330
6	2.547893	4.282030	-0.769702	1	1.041804	-3.431418	-2.617107
6	3.675542	4.177080	0.112404	1	4.372888	1.668262	-2.511878
6	3.674262	3.185131	1.129457	15	-2.913047	-0.225948	1.954248
6	2.646446	2.281916	1.221122	6	-2.234787	-0.475289	3.673343
6	1.541408	2.381702	0.345840	6	-1.786876	-1.738564	4.096916
6	4.784969	5.048289	-0.064293	6	-2.124260	0.597159	4.573339
6	4.808605	5.969754	-1.087968	6	-1.282580	-1.932218	5.381198
6	3.714223	6.052311	-1.981848	1	-1.798242	-2.576701	3.415635
6	2.614763	5.235519	-1.824700	6	-1.608844	0.404820	5.858609
8	0.532499	1.455702	0.499840	1	-2.433099	1.593942	4.286158
1	-0.652809	7.890157	0.197088	6	-1.190284	-0.859140	6.270703
1	0.645589	5.815987	0.169836	1	-0.941782	-2.920169	5.677724
1	-3.344289	6.293781	-2.754812	1	-1.534110	1.253466	6.532828
1	-2.650160	8.159570	-1.276206	1	-0.784068	-1.006183	7.267221
1	-3.032532	4.017340	-3.603768	6	-3.278385	1.585128	2.003399
1	-1.850328	1.831613	-3.481388	6	-2.334179	2.474890	1.474236
1	1.790122	5.306586	-2.524617	6	-4.410278	2.105435	2.655071
1	2.657939	1.473814	1.940709	6	-2.536570	3.854338	1.552900
1	3.743142	6.762297	-2.803743	1	-1.440559	2.094707	0.995139
1	5.623838	4.962826	0.622165	6	-4.616225	3.483813	2.722936
1	4.519478	3.123686	1.807680	1	-5.131543	1.442422	3.119372
1	5.665551	6.624527	-1.217983	6	-3.683993	4.362259	2.164535
1	-1.039043	-3.405019	-1.236960	1	-1.801321	4.528449	1.127237
1	0.473092	-4.295951	1.233860	1	-5.502754	3.868885	3.218978
1	1.179310	-4.002909	-0.432514	1	-3.846264	5.435442	2.212643
1	0.664136	0.550876	3.498853	6	-4.586063	-1.021439	2.016939
1	3.124067	-2.945543	3.174013	6	-4.743999	-2.287756	2.606033
1	1.899615	1.239395	5.551613	6	-5.699900	-0.432045	1.394706
1	4.330097	-2.304669	5.255807	6	-5.978676	-2.937261	2.585131
1	3.726057	-0.199635	6.435239	1	-3.908574	-2.777506	3.089165
1	-1.756723	-3.478146	1.791068	6	-6.936195	-1.081632	1.380059
1	-2.977706	-3.501590	0.457068	1	-5.614179	0.533661	0.914692
15	-2.969075	-1.158686	-1.536318	6	-7.082066	-2.336292	1.973765
8	4.095067	-0.350006	0.562193	1	-6.075618	-3.914866	3.048577
7	3.986023	-3.213652	-1.105541	1	-7.779638	-0.603580	0.890645
6	5.079710	0.399043	0.390004	1	-8.043023	-2.842294	1.958706
6	7.055969	1.605164	1.308752	6	-2.255310	-0.879751	-3.217719
6	6.544189	1.755360	-1.114176	6	-3.079350	-0.417885	-4.259863
6	7.641017	1.499208	-0.091368	6	-0.918124	-1.183327	-3.492276
1	6.763376	2.644732	1.526510	6	-2.562867	-0.243146	-5.542817
1	6.898180	1.506334	-2.120646	1	-4.121164	-0.181465	-4.074575
1	8.449692	2.224602	-0.220127	6	-0.403898	-1.009835	-4.779667
7	5.368823	0.930282	-0.835854	1	-0.263204	-1.536150	-2.706572
7	5.909389	0.713377	1.441881	6	-1.220969	-0.534840	-5.804767
1	8.055298	0.495827	-0.237399	1	-3.208415	0.124356	-6.335521
1	7.797088	1.313589	2.060909	1	0.638555	-1.239687	-4.970465
1	6.256455	2.816802	-1.120479	1	-0.816528	-0.391473	-6.802775
6	5.495358	0.399121	2.799381	6	-3.847792	-2.764725	-1.786253
1	5.342118	1.321387	3.376962	6	-3.394633	-3.686672	-2.741887
1	4.564192	-0.158234	2.773372	6	-4.919323	-3.124274	-0.951172
1	6.257959	-0.202199	3.308404	6	-4.004870	-4.938097	-2.861645
6	4.450758	0.731171	-1.949798	1	-2.568336	-3.435921	-3.398453
1	4.813086	-0.053927	-2.626337	6	-5.533306	-4.369151	-1.080818
1	3.460799	0.460696	-1.585863	1	-5.274353	-2.434253	-0.197868
14	5.526019	-3.465659	-0.426708	6	-5.075865	-5.281923	-2.035236
14	3.521877	-3.882566	-2.594367	1	-3.641344	-5.640333	-3.606353
3	2.954545	-1.684822	-0.273002	1	-6.364373	-4.623239	-0.429321
6	6.242338	-5.228384	-0.662252	1	-5.550882	-6.253832	-2.133592
1	5.579553	-5.992543	-0.236510	6	-4.301225	0.109555	-1.498117

6	-5.625372	-0.134515	-1.898769	1	3.061238	-3.145845	3.378639
6	-3.934027	1.406518	-1.121843	1	1.738372	1.152133	5.481270
6	-6.564561	0.897278	-1.879781	1	4.089909	-2.454855	5.541106
1	-5.931847	-1.122618	-2.220798	1	3.445820	-0.287388	6.578644
6	-4.873192	2.437884	-1.100649	1	-1.064226	-3.501945	1.713111
1	-2.911630	1.612275	-0.840524	1	-2.820601	-3.909487	1.280858
6	-6.194789	2.182126	-1.469643	15	-2.968990	-1.106034	-1.653552
1	-7.587855	0.694454	-2.182568	8	4.079628	-0.425770	0.672751
1	-4.566238	3.430724	-0.787395	7	4.131364	-2.992450	-1.384607
1	-6.932325	2.979386	-1.445621	6	5.078213	0.313421	0.556770
				6	7.028044	1.471841	1.581624
4BI-LiHMDS.IDMPU				6	6.572170	1.754166	-0.841333
				6	7.648456	1.458112	0.192513
Number of imaginary frequencies : 0				1	6.703687	2.490205	1.850634
Electronic energy : HF=-5359.2657734				1	6.948967	1.555718	-1.851361
Zero-point correction= 1.420281 (Hartree/Particle)				1	8.445312	2.204639	0.124323
Thermal correction to Energy= 1.514117				7	5.392349	0.916450	-0.630951
Thermal correction to Enthalpy= 1.515061				7	5.902598	0.545266	1.634514
Thermal correction to Gibbs Free Energy= 1.290396				1	8.087332	0.473003	0.002062
Sum of electronic and zero-point Energies= -5357.845492				1	7.758370	1.156435	2.334279
Sum of electronic and thermal Energies= -5357.751656				1	6.279647	2.813923	-0.805312
Sum of electronic and thermal Enthalpies= -5357.750712				6	5.484220	0.113282	2.958380
Sum of electronic and thermal Free Energies= -5357.975377				1	5.259654	0.979806	3.596100
Standard State and RRHO Corrected G= -5357.95333				1	4.591540	-0.499136	2.874074
				1	6.277555	-0.470579	3.439899
Cartesian Coordinates				6	4.457788	0.864423	-1.746721
				1	4.846615	0.230945	-2.553101
6	2.983811	-0.603549	5.647254	1	3.494785	0.479030	-1.419569
6	2.025571	0.206429	5.030392	14	5.515465	-3.512351	-0.547574
6	1.422252	-0.205714	3.841822	14	3.920450	-3.162589	-3.057022
6	1.797263	-1.415837	3.245424	3	3.001372	-1.754210	-0.265833
6	2.765283	-2.220750	3.860043	6	6.123126	-5.274133	-0.993515
6	3.345739	-1.822623	5.064691	1	5.335526	-6.021806	-0.834035
6	1.193338	-1.854148	1.936104	1	6.434427	-5.345908	-2.043516
8	1.836550	-2.629432	1.200807	1	6.985399	-5.568228	-0.378725
6	-0.325772	-3.023185	-0.900644	6	5.236082	-3.553650	1.333964
6	-1.497380	-3.642274	-0.383989	1	4.902076	-2.575958	1.691396
6	-1.835273	-3.588742	0.958908	1	4.462271	-4.285174	1.595750
45	-1.386231	-1.367259	0.097604	1	6.153769	-3.825989	1.872937
8	0.020361	-1.368871	1.712578	6	7.048448	-2.398786	-0.828945
15	0.249210	0.131053	-0.659236	1	7.849129	-2.592998	-0.101873
8	1.554309	-0.564656	-0.949957	1	7.470515	-2.547191	-1.830822
8	0.087989	1.156417	-1.990150	1	6.767789	-1.343952	-0.749706
6	-0.456958	2.417507	-2.002306	6	5.438366	-2.666609	-4.117720
6	0.078464	3.458029	-1.248593	1	5.221909	-2.732353	-5.192955
6	-0.626511	4.716236	-1.243498	1	5.756176	-1.637310	-3.907546
6	-1.744267	4.909422	-2.122272	1	6.299142	-3.318069	-3.919545
6	-2.138770	3.851423	-2.983515	6	2.478666	-2.119360	-3.729755
6	-1.521802	2.629705	-2.911465	1	2.524146	-1.077161	-3.399805
6	-2.449692	6.143231	-2.101546	1	2.472344	-2.142412	-4.827763
6	-2.090011	7.152010	-1.236373	6	3.502760	-4.943023	-3.625718
6	-1.002484	6.959965	-0.351446	1	2.604981	-5.312765	-3.112192
6	-0.288751	5.780329	-0.358414	1	3.309958	-4.996738	-4.706479
6	1.327821	3.272185	-0.462903	1	4.315078	-5.645163	-3.400994
6	2.460112	4.152682	-0.609042	1	1.522728	-2.525706	-3.383636
6	3.570003	4.026086	0.292260	1	4.315027	1.878745	-2.139321
6	3.557091	3.001097	1.275278	15	-2.803663	-0.307757	2.024351
6	2.531596	2.091561	1.322078	6	-2.096675	-0.639341	3.714987
6	1.440319	2.224691	0.437591	6	-1.670450	-1.928376	4.073837
6	4.679704	4.905444	0.162858	6	-1.986798	0.381141	4.673991
6	4.722455	5.851908	-0.836713	6	-1.184640	-2.198854	5.351893
6	3.649337	5.951412	-1.754088	1	-1.705465	-2.731978	3.355120
6	2.548636	5.129107	-1.641018	6	-1.492794	0.111635	5.953103
8	0.421129	1.289490	0.542311	1	-2.281258	1.395521	4.438005
1	-0.729563	7.747708	0.345071	6	-1.094101	-1.178515	6.300364
1	0.530631	5.650411	0.338133	1	-0.860944	-3.206156	5.597632
1	-3.290304	6.268844	-2.779378	1	-1.417440	0.920657	6.674335
1	-2.641180	8.087834	-1.223702	1	-0.703822	-1.384975	7.292637
1	-2.961067	4.009299	-3.675819	6	-3.172894	1.500650	2.172413
1	-1.834360	1.801780	-3.533301	6	-2.247989	2.427951	1.675373
1	1.741308	5.214779	-2.358877	6	-4.297960	1.976523	2.869168
1	2.542882	1.255237	2.006729	6	-2.459674	3.799414	1.832166
1	3.695501	6.679244	-2.559296	1	-1.363959	2.082060	1.157254
1	5.503441	4.804165	0.865081	6	-4.512714	3.347004	3.017291
1	4.395775	2.913632	1.958903	1	-5.008678	1.284552	3.306111
1	5.579519	6.512492	-0.931190	6	-3.597866	4.263707	2.492847
1	-2.256932	-3.967085	-1.084838	1	-1.739397	4.501376	1.425629
1	0.595094	-3.022503	-0.328669	1	-5.393268	3.695587	3.549616
1	-0.211584	-3.018263	-1.978460	1	-3.767757	5.330999	2.604193
1	0.659490	0.397936	3.365499	6	-4.490249	-1.080619	2.122246

6	-4.683099	-2.325139	2.746016	6	-3.912271	2.416466	-2.257604
6	-5.587827	-0.480699	1.481415	6	-2.851571	1.569146	-2.460369
6	-5.930601	-2.951295	2.722351	6	-4.891233	4.391752	-1.138017
1	-3.866181	-2.818261	3.257221	6	-4.773198	5.466000	-0.285774
6	-6.835392	-1.106748	1.462140	6	-3.522469	5.749426	0.314338
1	-5.479854	0.479105	0.995107	6	-2.418692	4.970224	0.043086
6	-7.012487	-2.346417	2.077703	6	-0.029932	3.256568	-0.534288
1	-6.053992	-3.912927	3.212318	6	0.700632	4.472303	-0.769236
1	-7.663839	-0.620917	0.955145	6	1.945186	4.689271	-0.085791
1	-7.982069	-2.835458	2.058791	6	2.446090	3.685802	0.787284
6	-2.348629	-0.754379	-3.356723	6	1.780522	2.495240	0.940864
6	-3.254094	-0.285105	-4.327771	6	0.560707	2.283140	0.261071
6	-1.014961	-0.963743	-3.722629	6	2.664788	5.894378	-0.312610
6	-2.824262	-0.024009	-5.627459	6	2.198207	6.844570	-1.193344
1	-4.293693	-0.112525	-4.072602	6	0.986852	6.620817	-1.891583
6	-0.586113	-0.701263	-5.025497	6	0.258584	5.469217	-1.684459
1	-0.288821	-1.299520	-2.997739	8	-0.066737	1.065235	0.432888
6	-1.486333	-0.228551	-5.979218	1	-3.433289	6.585891	1.002040
1	-3.534027	0.344152	-6.362641	1	-1.475797	5.195458	0.526723
1	0.457227	-0.858611	-5.278034	1	-5.848069	4.149913	-1.593994
1	-1.150118	-0.016634	-6.990160	1	-5.634831	6.089081	-0.063863
6	-4.003684	-2.613817	-1.913272	1	-4.878195	2.197018	-2.702221
6	-3.967556	-3.345449	-3.109074	1	-2.952321	0.670921	-3.059060
6	-4.805265	-3.072689	-0.854365	1	-0.662131	5.309006	-2.233822
6	-4.722541	-4.514699	-3.240068	1	2.173372	1.693150	1.551961
1	-3.350453	-3.017632	-3.937697	1	0.630674	7.361855	-2.601794
6	-5.562570	-4.233924	-0.992529	1	3.601021	6.046258	0.219275
1	-4.832779	-2.526700	0.078067	1	3.379598	3.862789	1.311769
6	-5.521014	-4.960967	-2.186121	1	2.759588	7.759003	-1.362796
1	-4.682863	-5.074136	-4.170209	1	0.460918	-3.773024	-1.123701
1	-6.180144	-4.568594	-0.164352	1	0.896510	-4.192251	1.783991
1	-6.105819	-5.870116	-2.292040	1	2.109733	-3.748524	0.522668
6	-4.224117	0.219107	-1.429192	1	-1.033600	0.558673	2.987367
6	-5.575106	0.038015	-1.773827	1	2.704366	-1.498875	3.557825
6	-3.801840	1.469501	-0.966457	1	-0.395842	2.206967	4.736775
6	-6.479586	1.091026	-1.638674	1	3.343461	0.144747	5.307215
1	-5.926675	-0.920058	-2.138393	1	1.798006	2.001595	5.887149
6	-4.708368	2.521135	-0.825938	1	-1.501855	-4.348655	1.214516
1	-2.765873	1.624534	-0.703553	1	-1.824096	-4.630238	-0.561120
6	-6.050435	2.332381	-1.157724	8	3.999007	0.201033	0.468667
1	-7.522097	0.938023	-1.902398	7	3.828156	-2.781167	-0.913637
1	-4.360126	3.475970	-0.446126	6	4.798444	1.139221	0.249463
1	-6.760296	3.146445	-1.042281	6	6.235199	2.998747	1.112093
				6	5.908399	2.681943	-1.329440
(3...4)_{B1} (after dissociation of PPh3 group)				6	6.936263	2.942088	-0.237312
				1	5.668760	3.937372	1.208700
Number of imaginary frequencies : 0				1	6.400267	2.558158	-2.297751
Electronic energy : HF=-4322.8133954				1	7.459864	3.884561	-0.422248
Zero-point correction= 1.141854 (Hartree/Particle)				7	5.184036	1.446594	-1.027526
Thermal correction to Energy= 1.219281				7	5.334463	1.859539	1.287046
Thermal correction to Enthalpy= 1.220225				1	7.676111	2.133941	-0.240369
Thermal correction to Gibbs Free Energy= 1.024463				1	6.966987	2.979758	1.927627
Sum of electronic and zero-point Energies= -4321.671541				1	5.211039	3.528936	-1.417042
Sum of electronic and thermal Energies= -4321.594115				6	4.871937	1.623174	2.645424
Sum of electronic and thermal Enthalpies= -4321.593171				1	4.337806	2.501144	3.032902
Sum of electronic and thermal Free Energies= -4321.788933				1	4.200320	0.769594	2.658753
Standard State and RRHO Corrected G= -4321.767225				1	5.724075	1.419972	3.304993
				6	4.518134	0.743610	-2.123397
Cartesian Coordinates				1	4.605994	-0.338168	-1.989194
				1	3.455699	1.002517	-2.193972
6	1.512592	1.275718	5.131166	14	5.168951	-3.090425	0.086530
6	0.275743	1.391455	4.486698	14	3.517559	-3.535408	-2.402562
6	-0.091599	0.467639	3.513836	3	2.957180	-1.071958	-0.494150
6	0.788367	-0.577128	3.181150	6	5.755916	-4.912240	0.107511
6	2.029162	-0.695643	3.828922	1	4.956477	-5.584298	0.445168
6	2.384749	0.232000	4.805547	1	6.075265	-5.257062	-0.883787
6	0.412549	-1.510365	2.110573	1	6.607015	-5.047937	0.788898
8	1.386750	-2.208419	1.589255	6	4.796811	-2.681603	1.909309
6	1.124418	-3.536879	0.938268	1	4.511976	-1.629820	2.004284
6	0.063965	-3.601637	-0.125021	1	3.970084	-3.294261	2.289248
6	-1.258555	-4.075848	0.188147	1	5.669526	-2.862287	2.551273
45	-1.285207	-1.978472	-0.187485	6	6.714334	-2.075228	-0.391687
8	-0.790097	-1.567645	1.733706	1	7.552080	-2.227965	0.302530
15	-0.015579	-0.061564	-0.846517	1	7.064017	-2.351181	-1.395062
8	1.437189	-0.273211	-1.242418	1	6.486269	-1.003053	-0.410457
8	-0.573142	0.958605	-2.099616	6	5.022152	-3.626417	-3.580747
6	-1.596662	1.847708	-1.869526	1	4.761887	-4.093254	-4.540633
6	-1.378413	2.997157	-1.113984	1	5.411425	-2.623308	-3.798553
6	-2.498983	3.856630	-0.842318	1	5.845305	-4.208161	-3.147136
6	-3.775615	3.560261	-1.428711	6	2.176582	-2.627627	-3.406083

1	1.277937	-2.437879	-2.810864	6	-2.873844	1.513263	-2.479712
1	2.534112	-1.648803	-3.748635	6	-4.973475	4.296687	-1.168116
6	2.911007	-5.342972	-2.242747	6	-4.874816	5.383408	-0.329341
1	2.022841	-5.415571	-1.602015	6	-3.625071	5.708425	0.251436
1	2.650321	-5.776486	-3.217958	6	-2.503716	4.956645	-0.024588
1	3.683308	-5.981431	-1.796230	6	-0.077609	3.293884	-0.602243
1	1.892732	-3.208474	-4.294312	6	0.628736	4.520915	-0.851402
1	5.016267	1.012040	-3.056996	6	1.880073	4.760088	-0.187426
15	-3.635292	-1.414266	0.145246	6	2.411198	3.768018	0.681196
6	-4.543649	-2.753870	1.027675	6	1.763858	2.570207	0.854105
6	-4.058256	-3.129933	2.293009	6	0.537107	2.337631	0.195219
6	-5.658748	-3.417705	0.499303	6	2.576305	5.976041	-0.428125
6	-4.685209	-4.141727	3.018305	6	2.080252	6.916753	-1.302847
1	-3.184096	-2.631465	2.704455	6	0.862238	6.671416	-1.981992
6	-6.279276	-4.439911	1.225357	6	0.156802	5.507972	-1.762307
1	-6.048933	-3.138785	-0.474590	8	-0.068444	1.111449	0.382976
6	-5.797366	-4.801976	2.484036	1	-3.550754	6.554689	0.928825
1	-4.302871	-4.420910	3.996302	1	-1.561708	5.212641	0.445205
1	-7.142625	-4.948499	0.805022	1	-5.929025	4.022889	-1.608393
1	-6.281872	-5.595314	3.046142	1	-5.750682	5.984728	-0.103131
6	-4.220415	0.081567	1.040662	1	-4.920094	2.082879	-2.703636
6	-3.310373	1.123284	1.267582	1	-2.957437	0.602801	-3.062915
6	-5.536385	0.201782	1.520720	1	-0.769323	5.331425	-2.297408
6	-3.712315	2.273991	1.950722	1	2.174547	1.776293	1.464267
1	-2.291092	1.039307	0.910793	1	0.482763	7.405249	-2.687616
6	-5.937552	1.358545	2.189529	1	3.518359	6.143617	0.088627
1	-6.244996	-0.608788	1.377081	1	3.351407	3.960929	1.187918
6	-5.026067	2.397598	2.404344	1	2.623563	7.840139	-1.482347
1	-3.000121	3.076637	2.111085	1	0.291821	-3.922793	-1.195270
1	-6.959571	1.446711	2.547694	1	0.963036	-4.045246	1.766316
1	-5.339541	3.297784	2.925494	1	2.104016	-3.693108	0.346009
6	-4.407304	-1.362444	-1.521402	1	-1.093107	0.562811	3.090383
6	-3.726861	-2.062853	-2.532101	1	2.690044	-1.420438	3.567004
6	-5.562801	-0.642642	-1.851138	1	-0.562680	2.048808	5.014514
6	-4.186893	-2.043892	-3.848870	1	3.220520	0.049011	5.506403
1	-2.822656	-2.622011	-2.283424	1	1.596716	1.790780	6.218402
6	-6.024348	-0.622375	-3.169680	1	-1.545989	-4.197689	1.320101
1	-6.091346	-0.080331	-1.088434	1	-2.011459	-4.567939	-0.403444
6	-5.338258	-1.318028	-4.168959	8	3.957597	0.162477	0.599326
1	-3.646647	-2.583865	-4.621095	7	3.755617	-2.761134	-0.940338
1	-6.917647	-0.055911	-3.417683	6	4.749265	1.108981	0.392872
1	-5.696726	-1.292178	-5.193925	6	6.139172	2.993287	1.295576
				6	5.871664	2.668845	-1.151345
(3-4)_{B1}⁺ (after dissociation of PPh3 group)				6	6.870442	2.951606	-0.038258
				1	5.570397	3.930686	1.390491
Number of imaginary frequencies : 1				1	6.384203	2.567256	-2.111376
Electronic energy : HF=-4322.8033158				1	7.378776	3.904705	-0.211180
Zero-point correction= 1.139675 (Hartree/Particle)				7	5.181530	1.409243	-0.871903
Thermal correction to Energy= 1.216809				7	5.233302	1.853913	1.440718
Thermal correction to Enthalpy= 1.217753				1	7.626593	2.158834	-0.026751
Thermal correction to Gibbs Free Energy= 1.022567				1	6.852928	2.967583	2.127127
Sum of electronic and zero-point Energies= -4321.663641				1	5.149584	3.494251	-1.246860
Sum of electronic and thermal Energies= -4321.586507				6	4.714424	1.632142	2.781175
Sum of electronic and thermal Enthalpies= -4321.585563				1	4.143669	2.504357	3.127527
Sum of electronic and thermal Free Energies= -4321.780749				1	4.062465	0.763397	2.780073
Standard State and RRHO Corrected G= -4321.758946				1	5.539711	1.460663	3.482626
				6	4.570534	0.699850	-1.995016
Cartesian Coordinates				1	4.544629	-0.373100	-1.794840
				1	3.547520	1.040890	-2.189550
6	1.360578	1.138688	5.382214	14	5.115923	-3.120761	0.016109
6	0.143745	1.283491	4.706967	14	3.468158	-3.371658	-2.498873
6	-0.162272	0.450858	3.633279	3	2.849361	-1.103596	-0.324252
6	0.759941	-0.526855	3.228193	6	5.713896	-4.936557	-0.086786
6	1.982075	-0.670395	3.902012	1	4.917202	-5.638669	0.190523
6	2.275727	0.159683	4.982702	1	6.045125	-5.201701	-1.098806
6	0.470782	-1.377708	2.049917	1	6.560675	-5.116528	0.589712
8	1.443494	-1.943252	1.455549	6	4.764466	-2.814636	1.863127
6	1.097319	-3.654710	0.760855	1	4.486710	-1.767592	2.017777
6	0.009234	-3.772328	-0.154974	1	3.936888	-3.439785	2.220095
6	-1.350208	-4.015741	0.264081	1	5.643197	-3.035041	2.484164
45	-1.242377	-1.946323	-0.195166	6	6.659355	-2.080602	-0.414817
8	-0.759668	-1.479120	1.700523	1	7.506839	-2.298903	0.249540
15	0.022274	-0.020992	-0.888650	1	6.988363	-2.279020	-1.443031
8	1.482213	-0.188724	-1.268474	1	6.446661	-1.007915	-0.343125
8	-0.575647	0.969690	-2.142873	6	4.957797	-3.221967	-3.689772
6	-1.619876	1.834802	-1.909665	1	4.724013	-3.601094	-4.694000
6	-1.423939	2.998631	-1.169953	1	5.268598	-2.174562	-3.796717
6	-2.563950	3.831189	-0.896412	1	5.826352	-3.783029	-3.322087
6	-3.838864	3.492982	-1.463485	6	2.037013	-2.489663	-3.393684
6	-3.954747	2.334304	-2.274838	1	1.097942	-2.571291	-2.835145

1	2.231535	-1.419279	-3.513391	6	-4.997672	4.303120	-1.107187
6	2.985362	-5.223357	-2.522671	6	-4.903041	5.335680	-0.202320
1	2.126857	-5.413465	-1.864814	6	-3.662822	5.606839	0.423991
1	2.710267	-5.563534	-3.530498	6	-2.545040	4.857956	0.126540
1	3.806150	-5.861289	-2.173464	6	-0.121852	3.236529	-0.528990
1	1.880946	-2.927937	-4.389102	6	0.573410	4.482443	-0.715463
1	5.184882	0.870075	-2.882478	6	1.817601	4.701372	-0.031824
15	-3.531408	-1.449996	0.168653	6	2.353283	3.676161	0.794601
6	-4.389637	-2.759520	1.133418	6	1.719236	2.463905	0.904901
6	-3.933387	-2.998769	2.441985	6	0.504921	2.254828	0.221868
6	-5.436798	-3.534076	0.618033	6	2.504451	5.932941	-0.212277
6	-4.524580	-3.990471	3.222351	6	2.006960	6.906403	-1.049334
1	-3.110197	-2.411934	2.841762	6	0.796905	6.681164	-1.748853
6	-6.022068	-4.533486	1.402615	6	0.099179	5.503889	-1.585640
1	-5.801256	-3.359438	-0.389575	8	-0.084458	1.001105	0.335350
6	-5.570253	-4.762246	2.702999	1	-3.592625	6.408803	1.153524
1	-4.166481	-4.166178	4.232938	1	-1.611087	5.072137	0.631745
1	-6.834319	-5.128807	0.994771	1	-5.945835	4.071168	-1.585641
1	-6.027266	-5.538462	3.310147	1	-5.775610	5.935036	0.040939
6	-4.131481	0.075325	0.990448	1	-4.929222	2.200112	-2.793600
6	-3.221530	1.105204	1.260552	1	-2.983400	0.712378	-3.188014
6	-5.472604	0.213589	1.391136	1	-0.820613	5.343804	-2.136287
6	-3.648652	2.265346	1.911830	1	2.133583	1.640730	1.470708
1	-2.185223	1.006134	0.963714	1	0.417398	7.441480	-2.425710
6	-5.897418	1.382316	2.022218	1	3.440535	6.085852	0.319324
1	-6.181135	-0.590882	1.216048	1	3.289911	3.852325	1.313842
6	-4.985384	2.410633	2.283257	1	2.543668	7.841116	-1.184044
1	-2.936251	3.059022	2.110497	1	-1.051341	-4.218912	-2.284374
1	-6.937694	1.487446	2.317304	1	1.008328	-3.335885	-0.129196
1	-5.317250	3.319787	2.776413	1	1.078587	-3.050757	-1.928022
6	-4.273145	-1.521068	-1.506395	1	-1.640180	-0.628243	3.305445
6	-3.612007	-2.342503	-2.438130	1	2.547133	-1.549994	3.538179
6	-5.381965	-0.771768	-1.920006	1	-1.621985	0.095094	5.683258
6	-4.043671	-2.403985	-3.763357	1	2.575164	-0.837966	5.928076
1	-2.758518	-2.943913	-2.119912	1	0.487283	-0.009989	6.995401
6	-5.816909	-0.839831	-3.245394	1	-1.368855	-4.211471	0.800500
1	-5.891923	-0.118678	-1.220412	1	-2.631031	-4.647057	-0.474903
6	-5.148054	-1.648627	-4.168332	8	3.937094	0.241969	0.718828
1	-3.520766	-3.036082	-4.475103	7	4.050778	-2.466773	-1.079133
1	-6.675650	-0.253072	-3.559015	6	4.755552	1.183211	0.703759
1	-5.485604	-1.690147	-5.199768	6	6.034696	2.948096	1.946691
4_{B1} (after dissociation of PPh3 group)				6	6.062401	2.869979	-0.536329
Number of imaginary frequencies : 0				6	6.920540	3.025404	0.711281
Electronic energy : HF=-4322.8371011				1	5.457456	3.878599	2.062490
Zero-point correction= 1.141480 (Hartree/Particle)				1	6.687316	2.850978	-1.433481
Thermal correction to Energy= 1.219164				1	7.451194	3.981903	0.695576
Thermal correction to Enthalpy= 1.220108				7	5.332397	1.605276	-0.466746
Thermal correction to Gibbs Free Energy= 1.024751				7	5.120737	1.808633	1.872947
Sum of electronic and zero-point Energies= -4321.695622				1	7.665587	2.222480	0.734682
Sum of electronic and thermal Energies= -4321.617937				1	6.644820	2.837291	2.850587
Sum of electronic and thermal Enthalpies= -4321.616993				1	5.365150	3.716388	-0.638287
Sum of electronic and thermal Free Energies= -4321.812350				6	4.457974	1.453582	3.118869
Standard State and RRHO Corrected G= -4321.791215				1	3.877757	2.303145	3.503739
Cartesian Coordinates				1	3.787589	0.613479	2.952102
				1	5.200106	1.173597	3.876277
6	0.476367	-0.331040	5.957481	6	4.828757	1.038627	-1.715465
6	-0.710905	-0.274825	5.221535	1	4.684749	-0.036695	-1.602833
6	-0.728066	-0.686988	3.888707	1	3.875864	1.493077	-2.015526
6	0.450613	-1.148723	3.285594	14	5.234892	-2.942246	0.042946
6	1.642707	-1.197633	4.022717	14	4.095285	-2.867068	-2.726502
6	1.651783	-0.795098	5.357427	3	2.860922	-1.041469	-0.291133
6	0.490625	-1.523410	1.835087	6	5.822316	-4.758929	-0.123080
8	1.552333	-1.524798	1.211761	1	4.984214	-5.458059	-0.004998
6	0.465996	-3.284147	-1.065874	1	6.278318	-4.958728	-1.100938
6	-0.723062	-4.039074	-1.258653	1	6.569642	-5.011524	0.642021
6	-1.655857	-4.230203	-0.246408	6	4.621693	-2.798232	1.840082
45	-1.185759	-1.914523	-0.590596	1	4.328687	-1.765891	2.051218
8	-0.693184	-1.825127	1.353055	1	3.746833	-3.436935	2.012122
15	0.061547	-0.016963	-0.988779	1	5.401380	-3.094610	2.555054
8	1.503581	-0.138346	-1.413573	6	6.839288	-1.903822	-0.048344
8	-0.633169	0.957509	-2.177339	1	7.548041	-2.155126	0.752979
6	-1.664629	1.837762	-1.911908	1	7.355628	-2.061709	-1.003774
6	-1.462859	2.960812	-1.114784	1	6.616215	-0.832770	0.025255
6	-2.600965	3.788828	-0.813003	6	5.825765	-2.769647	-3.543504
6	-3.866580	3.503501	-1.426255	1	5.777238	-2.999581	-4.616928
6	-3.975524	2.404492	-2.317307	1	6.251207	-1.762823	-3.442703
6	-2.903053	1.577834	-2.540945	1	6.537767	-3.471603	-3.091892
				6	3.021428	-1.711278	-3.795605
				1	2.007351	-1.601844	-3.400375
				1	3.448819	-0.701324	-3.826081

6	3.484809	-4.640873	-3.112502
1	2.467455	-4.805874	-2.734558
1	3.478229	-4.853822	-4.190505
1	4.128315	-5.389664	-2.633298
1	2.960160	-2.076049	-4.830237
1	5.570250	1.215663	-2.499019
15	-3.487428	-1.375913	0.063615
6	-4.256790	-2.770262	0.985159
6	-3.680621	-3.126447	2.217088
6	-5.365922	-3.481380	0.510376
6	-4.212471	-4.177950	2.961099
1	-2.807557	-2.592554	2.580423
6	-5.892314	-4.538889	1.259661
1	-5.824032	-3.214005	-0.436648
6	-5.319337	-4.888093	2.483349
1	-3.759942	-4.446718	3.911547
1	-6.753272	-5.085205	0.884677
1	-5.730601	-5.709486	3.063066
6	-3.994807	0.049183	1.102091
6	-3.082221	1.077593	1.362778
6	-5.281063	0.105708	1.671161
6	-3.454436	2.161958	2.161962
1	-2.083733	1.031123	0.952338
6	-5.652401	1.197988	2.453435
1	-5.987046	-0.703562	1.510866
6	-4.740015	2.230346	2.697670
1	-2.738005	2.954237	2.352124
1	-6.650946	1.239734	2.879193
1	-5.030701	3.079256	3.309979
6	-4.411467	-1.270374	-1.519033
6	-3.841120	-1.901955	-2.639235
6	-5.615002	-0.568831	-1.672919
6	-4.460094	-1.830648	-3.887960
1	-2.902137	-2.447585	-2.548535
6	-6.236576	-0.504600	-2.921205
1	-6.060068	-0.053277	-0.829308
6	-5.661029	-1.131001	-4.029978
1	-4.003206	-2.315466	-4.745676
1	-7.168224	0.043426	-3.028549
1	-6.144370	-1.071352	-5.000671

(3...4)B2-LiHMDS.IDMPU

Number of imaginary frequencies : 0
 Electronic energy : HF=-5699.3381594
 Zero-point correction= 1.454487 (Hartree/Particle)
 Thermal correction to Energy= 1.551046
 Thermal correction to Enthalpy= 1.551990
 Thermal correction to Gibbs Free Energy= 1.320574
 Sum of electronic and zero-point Energies= -5697.883673
 Sum of electronic and thermal Energies= -5697.787114
 Sum of electronic and thermal Enthalpies= -5697.786170
 Sum of electronic and thermal Free Energies= -5698.017586
 Standard State and RRHO Corrected G= -5697.993981

Cartesian Coordinates

6	-3.769214	1.598670	-4.440326
6	-2.788049	1.996889	-3.527359
6	-1.726101	1.146229	-3.231514
6	-1.645835	-0.111482	-3.845719
6	-2.634277	-0.514258	-4.755341
6	-3.689123	0.345904	-5.056801
6	-0.531653	-1.006817	-3.460630
8	-0.759420	-2.268140	-3.736202
6	0.182386	-3.385885	-3.605161
6	1.429364	-3.273318	-2.762209
6	2.565216	-2.490183	-3.149064
45	1.653179	-1.591615	-1.438480
8	0.505481	-0.546808	-2.943894
15	-0.287707	-0.945736	-0.109518
8	-1.557916	-0.950703	-0.943823
8	-0.926545	-1.461345	1.395835
6	-0.342418	-1.191797	2.608047
6	-0.255429	0.104718	3.112567
6	0.516351	0.297893	4.316487
6	0.993539	-0.839445	5.050376
6	0.722946	-2.144785	4.560568
6	0.093999	-2.313505	3.354730
6	1.769398	-0.642963	6.224403

6	2.103259	0.622360	6.652409
6	1.670943	1.747521	5.910441
6	0.895726	1.590245	4.781095
6	-0.892761	1.256422	2.414942
6	-1.755875	2.183911	3.103077
6	-2.194082	3.374488	2.430857
6	-1.820320	3.589733	1.076926
6	-1.094125	2.645671	0.400317
6	-0.653206	1.478827	1.066415
6	-3.005267	4.312513	3.125275
6	-3.404378	4.085713	4.424117
6	-3.014839	2.891178	5.075347
6	-2.215868	1.968644	4.433085
8	0.137946	0.619496	0.348638
1	1.957430	2.745846	6.229515
1	0.589857	2.464706	4.219701
1	2.114766	-1.519379	6.767114
1	2.707379	0.759739	7.544663
1	1.058083	-3.006915	5.130692
1	-0.089530	-3.296592	2.940981
1	-1.935984	1.056878	4.947073
1	-0.818549	2.778280	-0.638903
1	-3.352116	2.695687	6.089453
1	-3.311434	5.215641	2.603137
1	-2.132715	4.501930	0.577102
1	-4.026377	4.809672	4.942694
1	1.629747	-4.231031	-2.284902
1	0.447447	-3.617198	-4.644137
1	-0.455826	-4.183141	-3.225749
1	-0.968739	1.427280	-2.513222
1	-2.575746	-1.493877	-5.216197
1	-2.848183	2.967861	-3.047187
1	-4.453416	0.035323	-5.762669
1	-4.600377	2.260662	-4.665838
1	2.479671	-1.817037	-4.001115
1	3.566265	-2.876147	-2.988412
6	2.178467	3.351070	-2.008992
6	1.066950	4.225034	-2.286153
6	2.345301	2.243850	-2.829924
6	0.653004	5.243094	-1.381733
6	0.307109	4.040916	-3.488345
6	1.608838	2.066918	-4.022161
6	-0.434371	6.043657	-1.659922
1	1.187251	5.369458	-0.447480
6	-0.794207	4.898479	-3.756740
6	0.637015	2.971839	-4.364943
1	1.825036	1.200253	-4.635025
6	-1.161387	5.880881	-2.863789
1	-0.739322	6.802504	-0.944940
1	-1.355997	4.746034	-4.674317
1	0.067538	2.845289	-5.280611
1	-2.012365	6.522327	-3.073900
8	3.308293	1.288070	-2.537364
6	3.129392	3.617239	-0.894983
6	3.829265	4.873433	-0.779159
6	3.405352	2.639024	0.046794
6	3.755567	5.890825	-1.772146
6	4.667375	5.112262	0.362084
6	4.228492	2.869212	1.173013
6	4.432503	7.082664	-1.625800
1	3.166155	5.720354	-2.664751
6	5.340347	6.357614	0.489362
6	4.830303	4.090553	1.336926
1	4.363075	2.061655	1.883715
6	5.223153	7.329415	-0.478692
1	4.361917	7.838106	-2.403348
1	5.960387	6.522993	1.366814
1	5.456166	4.283160	2.203973
1	5.744653	8.276246	-0.372661
8	2.815491	1.390273	-0.036777
15	3.088466	0.264128	-1.222191
8	4.637716	-0.188308	-1.060135
6	5.776727	0.701667	-1.007228
1	6.629033	0.136350	-1.390302
1	5.618657	1.588309	-1.624117
1	5.964072	0.992981	0.028719
8	-3.799947	0.827287	0.180311
7	-4.781226	-2.146411	-1.061119
6	-4.593295	1.336802	1.003722
6	-6.154714	3.156982	1.654699

6	-5.823241	1.221983	3.178138
6	-6.859777	2.109714	2.504153
1	-5.600587	3.862438	2.290394
1	-6.308254	0.345796	3.622923
1	-7.483469	2.593439	3.261672
7	-4.834886	0.742715	2.210363
7	-5.247239	2.506292	0.713771
1	-7.509054	1.501858	1.864968
1	-6.881780	3.734029	1.073930
1	-5.311403	1.763334	3.984304
6	-4.909830	3.253699	-0.486661
1	-4.135322	2.723969	-1.035315
1	-5.791385	3.369907	-1.128827
1	-4.539615	4.251891	-0.220943
6	-4.101491	-0.458763	2.585761
1	-4.712685	-1.356038	2.437447
1	-3.192596	-0.546438	1.994527
14	-6.357936	-1.545073	-1.207503
14	-4.235186	-3.702547	-0.664801
3	-3.403146	-0.773115	-0.719796
6	-7.561089	-2.606300	-2.250077
1	-7.135004	-2.840415	-3.234302
1	-7.807726	-3.557829	-1.765064
1	-8.506054	-2.071796	-2.420670
6	-6.354923	0.154269	-2.068133
1	-5.644339	0.831188	-1.586741
1	-6.051187	0.052558	-3.117050
1	-7.345250	0.629097	-2.050532
6	-7.255852	-1.301965	0.463513
1	-8.256780	-0.864064	0.345108
1	-7.376974	-2.260154	0.986427
1	-6.675473	-0.644259	1.118617
6	-5.484589	-5.127283	-0.927124
1	-5.025881	-6.096243	-0.685813
1	-6.369527	-5.019708	-0.287031
1	-5.834082	-5.178782	-1.965380
6	-3.706160	-3.862947	1.164293
1	-4.551899	-3.636486	1.826593
1	-3.362104	-4.874641	1.415738
6	-2.708444	-4.154586	-1.705058
1	-1.951637	-3.375915	-1.573500
1	-2.276465	-5.128122	-1.438854
1	-2.966615	-4.180258	-2.771288
1	-2.896506	-3.164222	1.406764
1	-3.825132	-0.389417	3.642546
15	2.719566	-2.915279	0.101909
6	3.594103	-2.073208	1.489183
6	3.047966	-0.904660	2.037605
6	4.768241	-2.606067	2.050024
6	3.664697	-0.280114	3.123490
1	2.150058	-0.468354	1.621606
6	5.382302	-1.976957	3.133847
1	5.208706	-3.510530	1.645550
6	4.832210	-0.811676	3.672850
1	3.222293	0.616800	3.543075
1	6.289308	-2.400893	3.555535
1	5.305636	-0.323556	4.520005
6	1.646346	-4.154129	0.946253
6	0.391129	-4.487826	0.421661
6	2.106832	-4.816762	2.096742
6	-0.393613	-5.464268	1.039603
1	0.018582	-3.980108	-0.459468
6	1.318249	-5.786056	2.715081
1	3.073274	-4.570026	2.522496
6	0.064358	-6.111196	2.188390
1	-1.365286	-5.707066	0.624847
1	1.681060	-6.282949	3.610319
1	-0.552664	-6.862332	2.673243
6	4.023716	-3.977804	-0.656018
6	5.236994	-3.396654	-1.065255
6	3.799501	-5.338431	-0.908723
6	6.208817	-4.168085	-1.700258
1	5.409600	-2.340522	-0.892918
6	4.773353	-6.106056	-1.554374
1	2.871581	-5.807880	-0.599991
6	5.978952	-5.525158	-1.948733
1	7.144617	-3.708090	-2.005194
1	4.586318	-7.159386	-1.742821
1	6.736148	-6.124159	-2.446628

(3-4)B2-LHMDS.IDMPU[‡]

Number of imaginary frequencies : 1
 Electronic energy : HF=-5699.3078852
 Zero-point correction= 1.450676 (Hartree/Particle)
 Thermal correction to Energy= 1.547593
 Thermal correction to Enthalpy= 1.548537
 Thermal correction to Gibbs Free Energy= 1.315314
 Sum of electronic and zero-point Energies= -5697.857209
 Sum of electronic and thermal Energies= -5697.760293
 Sum of electronic and thermal Enthalpies= -5697.759348
 Sum of electronic and thermal Free Energies= -5697.992571
 Standard State and RRHO Corrected G= -5697.968039

Cartesian Coordinates

6	0.489924	-4.837735	-2.805846
6	-0.485108	-4.096381	-2.132267
6	-0.339162	-2.719055	-1.988771
6	0.798996	-2.079408	-2.499899
6	1.775643	-2.821671	-3.175732
6	1.615087	-4.198334	-3.335642
6	0.973298	-0.618727	-2.259398
8	2.151965	-0.144271	-2.201569
6	2.308072	1.765565	-2.754366
6	1.386802	2.720905	-2.251179
6	0.064921	2.876005	-2.803181
45	-0.245028	1.841843	-0.950495
8	-0.087604	0.066406	-2.118593
15	0.874013	0.556325	0.793945
8	2.388585	0.545986	0.662932
8	0.697837	0.642648	2.491771
6	-0.451485	0.252703	3.131340
6	-0.861439	-1.079066	3.145453
6	-2.167419	-1.373126	3.671086
6	-2.909887	-0.346828	4.346831
6	-2.338913	0.947224	4.475888
6	-1.153890	1.247812	3.852261
6	-4.211406	-0.635794	4.841413
6	-4.779550	-1.877092	4.657772
6	-4.058787	-2.885869	3.973263
6	-2.786390	-2.644227	3.502393
6	0.045639	-2.146869	2.643826
6	0.446623	-3.254917	3.473692
6	1.288993	-4.279149	2.920498
6	1.745373	-4.158456	1.580543
6	1.420239	-3.060128	0.827366
6	0.586461	-2.055955	1.370433
6	1.680848	-5.378663	3.732228
6	1.287096	-5.466040	5.048888
6	0.486087	-4.442310	5.608669
6	0.077684	-3.370041	4.844374
8	0.249737	-0.995446	0.560314
1	-4.516542	-3.857755	3.811882
1	-2.251160	-3.423244	2.971076
1	-4.755946	0.151812	5.356709
1	-5.779477	-2.083357	5.028716
1	-2.880684	1.713934	5.021941
1	-0.734906	2.247868	3.875530
1	-0.524970	-2.592253	5.297830
1	1.805470	-2.924029	-0.172568
1	0.194832	-4.498134	6.653902
1	2.309202	-6.148163	3.290149
1	2.383652	-4.934588	1.167141
1	1.596861	-6.308507	5.660708
1	1.812372	3.496221	-1.619150
1	2.148481	1.380745	-3.756184
1	3.340087	1.764604	-2.399995
1	-1.080712	-2.129564	-1.465380
1	2.648540	-2.319192	-3.573599
1	-1.367458	-4.586838	-1.734346
1	2.368548	-4.770424	-3.869333
1	0.368394	-5.910898	-2.924439
1	-0.201153	2.230910	-3.639511
1	-0.378542	3.863353	-2.850826
6	-3.776685	-1.471964	-2.464823
6	-3.664363	-2.824739	-2.958449
6	-3.010939	-0.499749	-3.091579
6	-4.220481	-3.941602	-2.273387
6	-2.928384	-3.079013	-4.162993

6	-2.262794	-0.751755	-4.263008
6	-4.097602	-5.220744	-2.773966
1	-4.735428	-3.786277	-1.333238
6	-2.838163	-4.405135	-4.663417
6	-2.251185	-2.009008	-4.807609
1	-1.713327	0.070788	-4.706187
6	-3.415521	-5.458200	-3.990363
1	-4.524419	-6.054603	-2.223866
1	-2.279727	-4.574106	-5.580352
1	-1.689277	-2.210439	-5.715152
1	-3.331893	-6.469680	-4.377062
8	-3.021522	0.814013	-2.652623
6	-4.652691	-1.146966	-1.302980
6	-6.044048	-1.527353	-1.260378
6	-4.151234	-0.471775	-0.202084
6	-6.732625	-2.036259	-2.396918
6	-6.787600	-1.359558	-0.043140
6	-4.863643	-0.328342	1.008836
6	-8.062711	-2.390626	-2.325412
1	-6.202719	-2.133705	-3.336985
6	-8.152371	-1.753719	0.001887
6	-6.151863	-0.791155	1.094600
1	-4.359619	0.128730	1.852092
6	-8.780077	-2.263595	-1.112270
1	-8.566078	-2.767598	-3.211157
1	-8.694782	-1.631927	0.935928
1	-6.703067	-0.708110	2.026782
1	-9.825140	-2.556006	-1.067750
8	-2.868519	0.067891	-0.217253
15	-2.439902	1.338225	-1.188257
8	-3.476917	2.554892	-0.998661
6	-4.916043	2.505125	-1.137251
1	-5.232974	3.527391	-1.350403
1	-5.210289	1.844889	-1.955266
1	-5.361869	2.169217	-0.199036
8	4.124429	-1.876309	-0.129649
7	5.249592	0.982995	-1.367701
6	4.622222	-2.773515	0.581777
6	5.516617	-5.081430	0.785886
6	5.220650	-3.703129	2.821772
6	6.173978	-4.626076	2.079824
1	4.642710	-5.717455	1.000463
1	5.728252	-3.220320	3.664287
1	6.421619	-5.488318	2.705922
7	4.712348	-2.649994	1.942416
7	5.122606	-3.916175	-0.002668
1	7.103823	-4.095506	1.846486
1	6.211990	-5.675941	0.185291
1	4.374530	-4.271190	3.236498
6	4.869512	-4.146814	-1.418133
1	4.754302	-3.195665	-1.931022
1	5.716816	-4.686989	-1.852073
1	3.958498	-4.741594	-1.573310
6	4.006680	-1.575165	2.629267
1	4.706391	-0.996024	3.242681
1	3.523308	-0.914183	1.915051
14	6.174965	0.099803	-2.482744
14	5.821847	2.141473	-0.267210
3	3.674447	-0.093312	-0.631174
6	7.332827	1.129038	-3.608044
1	6.802888	1.976910	-4.061766
1	8.192476	1.533858	-3.061682
1	7.729303	0.513879	-4.427929
6	5.043667	-0.838057	-3.691157
1	4.288493	-1.386813	-3.125679
1	4.511051	-0.150042	-4.359955
1	5.600172	-1.549922	-4.314689
6	7.314793	-1.220472	-1.701700
1	7.850795	-1.814033	-2.455372
1	8.069910	-0.751684	-1.056750
1	6.736559	-1.910561	-1.077825
6	7.687740	2.562235	-0.342617
1	7.955300	3.258139	0.464570
1	8.316999	1.671070	-0.224256
1	7.966517	3.040473	-1.288958
6	5.540619	1.593658	1.536968
1	6.090006	0.659861	1.716339
1	5.898694	2.328958	2.270143
6	4.970199	3.832035	-0.528305
1	3.882115	3.733485	-0.588787

1	5.196892	4.559708	0.261833
1	5.304666	4.266097	-1.480339
1	4.482462	1.392930	1.730884
1	3.238585	-2.001538	3.287223
15	-0.562661	3.764860	0.349194
6	-2.176657	3.991260	1.216321
6	-2.836599	2.886118	1.766232
6	-2.736824	5.268479	1.385015
6	-4.041740	3.046131	2.449693
1	-2.420620	1.893666	1.651549
6	-3.944367	5.427306	2.067468
1	-2.237344	6.145046	0.988700
6	-4.603349	4.315785	2.596494
1	-4.538937	2.177205	2.868238
1	-4.365789	6.421548	2.184767
1	-5.545787	4.438907	3.122594
6	0.658267	4.052795	1.699043
6	1.992834	3.664038	1.520773
6	0.290874	4.713296	2.884153
6	2.946166	3.944656	2.500738
1	2.289705	3.118726	0.634743
6	1.244022	4.975044	3.868864
1	-0.735035	5.020849	3.048910
6	2.574587	4.596046	3.677247
1	3.973882	3.641843	2.342882
1	0.943867	5.477464	4.784080
1	3.316873	4.803022	4.442905
6	-0.436216	5.279095	-0.690465
6	-1.506964	5.602525	-1.543918
6	0.727762	6.057046	-0.724502
6	-1.415889	6.696084	-2.402493
1	-2.406579	4.993581	-1.535878
6	0.817987	7.147577	-1.595170
1	1.565242	5.822187	-0.076001
6	-0.250895	7.470487	-2.431547
1	-2.251097	6.940775	-3.052495
1	1.725421	7.744233	-1.612409
1	-0.179138	8.320095	-3.104492

4B2-LiHMDs.IDMPU

Number of imaginary frequencies : 0
 Electronic energy : HF=-5699.3415377
 Zero-point correction= 1.451477 (Hartree/Particle)
 Thermal correction to Energy= 1.549258
 Thermal correction to Enthalpy= 1.550202
 Thermal correction to Gibbs Free Energy= 1.315276
 Sum of electronic and zero-point Energies= -5697.890061
 Sum of electronic and thermal Energies= -5697.792280
 Sum of electronic and thermal Enthalpies= -5697.791335
 Sum of electronic and thermal Free Energies= -5698.026262
 Standard State and RRHO Corrected G= -5698.001857

Cartesian Coordinates

6	-1.047192	5.700408	0.123059
6	-0.253176	4.710573	0.460882
6	-0.144503	3.454473	-0.138457
6	-0.873127	3.167916	-1.298560
6	-1.686317	4.155108	-1.871427
6	-1.756673	5.423741	-1.296952
6	-0.831079	1.795162	-1.913348
8	-1.808317	1.395222	-2.574642
6	-0.683703	-1.383970	-3.313405
6	0.581434	-1.488824	-3.923681
6	1.521908	-0.443601	-3.871987
45	0.889936	-0.931536	-1.739254
8	0.260449	1.141640	-1.690530
15	-0.693625	-1.107926	0.000630
8	-2.048197	-0.620477	-0.435782
8	-1.064042	-2.544275	0.822784
6	-0.483299	-3.013562	1.978004
6	-0.450050	-2.268872	3.154243
6	0.327326	-2.783965	4.252855
6	0.876986	-4.107174	4.181090
6	0.649973	-4.884928	3.015048
6	0.007668	-4.342452	1.933182
6	1.657043	-4.602405	5.260300
6	1.916316	-3.821763	6.364674
6	1.400462	-2.505111	6.428776

6	0.623625	-2.002940	5.406383
6	-1.180697	-0.977404	3.268124
6	-2.153177	-0.734049	4.302954
6	-2.753493	0.566202	4.407671
6	-2.413763	1.572506	3.464084
6	-1.560140	1.298598	2.425949
6	-0.960150	0.024331	2.339227
6	-3.707071	0.814769	5.432610
6	-4.087377	-0.180562	6.305356
6	-3.526330	-1.473991	6.180870
6	-2.584422	-1.742141	5.210586
8	-0.094024	-0.214989	1.281154
1	1.622390	-1.881721	7.290505
1	0.245963	-0.988992	5.469711
1	2.059534	-5.609643	5.187289
1	2.522005	-4.206882	7.179983
1	1.027293	-5.902948	2.973002
1	-0.141400	-4.911042	1.027019
1	-2.173996	-2.741404	5.125502
1	-1.346141	2.028554	1.657307
1	-3.844888	-2.265460	6.853430
1	-4.140054	1.809369	5.504827
1	-2.875852	2.551308	3.547076
1	-4.822535	0.019241	7.079647
1	0.926598	-2.473304	-4.228325
1	-1.201395	-0.432690	-3.235534
1	-1.306757	-2.268856	-3.267100
1	0.493591	2.686684	0.282662
1	-2.261806	3.912803	-2.758191
1	0.301737	4.924174	1.368737
1	-2.376436	6.190696	-1.753037
1	-1.109842	6.684918	0.331504
1	1.195604	0.590169	-3.864287
1	2.537001	-0.631841	-4.207941
6	3.263605	3.568839	-0.745000
6	2.842720	4.948222	-0.760064
6	2.943523	2.788385	-1.846118
6	2.972659	5.806382	0.368059
6	2.219692	5.482752	-1.936522
6	2.326144	3.308516	-3.003017
6	2.555222	7.119195	0.319432
1	3.391140	5.417492	1.288001
6	1.808925	6.842474	-1.957697
6	1.987058	4.635946	-3.052703
1	2.132953	2.638777	-3.832655
6	1.979191	7.651892	-0.857527
1	2.661478	7.747917	1.198949
1	1.340585	7.225903	-2.860266
1	1.511936	5.048096	-3.938092
1	1.656382	8.688536	-0.882824
8	3.295003	1.444524	-1.899196
6	3.959796	2.979584	0.434818
6	5.170435	3.537352	0.981888
6	3.455460	1.842023	1.045087
6	5.888710	4.583492	0.337543
6	5.711292	2.997114	2.197716
6	3.972496	1.306519	2.243799
6	7.048709	5.090374	0.881729
1	5.519509	4.978183	-0.601502
6	6.899560	3.556701	2.741871
6	5.068044	1.895166	2.825042
1	3.494857	0.429034	2.666089
6	7.554916	4.584826	2.103072
1	7.581931	5.883705	0.365819
1	7.287820	3.144978	3.669827
1	5.475411	1.502939	3.752530
1	8.465128	5.000785	2.525021
8	2.389538	1.146111	0.465907
15	2.706064	0.273899	-0.892835
8	4.069427	-0.541125	-0.642884
6	5.426919	-0.037180	-0.561404
1	6.063819	-0.815053	-0.987589
1	5.539327	0.889091	-1.125637
1	5.686762	0.120035	0.485801
8	-3.751597	1.657429	0.155075
7	-4.944091	-0.090460	-2.418286
6	-4.573618	1.817040	1.079920
6	-5.710500	3.300153	2.715458
6	-6.286574	0.887149	2.654479
6	-6.855410	2.298047	2.688188

1	-5.146130	3.216284	3.658304
1	-7.076329	0.165524	2.415088
1	-7.493050	2.420869	3.568667
7	-5.239460	0.761846	1.640529
7	-4.837330	3.077772	1.569225
1	-7.467063	2.475065	1.796648
1	-6.090855	4.325173	2.655199
1	-5.876961	0.610663	3.636776
6	-3.978929	4.183226	1.177122
1	-3.359708	3.878726	0.338713
1	-4.584317	5.048643	0.883604
1	-3.324829	4.487198	2.006832
6	-4.894849	-0.600664	1.254546
1	-5.611079	-0.997752	0.525128
1	-3.896043	-0.631353	0.823932
14	-6.104634	1.130786	-2.593709
14	-5.022168	-1.689702	-2.961524
3	-3.321777	0.540253	-1.401168
6	-7.070047	1.129958	-4.249124
1	-6.384266	1.196211	-5.104060
1	-7.673129	0.224043	-4.384405
1	-7.753362	1.988427	-4.312019
6	-5.332541	2.872749	-2.520112
1	-4.730940	3.000890	-1.615440
1	-4.677730	3.040317	-3.384701
1	-6.104253	3.654845	-2.534108
6	-7.453316	1.093633	-1.237177
1	-8.156117	1.934995	-1.313183
1	-8.040656	0.167615	-1.294827
1	-6.994468	1.126831	-0.242725
6	-6.770991	-2.467174	-3.052068
1	-6.717332	-3.526456	-3.339934
1	-7.272403	-2.420730	-2.076389
1	-7.421812	-1.965874	-3.778357
6	-4.054417	-2.891275	-1.842524
1	-4.583470	-3.067948	-0.896862
1	-3.925559	-3.864001	-2.335805
6	-4.284208	-1.922284	-4.712153
1	-3.258591	-1.532985	-4.754199
1	-4.257280	-2.974029	-5.030111
1	-4.868222	-1.366979	-5.458134
1	-3.073232	-2.487156	-1.583245
1	-4.913993	-1.232807	2.149356
15	1.900903	-3.028334	-1.466215
6	2.966566	-3.164615	0.031774
6	2.628440	-2.469910	1.201780
6	4.112483	-3.975315	0.027739
6	3.408493	-2.593904	2.350599
1	1.772628	-1.809478	1.226417
6	4.893015	-4.095859	1.179295
1	4.410594	-4.503947	-0.871407
6	4.542250	-3.408753	2.343404
1	3.121830	-2.057414	3.249537
1	5.777853	-4.725738	1.161773
1	5.149595	-3.505534	3.238711
6	0.817899	-4.512827	-1.371546
6	-0.565265	-4.432221	-1.560666
6	1.397630	-5.762895	-1.084219
6	-1.362236	-5.575011	-1.458114
1	-1.034996	-3.480690	-1.751769
6	0.601431	-6.901589	-0.984600
1	2.467129	-5.851228	-0.929655
6	-0.782562	-6.809714	-1.168565
1	-2.436088	-5.485235	-1.586161
1	1.060947	-7.858999	-0.757091
1	-1.403222	-7.696695	-1.080598
6	3.022265	-3.422040	-2.877486
6	4.196306	-2.672695	-3.061389
6	2.689759	-4.408406	-3.819646
6	5.024888	-2.914225	-4.156580
1	4.461614	-1.905740	-2.346703
6	3.519840	-4.642155	-4.918652
1	1.786634	-4.997340	-3.705234
6	4.688400	-3.898621	-5.089764
1	5.932850	-2.330897	-4.280042
1	3.249036	-5.409233	-5.638178
1	5.332997	-4.084317	-5.943949

(3-4)_{B3}[‡]

Number of imaginary frequencies : 1
 Electronic energy : HF=-4397.5981747
 Zero-point correction= 1.032830 (Hartree/Particle)
 Thermal correction to Energy= 1.100406
 Thermal correction to Enthalpy= 1.101351
 Thermal correction to Gibbs Free Energy= 0.929180
 Sum of electronic and zero-point Energies= -4396.565345
 Sum of electronic and thermal Energies= -4396.497768
 Sum of electronic and thermal Enthalpies= -4396.496824
 Sum of electronic and thermal Free Energies= -4396.668995
 Standard State and RRHO Corrected G= -4396.65104

Cartesian Coordinates

```

6      6.193976 -4.476283 -0.075489
6      5.267564 -3.872797  0.779690
6      4.001819 -3.526258  0.307242
6      3.650820 -3.792276 -1.023041
6      4.580428 -4.401227 -1.877287
6      5.848604 -4.738660 -1.405511
6      2.294396 -3.398238 -1.541552
8      2.041131 -3.605261 -2.751362
6      0.008726 -3.741535 -3.230075
6     -0.915698 -2.878696 -2.639827
6     -1.406550 -3.076521 -1.297210
45    -0.022846 -1.473463 -0.974855
8      1.499470 -2.900055 -0.664479
15     1.897393 -0.093269 -1.561376
8      2.609558 -0.569297 -2.796133
8      1.830123  1.606760 -1.756145
6      1.955138  2.536213 -0.765285
6      3.156209  2.717092 -0.080041
6      3.200679  3.704551  0.966525
6      2.075724  4.571160  1.178176
6      0.912359  4.399888  0.382833
6      0.844497  3.389560 -0.541613
6      2.117378  5.535162  2.221088
6      3.207165  5.630343  3.057415
6      4.304244  4.753364  2.878558
6      4.303357  3.823212  1.861104
6      4.336493  1.877813 -0.423191
6      5.612986  2.447318 -0.772816
6      6.728416  1.578460 -1.024683
6      6.540111  0.170692 -0.976412
6      5.299374 -0.359657 -0.728410
6      4.204723  0.494788 -0.459591
6      7.993457  2.139240 -1.350747
6      8.160011  3.501470 -1.460733
6      7.052833  4.360158 -1.260101
6      5.817225  3.848512 -0.926555
8      2.974358 -0.089294 -0.225876
1      5.153737  4.809609  3.553608
1      5.147068  3.152436  1.750736
1      1.256246  6.184195  2.360069
1      3.223149  6.362757  3.859461
1      0.062439  5.059077  0.539794
1     -0.046237  3.221719 -1.130249
1      4.980099  4.522728 -0.790770
1      5.125604 -1.427870 -0.730774
1      7.175949  5.433376 -1.377220
1      8.827735  1.464415 -1.526380
1      7.386547 -0.482600 -1.171592
1      9.130341  3.917772 -1.716317
1     -1.369695 -2.131787 -3.286488
1      0.152139 -4.732566 -2.816693
1      0.281048 -3.609250 -4.270125
1      3.284962 -3.034992  0.950166
1      4.299817 -4.596201 -2.906707
1      5.531453 -3.662504  1.812202
1      6.568147 -5.204083 -2.073339
1      7.182739 -4.739195  0.290816
1     -1.068590 -3.978550 -0.788428
1     -2.439712 -2.833925 -1.079297
6     -4.811758  0.173496 -0.992469
6     -6.008155 -0.391114 -0.418286
6     -4.065092 -0.637558 -1.836284
6     -6.730314  0.253220  0.624838
6     -6.466268 -1.678386 -0.856956
6     -4.522421 -1.896591 -2.287117
6     -7.849666 -0.327814  1.180541

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1     -6.380437  1.205826  1.003534
6     -7.636535 -2.240038 -0.278264
6     -5.713541 -2.395058 -1.825317
1     -3.908251 -2.445355 -2.992307
6     -8.318410 -1.580910  0.719816
1     -8.372828  0.178946  1.986292
1     -7.971261 -3.212917 -0.628517
1     -6.074560 -3.360004 -2.169209
1     -9.205237 -2.023910  1.163309
8     -2.838486 -0.225879 -2.338041
6     -4.372620  1.556541 -0.651048
6     -5.222396  2.703850 -0.844782
6     -3.110238  1.783087 -0.132644
6     -6.474790  2.626055 -1.515345
6     -4.782720  3.990262 -0.380873
6     -2.672406  3.035410  0.346794
6     -7.258871  3.745960 -1.688999
1     -6.810099  1.672323 -1.905099
6     -5.623560  5.121773 -0.563331
6     -3.509523  4.118345  0.239802
1     -1.683996  3.106128  0.785424
6     -6.838610  5.005644 -1.199640
1     -8.207396  3.661281 -2.211448
1     -5.280137  6.085833 -0.197411
1     -3.197335  5.091410  0.608367
1     -7.470544  5.877987 -1.337974
8     -2.198419  0.729964 -0.049055
15    -1.503994  0.125439 -1.409712
8     -0.954551  1.342828 -2.289750
6     -1.726078  2.293351 -3.068378
1     -1.007055  2.769016 -3.736346
1     -2.497633  1.783825 -3.646986
1     -2.179325  3.040972 -2.414675
15    -0.344476 -1.493570  1.384443
6     0.882342 -2.603395  2.204755
6     0.812829 -3.972063  1.887439
6     1.825890 -2.174472  3.146055
6     1.660382 -4.887641  2.503970
1     0.090619 -4.320237  1.157898
6     2.683557 -3.096224  3.757706
1     1.893987 -1.130326  3.425437
6     2.603021 -4.451558  3.441363
1     1.593268 -5.940590  2.245833
1     3.408329 -2.745928  4.487089
1     3.269899 -5.164918  3.916947
6     -0.226512  0.112371  2.276693
6     0.981500  0.828737  2.250449
6     -1.312359  0.628649  3.001531
6     1.117137  1.998792  2.998884
1     1.816527  0.472078  1.657290
6     -1.185131  1.827879  3.704295
1     -2.260480  0.104489  3.019469
6     0.034922  2.506544  3.720053
1     2.067393  2.518130  3.009205
1     -2.038649  2.220792  4.249763
1     0.143814  3.429346  4.282773
6     -1.920162 -2.193640  2.070808
6     -1.909665 -2.834041  3.323990
6     -3.149494 -2.017422  1.421574
6     -3.093251 -3.300879  3.895270
1     -0.978803 -2.965734  3.863492
6     -4.335541 -2.481406  1.996638
1     -3.197114 -1.496854  0.478026
6     -4.310146 -3.129508  3.231631
1     -3.061454 -3.794532  4.862484
1     -5.275995 -2.332323  1.477922
1     -5.232316 -3.493160  3.676066

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(3...4)B3-LiHMDS.IDMPU

Number of imaginary frequencies : 0
 Electronic energy : HF=-5699.336315
 Zero-point correction= 1.452778 (Hartree/Particle)
 Thermal correction to Energy= 1.550265
 Thermal correction to Enthalpy= 1.551209
 Thermal correction to Gibbs Free Energy= 1.315268
 Sum of electronic and zero-point Energies= -5697.883537
 Sum of electronic and thermal Energies= -5697.786050
 Sum of electronic and thermal Enthalpies= -5697.785106
 Sum of electronic and thermal Free Energies= -5698.021047

6	0.526911	-0.699118	6.221433	1	2.446244	7.984533	-0.056721
1	-0.363967	-2.658266	6.400408	1	3.032892	5.606254	-0.077662
1	1.245818	1.279642	5.748381	1	-1.186242	7.149646	-2.204767
1	1.137500	-0.801126	7.114156	1	0.347122	8.784936	-1.144287
6	-2.591687	1.460356	2.243413	1	-1.799797	4.841153	-2.730395
6	-1.620664	2.406906	1.874693	1	-1.315109	2.402716	-2.567122
6	-3.917993	1.890868	2.409402	1	3.361036	4.695540	-2.818303
6	-1.958651	3.754644	1.735950	1	4.013850	0.787822	1.623913
1	-0.600482	2.097320	1.682720	1	5.546208	5.397549	-3.675579
6	-4.258705	3.233928	2.235590	1	7.526552	3.052494	-0.661059
1	-4.698994	1.183007	2.659658	1	6.219448	1.670100	0.879499
6	-3.278889	4.173530	1.911302	1	7.649914	4.608345	-2.587760
1	-1.188822	4.473272	1.479990	1	-1.021366	-3.209157	-0.474365
1	-5.293580	3.541850	2.358527	1	0.651540	-4.118703	1.888670
1	-3.540661	5.220637	1.786316	1	1.141648	-4.143339	0.103199
6	-3.688407	-1.096846	2.984662	1	1.947166	0.548629	3.778748
6	-4.194262	-0.825578	4.269954	1	4.056105	-3.074603	2.871341
6	-4.422888	-1.932899	2.135143	1	3.708385	1.173588	5.424813
6	-5.401485	-1.382010	4.689307	1	5.807736	-2.482552	4.541586
1	-3.644607	-0.174649	4.942641	1	5.639647	-0.348750	5.806058
6	-5.634395	-2.490269	2.555236	1	-1.363117	-2.818636	2.603881
1	-4.048846	-2.153222	1.144146	1	-2.699247	-2.749120	1.380164
6	-6.125455	-2.216731	3.831384	6	-5.394019	-1.404597	-1.052055
1	-5.778504	-1.162161	5.684294	6	-6.612371	-1.850953	-0.425660
1	-6.190348	-3.131760	1.880031	6	-4.283271	-2.230943	-0.949040
1	-7.067016	-2.649416	4.157958	6	-7.747116	-1.005179	-0.278677
				6	-6.679162	-3.170934	0.133882
(3-4)B3-LiHMDS.1DMPL [‡]				6	-4.349459	-3.540892	-0.424236
				6	-8.885507	-1.446381	0.360475
Number of imaginary frequencies : 1				1	-7.706015	0.009291	-0.656460
Electronic energy : HF=-5699.3123356				6	-7.875689	-3.601978	0.768404
Zero-point correction= 1.450262 (Hartree/Particle)				6	-5.533392	-4.009613	0.086319
Thermal correction to Energy= 1.547566				1	-3.450220	-4.147031	-0.434729
Thermal correction to Enthalpy= 1.548510				6	-8.959489	-2.760325	0.880848
Thermal correction to Gibbs Free Energy= 1.314357				1	-9.732168	-0.775208	0.472038
Sum of electronic and zero-point Energies= -5697.862073				1	-7.910135	-4.607513	1.179268
Sum of electronic and thermal Energies= -5697.764770				1	-5.596504	-5.016058	0.489753
Sum of electronic and thermal Enthalpies= -5697.763826				1	-9.865285	-3.096039	1.377082
Sum of electronic and thermal Free Energies= -5697.997979				8	-3.037330	-1.825731	-1.412906
Standard State and RRHO Corrected G= -5697.973588				6	-5.313098	-0.084923	-1.741023
				6	-6.184248	0.274722	-2.829757
Cartesian Coordinates				6	-4.362587	0.842267	-1.354176
				6	-7.103201	-0.641887	-3.412295
6	4.870366	-0.615393	5.086507	6	-6.104377	1.597845	-3.383934
6	3.786031	0.241659	4.872593	6	-4.276595	2.147366	-1.882068
6	2.796086	-0.100759	3.952823	6	-7.917374	-0.263542	-4.457749
6	2.896555	-1.299785	3.233047	1	-7.153866	-1.655654	-3.033117
6	3.985439	-2.156699	3.444322	6	-6.969228	1.958379	-4.453013
6	4.965908	-1.816414	4.376097	6	-5.152203	2.521807	-2.871402
6	1.841895	-1.660493	2.238103	1	-3.519769	2.817480	-1.490394
8	2.107795	-2.560090	1.384153	6	-7.861327	1.051356	-4.978499
6	0.520614	-3.719001	0.888660	1	-8.606058	-0.983899	-4.889746
6	-0.707505	-3.110642	0.561409	1	-6.902929	2.966145	-4.854570
6	-1.636109	-2.647040	1.563396	1	-5.111346	3.523591	-3.289600
45	-0.756103	-0.828216	0.850922	1	-8.513757	1.336402	-5.798590
8	0.733139	-1.046186	2.343238	8	-3.421141	0.491375	-0.384675
15	1.013893	0.331733	-0.325808	15	-2.201752	-0.528674	-0.802293
8	2.102263	-0.609038	-0.788364	8	-1.575059	0.011580	-2.165464
8	0.830971	1.335233	-1.676985	6	-2.060409	-0.170603	-3.517818
6	0.606713	2.683139	-1.648169	1	-1.206491	0.042394	-4.160832
6	1.583528	3.562683	-1.188471	1	-2.400249	-1.194654	-3.673064
6	1.276714	4.969094	-1.180818	1	-2.871327	0.531813	-3.721668
6	0.049201	5.432157	-1.765595	8	4.856907	-1.543361	-0.176928
6	-0.871184	4.486368	-2.290958	7	2.838205	-3.877906	-1.573681
6	-0.611564	3.142510	-2.207937	6	5.896924	-1.046076	-0.656512
6	-0.254555	6.820097	-1.751357	6	8.240491	-0.278057	-0.379646
6	0.594506	7.727358	-1.157813	6	7.145651	-0.061438	-2.593664
6	1.787918	7.272729	-0.546995	6	8.403953	-0.520888	-1.873027
6	2.120710	5.934947	-0.561455	1	8.178897	0.801516	-0.170338
6	2.884224	3.031766	-0.689826	1	7.147839	-0.418809	-3.629725
6	4.152521	3.471919	-1.211655	1	9.271667	0.023609	-2.257048
6	5.366857	2.980937	-0.622292	7	5.941538	-0.577099	-1.940068
6	5.297996	2.037888	0.438174	7	7.047770	-0.968871	0.098843
6	4.086988	1.553015	0.861646	1	8.567833	-1.590086	-2.048057
6	2.892970	2.042133	0.284987	1	9.100346	-0.668412	0.174070
6	6.618969	3.421711	-1.131865	1	7.098719	1.036675	-2.625603
6	6.686917	4.284362	-2.203465	6	6.974402	-1.236281	1.525281
6	5.493137	4.737823	-2.813986	1	6.922346	-0.305136	2.108436
6	4.263232	4.345553	-2.330607	1	6.085530	-1.822850	1.737923
8	1.699933	1.490305	0.720762	1	7.862385	-1.792873	1.844439

6	4.715154	-0.508551	-2.726308
1	4.606501	-1.386837	-3.375811
1	3.845776	-0.433118	-2.074995
14	4.181392	-4.887532	-1.330829
14	1.744007	-4.006634	-2.863483
3	3.047804	-2.214676	-0.478173
6	3.880356	-6.743062	-1.699896
1	3.076509	-7.147266	-1.070870
1	3.593881	-6.914889	-2.745079
1	4.780231	-7.343224	-1.506323
6	4.773652	-4.842077	0.479864
1	5.035372	-3.817515	0.761669
1	3.988451	-5.192691	1.161356
1	5.657062	-5.476633	0.633506
6	5.695464	-4.408205	-2.395018
1	6.589341	-4.999612	-2.152515
1	5.484973	-4.552110	-3.462600
1	5.943895	-3.349934	-2.252528
6	2.544425	-4.335050	-4.571707
1	1.793062	-4.386797	-5.371758
1	3.248389	-3.534546	-4.834007
1	3.104324	-5.278625	-4.588225
6	0.694146	-2.440806	-3.108037
1	1.313195	-1.565224	-3.329638
1	-0.016262	-2.579466	-3.934379
6	0.462504	-5.412596	-2.637440
1	-0.119175	-5.270270	-1.716681
1	-0.251069	-5.460019	-3.471768
1	0.948940	-6.393374	-2.563170
1	0.124418	-2.194604	-2.208391
1	4.756636	0.388419	-3.353484
15	-1.852154	0.648052	2.376295
6	-0.902849	0.794047	3.955391
6	-0.759833	-0.381312	4.713742
6	-0.370584	1.989619	4.453168
6	-0.102535	-0.359358	5.940311
1	-1.165466	-1.315470	4.340386
6	0.294315	2.008122	5.684750
1	-0.480750	2.916069	3.902955
6	0.430786	0.837816	6.429901
1	0.001767	-1.277651	6.511106
1	0.698030	2.945083	6.057973
1	0.949661	0.853997	7.383980
6	-2.123545	2.378037	1.812427
6	-1.010868	3.183079	1.514974
6	-3.412511	2.915419	1.675222
6	-1.187692	4.520270	1.160256
1	-0.008895	2.771712	1.566339
6	-3.583707	4.241547	1.272623
1	-4.285157	2.305232	1.877366
6	-2.472506	5.051873	1.030817
1	-0.320211	5.140634	0.968244
1	-4.587978	4.640449	1.159865
1	-2.602810	6.088499	0.733361
6	-3.510782	0.183165	3.059973
6	-3.937399	0.772535	4.265314
6	-4.377336	-0.694999	2.398955
6	-5.194429	0.481628	4.792451
1	-3.288733	1.464127	4.792881
6	-5.637245	-0.988769	2.929309
1	-4.086415	-1.143224	1.462120
6	-6.047363	-0.403415	4.126713
1	-5.506402	0.947083	5.723165
1	-6.293653	-1.673330	2.402985
1	-7.026063	-0.633175	4.538519

4B3-LHMD5.IDMPU			

Number of imaginary frequencies : 0			
Electronic energy : HF=-5699.3352401			
Zero-point correction= 1.451521 (Hartree/Particle)			
Thermal correction to Energy= 1.549382			
Thermal correction to Enthalpy= 1.550326			
Thermal correction to Gibbs Free Energy= 1.314944			
Sum of electronic and zero-point Energies= -5697.883719			
Sum of electronic and thermal Energies= -5697.785858			
Sum of electronic and thermal Enthalpies= -5697.784914			
Sum of electronic and thermal Free Energies= -5698.020296			
Standard State and RRHO Corrected G= -5697.995872			

Cartesian Coordinates			

6	4.685262	-1.183176	5.161408
6	3.607574	-0.332689	4.899862
6	2.736599	-0.609392	3.844836
6	2.954252	-1.726115	3.028615
6	4.042102	-2.572161	3.287169
6	4.896629	-2.308663	4.357496
6	2.068972	-2.015825	1.843895
8	2.494343	-2.773823	0.951065
6	0.030037	-2.890510	-0.777154
6	-1.089980	-3.419991	-0.079366
6	-1.190747	-3.407603	1.309045
45	-0.698343	-1.217639	0.484647
8	0.914376	-1.436422	1.882489
15	0.926567	0.221365	-0.408923
8	2.114832	-0.536234	-0.933872
8	0.613583	1.345695	-1.611157
6	0.273795	2.664644	-1.427008
6	1.135393	3.564264	-0.806503
6	0.680758	4.920530	-0.629590
6	-0.562655	5.336321	-1.212401
6	-1.344758	4.390330	-1.924941
6	-0.947147	3.080823	-2.007746
6	-1.019228	6.668356	-1.021870
6	-0.302323	7.561408	-0.257987
6	0.906903	7.147389	0.350421
6	1.386340	5.868004	0.166720
6	2.458081	3.119071	-0.291793
6	3.688152	3.781227	-0.643683
6	4.906331	3.392554	0.008193
6	4.886785	2.328635	0.948667
6	3.732059	1.627516	1.186997
6	2.534446	2.022474	0.554251
6	6.119732	4.053900	-0.326737
6	6.149945	5.035692	-1.292064
6	4.958194	5.391275	-1.968242
6	3.761776	4.784850	-1.650487
8	1.391384	1.273389	0.816969
1	1.460775	7.843063	0.974516
1	2.305378	5.569974	0.656202
1	-1.961074	6.961865	-1.478630
1	-0.665419	8.574274	-0.109784
1	-2.278866	4.709722	-2.378980
1	-1.543114	2.338659	-2.519543
1	2.861200	5.064087	-2.184937
1	3.714638	0.763716	1.837139
1	4.987388	6.146134	-2.748996
1	7.028965	3.756766	0.189844
1	5.812315	2.037769	1.435735
1	7.084344	5.528510	-1.545021
1	-1.993838	-3.613431	-0.644521
1	1.029749	-3.006823	-0.376404
1	-0.046931	-2.794587	-1.855261
1	1.891080	0.034590	3.638902
1	4.214016	-3.418869	2.631591
1	3.437023	0.541129	5.522009
1	5.734795	-2.970897	4.555982
1	5.358287	-0.971112	5.987895
1	-0.309507	-3.426841	1.938738
1	-2.131326	-3.671087	1.780110
6	-5.589578	-1.329258	-1.137181
6	-6.823805	-1.782454	-0.544335
6	-4.543308	-2.237693	-1.210220
6	-7.881580	-0.891517	-0.209619
6	-6.991884	-3.171647	-0.230525
6	-4.705406	-3.608744	-0.906865
6	-9.043227	-1.352780	0.370868
1	-7.762992	0.169011	-0.396256
6	-8.210927	-3.619007	0.346800
6	-5.916345	-4.070731	-0.456862
1	-3.872063	-4.284463	-1.059627
6	-9.220354	-2.730592	0.640467
1	-9.829337	-0.649279	0.629319
1	-8.321298	-4.677242	0.568394
1	-6.052128	-5.126153	-0.239356
1	-10.144842	-3.079764	1.090720
8	-3.283148	-1.863253	-1.670749
6	-5.447037	0.068030	-1.631080
6	-6.358224	0.639413	-2.591367

6	-4.415731	0.871564	-1.182373
6	-7.351896	-0.129787	-3.258475
6	-6.243409	2.031197	-2.926830
6	-4.303342	2.243969	-1.483507
6	-8.201217	0.449091	-4.176395
1	-7.432710	-1.189816	-3.050031
6	-7.146873	2.599666	-3.865536
6	-5.220782	2.817235	-2.328657
1	-3.498314	2.809429	-1.033035
6	-8.109983	1.829103	-4.476309
1	-8.945754	-0.162070	-4.678279
1	-7.052906	3.656831	-4.099568
1	-5.160642	3.875595	-2.565963
1	-8.791695	2.272316	-5.196196
8	-3.417949	0.326295	-0.364430
15	-2.313915	-0.696692	-1.004205
8	-1.732341	-0.084593	-2.356795
6	-2.393859	0.004198	-3.648384
1	-1.593298	0.173853	-4.368622
1	-2.917017	-0.924713	-3.877737
1	-3.092610	0.842787	-3.654283
8	4.943213	-0.970469	-0.035404
7	3.831580	-3.249778	-2.214032
6	5.975918	-0.358012	-0.374561
6	8.229504	0.524432	0.172243
6	7.286069	0.919700	-2.087174
6	8.518137	0.462404	-1.320812
1	8.075151	1.567354	0.493208
1	7.388416	0.678714	-3.151734
1	9.371231	1.098846	-1.573875
7	6.078042	0.261220	-1.589882
7	7.057367	-0.288291	0.476334
1	8.767572	-0.568516	-1.595674
1	9.072513	0.128646	0.747600
1	7.162929	2.009674	-2.008492
6	6.909407	-0.737837	1.850484
1	6.827140	0.113121	2.542605
1	6.010198	-1.340255	1.938154
1	7.778057	-1.337321	2.145666
6	4.915751	0.338332	-2.466096
1	4.984497	-0.398075	-3.275253
1	4.000405	0.167952	-1.903551
14	5.277239	-4.083998	-1.912606
14	2.925322	-3.309245	-3.643739
3	3.417403	-1.982432	-0.706382
6	5.340631	-5.886707	-2.559687
1	4.539962	-6.490450	-2.112513
1	5.223766	-5.946570	-3.648619
1	6.294177	-6.371335	-2.307259
6	5.635867	-4.248683	-0.048011
1	5.634914	-3.266599	0.433773
1	4.870109	-4.862912	0.441842
1	6.610625	-4.722408	0.132831
6	6.808615	-3.220370	-2.668590
1	7.756026	-3.699577	-2.384924
1	6.755333	-3.217434	-3.765142
1	6.849079	-2.174230	-2.342668
6	3.942241	-3.504238	-5.258064
1	3.288746	-3.507813	-6.141708
1	4.648371	-2.672493	-5.379996
1	4.525560	-4.432751	-5.281932
6	1.908863	-1.728080	-3.957919
1	2.569011	-0.887767	-4.209916
1	1.214338	-1.865025	-4.798766
6	1.673462	-4.757535	-3.686489
1	1.035252	-4.753290	-2.793737
1	1.018157	-4.727991	-4.568230
1	2.198373	-5.721954	-3.698781
1	1.341022	-1.423281	-3.076505
1	4.875531	1.341116	-2.906876
15	-1.797954	0.015771	2.320275
6	-0.861693	-0.036404	3.909852
6	-0.603044	-1.310703	4.443457
6	-0.490449	1.096037	4.644601
6	0.006094	-1.447284	5.687187
1	-0.883475	-2.197191	3.885508
6	0.129315	0.955149	5.891557
1	-0.693491	2.091321	4.268053
6	0.376317	-0.312475	6.416308
1	0.202496	-2.439217	6.083667

1	0.409164	1.843368	6.451042
1	0.858369	-0.419645	7.383660
6	-2.223407	1.791650	2.059031
6	-1.198327	2.742238	1.920618
6	-3.558989	2.218939	1.985742
6	-1.507298	4.094802	1.766507
1	-0.161686	2.429923	1.936759
6	-3.861767	3.568481	1.799670
1	-4.368969	1.503548	2.061062
6	-2.837664	4.512132	1.700901
1	-0.705793	4.820047	1.686135
1	-4.901034	3.877760	1.733351
1	-3.070144	5.564274	1.564033
6	-3.397322	-0.698341	2.916488
6	-3.946954	-0.225721	4.123141
6	-4.073057	-1.700925	2.215722
6	-5.147196	-0.742757	4.605514
1	-3.435293	0.549428	4.685037
6	-5.271552	-2.228469	2.705423
1	-3.667914	-2.084905	1.290378
6	-5.812809	-1.748168	3.896783
1	-5.559878	-0.364254	5.536330
1	-5.777867	-3.009891	2.151072
1	-6.746613	-2.155684	4.273472

(3-4)_{B4}[‡]

Number of imaginary frequencies : 1
 Electronic energy : HF=-4737.6683188
 Zero-point correction= 1.064567 (Hartree/Particle)
 Thermal correction to Energy= 1.135827
 Thermal correction to Enthalpy= 1.136771
 Thermal correction to Gibbs Free Energy= 0.956754
 Sum of electronic and zero-point Energies= -4736.603752
 Sum of electronic and thermal Energies= -4736.532492
 Sum of electronic and thermal Enthalpies= -4736.531548
 Sum of electronic and thermal Free Energies= -4736.711565
 Standard State and RRHO Corrected G= -4736.692725

 Cartesian Coordinates

6	-6.481315	-0.869468	-2.182941
6	-5.474744	-0.184563	-1.495778
6	-4.135242	-0.429298	-1.793343
6	-3.795168	-1.380346	-2.764962
6	-4.805832	-2.071131	-3.447525
6	-6.146144	-1.807454	-3.164899
6	-2.357846	-1.728346	-2.998921
8	-2.101421	-2.865536	-3.483439
6	-0.338267	-2.956640	-4.509931
6	0.858707	-2.503521	-3.929554
6	1.231078	-1.109991	-3.917821
45	0.431050	-1.403152	-1.948148
8	-1.484019	-0.846420	-2.683796
15	-0.682165	-2.714988	-0.227479
8	-0.665353	-4.213892	-0.313032
8	-0.376244	-2.385022	1.433008
6	-0.849633	-1.281783	2.096117
6	-2.213013	-1.058522	2.289256
6	-2.618891	0.193689	2.873127
6	-1.631864	1.070161	3.433380
6	-0.263565	0.695221	3.368171
6	0.118430	-0.423889	2.675042
6	-2.034745	2.306541	4.006211
6	-3.359634	2.684627	4.016629
6	-4.335290	1.834541	3.442044
6	-3.976072	0.624671	2.888195
6	-3.213391	-2.085509	1.891962
6	-4.184911	-2.621297	2.809173
6	-5.165339	-3.554138	2.326584
6	-5.132944	-3.964014	0.965092
6	-4.154236	-3.503695	0.120479
6	-3.197760	-2.578617	0.597795
6	-6.140140	-4.069159	3.224024
6	-6.144395	-3.708825	4.553039
6	-5.156177	-2.820772	5.041146
6	-4.205124	-2.292918	4.194434
8	-2.254734	-2.107588	-0.282446
1	-5.375983	2.145090	3.423662
1	-4.733423	-0.002577	2.432127

1	-1.269546	2.959312	4.419114
1	-3.655945	3.636807	4.447742
1	0.480049	1.340090	3.825931
1	1.162021	-0.677647	2.539910
1	-3.450770	-1.622860	4.589473
1	-4.097531	-3.810447	-0.917715
1	-5.143367	-2.556579	6.095068
1	-6.880234	-4.766208	2.838428
1	-5.884228	-4.663267	0.607716
1	-6.892385	-4.112859	5.229413
1	1.572491	-3.268574	-3.632829
1	-0.852479	-2.319030	-5.219889
1	-0.501153	-4.021855	-4.618756
1	-3.345325	0.082225	-1.259747
1	-4.530551	-2.816922	-4.185981
1	-5.728989	0.542400	-0.730841
1	-6.927513	-2.340338	-3.699520
1	-7.525275	-0.676892	-1.950486
1	0.607631	-0.421761	-4.487014
1	2.286526	-0.855167	-3.926402
6	5.026958	-0.162280	-0.348756
6	5.645993	1.136336	-0.268433
6	4.537671	-0.559758	-1.584596
6	5.975927	1.747237	0.973901
6	5.904247	1.874071	-1.471216
6	4.801763	0.153138	-2.774034
6	6.547782	3.000623	1.021058
1	5.756738	1.223398	1.896979
6	6.515729	3.153950	-1.389030
6	5.503543	1.330336	-2.721545
1	4.445991	-0.255184	-3.713162
6	6.833948	3.709382	-0.170004
1	6.776911	3.450481	1.982878
1	6.710772	3.694766	-2.311508
1	5.723594	1.879508	-3.632622
1	7.291131	4.693133	-0.117939
8	3.814233	-1.739190	-1.728227
6	4.905492	-1.044149	0.846213
6	6.048808	-1.440590	1.630254
6	3.674814	-1.553686	1.217889
6	7.384028	-1.109819	1.266111
6	5.849535	-2.235720	2.810166
6	3.466142	-2.345308	2.366862
6	8.452138	-1.504646	2.042367
1	7.563841	-0.547458	0.357990
6	6.972773	-2.613062	3.595802
6	4.539086	-2.659067	3.163571
1	2.460774	-2.690867	2.581499
6	8.248558	-2.251878	3.226740
1	9.461761	-1.243561	1.738350
1	6.801797	-3.204658	4.491348
1	4.400983	-3.258419	4.058841
1	9.099736	-2.549142	3.832269
8	2.547686	-1.269954	0.442726
15	2.349440	-2.013564	-1.003771
8	2.471973	-3.594881	-0.812540
6	3.658764	-4.346533	-0.442881
1	3.601558	-5.289744	-0.988261
1	4.569863	-3.812512	-0.715724
1	3.636745	-4.532915	0.631871
6	-1.808216	2.980226	-0.959155
6	-3.209812	3.262537	-0.784700
6	-1.428145	2.317676	-2.119343
6	-3.742816	3.722624	0.450796
6	-4.115587	3.044092	-1.874353
6	-2.316916	2.093439	-3.192880
6	-5.089087	3.982930	0.589322
1	-3.082752	3.838905	1.302138
6	-5.494595	3.340567	-1.704370
6	-3.625989	2.486819	-3.086428
1	-1.936736	1.597591	-4.077704
6	-5.974990	3.806023	-0.500185
1	-5.474310	4.316108	1.548587
1	-6.167640	3.169621	-2.540405
1	-4.316635	2.322666	-3.908337
1	-7.032929	4.019855	-0.377933
8	-0.111008	1.920233	-2.323133
6	-0.787527	3.406879	0.038639
6	-0.647581	4.779922	0.458640
6	0.126362	2.493184	0.531017

6	-1.430838	5.838076	-0.082302
6	0.353802	5.117883	1.432060
6	1.137771	2.822924	1.458321
6	-1.271854	7.137309	0.349549
1	-2.158708	5.620210	-0.853701
6	0.481130	6.465524	1.866180
6	1.231031	4.111202	1.920155
1	1.814924	2.042435	1.783306
6	-0.318629	7.457115	1.344999
1	-1.882082	7.924607	-0.083868
1	1.235320	6.698383	2.613508
1	1.994185	4.381707	2.644455
1	-0.210440	8.483892	1.682218
8	0.071179	1.167828	0.102005
15	0.644075	0.775708	-1.386240
8	2.149917	1.327189	-1.494517
6	2.570280	2.716172	-1.545693
1	1.718295	3.392932	-1.604752
1	3.157101	2.925469	-0.651112
1	3.192852	2.824708	-2.434080

(3...4)_{B4-LiH}MDS.IDMPU

Number of imaginary frequencies : 0
 Electronic energy : HF=-6039.3970084
 Zero-point correction= 1.485860 (Hartree/Particle)
 Thermal correction to Energy= 1.586508
 Thermal correction to Enthalpy= 1.587452
 Thermal correction to Gibbs Free Energy= 1.346877
 Sum of electronic and zero-point Energies= -6037.911148
 Sum of electronic and thermal Energies= -6037.810501
 Sum of electronic and thermal Enthalpies= -6037.809556
 Sum of electronic and thermal Free Energies= -6038.050131
 Standard State and RRHO Corrected G= -6038.025129

Cartesian Coordinates

6	-4.382236	3.694088	-3.431394
6	-3.060728	3.762128	-2.978835
6	-2.309011	2.597836	-2.851873
6	-2.877354	1.359136	-3.181454
6	-4.203705	1.289160	-3.637116
6	-4.951246	2.459094	-3.761318
6	-2.075512	0.136496	-2.973205
8	-2.795915	-0.955161	-2.852910
6	-2.268793	-2.319768	-3.085162
6	-0.903941	-2.708115	-2.568758
6	0.302222	-2.463376	-3.303839
45	0.228809	-1.181393	-1.578681
8	-0.830792	0.184064	-2.887721
15	-1.109366	-0.321420	0.205558
8	-2.408501	-1.050602	0.495299
8	-0.488831	-0.045682	1.763750
6	0.207094	1.086263	2.125530
6	-0.409525	2.333550	2.175788
6	0.393771	3.475504	2.534376
6	1.748571	3.282721	2.966654
6	2.292551	1.971340	2.973246
6	1.548715	0.906149	2.537065
6	2.526664	4.404142	3.363432
6	2.005073	5.677863	3.327445
6	0.684452	5.879043	2.859901
6	-0.094187	4.811952	2.468377
6	-1.853280	2.473583	1.840273
6	-2.800436	3.092468	2.731409
6	-4.148023	3.311132	2.286629
6	-4.540781	2.850896	1.002072
6	-3.660124	2.162026	0.207420
6	-2.326339	1.973525	0.635425
6	-5.077329	3.945516	3.156238
6	-4.716992	4.316830	4.432603
6	-3.403482	4.057904	4.892809
6	-2.472445	3.466967	4.065660
8	-1.466857	1.284211	-0.203087
1	0.285371	6.887037	2.792298
1	-1.094326	4.992449	2.093381
1	3.548793	4.233220	3.692483
1	2.607870	6.527953	3.634336
1	3.320791	1.828534	3.292850
1	1.966543	-0.087700	2.474785

1	-1.473673	3.270855	4.437719
1	-3.966379	1.741665	-0.739884
1	-3.127181	4.324348	5.909195
1	-6.087590	4.119469	2.793763
1	-5.564884	3.007714	0.675040
1	-5.438083	4.793733	5.090361
1	-0.960684	-3.618064	-1.976607
1	-2.323103	-2.435057	-4.173492
1	-3.035465	-2.927694	-2.603854
1	-1.304336	2.625464	-2.456153
1	-4.640926	0.328570	-3.881708
1	-2.621646	4.716796	-2.705446
1	-5.976832	2.407502	-4.114209
1	-4.971860	4.602094	-3.521331
1	0.262034	-1.871990	-4.217702
1	1.099393	-3.199995	-3.282961
6	4.316051	-3.372341	0.022878
6	5.661548	-3.003827	-0.329991
6	3.437202	-3.655283	-1.012588
6	6.573871	-2.459727	0.617241
6	6.094964	-3.131516	-1.690669
6	3.859738	-3.800448	-2.350976
6	7.844217	-2.078369	0.242251
1	6.254234	-2.325825	1.644342
6	7.420453	-2.755344	-2.038286
6	5.174103	-3.579066	-2.676044
1	3.130359	-4.087813	-3.099568
6	8.279913	-2.237650	-1.095260
1	8.516500	-1.648925	0.979561
1	7.735181	-2.863772	-3.073010
1	5.513068	-3.697523	-3.701260
1	9.286075	-1.939760	-1.375379
8	2.085093	-3.874811	-0.756682
6	3.869025	-3.444745	1.441165
6	4.529135	-4.279411	2.413393
6	2.751878	-2.743326	1.856210
6	5.600102	-5.154049	2.077334
6	4.073159	-4.264945	3.775561
6	2.284232	-2.733802	3.187594
6	6.209025	-5.934538	3.036150
1	5.934850	-5.214121	1.048991
6	4.733065	-5.072464	4.741710
6	2.952728	-3.467886	4.135518
1	1.402413	-2.150004	3.426835
6	5.783611	-5.886974	4.385066
1	7.021103	-6.597474	2.751643
1	4.381061	-5.040621	5.769472
1	2.615283	-3.466604	5.167899
1	6.277782	-6.502884	5.130711
8	2.048200	-1.963838	0.935255
15	1.096762	-2.664238	-0.200663
8	-0.001910	-3.565091	0.530171
6	0.241880	-4.749490	1.336647
1	-0.543479	-5.459422	1.081493
1	1.220049	-5.182019	1.123369
1	0.171675	-4.472092	2.388995
8	-5.414563	-0.426606	0.171612
7	-4.600284	-3.475780	-0.713670
6	-6.203467	0.095743	0.989437
6	-8.199188	1.478624	1.429627
6	-6.845237	0.668724	3.344210
6	-8.258951	0.827544	2.804568
1	-7.788961	2.498580	1.502823
1	-6.836196	-0.013474	4.202604
1	-8.850489	1.436806	3.494265
7	-5.936013	0.132755	2.328589
7	-7.382186	0.649894	0.546425
1	-8.743150	-0.151032	2.713910
1	-9.198539	1.557396	0.992732
1	-6.454680	1.634656	3.693202
6	-7.581849	0.785185	-0.890063
1	-7.073914	1.671098	-1.298272
1	-7.200797	-0.095242	-1.402672
1	-8.653068	0.875982	-1.089225
6	-4.631628	-0.281056	2.829693
1	-4.698522	-1.245105	3.350341
1	-3.911907	-0.362726	2.018018
14	-5.981576	-3.466291	-1.699411
14	-4.039172	-4.733992	0.278769
3	-4.041724	-1.684857	-0.150407

6	-6.239529	-5.049869	-2.741036
1	-5.369218	-5.243123	-3.382013
1	-6.385951	-5.938604	-2.114804
1	-7.116704	-4.964641	-3.397198
6	-5.898471	-2.051827	-2.974483
1	-5.602074	-1.121152	-2.482898
1	-5.161936	-2.260265	-3.759491
1	-6.867694	-1.887464	-3.463966
6	-7.612485	-3.204555	-0.740599
1	-8.489314	-3.152574	-1.400619
1	-7.784883	-4.020236	-0.026573
1	-7.568307	-2.270457	-0.167667
6	-5.393541	-5.896717	0.969975
1	-4.962696	-6.665868	1.625758
1	-6.126513	-5.335262	1.563660
1	-5.945441	-6.416765	0.177336
6	-3.152752	-4.058897	1.822310
1	-3.862902	-3.520555	2.464688
1	-2.713449	-4.864358	2.425601
6	-2.799092	-5.887393	-0.606975
1	-1.905505	-5.334612	-0.921212
1	-2.470441	-6.722158	0.027119
1	-3.249091	-6.319995	-1.510412
1	-2.361315	-3.355693	1.545937
1	-4.270696	0.470970	3.540439
6	2.629209	3.448319	-1.570145
6	2.136151	4.781939	-1.337209
6	1.986367	2.684626	-2.538039
6	2.600689	5.592665	-0.264527
6	1.122037	5.324200	-2.197082
6	0.991847	3.216858	-3.387139
6	2.124754	6.872361	-0.080915
1	3.319346	5.186155	0.436054
6	0.657366	6.650337	-1.983887
6	0.587219	4.519402	-3.237138
1	0.562815	2.566893	-4.141145
6	1.152392	7.416239	-0.952962
1	2.488109	7.462105	0.754989
1	-0.105894	7.044041	-2.650427
1	-0.173445	4.934920	-3.891850
1	0.788667	8.427681	-0.796327
8	2.350664	1.370832	-2.786897
6	3.782798	2.893708	-0.803776
6	5.068287	3.543059	-0.752465
6	3.653554	1.681992	-0.147079
6	5.375588	4.703655	-1.516865
6	6.109361	2.979809	0.062380
6	4.670439	1.120169	0.655637
6	6.618443	5.295301	-1.447581
1	4.620900	5.121488	-2.172153
6	7.374842	3.624412	0.122535
6	5.872120	1.771523	0.773791
1	4.473743	0.176252	1.150986
6	7.627072	4.762166	-0.610213
1	6.827258	6.177353	-2.046348
1	8.146208	3.190413	0.753702
1	6.666223	1.353281	1.385966
1	8.599407	5.243487	-0.559355
8	2.478235	0.954599	-0.270005
15	2.157809	0.137739	-1.673080
8	3.488703	-0.700105	-2.043769
6	4.770043	-0.173132	-2.469658
1	4.689091	0.866480	-2.787682
1	5.479059	-0.259795	-1.646078
1	5.097637	-0.791296	-3.306425

(3-4)B4-LiHMDS.IDMPU[‡]

Number of imaginary frequencies : 1
 Electronic energy : HF=-6039.3776384
 Zero-point correction= 1.483365 (Hartree/Particle)
 Thermal correction to Energy= 1.583781
 Thermal correction to Enthalpy= 1.584725
 Thermal correction to Gibbs Free Energy= 1.345302
 Sum of electronic and zero-point Energies= -6037.894274
 Sum of electronic and thermal Energies= -6037.793858
 Sum of electronic and thermal Enthalpies= -6037.792913
 Sum of electronic and thermal Free Energies= -6038.032337
 Standard State and RRHO Corrected G= -6038.007915

Cartesian Coordinates

6	-4.490131	3.758751	-3.448517	6	2.844703	-2.700918	1.835210
6	-3.245753	3.843625	-2.816416	6	5.710719	-5.093852	1.992964
6	-2.510157	2.686527	-2.565172	6	4.187749	-4.245602	3.716333
6	-3.025444	1.437380	-2.933355	6	2.382590	-2.717947	3.167795
6	-4.279369	1.349928	-3.554139	6	6.332442	-5.884877	2.934709
6	-5.003148	2.511852	-3.821882	1	6.039086	-5.133915	0.961605
6	-2.264778	0.197820	-2.603317	6	4.860863	-5.063677	4.664383
8	-2.937142	-0.837004	-2.297728	6	3.063001	-3.464555	4.097585
6	-2.128624	-2.533469	-2.993860	1	1.497794	-2.145010	3.421772
6	-0.800741	-2.858235	-2.633354	6	5.915582	-5.863222	4.286983
6	0.364979	-2.312787	-3.284131	1	7.148149	-6.536100	2.634065
45	0.146074	-1.147519	-1.500459	1	4.515710	-5.051909	5.694832
8	-0.991594	0.248720	-2.652338	1	2.731684	-3.485310	5.131679
15	-1.086445	-0.328867	0.396892	1	6.419854	-6.487303	5.018912
8	-2.356270	-1.083612	0.736267	8	2.129468	-1.913152	0.926303
8	-0.349265	-0.081006	1.905462	15	1.155865	-2.625627	-0.175957
6	0.348955	1.058737	2.246361	8	0.100776	-3.553871	0.578655
6	-0.281486	2.294511	2.361583	6	0.372558	-4.771304	1.327138
6	0.528928	3.446417	2.668665	1	-0.389233	-5.490633	1.029464
6	1.917014	3.273301	2.988141	1	1.365615	-5.162047	1.103385
6	2.476615	1.969420	2.951649	1	0.284522	-4.544098	2.389861
6	1.717998	0.895909	2.564080	8	-5.290656	-0.432642	-0.003931
6	2.711479	4.406245	3.312829	7	-4.459975	-3.499129	-0.776347
6	2.172625	5.673267	3.313057	6	-6.181973	0.031381	0.736763
6	0.813042	5.854473	2.963754	6	-8.227108	1.405611	1.005082
6	0.016886	4.775309	2.647132	6	-7.123436	0.465236	3.015283
6	-1.746000	2.418028	2.126356	6	-8.458113	0.667318	2.315192
6	-2.645648	2.997304	3.089037	1	-7.855841	2.425653	1.196045
6	-4.025766	3.185276	2.738089	1	-7.229544	-0.239068	3.848161
6	-4.486328	2.756765	1.464429	1	-9.134452	1.234968	2.961051
6	-3.639799	2.118979	0.593063	7	-6.115168	-0.068831	2.098707
6	-2.282791	1.940999	0.940422	7	-7.280548	0.654867	0.184268
6	-4.914419	3.765663	3.684532	1	-8.921963	-0.302589	2.104189
6	-4.479367	4.122395	4.941411	1	-9.160925	1.499717	0.442536
6	-3.128317	3.904525	5.304137	1	-6.759454	1.413413	3.438243
6	-2.237521	3.360750	4.403736	6	-7.259384	0.964173	-1.238750
8	-1.463258	1.279995	0.040269	1	-6.809183	1.947072	-1.437127
1	0.395604	6.856689	2.929198	1	-6.687650	0.208603	-1.771590
1	-1.014919	4.940855	2.361638	1	-8.285945	0.969442	-1.617589
1	3.760007	4.249845	3.554340	6	-4.917160	-0.593611	2.741048
1	2.788593	6.532953	3.561470	1	-5.119128	-1.570478	3.198564
1	3.527269	1.838981	3.193939	1	-4.103632	-0.690283	2.025798
1	2.146889	-0.089812	2.468303	14	-5.835880	-3.553225	-1.772345
1	-1.209056	3.192850	4.701733	14	-3.948639	-4.738243	0.268852
1	-3.990257	1.719314	-0.347701	3	-3.848592	-1.629321	-0.377809
1	-2.791386	4.163939	6.303950	6	-6.084224	-5.201541	-2.716263
1	-5.952181	3.913798	3.395803	1	-5.202117	-5.437143	-3.326459
1	-5.531061	2.901733	1.204518	1	-6.251375	-6.052723	-2.045297
1	-5.169369	4.558797	5.658015	1	-6.945910	-5.148248	-3.396063
1	-0.706696	-3.714660	-1.970400	6	-5.754640	-2.233620	-3.144086
1	-2.318647	-2.114508	-3.976297	1	-5.454222	-1.276230	-2.713502
1	-2.940867	-3.075302	-2.511781	1	-5.018421	-2.490583	-3.915742
1	-1.559452	2.729762	-2.052822	1	-6.726354	-2.106447	-3.639536
1	-4.676789	0.376914	-3.819818	6	-7.482961	-3.222876	-0.863370
1	-2.850419	4.807843	-2.510440	1	-8.352642	-3.312352	-1.529009
1	-5.969676	2.444082	-4.312792	1	-7.629550	-3.923646	-0.031792
1	-5.062310	4.661198	-3.645529	1	-7.487058	-2.208837	-0.445447
1	0.211570	-1.683434	-4.159673	6	-5.339693	-5.842749	0.986899
1	1.267364	-2.914152	-3.322492	1	-4.927961	-6.604828	1.663078
6	4.387694	-3.295323	-0.025066	1	-6.051591	-5.243118	1.568935
6	5.725850	-2.910788	-0.390233	1	-5.912070	-6.368774	0.213561
6	3.499272	-3.575426	-1.053259	6	-3.051480	-4.077899	1.809563
6	6.644334	-2.370097	0.552811	1	-3.748287	-3.517810	2.446679
6	6.144228	-3.019121	-1.757336	1	-2.640082	-4.897816	2.413803
6	3.910669	-3.714356	-2.395922	6	-2.736208	-5.954502	-0.575706
6	7.906120	-1.971465	0.166772	1	-1.840747	-5.428794	-0.930478
1	6.336418	-2.253118	1.585560	1	-2.407059	-6.760751	0.094137
6	7.460405	-2.622682	-2.117239	1	-3.202048	-6.425995	-1.451117
6	5.218548	-3.475624	-2.734317	1	-2.243251	-3.394649	1.537940
1	3.178139	-4.011858	-3.137377	1	-4.603398	0.098847	3.531333
6	8.325926	-2.107536	-1.178210	6	2.420103	3.464800	-1.650339
1	8.583882	-1.546128	0.901419	6	1.928388	4.794592	-1.394342
1	7.763647	-2.715994	-3.156811	6	1.729763	2.694640	-2.578736
1	5.547828	-3.587563	-3.763351	6	2.434834	5.607503	-0.342689
1	9.325216	-1.795245	-1.467013	6	0.870616	5.327108	-2.205838
8	2.148327	-3.801703	-0.790833	6	0.686962	3.211551	-3.375196
6	3.960458	-3.389272	1.398141	6	1.956052	6.882518	-0.135444
6	4.635055	-4.234055	2.351067	1	3.188555	5.206288	0.323519
				6	0.406388	6.649916	-1.971516
				6	0.288315	4.514365	-3.213753

1	0.212106	2.550319	-4.090226	6	-4.712587	4.010785	4.393953
6	0.941363	7.418835	-0.962975	6	-3.443944	3.689052	4.934236
1	2.351240	7.474447	0.684329	6	-2.451227	3.168556	4.132191
1	-0.389986	7.037619	-2.601737	8	-1.186776	1.199754	-0.156160
1	-0.511058	4.920463	-3.826235	1	0.054018	6.786276	3.400560
1	0.576659	8.427053	-0.788952	1	-1.124992	4.883012	2.445324
8	2.091884	1.377761	-2.841208	1	3.553391	4.365920	4.017077
6	3.620520	2.925075	-0.948995	1	2.396527	6.551830	4.234027
6	4.900571	3.587407	-0.973014	1	3.560227	2.023763	3.333834
6	3.543613	1.715151	-0.282905	1	2.370419	0.073252	2.368131
6	5.150390	4.751503	-1.752420	1	-1.486293	2.923909	4.561281
6	5.993265	3.032829	-0.222361	1	-3.580257	1.805807	-0.878343
6	4.610196	1.159519	0.455606	1	-3.251939	3.851429	5.991118
6	6.389753	5.354459	-1.756267	1	-5.944650	3.989724	2.638495
1	4.354224	5.163521	-2.360427	1	-5.264327	3.059124	0.478310
6	7.254192	3.688746	-0.237047	1	-5.482475	4.433924	5.032907
6	5.811007	1.821594	0.500259	1	0.466336	-4.230080	-2.173079
1	4.451187	0.215312	0.963061	1	-2.089876	-2.499736	-2.464258
6	7.451415	4.829549	-0.981793	1	-1.710217	-3.690815	-1.143463
1	6.554181	6.239310	-2.364563	1	-4.764082	0.951062	-2.796659
1	8.065884	3.261079	0.345852	1	-1.135410	0.754813	-5.068271
1	6.644517	1.409707	1.062101	1	-5.816634	2.344466	-4.581298
1	8.420580	5.319745	-0.988595	1	-2.177708	2.120034	-6.871385
8	2.364163	0.977199	-0.335447	1	-4.516256	2.923807	-6.621088
15	1.993588	0.163129	-1.716821	1	-0.018165	-1.826228	-4.066528
8	3.296379	-0.676707	-2.151205	1	1.562756	-2.725470	-3.754491
6	4.549450	-0.149661	-2.661726	6	4.540146	-2.998880	0.015133
1	4.442117	0.884288	-2.989831	6	5.778971	-2.452807	-0.472615
1	5.304077	-0.220391	-1.878731	6	3.623322	-3.445480	-0.925048
1	4.828087	-0.780901	-3.506036	6	6.704660	-1.784647	0.377364
-----				6	6.078467	-2.527697	-1.873710
4B4-LHMDS.IDMPU				6	3.928110	-3.565474	-2.295848
-----				6	7.860701	-1.229982	-0.128030
Number of imaginary frequencies : 0				1	6.484943	-1.694664	1.434672
Electronic energy : HF=-6039.4125786				6	7.287521	-1.959223	-2.359238
Zero-point correction= 1.483437 (Hartree/Particle)				6	5.147353	-3.137140	-2.756899
Thermal correction to Energy= 1.584848				1	3.184165	-3.992440	-2.958087
Thermal correction to Enthalpy= 1.585792				6	8.161497	-1.320851	-1.508432
Thermal correction to Gibbs Free Energy= 1.343392				1	8.545589	-0.714810	0.539302
Sum of electronic and zero-point Energies= -6037.929142				1	7.500308	-2.026032	-3.422933
Sum of electronic and thermal Energies= -6037.827731				1	5.395861	-3.222859	-3.810682
Sum of electronic and thermal Enthalpies= -6037.826787				1	9.076861	-0.880474	-1.892450
Sum of electronic and thermal Free Energies= -6038.069187				8	2.343760	-3.848489	-0.527412
Standard State and RRHO Corrected G= -6038.043825				6	4.220899	-3.072610	1.467115
-----				6	5.058687	-3.763931	2.412968
Cartesian Coordinates				6	3.051600	-2.510182	1.943867
-----				6	6.212229	-4.500290	2.024181
6	-4.061780	2.322123	-5.838775	6	4.704583	-3.746619	3.805008
6	-4.793202	1.996733	-4.691965	6	2.687001	-2.491393	3.305941
6	-4.211352	1.221347	-3.689968	6	6.989794	-5.147972	2.959612
6	-2.888213	0.774972	-3.822238	1	6.476679	-4.559787	0.975283
6	-2.158825	1.102125	-4.973697	6	5.536745	-4.414583	4.744260
6	-2.745987	1.871091	-5.979547	6	3.517379	-3.086104	4.223462
6	-2.295619	-0.050522	-2.711682	1	1.760628	-2.006008	3.591750
8	-3.043658	-0.486784	-1.826382	6	6.659646	-5.097112	4.334908
6	-1.331444	-3.061996	-1.938521	1	7.862671	-5.708103	2.636881
6	-0.107626	-3.395137	-2.571299	1	5.259861	-4.383283	5.794688
6	0.543455	-2.518184	-3.448998	1	3.262935	-3.076224	5.279277
45	0.128824	-1.433525	-1.444479	1	7.285932	-5.607289	5.060802
8	-1.015777	-0.240647	-2.789353	8	2.183526	-1.871135	1.050511
15	-0.976052	-0.382260	0.350585	15	1.258870	-2.723054	0.018967
8	-2.235183	-1.004091	0.894629	8	0.260086	-3.670352	0.817190
8	-0.051630	-0.088166	1.717902	6	0.615251	-4.751431	1.725783
6	0.506483	1.102086	2.128918	1	-0.143965	-5.520636	1.587727
6	-0.222592	2.280424	2.272228	1	1.603609	-5.150897	1.494019
6	0.479993	3.452467	2.751194	1	0.585799	-4.369965	2.746934
6	1.848957	3.345189	3.169252	8	-5.215009	-0.315962	0.148570
6	2.518552	2.100900	3.034072	7	-4.339526	-3.435921	-0.260936
6	1.867492	1.016532	2.512450	6	-6.141603	0.128957	0.849636
6	2.519282	4.479569	3.700974	6	-8.320031	1.295257	1.007911
6	1.878891	5.692319	3.817615	6	-7.112523	0.690967	3.092067
6	0.547827	5.819781	3.358952	6	-8.463433	0.676761	2.391599
6	-0.123278	4.740107	2.827530	1	-8.051056	2.361402	1.086427
6	-1.659147	2.370021	1.885788	1	-7.136663	0.049957	3.981178
6	-2.672024	2.925080	2.747078	1	-9.195387	1.230887	2.986732
6	-3.977321	3.199667	2.216386	7	-6.047433	0.206622	2.212972
6	-4.272907	2.852037	0.871584	7	-7.311921	0.555535	0.254705
6	-3.349445	2.184240	0.108074	1	-8.820598	-0.353554	2.285210
6	-2.064243	1.933795	0.632424	1	-9.264218	1.237882	0.457973
6	-4.968886	3.767313	3.062976	1	-6.862548	1.705860	3.433299

6	-7.341922	0.669584	-1.196188	Zero-point correction=	0.664096 (Hartree/Particle)
1	-6.979410	1.650368	-1.539951	Thermal correction to Energy=	0.705976
1	-6.719590	-0.105778	-1.638464	Thermal correction to Enthalpy=	0.706920
1	-8.371651	0.542559	-1.543076	Thermal correction to Gibbs Free Energy=	0.587281
6	-4.800479	-0.142434	2.880491	Sum of electronic and zero-point Energies=	-1808.863493
1	-4.914188	-1.074714	3.448732	Sum of electronic and thermal Energies=	-1808.821613
1	-3.998742	-0.263421	2.155152	Sum of electronic and thermal Enthalpies=	-1808.820669
14	-5.586318	-3.639358	-1.390881	Sum of electronic and thermal Free Energies=	-1808.940308
14	-3.913773	-4.542288	0.948835	Standard State and RRHO Corrected G=	-1808.927945
3	-3.751274	-1.507374	-0.208780	-----	
6	-5.766385	-5.413705	-2.094432	Cartesian Coordinates	
1	-4.838929	-5.741487	-2.582033	-----	
1	-6.000769	-6.147536	-1.313002	6	1.020923 -2.033929 0.627948
1	-6.567445	-5.470516	-2.844637	6	1.910712 -1.406927 -0.412634
6	-5.331532	-2.550234	-2.935398	1	1.466201 -0.418829 -0.595615
1	-5.126745	-1.510554	-2.665500	3	-1.138577 -0.095622 0.084577
1	-4.471468	-2.901756	-3.521319	7	0.039398 1.460086 -0.223640
1	-6.209863	-2.573088	-3.594867	14	0.093576 2.101299 -1.794350
6	-7.325416	-3.202805	-0.724448	14	0.532363 2.146975 1.251911
1	-8.106341	-3.289715	-1.492863	6	1.668029 3.079285 -2.263161
1	-7.603344	-3.867772	0.103814	1	1.651602 3.328966 -3.333162
1	-7.347570	-2.176936	-0.339120	1	1.766273 4.019971 -1.710301
6	-5.393853	-5.377462	1.836444	1	2.578726 2.494604 -2.081567
1	-5.060905	-6.068730	2.623300	6	0.028097 0.713683 -3.102821
1	-6.035965	-4.624565	2.312147	1	-0.676911 -0.077733 -2.831914
1	-6.023404	-5.950672	1.144158	1	-0.256924 1.101882 -4.089732
6	-2.888360	-3.767521	2.350818	1	1.016277 0.250022 -3.212135
1	-3.478273	-3.031608	2.911047	6	-1.338569 3.306377 -2.181632
1	-2.551650	-4.534447	3.062284	1	-2.319075 2.842701 -2.016911
6	-2.846545	-6.006419	0.316485	1	-1.285953 4.186412 -1.526706
1	-1.893799	-5.653867	-0.099250	1	-1.313750 3.667606 -3.218784
1	-2.611831	-6.722334	1.116735	6	-0.865706 3.075037 2.160811
1	-3.359598	-6.561446	-0.479333	1	-1.685379 2.382880 2.384244
1	-2.016696	-3.242533	1.952946	1	-0.530186 3.517558 3.108577
1	-4.529109	0.657341	3.579108	1	-1.276421 3.884771 1.543567
6	1.930645	3.401509	-1.371945	6	1.129518 0.819883 2.485663
6	1.390104	4.641838	-0.873570	1	2.019999 0.299797 2.112387
6	1.106746	2.618905	-2.165977	1	1.397178 1.276393 3.447901
6	2.104604	5.495546	0.012695	1	0.360150 0.066424 2.683253
6	0.070786	5.045844	-1.273561	6	1.978226 3.392115 1.157443
6	-0.198309	2.994576	-2.536864	1	2.300274 3.679755 2.167470
6	1.582321	6.705065	0.413288	1	2.850097 2.970323 0.643550
1	3.071564	5.186356	0.387762	1	1.697731 4.312743 0.631938
6	-0.445551	6.292420	-0.826206	6	-2.917750 -2.172448 -0.917219
6	-0.702813	4.194180	-2.106320	6	-3.358007 -0.134830 -2.054488
1	-0.772430	2.312092	-3.145858	6	-4.193008 -2.336181 -1.745272
6	0.299100	7.117746	-0.015432	1	-3.123287 -2.196000 0.158316
1	2.151962	7.334675	1.089454	1	-2.149954 -2.916700 -1.145621
1	-1.444806	6.580223	-1.142879	6	-4.676137 -0.885141 -1.886442
1	-1.707201	4.497372	-2.388370	1	-3.021778 -0.139770 -3.098880
1	-0.101916	8.071719	0.314635	1	-3.389586 0.899962 -1.705701
8	1.579468	1.416648	-2.698862	1	-3.958960 -2.754437 -2.730454
6	3.299436	2.930412	-1.012113	1	-4.919632 -2.991407 -1.257500
6	4.487964	3.712415	-1.236499	1	-5.351710 -0.731015 -2.731845
6	3.467063	1.674115	-0.451134	1	-5.185500 -0.560823 -0.972430
6	4.473934	4.927070	-1.977965	6	-3.724829 0.517377 1.599578
6	5.751369	3.235061	-0.747080	6	-2.345118 -0.794734 2.873086
6	4.698800	1.199767	0.045430	6	-4.658410 -0.577597 2.143073
6	5.630512	5.645931	-2.188312	1	-3.929006 0.813804 0.569820
1	3.537691	5.283077	-2.391240	1	-3.753182 1.413735 2.234955
6	6.922181	4.011100	-0.966006	6	-3.720381 -1.471481 3.001265
6	5.819666	1.981552	-0.080008	1	-2.161787 -0.099214 3.704369
1	4.732752	0.214452	0.495299	1	-1.509701 -1.490769 2.794738
6	6.866690	5.194475	-1.666849	1	-5.477391 -0.146369 2.724652
1	5.593888	6.566045	-2.764477	1	-5.097028 -1.153089 1.323519
1	7.867759	3.641016	-0.578214	1	-4.037618 -1.533766 4.045500
1	6.776947	1.628312	0.291688	1	-3.684386 -2.488897 2.601454
1	7.768888	5.775724	-1.833761	8	-2.396451 -0.858250 -1.247137
8	2.386685	0.790156	-0.370989	8	-2.407435 -0.053794 1.642999
15	1.838950	0.096859	-1.754648	8	-0.181846 -1.807878 0.691128
8	3.086071	-0.555442	-2.525810	1	1.469574 -2.737155 1.352904
6	4.177216	0.143258	-3.183146	6	1.777627 -2.206986 -1.748405
1	3.864577	1.134208	-3.514720	1	2.357215 -1.663587 -2.502642
1	5.020841	0.220549	-2.497457	1	0.727779 -2.147387 -2.055737
1	4.450774	-0.469132	-4.043248	6	2.224800 -3.669934 -1.707662
-----				1	2.068026 -4.137478 -2.685641
(5...6) _{E-LHMDS,2THF}				1	3.287329 -3.762052 -1.464198
-----				1	1.657808 -4.250676 -0.970114
Number of imaginary frequencies : 0				6	3.341467 -1.216819 0.053202
Electronic energy : HF=-1809.5275883				6	4.088793 -2.230829 0.672828

6	3.948641	0.033389	-0.144631
6	5.406924	-2.000863	1.076479
1	3.646232	-3.207386	0.844202
6	5.265956	0.263854	0.253913
1	3.375693	0.831826	-0.607421
6	6.000736	-0.754378	0.867229
1	5.968633	-2.798437	1.555239
1	5.714464	1.240158	0.091334
1	7.025300	-0.577043	1.182181

(5-6)*E*-LiHMDs.2THF[‡]

Number of imaginary frequencies : 1
 Electronic energy : HF=-1809.517817
 Zero-point correction= 0.660190 (Hartree/Particle)
 Thermal correction to Energy= 0.700855
 Thermal correction to Enthalpy= 0.701799
 Thermal correction to Gibbs Free Energy= 0.586581
 Sum of electronic and zero-point Energies= -1808.857627
 Sum of electronic and thermal Energies= -1808.816962
 Sum of electronic and thermal Enthalpies= -1808.816018
 Sum of electronic and thermal Free Energies= -1808.931236
 Standard State and RRHO Corrected G= -1808.920316

Cartesian Coordinates

6	-0.919991	1.753788	-0.934225
6	-1.869995	0.696822	-1.152073
1	-1.248841	-0.121622	-0.339063
3	1.200285	0.302931	-0.167516
7	-0.322830	-0.981134	0.437074
14	-0.187317	-2.595764	-0.188485
14	-0.681270	-0.694051	2.114006
6	-1.852614	-3.503075	-0.347777
1	-1.696265	-4.516997	-0.740362
1	-2.376704	-3.597389	0.609162
1	-2.523202	-2.988138	-1.045802
6	0.557697	-2.642001	-1.940033
1	1.279730	-1.838608	-2.109234
1	1.071989	-3.598415	-2.100342
1	-0.221102	-2.562953	-2.705608
6	0.905285	-3.708692	0.903487
1	1.892114	-3.267660	1.084048
1	0.443606	-3.894925	1.880255
1	1.060313	-4.684765	0.425591
6	0.812310	-0.996520	3.249428
1	1.679576	-0.416040	2.920007
1	0.583242	-0.693107	4.279690
1	1.103646	-2.052079	3.274790
6	-1.210422	1.108215	2.373614
1	-2.128535	1.349456	1.827852
1	-1.405046	1.285946	3.439082
1	-0.429733	1.808507	2.060995
6	-2.090295	-1.760735	2.819440
1	-2.297337	-1.474918	3.859262
1	-3.018826	-1.630971	2.252229
1	-1.841686	-2.828405	2.819181
6	3.499699	0.460166	-1.992160
6	3.675260	-1.461736	-0.608142
6	4.858168	-0.206089	-2.234760
1	3.602408	1.461897	-1.562264
1	2.882823	0.525710	-2.893315
6	5.086927	-0.984795	-0.929914
1	3.415199	-2.365019	-1.174445
1	3.495947	-1.651930	0.452976
1	4.797961	-0.899224	-3.080612
1	5.642114	0.525583	-2.446261
1	5.792774	-1.812526	-1.036562
1	5.449661	-0.316774	-0.140677
6	3.369489	1.352990	1.742907
6	1.913082	2.994978	1.094466
6	4.278948	2.457525	1.170158
1	3.690312	0.340368	1.498123
1	3.280608	1.440962	2.834664
6	3.280380	3.523689	0.643318
1	1.650155	3.365997	2.095760
1	1.103025	3.205210	0.397487
1	4.944817	2.854212	1.941113
1	4.900626	2.069932	0.358918
1	3.478861	4.523588	1.038076

1	3.316829	3.578508	-0.448669
8	2.814787	-0.375220	-1.020889
8	2.076345	1.565116	1.149093
8	0.280864	1.704330	-1.296747
1	-1.226034	2.579930	-0.264189
6	-1.742769	-0.062440	-2.483481
1	-2.225840	-1.041174	-2.386578
1	-0.682613	-0.249887	-2.669839
6	-2.348725	0.695288	-3.670690
1	-2.248539	0.121074	-4.599353
1	-3.414175	0.895813	-3.513430
1	-1.846726	1.659320	-3.814618
6	-3.277642	0.928012	-0.684586
6	-3.904416	2.184802	-0.739114
6	-4.020246	-0.153782	-0.177070
6	-5.213420	2.359708	-0.280989
1	-3.366545	3.032984	-1.154565
6	-5.330317	0.014621	0.271955
1	-3.555924	-1.133770	-0.128092
6	-5.932462	1.275915	0.227615
1	-5.674397	3.342821	-0.333097
1	-5.879300	-0.838137	0.663222
1	-6.951343	1.410442	0.580337

6E-LiHMDs.2THF

Number of imaginary frequencies : 0
 Electronic energy : HF=-1809.5559251
 Zero-point correction= 0.665258 (Hartree/Particle)
 Thermal correction to Energy= 0.706515
 Thermal correction to Enthalpy= 0.707460
 Thermal correction to Gibbs Free Energy= 0.589930
 Sum of electronic and zero-point Energies= -1808.890668
 Sum of electronic and thermal Energies= -1808.849410
 Sum of electronic and thermal Enthalpies= -1808.848465
 Sum of electronic and thermal Free Energies= -1808.965995
 Standard State and RRHO Corrected G= -1808.954395

Cartesian Coordinates

6	1.062962	1.459075	1.189035
6	2.221028	0.777601	1.508322
1	0.874673	-0.565095	0.020413
3	-1.230471	0.343262	0.454344
7	0.164875	-1.074452	-0.522320
14	0.074349	-2.741119	0.093060
14	0.408251	-0.682971	-2.240752
6	1.785945	-3.543920	0.099196
1	1.775813	-4.480975	0.670014
1	2.130037	-3.773789	-0.914611
1	2.531452	-2.884710	0.558606
6	-0.590532	-2.747894	1.856203
1	-1.530729	-2.195156	1.937691
1	-0.765982	-3.781081	2.181792
1	0.123540	-2.299168	2.553515
6	-1.066908	-3.756148	-1.014225
1	-2.054185	-3.299089	-1.130413
1	-0.642160	-3.906070	-2.012667
1	-1.211920	-4.748805	-0.570152
6	-1.207984	-0.948676	-3.175657
1	-2.033489	-0.403790	-2.707789
1	-1.109679	-0.578401	-4.203837
1	-1.488220	-2.004938	-3.232949
6	0.933524	1.119336	-2.368907
1	1.873998	1.306866	-1.839760
1	1.086272	1.387141	-3.421932
1	0.165923	1.780609	-1.957677
6	1.757361	-1.748254	-3.027040
1	1.945611	-1.424981	-4.058768
1	2.699371	-1.656097	-2.473703
1	1.486277	-2.809338	-3.059280
6	-3.707938	0.308917	1.964643
6	-3.752391	-1.373658	0.285480
6	-5.103070	-0.315699	1.927620
1	-3.718305	1.350366	1.623782
1	-3.230891	0.263058	2.947799
6	-5.174930	-0.862102	0.493693
1	-3.625562	-2.386984	0.687380
1	-3.425275	-1.368391	-0.757838
1	-5.173589	-1.136484	2.649630

1	-5.886184	0.412045	2.155091
1	-5.921923	-1.649448	0.364409
1	-5.396006	-0.054029	-0.212528
6	-3.154215	1.848128	-1.505989
6	-1.710120	3.182649	-0.317859
6	-4.057677	2.939744	-0.899484
1	-3.599916	0.852471	-1.498016
1	-2.864994	2.096745	-2.536593
6	-3.090989	3.781709	-0.022779
1	-1.223625	3.692590	-1.162031
1	-1.037774	3.154249	0.539201
1	-4.533428	3.533399	-1.684497
1	-4.850315	2.496308	-0.290706
1	-3.126818	4.848601	-0.258221
1	-3.331681	3.663791	1.037797
8	-2.907175	-0.465487	1.031940
8	-1.976971	1.813428	-0.682810
8	-0.128135	1.261670	1.670309
1	1.143156	2.218794	0.391453
6	2.184996	-0.279342	2.593303
1	2.426025	-1.276693	2.196776
1	1.154144	-0.337745	2.953592
6	3.122044	0.015479	3.776606
1	3.062446	-0.770718	4.539357
1	4.166024	0.087856	3.452496
1	2.858273	0.967809	4.251086
6	3.463472	1.018265	0.760143
6	3.755380	2.251946	0.124699
6	4.434960	-0.003032	0.617166
6	4.907186	2.430486	-0.638955
1	3.074862	3.088695	0.249963
6	5.593746	0.182199	-0.137098
1	4.270596	-0.964850	1.093375
6	5.840016	1.397394	-0.781722
1	5.087851	3.393712	-1.110919
1	6.307614	-0.633858	-0.224592
1	6.742642	1.542103	-1.368715

(5...6)_{E-LIHMS,2DMPU}

Number of imaginary frequencies : 0
 Electronic energy : HF=-2185.90374
 Zero-point correction= 0.801155 (Hartree/Particle)
 Thermal correction to Energy= 0.851605
 Thermal correction to Enthalpy= 0.852549
 Thermal correction to Gibbs Free Energy= 0.716670
 Sum of electronic and zero-point Energies= -2185.102585
 Sum of electronic and thermal Energies= -2185.052135
 Sum of electronic and thermal Enthalpies= -2185.051191
 Sum of electronic and thermal Free Energies= -2185.187070
 Standard State and RRHO Corrected G= -2185.174197

Cartesian Coordinates

6	-6.125849	-0.771106	-1.455258
6	-4.736182	-0.807421	-1.330073
6	-4.114376	-1.545191	-0.307601
6	-4.933684	-2.240610	0.593072
6	-6.325417	-2.203746	0.473101
6	-6.928170	-1.472631	-0.552427
1	-6.579119	-0.189727	-2.253464
1	-4.128013	-0.237769	-2.029160
1	-6.938443	-2.749922	1.185137
1	-8.010326	-1.445855	-0.644524
1	-4.492169	-2.814596	1.400721
6	-2.599270	-1.503048	-0.190390
6	-1.943388	-2.596050	0.699145
1	-0.887594	-2.331042	0.802329
1	-2.375142	-2.521664	1.702275
6	-2.074326	-4.030360	0.172498
1	-1.545525	-4.162703	-0.778303
1	-1.644758	-4.741058	0.886773
1	-3.119288	-4.312162	0.009216
6	-1.940507	-1.565733	-1.548556
8	-0.880857	-1.012582	-1.810241
1	-2.441278	-2.175077	-2.325712
3	0.085781	0.339727	-0.522977
7	-1.218479	1.566436	0.385798
6	2.679267	1.110643	-1.441385
6	4.926842	0.119882	-1.847412

6	4.713743	2.246237	-0.577048
6	5.394792	0.885778	-0.618626
1	5.283569	-0.914750	-1.812976
1	5.082565	2.889780	-1.390798
1	5.132625	0.321606	0.281240
6	2.246174	-1.548720	0.703603
6	3.654645	-3.596307	0.542035
6	4.312111	-1.752838	2.069022
6	4.814166	-2.737611	1.023595
1	3.328967	-4.284673	1.337062
1	5.100114	-1.042661	2.338542
1	5.597507	-3.371764	1.448606
6	1.492842	-3.432036	-0.647126
1	0.787379	-2.702369	-1.035736
1	1.953004	-3.967939	-1.483227
1	0.950528	-4.159497	-0.027568
6	2.838514	0.244017	2.233749
1	3.756835	0.803614	2.433197
1	2.187489	0.846670	1.607181
1	2.332005	0.050416	3.188611
6	2.450202	3.227916	-0.266966
1	2.497576	4.042730	-1.003787
1	1.413074	2.922117	-0.146278
1	2.823510	3.605481	0.689083
6	2.878568	-0.924231	-2.770540
1	3.279975	-1.904637	-2.497133
1	1.798504	-0.933768	-2.642820
1	3.113424	-0.731226	-3.827111
7	3.262702	2.087505	-0.674419
7	3.465955	0.088676	-1.905706
7	2.533314	-2.756732	0.117233
7	3.181288	-0.990186	1.538665
1	3.958124	-4.209123	-0.313174
1	5.242661	-2.188060	0.178412
1	4.019364	-2.280937	2.989332
1	5.332283	0.573095	-2.765106
1	6.481350	1.009155	-0.644453
1	4.934361	2.757004	0.365621
8	1.176339	-0.952389	0.452665
8	1.447705	1.129145	-1.667488
1	-2.303681	-0.523621	0.224070
14	-1.192428	1.743420	2.075900
14	-1.965113	2.650376	-0.692406
6	-2.798760	2.433119	2.855075
1	-3.676042	1.849220	2.550081
1	-2.746371	2.401634	3.952217
1	-2.983222	3.476223	2.569519
6	-0.911538	0.077725	2.953857
1	-0.658019	0.215906	4.013713
1	-1.819287	-0.537125	2.913546
1	-0.105896	-0.485549	2.474752
6	0.165377	2.930589	2.718805
1	0.038592	3.932504	2.288676
1	0.127968	3.035355	3.812032
1	1.173983	2.593980	2.456567
6	-1.701553	2.135835	-2.506636
1	-2.118247	2.888953	-3.188786
1	-0.635400	2.022580	-2.731489
1	-2.187030	1.179723	-2.733376
6	-1.327586	4.451602	-0.579557
1	-1.490963	4.870652	0.421816
1	-0.252249	4.513651	-0.787438
1	-1.839467	5.110234	-1.294771
6	-3.862282	2.808483	-0.499136
1	-4.300676	3.364148	-1.339839
1	-4.346415	1.825240	-0.467072
1	-4.139566	3.336896	0.420382

(5-6)_{E-LIHMS,2DMPU}[‡]

Number of imaginary frequencies : 1
 Electronic energy : HF=-2185.8927857
 Zero-point correction= 0.796942 (Hartree/Particle)
 Thermal correction to Energy= 0.846496
 Thermal correction to Enthalpy= 0.847440
 Thermal correction to Gibbs Free Energy= 0.715022
 Sum of electronic and zero-point Energies= -2185.095844
 Sum of electronic and thermal Energies= -2185.046290
 Sum of electronic and thermal Enthalpies= -2185.045346
 Sum of electronic and thermal Free Energies= -2185.177764

Standard State and RRHO Corrected G=-2185.165972

Cartesian Coordinates

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6      6.229214  0.700575 -1.543373
6      4.836006  0.672222 -1.480642
6      4.120524  1.394488 -0.500347
6      4.886707  2.116737  0.436950
6      6.281980  2.136157  0.383579
6      6.966471  1.435550 -0.611409
1      6.739689  0.130869 -2.315945
1      4.299212  0.056045 -2.194558
1      6.834931  2.706712  1.125895
1      8.051967  1.452076 -0.653580
1      4.392458  2.676627  1.223096
6      2.625140  1.324752 -0.430915
6      1.917049  2.278069  0.550407
1      0.881534  1.951781  0.664859
1      2.370830  2.183047  1.540101
6      1.935924  3.747812  0.106770
1      1.404617  3.873872 -0.843017
1      1.450020  4.391660  0.849870
1      2.957266  4.115860 -0.036190
6      1.929777  1.222356 -1.703968
8      0.693770  1.088507 -1.806584
1      2.531366  1.191461 -2.631309
3      -0.152266 -0.219951 -0.451130
7      1.550473 -1.087793  0.456923
6      -2.629485 -1.266092 -1.396256
6      -4.786686 -0.205065 -2.053439
6      -4.789275 -2.321572 -0.756082
6      -5.407726 -0.936823 -0.873417
1      -5.094767  0.845870 -2.057568
1      -5.092061 -2.957094 -1.602401
1      -5.213917 -0.375219  0.045145
6      -2.455719  1.433062  0.763551
6      -3.828846  3.478920  0.432851
6      -4.618271  1.687311  1.960628
6      -5.028258  2.640482  0.847758
1      -3.561511  4.189013  1.230572
1      -5.430720  0.990618  2.187860
1      -5.838610  3.291466  1.188285
6      -1.563288  3.289925 -0.537880
1      -0.833154  2.558588 -0.875729
1      -1.939749  3.844986 -1.402793
1      -1.071819  4.001484  0.139725
6      -3.155963 -0.321176  2.272349
1      -4.093789 -0.741103  2.643205
1      -2.686977 -1.043405  1.606822
1      -2.487255 -0.143499  3.124269
6      -2.621324 -3.376323 -0.176170
1      -2.700532 -4.235874 -0.856880
1      -1.571998 -3.129915 -0.040572
1      -3.050665 -3.659032  0.790050
6      -2.629592  0.730954 -2.808262
1      -2.975216  1.737401 -2.552765
1      -1.557009  0.672348 -2.640580
1      -2.838492  0.549901 -3.872171
7      -3.331256 -2.216803 -0.697996
7      -3.326018 -0.239955 -1.974979
7      -2.681541  2.623937  0.120689
7      -3.455630  0.903597  1.538744
1      -4.061611  4.067694 -0.460461
1      -5.391865  2.065204 -0.010936
1      -4.393854  2.243704  2.883227
1      -5.121524 -0.646318 -3.004558
1      -6.490221 -1.015714 -1.008871
1      -5.126325 -2.817097  0.159880
8      -1.378331  0.811833  0.624354
8      -1.377458 -1.318507 -1.460091
1      2.247737  0.147299  0.033565
14     1.348125 -1.318647  2.165921
14     2.205458 -2.373571 -0.515048
6      2.906551 -1.987463  3.034659
1      3.787157 -1.378542  2.795911
1      2.780056 -1.975463  4.125518
1      3.131258 -3.020430  2.744022
6      0.892353  0.273773  3.088982
1      0.559744  0.013694  4.102793
1      1.740841  0.957840  3.191959

```

```

1      0.077340  0.803279  2.588646
6      -0.051589 -2.540515  2.587519
1      0.172989 -3.564792  2.274136
1      -0.228359 -2.559817  3.671310
1      -0.990002 -2.249286  2.107204
6      1.900281 -2.055907 -2.361181
1      2.193701 -2.941954 -2.939218
1      0.839292 -1.861645 -2.550261
1      2.471047 -1.209530 -2.755620
6      1.465381 -4.093759 -0.173687
1      1.707299 -4.457411  0.831193
1      0.376668 -4.117417 -0.287321
1      1.885745 -4.814658 -0.887843
6      4.080409 -2.617218 -0.289020
1      4.489298 -3.249063 -1.089137
1      4.625611 -1.668535 -0.306228
1      4.306436 -3.109609  0.663734

```

6E-LiHMDs.2DMPU

```

Number of imaginary frequencies : 0
Electronic energy : HF=-2185.9333753
Zero-point correction= 0.801089 (Hartree/Particle)
Thermal correction to Energy= 0.851623
Thermal correction to Enthalpy= 0.852567
Thermal correction to Gibbs Free Energy= 0.715487
Sum of electronic and zero-point Energies= -2185.132287
Sum of electronic and thermal Energies= -2185.081752
Sum of electronic and thermal Enthalpies= -2185.080808
Sum of electronic and thermal Free Energies= -2185.217888
Standard State and RRHO Corrected G= -2185.204266

```

Cartesian Coordinates

```

6      -6.433843 -0.490748 -1.757000
6      -5.056288 -0.579127 -1.577429
6      -4.473682 -1.468320 -0.632876
6      -5.388213 -2.225283  0.143125
6      -6.769190 -2.123187 -0.029123
6      -7.311532 -1.262386 -0.986009
1      -6.827828  0.206037 -2.493760
1      -4.416845  0.071732 -2.164742
1      -7.426458 -2.728968  0.591146
1      -8.386729 -1.182885 -1.119654
1      -5.013147 -2.914434  0.892283
6      -3.025422 -1.571444 -0.429930
6      -2.473905 -2.272722  0.796674
1      -1.489121 -1.854281  1.023027
1      -3.103544 -2.077450  1.674999
6      -2.313646 -3.794253  0.615643
1      -1.636426 -4.008003 -0.217910
1      -1.903408 -4.267786  1.516895
1      -3.270395 -4.277976  0.390289
6      -2.128581 -1.134514 -1.389694
8      -0.839746 -1.102822 -1.294672
1      -2.552914 -0.783524 -2.345549
3      0.208492  0.161747 -0.364971
7      -1.376653  1.359450  0.645114
6      2.628089  1.032697 -1.593552
6      4.570544 -0.300297 -2.402485
6      4.938920  1.935887 -1.388011
6      5.416757  0.491789 -1.417808
1      4.790139 -1.370154 -2.320663
1      5.170966  2.443071 -2.336988
1      5.315511  0.054773 -0.420082
6      2.512026 -1.384161  0.907049
6      3.521682 -3.643329  0.674062
6      4.818885 -1.813786  1.731328
6      4.875179 -2.952718  0.725000
1      3.333509 -4.188726  1.611958
1      5.741967 -1.227307  1.699866
1      5.650719 -3.669888  1.008873
6      1.143228 -3.246318  0.133500
1      0.463287 -2.491390 -0.260094
1      1.274135 -4.028529 -0.620404
1      0.697615 -3.705088  1.027385
6      3.714782  0.412553  1.996614
1      4.753143  0.714621  2.150899
1      3.241910  1.122617  1.320538
1      3.193041  0.443279  2.961810

```


6	2.972366	3.252933	-0.645451	1	-4.377550	0.296616	2.811828
1	3.033663	4.032805	-1.417602	1	-3.213544	1.177940	3.809518
1	1.932628	3.126251	-0.354409	1	-3.380477	1.558436	2.090304
1	3.551563	3.580483	0.223977	6	-1.306199	-1.843232	0.799618
6	2.259987	-1.110165	-2.723426	8	-0.116182	-1.685264	1.167314
1	2.538623	-2.104343	-2.358492	1	-1.525061	-2.659587	0.085919
1	1.223463	-0.918209	-2.452232	3	0.656988	-0.118185	0.129795
1	2.353559	-1.102102	-3.818522	7	-1.057771	0.959265	-0.473335
7	3.500555	1.984310	-1.126514	6	3.082971	-1.039275	-1.016172
7	3.145000	-0.115699	-2.128728	6	4.902968	-2.613417	-0.404221
7	2.451405	-2.671598	0.437447	6	5.459517	-0.402369	-1.386455
7	3.704585	-0.920959	1.406541	6	5.809819	-1.397705	-0.291008
1	3.493450	-4.376908	-0.138213	1	5.048451	-3.282380	0.449404
1	5.125122	-2.554661	-0.265013	1	5.745896	-0.796538	-2.373326
1	4.713687	-2.207007	2.753919	1	5.674159	-0.928177	0.689893
1	4.794607	-0.000686	-3.437622	6	3.598313	1.082197	-2.091795
1	6.470203	0.448217	-1.708892	1	3.588791	0.910133	-3.176790
1	5.443104	2.491236	-0.590626	1	2.598375	1.374881	-1.780107
8	1.519778	-0.621304	0.854929	1	4.292790	1.899201	-1.876315
8	1.389931	1.201963	-1.486620	6	2.514345	-3.261325	-0.204975
1	-1.961971	0.525967	0.526712	1	2.867006	-3.900466	0.609660
14	-0.987910	1.611999	2.358463	1	1.551604	-2.835787	0.075430
14	-2.014906	2.642399	-0.408011	1	2.392416	-3.883622	-1.103239
6	-2.333597	2.586931	3.265084	7	4.025892	-0.103562	-1.359212
1	-3.299599	2.071397	3.207573	7	3.497036	-2.201418	-0.418294
1	-2.078395	2.692864	4.327459	1	5.138654	-3.187029	-1.313809
1	-2.467688	3.595149	2.858070	1	6.856970	-1.700914	-0.379902
6	-0.820911	-0.064924	3.196512	1	6.001723	0.537034	-1.241220
1	-0.519294	0.073157	4.242708	8	1.862692	-0.813060	-1.204988
1	-1.766435	-0.617247	3.195578	1	-1.855039	0.034992	0.302170
1	-0.059888	-0.671288	2.697264	14	-0.970710	2.589676	0.120401
6	0.645356	2.545144	2.475584	14	-1.390257	0.626044	-2.152705
1	0.558246	3.590292	2.163855	6	-2.604846	3.560096	-0.004199
1	1.018306	2.536990	3.507333	1	-3.456156	2.984152	0.376904
1	1.391746	2.057750	1.844171	1	-2.545911	4.484843	0.585335
6	-1.714883	2.251429	-2.224852	1	-2.839367	3.843724	-1.035752
1	-2.026619	3.107664	-2.837081	6	-0.472579	2.664921	1.954393
1	-0.654304	2.058770	-2.411459	1	-0.035281	3.648072	2.172258
1	-2.283706	1.379692	-2.559575	1	-1.333769	2.544136	2.617811
6	-1.151899	4.275383	-0.018794	1	0.266238	1.903061	2.215810
1	-1.333299	4.625339	1.002446	6	0.314062	3.632709	-0.823080
1	-0.069519	4.211977	-0.171348	1	-0.016643	3.854292	-1.844234
1	-1.533435	5.046083	-0.700292	1	0.477647	4.594474	-0.319320
6	-3.873946	2.833905	-0.129226	1	1.283672	3.126510	-0.894670
1	-4.303510	3.567106	-0.823711	6	-1.697448	-1.226837	-2.414708
1	-4.395101	1.882755	-0.291014	1	-1.853444	-1.416098	-3.484669
1	-4.097910	3.166924	0.890360	1	-0.835561	-1.825123	-2.099109
-----				1	-2.583492	-1.589718	-1.884863
(5-6) _{E-LiHMDS.1THF.IDMPU[‡]}				6	0.038489	1.055146	-3.326508
-----				1	0.333160	2.108818	-3.284296
Number of imaginary frequencies : 1				1	0.911708	0.443716	-3.083830
Electronic energy : HF=-1997.7021209				1	-0.253800	0.836678	-4.362618
Zero-point correction= 0.728710 (Hartree/Particle)				6	-2.915324	1.526531	-2.852504
Thermal correction to Energy= 0.773631				1	-3.161705	1.123283	-3.843787
Thermal correction to Enthalpy= 0.774575				1	-3.801371	1.406558	-2.220147
Thermal correction to Gibbs Free Energy= 0.650767				1	-2.735265	2.600603	-2.976572
Sum of electronic and zero-point Energies= -1996.973411				6	2.389787	-0.369902	2.530406
Sum of electronic and thermal Energies= -1996.928490				6	2.909942	1.662474	1.418842
Sum of electronic and thermal Enthalpies= -1996.927546				6	3.666012	0.217040	3.136944
Sum of electronic and thermal Free Energies= -1997.051354				1	2.520910	-1.378267	2.131033
Standard State and RRHO Corrected G= -1997.039752				1	1.561168	-0.378085	3.246668
-----				6	3.524692	1.711707	2.813858
Cartesian Coordinates				1	2.314979	2.542624	1.164613
-----				1	3.676769	1.512114	0.649905
6	-5.470717	-3.037196	0.309111	1	3.748322	0.007218	4.206664
6	-4.203282	-2.665921	0.766397	1	4.550326	-0.194461	2.636951
6	-3.738417	-1.345810	0.633924	1	2.833454	2.192243	3.515452
6	-4.601038	-0.405402	0.041846	1	4.473430	2.254747	2.833075
6	-5.871484	-0.768161	-0.406956	8	2.030915	0.514969	1.436275
6	-6.310995	-2.089325	-0.279535	-----			
1	-5.803882	-4.066074	0.420010	(5...6) _{Z-LiHMDS.2THF}			
1	-3.564820	-3.409169	1.238091	-----			
1	-6.515397	-0.020974	-0.863885	Number of imaginary frequencies : 0			
1	-7.297665	-2.375902	-0.633342	Electronic energy : HF=-1809.5313609			
1	-4.260288	0.618704	-0.072137	Zero-point correction= 0.663723 (Hartree/Particle)			
6	-2.372153	-0.928791	1.099096	Thermal correction to Energy= 0.705657			
6	-2.298684	-0.296637	2.506916	Thermal correction to Enthalpy= 0.706601			
1	-2.367431	-1.099866	3.255725	Thermal correction to Gibbs Free Energy= 0.587474			
1	-1.307955	0.147541	2.628233	Sum of electronic and zero-point Energies= -1808.867638			
6	-3.377862	0.742185	2.817300	Sum of electronic and thermal Energies= -1808.825704			

Sum of electronic and thermal Enthalpies= -1808.824760
 Sum of electronic and thermal Free Energies= -1808.943887
 Standard State and RRHO Corrected G= -1808.931809

 Cartesian Coordinates

```

6      3.619411  0.386931 -1.261766
8      2.300052  0.701294 -1.746233
6      2.369431  1.911978 -2.535964
6      3.740973  2.555901 -2.234661
6      4.263244  1.748723 -1.030541
3      0.698558  0.303010 -0.653001
8      0.229353  2.163300 -0.084199
6      1.110076  3.065068  0.626830
6      0.195568  4.096482  1.285183
6      -0.957406  4.184623  0.274518
6      -1.105943  2.727616 -0.158062
8      -0.676165  0.199214 -2.160185
6      -1.703104 -0.463689 -2.222122
6      -2.269017 -1.229319 -1.048183
6      -3.021371 -2.510585 -1.484488
6      -4.340065 -2.298069 -2.233682
6      -3.090399 -0.281721 -0.180003
6      -3.995787  0.641595 -0.726860
6      -4.698909  1.521608  0.098695
6      -4.513048  1.486740  1.483284
6      -3.621487  0.564071  2.036608
6      -2.913522 -0.309571  1.209252
7      0.963500 -1.196766  0.602139
14     1.366244 -2.683993 -0.120139
6      0.245832 -4.134037  0.421449
14     1.298747 -0.794166  2.221097
6      3.045275 -0.051326  2.461300
6      0.077028  0.494060  2.920607
6      1.217628 -2.245609  3.462989
6      3.155631 -3.281720  0.195598
6      1.205189 -2.617152 -2.018814
1      -2.337431 -3.108204 -2.100941
1      -3.209445 -3.098261 -0.578516
1      -4.773885 -3.263635 -2.514343
1      -5.071826 -1.770900 -1.614273
1      -4.204498 -1.720830 -3.155147
1      -4.148828  0.682751 -1.801490
1      -2.200187 -1.006535  1.637225
1      -5.390043  2.235577 -0.340801
1      -3.463130  0.533586  3.110942
1      -5.057449  2.173889  2.124924
1      -2.254041 -0.506618 -3.179798
1      0.159957 -2.549634 -2.341654
1      1.734834 -1.751788 -2.433302
1      1.626923 -3.524007 -2.471995
1      0.466332 -5.053335 -0.138116
1      0.365653 -4.360940  1.487763
1      -0.812957 -3.894923  0.257410
1      3.373531 -3.374990  1.266669
1      3.337771 -4.264175 -0.260882
1      3.890076 -2.584659 -0.227188
1      0.226712 -2.716987  3.456317
1      1.954950 -3.027762  3.244793
1      1.406510 -1.896255  4.487352
1      3.237652  0.221045  3.508027
1      3.819441 -0.769636  2.162088
1      3.192334  0.851987  1.856138
1      -0.815962  0.005548  3.328115
1      0.527771  1.076717  3.735079
1      -0.255676  1.189540  2.146529
1      1.525368  2.537380 -2.234629
1      2.258568  1.657440 -3.596597
1      4.166826 -0.191996 -2.020497
1      3.495602 -0.220445 -0.365079
1      4.413622  2.437170 -3.089990
1      3.655162  3.624950 -2.022355
1      5.354640  1.700024 -0.987029
1      3.896686  2.172407 -0.089965
1      1.791686  3.534560 -0.093937
1      1.697445  2.483364  1.341315
1      -1.759168  2.171750  0.521763
1      -1.472210  2.603732 -1.179804
1      -0.169488  3.717865  2.246187
1      0.701631  5.050200  1.456866

```

1 -1.882100 4.581974 0.701316
 1 -0.670501 4.812022 -0.577209
 1 -1.396172 -1.522458 -0.452734

 (5-6)Z-LiHMDS.2THF[‡]

Number of imaginary frequencies : 1
 Electronic energy : HF=-1809.5183319
 Zero-point correction= 0.659785 (Hartree/Particle)
 Thermal correction to Energy= 0.700472
 Thermal correction to Enthalpy= 0.701417
 Thermal correction to Gibbs Free Energy= 0.586247
 Sum of electronic and zero-point Energies= -1808.858547
 Sum of electronic and thermal Energies= -1808.817859
 Sum of electronic and thermal Enthalpies= -1808.816915
 Sum of electronic and thermal Free Energies= -1808.932085
 Standard State and RRHO Corrected G= -1808.921214

 Cartesian Coordinates

```

6      3.666889 -1.244208 -0.095707
8      2.717826 -0.489138 -0.886317
6      3.413255  0.288576 -1.891989
6      4.838097 -0.260541 -1.917405
6      5.040638 -0.679024 -0.453664
3      0.915391  0.142873 -0.405355
8      1.504268  1.913676  0.239124
6      2.526392  2.095270  1.248421
6      2.828579  3.595776  1.273593
6      2.487108  4.020496 -0.162416
6      1.260806  3.161360 -0.453465
8      0.037130  0.603396 -2.133881
6      -0.966583 -0.110678 -2.349781
6      -2.085254 -0.299591 -1.449038
6      -3.085082 -1.347018 -1.967076
6      -4.062517 -0.812587 -3.021250
6      -2.697937  0.897931 -0.768772
6      -2.195744  2.204378 -0.908070
6      -2.796952  3.284981 -0.260906
6      -3.920248  3.097060  0.547912
6      -4.432736  1.806450  0.698873
6      -3.828529  0.725804  0.054184
7      -0.342893 -1.190954  0.550218
14     -0.039417 -2.862516  0.183117
6      -1.595034 -3.951781  0.296304
14     -0.587655 -0.656607  2.186334
6      0.979321 -0.881834  3.251096
6      -1.009494  1.186718  2.299229
6      -1.988090 -1.576105  3.088088
6      1.228586 -3.713475  1.318152
6      0.603838 -3.042285 -1.594283
1      -2.517628 -2.184805 -2.389870
1      -3.644676 -1.776092 -1.129536
1      -4.737005 -1.599642 -3.378132
1      -4.676627 -0.001565 -2.616212
1      -3.520646 -0.415002 -3.888095
1      -1.323182  2.374460 -1.525019
1      -4.245374 -0.265730  0.197279
1      -2.384138  4.282023 -0.395037
1      -5.304509  1.634954  1.325220
1      -4.386452  3.939094  1.051842
1      -0.948524 -0.763966 -3.244405
1      -0.168214 -2.799140 -2.332809
1      1.461430 -2.386647 -1.777248
1      0.915802 -4.077736 -1.781581
1      -1.367099 -4.984397 -0.000270
1      -1.993603 -3.983662  1.316712
1      -2.395844 -3.591442 -0.357803
1      0.808924 -3.910294  2.311447
1      1.513401 -4.683691  0.889889
1      2.143340 -3.129576  1.454888
1      -2.917778 -1.544752  2.506848
1      -1.742804 -2.629663  3.266468
1      -2.193433 -1.117559  4.064411
1      0.890745 -0.321987  4.191462
1      1.161974 -1.929497  3.510523
1      1.872586 -0.513755  2.732528
1      -2.031450  1.393232  1.973127
1      -0.922277  1.511513  3.344592
1      -0.332891  1.798573  1.697084

```

1	3.390319	1.343823	-1.592449
1	2.876952	0.179186	-2.837819
1	3.582413	-2.303682	-0.366833
1	3.405972	-1.130524	0.960159
1	4.897367	-1.135332	-2.574506
1	5.562467	0.481553	-2.263227
1	5.838873	-1.412731	-0.314854
1	5.266306	0.197840	0.164068
1	3.404006	1.506383	0.956003
1	2.146992	1.715965	2.201381
1	0.346393	3.616974	-0.053038
1	1.109139	2.932206	-1.510013
1	2.167671	4.104013	1.984232
1	3.863584	3.803797	1.556986
1	2.279753	5.089221	-0.262124
1	3.305007	3.760665	-0.844424
1	-1.353796	-0.794341	-0.473213

6Z-LiHMDs.2THF

Number of imaginary frequencies : 0
Electronic energy : HF=-1809.5612781
Zero-point correction= 0.664848 (Hartree/Particle)
Thermal correction to Energy= 0.706164
Thermal correction to Enthalpy= 0.707108
Thermal correction to Gibbs Free Energy= 0.588554
Sum of electronic and zero-point Energies= -1808.896430
Sum of electronic and thermal Energies= -1808.855114
Sum of electronic and thermal Enthalpies= -1808.854170
Sum of electronic and thermal Free Energies= -1808.972724
Standard State and RRHO Corrected G= -1808.960424

Cartesian Coordinates

6	3.205465	-0.031559	-2.111159
8	2.489370	0.708931	-1.093540
6	2.921662	2.095254	-1.092006
6	3.644083	2.287366	-2.421049
6	4.298386	0.911299	-2.616927
3	0.915269	0.480152	0.084855
8	1.873500	0.583405	1.821642
6	3.246080	0.163833	2.016009
6	3.869153	1.159065	3.011493
6	2.899187	2.352030	2.965495
6	1.563639	1.654171	2.741977
8	-0.123690	1.999252	0.146773
6	-1.129052	2.528943	-0.468771
6	-2.467958	2.185980	-0.429674
6	-3.421738	2.956289	-1.326693
6	-4.479034	3.777357	-0.568017
6	-2.991449	1.090734	0.392814
6	-2.321744	0.618220	1.552853
6	-2.841027	-0.419080	2.327244
6	-4.040988	-1.048254	1.979923
6	-4.724885	-0.596516	0.847473
6	-4.219232	0.452265	0.079355
7	-0.168882	-1.373998	-0.211114
14	-0.622457	-1.576220	-1.922594
6	-2.371122	-2.274431	-2.035155
14	0.461970	-2.704516	0.786578
6	2.264192	-3.010970	0.319085
6	0.337381	-2.218347	2.601998
6	-0.530258	-4.297959	0.557607
6	0.584508	-2.756736	-2.766357
6	-0.564772	0.080824	-2.813301
1	-2.836305	3.637167	-1.957655
1	-3.937548	2.285264	-2.030778
1	-5.149078	4.307096	-1.256744
1	-5.096164	3.138184	0.072567
1	-3.997065	4.521412	0.076954
1	-1.391653	1.090714	1.841846
1	-4.784233	0.775789	-0.788913
1	-2.304488	-0.730449	3.219548
1	-5.663999	-1.062681	0.557853
1	-4.438391	-1.859688	2.583161
1	-0.889955	3.372004	-1.147727
1	-1.335667	0.759546	-2.435820
1	0.402944	0.575541	-2.683557
1	-0.734120	-0.066806	-3.887391
1	-2.713828	-2.323057	-3.076312

1	-2.426463	-3.285000	-1.615018
1	-3.075271	-1.643413	-1.480311
1	0.521010	-3.778499	-2.378579
1	0.345066	-2.798830	-3.836318
1	1.622353	-2.423670	-2.676270
1	-1.585610	-4.131553	0.804632
1	-0.482446	-4.687432	-0.464795
1	-0.153936	-5.082108	1.227151
1	2.741030	-3.663466	1.060946
1	2.360011	-3.498723	-0.655807
1	2.830109	-2.075147	0.285233
1	-0.693770	-2.296823	2.959835
1	0.949227	-2.894941	3.211585
1	0.688384	-1.196179	2.765767
1	3.601597	2.251096	-0.243418
1	2.031458	2.712222	-0.952444
1	2.504290	-0.292381	-2.911975
1	3.590321	-0.953805	-1.666530
1	2.922542	2.484893	-3.221940
1	4.361976	3.111227	-2.389636
1	4.576693	0.701732	-3.653019
1	5.196220	0.826933	-1.994098
1	3.731448	0.184986	1.035908
1	3.255120	-0.865304	2.391668
1	1.172374	1.230183	3.678486
1	0.797613	2.266777	2.265560
1	3.887991	0.729653	4.018663
1	4.893700	1.425184	2.738387
1	2.914294	2.954873	3.877532
1	3.123850	3.003065	2.113233
1	-0.944748	-0.919123	0.281664

(5...6)Z-LiHMDs.2DMPU

Number of imaginary frequencies : 0
Electronic energy : HF=-2185.9001543
Zero-point correction= 0.799696 (Hartree/Particle)
Thermal correction to Energy= 0.850767
Thermal correction to Enthalpy= 0.851711
Thermal correction to Gibbs Free Energy= 0.713080
Sum of electronic and zero-point Energies= -2185.100459
Sum of electronic and thermal Energies= -2185.049388
Sum of electronic and thermal Enthalpies= -2185.048443
Sum of electronic and thermal Free Energies= -2185.187074
Standard State and RRHO Corrected G= -2185.173127

Cartesian Coordinates

6	-3.283244	3.583363	-0.695048
6	-2.842956	2.377627	-1.248969
6	-3.596600	1.204751	-1.111354
6	-4.805199	1.275694	-0.398289
6	-5.246803	2.478039	0.154306
6	-4.486454	3.641466	0.008104
1	-2.677170	4.477472	-0.814557
1	-1.895973	2.360726	-1.776071
1	-6.182584	2.502343	0.706165
1	-4.826413	4.578014	0.441034
1	-5.404625	0.380872	-0.263170
6	-3.142930	-0.155237	-1.650105
6	-4.247118	-0.938969	-2.397190
1	-3.797849	-1.858110	-2.794524
1	-4.998809	-1.270379	-1.673472
6	-4.925064	-0.163314	-3.531045
1	-4.198103	0.192851	-4.270570
1	-5.648703	-0.795568	-4.056521
1	-5.458276	0.712394	-3.148052
6	-1.898127	-0.080597	-2.494072
8	-0.782464	0.152886	-2.048118
1	-2.006436	-0.286428	-3.577159
3	-0.067565	-0.143404	-0.085626
7	-1.396042	-1.238373	0.941192
6	1.871459	1.939950	0.524692
6	3.985718	2.800479	-0.478302
6	3.739841	2.665625	1.989761
6	4.668194	2.387568	0.816933
1	4.562654	2.454460	-1.342835
1	3.605502	3.749067	2.131611
1	4.897188	1.318469	0.785161
6	2.801792	-1.090684	-0.756092

6	4.658191	-1.323862	-2.395568	6	3.364883	1.149615	1.247705
6	5.138290	-1.407911	0.038722	6	4.632033	1.474779	0.722420
6	5.586650	-0.831164	-1.295827	6	4.987688	2.792306	0.428223
1	4.796946	-2.403571	-2.561811	6	4.087119	3.835760	0.651373
1	5.704994	-0.959505	0.861356	1	2.106739	4.328545	1.349525
1	6.615813	-1.133986	-1.509383	1	1.476158	2.008821	1.837664
6	2.298198	-1.174365	-3.133881	1	5.974886	2.999462	0.022601
1	1.338132	-0.761149	-2.831399	1	4.360637	4.861870	0.421546
1	2.666917	-0.626569	-4.006670	1	5.358595	0.691187	0.538906
1	2.159182	-2.226642	-3.421538	6	3.016730	-0.290750	1.532447
6	3.254954	-1.263722	1.638510	6	4.193373	-1.220573	1.868335
1	3.852467	-0.615754	2.287807	1	3.802872	-2.239518	1.974108
1	2.210540	-0.970634	1.706653	1	4.881441	-1.270585	1.016974
1	3.355790	-2.299082	1.991033	6	4.961950	-0.844080	3.141428
6	1.613501	1.786550	2.938235	1	4.293825	-0.844761	4.011249
1	1.130550	2.710089	3.286833	1	5.775547	-1.550853	3.342630
1	0.839189	1.059601	2.706470	1	5.397901	0.156991	3.063498
1	2.238843	1.396321	3.746274	6	1.833680	-0.581382	2.323229
6	2.044795	2.229665	-1.895392	8	0.711167	-0.059099	2.174380
1	2.720000	1.736362	-2.601401	1	1.916030	-1.434266	3.025501
1	1.100168	1.693131	-1.880177	3	0.044967	-0.127615	0.180722
1	1.870601	3.259344	-2.239598	7	1.672482	-1.000129	-0.815729
7	2.448198	2.016111	1.766833	6	-1.938965	1.924712	-0.337705
7	2.647404	2.216811	-0.570561	6	-4.076223	2.629243	0.733545
7	3.264726	-1.040472	-2.050079	6	-3.807006	2.776742	-1.731759
7	3.720199	-1.127583	0.264464	6	-4.738619	2.349809	-0.607008
1	4.880048	-0.819000	-3.341477	1	-4.650395	2.173884	1.547601
1	5.555760	0.262940	-1.252486	1	-3.694336	3.871577	-1.749372
1	5.320080	-2.493050	0.072437	1	-4.945766	1.279432	-0.696755
1	3.921368	3.897169	-0.549023	6	-2.757012	-1.279315	0.547526
1	5.606453	2.936889	0.936873	6	-4.577665	-1.727970	2.180832
1	4.161984	2.266576	2.917009	6	-5.104757	-1.515860	-0.234457
8	1.577796	-1.060700	-0.518595	6	-5.530821	-1.111444	1.168498
8	0.676811	1.583153	0.399525	1	-4.710402	-2.820269	2.219136
1	-2.809501	-0.723647	-0.759957	1	-5.694753	-0.982150	-0.986510
14	-1.218915	-2.892650	0.588463	1	-6.553294	-1.447607	1.363332
14	-2.061175	-0.566317	2.353744	6	-2.203840	-1.667541	2.886425
6	-2.693313	-3.999444	1.102691	1	-1.252404	-1.200490	2.637910
1	-3.644517	-3.611300	0.717063	1	-2.569176	-1.250177	3.829812
1	-2.572327	-5.020546	0.715539	1	-2.049655	-2.747330	3.025891
1	-2.789212	-4.075722	2.192922	6	-3.253153	-1.144549	-1.837841
6	-1.011781	-3.190445	-1.283797	1	-3.931355	-0.504219	-2.409925
1	-0.797948	-4.247554	-1.491891	1	-2.247996	-0.735201	-1.895405
1	-1.916869	-2.925332	-1.844376	1	-3.256126	-2.146064	-2.289561
1	-0.181235	-2.594421	-1.675347	1	-1.651716	2.057809	-2.749385
6	0.315741	-3.701080	1.386397	1	-1.186198	3.025683	-2.981576
1	0.335783	-3.545277	2.472594	1	-0.862531	1.325671	-2.593900
1	0.363007	-4.783615	1.204146	1	-2.259567	1.751183	-3.605442
1	1.220015	-3.246642	0.968704	6	-2.138142	1.939998	2.100495
6	-2.104101	1.337088	2.297906	1	-2.780607	1.304645	2.718855
1	-2.232271	1.753873	3.306493	1	-1.153649	1.484328	2.033939
1	-1.191704	1.757118	1.866813	1	-2.048548	2.922714	2.584438
1	-2.946484	1.688121	1.692366	7	-2.503581	2.132360	-1.569751
6	-1.113116	-1.043881	3.948667	7	-2.724445	2.070820	0.773729
1	-1.174132	-2.124884	4.131586	7	-3.190418	-1.401878	1.844262
1	-0.047802	-0.790048	3.876968	7	-3.695915	-1.183327	-0.450212
1	-1.513809	-0.539433	4.838760	1	-4.779821	-1.341392	3.184920
6	-3.876795	-1.056609	2.707368	1	-5.508078	-0.020005	1.258424
1	-4.281469	-0.481623	3.551918	1	-5.270314	-2.592242	-0.394712
1	-4.512771	-0.847072	1.837758	1	-4.038202	3.711666	0.929055
1	-3.989894	-2.119552	2.949472	1	-5.687240	2.890110	-0.674812
-----				1	-4.213026	2.475830	-2.702246
(5-6)Z-LiHMDS.2DMPU [‡]				8	-1.536682	-1.214089	0.284248
-----				8	-0.740433	1.568581	-0.243068
Number of imaginary frequencies : 1				1	2.487606	-0.673997	0.414690
Electronic energy : HF=-2185.8932169				14	1.445745	-2.719216	-0.852392
Zero-point correction= 0.796180 (Hartree/Particle)				14	2.244990	-0.132860	-2.204268
Thermal correction to Energy= 0.845987				6	2.973707	-3.685390	-1.456942
Thermal correction to Enthalpy= 0.846931				1	3.881202	-3.379337	-0.922375
Thermal correction to Gibbs Free Energy= 0.712607				1	2.841304	-4.763592	-1.295332
Sum of electronic and zero-point Energies= -2185.097037				1	3.155980	-3.537266	-2.527998
Sum of electronic and thermal Energies= -2185.047230				6	1.055461	-3.395964	0.879366
Sum of electronic and thermal Enthalpies= -2185.046285				1	0.766727	-4.452112	0.796988
Sum of electronic and thermal Free Energies= -2185.180610				1	1.909786	-3.348937	1.562578
Standard State and RRHO Corrected G= -2185.168023				1	0.218533	-2.855813	1.332196
-----				6	-0.010257	-3.288935	-1.932153
Cartesian Coordinates				1	0.108477	-3.033137	-2.989745
-----				1	-0.130807	-4.378821	-1.866580
6	2.826481	3.533109	1.171007	1	-0.930902	-2.824513	-1.567892
6	2.468032	2.215506	1.458131	6	2.084828	1.747220	-2.020726

1	2.152943	2.218902	-3.010447
1	1.135046	2.038554	-1.566681
1	2.891045	2.157433	-1.406260
6	1.307199	-0.592541	-3.800966
1	1.542785	-1.609212	-4.136690
1	0.220229	-0.533628	-3.669132
1	1.579420	0.090333	-4.616539
6	4.087629	-0.438994	-2.577726
1	4.429956	0.205917	-3.398371
1	4.704320	-0.205209	-1.701766
1	4.294982	-1.476104	-2.863352

6Z-LiHMDS.2DMPU

Number of imaginary frequencies : 0
 Electronic energy : HF=-2185.934803
 Zero-point correction= 0.801637 (Hartree/Particle)
 Thermal correction to Energy= 0.851669
 Thermal correction to Enthalpy= 0.852613
 Thermal correction to Gibbs Free Energy= 0.718225
 Sum of electronic and zero-point Energies= -2185.133166
 Sum of electronic and thermal Energies= -2185.083134
 Sum of electronic and thermal Enthalpies= -2185.082190
 Sum of electronic and thermal Free Energies= -2185.216578
 Standard State and RRHO Corrected G= -2185.204084

Cartesian Coordinates

6	-3.138245	0.809845	-1.861668
6	-2.068489	0.051950	-2.309281
6	-4.518474	0.440847	-2.381535
1	-4.453395	-0.527678	-2.893489
1	-5.224921	0.279867	-1.553394
6	-5.124572	1.467305	-3.355374
1	-6.123993	1.164018	-3.691994
1	-5.213387	2.455322	-2.891439
1	-4.486590	1.576158	-4.240298
6	-2.999280	1.973314	-0.975988
6	-1.756419	2.625810	-0.767190
6	-4.117749	2.532794	-0.306767
6	-1.646023	3.746678	0.051091
1	-0.878956	2.225027	-1.253472
6	-4.000296	3.651457	0.519301
1	-5.098012	2.083185	-0.429060
6	-2.762930	4.272591	0.709657
1	-0.671103	4.213280	0.179619
1	-4.886121	4.039899	1.017252
1	-2.672119	5.143839	1.352733
8	-0.817143	0.113996	-1.987702
1	-2.341450	-0.734959	-3.038517
3	-0.055702	-0.519066	-0.379143
7	-1.803886	-1.419366	0.679529
1	-2.367495	-0.866954	0.023220
14	-1.858723	-3.134871	0.208403
14	-2.061007	-0.827865	2.334468
6	-1.715260	-3.247285	-1.665366
1	-0.864250	-2.663519	-2.027314
1	-1.570692	-4.294086	-1.961230
1	-2.621277	-2.884443	-2.161464
6	-3.483230	-3.960798	0.723542
1	-3.546153	-4.106141	1.807637
1	-4.352821	-3.369268	0.413611
1	-3.570862	-4.949651	0.254925
6	-0.431791	-4.073145	1.002622
1	-0.523273	-4.156642	2.089457
1	-0.401945	-5.092491	0.596487
1	0.515996	-3.584534	0.761258
6	-3.826264	-1.153609	2.934585
1	-4.557192	-0.746241	2.225107
1	-4.042917	-2.218881	3.063497
1	-3.997344	-0.659710	3.899917
6	-0.848850	-1.705144	3.488059
1	-0.752129	-1.139622	4.422958
1	-1.189250	-2.712352	3.751226
1	0.148564	-1.794306	3.045862
6	-1.796458	1.030441	2.398660
1	-2.602893	1.559852	1.882458
1	-1.795922	1.366198	3.443862
1	-0.850233	1.320293	1.938964
8	1.310676	-1.861446	-0.737313

8	0.996444	0.757982	0.577954
6	2.053453	1.410014	0.719120
6	3.798502	2.930219	-0.194585
6	3.767885	2.403000	2.226890
6	4.653997	2.531385	0.997742
1	4.384367	2.895768	-1.119000
1	3.389338	3.389820	2.535197
1	5.143871	1.572231	0.796593
6	2.500819	-1.551247	-0.985316
6	4.289681	-1.108428	-2.643911
6	4.863058	-1.323169	-0.233197
6	5.094336	-0.510407	-1.498880
1	4.692535	-2.092709	-2.928691
1	5.302590	-0.816850	0.632635
1	6.159210	-0.502602	-1.748930
7	2.668275	2.012520	-0.347612
7	2.652832	1.496409	1.953501
6	1.999640	2.057034	-1.642529
1	1.582278	3.056534	-1.828157
1	2.725081	1.835802	-2.432422
1	1.193441	1.329238	-1.688650
6	1.925597	1.017746	3.121610
1	1.386604	1.834947	3.621153
1	1.207984	0.259423	2.823156
1	2.633472	0.583769	3.834854
6	1.903832	-1.383060	-3.332592
1	0.918717	-1.055952	-2.995713
1	2.214963	-0.758544	-4.174557
1	1.843852	-2.424623	-3.679340
6	3.049898	-1.896902	1.361484
1	3.600599	-1.292714	2.087561
1	1.984471	-1.735874	1.505902
1	3.280148	-2.956830	1.540135
7	3.430834	-1.481249	0.019253
7	2.882347	-1.224657	-2.259461
1	3.432504	3.961937	-0.080579
1	5.431465	3.281225	1.169706
1	4.333567	1.994442	3.070586
1	4.772767	0.521914	-1.332473
1	4.346027	-0.465862	-3.527683
1	5.344769	-2.309711	-0.313509

(5-6)Z-LiHMDS.1THF.1DMPU[‡]

Number of imaginary frequencies : 1
 Electronic energy : HF=-1997.7049174
 Zero-point correction= 0.728005 (Hartree/Particle)
 Thermal correction to Energy= 0.773392
 Thermal correction to Enthalpy= 0.774336
 Thermal correction to Gibbs Free Energy= 0.649084
 Sum of electronic and zero-point Energies= -1996.976912
 Sum of electronic and thermal Energies= -1996.931526
 Sum of electronic and thermal Enthalpies= -1996.930582
 Sum of electronic and thermal Free Energies= -1997.055834
 Standard State and RRHO Corrected G= -1997.043842

Cartesian Coordinates

6	-0.006939	3.541522	-2.143615
8	0.042091	3.073591	-0.783612
6	-0.879431	3.908031	-0.058697
6	-2.079310	4.105287	-0.999439
6	-1.490550	3.841422	-2.412592
3	0.023861	1.093095	-0.345915
8	-1.804329	1.025238	0.144832
6	-2.833635	0.325215	0.300730
7	-3.330708	0.090708	1.552948
6	-4.540882	-0.691414	1.809545
6	-4.768319	-1.698424	0.692548
6	-4.722386	-0.977855	-0.646374
7	-3.463847	-0.242628	-0.775041
6	-2.759322	0.775074	2.704697
6	-3.108270	0.188364	-2.121523
7	1.661689	0.350572	0.737784
14	2.919313	1.548066	0.728719
6	2.450158	3.155476	1.627420
14	1.326577	-0.552653	2.182680
6	-0.254480	-1.589958	2.066485
6	2.687021	-1.814834	2.612710
6	1.119597	0.560384	3.715648

6	3.373697	2.068325	-1.040461	8	-4.435543	-1.278795	-2.589649
6	4.557839	0.970339	1.511398	3	-3.839932	-2.299705	-1.129351
8	0.386503	0.397146	-2.249086	8	-4.685984	-1.898647	0.481650
6	1.454690	-0.240254	-2.354808	6	-4.972860	-0.741135	0.902567
6	1.882572	-1.327390	-1.493167	6	-4.943591	-0.249955	2.224680
6	3.318372	-1.787266	-1.789917	6	-2.766363	0.553768	1.661211
6	3.454557	-2.708194	-3.009051	6	-2.522188	0.927247	0.332632
6	0.893665	-2.412804	-1.143434	6	-1.989045	0.046431	-0.671303
6	-0.492081	-2.288534	-1.362407	45	-0.173219	0.822667	0.142572
6	-1.379480	-3.306320	-1.011393	15	1.312528	-0.536047	-1.006567
6	-0.917468	-4.485578	-0.423014	8	0.685612	-1.650912	-1.799663
6	0.453139	-4.628107	-0.195535	8	-0.040425	-0.807760	1.518616
6	1.340944	-3.610015	-0.548595	6	-0.415700	-2.043777	1.538934
1	3.937489	-0.895819	-1.943880	6	0.360893	-2.885426	2.530802
1	3.741664	-2.273330	-0.903798	6	-0.156403	-4.117369	2.953102
1	4.499665	-2.989041	-3.183979	6	0.555242	-4.911931	3.852737
1	2.875905	-3.628704	-2.881952	6	1.799903	-4.486423	4.328910
1	3.085057	-2.209714	-3.913429	6	2.326376	-3.263678	3.902526
1	-0.878260	-1.383281	-1.807875	6	1.609632	-2.464409	3.010300
1	2.397474	-3.757029	-0.354384	8	-1.323704	-2.569245	0.873648
1	-2.441687	-3.169463	-1.198650	15	0.763975	1.892091	2.337061
1	0.839225	-5.535575	0.261880	6	-0.455297	1.617413	3.712780
1	-1.609613	-5.275647	-0.145254	6	-0.638737	0.322878	4.231777
1	2.207653	0.134319	-3.075106	6	-1.615651	0.071471	5.193906
1	3.869838	1.268781	-1.600745	6	-2.429503	1.105917	5.661299
1	2.500989	2.395231	-1.612272	6	-2.250150	2.396717	5.162966
1	4.073711	2.912840	-0.995559	6	-1.269818	2.651966	4.200235
1	5.347196	1.713313	1.335784	6	-4.635106	-1.113088	3.377837
1	4.474280	0.835298	2.596039	6	-5.152111	-0.836427	4.663447
1	4.897698	0.019399	1.083753	6	-4.845143	-1.637553	5.763834
1	1.585749	3.619880	1.143439	6	-3.996453	-2.738432	5.625670
1	2.204297	2.993665	2.681910	6	-3.458411	-3.020052	4.365405
1	3.280360	3.873510	1.587771	6	-3.768180	-2.228322	3.261010
1	2.896566	-2.462440	1.752712	6	-5.645086	1.083269	2.436255
1	3.629571	-1.345669	2.913003	6	-7.177620	0.977422	2.528291
1	2.362358	-2.464483	3.436758	6	2.313727	1.132940	2.990025
1	0.786028	-0.030627	4.578715	6	3.344010	0.849283	2.082118
1	2.058351	1.049657	4.000220	6	4.554338	0.311939	2.523319
1	0.375144	1.347608	3.546243	6	4.749563	0.044700	3.879736
1	-1.069205	-1.064364	1.569703	6	3.734117	0.333322	4.795371
1	-0.080589	-2.522374	1.524431	6	2.528059	0.881232	4.355342
1	-0.591865	-1.855612	3.077080	6	1.125812	3.694180	2.527119
1	0.409015	2.755551	-2.773736	6	2.268941	4.196528	3.164290
1	0.606327	4.450319	-2.231883	6	2.486026	5.574894	3.241262
1	-0.389691	4.865541	0.171131	6	1.564566	6.467775	2.690967
1	-1.127522	3.396835	0.872217	6	0.415678	5.976943	2.063873
1	-1.609355	4.693774	-3.087211	6	0.206219	4.601921	1.980640
1	-1.975283	2.976802	-2.873976	8	2.409786	-1.185454	0.110783
1	-2.503270	5.108384	-0.899862	6	3.258273	-2.159342	-0.367723
1	-2.858398	3.376327	-0.768266	6	4.386311	-1.792888	-1.087369
1	1.887238	-0.593369	-0.425631	6	5.193617	-2.838334	-1.661430
1	-5.577594	-0.292312	-0.748873	6	4.884452	-4.209523	-1.365803
1	-5.405929	-0.019285	1.910601	6	3.762553	-4.511451	-0.546340
1	-5.735226	-2.192250	0.823528	6	2.948258	-3.509457	-0.080956
1	-4.776974	-1.693443	-1.473088	6	5.690160	-5.242570	-1.917301
1	-3.984785	-2.463599	0.722158	6	6.744396	-4.951472	-2.753850
1	-4.410765	-1.202960	2.768869	6	7.027170	-3.603800	-3.081643
1	-2.475829	0.047937	3.472951	6	6.274851	-2.578139	-2.550641
1	-1.875089	1.330005	2.401060	6	4.699164	-0.348739	-1.266668
1	-3.491529	1.470872	3.135029	6	3.739308	0.521996	-1.783867
1	-2.103362	0.602396	-2.130235	6	4.067373	1.860824	-2.116272
1	-3.142727	-0.671538	-2.797684	6	5.310706	2.368143	-1.840674
1	-3.814585	0.945293	-2.491365	6	6.285904	1.567414	-1.188499
(4-7) _{re-a*} ($\Phi_1=153.1^\circ$)				6	5.979074	0.196597	-0.892629
Number of imaginary frequencies : 1				6	6.958748	-0.562137	-0.187684
Electronic energy : HF=-5369.5020265				6	8.167873	-0.009612	0.177137
Zero-point correction= 1.563333 (Hartree/Particle)				6	8.475718	1.333618	-0.146087
Thermal correction to Energy= 1.661488				6	7.548035	2.102144	-0.812815
Thermal correction to Enthalpy= 1.662432				8	2.472646	0.119370	-2.094639
Thermal correction to Gibbs Free Energy= 1.425073				8	-3.250439	-3.953022	-1.723628
Sum of electronic and zero-point Energies= -5367.938693				1	8.889184	-0.610836	0.723704
Sum of electronic and thermal Energies= -5367.840538				1	6.738026	-1.587671	0.083088
Sum of electronic and thermal Enthalpies= -5367.839594				1	7.761567	3.140473	-1.054819
Sum of electronic and thermal Free Energies= -5368.076954				1	9.434456	1.755210	0.142038
Standard State and RRHO Corrected G= -5368.051085				1	5.552265	3.396875	-2.094331
Cartesian Coordinates				1	3.302242	2.460370	-2.593696
				1	6.500140	-1.553607	-2.822453
				1	2.069386	-3.716647	0.516166
				1	7.841971	-3.375324	-3.763154
				1	5.447031	-6.273778	-1.672828

1	3.543691	-5.550086	-0.313533
1	7.349470	-5.750168	-3.173465
1	-0.022862	-0.490677	3.875834
1	-1.149181	3.666694	3.839737
1	-1.752673	-0.939137	5.565048
1	-2.868697	3.214109	5.524213
1	-3.197462	0.902957	6.400879
1	3.197051	1.014465	1.022726
1	1.754128	1.106615	5.080427
1	5.336215	0.092125	1.804676
1	3.878794	0.134703	5.853785
1	5.687443	-0.384857	4.221199
1	2.997450	3.519106	3.596179
1	-0.676995	4.216287	1.484221
1	3.380531	5.949266	3.731619
1	-0.305941	6.661709	1.627502
1	1.741188	7.538240	2.745951
1	2.012637	-1.524849	2.655633
1	-1.114923	-4.440004	2.564939
1	3.296116	-2.929492	4.260780
1	0.142233	-5.862248	4.180845
1	2.357025	-5.107024	5.025887
1	-5.275490	0.015139	0.152267
1	-5.806804	0.014938	4.813161
1	-3.319180	-2.451979	2.301708
1	-5.269892	-1.394943	6.735047
1	-2.775250	-3.856043	4.242509
1	-3.752806	-3.360010	6.483010
1	-5.249809	1.576791	3.332280
1	-5.396492	1.745682	1.596821
1	-7.492611	0.316038	3.341696
1	-7.635506	1.960211	2.695093
1	-7.586941	0.567412	1.597659
1	-1.920041	-1.013267	-0.446903
1	-2.206101	0.285795	-1.706256
1	-2.896683	1.897293	0.023911
1	-2.988320	1.316338	2.396081
1	-2.374016	-0.377457	2.036243
15	-0.146701	2.524233	-1.448240
6	0.273269	2.025668	-3.188178
6	0.955112	2.891215	-4.057929
6	-0.142537	0.776674	-3.672637
6	1.214718	2.512891	-5.376889
1	1.298482	3.860168	-3.714819
6	0.110476	0.403902	-4.992864
1	-0.631184	0.070107	-3.017049
6	0.790714	1.269676	-5.850722
1	1.753115	3.192735	-6.031427
1	-0.217259	-0.571602	-5.341375
1	0.995365	0.976545	-6.876628
6	0.971069	3.958166	-1.157477
6	0.698110	5.239206	-1.669760
6	2.166788	3.751468	-0.460497
6	1.598788	6.285555	-1.471679
1	-0.214371	5.423917	-2.225880
6	3.072650	4.795210	-0.270994
1	2.390470	2.770904	-0.061148
6	2.787623	6.066172	-0.769603
1	1.371609	7.271414	-1.867271
1	3.991747	4.611653	0.276275
1	3.485529	6.883332	-0.611001
6	-1.810357	3.304661	-1.704375
6	-2.692855	2.784150	-2.662477
6	-2.267596	4.334661	-0.864274
6	-3.999445	3.265277	-2.765578
1	-2.370791	1.998005	-3.333090
6	-3.571702	4.818063	-0.970813
1	-1.603115	4.775415	-0.132441
6	-4.446887	4.278655	-1.917655
1	-4.661664	2.838145	-3.510822
1	-3.901207	5.618454	-0.314270
1	-5.464372	4.650619	-1.997048
6	-2.101735	-4.469985	-1.662623
6	-0.395273	-5.638779	-0.341272
6	0.215420	-4.706106	-2.558630
6	0.341689	-5.916265	-1.644244
1	0.064112	-4.802223	0.199944
1	0.540560	-4.958337	-3.575321
1	1.399802	-6.112926	-1.449164
6	-5.226600	-0.606092	-3.287959

6	-5.644578	0.734331	-5.346042
6	-7.539961	0.064505	-3.891605
6	-6.923926	1.211954	-4.675762
1	-5.104067	1.575964	-5.791540
1	-7.918265	-0.712337	-4.573674
1	-6.703470	2.041317	-3.995276
7	-6.557142	-0.513836	-2.971590
7	-4.757636	0.100150	-4.368229
7	-1.794033	-5.324356	-0.638849
7	-1.175764	-4.241934	-2.636337
1	0.835348	-3.876367	-2.201669
1	-0.088173	-6.805149	-2.120501
1	-0.374902	-6.515219	0.313212
1	-5.876215	0.028046	-6.157874
1	-7.628471	1.572638	-5.430587
1	-8.388523	0.415992	-3.296279
6	-3.393275	-0.148930	-4.819270
1	-2.992329	0.762121	-5.270877
1	-2.770111	-0.432913	-3.975886
1	-3.357403	-0.951502	-5.569887
6	-7.111317	-1.379961	-1.937276
1	-6.338492	-1.688440	-1.237451
1	-7.884199	-0.832493	-1.388358
1	-7.571044	-2.276080	-2.378388
6	-2.759157	-5.424935	0.451976
1	-2.780110	-4.506995	1.046984
1	-3.758514	-5.609570	0.054535
1	-2.473575	-6.267174	1.087544
6	-1.424149	-3.216629	-3.644318
1	-2.464132	-2.899344	-3.600289
1	-0.768898	-2.359831	-3.456038
1	-1.213088	-3.622225	-4.641662

(4-7)_{re-a}[‡] ($\Phi_1 = -174.8^\circ$)

Number of imaginary frequencies : 1

Electronic energy : HF=-5369.516392

Zero-point correction= 1.563748 (Hartree/Particle)

Thermal correction to Energy= 1.661105

Thermal correction to Enthalpy= 1.662049

Thermal correction to Gibbs Free Energy= 1.426472

Sum of electronic and zero-point Energies= -5367.952644

Sum of electronic and thermal Energies= -5367.855287

Sum of electronic and thermal Enthalpies= -5367.854343

Sum of electronic and thermal Free Energies= -5368.089920

Standard State and RRHO Corrected G= -5368.064335

Cartesian Coordinates

8	-5.085144	3.270453	-0.543232
3	-3.930315	2.197626	0.581607
8	-2.448160	1.483081	-0.394066
6	-1.303234	1.637438	-0.879430
8	-0.327279	0.812790	-0.786210
45	0.289341	-0.828879	0.462139
15	0.994098	-1.596073	-1.931938
6	-0.490439	-2.349335	-2.751854
6	-1.687693	-1.611796	-2.752739
6	-2.855877	-2.143847	-3.294875
6	-2.852385	-3.431661	-3.838824
6	-1.669909	-4.172475	-3.847002
6	-0.493815	-3.634215	-3.314089
6	-1.017275	2.888647	-1.671798
6	0.291536	3.204280	-2.056673
6	0.554167	4.395409	-2.734999
6	-0.489283	5.272907	-3.042560
6	-1.799407	4.954632	-2.668080
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6	-1.815515	-1.460979	1.308845
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6	-4.936045	-1.712850	0.819151
6	-5.508543	-1.850823	-0.529068
6	-5.734828	-3.129430	-1.094243
6	-6.242807	-3.285022	-2.383792
6	-6.546679	-2.170137	-3.168828
6	-6.323448	-0.896573	-2.635265
6	-5.810713	-0.734322	-1.348992
6	-1.209282	-0.277446	1.855229
15	1.918948	0.633669	1.240713
8	1.677124	1.271073	2.589877

8	2.217004	1.833578	0.075776	1	-6.005397	-4.329513	2.901522
6	3.158302	2.795449	0.376930	1	-6.606716	-2.660288	2.897599
6	4.515349	2.504791	0.290690	1	-1.594163	0.681973	1.535219
6	5.451779	3.507124	0.722731	1	-0.886870	-0.297063	2.886829
6	4.973752	4.809181	1.094387	1	-1.713037	-2.387705	1.865790
6	3.578010	5.075162	1.055802	1	-2.886691	-2.449950	-0.264758
6	2.688628	4.083476	0.724494	1	-2.875776	-0.603649	-0.349617
6	5.903391	5.801766	1.508602	6	-2.256742	3.245611	2.760091
6	7.250290	5.525754	1.583991	6	0.042234	4.072259	3.244701
6	7.721812	4.232177	1.253576	6	-0.922877	2.270266	4.630136
6	6.848334	3.252250	0.834132	6	-0.188395	3.601665	4.672848
6	4.935942	1.181388	-0.243829	1	0.741260	3.393162	2.744013
6	4.393577	0.018569	0.298468	1	-1.224288	1.956895	5.635254
6	4.742219	-1.263955	-0.187297	1	0.771750	3.481426	5.183263
6	5.612380	-1.392752	-1.239313	6	-6.273838	2.983453	-0.829670
6	6.143555	-0.244106	-1.882365	6	-7.984339	2.483335	-2.544971
6	5.796739	1.060844	-1.392443	6	-8.662559	2.687285	-0.162120
6	6.279727	2.187840	-2.119532	6	-8.798525	1.848913	-1.425435
6	7.075196	2.034494	-3.234837	1	-8.402009	3.463438	-2.822366
6	7.437477	0.745402	-3.694033	1	-9.058125	2.141166	0.701582
6	6.974330	-0.367242	-3.029337	1	-9.851993	1.779007	-1.711726
8	3.532352	0.080318	1.361323	7	-7.261445	3.010374	0.111741
6	1.398276	-0.176023	-3.047478	7	-6.594057	2.614262	-2.109967
6	2.576357	0.536794	-2.778707	7	-1.230861	4.118529	2.517033
6	2.999356	1.563015	-3.622574	7	-2.136752	2.384258	3.815982
6	2.237400	1.909733	-4.740875	1	0.469884	5.080574	3.230919
6	1.056394	1.216692	-5.009526	1	-0.780687	4.341371	5.224532
6	0.643421	0.174091	-4.175524	1	-0.266934	1.497811	4.211414
6	2.329667	-2.792837	-2.399922	1	-9.241981	3.618439	-0.251003
6	2.438482	-3.981226	-1.664432	1	-8.423627	0.836125	-1.243748
6	3.410413	-4.934033	-1.971923	1	-8.004249	1.853274	-3.438145
6	4.297394	-4.711153	-3.027317	15	0.962518	-2.624793	1.851054
6	4.190509	-3.537671	-3.777502	6	2.748555	-3.054115	2.147323
6	3.213389	-2.588246	-3.471996	6	3.348839	-4.161737	1.524462
6	-4.818095	-0.473793	1.500252	6	3.540981	-2.263219	2.995198
8	-5.046476	0.696587	1.092104	6	4.696272	-4.462342	1.733423
6	-4.806866	-2.943061	1.704155	1	2.773426	-4.808246	0.878599
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1	7.420061	2.913706	-3.772017	6	5.471443	-3.663990	2.574132
1	6.000527	3.184220	-1.800188	1	5.133784	-5.321277	1.232861
1	7.223814	-1.365803	-3.379692	1	5.475144	-1.932415	3.862357
1	8.065864	0.639491	-4.573709	1	6.520980	-3.893109	2.734883
1	5.869426	-2.378166	-1.615535	6	0.331173	-2.426776	3.594084
1	4.296298	-2.129207	0.280470	6	-0.578168	-3.325894	4.172396
1	7.224072	2.264292	0.593056	6	0.719133	-1.296290	4.337040
1	1.619712	4.255749	0.713896	6	-1.056479	-3.122089	5.469993
1	8.781787	4.008385	1.336640	1	-0.933431	-4.186996	3.619943
1	5.525064	6.785228	1.776722	6	0.251030	-1.105057	5.637121
1	3.222161	6.068670	1.315821	1	1.327932	-0.521025	3.884613
1	7.950059	6.291145	1.907346	6	-0.635403	-2.018596	6.212051
1	-1.704650	-0.620595	-2.315770	1	-1.760986	-3.831708	5.894745
1	0.413110	-4.227650	-3.335236	1	0.564747	-0.224046	6.189586
1	-3.771907	-1.563077	-3.271098	1	-1.005397	-1.863379	7.221591
1	-1.654284	-5.173434	-4.269993	6	0.251198	-4.252385	1.326787
1	-3.768115	-3.850818	-4.244999	6	0.540193	-5.430209	2.041785
1	3.170759	0.283842	-1.913362	6	-0.594741	-4.334268	0.212845
1	-0.265138	-0.362779	-4.420746	6	-0.006882	-6.650685	1.647499
1	3.921758	2.089563	-3.400300	1	1.193555	-5.395898	2.907548
1	0.453806	1.478141	-5.875102	6	-1.139974	-5.557309	-0.184298
1	2.560201	2.715121	-5.394746	1	-0.822258	-3.443410	-0.354832
1	1.743351	-4.171679	-0.858174	6	-0.848813	-6.717822	0.532834
1	3.153595	-1.686684	-4.069331	1	0.226326	-7.549401	2.211193
1	3.473121	-5.846323	-1.385193	1	-1.783233	-5.592497	-1.058450
1	4.870917	-3.354833	-4.604656	1	-1.271599	-7.670570	0.226867
1	5.060869	-5.446258	-3.265847	6	-6.965699	3.432027	1.473020
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1	-2.613854	5.634335	-2.905337	6	-5.537968	2.681717	-3.113722
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1	-4.426765	-0.584545	2.529762	1	-4.641246	2.175805	-2.753219
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1	-6.402353	-4.286930	-2.775051	1	-0.621478	4.480548	0.520808
1	-6.541950	-0.013731	-3.228392	1	-2.267430	4.993529	0.924126
1	-6.944272	-2.290141	-4.172794	1	-0.875912	5.926889	1.526709
1	-4.314030	-3.761449	1.163597	6	-3.199974	1.436616	4.111341
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1	-6.853931	-3.689445	1.483192	1	-3.972470	1.499756	3.347299


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1      -2.798259  0.417457  4.132183
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(4-7)re-a2 ( $\Phi_1 = -82.8^\circ$ )
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Number of imaginary frequencies : 1
Electronic energy : HF=-5369.5003126
Zero-point correction= 1.562803 (Hartree/Particle)
Thermal correction to Energy= 1.661713
Thermal correction to Enthalpy= 1.662657
Thermal correction to Gibbs Free Energy= 1.420746
Sum of electronic and zero-point Energies= -5367.937510
Sum of electronic and thermal Energies= -5367.838600
Sum of electronic and thermal Enthalpies= -5367.837656
Sum of electronic and thermal Free Energies= -5368.079567
Standard State and RRHO Corrected G= -5368.051731
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Cartesian Coordinates
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8      7.903777  1.721666  0.188513
3      6.104301  2.230941  0.238178
8      5.144484  0.795075 -0.411943
6      4.692997  0.274119 -1.472183
6      4.400359 -1.088295 -1.724518
6      2.389284 -0.618899 -0.777141
6      1.458672 -1.540003 -1.283290
45     -0.644008 -0.802396 -0.580954
6      4.865776 -2.183502 -0.844579
6      4.873150 -3.522942 -1.295360
6      5.290242 -4.571158 -0.473920
6      5.694292 -4.330105  0.840341
6      5.674023 -3.015296  1.316312
6      5.274598 -1.962065  0.494667
6      3.998128 -1.402032 -3.155765
6      5.179550 -1.644581 -4.109929
6      0.510534 -1.242610 -2.323263
8      -0.074605  1.259293 -0.586766
6      0.372941  2.092478 -1.462128
6      -0.066210  3.519138 -1.204093
6      -0.445283  3.944322  0.076188
6      -0.879265  5.254649  0.281467
6      -0.964966  6.144428 -0.795017
6      -0.591695  5.723593 -2.075851
6      -0.127801  4.420937 -2.274662
15     -0.607606 -0.358837  1.985099
6      0.364996  1.157826  2.456065
6      1.585105  1.416070  1.812519
6      2.366504  2.517448  2.153313
6      1.923078  3.417645  3.125401
6      0.692610  3.198995  3.746550
6      -0.077374  2.076864  3.421988
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8      1.113930  1.855186 -2.431068
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6      1.723130 -1.772412  2.803469
6      2.421276 -2.865278  3.318869
6      1.732646 -3.933568  3.898892
6      0.338141 -3.897781  3.951945
6      -0.362516 -2.811208  3.423139
6      -2.103685 -0.119650  3.050007
6      -2.124807 -0.410065  4.424726
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6      -5.384290  1.813328 -1.097036
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1	1.480114	-6.298672	-2.961615	6	-1.350346	-6.079330	3.908020
1	2.494317	-5.476257	1.140931	6	-1.532403	-5.943500	2.532790
1	2.951536	-6.681419	-0.993029	6	-1.440370	-4.682978	1.934348
6	-2.379277	-3.548501	0.871364	6	-2.259309	-0.866816	2.803894
6	-2.262258	-4.836985	1.421587	6	-3.246813	-1.420939	3.634024
6	-3.284016	-2.649636	1.445272	6	-4.218921	-0.604621	4.219110
6	-3.022323	-5.198629	2.534069	6	-4.214771	0.772778	3.992808
1	-1.573308	-5.556598	0.994608	6	-3.240097	1.329355	3.161711
6	-4.044238	-3.009393	2.559110	6	-2.280088	0.517029	2.560446
1	-3.389152	-1.658489	1.029709	8	-3.977191	0.348760	-1.398361
6	-3.910099	-4.283818	3.110426	6	-4.883647	0.668459	-0.433819
1	-2.915951	-6.194908	2.954033	6	-5.024123	1.947263	0.111457
1	-4.726139	-2.285189	2.992994	6	-5.937731	2.115640	1.213837
1	-4.491932	-4.565295	3.983670	6	-6.801867	1.038990	1.603345
6	-2.507959	-3.506167	-2.013231	6	-6.729006	-0.190577	0.896077
6	-2.530604	-2.790208	-3.217011	6	-5.786286	-0.370889	-0.080953
6	-3.268266	-4.683699	-1.910064	6	-7.689042	1.207787	2.699591
6	-3.300203	-3.237712	-4.292799	6	-7.716439	2.382666	3.418297
1	-1.978398	-1.864432	-3.317758	6	-6.842215	3.437441	3.062340
6	-4.042308	-5.125323	-2.983360	6	-5.983281	3.308724	1.991301
1	-3.267155	-5.257514	-0.989480	6	-4.229072	3.094592	-0.406653
6	-4.059534	-4.402793	-4.179545	6	-2.851518	2.980928	-0.503762
1	-3.313458	-2.662098	-5.213899	6	-2.019098	4.045339	-0.916487
1	-4.631796	-6.032380	-2.883024	6	-2.576903	5.250832	-1.258815
1	-4.664569	-4.744487	-5.014723	6	-3.989886	5.418561	-1.252944
-----				6	-4.832461	4.326805	-0.847645
(4-7) _{re-a} [‡] ($\Phi_1 = -159.6^\circ$)				6	-6.241835	4.507254	-0.938881
-----				6	-6.785736	5.701416	-1.361173
Number of imaginary frequencies : 1				6	-5.952076	6.788150	-1.717522
Electronic energy : HF=-5369.4865077				6	-4.583722	6.641375	-1.668643
Zero-point correction= 1.560767 (Hartree/Particle)				8	-2.245164	1.790536	-0.176672
Thermal correction to Energy= 1.660335				8	4.915260	3.978675	-1.368729
Thermal correction to Enthalpy= 1.661279				1	-6.842647	4.356307	3.642366
Thermal correction to Gibbs Free Energy= 1.415863				1	-5.312983	4.124156	1.746899
Sum of electronic and zero-point Energies= -5367.925741				1	-8.338859	0.379054	2.970545
Sum of electronic and thermal Energies= -5367.826173				1	-8.393591	2.497910	4.259882
Sum of electronic and thermal Enthalpies= -5367.825229				1	-7.411584	-0.995305	1.156723
Sum of electronic and thermal Free Energies= -5368.070644				1	-5.701991	-1.307197	-0.618566
Standard State and RRHO Corrected G= -5368.041275				1	-6.896521	3.683359	-0.680903
-----				1	-0.954190	3.852747	-0.953213
Cartesian Coordinates				1	-7.865212	5.806801	-1.426876
-----				1	-3.930186	7.459712	-1.961385
8	7.249622	1.992491	-0.712180	1	-1.949303	6.081788	-1.571060
3	5.498512	2.245831	-1.240420	1	-6.392763	7.726584	-2.042119
8	4.426169	0.773823	-1.520772	1	-0.003744	0.491306	3.590885
6	4.091186	-0.344353	-1.991834	1	1.554944	-3.221165	2.062577
6	4.284500	-1.642567	-1.441736	1	2.185713	1.005630	4.568193
6	2.223396	-1.650098	-0.587504	1	3.754593	-2.694729	3.034445
6	1.222036	-1.904046	-1.547159	1	4.089265	-0.580089	4.301649
45	-0.863160	-1.084788	-0.670281	1	-3.272827	-2.488094	3.820619
6	5.077839	-1.873311	-0.213228	1	-1.562456	0.946895	1.874724
6	5.560403	-3.163991	0.108495	1	-4.983733	-1.051326	4.849008
6	6.255597	-3.415998	1.292089	1	-3.247499	2.394815	2.953326
6	6.498646	-2.387880	2.206843	1	-4.980857	1.403687	4.433035
6	6.022694	-1.106995	1.914276	1	-0.744903	-2.826452	4.692802

1	-1.602231	-4.596493	0.871586
1	-0.923201	-5.042877	5.754631
1	-1.752244	-6.811670	1.917760
1	-1.423434	-7.056675	4.377020
1	-0.344805	2.948583	2.081227
1	3.396076	1.724733	0.378896
1	0.862839	4.192573	3.859805
1	4.622649	2.916491	2.191651
1	3.349376	4.169226	3.929103
1	3.531562	-0.341119	-2.945111
1	5.391961	-3.990633	-0.572050
1	4.950448	0.140813	0.551949
1	6.608792	-4.423483	1.497077
1	6.182281	-0.293607	2.616226
1	7.038983	-2.582145	3.129037
1	3.805642	-3.694744	-1.933406
1	3.301828	-2.524392	-3.122715
1	6.249755	-3.283047	-2.655729
1	5.223555	-3.901740	-3.960727
1	5.637437	-2.180052	-3.892334
1	0.837864	0.119940	-2.276644
1	0.099776	-1.229202	-3.254465
1	1.127005	-2.935294	-1.863788
1	2.563831	-2.482343	0.015508
1	2.298629	-0.683690	-0.106681
6	7.978814	1.076327	-0.248833
6	9.306462	0.133629	1.653467
6	8.997924	-1.160325	-0.444466
6	10.009032	-0.713247	0.602108
1	10.038567	0.655599	2.280329
1	9.494862	-1.703236	-1.252913
1	10.798999	-0.131138	0.114797
6	3.829249	4.618257	-1.279943
6	2.446217	6.363574	-0.188456
6	1.493667	5.018922	-2.055961
6	1.246411	5.552660	-0.654140
1	2.332515	6.643531	0.863684
1	0.751050	4.257662	-2.300902
1	1.094269	4.713096	0.028426
1	8.245335	-1.827792	-0.004175
1	10.472523	-1.581104	1.080023
1	8.700814	-0.502148	2.312334
1	2.544700	7.293268	-0.769295
1	0.343814	6.170139	-0.642266
1	1.422003	5.824914	-2.800560
6	4.763815	5.916916	0.575118
1	5.609129	5.258222	0.387231
1	5.076973	6.955658	0.404178
1	4.453488	5.814801	1.621197
6	2.964998	3.352372	-3.169710
1	3.993888	3.322690	-3.530758
1	2.687858	2.373406	-2.769608
1	2.308182	3.598538	-4.008401
6	7.762993	-0.129609	-2.351650
1	6.795473	-0.640580	-2.307612
1	7.624381	0.848553	-2.812319
1	8.443002	-0.718052	-2.973573
6	7.954737	2.176469	1.934564
1	7.260924	2.828534	1.408447
1	7.442784	1.721729	2.792470
1	8.790828	2.776813	2.313320
7	8.441115	1.141057	1.035614
7	8.352830	0.018673	-1.026657
7	3.663352	5.562882	-0.305918
7	2.814035	4.387200	-2.150517
15	-2.147369	-2.717388	-1.699275
6	-1.177619	-4.114174	-2.436934
6	-1.291999	-4.491940	-3.781351
6	-0.294283	-4.829442	-1.607938
6	-0.537165	-5.556470	-4.285878
1	-1.969585	-3.964697	-4.443120
6	0.448076	-5.896915	-2.108358
1	-0.169432	-4.537458	-0.571187
6	0.331045	-6.262217	-3.453426
1	-0.636069	-5.832298	-5.331990
1	1.124102	-6.436234	-1.450772
1	0.914369	-7.089709	-3.847180
6	-3.320582	-3.609849	-0.591392
6	-3.656948	-4.957884	-0.802276
6	-3.913012	-2.919011	0.472455

6	-4.551126	-5.601464	0.054209
1	-3.215799	-5.508728	-1.626394
6	-4.817281	-3.560465	1.320242
1	-3.665964	-1.879441	0.646722
6	-5.131155	-4.905025	1.119021
1	-4.794652	-6.647210	-0.111092
1	-5.262536	-3.004410	2.139043
1	-5.823406	-5.409942	1.786807
6	-3.248421	-2.209144	-3.094516
6	-2.732975	-1.402796	-4.120938
6	-4.589657	-2.617260	-3.162002
6	-3.538887	-1.023141	-5.194526
1	-1.714341	-1.042948	-4.073949
6	-5.396892	-2.224730	-4.230762
1	-5.016386	-3.235252	-2.380809
6	-4.873353	-1.429157	-5.251667
1	-3.124294	-0.394229	-5.977166
1	-6.435551	-2.541973	-4.262105
1	-5.502343	-1.122940	-6.082969

(4-7)_{re→*}(re_1)

Number of imaginary frequencies : 1

Electronic energy : HF=-5369.5154605

Zero-point correction= 1.564122 (Hartree/Particle)

Thermal correction to Energy= 1.661952

Thermal correction to Enthalpy= 1.662897

Thermal correction to Gibbs Free Energy= 1.427151

Sum of electronic and zero-point Energies= -5367.951339

Sum of electronic and thermal Energies= -5367.853508

Sum of electronic and thermal Enthalpies= -5367.852564

Sum of electronic and thermal Free Energies= -5368.088309

Standard State and RRHO Corrected G= -5368.063195

Cartesian Coordinates

8	-5.471655	2.199535	0.058608
3	-4.223221	1.444729	1.330965
8	-2.579346	1.095046	0.367432
6	-1.500008	1.455496	-0.159650
8	-0.451551	0.732555	-0.291369
45	0.457922	-1.004540	0.612100
15	0.903580	-1.341897	-1.941177
6	-0.580936	-2.152856	-2.702551
6	-1.849897	-1.615809	-2.422996
6	-3.006923	-2.233955	-2.894415
6	-2.917185	-3.402120	-3.656924
6	-1.662902	-3.937942	-3.951279
6	-0.501132	-3.317149	-3.481002
6	-1.398182	2.850952	-0.728702
6	-0.165828	3.353798	-1.164621
6	-0.071612	4.656549	-1.655856
6	-1.211808	5.461620	-1.734834
6	-2.447538	4.956562	-1.317374
6	-2.540644	3.660931	-0.807480
6	-1.464203	-1.978809	1.596007
6	-2.465584	-1.981571	0.621280
6	-4.577596	-2.524856	1.468549
6	-5.288428	-2.654702	0.185721
6	-5.373329	-3.908808	-0.467862
6	-6.003243	-4.055689	-1.703064
6	-6.578904	-2.955526	-2.343866
6	-6.499969	-1.704957	-1.723237
6	-5.863973	-1.549710	-0.492001
6	-0.915985	-0.805285	2.217150
15	2.043071	0.501634	1.392881
8	1.909175	0.968811	2.822620
8	2.111082	1.837520	0.348952
6	3.000343	2.842333	0.663050
6	4.353394	2.697999	0.381980
6	5.250147	3.732708	0.821571
6	4.715994	4.928973	1.410234
6	3.309776	5.055383	1.577593
6	2.473117	4.023852	1.231680
6	5.604566	5.956118	1.830286
6	6.968220	5.810252	1.706461
6	7.500361	4.616537	1.161903
6	6.665645	3.608021	0.731389
6	4.803875	1.487676	-0.355041
6	4.422479	0.227232	0.100662

6	4.807259	-0.954257	-0.576608
6	5.544984	-0.884825	-1.730291
6	5.900349	0.371892	-2.286157
6	5.517775	1.575924	-1.603153
6	5.812447	2.816807	-2.239968
6	6.469148	2.863363	-3.451157
6	6.871658	1.672778	-4.102557
6	6.586164	0.454822	-3.528503
8	3.698625	0.087627	1.255532
6	1.015418	0.261073	-2.858213
6	2.176522	1.026911	-2.672980
6	2.370955	2.212210	-3.380767
6	1.395224	2.664044	-4.272983
6	0.230758	1.916756	-4.454490
6	0.043935	0.719115	-3.758708
6	2.283038	-2.292481	-2.730435
6	2.659786	-3.509141	-2.146565
6	3.674056	-4.291247	-2.700111
6	4.331156	-3.864935	-3.856362
6	3.953695	-2.661643	-4.457900
6	2.935450	-1.883002	-3.904766
6	-4.539396	-1.323684	2.221815
8	-4.989234	-0.183654	1.925743
6	-4.170666	-3.777984	2.227884
6	-5.348822	-4.514478	2.885830
8	-3.782278	2.717493	2.712878
1	6.671726	3.825082	-3.914431
1	5.498654	3.741121	-1.770984
1	6.866841	-0.470871	-4.024833
1	7.390013	1.724217	-5.055763
1	5.827314	-1.794753	-2.251011
1	4.494582	-1.904076	-0.170155
1	7.088829	2.696488	0.324828
1	1.401235	4.081215	1.364643
1	8.577171	4.491957	1.087894
1	5.182922	6.859354	2.264534
1	2.908634	5.970353	2.005710
1	7.636840	6.600286	2.036433
1	-1.929981	-0.719976	-1.818061
1	0.462371	-3.754176	-3.717485
1	-3.977655	-1.823357	-2.639918
1	-1.580716	-4.844126	-4.545488
1	-3.821615	-3.890354	-4.007511
1	2.937484	0.690379	-1.983654
1	-0.860134	0.147726	-3.933483
1	3.284976	2.777975	-3.230229
1	-0.536365	2.258922	-5.143846
1	1.540812	3.591781	-4.819315
1	2.141388	-3.855866	-1.263566
1	2.660990	-0.953919	-4.389991
1	3.950085	-5.228778	-2.225720
1	4.453933	-2.322823	-5.360933
1	5.126426	-4.466358	-4.287707
1	0.702605	2.714333	-1.102485
1	-3.493359	3.269346	-0.473312
1	0.892069	5.038247	-1.981376
1	-3.338790	5.575073	-1.382051
1	-1.139430	6.474837	-2.121791
1	-3.998647	-1.422910	3.184143
1	-4.940436	-4.789289	-0.006268
1	-5.803648	-0.570197	-0.039222
1	-6.044627	-5.039119	-2.165250
1	-6.928276	-0.829629	-2.202547
1	-7.074067	-3.069384	-3.304374
1	-3.623767	-4.470705	1.574742
1	-3.454950	-3.492811	3.008454
1	-6.095525	-4.820021	2.145479
1	-5.010421	-5.413887	3.414690
1	-5.851278	-3.863892	3.610800
1	-1.432732	0.128394	2.041718
1	-0.484981	-0.892773	3.206216
1	-1.202830	-2.948682	2.007954
1	-2.636638	-2.878309	0.040767
1	-2.804795	-1.045000	0.204895
6	-2.932649	3.641410	2.671853
6	-0.710521	4.559813	3.287341
6	-2.353122	6.007404	2.127820
6	-0.900770	5.555957	2.154739
1	-0.836933	5.053612	4.263629
1	-2.548260	6.597499	1.226728

1	-0.242241	6.418680	2.293016
6	-6.301101	2.190994	-0.878686
6	-6.844317	1.816180	-3.277812
6	-8.504132	2.901335	-1.783965
6	-8.307638	1.847372	-2.863224
1	-6.578213	2.730322	-3.830135
1	-9.520981	2.855930	-1.382193
1	-8.936914	2.072768	-3.729051
7	-7.571731	2.669208	-0.679993
7	-5.979651	1.670694	-2.105286
7	-1.664019	3.459148	3.153600
7	-3.247270	4.850209	2.106511
1	0.295378	4.131938	3.269787
1	-0.651118	5.083007	1.199761
1	-2.578769	6.645746	2.995937
1	-8.360344	3.911266	-2.198387
1	-8.602823	0.867047	-2.473153
1	-6.651128	0.967828	-3.942401
15	1.451955	-2.890631	1.639497
6	3.292045	-3.174604	1.698432
6	3.920202	-4.137687	0.889804
6	4.096087	-2.413846	2.563132
6	5.303173	-4.325394	0.935832
1	3.342393	-4.760893	0.222954
6	5.476256	-2.603512	2.610647
1	3.664823	-1.650991	3.193754
6	6.088269	-3.555982	1.793941
1	5.760063	-5.074184	0.295258
1	6.072600	-1.993997	3.283259
1	7.164734	-3.697145	1.827822
6	1.021777	-3.000976	3.450119
6	0.324810	-4.088941	3.997692
6	1.361245	-1.927779	4.295216
6	0.012825	-4.123605	5.359695
1	0.005457	-4.913772	3.372975
6	1.058643	-1.972745	5.656135
1	1.802308	-1.022623	3.890253
6	0.388701	-3.072917	6.196428
1	-0.528824	-4.976103	5.759905
1	1.330590	-1.132147	6.288477
1	0.147733	-3.102383	7.255310
6	0.829527	-4.492550	0.947478
6	1.296234	-5.726312	1.440186
6	-0.127291	-4.498933	-0.075899
6	0.811358	-6.926180	0.920812
1	2.040212	-5.752106	2.229533
6	-0.610197	-5.700414	-0.599125
1	-0.494184	-3.563168	-0.471682
6	-0.143406	-6.916794	-0.100854
1	1.181563	-7.868459	1.314243
1	-1.344465	-5.673725	-1.398659
1	-0.517611	-7.853323	-0.504545
6	-7.875579	3.333150	0.581538
1	-7.286971	2.892552	1.384488
1	-7.662470	4.410832	0.536979
1	-8.938140	3.200481	0.804582
6	-4.604597	1.267079	-2.378684
1	-4.051156	2.064343	-2.892862
1	-4.088660	1.027194	-1.452369
1	-4.616593	0.383556	-3.022710
6	-1.323238	2.242668	3.882505
1	-1.240621	2.451307	4.959293
1	-2.098437	1.496307	3.730167
1	-0.363231	1.854065	3.526228
6	-4.617439	5.093576	1.677739
1	-4.603621	5.774701	0.821334
1	-5.086732	4.160595	1.374491
1	-5.215337	5.557437	2.475708

(4...7)_{re-a} (re_2)

Number of imaginary frequencies : 0
Electronic energy : HF=-5369.5222167
Zero-point correction= 1.563116 (Hartree/Particle)
Thermal correction to Energy= 1.662192
Thermal correction to Enthalpy= 1.663136
Thermal correction to Gibbs Free Energy= 1.421419
Sum of electronic and zero-point Energies= -5367.959101
Sum of electronic and thermal Energies= -5367.860025
Sum of electronic and thermal Enthalpies= -5367.859081

Sum of electronic and thermal Free Energies=				-5368.100798	1	-4.857206	1.239719	-1.152889
Standard State and RRHO Corrected G=				-5368.073086	1	-6.779624	-3.199758	0.535765
.....					1	-1.564068	-2.945531	3.409801
Cartesian Coordinates					1	-8.314171	-4.728688	1.673023
.....					1	-5.276723	-5.702883	4.557976
8	4.730316	-3.226238	-1.853561		1	-3.103127	-4.593756	4.478276
3	3.770468	-1.919514	-0.757871		1	-7.570405	-6.021886	3.673772
8	2.011006	-1.205655	-1.306896		1	1.705816	0.797078	-2.412967
6	0.807426	-1.516885	-1.126116		1	-0.379983	4.428332	-3.455251
8	-0.077656	-0.831632	-0.508528		1	3.740551	1.673382	-3.454466
45	-0.442186	1.080312	0.425408		1	1.661327	5.292193	-4.500551
15	-0.956520	1.802827	-1.976238		1	3.752914	3.934093	-4.495081
6	0.513572	2.563069	-2.812210		1	-2.241916	-0.860175	-1.651718
6	1.686504	1.788964	-2.850676		1	-0.418498	1.375591	-4.848982
6	2.840593	2.278042	-3.457300		1	-2.844358	-2.634969	-3.242551
6	2.845191	3.547964	-4.042259		1	-0.998031	-0.415551	-6.430881
6	1.677304	4.310026	-4.035916		1	-2.226119	-2.437549	-5.639105
6	0.515133	3.819779	-3.431473		1	-1.482632	4.677172	-1.451019
6	0.311847	-2.816616	-1.709773		1	-3.529489	1.455285	-3.441865
6	-0.813327	-3.465774	-1.185149		1	-3.368796	6.166718	-1.907804
6	-1.255093	-4.664379	-1.743698		1	-5.426508	2.946591	-3.888379
6	-0.599717	-5.203488	-2.855567		1	-5.377430	5.314820	-3.120272
6	0.507999	-4.545244	-3.397099		1	-1.334360	-3.009725	-0.354078
6	0.971416	-3.362761	-2.817013		1	1.840835	-2.851763	-3.216257
6	1.591463	1.386878	1.521690		1	-2.123773	-5.164887	-1.326775
6	2.096167	1.381354	0.240461		1	1.014857	-4.955001	-4.266416
6	5.087928	1.711373	0.667812		1	-0.955009	-6.128557	-3.301710
6	5.463575	2.522424	-0.487914		1	4.492891	-0.088932	1.560591
6	5.341450	3.938213	-0.470946		1	4.969150	4.435607	0.418827
6	5.680841	4.723269	-1.572785		1	6.046590	0.877270	-1.750757
6	6.174353	4.138943	-2.742874		1	5.563534	5.803371	-1.511833
6	6.309611	2.745935	-2.784719		1	6.690994	2.267089	-3.684500
6	5.958065	1.954374	-1.694050		1	6.449661	4.751347	-3.597318
6	0.776400	0.326265	2.035237		1	4.098031	3.205790	1.899207
15	-2.249211	0.034249	1.497458		1	4.357316	1.665614	2.676018
8	-2.404506	0.317378	2.967157		1	6.610850	3.666669	2.053257
8	-2.025212	-1.613935	1.243817		1	5.849685	3.439618	3.637098
6	-2.935820	-2.479672	1.819272		1	6.797693	2.130070	2.902568
6	-4.159757	-2.693126	1.204217		1	0.988301	-0.688162	1.718608
6	-5.097017	-3.574386	1.854575		1	0.393488	0.421773	3.045021
6	-4.693171	-4.280185	3.038675		1	1.680403	2.296814	2.104359
6	-3.398059	-4.057292	3.580468		1	2.572999	2.264946	-0.160116
6	-2.544168	-3.155430	2.997395		1	2.200164	0.466949	-0.327190
6	-5.605422	-5.169344	3.669598		6	3.237683	-2.763595	2.031901
6	-6.880616	-5.342804	3.180893		6	4.036748	-2.108938	4.286665
6	-7.298481	-4.614911	2.041530		6	1.616260	-2.529263	3.927538
6	-6.433435	-3.756020	1.398262		6	2.633316	-1.574098	4.533759
6	-4.493939	-1.966540	-0.050995		1	4.199348	-3.045353	4.843155
6	-4.380744	-0.579032	-0.110591		1	0.621192	-2.070041	3.916222
6	-4.907291	0.159781	-1.197642		1	2.449682	-1.465456	5.606571
6	-5.454403	-0.483516	-2.277403		6	5.348806	-4.128716	-1.236779
6	-5.447237	-1.901508	-2.347315		6	7.426490	-5.006147	-0.233279
6	-4.947691	-2.653591	-1.232194		6	5.386987	-6.428097	-0.236595
6	-4.872211	-4.069002	-1.364939		6	6.544276	-5.917173	0.609631
6	-5.273765	-4.700541	-2.522601		1	7.906657	-5.575489	-1.044901
6	-5.790530	-3.955305	-3.609641		1	4.614750	-6.868636	0.404796
6	-5.874847	-2.584004	-3.517732		1	7.122957	-6.761313	0.996204
8	-3.843106	0.150170	0.915957		7	4.773678	-5.348085	-1.011229
6	-1.297122	0.394520	-3.128362		7	6.619638	-3.911900	-0.768164
6	-1.991459	-0.741372	-2.695740		7	4.242487	-2.320157	2.854848
6	-2.327147	-1.752694	-3.600062		1	1.971747	-2.861335	2.548357
6	-1.972203	-1.642950	-4.943037		7	4.787534	-1.390600	4.629943
6	-1.280831	-0.511513	-5.386187		1	2.536309	-0.586819	4.069429
6	-0.948090	0.500856	-4.487664		1	1.543982	-3.450865	4.524685
6	-2.354456	2.944775	-2.401772		1	5.728706	-7.218412	-0.921054
6	-2.336553	4.286685	-1.983822		1	6.158827	-5.348424	1.462493
6	-3.411788	5.135013	-2.244776		1	8.223403	-4.571793	0.377083
6	-4.535093	4.657785	-2.923595		15	-1.014360	3.091748	1.541665
6	-4.562823	3.329552	-3.351780		6	-2.801731	3.438714	1.807498
6	-3.481130	2.481440	-3.100425		6	-3.716183	3.118351	0.796796
6	4.850392	0.341945	0.606409		6	-3.261370	4.094682	2.961823
8	4.953153	-0.472207	-0.383146		6	-5.064484	3.448687	0.928682
6	4.831470	2.389525	2.000715		1	-3.379782	2.600570	-0.088448
6	6.091994	2.941628	2.689408		6	-4.612421	4.417207	3.094647
8	3.463190	-3.052870	0.834518		1	-2.572826	4.357364	3.756606
1	-5.186839	-5.780448	-2.603149		6	-5.516607	4.097128	2.078472
1	-4.472826	-4.654621	-0.545256		1	-5.758492	3.188472	0.135131
1	-6.249787	-1.995724	-4.351387		1	-4.956412	4.920013	3.993972
1	-6.106482	-4.465777	-4.514801		1	-6.567870	4.349235	2.185638
1	-5.855309	0.086027	-3.111322		6	-0.277795	3.287057	3.232332

6	0.707407	4.257453	3.483190	6	-5.892548	-2.873585	-3.045847
6	-0.685189	2.441086	4.278148	6	-5.519224	-2.164525	-1.904963
6	1.280911	4.370604	4.751265	6	-1.066859	-0.549929	1.674763
1	1.040221	4.923848	2.696086	15	2.084706	0.310019	1.529062
6	-0.111307	2.565941	5.544672	8	2.112121	0.210132	3.034042
1	-1.439117	1.684152	4.087492	8	1.783341	1.921571	1.090164
6	0.874613	3.525674	5.785626	6	2.580194	2.894945	1.657420
1	2.044043	5.123585	4.926219	6	3.827055	3.157913	1.109989
1	-0.438368	1.907027	6.344436	6	4.647053	4.164093	1.735566
1	1.320750	3.616753	6.772016	6	4.113847	4.922761	2.832515
6	-0.407053	4.624664	0.712994	6	2.811933	4.626802	3.319701
6	-1.060014	5.853529	0.914745	6	2.069682	3.616768	2.761295
6	0.751029	4.591701	-0.073527	6	4.909367	5.933531	3.437978
6	-0.564740	7.015995	0.325197	6	6.194656	6.177554	3.009470
1	-1.959150	5.906049	1.518238	6	6.741230	5.401505	1.959720
6	1.252256	5.759385	-0.653148	6	5.991090	4.423611	1.342594
1	1.250826	3.654562	-0.260959	6	4.310526	2.339730	-0.034121
6	0.592737	6.973068	-0.459364	6	4.312000	0.947883	0.062608
1	-1.084430	7.957333	0.479592	6	4.971649	0.148862	-0.904126
1	2.147166	5.705269	-1.265075	6	5.550528	0.720683	-2.007942
1	0.973942	7.881179	-0.917534	6	5.440314	2.117373	-2.236292
6	3.404820	-5.576888	-1.444877	6	4.796049	2.935362	-1.249611
1	3.313151	-6.595328	-1.838725	6	4.615970	4.317101	-1.544314
1	2.701116	-5.452706	-0.612343	6	5.055383	4.856641	-2.734488
1	3.143321	-4.866688	-2.223785	6	5.715836	4.049743	-3.692583
6	7.300317	-2.678380	-1.150068	6	5.902954	2.708624	-3.442449
1	7.724680	-2.739529	-2.162677	8	3.759833	0.299002	1.129788
1	6.607985	-1.837826	-1.094933	6	1.724827	-0.518851	-3.150822
1	8.118920	-2.505123	-0.445910	6	2.168085	0.742759	-2.741963
6	5.624065	-2.389400	2.395755	6	2.481917	1.722845	-3.689000
1	6.115501	-3.305670	2.753307	6	2.364202	1.450506	-5.050395
1	5.655790	-2.361810	1.309426	6	1.928147	0.189314	-5.470152
1	6.174016	-1.527279	2.785491	6	1.609490	-0.786688	-4.528096
6	0.911430	-3.463975	1.751332	6	2.830167	-2.970865	-2.194163
1	0.104069	-2.747796	1.576191	6	2.835161	-4.296639	-1.725333
1	1.314152	-3.780821	0.793398	6	3.975935	-5.092594	-1.831455
1	0.497776	-4.335340	2.275761	6	5.143860	-4.578593	-2.398429
				6	5.152486	-3.265618	-2.873107
(4-7) _{re-a*} (re_2)				6	4.007147	-2.471611	-2.778415
				6	-4.687757	-0.698511	0.607865
Number of imaginary frequencies : 1				8	-4.998429	0.171921	-0.252708
Electronic energy : HF=-5369.5179146				6	-4.452437	-2.877345	1.772199
Zero-point correction= 1.562790 (Hartree/Particle)				6	-5.773260	-3.319411	2.421555
Thermal correction to Energy= 1.661269				8	-3.930296	2.864781	0.940984
Thermal correction to Enthalpy= 1.662213				1	4.888897	5.910239	-2.940933
Thermal correction to Gibbs Free Energy= 1.421178				1	4.107587	4.947229	-0.823420
Sum of electronic and zero-point Energies= -5367.955124				1	6.387934	2.071672	-4.177942
Sum of electronic and thermal Energies= -5367.856646				1	6.060339	4.487987	-4.624819
Sum of electronic and thermal Enthalpies= -5367.855702				1	6.055767	0.102524	-2.745107
Sum of electronic and thermal Free Energies= -5368.096737				1	5.000882	-0.920845	-0.746501
Standard State and RRHO Corrected G= -5368.068872				1	6.435199	3.833460	0.550410
				1	1.092078	3.352216	3.143797
Cartesian Coordinates				1	7.765605	5.573165	1.640751
				1	4.482693	6.504099	4.259277
8	-4.968308	2.854913	-1.875531	1	2.422511	5.196005	4.159669
3	-3.943859	1.743949	-0.654250	1	6.794496	6.949874	3.482485
8	-2.184147	1.059622	-1.055661	1	-1.240488	-0.914625	-2.579032
6	-0.973719	1.381515	-1.158775	1	0.890537	-4.596945	-3.267219
8	0.030499	0.703530	-0.761954	1	-3.219866	-1.854668	-3.692027
45	0.549442	-1.041951	0.390287	1	-1.097324	-5.537158	-4.359128
15	1.368652	-1.860238	-1.922283	1	-3.179465	-4.182516	-4.569994
6	-0.031303	-2.692364	-2.813319	1	2.246010	0.972178	-1.689578
6	-1.200126	-1.926144	-2.968677	1	1.271487	-1.761169	-4.866312
6	-2.320878	-2.455340	-3.603247	1	2.810956	2.699769	-3.354384
6	-2.297053	-3.763963	-4.095957	1	1.833439	-0.033697	-6.529506
6	-1.134303	-4.523836	-3.968084	1	2.608591	2.216409	-5.781424
6	-0.004020	-3.990323	-3.338376	1	1.950613	-4.715163	-1.269379
6	-0.634301	2.686253	-1.837954	1	4.040673	-1.456282	-3.152830
6	0.543611	3.375327	-1.520030	1	3.947420	-6.113002	-1.460096
6	0.834175	4.591328	-2.138861	1	6.051355	-2.853392	-3.323587
6	-0.034696	5.113769	-3.101780	1	6.035642	-5.194532	-2.471786
6	-1.204529	4.422679	-3.431133	1	1.213986	2.944746	-0.787827
6	-1.511069	3.219753	-2.791544	1	-2.432854	2.694355	-3.017874
6	-1.594209	-1.740052	1.069342	1	1.748307	5.119462	-1.882981
6	-2.397927	-1.804980	-0.076372	1	-1.881931	4.823102	-4.180525
6	-4.636881	-2.109913	0.474013	1	0.199024	6.053765	-3.594704
6	-5.085153	-2.829866	-0.732046	1	-4.355481	-0.336583	1.598934
6	-5.036156	-4.244229	-0.787131	1	-4.706111	-4.808328	0.078454
6	-5.399317	-4.947691	-1.934857	1	-5.551815	-1.083878	-1.903666
6	-5.834864	-4.270023	-3.076700	1	-5.343776	-6.033663	-1.933713

1	-6.224772	-2.325014	-3.924237
1	-6.123808	-4.817969	-3.969390
1	-3.806453	-3.751567	1.621317
1	-3.908768	-2.238955	2.478499
1	-6.353341	-3.964005	1.752952
1	-5.592452	-3.872351	3.351331
1	-6.394495	-2.448160	2.660185
1	-1.454382	0.405803	1.337925
1	-0.820768	-0.584053	2.729897
1	-1.506694	-2.663394	1.630751
1	-2.538872	-2.761979	-0.560578
1	-2.541273	-0.921781	-0.680717
6	-3.547104	2.489380	2.074996
6	-4.068881	1.683676	4.354949
6	-1.710016	2.209755	3.754635
6	-2.626578	1.203736	4.437776
1	-4.210629	2.601984	4.945835
1	-0.718088	1.772388	3.597768
1	-2.323037	1.077553	5.481112
6	-5.791723	3.621337	-1.312488
6	-8.084321	4.124052	-0.553481
6	-6.297829	5.815924	-0.211606
6	-7.459675	5.086053	0.447345
1	-8.530217	4.675548	-1.396264
1	-5.678301	6.305642	0.548631
1	-8.200286	5.809692	0.800260
7	-5.444905	4.896163	-0.968658
7	-7.062176	3.191204	-1.022751
7	-4.427813	1.912424	2.955500
7	-2.238345	2.611088	2.449407
1	-4.749067	0.927245	4.757476
1	-2.546258	0.230958	3.943480
1	-1.578747	3.102518	4.384510
1	-6.667595	6.602764	-0.884813
1	-7.100995	4.515459	1.310839
1	-8.882509	3.542381	-0.083820
15	1.204120	-2.858080	1.709693
6	2.984672	-2.994088	2.156528
6	3.938171	-2.759990	1.156826
6	3.415474	-3.400676	3.428876
6	5.296354	-2.937114	1.416117
1	3.619093	-2.435028	0.177005
6	4.777182	-3.565022	3.690061
1	2.696890	-3.592263	4.217530
6	5.720059	-3.337016	2.684826
1	6.020171	-2.752222	0.627876
1	5.098602	-3.874509	4.680570
1	6.778682	-3.468178	2.890832
6	0.324365	-3.006979	3.336884
6	-0.560193	-4.067550	3.592517
6	0.500358	-2.015232	4.317894
6	-1.261941	-4.130187	4.798756
1	-0.715598	-4.845877	2.854091
6	-0.198512	-2.088904	5.524077
1	1.168109	-1.182314	4.117482
6	-1.084472	-3.141451	5.767816
1	-1.945984	-4.955242	4.976594
1	-0.052199	-1.314551	6.272422
1	-1.631097	-3.191310	6.705506
6	0.857504	-4.511316	0.958203
6	1.614991	-5.636364	1.325518
6	-0.191811	-4.670194	0.042379
6	1.331783	-6.886857	0.775814
1	2.433736	-5.539705	2.030220
6	-0.481240	-5.924865	-0.498237
1	-0.761519	-3.811979	-0.281025
6	0.282850	-7.035420	-0.136997
1	1.933189	-7.745687	1.060163
1	-1.289777	-6.019757	-1.216469
1	0.067339	-8.010069	-0.565583
6	-4.083434	5.352956	-1.202729
1	-4.104860	6.397275	-1.533373
1	-3.484722	5.278205	-0.286964
1	-3.615001	4.743976	-1.970874
6	-7.509690	1.912728	-1.563032
1	-7.889066	2.012550	-2.590485
1	-6.690675	1.197097	-1.545983
1	-8.318851	1.532515	-0.932911
6	-5.843981	1.881199	2.613446
1	-6.373717	2.763563	3.000968

1	-5.960041	1.837686	1.532440
1	-6.295311	0.987140	3.054541
6	-1.303282	3.310555	1.577022
1	-0.449194	2.669768	1.345373
1	-1.803545	3.586081	0.653144
1	-0.933595	4.219775	2.069493

7_R (re_2)

Number of imaginary frequencies : 0
 Electronic energy : HF=-5369.5410488
 Zero-point correction= 1.566038 (Hartree/Particle)
 Thermal correction to Energy= 1.664320
 Thermal correction to Enthalpy= 1.665264
 Thermal correction to Gibbs Free Energy= 1.426131
 Sum of electronic and zero-point Energies= -5367.975011
 Sum of electronic and thermal Energies= -5367.876729
 Sum of electronic and thermal Enthalpies= -5367.875785
 Sum of electronic and thermal Free Energies= -5368.114918
 Standard State and RRHO Corrected G= -5368.088106

Cartesian Coordinates

8	-5.358869	2.143897	-1.423682
3	-4.164023	1.449195	-0.137658
8	-2.460961	0.811492	-0.634554
6	-1.303776	1.152446	-1.006215
8	-0.225797	0.504519	-0.822500
45	0.645833	-1.095789	0.394038
15	1.584963	-1.844731	-1.857153
6	0.345638	-2.858013	-2.802663
6	-0.837370	-2.198682	-3.185213
6	-1.847179	-2.877567	-3.863469
6	-1.700497	-4.233991	-4.168544
6	-0.526039	-4.894748	-3.807439
6	0.493369	-4.210823	-3.136053
6	-1.167899	2.457502	-1.755305
6	-0.014933	3.241636	-1.619030
6	0.081058	4.469621	-2.275334
6	-0.963206	4.912928	-3.092053
6	-2.113245	4.130074	-3.235992
6	-2.222189	2.913379	-2.559303
6	-1.297590	-2.068045	0.843088
6	-2.267793	-2.225600	-0.300014
6	-3.800491	-2.440606	0.067916
6	-4.543639	-2.590818	-1.261091
6	-5.034126	-3.825707	-1.711257
6	-5.643474	-3.952528	-2.963595
6	-5.780183	-2.843078	-3.798275
6	-5.280712	-1.608931	-3.373439
6	-4.658319	-1.489592	-2.130676
6	-1.083663	-0.891395	1.621093
15	2.065853	0.563545	1.437553
8	2.081979	0.555980	2.951599
8	1.592797	2.144032	0.935085
6	2.274684	3.217067	1.461169
6	3.476086	3.612582	0.888629
6	4.175674	4.733579	1.461250
6	3.575258	5.458495	2.546256
6	2.333633	5.015153	3.075539
6	1.710427	3.905651	2.561974
6	4.249954	6.581099	3.099033
6	5.485256	6.968989	2.631166
6	6.102766	6.230663	1.593296
6	5.468663	5.145549	1.027351
6	4.050171	2.803903	-0.218571
6	4.228544	1.430594	-0.033132
6	4.970141	0.666926	-0.971597
6	5.454375	1.239470	-2.120483
6	5.166968	2.595665	-2.426448
6	4.440833	3.383802	-1.472414
6	4.083750	4.713395	-1.839966
6	4.431174	5.232459	-3.068998
6	5.171157	4.458421	-3.996248
6	5.530352	3.168268	-3.674797
8	3.771809	0.794945	1.077936
6	1.810016	-0.488824	-3.104253
6	2.012954	0.834317	-2.703283
6	2.217303	1.838700	-3.655428
6	2.233524	1.529841	-5.013790

6	2.042019	0.206630	-5.426077
6	1.829055	-0.792960	-4.479161
6	3.190977	-2.761514	-2.073560
6	3.379025	-4.042318	-1.524001
6	4.617062	-4.682311	-1.588288
6	5.706439	-4.050944	-2.191273
6	5.537655	-2.778499	-2.740038
6	4.294640	-2.143141	-2.687192
6	-4.233349	-1.223360	0.858671
8	-5.017913	-0.356872	0.500168
6	-3.940713	-3.647188	1.035339
6	-5.353764	-3.873731	1.588232
8	-4.242762	2.431749	1.491098
1	4.130904	6.243490	-3.330435
1	3.511954	5.315538	-1.142591
1	6.079044	2.554624	-4.385138
1	5.441553	4.880144	-4.960116
1	6.020893	0.645701	-2.833152
1	5.137254	-0.380155	-0.756493
1	5.966750	4.587922	0.243707
1	0.787540	3.533506	2.984388
1	7.090521	6.517795	1.243052
1	3.772227	7.122131	3.912367
1	1.895954	5.553244	3.912577
1	5.993029	7.826253	3.064149
1	-0.969354	-1.148479	-2.943689
1	1.401417	-4.744449	-2.884909
1	-2.756526	-2.353157	-4.136566
1	-0.390900	-5.945060	-4.052391
1	-2.495021	-4.764758	-4.685374
1	1.994875	1.085674	-1.653087
1	1.681202	-1.815949	-4.810803
1	2.363394	2.861285	-3.328359
1	2.056731	-0.046223	-6.482953
1	2.397699	2.314282	-5.747610
1	2.563287	-4.545746	-1.027992
1	4.196073	-1.154067	-3.115174
1	4.725979	-5.671784	-1.153111
1	6.374322	-2.272972	-3.214945
1	6.673925	-4.543304	-2.232186
1	0.784508	2.884623	-0.983114
1	-3.127710	2.321385	-2.638172
1	0.977935	5.071928	-2.157398
1	-2.928267	4.469594	-3.869728
1	-0.883072	5.863611	-3.612609
1	-3.765793	-1.148515	1.858106
1	-4.941950	-4.711287	-1.092939
1	-4.244165	-0.531692	-1.845579
1	-6.011451	-4.924334	-3.281985
1	-5.362083	-0.734472	-4.013591
1	-6.260320	-2.939341	-4.768183
1	-3.570780	-4.544814	0.527634
1	-3.262396	-3.482246	1.878981
1	-6.095592	-4.000984	0.794970
1	-5.379604	-4.767353	2.221000
1	-5.678688	-3.027662	2.205995
1	-1.584276	0.031294	1.354944
1	-0.864977	-0.993029	2.676987
1	-1.152176	-3.000386	1.383500
1	-2.000596	-3.109176	-0.887155
1	-2.216602	-1.367553	-0.960150
6	-3.613078	2.047303	2.511163
6	-3.638686	1.190274	4.819918
6	-1.469775	1.884390	3.800688
6	-2.171200	0.827752	4.644656
1	-3.749081	2.111786	5.412414
1	-0.505688	1.506683	3.440793
1	-1.675227	0.748516	5.615989
6	-6.390488	2.730424	-0.997527
6	-8.820186	2.762108	-0.589034
6	-7.465909	4.769177	-0.023985
6	-8.544045	3.816891	0.474293
1	-9.241600	3.224767	-1.494925
1	-7.077669	5.371130	0.805270
1	-9.454683	4.377168	0.705175
7	-6.342934	4.039071	-0.619553
7	-7.577346	2.056322	-0.896272
7	-4.256784	1.349860	3.502119
7	-2.274311	2.272145	2.636459
1	-4.171631	0.394529	5.347787

1	-2.104342	-0.148291	4.157272
1	-1.266304	2.781654	4.404334
1	-7.878266	5.465922	-0.767653
1	-8.208642	3.318820	1.391013
1	-9.545320	2.028401	-0.226607
15	1.519886	-2.738127	1.754138
6	3.303498	-2.633034	2.210751
6	4.220631	-2.236375	1.229122
6	3.782347	-3.007630	3.477058
6	5.589164	-2.227087	1.497920
1	3.863490	-1.924088	0.258678
6	5.151213	-2.985132	3.748324
1	3.093550	-3.319258	4.254095
6	6.058539	-2.599230	2.758297
1	6.284380	-1.916581	0.723587
1	5.506894	-3.272025	4.734014
1	7.123896	-2.584326	2.970998
6	0.667347	-2.890296	3.393856
6	-0.178020	-3.971276	3.685568
6	0.818080	-1.864428	4.344187
6	-0.860963	-4.028338	4.904205
1	-0.310042	-4.774982	2.969515
6	0.145106	-1.935366	5.564339
1	1.432414	-1.001208	4.101603
6	-0.698586	-3.013565	5.848264
1	-1.513238	-4.871816	5.113315
1	0.274373	-1.138366	6.291587
1	-1.225370	-3.061227	6.797473
6	1.382987	-4.481016	1.129464
6	2.216648	-5.490405	1.640170
6	0.428700	-4.822682	0.161139
6	2.101199	-6.803795	1.184059
1	2.967836	-5.255886	2.386240
6	0.306989	-6.139776	-0.287710
1	-0.192578	-4.054527	-0.275499
6	1.144909	-7.133744	0.219109
1	2.761881	-7.568942	1.581994
1	-0.427620	-6.374933	-1.051847
1	1.059503	-8.156361	-0.137486
6	-5.081684	4.766443	-0.697141
1	-5.283981	5.796488	-1.008798
1	-4.576014	4.775507	0.275325
1	-4.421865	4.298689	-1.425286
6	-7.668339	0.713634	-1.459980
1	-7.886846	0.735512	-2.537066
1	-6.735108	0.178177	-1.299958
1	-8.475701	0.176549	-0.954741
6	-5.704443	1.199867	3.416052
1	-6.233571	2.066400	3.838762
1	-5.997485	1.073579	2.375943
1	-5.996911	0.308712	3.978844
6	-1.591923	3.112814	1.659584
1	-0.684216	2.615764	1.312363
1	-2.244885	3.301846	0.813039
1	-1.313500	4.073343	2.113373

(4...7)_{re} (re_2) (after dissociation of PPh₃ group)

Number of imaginary frequencies : 0
 Electronic energy : HF=-4333.1406885
 Zero-point correction= 1.285515 (Hartree/Particle)
 Thermal correction to Energy= 1.367645
 Thermal correction to Enthalpy= 1.368589
 Thermal correction to Gibbs Free Energy= 1.161644
 Sum of electronic and zero-point Energies= -4331.855174
 Sum of electronic and thermal Energies= -4331.773043
 Sum of electronic and thermal Enthalpies= -4331.772099
 Sum of electronic and thermal Free Energies= -4331.979045
 Standard State and RRHO Corrected G= -4331.955206

Cartesian Coordinates

8	-3.709597	0.334245	1.694767
3	-2.541271	-0.853960	0.784980
8	-0.730265	-0.085004	0.754156
6	0.308235	-0.155923	1.492830
8	1.459058	-0.128274	0.946857
45	0.757587	0.072362	-1.091598
15	0.317234	2.423254	-1.045691
6	-1.197770	2.766249	-2.037864

6	-2.334542	1.970776	-1.810006
6	-3.513233	2.208629	-2.515703
6	-3.573389	3.243362	-3.453703
6	-2.449613	4.039769	-3.681022
6	-1.265666	3.806613	-2.975321
6	0.223418	-0.220076	2.975825
6	1.397621	-0.409405	3.720684
6	1.343539	-0.432894	5.112983
6	0.118609	-0.264436	5.767504
6	-1.051019	-0.072430	5.025261
6	-1.003408	-0.049415	3.631541
6	0.414442	-1.487403	-2.644346
6	-0.322652	-0.301729	-2.927957
6	-4.466734	-1.981771	-2.680443
6	-5.669716	-1.232370	-2.315266
6	-6.857099	-1.322023	-3.091592
6	-8.012950	-0.612854	-2.768835
6	-8.049839	0.226599	-1.652047
6	-6.895610	0.336716	-0.870231
6	-5.734394	-0.369336	-1.184629
6	0.261499	-2.120747	-1.405872
15	2.787118	0.107542	-2.046070
8	2.957097	0.282761	-3.523013
8	3.352344	-1.370498	-1.494739
6	4.708810	-1.646208	-1.511594
6	5.544130	-1.070072	-0.567237
6	6.951998	-1.368218	-0.642348
6	7.418497	-2.321696	-1.610006
6	6.493533	-2.918173	-2.509310
6	5.166069	-2.571550	-2.476304
6	8.803905	-2.634563	-1.673009
6	9.709113	-2.018311	-0.839000
6	9.259786	-1.047340	0.087355
6	7.921804	-0.730727	0.182518
6	4.992452	-0.115205	0.432101
6	4.258378	0.985230	0.009505
6	3.920256	2.043782	0.879203
6	4.203120	1.949038	2.218346
6	4.794469	0.770003	2.745183
6	5.191985	-0.277560	1.848038
6	5.727071	-1.471097	2.410130
6	5.870324	-1.615297	3.773356
6	5.499082	-0.569845	4.653247
6	4.973153	0.597028	4.144754
8	3.886719	1.130851	-1.314742
6	-0.131048	3.100665	0.610838
6	0.686889	2.824434	1.716857
6	0.375242	3.334818	2.976881
6	-0.756973	4.133400	3.150108
6	-1.570779	4.423112	2.052770
6	-1.262428	3.912399	0.790226
6	1.566094	3.603595	-1.691009
6	2.119795	3.365681	-2.959390
6	3.065837	4.242429	-3.488207
6	3.475590	5.360341	-2.756381
6	2.926628	5.603708	-1.496140
6	1.970132	4.734465	-0.965817
6	-3.260817	-1.902156	-2.002955
8	-2.925900	-1.193448	-0.981751
6	-4.517590	-2.937916	-3.861648
6	-5.252695	-4.261908	-3.581319
8	-2.401899	-2.558513	1.744652
1	6.266937	-2.542540	4.177124
1	6.007535	-2.284776	1.750948
1	4.667918	1.401906	4.808563
1	5.622407	-0.694863	5.725200
1	3.939914	2.758125	2.894069
1	3.432964	2.913785	0.455153
1	7.602749	0.024595	0.890272
1	4.445694	-2.992933	-3.169602
1	9.977673	-0.540915	0.726501
1	9.135949	-3.366185	-2.405250
1	6.856313	-3.637187	-3.238663
1	10.765822	-2.262489	-0.898889
1	-2.308606	1.151720	-1.098498
1	-0.403541	4.438057	-3.159999
1	-4.377801	1.579076	-2.329686
1	-2.488854	4.847083	-4.407106
1	-4.491681	3.425108	-4.005172
1	1.554281	2.190407	1.603608

1	-1.908876	4.146865	-0.047469
1	1.009234	3.088285	3.823714
1	-2.451814	5.046468	2.175775
1	-1.005459	4.524456	4.132686
1	1.833681	2.486826	-3.526605
1	1.547032	4.939394	0.011547
1	3.490650	4.043877	-4.467937
1	3.237702	6.472248	-0.922575
1	4.219932	6.037044	-3.166407
1	2.341745	-0.526825	3.201703
1	-1.905665	0.109722	3.052170
1	2.256521	-0.578612	5.683197
1	-2.001650	0.065146	5.533176
1	0.076490	-0.280213	6.853271
1	-2.461779	-2.543775	-2.425308
1	-6.879347	-1.956867	-3.970579
1	-4.854623	-0.255000	-0.566347
1	-8.892882	-0.718345	-3.400098
1	-6.890096	0.982416	0.002440
1	-8.950550	0.779271	-1.398449
1	-4.973968	-2.455753	-4.738119
1	-3.491034	-3.177248	-4.167164
1	-6.271286	-4.090142	-3.217749
1	-5.317914	-4.888398	-4.480190
1	-4.722366	-4.833003	-2.811221
1	-0.690925	-2.085919	-0.885473
1	0.972089	-2.884066	-1.109145
1	1.266212	-1.741097	-3.270112
1	-0.074384	0.260923	-3.823208
1	-1.351634	-0.231887	-2.593171
6	-2.169419	-3.601820	1.081692
6	-2.963306	-5.532730	-0.231673
6	-0.533531	-5.284979	0.209626
1	-1.577263	-5.563543	-0.862298
1	-3.073416	-6.349557	0.498227
1	0.443828	-5.089299	-0.246650
1	-1.386118	-6.537594	-1.321826
6	-4.790934	0.712259	2.203463
6	-6.596898	2.434254	2.392396
6	-6.584836	0.455764	3.890092
6	-7.449999	1.326040	2.991001
1	-6.346128	3.187171	3.154095
1	-7.153358	-0.404108	4.256530
1	-8.276231	1.759060	3.562081
7	-5.438288	-0.053636	3.137318
7	-5.365146	1.892176	1.815637
7	-3.172418	-4.233796	0.405789
7	-0.901743	-4.115342	1.008525
1	-3.736263	-5.665311	-0.991891
1	-1.524679	-4.798630	-1.645183
1	-0.415458	-6.156884	0.869993
1	-6.244171	1.023609	4.769997
1	-7.874107	0.709241	2.191339
1	-7.141963	2.949466	1.593777
6	-4.761813	-1.219200	3.694498
1	-4.214345	-0.963097	4.613553
1	-5.512201	-1.975815	3.944118
1	-4.063228	-1.638880	2.973715
6	-4.690649	2.746116	0.848748
1	-4.547317	3.747221	1.272421
1	-3.722430	2.323548	0.598751
1	-5.287970	2.835674	-0.065949
6	-4.532596	-3.727299	0.554321
1	-4.971364	-4.008189	1.521170
1	-4.539917	-2.641807	0.460599
1	-5.146816	-4.143909	-0.245471
6	0.155162	-3.556213	1.838609
1	0.898827	-3.026106	1.232213
1	-0.271807	-2.859456	2.555249
1	0.662952	-4.364251	2.379156

(4-7)_{re}[‡](re_2) (after dissociation of PPh₃ group)

Number of imaginary frequencies : 1
Electronic energy : HF=-4333.1147511
Zero-point correction= 1.284903 (Hartree/Particle)
Thermal correction to Energy= 1.366501
Thermal correction to Enthalpy= 1.367445
Thermal correction to Gibbs Free Energy= 1.161127
Sum of electronic and zero-point Energies= -4331.829848

Sum of electronic and thermal Energies=	-4331.748250	1	5.743374	-1.611231	5.191865
Sum of electronic and thermal Enthalpies=	-4331.747306	1	3.868343	2.331012	3.266209
Sum of electronic and thermal Free Energies=	-4331.953624	1	3.125110	2.959556	0.975231
Standard State and RRHO Corrected G=	-4331.929405	1	7.277168	0.003074	0.391629
.....					
Cartesian Coordinates		1	3.602603	-2.140803	-3.783578
.....					
8	-3.578257	-2.035762	2.346238	9.599622	-0.573673
3	-2.353226	-1.942525	0.891115	8.329694	-2.747553
8	-1.039228	-0.351448	1.115781	5.965547	-2.813786
6	0.098229	-0.494244	1.683242	10.147698	-1.978548
8	1.168471	-0.186388	1.067399	1	-2.629421
45	0.268395	0.590676	-0.742139	1	2.218702
15	0.022395	2.904741	0.013569	1	0.932967
6	-1.649586	3.480519	-0.525275	1	-1.004867
6	-2.767986	2.922439	0.118138	1	4.825528
6	-4.056916	3.261195	-0.284807	1	-2.091548
6	-4.252855	4.146239	-1.349138	1	2.817965
6	-3.147580	4.699846	-1.996372	1	0.215699
6	-1.851286	4.375564	-1.583951	1	-3.288221
6	0.221842	-0.960946	3.093495	1	5.393155
6	1.498416	-1.191429	3.631444	1	-5.259404
6	1.635636	-1.581353	4.962153	1	4.391423
6	0.500725	-1.740558	5.764790	1	-1.672657
6	-0.770798	-1.511386	5.230637	1	1.305227
6	-0.913852	-1.121337	3.898293	1	1.665535
6	-0.812542	-0.074908	-2.554368	1	2.335717
6	-2.002114	0.538741	-2.118360	1	-1.403159
6	-3.905190	-0.754052	-2.787764	1	4.944795
6	-4.988376	0.204850	-2.505410	1	2.086304
6	-5.452422	1.083472	-3.514014	1	4.759403
6	-6.505290	1.969014	-3.291083	1	-1.450122
6	-7.147790	2.010772	-2.050919	1	5.387241
6	-6.698689	1.160915	-1.036555	1	4.101545
6	-5.633169	0.285777	-1.246265	1	-0.141395
6	-0.209666	-1.160928	-1.830038	1	3.958514
15	2.149270	0.718643	-1.916991	1	5.663704
8	2.166161	1.148158	-3.354258	1	1.143075
8	2.757123	-0.845284	-1.725739	1	3.335804
6	4.086909	-1.127596	-1.947845	1	5.277777
6	5.040685	-0.755790	-1.012223	1	1.446008
6	6.419326	-1.064364	-1.291894	1	2.634012
6	6.745634	-1.832323	-2.461273	1	5.034462
6	5.709189	-2.233267	-3.347606	1	-3.603907
6	4.407394	-1.869793	-3.108140	1	2.981441
6	8.103596	-2.157672	-2.728325	1	6.941063
6	9.113369	-1.727032	-1.897605	1	0.239363
6	8.800448	-0.936168	-0.766270	1	6.841462
6	7.493102	-0.613536	-0.472557	1	-2.173944
6	4.626417	-0.001103	0.200676	1	2.370173
6	3.881660	1.165507	0.070263	1	-1.054728
6	3.645139	2.027979	1.163006	1	-1.897236
6	4.058211	1.673692	2.422330	1	-0.954342
6	4.675815	0.415374	2.648762	1	2.627171
6	4.955143	-0.439943	1.530470	1	-1.755822
6	5.501028	-1.728035	1.795898	1	-1.633951
6	5.769320	-2.138002	3.084206	1	-1.073077
6	5.520881	-1.278549	4.181994	1	-5.289709
6	4.984819	-0.028834	3.963252	1	-6.828724
8	3.393621	1.563487	-1.157894	1	2.625095
6	-0.047559	3.262552	1.827364	1	-7.181748
6	0.698513	2.474539	2.715051	1	-7.976315
6	0.664344	2.722180	4.089795	1	-3.326003
6	-0.110026	3.767214	4.594605	1	-2.592018
6	-0.848916	4.567772	3.717300	1	-5.560822
6	-0.821092	4.317531	2.345200	1	-1.341747
6	1.162662	4.194888	-0.643720	1	-5.289709
6	1.515469	4.138480	-2.002365	1	-6.828724
6	2.371007	5.093637	-2.551536	1	2.625095
6	2.902972	6.105563	-1.748357	1	-7.181748
6	2.568048	6.161039	-0.394068	1	-7.976315
6	1.698068	5.216354	0.155910	1	-3.326003
6	-3.430048	-1.695289	-1.842561	1	-2.592018
8	-3.589562	-1.705891	-0.585722	1	-5.560822
6	-3.536434	-1.053413	-4.232294	1	-1.341747
6	-4.599969	-1.866228	-4.988206	1	-5.289709
8	-1.194305	-3.479971	0.735991	1	-6.828724
1	6.170394	-3.132304	3.259595	1	2.625095
1	5.688550	-2.401847	0.967614	1	-7.181748
1	4.768247	0.634008	4.797260	1	-7.976315
				1	-3.326003
				1	-2.592018
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				1	-5.289709
				1	-6.828724
				1	2.625095
				1	-7.181748
				1	-7.976315
				1	-3.326003

1	-3.376503	-5.171908	-1.777302	6	-0.970051	4.462177	2.261433
6	1.545827	-3.340330	0.527153	6	0.969014	4.204006	-0.726518
1	1.849889	-2.356201	0.158958	6	1.329681	4.078337	-2.078910
1	1.017829	-3.219470	1.469982	6	2.151805	5.027329	-2.686836
1	2.439512	-3.952474	0.694809	6	2.646873	6.105719	-1.949423
7_R (re_2) (after dissociation of PPh₃ group)							
Number of imaginary frequencies : 0							
Electronic energy : HF=-4333.148573							
Zero-point correction= 1.287904 (Hartree/Particle)							
Thermal correction to Energy= 1.369242							
Thermal correction to Enthalpy= 1.370187							
Thermal correction to Gibbs Free Energy= 1.165992							
Sum of electronic and zero-point Energies= -4331.860669							
Sum of electronic and thermal Energies= -4331.779331							
Sum of electronic and thermal Enthalpies= -4331.778386							
Sum of electronic and thermal Free Energies= -4331.982581							
Standard State and RRHO Corrected G= -4331.959471							
Cartesian Coordinates							
8	-3.429970	-2.165932	2.234092	1	5.885196	-2.808180	-4.259581
3	-2.031707	-1.960101	0.971572	1	10.071857	-1.890180	-2.185138
8	-1.004110	-0.282848	1.233444	1	-2.757126	2.364848	1.112693
6	0.107724	-0.358321	1.883943	1	-1.210339	4.454625	-2.323511
8	1.200540	-0.075143	1.328657	1	-5.057169	2.772556	0.315956
45	0.216237	0.575158	-0.638573	1	-3.506675	4.838902	-3.119031
15	-0.109503	2.896406	0.015084	1	-5.449402	3.988304	-1.811564
6	-1.809474	3.380169	-0.544551	1	1.229416	1.876085	2.389534
6	-2.914500	2.915947	0.190981	1	-1.582749	5.024631	1.564130
6	-4.214289	3.145181	-0.257260	1	1.203778	2.472476	4.781625
6	-4.436707	3.830868	-1.454178	1	-1.595273	5.638011	3.951007
6	-3.346542	4.298925	-2.189595	1	-0.210733	4.364661	5.581136
6	-2.042380	4.079644	-1.737314	1	0.994906	3.222813	-2.655471
6	0.120901	-0.733193	3.331591	1	1.218641	5.409285	1.054460
6	1.356973	-0.897490	3.977082	1	2.419398	4.910700	-3.733429
6	1.403078	-1.204859	5.335421	1	2.693905	7.061391	-0.015604
6	0.215292	-1.347112	6.061358	1	3.298135	6.837233	-2.419844
6	-1.016889	-1.184998	5.421182	1	2.268378	-0.773036	3.404120
6	-1.066910	-0.879070	4.059919	1	-2.017827	-0.766120	3.554502
6	-1.041651	0.129736	-2.276721	1	2.364415	-1.330851	5.825912
6	-2.501228	0.412875	-1.966725	1	-1.940473	-1.294946	5.983228
6	-3.556312	-0.557567	-2.593812	1	0.250466	-1.583481	7.121510
6	-4.926354	0.146165	-2.517837	1	-4.327225	-2.616850	-2.211246
6	-5.416846	0.912082	-3.586974	1	-4.859131	0.974315	-4.514712
6	-6.616559	1.616121	-3.474969	1	-5.302382	-0.420769	-0.460546
6	-7.357596	1.567088	-2.291512	1	-6.971602	2.204128	-4.316901
6	-6.875903	0.818484	-1.217315	1	-7.436143	0.776439	-0.288248
6	-5.668674	0.122679	-1.326252	1	-8.295177	2.109309	-2.207854
6	-0.375178	-1.069075	-1.844974	1	-2.971510	-0.036477	-4.599954
15	1.995562	0.692512	-1.941777	1	-2.178259	-1.459028	-3.981084
8	1.972214	1.070970	-3.396587	1	-5.134064	-1.445860	-4.858605
8	2.668020	-0.864052	-1.751988	1	-3.770835	-1.969527	-5.854207
6	3.995712	-1.114180	-1.985988	1	-4.188394	-2.865158	-4.397066
6	4.956558	-0.711933	-1.067629	1	-0.911454	-1.805472	-1.259711
6	6.336511	-1.007010	-1.353155	1	0.394854	-1.506687	-2.474258
6	6.665610	-1.790086	-2.512011	1	-0.702900	0.562814	-3.217136
6	5.627833	-2.217877	-3.384036	1	-2.743857	1.418173	-2.316055
6	4.323162	-1.869585	-3.138227	1	-2.676884	0.413598	-0.887283
6	8.025712	-2.103026	-2.782825	6	-0.194214	-3.977714	-0.109421
6	9.035957	-1.647455	-1.965902	6	-0.078633	-5.448822	-2.095074
6	8.720369	-0.842266	-0.845341	6	1.986594	-4.345028	-1.278573
6	7.411003	-0.530324	-0.548829	6	1.151434	-4.655503	-2.510319
6	4.542674	0.067483	0.129850	1	0.210942	-6.434429	-1.697353
6	3.784950	1.222739	-0.032696	1	2.739262	-3.586029	-1.509498
6	3.542518	2.110790	1.039570	1	1.747718	-5.223040	-3.230606
6	3.963119	1.794725	2.306255	6	-4.673515	-2.077689	2.092617
6	4.594087	0.549070	2.564678	6	-6.734716	-0.718889	2.247091
6	4.880414	-0.332136	1.468676	6	-6.905396	-3.172067	1.890631
6	5.440574	-1.606952	1.766520	6	-7.434309	-1.813334	1.453785
6	5.713832	-1.981999	3.064743	1	-7.014467	-0.771761	3.310398
6	5.457120	-1.097503	4.140430	1	-7.252845	-3.956556	1.210237
6	4.909876	0.141665	3.889527	1	-8.514842	-1.766584	1.617181
8	3.287135	1.570821	-1.267337	7	-5.440539	-3.190260	1.888193
6	-0.176691	3.395310	1.800904	7	-5.283799	-0.848707	2.094391
6	0.611131	2.696033	2.726645	7	-0.834491	-4.691833	-1.096985
6	0.598815	3.041561	4.080878	7	1.155259	-3.829141	-0.187371
6	-0.196299	4.097354	4.527996	1	-0.735497	-5.622102	-2.952870
6	-0.977988	4.810045	3.612653	1	0.833400	-3.723667	-2.989596

1	2.518454	-5.243778	-0.933943	6	-3.770972	2.137219	0.294632
1	-7.273841	-3.426174	2.895714	6	-4.470162	1.671108	1.435825
1	-7.246318	-1.665790	0.385433	6	-4.589809	2.456179	2.553227
1	-7.023370	0.270902	1.883703	6	-3.959785	3.727138	2.609029
6	-4.824533	-4.509653	1.936935	6	-3.272323	4.216234	1.448559
1	-5.147998	-5.054745	2.834031	6	-2.576528	5.453705	1.561493
1	-5.121175	-5.089624	1.055805	6	-2.570646	6.166179	2.741912
1	-3.741602	-4.410391	1.952990	6	-3.273571	5.691131	3.875410
6	-4.473968	0.319841	2.426803	6	-3.953590	4.495838	3.803744
1	-4.352197	0.439782	3.512348	8	-3.704550	1.288767	-0.772235
1	-3.487179	0.239872	1.972380	6	-1.261413	-0.131752	3.148437
1	-4.973536	1.208681	2.035590	6	-1.346806	1.197205	2.721961
6	-2.215828	-5.105619	-0.883989	6	-1.144450	2.243477	3.627990
1	-2.273364	-6.069078	-0.355925	6	-0.856354	1.973502	4.964112
1	-2.748879	-4.352449	-0.310780	6	-0.769470	0.647298	5.400468
1	-2.704032	-5.218255	-1.856920	6	-0.970832	-0.396784	4.500032
6	1.878953	-3.073221	0.830710	6	-3.295133	-2.051704	2.617763
1	2.155867	-2.086763	0.451564	6	-3.830396	-3.317553	2.321253
1	1.257152	-2.950995	1.713917	6	-5.136019	-3.648886	2.684559
1	2.784007	-3.627384	1.105120	6	-5.942160	-2.719128	3.344061
				6	-5.421646	-1.460781	3.652621
(4-7) _{re-a} ⁺ (re_3)				6	-4.110787	-1.131922	3.300037
				6	3.720809	-2.382207	-2.105166
Number of imaginary frequencies : 1				8	4.387183	-1.387638	-1.708386
Electronic energy : HF=-5369.5163894				6	2.854195	-4.689801	-2.363492
Zero-point correction= 1.563079 (Hartree/Particle)				6	3.868806	-5.560779	-3.122658
Thermal correction to Energy= 1.661416				8	4.586156	1.842271	-1.695722
Thermal correction to Enthalpy= 1.662360				1	-2.017283	7.099157	2.803412
Thermal correction to Gibbs Free Energy= 1.422895				1	-2.028571	5.829667	0.705222
Sum of electronic and zero-point Energies= -5367.953311				1	-4.480498	4.106708	4.671356
Sum of electronic and thermal Energies= -5367.854974				1	-3.264383	6.263898	4.798239
Sum of electronic and thermal Enthalpies= -5367.854030				1	-5.128436	2.094102	3.424825
Sum of electronic and thermal Free Energies= -5368.093494				1	-4.902044	0.680199	1.396087
Standard State and RRHO Corrected G= -5368.066327				1	-4.807961	5.571178	-0.149124
				1	-0.549239	3.103022	-3.505611
Cartesian Coordinates				1	-5.608313	7.646776	-1.165821
				1	-2.737391	7.248812	-4.343819
8	5.781431	0.174377	0.561157	1	-1.292622	5.283021	-4.456008
3	4.261871	0.219676	-0.665820	1	-4.559707	8.527967	-3.252732
8	2.457955	0.082235	0.103745	1	1.218872	-1.612524	1.971011
6	1.449972	0.729509	0.480666	1	-1.847416	-4.167924	3.592483
8	0.228322	0.376696	0.377871	1	2.943601	-3.164389	2.791313
45	-1.078846	-1.089080	-0.516559	1	-0.122793	-5.718325	4.401286
15	-1.624451	-1.536091	1.995814	1	2.291280	-5.239057	3.997585
6	-0.445605	-2.788237	2.689557	1	-1.548177	1.418506	1.684052
6	0.919133	-2.511653	2.498867	1	-0.904538	-1.421528	4.851556
6	1.896834	-3.384708	2.969578	1	-1.202974	3.267624	3.279552
6	1.527435	-4.551803	3.645501	1	-0.544890	0.425657	6.440354
6	0.176397	-4.822310	3.863933	1	-0.697523	2.790922	5.662255
6	-0.806319	-3.942705	3.395866	1	-3.233967	-4.052735	1.802286
6	1.669483	2.058146	1.162675	1	-3.731397	-0.149120	3.550498
6	0.742951	3.100564	1.035019	1	-5.520364	-4.635121	2.440507
6	0.969504	4.320637	1.673013	1	-6.033399	-0.729225	4.173622
6	2.106037	4.497664	2.468562	1	-6.962316	-2.973148	3.617474
6	3.027500	3.455313	2.605254	1	-0.146036	2.936134	0.440287
6	2.816952	2.244611	1.942669	1	3.534805	1.435452	2.023612
6	0.539675	-2.479030	-1.554980	1	0.247903	5.124762	1.566029
6	1.511810	-2.723965	-0.583103	1	3.910617	3.585714	3.224693
6	3.493816	-3.633202	-1.476700	1	2.271747	5.442365	2.979613
6	4.117237	-4.039448	-0.206480	1	3.194883	-2.280481	-3.075365
6	3.976830	-5.362256	0.281560	1	3.432440	-6.099082	-0.298488
6	4.523705	-5.759996	1.501638	1	4.947973	-2.109685	0.311366
6	5.240872	-4.856820	2.290330	1	4.390339	-6.786847	1.833942
6	5.384003	-3.542246	1.834618	1	5.928058	-2.814403	2.432423
6	4.826935	-3.135353	0.623068	1	5.673157	-5.168470	3.237238
6	0.269285	-1.200596	-2.153384	1	2.183317	-5.332624	-1.778855
15	-2.258004	0.679658	-1.473502	1	2.208274	-4.187953	-3.094119
8	-2.637441	0.549643	-2.926175	1	4.544567	-6.082387	-2.436836
8	-1.317163	2.076108	-1.257571	1	3.364457	-6.315454	-3.738645
6	-1.807450	3.260179	-1.767741	1	4.485742	-4.941217	-3.783706
6	-2.751713	3.978345	-1.048248	1	0.997774	-0.413952	-1.989832
6	-3.261747	5.196769	-1.625787	1	-0.197689	-1.180836	-3.133195
6	-2.702392	5.679817	-2.857595	1	0.058177	-3.351868	-1.983395
6	-1.702084	4.916633	-3.518390	1	1.500776	-3.665113	-0.048808
6	-1.283132	3.717577	-2.999239	1	2.038874	-1.897015	-0.130012
6	-3.182514	6.895360	-3.416927	6	4.093257	2.995114	-1.702450
6	-4.197680	7.602766	-2.813501	6	2.132351	4.516458	-2.024900
6	-4.785779	7.106181	-1.625908	6	4.386950	5.455321	-1.592219
6	-4.332739	5.938516	-1.050391	6	2.916799	5.534515	-1.213653
6	-3.264045	3.435926	0.239377	1	2.041036	4.840635	-3.072957

1	4.986640	6.113537	-0.955489	Sum of electronic and thermal Enthalpies=	-5367.840409
1	2.526821	6.539069	-1.402315	Sum of electronic and thermal Free Energies=	-5368.079442
6	6.964520	0.583892	0.490468	Standard State and RRHO Corrected G=	-5368.052585
6	9.348536	0.216824	-0.072867		
6	8.687306	2.253862	1.185636		
6	9.526683	1.724253	0.032361		
1	9.789778	-0.285631	0.802202		
1	8.671973	3.347972	1.174038		
1	10.580580	1.969380	0.193369		
7	7.307781	1.777542	1.067583		
7	7.928053	-0.116582	-0.190059		
7	2.768364	3.199385	-1.974401		
7	4.872551	4.088726	-1.402363		
1	1.116561	4.412694	-1.630159		
1	2.805243	5.319859	-0.146632		
1	4.541455	5.777088	-2.634355		
1	9.116989	1.941676	2.149243		
1	9.205777	2.195165	-0.903767		
1	9.858780	-0.168691	-0.960542		
15	-2.575281	-2.593738	-1.491216		
6	-4.350936	-2.112652	-1.556481		
6	-4.915492	-1.510545	-0.424389		
6	-5.173747	-2.406716	-2.655108		
6	-6.277778	-1.217614	-0.381134		
1	-4.289226	-1.267561	0.421649		
6	-6.535000	-2.098861	-2.615378		
1	-4.762149	-2.877335	-3.540525		
6	-7.090866	-1.507434	-1.478374		
1	-6.697421	-0.754853	0.507156		
1	-7.160099	-2.325959	-3.474341		
1	-8.151225	-1.272697	-1.449459		
6	-2.188846	-3.099181	-3.232181		
6	-1.774499	-4.406606	-3.535025		
6	-2.281064	-2.155238	-4.269959		
6	-1.455062	-4.762254	-4.847411		
1	-1.693551	-5.154408	-2.754387		
6	-1.969090	-2.520964	-5.580427		
1	-2.577200	-1.136743	-4.037699		
6	-1.552843	-3.821920	-5.874178		
1	-1.133026	-5.777252	-5.062602		
1	-2.047752	-1.781511	-6.372784		
1	-1.306461	-4.100410	-6.895071		
6	-2.638862	-4.235956	-0.643926		
6	-3.792651	-5.034287	-0.718066		
6	-1.520945	-4.721536	0.048921		
6	-3.826940	-6.283406	-0.098278		
1	-4.670876	-4.680378	-1.246617		
6	-1.554630	-5.976100	0.661999		
1	-0.633986	-4.111644	0.140884		
6	-2.709024	-6.757558	0.595100		
1	-4.729969	-6.884647	-0.154008		
1	-0.684109	-6.324372	1.209106		
1	-2.740710	-7.728251	1.081661		
6	6.258965	2.500052	1.777427		
1	5.402980	2.668237	1.123806		
1	5.914828	1.956690	2.665168		
1	6.655778	3.466666	2.093059		
6	7.609054	-1.451314	-0.685914		
1	7.740503	-2.218474	0.089781		
1	6.581347	-1.487890	-1.042655		
1	8.282609	-1.681179	-1.516480		
6	1.958530	2.105789	-2.494106		
1	1.707400	2.289595	-3.548434		
1	2.509760	1.172973	-2.422894		
1	1.028611	2.020992	-1.926675		
6	6.319472	3.932390	-1.352285		
1	6.727547	4.585722	-0.574460		
1	6.571129	2.902049	-1.119087		
1	6.782403	4.207151	-2.311465		
(4-7) _{st-a} [‡] ($\Phi_1 = -20.8^\circ$)					
Number of imaginary frequencies : 1					
Electronic energy : HF=-5369.5030591					
Zero-point correction= 1.563372 (Hartree/Particle)					
Thermal correction to Energy= 1.661706					
Thermal correction to Enthalpy= 1.662650					
Thermal correction to Gibbs Free Energy= 1.423617					
Sum of electronic and zero-point Energies= -5367.939687					
Sum of electronic and thermal Energies= -5367.841353					
Cartesian Coordinates					
8	-3.299241	-3.636959	-2.062329		
3	-3.797006	-2.525442	-0.557717		
8	-4.475192	-0.882396	-1.407578		
6	-4.790219	0.147598	-0.752471		
6	-4.602699	1.519831	-1.076046		
6	-2.587245	1.300296	0.079186		
6	-1.594340	1.204192	-0.906633		
6	-0.966537	-0.007619	-1.338297		
45	0.276394	0.586431	0.293768		
15	0.430415	1.668156	2.590474		
6	-1.283500	2.261718	2.940034		
6	-1.692084	3.532564	2.498247		
6	-3.013619	3.952985	2.651107		
6	-3.959029	3.104185	3.232452		
6	-3.570552	1.828947	3.648339		
6	-2.247032	1.407031	3.500393		
6	-5.324574	2.496449	-0.159517		
6	-6.724202	2.897213	-0.654462		
6	-4.100637	1.993628	-2.372861		
6	-3.575338	1.111464	-3.349128		
6	-3.024566	1.592400	-4.537291		
6	-2.960137	2.963360	-4.799877		
6	-3.464028	3.852263	-3.846121		
6	-4.022047	3.377678	-2.659373		
8	-0.789047	-0.740604	1.647211		
6	-1.551104	-1.759604	1.471601		
6	-1.568339	-2.774665	2.589155		
6	-1.095360	-2.469770	3.871062		
6	-1.156170	-3.420480	4.891798		
6	-1.674480	-4.692278	4.635785		
6	-2.137543	-5.007627	3.353993		
6	-2.092368	-4.052096	2.339080		
8	-2.303272	-1.955114	0.493375		
15	1.594458	-1.341698	-0.006741		
8	0.869325	-2.642041	0.194914		
8	3.012032	-1.355109	0.967634		
6	3.734393	-2.530572	0.950341		
6	4.625085	-2.754552	-0.086293		
6	5.320982	-4.013765	-0.125412		
6	5.137608	-4.949747	0.948883		
6	4.235900	-4.638172	2.003397		
6	3.527520	-3.462535	1.993161		
6	5.836899	-6.187179	0.923711		
6	6.666716	-6.513334	-0.125584		
6	6.819586	-5.610738	-1.205230		
6	6.165522	-4.397465	-1.205571		
6	4.788058	-1.714065	-1.137639		
6	3.678035	-1.226570	-1.830739		
6	3.838362	-0.386521	-2.960402		
6	5.077174	0.072394	-3.326141		
6	6.222230	-0.256215	-2.554032		
6	6.078118	-1.156227	-1.445869		
6	7.231376	-1.417431	-0.650503		
6	8.448275	-0.839198	-0.942301		
6	8.589129	0.027005	-2.053356		
6	7.494150	0.309283	-2.839183		
8	2.394302	-1.576813	-1.524284		
6	0.822048	0.538992	4.004388		
6	1.751271	-0.490393	3.810927		
6	2.160048	-1.282810	4.886461		
6	1.635545	-1.066496	6.161927		
6	0.713775	-0.035132	6.363433		
6	0.320755	0.772844	5.295322		
6	1.541994	3.042527	3.158115		
6	1.130096	4.191073	3.849140		
6	2.064256	5.155042	4.238012		
6	3.421139	4.980320	3.956988		
6	3.845556	3.817652	3.308153		
6	2.913244	2.856503	2.919700		
8	-5.208236	-3.283317	0.564983		
1	9.306821	-1.046697	-0.309472		
1	7.141545	-2.068255	0.211463		
1	7.580800	0.985395	-3.686368		
1	9.554665	0.472839	-2.274787		

1	5.185431	0.725948	-4.187077
1	2.947744	-0.111040	-3.511185
1	6.286827	-3.724528	-2.046134
1	2.795074	-3.229190	2.757178
1	7.454029	-5.879405	-2.045434
1	5.692467	-6.879572	1.749478
1	4.092567	-5.359601	2.803487
1	7.192418	-7.463938	-0.135031
1	-0.985699	4.193989	2.012369
1	-1.972704	0.406408	3.810369
1	-3.301869	4.941649	2.304754
1	-4.297498	1.154188	4.090587
1	-4.988763	3.429271	3.350303
1	2.147327	-0.684555	2.822704
1	-0.378179	1.583604	5.473482
1	2.882662	-2.076640	4.721600
1	0.307028	0.148565	7.354177
1	1.945094	-1.692166	6.994464
1	0.084249	4.348412	4.085118
1	3.255235	1.959773	2.417689
1	1.726697	6.043945	4.764224
1	4.898034	3.658621	3.092918
1	4.142323	5.737384	4.251777
1	-1.430132	2.112915	-1.468413
1	-1.416029	-0.940957	-1.036325
1	-0.470922	-0.031111	-2.301199
1	-0.679144	-1.490867	4.060266
1	-2.459344	-4.282547	1.345274
1	-0.790014	-3.166459	5.882652
1	-2.534937	-5.997453	3.146036
1	-1.715533	-5.435101	5.428131
1	-5.243511	-0.001509	0.243931
1	-3.603375	0.049001	-3.150200
1	-4.393024	4.100936	-1.941900
1	-2.631984	0.884723	-5.263059
1	-3.424498	4.923897	-4.025889
1	-2.522650	3.331637	-5.723334
1	-5.415302	2.038468	0.832390
1	-4.723345	3.399915	-0.001245
1	-7.370069	2.017319	-0.749547
1	-7.204694	3.596092	0.040933
1	-6.679716	3.377420	-1.637241
1	-2.817532	2.270336	0.494144
1	-2.813718	0.441749	0.693177
6	-6.207635	-2.586852	0.869545
6	-7.215203	-0.733532	2.224411
6	-8.597501	-1.985323	0.585564
6	-8.210592	-0.599697	1.081458
1	-7.717010	-1.082354	3.138743
1	-9.156801	-2.535019	1.357896
1	-9.094706	-0.050991	1.418278
6	-2.999763	-3.106347	-3.162585
6	-1.293194	-2.128380	-4.693102
6	-3.696809	-2.132161	-5.343882
6	-2.278191	-2.417104	-5.816927
1	-1.208656	-1.046212	-4.516737
1	-3.852724	-1.054054	-5.201623
1	-2.042354	-1.802387	-6.690909
1	-4.421575	-2.466396	-6.094157
1	-2.197947	-3.469596	-6.111671
1	-0.296365	-2.492430	-4.960629
1	-9.241632	-1.913673	-0.296130
1	-7.754788	-0.040605	0.257465
1	-6.764561	0.239813	2.451645
6	-4.916510	-1.538894	2.661713
1	-4.287494	-2.410004	2.503798
1	-4.349582	-0.643538	2.380869
1	-5.177625	-1.468006	3.723948
6	-7.555354	-3.766925	-0.797266
1	-7.882530	-3.334645	-1.750088
1	-6.605680	-4.276972	-0.941437
1	-8.307753	-4.497460	-0.471620
6	-5.368513	-2.955607	-3.706934
1	-5.967519	-3.213956	-4.585706
1	-5.479415	-3.736662	-2.957811
1	-5.730845	-2.012317	-3.281430
6	-0.648438	-3.148862	-2.509522
1	-0.253625	-4.153355	-2.715917
1	0.169815	-2.434590	-2.602573
1	-1.006474	-3.112440	-1.484541

7	-3.969562	-2.852966	-4.102190
7	-1.704692	-2.795533	-3.456535
7	-6.135145	-1.657227	1.873506
7	-7.395078	-2.722319	0.202430
15	1.432656	2.276692	-0.898328
6	1.558523	2.241882	-2.767285
6	2.772083	2.560642	-3.402484
6	0.452079	1.954580	-3.588103
6	2.878281	2.582921	-4.793846
1	3.659003	2.769131	-2.821514
6	0.562138	1.967655	-4.980004
1	-0.519168	1.735763	-3.172226
6	1.776278	2.277850	-5.592086
1	3.833264	2.830924	-5.248480
1	-0.314724	1.742973	-5.578496
1	1.860494	2.287012	-6.675023
6	0.619211	3.934955	-0.632791
6	-0.417809	4.392531	-1.464863
6	1.012334	4.750352	0.441181
6	-1.065540	5.600634	-1.203578
1	-0.728023	3.829738	-2.335980
6	0.377825	5.969282	0.689205
1	1.822211	4.447377	1.088659
6	-0.674552	6.394007	-0.122986
1	-1.870447	5.920916	-1.858670
1	0.706128	6.574366	1.529200
1	-1.175416	7.337463	0.074775
6	3.189458	2.603443	-0.427353
6	3.789010	3.859384	-0.640115
6	3.980973	1.556088	0.055676
6	5.140182	4.056400	-0.358828
1	3.209001	4.684048	-1.038811
6	5.337352	1.751168	0.327546
1	3.549226	0.585767	0.245959
6	5.920463	3.001399	0.124331
1	5.584303	5.033657	-0.525419
1	5.931890	0.919506	0.691483
1	6.975486	3.153215	0.333960

(4-7)_{st-a}[±] (Φ₁=58.9°)

Number of imaginary frequencies : 1
 Electronic energy : HF=-5369.4762878
 Zero-point correction= 1.562633 (Hartree/Particle)
 Thermal correction to Energy= 1.661520
 Thermal correction to Enthalpy= 1.662464
 Thermal correction to Gibbs Free Energy= 1.419829
 Sum of electronic and zero-point Energies= -5367.913655
 Sum of electronic and thermal Energies= -5367.814768
 Sum of electronic and thermal Enthalpies= -5367.813824
 Sum of electronic and thermal Free Energies= -5368.056458
 Standard State and RRHO Corrected G= -5368.028001

Cartesian Coordinates

8	5.976101	2.924202	1.358546
3	6.374964	1.154105	0.990903
8	5.466960	0.473062	-0.477270
6	5.036217	-0.684808	-0.744215
6	4.187477	-1.100910	-1.802564
6	2.396454	-0.810851	-0.449422
6	1.295563	-1.228817	-1.218826
6	0.440450	-0.331971	-1.932974
45	-0.673784	-0.605031	-0.119507
15	-0.510766	-0.961326	2.420009
6	1.309190	-1.106253	2.687701
6	1.945173	-2.356388	2.580478
6	3.334079	-2.459692	2.672998
6	4.114729	-1.312941	2.844336
6	3.495734	-0.062811	2.908211
6	2.105812	0.041318	2.831369
6	4.097648	-2.613904	-1.966152
6	5.174666	-3.210601	-2.885224
6	3.832698	-0.239542	-2.949874
6	4.126674	1.144188	-2.993442
6	3.731626	1.932623	-4.072165
6	3.018679	1.384660	-5.143158
6	2.710284	0.024346	-5.117026
6	3.111018	-0.771439	-4.042807
8	0.063407	1.225709	0.723521

6	0.587600	2.286391	0.199728	1	5.293107	-1.495427	-0.039460
6	0.066850	3.581817	0.780519	1	4.654742	1.592074	-2.163312
6	-0.150828	3.739779	2.153405	1	2.854400	-1.824420	-4.061641
6	-0.609567	4.959324	2.659450	1	3.978707	2.991304	-4.074223
6	-0.882177	6.020972	1.792366	1	2.153398	-0.425679	-5.935275
6	-0.681669	5.861071	0.416194	1	2.708229	2.006926	-5.977919
6	-0.197414	4.652455	-0.083701	1	4.179418	-3.078439	-0.975253
8	1.462657	2.331079	-0.676901	1	3.108435	-2.900907	-2.337449
15	-2.271572	0.864405	-0.985112	1	6.175098	-3.041062	-2.473893
8	-1.697559	2.117539	-1.583048	1	5.037705	-4.292381	-3.003379
8	-3.403251	1.273905	0.230873	1	5.146725	-2.757448	-3.881354
6	-4.203666	2.360650	-0.047066	1	2.794046	-1.488338	0.291329
6	-5.325144	2.173178	-0.836078	1	2.531144	0.250620	-0.277365
6	-6.097112	3.334181	-1.195731	6	8.415212	-0.556520	0.504017
6	-5.737055	4.612786	-0.646399	6	8.587591	-2.789511	-0.599958
6	-4.602891	4.718666	0.205947	6	9.828567	-0.852958	-1.516584
6	-3.831832	3.617439	0.482193	6	8.904833	-2.009185	-1.865525
6	-6.505919	5.759001	-0.986941	1	9.471946	-3.342264	-0.250975
6	-7.572572	5.668884	-1.853175	1	10.813180	-1.220753	-1.191593
6	-7.906550	4.418402	-2.425999	1	9.376880	-2.665523	-2.601728
6	-7.190049	3.284932	-2.106566	6	5.311381	3.726822	0.642633
6	-5.662127	0.799811	-1.306764	6	3.235008	5.016995	0.214567
6	-4.729428	0.012553	-1.987382	6	4.976870	4.872052	-1.533538
6	-5.126189	-1.194332	-2.620666	6	4.041801	5.817041	-0.794285
6	-6.392443	-1.692773	-2.471681	1	2.549231	4.330553	-0.293645
6	-7.329385	-1.025595	-1.638257	1	4.398902	4.171931	-2.151986
6	-6.959475	0.227386	-1.044161	1	3.365155	6.304668	-1.502120
6	-7.894282	0.837699	-0.158529	1	5.650448	5.425165	-2.194782
6	-9.118130	0.259047	0.104021	1	4.626010	6.594000	-0.287742
6	-9.487826	-0.960723	-0.510973	1	2.639761	5.677939	0.851796
6	-8.604920	-1.586344	-1.363166	1	9.989149	-0.209670	-2.387172
8	-3.421967	0.353923	-2.171862	1	7.980592	-1.615406	-2.302399
6	-1.025915	0.475664	3.467098	1	7.795586	-3.523163	-0.785120
6	-2.159386	1.202545	3.086638	6	7.436950	-2.530365	1.569513
6	-2.666338	2.207265	3.913651	1	7.322218	-1.822210	2.386662
6	-2.038412	2.505476	5.124416	1	6.449710	-2.899164	1.266509
6	-0.905555	1.782834	5.511115	1	8.030256	-3.384060	1.919015
6	-0.409205	0.764158	4.694915	6	9.727040	1.328150	-0.354625
6	-1.256978	-2.256543	3.527634	1	9.490403	1.894053	-1.261991
6	-0.552817	-3.064508	4.431691	1	9.279676	1.820700	0.505483
6	-1.227169	-4.004625	5.216446	1	10.817500	1.316544	-0.228299
6	-2.612988	-4.144905	5.120413	6	7.022907	3.513393	-1.062748
6	-3.328814	-3.313669	4.254243	1	7.427326	4.134235	-1.865410
6	-2.655707	-2.374902	3.474134	1	7.760743	3.456137	-0.262903
8	7.934342	0.178751	1.413205	1	6.843756	2.503541	-1.453324
1	-9.803113	0.743053	0.794851	6	3.499705	3.629016	2.251994
1	-7.627403	1.766249	0.332451	1	2.844719	4.364586	2.725535
1	-8.864531	-2.533043	-1.830825	1	2.894756	2.762928	1.960603
1	-10.457328	-1.403399	-0.300728	1	4.259879	3.313109	2.964758
1	-6.679661	-2.620570	-2.959824	7	5.797983	4.131895	-0.569521
1	-4.383857	-1.705222	-3.219597	7	4.129021	4.239329	1.085884
1	-7.453783	2.338538	-2.563727	7	8.119234	-1.888785	0.455826
1	-2.934607	3.679229	1.088101	7	9.224176	-0.034238	-0.464269
1	-8.732104	4.351890	-3.129377	15	-1.619364	-2.675950	-0.638764
1	-6.224527	6.716532	-0.555371	6	-1.876034	-3.194886	-2.412409
1	-4.333119	5.691637	0.607870	6	-3.077675	-3.789719	-2.832886
1	-8.148774	6.553695	-2.108747	6	-0.850233	-3.047460	-3.364465
1	1.361246	-3.252553	2.404426	6	-3.249341	-4.212791	-4.152803
1	1.641280	1.018847	2.862465	1	-3.900824	-3.913144	-2.141940
1	3.802841	-3.437336	2.599361	6	-1.022491	-3.470219	-4.683221
1	4.093440	0.837430	3.015514	1	0.101796	-2.615163	-3.093629
1	5.193604	-1.390313	2.918638	6	-2.224870	-4.052498	-5.085791
1	-2.626019	1.009442	2.130331	1	-4.193225	-4.662964	-4.447390
1	0.456885	0.196609	5.020583	1	-0.210328	-3.340111	-5.392871
1	-3.538186	2.771473	3.594018	1	-2.360869	-4.377910	-6.113135
1	-0.412330	2.003686	6.453990	6	-0.565901	-4.075681	0.003117
1	-2.425418	3.295090	5.762745	6	0.479531	-4.624333	-0.760129
1	0.522030	-2.973637	4.532876	6	-0.759927	-4.565637	1.304749
1	-3.224310	-1.733967	2.812180	6	1.326568	-5.595317	-0.223837
1	-0.662721	-4.627229	5.905568	1	0.636627	-4.317284	-1.786216
1	-4.409057	-3.396835	4.176801	6	0.078446	-5.547986	1.836113
1	-3.131412	-4.884998	5.723512	1	-1.570110	-4.191059	1.913608
1	1.216227	-2.295699	-1.385890	6	1.134894	-6.057545	1.080042
1	0.725629	0.714093	-1.957839	1	2.130051	-5.996587	-0.835171
1	-0.093165	-0.669367	-2.813943	1	-0.097191	-5.901574	2.847704
1	0.033092	2.907150	2.821545	1	1.792487	-6.815830	1.495508
1	-0.034089	4.514224	-1.146242	6	-3.265299	-3.022423	0.124891
1	-0.767170	5.071552	3.728581	6	-3.735451	-4.339678	0.283500
1	-0.904429	6.678099	-0.264984	6	-4.097320	-1.962860	0.504969
1	-1.251724	6.965062	2.184053	6	-5.003195	-4.581116	0.811383

1	-3.115045	-5.180219	-0.009042	6	-0.117664	2.208174	1.893618
6	-5.370848	-2.204409	1.025768	6	-0.764556	2.969599	2.876681
1	-3.754880	-0.942227	0.419409	6	-0.407535	4.305322	3.094641
6	-5.826848	-3.512882	1.181278	6	0.605372	4.896929	2.341190
1	-5.348585	-5.604221	0.929512	6	1.262636	4.142955	1.365143
1	-6.000894	-1.365058	1.302267	6	0.902471	2.816364	1.143414
1	-6.818212	-3.701278	1.583454	8	-0.045603	2.660040	-3.097661
				6	4.241328	-0.004008	-2.913490
(4-7) _{st-a*} ($\Phi_1=174.6^\circ$)				8	5.056765	-0.399100	-2.021333
				6	2.828027	1.462846	-4.345581
Number of imaginary frequencies : 1				6	3.604813	2.140040	-5.485847
Electronic energy : HF=-5369.4906473				3	5.365715	-0.762051	-0.272900
Zero-point correction= 1.563647 (Hartree/Particle)				1	-8.444459	-1.085688	3.870864
Thermal correction to Energy= 1.661897				1	-7.263463	0.276393	2.207551
Thermal correction to Enthalpy= 1.662841				1	-7.566792	-4.650808	1.627093
Thermal correction to Gibbs Free Energy= 1.423529				1	-8.631727	-3.558674	3.582916
Sum of electronic and zero-point Energies= -5367.927001				1	-6.220628	-4.510180	-0.431928
Sum of electronic and thermal Energies= -5367.828751				1	-4.759177	-3.170270	-1.918988
Sum of electronic and thermal Enthalpies= -5367.827807				1	-8.583255	-0.251188	-0.442358
Sum of electronic and thermal Free Energies= -5368.067118				1	-4.073650	3.620247	-0.058095
Standard State and RRHO Corrected G= -5368.040437				1	-10.717175	0.930443	-0.620978
				1	-8.703647	4.712401	-0.243993
Cartesian Coordinates				1	-6.266043	4.798747	-0.092386
				1	-10.806529	3.421780	-0.487828
6	4.912806	4.811836	-0.958822	1	1.696157	-1.365614	0.523315
6	5.767166	3.708962	-1.050479	1	0.991695	0.850014	4.136151
6	5.369475	2.553474	-1.722608	1	3.837137	-2.203163	1.453247
6	4.104512	2.465539	-2.344610	1	3.129234	0.034206	5.058032
6	3.255328	3.592627	-2.243960	1	4.558073	-1.508215	3.723066
6	3.651317	4.741558	-1.559119	1	-1.541485	2.533234	3.492344
6	3.667301	1.266883	-3.092717	1	1.418138	2.250757	0.378778
6	1.961069	0.566579	-1.591382	1	-0.924026	4.875920	3.861939
6	1.196991	-0.521435	-2.018028	1	2.053349	4.585477	0.767183
6	0.044720	-0.419049	-2.874773	1	0.878392	5.935247	2.507468
45	-0.867692	-0.172253	-0.955552	1	-3.136384	1.294264	2.158087
8	-0.730324	1.961672	-1.048924	1	-0.389958	-1.524990	3.903231
6	-0.564585	2.836563	-1.981344	1	-4.778323	0.787354	3.922146
6	-1.004368	4.234262	-1.595805	1	-2.040839	-2.051399	5.643708
6	-1.652892	4.484530	-0.380728	1	-4.238483	-0.883521	5.691384
6	-2.047097	5.779769	-0.042718	1	1.593812	-1.506756	-1.797982
6	-1.788422	6.841155	-0.915231	1	-0.124906	0.518283	-3.394555
6	-1.133938	6.599485	-2.127399	1	-0.216875	-1.312101	-3.435547
6	-0.746423	5.301989	-2.465398	1	-1.825387	3.655528	0.293414
15	-3.066336	0.454652	-1.461084	1	-0.243713	5.093960	-3.404251
8	-3.209981	1.444101	-2.580793	1	-2.547409	5.960918	0.904891
15	-0.429283	0.399783	1.572605	1	-0.929031	7.421366	-2.808534
6	-1.621452	-0.042685	2.918219	1	-2.092379	7.850952	-0.651883
6	-2.882048	0.582759	2.933101	1	3.879343	-0.768186	-3.625918
6	-3.812772	0.289537	3.929178	1	6.042272	1.707782	-1.779369
6	-3.511409	-0.650608	4.918538	1	2.265894	3.564165	-2.690239
6	-2.278329	-1.303271	4.892444	1	6.753820	3.746074	-0.595587
6	-1.340279	-1.003132	3.901553	1	2.967702	5.584824	-1.498864
8	-4.329121	-0.669899	-1.806978	1	5.224460	5.710205	-0.433055
6	-5.188923	-1.296168	-0.954263	1	2.471207	0.481774	-4.683327
6	-5.987626	-0.610793	-0.038045	1	1.926483	2.038885	-4.123237
6	-6.722664	-1.387804	0.926487	1	4.484043	1.549373	-5.770310
6	-6.804223	-2.812504	0.786937	1	2.974674	2.262357	-6.374927
6	-6.129194	-3.435842	-0.296305	1	3.955857	3.133630	-5.185398
6	-5.318662	-2.701871	-1.120800	1	2.709140	0.436358	-0.818604
6	-7.515107	-3.572177	1.753695	1	1.595620	1.565208	-1.763657
6	-8.102354	-2.965797	2.842384	8	5.968766	0.387926	1.007821
6	-8.000382	-1.562834	3.001493	8	5.811519	-2.539041	0.145478
6	-7.338344	-0.795847	2.066147	6	6.380834	1.447409	1.538071
6	-6.097239	0.872058	-0.077236	6	5.919064	3.662944	2.564482
6	-7.373680	1.534124	-0.196678	6	8.253492	2.987024	2.038245
6	-7.427425	2.969343	-0.177733	6	7.346171	3.610418	3.089590
6	-6.218909	3.712932	-0.098463	1	5.825284	4.409372	1.763685
6	-5.006738	3.071440	-0.068809	1	8.339444	3.646380	1.161349
6	-4.956492	1.658716	-0.064095	1	7.689814	4.619830	3.332900
6	-8.685056	3.625616	-0.271375	6	6.984655	-2.994443	0.138296
6	-9.851976	2.908840	-0.411431	6	9.020526	-3.663246	1.389884
6	-9.800566	1.496261	-0.478466	6	8.776655	-4.259409	-1.015050
6	-8.598616	0.829557	-0.374274	6	9.725288	-3.710067	0.041461
8	-3.713944	1.057675	-0.009880	1	9.638017	-3.142912	2.128189
6	1.177475	-0.223428	2.266908	1	9.220434	-4.173200	-2.011076
6	2.000443	-1.070726	1.518498	1	10.043136	-2.700129	-0.241340
6	3.210992	-1.540453	2.042053	1	8.573919	-5.326165	-0.836202
6	3.616796	-1.149495	3.317777	1	10.616732	-4.340354	0.107217
6	2.813781	-0.283966	4.068126	1	8.840972	-4.680635	1.768799
6	1.606821	0.177047	3.546484	1	7.383244	3.009023	4.004790

1	5.225581	3.951115	3.361244	6	2.008299	0.496812	-1.115216
1	9.261452	2.839718	2.437424	6	1.095580	-0.553669	-1.342799
6	4.084282	2.212006	1.752569	6	-0.073260	-0.473681	-2.172422
1	3.835281	2.739560	0.825525	45	-0.873233	0.159496	-0.293573
1	3.821349	1.162606	1.650999	8	-0.522880	2.238935	-0.770183
1	3.500797	2.643084	2.567788	6	-0.216987	2.880248	-1.852174
6	8.634481	0.780020	0.937335	6	-0.257378	4.394106	-1.730954
1	8.289775	-0.250423	1.020867	6	-0.757025	5.042805	-0.596222
1	8.716105	1.035377	-0.128754	6	-0.742886	6.436792	-0.510525
1	9.626492	0.859408	1.389145	6	-0.227153	7.199449	-1.561032
6	6.654939	-3.632339	-2.180239	6	0.264274	6.559706	-2.704253
1	5.987237	-2.773069	-2.251055	6	0.244722	5.167435	-2.788778
1	7.282802	-3.669037	-3.074188	15	-2.942338	0.603970	-1.317268
1	6.053748	-4.551284	-2.139510	8	-2.925047	1.670026	-2.373393
6	7.115359	-2.494083	2.507315	15	-0.495232	1.316886	1.924897
1	7.896036	-2.175308	3.202379	6	-0.830189	0.706364	3.646320
1	6.459169	-1.650283	2.301954	6	0.093166	0.708989	4.701100
1	6.535395	-3.298862	2.979817	6	-0.273348	0.232573	5.962715
7	7.752594	-2.938354	1.270276	6	-1.566904	-0.241419	6.192329
7	7.522414	-3.501192	-1.011218	6	-2.506807	-0.205617	5.158318
7	5.504020	2.351514	2.061897	6	-2.141007	0.273426	3.901372
7	7.727249	1.678944	1.642609	8	-3.784160	-0.699795	-2.087197
15	-1.238935	-2.465173	-0.855752	6	-4.737030	-1.497083	-1.525173
6	-2.150652	-3.209418	-2.296564	6	-5.941180	-1.004477	-1.017146
6	-2.567151	-2.445942	-3.393688	6	-6.808735	-1.918310	-0.321665
6	-2.431806	-4.587398	-2.291682	6	-6.509238	-3.321665	-0.310733
6	-3.258287	-3.038666	-4.453771	6	-5.346721	-3.781880	-0.982910
1	-2.376877	-1.382744	-3.423922	6	-4.477450	-2.889985	-1.555186
6	-3.126423	-5.178216	-3.345615	6	-7.357061	-4.216280	0.396231
1	-2.118141	-5.208004	-1.460518	6	-8.450007	-3.755909	1.095904
6	-3.544997	-4.403080	-4.431719	6	-8.735497	-2.369281	1.113143
1	-3.579787	-2.423230	-5.288983	6	-7.942642	-1.478687	0.421403
1	-3.341131	-6.242777	-3.317430	6	-6.286673	0.436032	-1.158694
1	-4.089624	-4.861612	-5.252283	6	-7.505440	0.885101	-1.779123
6	0.297755	-3.496427	-0.882534	6	-7.790586	2.292166	-1.830505
6	0.985473	-3.801796	0.302028	6	-6.842964	3.217802	-1.313633
6	0.849495	-3.907492	-2.108263	6	-5.652306	2.779193	-0.790519
6	2.194847	-4.497648	0.263610	6	-5.386306	1.392532	-0.716829
1	0.580709	-3.496236	1.260290	6	-9.002258	2.738122	-2.425386
6	2.064713	-4.592858	-2.145926	6	-9.894436	1.845452	-2.975967
1	0.335157	-3.688201	-3.037965	6	-9.598778	0.461210	-2.963246
6	2.741049	-4.890547	-0.960171	6	-8.438877	-0.004864	-2.382610
1	2.711173	-4.724604	1.191674	8	-4.183484	0.987142	-0.180445
1	2.479798	-4.895903	-3.102860	6	1.309741	1.687971	1.900391
1	3.685600	-5.426007	-0.989074	6	2.217846	0.694087	2.306246
6	-2.165948	-3.117495	0.600599	6	3.591674	0.885261	2.166857
6	-2.031313	-4.445840	1.047292	6	4.083509	2.065168	1.604150
6	-3.103483	-2.288639	1.229043	6	3.189769	3.044790	1.169654
6	-2.826392	-4.928286	2.086219	6	1.812638	2.860510	1.313868
1	-1.303671	-5.109334	0.594118	6	-1.331265	2.947561	2.171161
6	-3.903220	-2.776627	2.263442	6	-2.646425	3.104480	1.714865
1	-3.218108	-1.260707	0.915295	6	-3.352603	4.278422	1.989942
6	-3.769328	-4.094896	2.693594	6	-2.750277	5.311048	2.711291
1	-2.708413	-5.956304	2.417626	6	-1.441999	5.155227	3.178663
1	-4.626791	-2.119690	2.728212	6	-0.741439	3.975432	2.923845
1	-4.396745	-4.471014	3.496755	8	0.158511	2.400683	-2.934147
-----				6	4.200594	-0.465762	-2.114480
(4-7) _{SR-a³} (Φ ₁ =167.5°)				8	4.981029	-0.612773	-1.127340
-----				6	2.879239	0.619968	-3.924944
Number of imaginary frequencies : 1				6	3.733422	0.885627	-5.173555
Electronic energy : HF=-5369.4806295				3	5.348185	-1.707244	0.289483
Zero-point correction= 1.564107 (Hartree/Particle)				1	-9.585286	-2.001848	1.681970
Thermal correction to Energy= 1.662578				1	-8.171197	-0.419948	0.458039
Thermal correction to Enthalpy= 1.663523				1	-7.113082	-5.275898	0.386134
Thermal correction to Gibbs Free Energy= 1.422725				1	-9.085534	-4.447765	1.641373
Sum of electronic and zero-point Energies= -5367.916522				1	-5.131017	-4.846548	-1.004168
Sum of electronic and thermal Energies= -5367.818051				1	-3.564309	-3.218960	-2.035092
Sum of electronic and thermal Enthalpies= -5367.817107				1	-8.225018	-1.067047	-2.392837
Sum of electronic and thermal Free Energies= -5368.057904				1	-4.893556	3.468078	-0.437294
Standard State and RRHO Corrected G= -5368.030502				1	-10.290020	-0.240893	-3.421396
-----				1	-9.205033	3.806147	-2.447231
Cartesian Coordinates				1	-7.062468	4.280901	-1.366961
-----				1	-10.814785	2.199363	-3.431878
6	5.152352	4.653981	-1.561618	1	1.857044	-0.243209	2.709544
6	5.922970	3.516110	-1.303070	1	1.133637	3.618593	0.942532
6	5.450409	2.245197	-1.630876	1	4.273864	0.101194	2.475622
6	4.191777	2.070643	-2.244365	1	3.562066	3.946027	0.693338
6	3.428534	3.230980	-2.499300	1	5.150967	2.199146	1.475056
6	3.898065	4.499369	-2.158818	1	-3.114618	2.322047	1.130991
6	3.667869	0.735709	-2.629784	1	0.266410	3.862322	3.309766

1	-4.371655	4.386491	1.629729
1	-0.967506	5.949262	3.748820
1	-3.296086	6.228510	2.913261
1	1.103440	1.070083	4.547792
1	-2.878996	0.300743	3.109299
1	0.457750	0.232237	6.766863
1	-3.521213	-0.557387	5.322160
1	-1.843928	-0.623055	7.171052
1	1.418989	-1.518636	-0.971799
1	-0.165332	0.384849	-2.826738
1	-0.513450	-1.390758	-2.551151
1	-1.155652	4.447724	0.210867
1	0.614644	4.658040	-3.671849
1	-1.136163	6.921950	0.378639
1	0.659272	7.146383	-3.529635
1	-0.212150	8.284190	-1.493833
1	3.818640	-1.378790	-2.603739
1	6.050390	1.375554	-1.401002
1	2.442382	3.137852	-2.940924
1	6.902633	3.616513	-0.842410
1	3.272284	5.366313	-2.354496
1	5.521132	5.642089	-1.299631
1	2.455172	-0.390197	-3.983189
1	2.020827	1.296518	-3.909990
1	4.570139	0.178804	-5.235924
1	3.136952	0.788635	-6.088377
1	4.154418	1.896835	-5.153554
1	2.714979	0.405630	-0.302293
1	1.729020	1.498258	-1.392051
8	6.668645	-1.118984	1.456335
8	5.275574	-3.530874	-0.194424
6	7.226595	-0.002357	1.638624
6	7.776522	1.908777	3.150935
6	8.777883	1.770761	0.883895
6	8.099495	2.689903	1.887057
1	7.111496	2.486610	3.801679
1	8.925735	2.283959	-0.070355
1	7.182243	3.093355	1.447054
6	5.628744	-3.785619	-1.379874
6	7.418418	-4.291001	-3.024734
6	5.033413	-4.437681	-3.702654
6	6.407816	-3.920432	-4.099493
1	8.384119	-3.817151	-3.225474
1	4.269679	-4.063992	-4.390775
1	6.370962	-2.830893	-4.211367
6	6.507736	-0.032546	3.979903
1	7.269882	-0.213303	4.749299
1	5.717760	0.589507	4.413670
1	6.084690	-0.985440	3.669786
6	8.251136	-0.177789	-0.565281
1	7.393627	-0.768277	-0.879040
1	8.495346	0.520121	-1.369649
1	9.111866	-0.840594	-0.404320
6	3.284414	-3.988952	-1.977380
1	2.967258	-4.973041	-1.608475
1	3.103574	-3.249448	-1.200976
1	2.683029	-3.734013	-2.852749
6	7.949724	-3.823578	-0.641780
1	8.890852	-3.439800	-1.043502
1	7.630073	-3.178432	0.174842
1	8.126139	-4.835500	-0.251016
1	9.768659	1.460096	1.248678
1	8.754179	3.531471	2.130452
1	8.692858	1.698818	3.721813
1	5.004785	-5.536511	-3.741577
1	6.707639	-4.350868	-5.059090
1	7.582843	-5.378883	-3.005663
7	7.937368	0.595491	0.633777
7	7.103196	0.645469	2.834995
7	4.692425	-3.971210	-2.355753
7	6.955830	-3.830139	-1.712163
15	-1.124988	-2.023302	0.632302
6	-1.192689	-3.539418	-0.470881
6	-2.124161	-4.565496	-0.233586
6	-0.287370	-3.722110	-1.532202
6	-2.147100	-5.719943	-1.018104
1	-2.862911	-4.467187	0.548692
6	-0.311287	-4.874951	-2.319329
1	0.461636	-2.980042	-1.759016
6	-1.243043	-5.881810	-2.067718

1	-2.883820	-6.489766	-0.806254
1	0.405991	-4.978790	-3.128359
1	-1.264048	-6.778543	-2.680288
6	-2.554483	-2.330355	1.764255
6	-2.541450	-3.391974	2.690132
6	-3.708802	-1.549177	1.659666
6	-3.652180	-3.648437	3.492084
1	-1.668786	-4.029290	2.780916
6	-4.824528	-1.809659	2.459930
1	-3.747560	-0.719012	0.971541
6	-4.800163	-2.857713	3.378458
1	-3.621957	-4.471028	4.200987
1	-5.711160	-1.193542	2.352669
1	-5.669461	-3.063601	3.996497
6	0.330120	-2.466431	1.720457
6	1.501969	-3.011941	1.172155
6	0.301124	-2.240638	3.106716
6	2.620876	-3.280788	1.961597
1	1.549280	-3.263675	0.123341
6	1.413781	-2.522528	3.903976
1	-0.586888	-1.848219	3.580259
6	2.583523	-3.028609	3.335619
1	3.507271	-3.698299	1.492790
1	1.358178	-2.330115	4.971206
1	3.449951	-3.240886	3.955892

(4-7)_{si-a*} ($\Phi_1 = -42.8^\circ$)

Number of imaginary frequencies : 1

Electronic energy : HF=-5369.5100977

Zero-point correction= 1.561417 (Hartree/Particle)

Thermal correction to Energy= 1.660062

Thermal correction to Enthalpy= 1.661006

Thermal correction to Gibbs Free Energy= 1.420604

Sum of electronic and zero-point Energies= -5367.948681

Sum of electronic and thermal Energies= -5367.850036

Sum of electronic and thermal Enthalpies= -5367.849092

Sum of electronic and thermal Free Energies= -5368.089494

Standard State and RRHO Corrected G= -5368.062245

Cartesian Coordinates

6	-0.605847	4.292787	2.154631
6	0.741702	4.002455	1.871760
6	1.566572	5.039691	1.407863
6	1.063751	6.335909	1.260960
6	-0.267772	6.617418	1.569845
6	-1.103344	5.587455	2.015128
15	1.286334	2.240648	1.899689
6	3.104734	2.294386	2.280309
6	3.689921	3.315326	3.045594
6	5.043032	3.259224	3.383999
6	5.822915	2.167952	2.991689
6	5.237742	1.126349	2.268779
6	3.888623	1.190743	1.914575
45	0.145942	1.066818	-0.062875
15	1.363876	-0.800325	-0.593812
8	0.679252	-1.925091	-1.312405
6	-2.145413	1.721708	-0.540913
6	-1.579159	0.563560	-1.187175
6	-2.761359	1.792859	0.709011
8	-0.681618	-0.109254	1.539806
6	-1.353691	-1.196622	1.625330
6	-1.866744	-1.512103	3.010366
6	-2.240783	-0.493661	3.895373
6	-2.784409	-0.810596	5.140923
6	-2.916286	-2.147456	5.528616
6	-2.514482	-3.167628	4.660273
6	-2.011627	-2.850841	3.397622
8	-1.632516	-1.988000	0.702085
8	2.027110	-1.359062	0.876958
6	2.462053	-2.667960	0.816938
6	3.661894	-2.954500	0.187306
6	3.988205	-4.341677	-0.027677
6	3.146101	-5.359551	0.537911
6	1.987286	-4.984072	1.271585
6	1.633922	-3.662688	1.382197
6	3.467353	-6.728323	0.327846
6	4.556640	-7.094412	-0.430536
6	5.368591	-6.095343	-1.018844

6	5.094517	-4.759162	-0.820588
6	4.562199	-1.849010	-0.250643
6	4.127345	-0.802299	-1.066501
6	5.057114	0.111065	-1.638511
6	6.385076	0.069012	-1.310827
6	6.856546	-0.866533	-0.351173
6	5.937193	-1.823393	0.194514
6	6.422606	-2.690649	1.215311
6	7.731450	-2.632598	1.645827
6	8.640375	-1.710392	1.076300
6	8.203420	-0.844293	0.098431
8	2.838172	-0.584527	-1.449590
6	0.803692	1.593979	3.570202
6	0.322252	2.380674	4.623853
6	0.127275	1.820721	5.891849
6	0.428253	0.478456	6.122885
6	0.916294	-0.309527	5.075580
6	1.094263	0.238789	3.807973
3	-3.220008	-2.448669	-0.319543
8	-4.315985	-0.834415	-0.507266
6	-4.620312	-0.100390	0.469436
6	-5.048831	1.255734	0.469955
6	-5.361171	2.004697	-0.753661
6	-4.977938	1.542506	-2.039376
6	-5.222118	2.298762	-3.184737
6	-5.852602	3.543544	-3.105250
6	-6.236901	4.020665	-1.848585
6	-5.995712	3.269962	-0.698859
6	-5.532690	1.768817	1.816604
6	-7.026524	1.511514	2.077007
8	-4.541251	-3.630972	0.551755
8	-2.685758	-3.131121	-2.015460
1	8.064801	-3.298590	2.436943
1	5.742732	-3.395392	1.678614
1	8.881015	-0.113736	-0.336749
1	9.670333	-1.678951	1.419858
1	7.083933	0.771723	-1.756687
1	4.671243	0.839683	-2.342448
1	5.721313	-4.009220	-1.288611
1	0.721125	-3.347492	1.875278
1	6.213523	-6.384210	-1.637842
1	2.822776	-7.483891	0.770355
1	1.362313	-5.760427	1.704468
1	4.787400	-8.143949	-0.589522
1	2.597922	4.843475	1.140506
1	-1.273306	3.498869	2.472950
1	1.718353	7.120705	0.892717
1	-2.146124	5.789203	2.243530
1	-0.655952	7.625349	1.454564
1	0.113683	3.434723	4.476395
1	1.449222	-0.383302	2.993456
1	-0.248098	2.443925	6.699289
1	1.137195	-1.360478	5.240765
1	0.278622	0.045898	7.108166
1	3.095629	4.156594	3.385994
1	3.446871	0.373605	1.357513
1	5.483921	4.064879	3.964918
1	5.826251	0.263463	1.975622
1	6.875351	2.123760	3.258017
1	-2.250150	2.610903	-1.147688
1	-1.833037	-0.430025	-0.849997
1	-1.494267	0.638946	-2.269351
1	-2.087775	0.540909	3.609593
1	-1.736740	-3.632086	2.696163
1	-3.084079	-0.014620	5.816761
1	-2.610161	-4.207604	4.959968
1	-3.325039	-2.393460	6.504893
1	-4.498705	-0.524207	1.485013
1	-4.487220	0.582752	-2.115946
1	-6.307444	3.678709	0.256317
1	-4.909964	1.909482	-4.151200
1	-6.728865	4.986574	-1.760086
1	-6.040835	4.129085	-4.001133
1	-4.950998	1.277312	2.607108
1	-5.322302	2.840263	1.921584
1	-7.232016	0.435880	2.072464
1	-7.339717	1.913102	3.048596
1	-7.652739	1.969261	1.304155
1	-3.091445	2.764280	1.060635
1	-2.606851	1.045347	1.468275

6	-1.638419	-3.539891	-2.572628
6	0.555056	-4.739954	-2.387181
6	-0.257230	-3.821635	-4.561311
6	0.955293	-3.980378	-3.650605
1	1.203882	-4.436456	-1.560204
1	-0.008283	-3.244018	-5.455078
1	1.309153	-2.986660	-3.369071
6	-5.749125	-3.286676	0.531815
6	-7.778922	-2.487856	1.719387
6	-7.918713	-3.049265	-0.688688
6	-8.282348	-2.013631	0.364821
1	-8.320417	-3.391306	2.040980
1	-8.539603	-3.951024	-0.574065
1	-9.366434	-1.868981	0.388621
1	-0.627058	-4.803021	-4.899270
1	1.761460	-4.514012	-4.164121
1	0.665215	-5.823647	-2.530094
1	-8.105078	-2.653902	-1.693119
1	-7.814266	-1.053767	0.120319
1	-7.942328	-1.722704	2.484320
7	-6.502915	-3.408733	-0.603270
7	-6.343115	-2.748318	1.646255
7	-0.840004	-4.484139	-1.995176
7	-1.292785	-3.104698	-3.823937
6	-2.167295	-2.182410	-4.526976
1	-2.912323	-2.703261	-5.146826
1	-2.695206	-1.562504	-3.802530
1	-1.566082	-1.538433	-5.176010
6	-1.190485	-4.941884	-0.656709
1	-0.875451	-4.218420	0.100807
1	-2.269530	-5.085149	-0.577335
1	-0.691802	-5.899377	-0.477873
6	-5.937097	-4.025210	-1.793936
1	-6.455746	-4.967153	-2.021014
1	-6.052861	-3.352830	-2.652195
1	-4.876931	-4.216996	-1.648244
6	-5.605386	-2.706069	2.898899
1	-5.904531	-3.524098	3.570012
1	-4.541925	-2.791418	2.697479
1	-5.798462	-1.755986	3.407449
15	0.923096	2.386470	-1.807945
6	2.377386	3.463599	-1.465477
6	2.467163	4.807724	-1.862641
6	3.470547	2.872647	-0.823535
6	3.622467	5.542907	-1.591698
1	1.642425	5.286934	-2.376936
6	4.626676	3.604919	-0.554733
1	3.411987	1.836541	-0.525533
6	4.701691	4.946858	-0.931891
1	3.676880	6.584447	-1.895730
1	5.452567	3.124506	-0.039392
1	5.595335	5.525652	-0.716003
6	-0.372688	3.567672	-2.370412
6	-1.098292	3.353808	-3.550043
6	-0.738728	4.627886	-1.523237
6	-2.180129	4.179818	-3.868809
1	-0.836912	2.536959	-4.214162
6	-1.809864	5.455821	-1.850784
1	-0.198909	4.793649	-0.599700
6	-2.540734	5.227907	-3.021397
1	-2.745544	3.994283	-4.777117
1	-2.080589	6.268081	-1.182488
1	-3.390731	5.857758	-3.265846
6	1.419130	1.560848	-3.388990
6	2.282656	2.223212	-4.278004
6	0.903253	0.307742	-3.750759
6	2.630799	1.640864	-5.497373
1	2.692369	3.194587	-4.022920
6	1.253020	-0.268854	-4.973422
1	0.263884	-0.248791	-3.077609
6	2.115910	0.391320	-5.849054
1	3.305729	2.164455	-6.168683
1	0.855971	-1.244272	-5.231748
1	2.389232	-0.065904	-6.795983

$$(4-7)_{st-a^*} (\Phi_1 = -44.4^\circ)$$

Number of imaginary frequencies : 1
Electronic energy : HF=-5369.5099114
Zero-point correction= 1.561886 (Hartree/Particle)

Thermal correction to Energy= 1.660285
 Thermal correction to Enthalpy= 1.661230
 Thermal correction to Gibbs Free Energy= 1.422326
 Sum of electronic and zero-point Energies= -5367.948026
 Sum of electronic and thermal Energies= -5367.849626
 Sum of electronic and thermal Enthalpies= -5367.848682
 Sum of electronic and thermal Free Energies= -5368.087585
 Standard State and RRHO Corrected G= -5368.061

.....
 Cartesian Coordinates

.....
 8 2.474652 2.438500 -3.014170
 3 3.219166 2.250070 -1.283733
 8 4.301684 0.633162 -1.202928
 6 4.695221 0.057351 -0.156609
 6 5.126539 -1.287577 0.015907
 6 2.892248 -1.775610 0.507617
 6 2.157779 -1.862576 -0.677467
 6 1.520330 -0.799825 -1.411984
 45 -0.056748 -1.120789 -0.032271
 8 0.951460 0.288818 1.252081
 6 1.640000 1.363222 1.151748
 8 1.854726 2.044230 0.128723
 15 -0.938518 -1.940813 2.219720
 6 -0.272659 -1.030451 3.693956
 6 -0.540341 0.349263 3.735798
 6 -0.231232 1.094799 4.870776
 6 0.369358 0.481906 5.974870
 6 0.648107 -0.884308 5.936603
 6 0.320535 -1.641038 4.805917
 6 -0.390686 -3.689309 2.431439
 6 0.981705 -3.947145 2.606237
 6 1.466920 -5.253706 2.631457
 6 0.591632 -6.332011 2.462991
 6 -0.767984 -6.087675 2.264940
 6 -1.257503 -4.778275 2.247468
 6 -2.699389 -1.900453 2.814753
 6 -3.185604 -2.769751 3.803825
 6 -4.486377 -2.631714 4.290996
 6 -5.308272 -1.603252 3.822607
 6 -4.816927 -0.706363 2.871732
 6 -3.522508 -0.855837 2.369406
 15 -1.312888 0.664429 -0.739904
 8 -2.873371 0.382534 -1.407256
 6 -4.108521 0.624985 -0.887087
 6 -4.467405 1.785046 -0.197628
 6 -5.771451 1.822172 0.420991
 6 -6.721409 0.777622 0.164733
 6 -6.347351 -0.299551 -0.682810
 6 -5.072384 -0.380935 -1.174703
 6 -6.149370 2.843818 1.339146
 6 -7.389114 2.844207 1.942917
 6 -8.332150 1.828318 1.659321
 6 -7.997246 0.815895 0.787449
 6 -3.542550 2.947839 -0.072660
 6 -2.263856 2.764439 0.426694
 6 -1.373518 3.833488 0.670510
 6 -1.755721 5.117441 0.373842
 6 -3.017279 5.370940 -0.231744
 6 -3.918356 4.278723 -0.477770
 6 -3.387955 6.684975 -0.627616
 6 -4.583974 6.924101 -1.266470
 6 -5.458209 5.846020 -1.543658
 6 -5.136078 4.562351 -1.158587
 8 -1.811757 1.483036 0.672138
 8 -0.680824 1.629118 -1.700225
 6 5.342385 -2.219337 -1.099915
 6 4.852317 -1.959537 -2.405725
 6 4.999620 -2.889536 -3.434110
 6 5.635394 -4.114187 -3.212266
 6 6.125864 -4.392116 -1.933056
 6 5.982808 -3.466603 -0.900160
 6 5.729048 -1.586810 1.379777
 6 7.237353 -1.298872 1.469135
 6 2.251707 1.818121 2.458745
 6 2.853045 0.906339 3.335425
 6 3.446116 1.351383 4.517437
 6 3.398844 2.706654 4.858490
 6 2.772603 3.616023 4.000817
 6 2.225125 3.176053 2.794600

8 4.467885 3.753170 -0.941968
 1 -7.640442 3.630157 2.649754
 1 -5.438659 3.624081 1.584059
 1 -8.701000 0.015409 0.572604
 1 -9.307287 1.842928 2.137608
 1 -7.074548 -1.074581 -0.909755
 1 -4.757659 -1.211090 -1.797045
 1 -5.813199 3.748582 -1.389788
 1 -0.393077 3.596955 1.067988
 1 -6.390393 6.030998 -2.070292
 1 -2.696924 7.499711 -0.425550
 1 -1.082544 5.950313 0.558530
 1 -4.852799 7.932055 -1.569488
 1 -2.313654 -4.614983 2.070691
 1 1.677161 -3.120985 2.710536
 1 -1.456565 -6.913770 2.111878
 1 2.529853 -5.428893 2.772208
 1 0.969442 -7.350329 2.475744
 1 -0.982306 0.835113 2.872412
 1 0.515155 -2.707963 4.812294
 1 -0.436212 2.161528 4.883752
 1 1.110824 -1.372188 6.790504
 1 0.623172 1.067795 6.853790
 1 -2.553221 -3.555182 4.203759
 1 -3.153503 -0.150200 1.634390
 1 -4.851949 -3.322337 5.046220
 1 -5.437233 0.109499 2.516981
 1 -6.319406 -1.493567 4.204837
 1 2.208272 -2.824289 -1.169283
 1 1.798678 0.230514 -1.250104
 1 1.307630 -1.024176 -2.455053
 1 2.838763 -0.151867 3.100819
 1 1.765688 3.878645 2.108776
 1 3.920471 0.637370 5.184713
 1 2.718788 4.667895 4.267785
 1 3.840413 3.050619 5.789708
 1 4.671074 0.637183 0.787462
 1 4.354448 -1.018503 -2.591654
 1 6.374982 -3.723953 0.077863
 1 4.606915 -2.652735 -4.420389
 1 6.625092 -5.337849 -1.734990
 1 5.746960 -4.835879 -4.017018
 1 5.212614 -0.975482 2.130892
 1 5.538010 -2.627835 1.667781
 1 7.434401 -0.235643 1.289146
 1 7.636020 -1.553514 2.458835
 1 7.798856 -1.868348 0.721260
 1 3.252211 -2.698026 0.950007
 1 2.796354 -0.938338 1.175586
 6 5.151388 3.831335 0.107104
 6 7.155040 3.192766 1.447961
 6 5.594673 4.923460 2.293457
 6 6.369391 3.666724 2.660340
 1 7.598763 2.208688 1.636371
 1 4.940259 5.222182 3.116899
 1 5.667189 2.889585 2.980351
 6 1.398802 2.794555 -3.549084
 6 -0.172271 2.753504 -5.411055
 6 -0.720381 4.125147 -3.403837
 6 -1.276104 3.143920 -4.433489
 1 0.187173 3.633703 -5.967740
 1 -0.816342 5.160312 -3.759133
 1 -2.123355 3.596041 -4.958912
 1 7.982473 3.885832 1.229175
 1 7.051984 3.871431 3.490397
 1 6.282717 5.759866 2.094904
 1 -0.527973 2.029051 -6.147733
 1 -1.617422 2.243711 -3.918063
 1 -1.282452 4.031180 -2.469350
 6 1.666075 1.042001 -5.224911
 1 2.360534 1.376797 -6.009675
 1 2.243071 0.552331 -4.440677
 1 0.972167 0.317384 -5.661724
 6 1.194103 4.565337 -1.920717
 1 0.917348 4.013527 -1.017185
 1 2.280106 4.657866 -1.956864
 1 0.753118 5.566627 -1.886912
 6 6.885038 2.412365 -0.872924
 1 7.237328 1.418368 -0.580582
 1 6.146663 2.297504 -1.660727

1	7.742892	2.991044	-1.245292	6	1.670949	0.188779	1.862087
6	3.648622	5.571089	0.870439	6	2.345236	-0.041501	3.199937
1	3.969627	6.455610	0.302356	6	1.929105	-1.067533	4.059519
1	2.866912	5.061878	0.310091	6	2.611790	-1.310163	5.252385
1	3.242149	5.904078	1.827941	6	3.712596	-0.523414	5.602624
7	6.283640	3.073923	0.278448	6	4.128953	0.505490	4.751715
7	4.754836	4.658274	1.126157	6	3.452487	0.742542	3.554836
7	0.912176	2.142467	-4.650297	8	2.210097	0.965856	1.045430
7	0.701781	3.886120	-3.112207	8	-1.333268	1.810772	0.890680
15	-1.025368	-2.706906	-1.420717	6	-1.219402	3.185409	0.846508
6	-2.410905	-3.698846	-0.721287	6	-2.190015	3.923394	0.189394
6	-3.428861	-2.997509	-0.067142	6	-1.951022	5.333609	0.013084
6	-2.530220	-5.090346	-0.869141	6	-0.804790	5.936863	0.635759
6	-4.537444	-3.663088	0.455453	6	0.096594	5.127864	1.381054
1	-3.348906	-1.926060	0.041929	6	-0.088356	3.770261	1.457428
6	-3.637958	-5.758439	-0.344642	6	-0.570306	7.328870	0.467461
1	-1.765096	-5.657286	-1.386438	6	-1.407892	8.102872	-0.304021
6	-4.640445	-5.049031	0.324093	6	-2.517191	7.505693	-0.949210
1	-5.303510	-3.094762	0.973844	6	-2.782001	6.162093	-0.793273
1	-3.715295	-6.836124	-0.457878	6	-3.420331	3.253774	-0.322403
1	-5.496590	-5.574659	0.737502	6	-3.369693	2.137507	-1.160823
6	0.211458	-3.972734	-1.928610	6	-4.543652	1.657592	-1.806647
6	0.792902	-3.954880	-3.203683	6	-5.772840	2.193162	-1.532268
6	0.695658	-4.876089	-0.966582	6	-5.906205	3.216959	-0.556260
6	1.852349	-4.815687	-3.504623	6	-4.723850	3.742282	0.064238
1	0.439025	-3.260551	-3.958200	6	-4.898665	4.706052	1.098777
6	1.742644	-5.741309	-1.275246	6	-6.153270	5.137286	1.475236
1	0.270024	-4.887246	0.028827	6	-7.311922	4.639473	0.834085
6	2.331668	-5.706318	-2.543490	6	-7.183472	3.695482	-0.160811
1	2.307603	-4.780306	-4.489877	8	-2.236739	1.463947	-1.501184
1	2.107347	-6.429709	-0.518394	6	-1.588855	-1.446767	3.544303
1	3.164688	-6.362446	-2.776850	6	-1.532759	-2.376562	4.589885
6	-1.730608	-2.172293	-3.046433	6	-1.187446	-1.965953	5.882618
6	-1.297133	-1.000721	-3.683296	6	-0.912410	-0.623854	6.144626
6	-2.676676	-2.987510	-3.691294	6	-0.980417	0.310792	5.106140
6	-1.809654	-0.653379	-4.935050	6	-1.308854	-0.095573	3.815151
1	-0.594961	-0.330572	-3.203034	3	3.884204	0.867575	0.042681
6	-3.186345	-2.634167	-4.941025	8	4.360167	-1.028942	-0.149927
1	-3.025334	-3.900408	-3.220975	6	4.331847	-1.905130	0.754871
6	-2.753373	-1.463651	-5.567239	6	4.185316	-3.316484	0.630427
1	-1.477823	0.263418	-5.407950	6	4.236651	-4.023463	-0.658093
1	-3.922422	-3.273290	-5.420623	6	4.113916	-3.344633	-1.897091
1	-3.152162	-1.182837	-6.538069	6	4.099360	-4.037905	-3.106749
-----				6	4.199323	-5.431269	-3.138363
(4-7) _{si-a} ⁺ (s _i -1)				6	4.317208	-6.122327	-1.928940
-----				6	4.334565	-5.434735	-0.716227
Number of imaginary frequencies : 1				6	4.418466	-4.086095	1.922383
Electronic energy : HF=-5369.5075979				6	5.896050	-4.426172	2.179855
Zero-point correction= 1.561664 (Hartree/Particle)				8	5.331858	1.696795	1.061449
Thermal correction to Energy= 1.660338				8	3.798828	1.708510	-1.670645
Thermal correction to Enthalpy= 1.661282				1	-6.251738	5.861837	2.278916
Thermal correction to Gibbs Free Energy= 1.420212				1	-4.027874	5.090527	1.616110
Sum of electronic and zero-point Energies= -5367.945934				1	-8.063055	3.285389	-0.651111
Sum of electronic and thermal Energies= -5367.847260				1	-8.294254	4.991286	1.136025
Sum of electronic and thermal Enthalpies= -5367.846316				1	-6.660710	1.817401	-2.033781
Sum of electronic and thermal Free Energies= -5368.087386				1	-4.424218	0.853094	-2.523564
Standard State and RRHO Corrected G= -5368.059804				1	-3.629869	5.721121	-1.304040
-----				1	0.621875	3.112751	1.946753
Cartesian Coordinates				1	-3.163569	8.111158	-1.578605
-----				1	0.297154	7.768955	0.953436
6	-1.226827	-4.444085	2.095121	1	0.958784	5.594427	1.849922
6	-2.348509	-3.660716	1.764370	1	-1.214051	9.164323	-0.429940
6	-3.478990	-4.299669	1.231479	1	-4.342282	-3.721906	0.923965
6	-3.497226	-5.687845	1.064608	1	-0.324963	-3.966393	2.464789
6	-2.389664	-6.457796	1.422314	1	-4.379516	-6.160579	0.642548
6	-1.250443	-5.828528	1.936291	1	-0.374971	-6.414244	2.202263
15	-2.177220	-1.826408	1.827881	1	-2.406428	-7.535938	1.291057
6	-3.889924	-1.165953	2.113200	1	-1.765688	-3.420986	4.413298
6	-4.880978	-1.886609	2.797468	1	-1.332996	0.629024	3.008041
6	-6.117742	-1.301231	3.074070	1	-1.144070	-2.699557	6.683295
6	-6.369609	0.021931	2.702056	1	-0.759138	1.357042	5.298878
6	-5.372511	0.760599	2.061294	1	-0.643573	-0.306837	7.148378
6	-4.142240	0.169636	1.766465	1	-4.694273	-2.904330	3.123261
45	-0.544795	-1.154029	-0.016874	1	-3.376188	0.754909	1.271041
15	-0.858343	1.046096	-0.557775	1	-6.879732	-1.877618	3.591869
8	0.261566	1.800255	-1.211844	1	-5.547938	1.795276	1.787429
6	1.359393	-2.658867	-0.413248	1	-7.330914	0.478495	2.921105
6	1.310056	-1.351728	-1.021056	1	1.140985	-3.498086	-1.059883
6	1.884995	-3.005255	0.834205	1	1.912634	-0.546106	-0.627803
8	0.594637	-0.483839	1.682246	1	1.266056	-1.352408	-2.108164

1	1.067824	-1.664506	3.788976
1	3.797098	1.505765	2.868037
1	2.277975	-2.107792	5.910187
1	4.987369	1.117488	5.016422
1	4.243906	-0.711730	6.531872
1	4.376202	-1.555645	1.804469
1	4.031465	-2.267219	-1.887887
1	4.424770	-6.009546	0.199122
1	4.002009	-3.479141	-4.034895
1	4.396291	-7.206992	-1.927183
1	4.186158	-5.967979	-4.083183
1	4.045399	-3.482943	2.759778
1	3.823294	-5.007127	1.936643
1	6.491883	-3.509305	2.255255
1	6.019819	-4.988488	3.113472
1	6.316074	-5.025891	1.365572
1	1.815331	-4.043230	1.143087
1	1.987361	-2.291286	1.632794
6	3.017813	2.432148	-2.334910
6	1.384534	4.334893	-2.364072
6	1.993429	3.093077	-4.441359
6	0.844809	3.709960	-3.649232
1	0.609391	4.305963	-1.592261
1	1.633871	2.604951	-5.350348
1	0.138659	2.919161	-3.389019
6	6.204397	2.507891	0.676138
6	8.293162	3.011751	-0.586699
6	7.276222	4.741091	0.875322
6	7.888774	4.475271	-0.491958
1	9.161140	2.807761	0.059036
1	8.036790	4.643055	1.665595
1	8.762222	5.115446	-0.646289
1	2.715486	3.865641	-4.750452
1	0.325351	4.469249	-4.242641
1	1.668917	5.383081	-2.528255
1	6.879703	5.759605	0.928611
1	7.153983	4.706915	-1.271322
1	8.585874	2.759426	-1.611322
7	6.169875	3.812905	1.110729
7	7.179436	2.140460	-0.210271
7	2.571179	3.629169	-1.854193
7	2.639243	2.087791	-3.603683
6	3.147139	0.865182	-4.200244
1	4.076129	1.030445	-4.765962
1	3.347479	0.136135	-3.415212
1	2.395105	0.455922	-4.881835
6	2.963946	3.978644	-0.495040
1	2.471106	3.329647	0.234844
1	4.044506	3.892096	-0.380150
1	2.674848	5.016304	-0.309772
6	5.233380	4.160174	2.172284
1	5.645343	3.948100	3.169346
1	5.011515	5.229160	2.110082
1	4.308185	3.599747	2.051978
6	7.305189	0.745621	-0.613387
1	8.199838	0.294028	-0.161842
1	6.426818	0.180944	-0.306734
1	7.402652	0.684975	-1.703073
15	-1.670293	-2.034623	-1.845325
6	-3.444144	-2.473656	-1.610415
6	-4.021795	-3.671773	-2.061551
6	-4.262131	-1.513904	-1.005588
6	-5.386019	-3.904479	-1.879090
1	-3.416529	-4.426034	-2.550402
6	-5.625935	-1.743425	-0.825113
1	-3.827636	-0.585110	-0.666895
6	-6.190169	-2.945575	-1.255110
1	-5.819639	-4.838884	-2.224173
1	-6.232087	-0.987219	-0.335907
1	-7.249756	-3.135209	-1.108364
6	-0.897591	-3.614757	-2.391131
6	-0.070524	-3.674406	-3.520840
6	-1.024026	-4.751212	-1.573722
6	0.627235	-4.848141	-3.819685
1	0.048294	-2.806655	-4.160552
6	-0.337422	-5.923066	-1.882881
1	-1.643393	-4.714064	-0.686648
6	0.498628	-5.971987	-3.003039
1	1.279347	-4.876798	-4.687251
1	-0.444998	-6.790556	-1.238184

1	1.052840	-6.877310	-3.231896
6	-1.727323	-1.065973	-3.421862
6	-2.744176	-1.320221	-4.357636
6	-0.730918	-0.131151	-3.739020
6	-2.769248	-0.649700	-5.581166
1	-3.524817	-2.039907	-4.137100
6	-0.756401	0.529988	-4.968809
1	0.044989	0.120289	-3.026758
6	-1.772095	0.276742	-5.891638
1	-3.568340	-0.853582	-6.288405
1	0.016052	1.254573	-5.197908
1	-1.789132	0.800984	-6.843084

(4-7)_{si-a}[‡] (si_2)

Number of imaginary frequencies : 1
 Electronic energy : HF=-5369.508571
 Zero-point correction= 1.562434 (Hartree/Particle)
 Thermal correction to Energy= 1.660760
 Thermal correction to Enthalpy= 1.661704
 Thermal correction to Gibbs Free Energy= 1.424069
 Sum of electronic and zero-point Energies= -5367.946137
 Sum of electronic and thermal Energies= -5367.847811
 Sum of electronic and thermal Enthalpies= -5367.846866
 Sum of electronic and thermal Free Energies= -5368.084502
 Standard State and RRHO Corrected G= -5368.058784

Cartesian Coordinates

6	-0.562082	-3.714130	3.198144
6	-1.769425	-3.085016	2.841816
6	-2.920755	-3.876662	2.703931
6	-2.869500	-5.253622	2.939901
6	-1.670810	-5.863203	3.312720
6	-0.514344	-5.086218	3.439489
15	-1.725415	-1.311715	2.342082
6	-3.408138	-0.633143	2.736905
6	-4.228731	-1.148391	3.751810
6	-5.432574	-0.519741	4.075061
6	-5.816171	0.650219	3.414210
6	-4.982712	1.194459	2.434606
6	-3.789313	0.554637	2.096339
45	-0.508807	-1.136787	0.094656
15	-1.142809	0.774894	-0.995366
8	-0.322354	1.251903	-2.159595
6	1.381481	-2.618370	-0.172331
6	1.188632	-1.535900	-1.104613
6	2.062853	-2.588081	1.048146
8	0.810978	0.059161	1.290497
6	1.789673	0.866043	1.131483
6	2.496346	1.231011	2.419159
6	2.598116	0.311312	3.471938
6	3.288625	0.643120	4.636896
6	3.844635	1.917733	4.779935
6	3.720473	2.849133	3.745494
6	3.068869	2.500342	2.561512
8	2.208505	1.352300	0.055912
8	-1.240997	1.985988	0.197473
6	-1.204241	3.261521	-0.333470
6	-2.351382	3.786414	-0.903657
6	-2.234255	5.044312	-1.600160
6	-0.986474	5.756580	-1.562494
6	0.126376	5.189853	-0.881580
6	0.029721	3.949089	-0.303981
6	-0.873011	7.004047	-2.234672
6	-1.928176	7.526653	-2.948219
6	-3.144395	6.807392	-3.025915
6	-3.293012	5.603855	-2.370541
6	-3.644194	3.046861	-0.814044
6	-3.783087	1.712672	-1.208659
6	-5.074621	1.127999	-1.346689
6	-6.206237	1.806884	-0.985783
6	-6.110302	3.100661	-0.406917
6	-4.818861	3.715835	-0.299855
6	-4.745323	4.971901	0.368337
6	-5.873049	5.587375	0.869517
6	-7.147610	4.991187	0.724964
6	-7.256503	3.768297	0.100288
8	-2.768344	0.871881	-1.556493
6	-0.897476	-0.415976	3.740947

6	-0.610262	-0.983503	4.988361
6	-0.142862	-0.183966	6.037563
6	0.024621	1.188887	5.856356
6	-0.267250	1.761646	4.614623
6	-0.715473	0.966971	3.562693
3	4.087347	1.107490	-0.604643
8	4.452017	-0.781987	-0.395328
6	4.491438	-1.549934	0.600343
6	4.332650	-2.964696	0.650680
6	4.257754	-3.810920	-0.549068
6	3.949192	-3.279261	-1.826788
6	3.807476	-4.105588	-2.941330
6	3.965450	-5.489846	-2.836727
6	4.264876	-6.036731	-1.585508
6	4.404566	-5.216667	-0.466744
6	4.699894	-3.587321	1.989952
6	6.201728	-3.880494	2.145406
8	5.362839	2.258091	0.239104
8	4.276142	1.453460	-2.494085
1	-5.778705	6.537888	1.387394
1	-3.778915	5.442465	0.504276
1	-8.223951	3.282481	-0.001103
1	-8.029186	5.489446	1.117996
1	-7.184241	1.348447	-1.105769
1	-5.126475	0.125967	-1.756478
1	-4.228875	5.064437	-2.452873
1	0.879237	3.447784	0.145928
1	-3.968150	7.204310	-3.612813
1	0.075599	7.533166	-2.184418
1	1.066162	5.735844	-0.862262
1	-1.826323	8.478148	-3.462427
1	-3.858535	-3.432131	2.394065
1	0.349010	-3.130458	3.276154
1	-3.771416	-5.846806	2.818810
1	0.428187	-5.549724	3.717284
1	-1.633365	-6.933469	3.494524
1	-0.765474	-2.042750	5.162421
1	-0.917945	1.414713	2.595488
1	0.077458	-0.639598	6.999391
1	-0.123290	2.827054	4.457818
1	0.386317	1.808271	6.672284
1	-3.933356	-2.036373	4.300326
1	-3.150360	0.989966	1.336530
1	-6.063910	-0.939321	4.853743
1	-5.258416	2.113338	1.929382
1	-6.750772	1.141922	3.669726
1	1.130193	-3.608898	-0.525593
1	1.800440	-0.645485	-1.034312
1	0.988699	-1.840312	-2.128617
1	2.113228	-0.653135	3.382522
1	3.001824	3.205451	1.740056
1	3.369795	-0.082178	5.441524
1	4.144197	3.841870	3.856043
1	4.365918	2.186213	5.694905
1	4.627916	-1.086535	1.598360
1	3.822273	-2.212133	-1.930603
1	4.631796	-5.683210	0.485611
1	3.563386	-3.657104	-3.901667
1	4.390419	-7.111487	-1.476873
1	3.856585	-6.129385	-3.708508
1	4.392422	-2.901183	2.789617
1	4.127204	-4.507428	2.157303
1	6.782307	-2.953973	2.068996
1	6.421169	-4.339108	3.117392
1	6.560052	-4.557858	1.363358
1	2.060840	-3.487386	1.653900
1	2.226295	-1.665818	1.576331
6	3.591409	0.914551	-3.401556
6	1.512373	0.892926	-4.790391
6	3.370261	-0.716315	-5.226202
6	1.863129	-0.563550	-5.072167
1	0.497451	0.972115	-4.394567
1	3.639778	-1.766830	-5.368460
1	1.532354	-1.194201	-4.241459
6	5.616373	3.373188	0.744228
6	5.452930	5.866443	0.704634
6	6.880672	4.736764	2.393668
6	5.846762	5.832226	2.172792
1	6.273379	6.274389	0.094546
1	7.832980	5.001822	1.909160

1	6.254284	6.802287	2.472074
1	3.730624	-0.160780	-6.107165
1	1.348430	-0.899846	-5.976778
1	1.570163	1.483981	-5.716466
1	7.084325	4.610779	3.461529
1	4.962842	5.633470	2.787845
1	4.585192	6.518291	0.555505
7	6.382545	3.462836	1.878097
7	5.099125	4.531329	0.221283
7	2.415021	1.469100	-3.790433
7	4.021133	-0.242969	-4.007044
6	5.382629	-0.691709	-3.742515
1	6.122248	-0.138069	-4.339938
1	5.608755	-0.568802	-2.684789
1	5.455245	-1.752637	-3.993102
6	2.014286	2.717590	-3.140442
1	1.894681	2.567717	-2.068443
1	2.750268	3.506281	-3.332384
1	1.049290	3.019603	-3.543828
6	6.964510	2.251279	2.435846
1	8.001140	2.107581	2.099628
1	6.959462	2.320071	3.528074
1	6.374157	1.388651	2.133817
6	4.365355	4.503925	-1.037290
1	4.850787	5.168345	-1.764452
1	4.340479	3.497481	-1.447175
1	3.336972	4.855548	-0.887480
15	-1.859476	-2.552115	-1.165359
6	-3.516404	-2.953415	-0.469985
6	-4.064466	-4.245789	-0.442208
6	-4.291437	-1.877683	-0.023557
6	-5.353667	-4.449111	0.053576
1	-3.494342	-5.094624	-0.800977
6	-5.580187	-2.079233	0.469936
1	-3.878847	-0.880148	-0.057691
6	-6.111898	-3.369385	0.516816
1	-5.764209	-5.454605	0.078852
1	-6.151897	-1.228419	0.827623
1	-7.111619	-3.534096	0.908729
6	-1.057923	-4.195017	-1.386240
6	-0.426642	-4.543708	-2.587637
6	-0.942323	-5.050948	-0.276856
6	0.319046	-5.722826	-2.673440
1	-0.495060	-3.892969	-3.452733
6	-0.210255	-6.232274	-0.371200
1	-1.405625	-4.783750	0.664916
6	0.431833	-6.566711	-1.568065
1	0.821054	-5.972483	-3.603163
1	-0.129520	-6.880994	0.496264
1	1.022457	-7.475555	-1.635093
6	-2.296239	-2.083678	-2.901793
6	-3.475345	-2.571087	-3.490764
6	-1.430361	-1.292877	-3.669960
6	-3.784193	-2.265405	-4.816372
1	-4.160765	-3.187299	-2.919767
6	-1.742908	-0.991116	-4.997331
1	-0.535963	-0.874581	-3.230427
6	-2.918348	-1.473428	-5.574026
1	-4.703464	-2.644864	-5.253780
1	-1.069706	-0.366315	-5.575576
1	-3.161144	-1.230830	-6.604864

(4...7)_{si-a} (si_3)

Number of imaginary frequencies : 0
 Electronic energy : HF=-5369.5159062
 Zero-point correction= 1.563563 (Hartree/Particle)
 Thermal correction to Energy= 1.662462
 Thermal correction to Enthalpy= 1.663407
 Thermal correction to Gibbs Free Energy= 1.423778
 Sum of electronic and zero-point Energies= -5367.952343
 Sum of electronic and thermal Energies= -5367.853444
 Sum of electronic and thermal Enthalpies= -5367.852500
 Sum of electronic and thermal Free Energies= -5368.092129
 Standard State and RRHO Corrected G= -5368.065624

Cartesian Coordinates

6	0.410499	-4.315444	2.225857
6	-0.915313	-3.970060	1.905386

6	-1.767466	-4.969386	1.410084	1	-2.784319	-4.730958	1.125532
6	-1.310989	-6.281557	1.257579	1	1.098172	-3.556000	2.581622
6	0.001104	-6.616384	1.593793	1	-1.986165	-7.035790	0.863986
6	0.861848	-5.626338	2.079115	1	1.888507	-5.871489	2.335728
15	-1.400075	-2.191045	1.929453	1	0.354639	-7.636260	1.472788
6	-3.220228	-2.162715	2.283288	1	-0.340816	-3.427874	4.519675
6	-3.862012	-3.169419	3.021167	1	-1.411447	0.461227	3.003368
6	-5.215051	-3.054116	3.344179	1	0.084345	-2.445696	6.733084
6	-5.936659	-1.919817	2.963093	1	-1.032899	1.432481	5.240407
6	-5.293161	-0.893081	2.268775	1	-0.266881	-0.012057	7.118303
6	-3.943964	-1.014310	1.931545	1	-3.313907	-4.045394	3.350710
45	-0.181660	-1.082497	-0.045944	1	-3.456251	-0.207533	1.398914
15	-1.306703	0.812139	-0.573977	1	-5.701504	-3.848689	3.903322
8	-0.619178	1.873653	-1.373008	1	-5.836181	0.002374	1.985818
6	2.099356	-1.755502	-0.801349	1	-6.989325	-1.830727	3.216578
6	1.512034	-0.489734	-1.189649	1	2.224273	-2.493878	-1.583332
6	2.346657	-2.177129	0.472385	1	1.832559	0.419901	-0.703473
8	0.727629	-0.057807	1.587406	1	1.386887	-0.365086	-2.260637
6	1.329544	1.060933	1.773354	1	2.282310	-0.888692	3.449021
6	1.937542	1.211983	3.146294	1	1.707347	3.345743	3.127732
6	2.392734	0.103283	3.870646	1	3.325472	-0.589368	5.682332
6	2.966087	0.274808	5.130665	1	2.654632	3.654771	5.412211
6	3.057604	1.552683	5.691316	1	3.490344	1.683823	6.679372
6	2.587794	2.660345	4.979539	1	4.815688	-0.151259	2.031540
6	2.047109	2.491485	3.704291	1	4.509792	0.140781	-1.712182
8	1.434997	1.999018	0.958428	1	6.290433	-3.664887	-0.762384
8	-1.896869	1.419857	0.887381	1	4.479727	-0.488896	-4.096295
6	-2.273961	2.752538	0.793618	1	6.224459	-4.293294	-3.114111
6	-3.465353	3.072700	0.166522	1	5.318675	-2.722260	-4.833745
6	-3.723737	4.468654	-0.091612	1	5.710528	-2.023711	2.412926
6	-2.827345	5.459783	0.436389	1	5.716192	-3.329048	1.251909
6	-1.678126	5.050586	1.166748	1	7.960750	-1.276892	1.687904
6	-1.386631	3.717889	1.313607	1	8.013099	-3.002653	2.094286
6	-3.082585	6.836305	0.189116	1	7.991659	-2.483231	0.400272
6	-4.157848	7.233805	-0.573045	1	2.661417	-3.202214	0.637736
6	-5.020062	6.259294	-1.129519	1	2.324367	-1.516030	1.323340
6	-4.811044	4.917475	-0.893581	6	1.912032	3.190703	-2.445894
6	-4.426321	2.006093	-0.237542	6	-0.101721	4.680671	-2.517813
6	-4.065714	0.903522	-1.013689	6	0.730757	3.506756	-4.555720
6	-5.054675	0.057301	-1.588357	6	-0.512363	3.889094	-3.759556
6	-6.380206	0.212577	-1.287912	1	-0.836229	4.521232	-1.721002
6	-6.789714	1.197285	-0.349560	1	0.473007	2.900050	-5.427553
6	-5.806229	2.089905	0.191335	1	-1.018554	2.973327	-3.448805
6	-6.233773	3.006139	1.194657	6	5.702173	3.192915	0.683612
6	-7.547527	3.054169	1.611317	6	7.483305	1.903774	1.894843
6	-8.518729	2.197204	1.043214	6	7.865530	2.748901	-0.410289
6	-8.139518	1.285592	0.082956	6	7.989076	1.539177	0.506301
8	-2.791549	0.538005	-1.351539	1	8.238565	2.483516	2.445326
6	-0.894473	-1.550140	3.594071	1	8.518108	3.567644	-0.067034
6	-0.476260	-2.360855	4.656748	1	9.029167	1.204941	0.567280
6	-0.245761	-1.804980	5.919805	1	1.252348	4.404275	-4.924897
6	-0.448521	-0.442279	6.137525	1	-1.198407	4.485271	-4.369727
6	-0.883474	0.367916	5.084407	1	-0.066945	5.756660	-2.736121
6	-1.097914	-0.178040	3.821175	1	8.169192	2.492312	-1.428968
3	3.210763	2.298007	0.085890	1	7.389392	0.719212	0.099299
8	4.157269	0.716375	0.318533	1	7.286767	0.992649	2.472857
6	4.773475	-0.220973	0.924409	7	6.470058	3.176300	-0.449430
6	5.398726	-1.353977	0.404249	7	6.239849	2.676631	1.830436
6	5.408281	-1.693242	-1.015637	7	1.222963	4.289270	-2.013620
6	4.900633	-0.819946	-2.020694	7	1.605630	2.719809	-3.694083
6	4.875268	-1.190129	-3.364395	6	2.366053	1.622362	-4.263257
6	5.343891	-2.439892	-3.784549	1	3.127570	1.976617	-4.973476
6	5.852063	-3.314307	-2.818641	1	2.864978	1.084279	-3.459966
6	5.890144	-2.950021	-1.473695	1	1.692588	0.938022	-4.791038
6	6.051677	-2.291772	1.404185	6	1.570053	4.843753	-0.711511
6	7.592044	-2.266898	1.396733	1	1.090091	4.287797	0.099177
8	4.542289	3.680304	0.673935	1	2.650555	4.813643	-0.563464
8	2.833256	2.678874	-1.767684	1	1.235048	5.885683	-0.680106
1	-7.836465	3.754092	2.390382	6	5.991263	3.850648	-1.646949
1	-5.507012	3.663294	1.656577	1	6.326718	4.897902	-1.687441
1	-8.866269	0.602631	-0.349971	1	6.381908	3.330296	-2.526645
1	-9.551655	2.250357	1.374849	1	4.903648	3.817965	-1.677795
1	-7.125346	-0.438171	-1.737336	6	5.447516	2.685857	3.049622
1	-4.716807	-0.710786	-2.274399	1	6.108367	2.866464	3.904868
1	-5.476577	4.187996	-1.339280	1	4.701710	3.474857	3.000561
1	-0.474513	3.368628	1.782008	1	4.931236	1.731140	3.201865
1	-5.852392	6.570937	-1.754421	15	-1.074769	-2.349214	-1.817185
1	-2.397790	7.571062	0.605222	6	-2.541970	-3.392286	-1.435335
1	-1.007694	5.807986	1.563478	6	-2.658611	-4.733682	-1.835201
1	-4.338320	8.288412	-0.760697	6	-3.616680	-2.783940	-0.779110

6	-3.825452	-5.447476	-1.557142	6	-1.975805	5.056419	1.061835
1	-1.847608	-5.226077	-2.358588	6	-1.603037	3.741997	1.189002
6	-4.783803	-3.495359	-0.502583	6	-3.494243	6.763615	0.111667
1	-3.536356	-1.751143	-0.477253	6	-4.603080	7.101050	-0.631762
6	-4.887798	-4.833575	-0.886210	6	-5.416987	6.080717	-1.179394
1	-3.902196	-6.486452	-1.864740	6	-5.124054	4.752216	-0.957558
1	-5.595253	-3.001884	0.023139	6	-4.553562	1.861240	-0.322113
1	-5.790636	-5.396114	-0.666068	6	-4.129621	0.792829	-1.114608
6	0.173568	-3.564737	-2.404181	6	-5.060629	-0.153208	-1.626447
6	0.823506	-3.415379	-3.636416	6	-6.378805	-0.117286	-1.260156
6	0.583306	-4.583382	-1.526573	6	-6.834752	0.845936	-0.320595
6	1.887361	-4.257197	-3.972838	6	-5.914399	1.834559	0.163756
1	0.525049	-2.631365	-4.323776	6	-6.381747	2.728921	1.169466
6	1.634878	-5.428292	-1.872501	6	-7.675363	2.665636	1.643085
1	0.095632	-4.701569	-0.566650	6	-8.586533	1.710917	1.133774
6	2.298961	-5.258312	-3.091921	6	-8.166586	0.819194	0.171717
1	2.400324	-4.119614	-4.919937	8	-2.848938	0.592198	-1.533706
1	1.944742	-6.206821	-1.181538	6	-0.732689	-1.370753	3.588226
1	3.135802	-5.900151	-3.351070	6	-0.237547	-2.101932	4.674911
6	-1.592352	-1.502791	-3.377082	6	-0.004502	-1.472057	5.903050
6	-2.543181	-2.112872	-4.212548	6	-0.280751	-0.114133	6.061497
6	-1.007881	-0.293836	-3.782516	6	-0.781297	0.619040	4.980910
6	-2.906867	-1.522162	-5.423535	6	-0.996702	0.000670	3.752039
1	-3.008845	-3.048540	-3.923655	3	3.344425	2.426604	-0.474299
6	-1.373361	0.290359	-4.996585	8	4.328573	0.740662	-0.781550
1	-0.303359	0.225910	-3.147618	6	4.626345	0.046563	0.228081
6	-2.321923	-0.318109	-5.819854	6	5.029140	-1.314861	0.300163
1	-3.648794	-2.004835	-6.053349	6	5.299777	-2.144253	-0.879672
1	-0.921791	1.231903	-5.289396	6	4.892272	-1.756669	-2.182530
1	-2.606784	0.144816	-6.760464	6	5.089273	-2.590683	-3.282161
				6	5.694391	-3.842279	-3.137969
(4-7) _{si-a*} (si_3)				6	6.103899	-4.245596	-1.863522
				6	5.911393	-3.416436	-0.759517
Number of imaginary frequencies : 1				6	5.524766	-1.756238	1.668302
Electronic energy : HF=-5369.5136874				6	7.024580	-1.502916	1.892746
Zero-point correction= 1.562061 (Hartree/Particle)				8	4.713608	3.393016	0.554315
Thermal correction to Energy= 1.660581				8	2.802079	3.400325	-2.024638
Thermal correction to Enthalpy= 1.661525				1	-7.994570	3.352719	2.421858
Thermal correction to Gibbs Free Energy= 1.421435				1	-5.699178	3.458540	1.587921
Sum of electronic and zero-point Energies= -5367.951626				1	-8.845558	0.064167	-0.217025
Sum of electronic and thermal Energies= -5367.853106				1	-9.604585	1.675393	1.510777
Sum of electronic and thermal Enthalpies= -5367.852162				1	-7.080375	-0.845489	-1.658265
Sum of electronic and thermal Free Energies= -5368.092252				1	-4.683730	-0.901737	-2.314367
Standard State and RRHO Corrected G= -5368.065044				1	-5.753004	3.984940	-1.393651
				1	-0.678187	3.447330	1.672466
Cartesian Coordinates				1	-6.278449	6.346931	-1.785592
				1	-2.849275	7.535617	0.524239
6	0.600906	-4.168732	2.301583	1	-1.352218	5.848330	1.467318
6	-0.751674	-3.878569	2.043427	1	-4.848434	8.144248	-0.809327
6	-1.603785	-4.931794	1.674716	1	-2.640991	-4.738071	1.429026
6	-1.121490	-6.241674	1.595818	1	1.288032	-3.365569	2.546776
6	0.216116	-6.521164	1.879248	1	-1.796944	-7.039474	1.300447
6	1.077984	-5.476562	2.230351	1	2.125188	-5.677815	2.438028
15	-1.274353	-2.111016	1.975089	1	0.588407	-7.539671	1.816707
6	-3.079203	-2.115240	2.420442	1	-0.047770	-3.165947	4.585165
6	-3.643885	-3.076407	3.273498	1	-1.362065	0.579036	2.910453
6	-4.981021	-2.980167	3.662226	1	0.380995	-2.052814	6.736920
6	-5.763552	-1.905108	3.232630	1	-0.982942	1.681231	5.089166
6	-5.196881	-0.920203	2.420924	1	-0.101943	0.372931	7.016005
6	-3.864599	-1.026024	2.015835	1	-3.044899	-3.901324	3.644314
45	-0.179643	-1.076090	-0.087334	1	-3.436822	-0.252671	1.389064
15	-1.361063	0.789888	-0.701442	1	-5.406305	-3.740511	4.311804
8	-0.653666	1.857637	-1.485665	1	-5.787373	-0.069023	2.099492
6	2.086002	-1.800829	-0.603770	1	-6.803204	-1.828292	3.538759
6	1.518538	-0.669627	-1.293684	1	2.157004	-2.724072	-1.162564
6	2.733352	-1.812690	0.630484	1	1.805033	0.335674	-1.020391
8	0.717024	0.173946	1.421236	1	1.393798	-0.806231	-2.365509
6	1.422926	1.243757	1.428043	1	2.146724	-0.395322	3.497761
6	1.977636	1.624148	2.781179	1	1.913935	3.725787	2.343258
6	2.337084	0.648732	3.718911	1	3.200929	0.256543	5.650863
6	2.913267	1.020743	4.934433	1	2.841696	4.404454	4.553895
6	3.091146	2.373017	5.240844	1	3.523909	2.663164	6.194397
6	2.707156	3.352216	4.318775	1	4.523264	0.524806	1.220319
6	2.174241	2.978111	3.084872	1	4.419423	-0.792909	-2.308810
8	1.702556	1.969620	0.452823	1	6.241565	-3.768926	0.211795
8	-1.984941	1.423540	0.753030	1	4.759647	-2.257691	-4.263773
6	-2.430947	2.726150	0.661514	1	6.578236	-5.214525	-1.725407
6	-3.649940	2.985818	0.056695	1	5.844903	-4.488789	-3.998346
6	-3.995539	4.364569	-0.181329	1	4.960655	-1.211405	2.436258
6	-3.153654	5.403254	0.344898	1	5.302404	-2.816753	1.838753

1	7.240595	-0.433401	1.809421	7s (si_3)			
1	7.345884	-1.840242	2.885980	-----			
1	7.634732	-2.021247	1.145565	Number of imaginary frequencies : 0			
1	3.064448	-2.767079	1.024940	Electronic energy : HF=-5369.5399521			
1	2.616625	-1.020139	1.349450	Zero-point correction= 1.565219 (Hartree/Particle)			
6	1.680490	3.727271	-2.486557	Thermal correction to Energy= 1.663348			
6	-0.140637	3.376271	-4.141921	Thermal correction to Enthalpy= 1.664292			
6	-0.484451	4.898781	-2.214349	Thermal correction to Gibbs Free Energy= 1.426663			
6	-0.678277	4.734658	-3.714585	Sum of electronic and zero-point Energies= -5367.974734			
1	-0.132849	3.291879	-5.234896	Sum of electronic and thermal Energies= -5367.876604			
1	-0.762510	5.909138	-1.898211	Sum of electronic and thermal Enthalpies= -5367.875660			
1	-0.149906	5.533438	-4.248695	Sum of electronic and thermal Free Energies= -5368.113290			
6	5.931135	3.093323	0.502984	Standard State and RRHO Corrected G= -5368.087172			
6	8.005932	2.342202	1.631027	-----			
6	8.090881	2.978738	-0.760418	Cartesian Coordinates			
6	8.511712	1.929347	0.257109	-----			
1	8.497666	3.269540	1.964449	6	0.556071	-4.288341	2.325547
1	8.689079	3.894806	-0.640444	6	-0.782715	-3.948691	2.056535
1	9.601149	1.830357	0.261811	6	-1.673164	-4.976492	1.706840
1	-1.103700	4.179718	-1.668439	6	-1.242705	-6.305812	1.656624
1	-1.741980	4.805808	-3.962196	6	0.081676	-6.632567	1.951960
1	-0.769902	2.578505	-3.731650	6	0.982291	-5.615031	2.284675
1	8.260486	2.613147	-1.779332	15	-1.232530	-2.161804	1.946995
1	8.080180	0.958008	-0.008500	6	-3.044862	-2.113596	2.382700
1	8.227000	1.571638	2.375300	6	-3.647892	-3.037248	3.251413
7	6.669312	3.302570	-0.629689	6	-4.987298	-2.896429	3.618888
7	6.555770	2.515945	1.581883	6	-5.736062	-1.812479	3.152001
7	1.234070	3.194767	-3.669304	6	-5.131352	-0.863203	2.325778
7	0.926647	4.690590	-1.872889	6	-3.797029	-1.015441	1.944075
6	1.350677	5.135963	-0.550368	45	-0.154985	-1.151587	-0.064605
1	1.091312	4.400709	0.218310	15	-1.414559	0.756537	-0.688980
1	2.430831	5.286005	-0.533889	8	-0.734979	1.822219	-1.511018
1	0.856298	6.085400	-0.327613	6	1.893420	-1.984508	-0.292070
6	1.931349	2.037910	-4.211430	6	1.597814	-0.955823	-1.243907
1	2.975438	2.056171	-3.904388	6	2.889178	-1.860457	0.844054
1	1.483853	1.098950	-3.860961	8	0.737679	0.176111	1.389564
1	1.875952	2.063113	-5.304932	6	1.460515	1.225485	1.325267
6	6.076156	3.966111	-1.781159	6	1.945904	1.753045	2.656619
1	6.638014	4.879872	-2.017716	6	2.237112	0.883068	3.714482
1	6.108407	3.305990	-2.656486	6	2.769268	1.378057	4.906596
1	5.038389	4.218815	-1.579198	6	2.971097	2.751565	5.067444
6	5.835507	2.396391	2.840852	6	2.655190	3.628003	4.024015
1	6.078761	3.221867	3.525032	6	2.166823	3.128204	2.816938
1	4.765783	2.406982	2.652512	8	1.831465	1.827360	0.292304
1	6.108147	1.454019	3.326262	8	-1.991847	1.483511	0.773033
15	-1.044046	-2.488430	-1.719062	6	-2.355739	2.800291	0.641849
6	-2.498082	-3.521001	-1.259619	6	-3.561802	3.120775	0.036591
6	-2.617965	-4.885539	-1.570324	6	-3.814261	4.507238	-0.261463
6	-3.561704	-2.876152	-0.620378	6	-2.899979	5.509940	0.211679
6	-3.772939	-5.585573	-1.217753	6	-1.743951	5.114940	0.938888
1	-1.816603	-5.407120	-2.080298	6	-1.460548	3.784950	1.121433
6	-4.717794	-3.573293	-0.270100	6	-3.149209	6.878161	-0.082770
1	-3.480600	-1.824921	-0.387340	6	-4.238529	7.256824	-0.835579
6	-4.822211	-4.934401	-0.561534	6	-5.124860	6.270069	-1.330329
1	-3.850576	-6.642895	-1.454950	6	-4.921016	4.936373	-1.047991
1	-5.519880	-3.050354	0.241483	6	-4.549483	2.046367	-0.275801
1	-5.715559	-5.485850	-0.282173	6	-4.217585	0.915046	-1.028564
6	0.218318	-3.721683	-2.246382	6	-5.232331	0.012124	-1.461671
6	0.908859	-3.592235	-3.459044	6	-6.535311	0.162123	-1.072195
6	0.600715	-4.729509	-1.344291	6	-6.901178	1.206131	-0.180444
6	1.972960	-4.448572	-3.756277	6	-5.897330	2.143295	0.237407
1	0.635545	-2.816804	-4.166472	6	-6.279853	3.122779	1.199541
6	1.653225	-5.589002	-1.650310	6	-7.568113	3.189893	1.687268
1	0.089654	-4.827666	-0.395127	6	-8.559979	2.286232	1.239702
6	2.349786	-5.444377	-2.854594	6	-8.223695	1.311741	0.325933
1	2.512010	-4.327714	-4.691124	8	-2.974506	0.600021	-1.467378
1	1.937225	-6.359528	-0.939499	6	-0.699461	-1.422670	3.567151
1	3.186295	-6.097675	-3.083479	6	-0.191317	-2.142252	4.655456
6	-1.580159	-1.768680	-3.336864	6	0.031021	-1.506840	5.883460
6	-2.465190	-2.483875	-4.160910	6	-0.270254	-0.154335	6.040886
6	-1.052134	-0.555609	-3.799806	6	-0.780281	0.568777	4.957458
6	-2.815852	-1.992611	-5.419119	6	-0.981922	-0.053849	3.728680
1	-2.886303	-3.425823	-3.826450	3	3.383453	2.495465	-0.556436
6	-1.396161	-0.073121	-5.064119	8	4.470398	0.639724	-0.844380
1	-0.402624	0.037627	-3.169740	6	4.336756	0.004511	0.190930
6	-2.278438	-0.787216	-5.876287	6	4.379234	-1.492945	0.423369
1	-3.507474	-2.554602	-6.040526	6	4.827394	-2.368079	-0.746492
1	-0.979347	0.868572	-5.406227	6	4.635243	-1.995571	-2.088618
1	-2.549437	-0.405649	-6.856766	6	4.975231	-2.858150	-3.133022
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6	5.694756	-4.511353	-1.541856
6	5.356955	-3.646651	-0.499108
6	5.257679	-1.658382	1.701461
6	6.724379	-1.262742	1.513097
8	4.764453	3.302137	0.501277
8	2.920253	3.379284	-2.143847
1	-7.820383	3.941972	2.429917
1	-5.536330	3.817088	1.571764
1	-8.965343	0.593079	-0.014703
1	-9.572894	2.353667	1.626316
1	-7.296378	-0.532957	-1.417399
1	-4.929329	-0.798651	-2.114831
1	-5.604274	4.193989	-1.443976
1	-0.555923	3.451878	1.618481
1	-5.971561	6.566207	-1.943592
1	-2.449985	7.622542	0.290813
1	-1.065766	5.879634	1.307859
1	-4.413757	8.305202	-1.060028
1	-2.700810	-4.747686	1.451425
1	1.271818	-3.507745	2.558497
1	-1.948037	-7.082294	1.374128
1	2.020249	-5.852448	2.501028
1	0.413494	-7.666180	1.912697
1	0.013255	-3.203755	4.569579
1	-1.352671	0.519022	2.885268
1	0.424309	-2.080708	6.718643
1	-0.999614	1.627702	5.063679
1	-0.103901	0.336356	6.995910
1	-3.076659	-3.868268	3.651589
1	-3.339736	-0.266895	1.310055
1	-5.441364	-3.629253	4.280749
1	-5.692868	-0.005295	1.970965
1	-6.777863	-1.702103	3.440492
1	1.890739	-2.991570	-0.690668
1	1.954390	0.057762	-1.117716
1	1.482951	-1.248183	-2.285829
1	2.029913	-0.175067	3.602361
1	1.961576	3.794413	1.986517
1	3.002687	0.693408	5.717006
1	2.807555	4.696971	4.145354
1	3.369719	3.138106	6.001485
1	4.114674	0.552431	1.125809
1	4.212082	-1.029397	-2.319878
1	5.505870	-3.986146	0.520173
1	4.812410	-2.539249	-4.159244
1	6.101360	-5.492876	-1.312698
1	5.767990	-4.791080	-3.682786
1	4.810753	-1.044088	2.493073
1	5.181880	-2.690579	2.055662
1	6.812896	-0.218593	1.195624
1	7.280017	-1.376446	2.450103
1	7.211257	-1.883326	0.754645
1	2.965822	-2.828174	1.350164
1	2.571207	-1.137725	1.596460
6	1.786403	3.666950	-2.613870
6	-0.048662	3.183403	-4.215776
6	-0.386227	4.832708	-2.398411
6	-0.587740	4.567039	-3.882378
1	-0.047215	3.021876	-5.299602
1	-0.671503	5.858317	-2.144903
1	-0.067102	5.329956	-4.473619
6	5.994696	3.052166	0.514224
6	8.013606	2.279556	1.747789
6	8.250275	3.249392	-0.521124
6	8.677749	2.109976	0.390728
1	8.419248	3.157948	2.272690
1	8.691057	4.200396	-0.184617
1	9.765902	2.106603	0.501479
1	-0.989608	4.140252	-1.802541
1	-1.653266	4.614682	-4.127161
1	-0.670913	2.418799	-3.739464
1	8.597594	3.074571	-1.544350
1	8.377429	1.152525	-0.049058
1	8.199899	1.406357	2.380691
7	6.790394	3.361889	-0.556039
7	6.564404	2.414214	1.588898
7	1.332384	3.040299	-3.741312
7	1.031907	4.661825	-2.058245
6	1.461495	5.215180	-0.781047
1	1.149151	4.577244	0.053443

1	2.546726	5.316572	-0.759898
1	1.010326	6.203531	-0.657269
6	2.036382	1.841309	-4.179642
1	3.110510	1.967135	-4.048713
1	1.720101	0.955691	-3.613928
1	1.823269	1.675434	-5.239505
6	6.249493	4.160293	-1.649868
1	6.545952	5.214354	-1.549122
1	6.643332	3.782434	-2.598982
1	5.163882	4.097582	-1.672045
6	5.777874	2.212856	2.799355
1	6.016476	2.972845	3.555880
1	4.718536	2.274751	2.568420
1	6.003626	1.227121	3.218172
15	-0.998714	-2.589779	-1.660096
6	-2.513683	-3.554338	-1.237934
6	-2.679364	-4.924303	-1.496624
6	-3.579442	-2.837446	-0.681955
6	-3.878047	-5.561294	-1.169577
1	-1.880478	-5.501179	-1.947016
6	-4.777513	-3.472315	-0.355297
1	-3.464754	-1.778473	-0.499884
6	-4.926414	-4.840474	-0.590350
1	-3.989738	-6.623991	-1.366356
1	-5.579878	-2.895121	0.093619
1	-5.854019	-5.342171	-0.329094
6	0.206721	-3.888474	-2.188802
6	0.893040	-3.807837	-3.408019
6	0.534487	-4.921326	-1.293520
6	1.885149	-4.740682	-3.724116
1	0.666160	-3.015606	-4.113177
6	1.514223	-5.857768	-1.616327
1	0.032967	-4.983530	-0.336755
6	2.198168	-5.766645	-2.832289
1	2.416235	-4.657261	-4.667846
1	1.750246	-6.647966	-0.909362
1	2.974725	-6.485105	-3.077729
1	-1.481004	-1.868849	-3.298164
6	-2.348895	-2.579973	-4.144378
6	-0.918877	-0.669380	-3.756288
6	-2.648724	-2.101859	-5.419966
1	-2.794199	-3.511901	-3.812630
6	-1.210420	-0.201590	-5.040234
1	-0.280616	-0.081378	-3.108939
6	-2.074314	-0.912436	-5.874135
1	-3.327591	-2.661319	-6.057715
1	-0.765790	0.725837	-5.384013
1	-2.302158	-0.540622	-6.869359

(4...7)_{si} (si_3) (after dissociation of PPh₃ group)

Number of imaginary frequencies : 0
 Electronic energy : HF=-4333.1392336
 Zero-point correction= 1.285422 (Hartree/Particle)
 Thermal correction to Energy= 1.367724
 Thermal correction to Enthalpy= 1.368668
 Thermal correction to Gibbs Free Energy= 1.161136
 Sum of electronic and zero-point Energies= -4331.853811
 Sum of electronic and thermal Energies= -4331.771510
 Sum of electronic and thermal Enthalpies= -4331.770566
 Sum of electronic and thermal Free Energies= -4331.978098
 Standard State and RRHO Corrected G= -4331.954104

Cartesian Coordinates

6	1.386814	-1.874206	-3.114955
6	0.594118	-0.740739	-2.863465
6	0.837448	0.430362	-3.591970
6	1.840965	0.459300	-4.564462
6	2.621544	-0.670398	-4.808911
6	2.396915	-1.837885	-4.073307
15	-0.793219	-0.920885	-1.653776
6	-1.894091	0.508982	-1.996544
6	-3.167388	0.365741	-2.566152
6	-3.957202	1.489641	-2.810198
6	-3.493423	2.763772	-2.478378
6	-2.236774	2.910541	-1.889919
6	-1.438050	1.791503	-1.648571
45	-0.099185	-1.132796	0.598032
15	-2.213395	-1.515499	1.296333

8	-2.361521	-2.825771	2.009910
6	0.088009	0.123078	2.438534
6	0.955747	-0.948946	2.631449
6	0.128663	0.888549	1.229601
8	0.781284	-3.192341	0.229021
6	1.911255	-2.702265	-0.079966
6	3.041505	-3.604353	-0.430794
6	2.962770	-4.968274	-0.112209
6	4.028022	-5.816878	-0.408810
6	5.171501	-5.311199	-1.036058
6	5.246060	-3.955212	-1.367657
6	4.185755	-3.100650	-1.065489
8	2.061740	-1.428069	-0.098073
8	-3.241331	-1.363906	-0.010134
6	-4.601399	-1.524568	0.203106
6	-5.330828	-0.491429	0.771027
6	-6.718287	-0.735746	1.068287
6	-7.320651	-1.970276	0.649602
6	-6.528425	-2.948369	-0.011326
6	-5.185737	-2.742435	-0.208521
6	-8.695246	-2.205305	0.926458
6	-9.448278	-1.281187	1.615005
6	-8.847084	-0.081968	2.066853
6	-7.521318	0.183554	1.800826
6	-4.656262	0.799570	1.074418
6	-3.489809	0.816749	1.831618
6	-2.882765	2.029105	2.237657
6	-3.381309	3.231949	1.807441
6	-4.504402	3.276950	0.941014
6	-5.152217	2.053299	0.565499
6	-6.242073	2.134467	-0.347185
6	-6.681730	3.347561	-0.830978
6	-6.052557	4.553431	-0.438826
6	-4.981256	4.512375	0.424944
8	-2.922309	-0.356230	2.297281
6	-1.600337	-2.416671	-2.371059
6	-1.936380	-2.434599	-3.735763
6	-2.509771	-3.569701	-4.307981
6	-2.732711	-4.709133	-3.529527
6	-2.377396	-4.706891	-2.179395
6	-1.815798	-3.566200	-1.599837
3	3.688983	-0.166169	0.257949
8	2.987735	1.574850	0.128269
6	2.638319	2.205338	-0.944893
6	1.865495	3.349549	-1.086372
6	1.239021	4.067070	0.027373
6	1.551505	3.799896	1.388199
6	0.899385	4.449744	2.433170
6	-0.090045	5.408757	2.183908
6	-0.397759	5.711711	0.854275
6	0.255497	5.066592	-0.196118
6	1.654021	3.854323	-2.503919
6	2.399206	5.161942	-2.827431
8	5.384454	-0.054369	-0.772427
8	4.235707	-0.796635	1.983566
1	-7.511681	3.376649	-1.531484
1	-6.721591	1.223215	-0.682384
1	-4.472890	5.426176	0.722018
1	-6.408401	5.502834	-0.828579
1	-2.898415	4.158586	2.103283
1	-2.019712	1.991910	2.891199
1	-7.075937	1.102328	2.163670
1	-4.551150	-3.484514	-0.679883
1	-9.435043	0.634139	2.634119
1	-9.137597	-3.140425	0.592261
1	-6.995617	-3.875190	-0.333022
1	-10.496279	-1.474402	1.825385
1	0.240425	1.318345	-3.428338
1	1.196476	-2.801148	-2.585144
1	2.006091	1.371342	-5.130790
1	3.000546	-2.723551	-4.248879
1	3.401731	-0.642796	-5.564214
1	-1.747784	-1.561514	-4.353329
1	-1.543952	-3.584932	-0.552252
1	-2.774264	-3.566037	-5.361527
1	-2.537061	-5.591639	-1.569603
1	-3.173616	-5.595892	-3.976194
1	-3.555674	-0.617285	-2.804009
1	-0.456665	1.928283	-1.205675
1	-4.945380	1.365255	-3.242812

1	-1.876694	3.890922	-1.597485
1	-4.120442	3.633143	-2.648141
1	-0.785479	0.191325	3.078616
1	1.946606	-0.955595	2.202145
1	0.751936	-1.666228	3.421631
1	2.070283	-5.345970	0.375278
1	4.250774	-2.049996	-1.320529
1	3.968136	-6.870545	-0.151823
1	6.130164	-3.561014	-1.860517
1	6.001184	-5.973462	-1.267373
1	2.983857	1.771275	-1.898064
1	2.303635	3.053438	1.598842
1	-0.014526	5.339086	-1.210593
1	1.171538	4.206241	3.458510
1	-1.154007	6.460526	0.628364
1	-0.596522	5.914041	3.001794
1	1.996707	3.083352	-3.203581
1	0.584303	3.988161	-2.723967
1	3.482102	5.016327	-2.735041
1	2.189129	5.505522	-3.848412
1	2.118755	5.966592	-2.139442
1	-0.651582	1.620783	1.063723
1	1.094568	1.123537	0.786038
6	4.113529	-0.943197	3.222377
6	3.620525	-0.001145	5.475583
6	3.853670	-2.451017	5.175203
6	4.254339	-1.263944	6.037782
1	4.015429	0.887973	5.978644
1	4.379241	-3.356784	5.493195
1	5.345465	-1.163697	6.038334
6	5.811426	1.113006	-0.975622
6	6.166968	3.042034	-2.513625
6	6.907899	3.195735	-0.156362
6	6.141110	3.904835	-1.261742
1	7.182692	2.994661	-2.935175
1	7.985134	3.174438	-0.382843
1	6.589553	4.881565	-1.465102
1	2.774324	-2.649202	5.266642
1	3.926673	-1.418871	7.069652
1	2.531585	-0.010058	5.634948
1	6.786541	3.724575	0.795072
1	5.101894	4.060922	-0.951851
1	5.513436	3.465570	-3.283608
7	6.405202	1.834267	0.023359
7	5.679661	1.698905	-2.205442
7	3.902768	0.129302	4.044751
7	4.203986	-2.194353	3.777726
6	4.182264	-3.349320	2.886683
1	3.154413	-3.683183	2.688698
1	4.653085	-3.100375	1.938503
1	4.729420	-4.171652	3.356539
6	3.629026	1.443604	3.476480
1	3.761195	1.430718	2.397860
1	2.594400	1.737795	3.695485
1	4.299087	2.189807	3.919076
6	6.723956	1.206183	1.296503
1	7.813386	1.129835	1.421287
1	6.325164	1.807586	2.121082
1	6.278339	0.216263	1.343358
6	5.174385	0.920727	-3.323646
1	5.988343	0.623857	-4.000692
1	4.675203	0.028491	-2.955778
1	4.453922	1.517071	-3.890399

(4-7)_{st}⁺ (si_3) (after dissociation of PPh₃ group)

Number of imaginary frequencies : 1
 Electronic energy : HF=-4333.1100921
 Zero-point correction= 1.284253 (Hartree/Particle)
 Thermal correction to Energy= 1.366420
 Thermal correction to Enthalpy= 1.367364
 Thermal correction to Gibbs Free Energy= 1.157636
 Sum of electronic and zero-point Energies= -4331.825839
 Sum of electronic and thermal Energies= -4331.743673
 Sum of electronic and thermal Enthalpies= -4331.742728
 Sum of electronic and thermal Free Energies= -4331.952456
 Standard State and RRHO Corrected G= -4331.926682

Cartesian Coordinates

6	-1.780144	2.647477	-2.734692	1	6.838628	3.581322	1.119092
6	-0.725285	1.725577	-2.835408	1	10.280364	0.544888	2.384471
6	-0.810423	0.702069	-3.792620	1	-0.008896	-0.023801	-3.886514
6	-1.916475	0.615117	-4.641043	1	-1.740530	3.442945	-1.998653
6	-2.952918	1.546924	-4.543889	1	-1.961536	-0.177123	-5.383403
6	-2.882899	2.560730	-3.584614	1	-3.688376	3.283368	-3.489457
15	0.668398	1.775294	-1.624919	1	-3.809815	1.482676	-5.208309
6	2.056975	1.032315	-2.594677	1	0.568688	4.106269	-3.525590
6	2.746143	1.745450	-3.586265	1	1.561389	3.405239	0.612836
6	3.758381	1.130276	-4.326700	1	1.147654	6.487794	-3.256905
6	4.086794	-0.207192	-4.094421	1	2.146573	5.781956	0.870687
6	3.405127	-0.925504	-3.109761	1	1.943522	7.341753	-1.059225
6	2.405732	-0.306234	-2.358297	1	2.508502	2.785437	-3.781177
45	0.016229	0.633968	0.388239	1	1.917245	-0.855987	-1.563552
15	2.006853	0.761072	1.358790	1	4.289587	1.699556	-5.084613
8	2.072949	1.738424	2.498148	1	3.667432	-1.958910	-2.907456
6	-0.132870	-1.525011	0.340345	1	4.877360	-0.684600	-4.666553
6	-0.646922	-1.023372	1.581817	1	0.777795	-2.109040	0.341755
6	-0.736745	-1.353564	-0.927517	1	-1.711524	-0.919718	1.718140
8	-0.927970	2.542940	1.186890	1	-0.104513	-1.295092	2.483930
6	-2.038333	2.301202	0.629342	1	-1.725998	4.876887	1.324807
6	-3.042500	3.397158	0.488870	1	-4.559745	2.145397	-0.393097
6	-2.705547	4.697573	0.894924	1	-3.351390	6.744845	1.047330
6	-3.618074	5.739165	0.734843	1	-6.184003	3.998464	-0.677345
6	-4.872955	5.489185	0.169859	1	-5.584301	6.301241	0.046014
6	-5.209991	4.194968	-0.237532	1	-3.611184	-1.822850	-1.626434
6	-4.297649	3.150165	-0.085024	1	-2.328296	-3.637997	1.409488
8	-2.268472	1.140088	0.126296	1	-0.281139	-5.151394	-2.052782
8	3.152278	1.124060	0.188003	1	-1.045707	-5.190854	2.840249
6	4.479278	1.199954	0.557700	1	0.993631	-6.681902	-0.640970
6	5.197817	0.031313	0.750180	1	0.646672	-6.723666	1.829543
6	6.562136	0.143495	1.195387	1	-2.405766	-2.480706	-3.243373
6	7.156074	1.445846	1.315357	1	-1.024046	-3.537494	-3.120268
6	6.377495	2.601308	1.031134	1	-3.967563	-4.431263	-3.113835
6	5.056124	2.483854	0.679062	1	-2.812666	-4.649768	-4.443072
6	8.508373	1.559989	1.738661	1	-2.602231	-5.537232	-2.922821
6	9.249151	0.444330	2.058187	1	-0.180624	-1.633983	-1.813102
6	8.656056	-0.838281	1.976792	1	-1.583294	-0.704198	-1.081912
6	7.351202	-0.984618	1.557902	6	-3.025877	0.097738	3.791784
6	4.534566	-1.283350	0.531670	6	-1.592122	-1.108372	5.445174
6	3.347448	-1.594806	1.189023	6	-1.604622	1.366720	5.382924
6	2.807456	-2.905369	1.157769	6	-1.664092	0.150877	6.294108
6	3.365289	-3.868978	0.356713	1	-1.808351	-1.994514	6.051110
6	4.479077	-3.559259	-0.469232	1	-1.769237	2.286202	5.952742
6	5.076815	-2.257970	-0.379237	1	-2.601646	0.163811	6.861542
6	6.156183	-1.959326	-1.258395	6	-6.094233	-0.800003	-0.480054
6	6.625201	-2.893426	-2.156665	6	-6.763329	-1.934950	-2.584057
6	6.047257	-4.183919	-2.225075	6	-7.515569	-2.845050	-0.398809
6	4.994962	-4.505012	-1.396434	6	-6.895169	-3.196958	-1.743144
8	2.682919	-0.672521	1.965412	1	-7.755558	-1.550956	-2.865034
6	1.059323	3.570509	-1.486260	1	-8.579397	-2.591500	-0.516627
6	0.932021	4.461139	-2.566220	1	-7.516002	-3.933962	-2.260524
6	1.251380	5.811264	-2.413138	1	-0.619125	1.447775	4.901822
6	1.697555	6.290190	-1.178672	1	-0.833909	0.169223	7.005981
6	1.814224	5.414958	-0.096453	1	-0.582878	-1.234963	5.026375
6	1.492321	4.063956	-0.244703	1	-7.458698	-3.699749	0.283239
3	-3.793669	-0.192764	0.907116	1	-5.902314	-3.634376	-1.587849
8	-3.463816	-2.084456	0.374693	1	-6.219373	-2.145994	-3.509639
6	-3.123441	-2.385064	-0.809104	7	-6.805275	-1.726350	0.223248
6	-2.137858	-3.289734	-1.278565	7	-6.011732	-0.924670	-1.839770
6	-1.421731	-4.256270	-0.435462	7	-2.568020	-1.061959	4.354029
6	-1.607200	-4.308223	0.966648	7	-2.649688	1.281420	4.361233
6	-0.873734	-5.183086	1.766218	6	-3.067658	2.547697	3.777600
6	0.074070	-6.044118	1.204474	1	-2.214828	3.059015	3.320263
6	0.267128	-6.016951	-0.180066	1	-3.821926	2.370707	3.015026
6	-0.464886	-5.143307	-0.983995	1	-3.490338	3.190325	4.558937
6	-2.064093	-3.420561	-2.792094	6	-2.935464	-2.354290	3.794934
6	-2.907625	-4.577687	-3.352898	1	-3.484667	-2.223456	2.866161
8	-5.502286	0.148848	0.101036	1	-2.030196	-2.935208	3.588265
8	-3.798681	0.071705	2.797513	1	-3.551828	-2.917032	4.508381
1	7.440326	-2.632586	-2.825830	6	-6.898054	-1.635278	1.673029
1	6.595497	-0.969272	-1.238109	1	-7.948851	-1.561602	1.981089
1	4.531015	-5.486985	-1.446069	1	-6.463259	-2.529405	2.136009
1	6.428391	-4.911644	-2.935764	1	-6.356906	-0.759905	2.025793
1	2.935627	-4.865837	0.324360	6	-5.326153	0.116369	-2.595355
1	1.943668	-3.122521	1.777170	1	-5.982387	0.969232	-2.817326
1	6.912090	-1.974183	1.512133	1	-4.461703	0.481300	-2.043350
1	4.431582	3.348997	0.482796	1	-4.979195	-0.308318	-3.539396
1	9.233254	-1.716438	2.252739				
1	8.943816	2.553222	1.815077				

7_s (si_3) (after dissociation of PPh₃ group)

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-----
Number of imaginary frequencies : 0
Electronic energy : HF=-4333.1456911
Zero-point correction= 1.287851 (Hartree/Particle)
Thermal correction to Energy= 1.369323
Thermal correction to Enthalpy= 1.370267
Thermal correction to Gibbs Free Energy= 1.164047
Sum of electronic and zero-point Energies= -4331.857840
Sum of electronic and thermal Energies= -4331.776368
Sum of electronic and thermal Enthalpies= -4331.775424
Sum of electronic and thermal Free Energies= -4331.981644
Standard State and RRHO Corrected G= -4331.957323

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Cartesian Coordinates

```

-----
6 -1.692790 2.810515 -2.458914
6 -0.594499 1.966983 -2.701084
6 -0.642400 1.106715 -3.810107
6 -1.761723 1.084127 -4.647543
6 -2.848800 1.923585 -4.393159
6 -2.806584 2.791605 -3.297548
15 0.775972 1.869275 -1.461866
6 2.198268 1.285656 -2.493385
6 2.988347 2.148220 -3.266681
6 4.047930 1.647279 -4.027815
6 4.325143 0.278474 -4.035592
6 3.539565 -0.589423 -3.273315
6 2.491197 -0.086789 -2.502244
45 0.078118 0.459173 0.376844
15 2.023875 0.411221 1.400320
8 2.120787 1.204446 2.675670
6 0.091673 -1.539652 -0.237242
6 -0.476681 -1.470462 1.084475
6 -0.650919 -1.805494 -1.552407
8 -0.759112 2.419026 1.381494
6 -1.892318 2.308205 0.852116
6 -2.819739 3.488565 0.869703
6 -2.396783 4.684313 1.470684
6 -3.225838 5.804968 1.467167
6 -4.485509 5.742806 0.862089
6 -4.910197 4.555659 0.258833
6 -4.080181 3.433421 0.257496
8 -2.249508 1.222964 0.254989
8 3.211318 0.915660 0.310399
6 4.527064 0.922898 0.709469
6 5.235444 -0.268187 0.746776
6 6.592980 -0.234148 1.224148
6 7.196944 1.031822 1.534272
6 6.432764 2.223908 1.402930
6 5.116571 2.170425 1.018109
6 8.543514 1.070739 1.988173
6 9.269793 -0.086485 2.158946
6 8.666384 -1.338450 1.890788
6 7.366837 -1.410163 1.437171
6 4.566374 -1.531764 0.332751
6 3.362550 -1.917647 0.916758
6 2.811305 -3.205375 0.684700
6 3.384943 -4.056985 -0.224358
6 4.521251 -3.647993 -0.974687
6 5.119625 -2.374160 -0.696458
6 6.216777 -1.964356 -1.505992
6 6.704353 -2.771181 -2.511702
6 6.127850 -4.039051 -2.763562
6 5.056896 -4.463403 -2.007993
8 2.690187 -1.112351 1.800700
6 1.161992 3.639538 -1.112751
6 0.997966 4.664510 -2.059155
6 1.316517 5.985602 -1.737287
6 1.803694 6.298440 -0.465770
6 1.963482 5.286217 0.484198
6 1.638993 3.965490 0.167554
3 -3.808490 0.248712 1.002649
8 -3.516162 -1.475912 0.050781
6 -2.985018 -1.515614 -1.046845
6 -2.020274 -2.574672 -1.529294
6 -2.004339 -3.843633 -0.683946
6 -3.183280 -4.366840 -0.127333
6 -3.168088 -5.551130 0.612797
6 -1.971806 -6.243367 0.811394
6 -0.794400 -5.744223 0.250235

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6 -0.813280 -4.560583 -0.490260
6 -2.373673 -2.886243 -3.019347
6 -3.787641 -3.418734 -3.261371
8 -5.582623 0.539950 0.314757
8 -3.711373 -0.051027 2.870059
1 7.533406 -2.425624 -3.122955
1 6.656029 -0.987461 -1.343357
1 4.593325 -5.428324 -2.198442
1 6.523821 -4.667442 -3.556234
1 2.959211 -5.041302 -0.400781
1 1.918315 -3.483347 1.234455
1 6.919500 -2.378772 1.247758
1 4.503162 3.061404 0.934430
1 9.231032 -2.253047 2.049824
1 8.986802 2.038729 2.208682
1 6.901217 3.177167 1.633003
1 10.296785 -0.043608 2.510344
1 0.195719 0.451923 -4.026908
1 -1.679685 3.492560 -1.616818
1 -1.776458 0.414929 -5.503750
1 -3.643295 3.452101 -3.087457
1 -3.717282 1.908449 -5.045710
1 0.612354 4.434509 -3.047754
1 1.735843 3.195048 0.923495
1 1.182866 6.768182 -2.479242
1 2.329603 5.523634 1.479421
1 2.049697 7.326602 -0.214551
1 2.793890 3.215454 -3.269539
1 1.916647 -0.756267 -1.875734
1 4.658103 2.330808 -4.612220
1 3.760675 -1.652146 -3.255293
1 5.155054 -0.109411 -4.619688
1 1.089469 -1.958488 -0.286720
1 -1.543146 -1.565406 1.232466
1 0.111847 -1.872114 1.905613
1 -1.412913 4.719944 1.925512
1 -4.412057 2.512828 -0.205705
1 -2.890031 6.727435 1.932689
1 -5.886907 4.503475 -0.214627
1 -5.131215 6.616815 0.859033
1 -3.134429 -0.686763 -1.763757
1 -4.121691 -3.840919 -0.256831
1 0.117232 -4.192563 -0.907753
1 -4.094394 -5.928399 1.037774
1 0.144344 -6.273712 0.390228
1 -1.957708 -7.160779 1.393208
1 -2.232997 -1.962825 -3.596154
1 -1.632219 -3.603772 -3.387841
1 -4.546849 -2.710020 -2.911865
1 -3.954928 -3.579310 -4.331650
1 -3.955732 -4.371068 -2.750347
1 0.015525 -2.376044 -2.210039
1 -0.833674 -0.870533 -2.092079
6 -2.716429 -0.322758 3.600558
6 -1.224411 -2.030255 4.666050
6 -0.715418 0.388661 4.866393
6 -0.812032 -0.925642 5.627538
1 -1.520047 -2.930344 5.217504
1 -0.515906 1.217056 5.551915
1 -1.554770 -0.827703 6.427848
6 -6.200914 -0.389417 -0.264506
6 -7.105648 -1.370650 -2.360395
6 -7.760493 -2.317318 -0.156079
6 -7.318101 -2.654750 -1.572190
1 -8.066775 -0.869699 -2.551152
1 -8.778501 -1.898977 -0.157305
1 -8.074244 -3.274037 -2.063303
1 0.095124 0.369550 4.124988
1 0.149855 -1.176075 6.084467
1 -0.381587 -2.306617 4.017847
1 -7.779351 -3.218553 0.463900
1 -6.383279 -3.224633 -1.538521
1 -6.651772 -1.587746 -3.332163
7 -6.827296 -1.368257 0.456349
7 -6.203905 -0.472904 -1.633374
7 -2.356249 -1.622544 3.829533
7 -1.991645 0.661523 4.199614
6 -2.390221 2.058193 4.100522
1 -1.599802 2.641563 3.622918
1 -3.295965 2.142345 3.504308

```

1	-2.582287	2.461714	5.103191	6	-1.405036	-1.192778	3.598490
6	-3.048772	-2.714309	3.159115	6	-1.177614	-1.992314	4.725542
1	-3.701780	-2.327692	2.382218	6	-0.902601	-1.404525	5.965486
1	-2.317649	-3.384888	2.695709	6	-0.870873	-0.016021	6.094704
1	-3.641792	-3.293947	3.879423	6	-1.107357	0.787048	4.974557
6	-6.883186	-1.242062	1.909852	6	-1.365227	0.206330	3.735145
1	-7.742996	-0.637479	2.231480	3	3.726591	1.802860	0.301521
1	-6.984686	-2.241929	2.340850	8	4.322894	-0.047777	0.193930
1	-5.968866	-0.788540	2.289798	6	4.354959	-1.015481	0.996379
6	-5.612306	0.618294	-2.399013	6	4.392512	-2.413195	0.720962
1	-6.327167	1.435101	-2.572320	6	4.564266	-2.965049	-0.630586
1	-4.745839	1.020100	-1.878786	6	4.312443	-2.195323	-1.794216
1	-5.287525	0.230974	-3.367904	6	4.398524	-2.756819	-3.068063
				6	4.739823	-4.100482	-3.241313
(4-7) _{si-a} ⁺ (si_4)				6	4.991703	-4.878946	-2.107717
				6	4.902481	-4.324985	-0.831541
Number of imaginary frequencies : 1				6	4.702629	-3.278419	1.934357
Electronic energy : HF=-5369.506331				6	6.206188	-3.424574	2.223881
Zero-point correction= 1.562700 (Hartree/Particle)				8	4.869458	2.940803	1.410127
Thermal correction to Energy= 1.660990				8	4.128370	2.522632	-1.425006
Thermal correction to Enthalpy= 1.661934				1	-6.903884	5.598001	2.102188
Thermal correction to Gibbs Free Energy= 1.422623				1	-4.700110	4.920020	1.288168
Sum of electronic and zero-point Energies= -5367.943631				1	-8.759702	2.474334	-0.200678
Sum of electronic and thermal Energies= -5367.845341				1	-8.963456	4.406068	1.344432
Sum of electronic and thermal Enthalpies= -5367.844397				1	-7.373631	0.933331	-1.523855
Sum of electronic and thermal Free Energies= -5368.083708				1	-5.121813	0.093376	-2.134069
Standard State and RRHO Corrected G= -5368.062245				1	-4.790745	5.128670	-1.717755
				1	0.187267	3.536125	1.138112
Cartesian Coordinates				1	-4.683008	7.477979	-2.395460
				1	-0.880118	7.912685	-0.433112
6	-0.578800	-4.221034	2.428453	1	0.188468	5.990137	0.624593
6	-1.819810	-3.669526	2.059316	1	-2.744914	8.904535	-1.730899
6	-2.830846	-4.535696	1.613835	1	-3.784750	-4.142434	1.284428
6	-2.613574	-5.915894	1.563627	1	0.230109	-3.569201	2.741390
6	-1.385654	-6.453181	1.952087	1	-3.407877	-6.565684	1.207441
6	-0.366110	-5.597815	2.383746	1	0.598875	-6.001486	2.677389
15	-1.966858	-1.835713	1.950779	1	-1.218701	-7.525725	1.911051
6	-3.755721	-1.447290	2.259354	1	-1.227594	-3.073464	4.655127
6	-4.603253	-2.266304	3.020620	1	-1.524741	0.836297	2.866420
6	-5.909003	-1.862033	3.304320	1	-0.725326	-2.038517	6.830234
6	-6.374510	-0.621026	2.861678	1	-1.072508	1.869482	5.062095
6	-5.521627	0.219698	2.143122	1	-0.658238	0.439012	7.058021
6	-4.222622	-0.192426	1.842084	1	-4.251291	-3.219143	3.400947
45	-0.557179	-1.036101	-0.033623	1	-3.570560	0.471966	1.286929
15	-1.346625	0.984537	-0.764672	1	-6.557850	-2.513992	3.883045
8	-0.497479	1.797715	-1.699923	1	-5.863112	1.194147	1.811940
6	1.525409	-2.200284	-0.380450	1	-7.389669	-0.305679	3.086381
6	1.287474	-0.956633	-1.068037	1	1.448117	-3.099011	-0.976627
6	2.072226	-2.393749	0.892864	1	1.763954	-0.046096	-0.727850
8	0.480007	-0.011592	1.545539	1	1.234179	-1.032153	-2.150856
6	1.385887	0.880695	1.679424	1	1.398312	-1.055209	3.614824
6	2.017693	0.925643	3.055724	1	2.760035	2.924190	2.797470
6	1.967864	-0.183708	3.912189	1	2.581738	-1.026196	5.794092
6	2.623101	-0.157535	5.142990	1	3.871892	3.007423	5.016674
6	3.311785	0.990981	5.544940	1	3.816731	1.015472	6.506967
6	3.342357	2.110151	4.708225	1	4.307094	-0.784777	2.077554
6	2.707480	2.073900	3.465753	1	4.046455	-1.154806	-1.684014
8	1.802795	1.673136	0.801018	1	5.099644	-4.966142	0.020620
8	-1.723496	1.885681	0.629090	1	4.187321	-2.133839	-3.934256
6	-1.796668	3.242955	0.373877	1	5.257978	-5.927805	-2.215636
6	-2.936299	3.754290	-0.222747	1	4.807583	-4.532958	-4.235925
6	-2.907645	5.134873	-0.640077	1	4.218816	-2.832570	2.812982
6	-1.769387	5.947049	-0.307917	1	4.252472	-4.272421	1.824591
6	-0.669317	5.367841	0.383105	1	6.653357	-2.445500	2.431479
6	-0.668101	4.030893	0.691509	1	6.385405	-4.069074	3.093140
6	-1.744958	7.312113	-0.704420	1	6.738913	-3.853911	1.369070
6	-2.778675	7.861483	-1.429163	1	2.126208	-3.409425	1.269218
6	-3.880535	7.053815	-1.798174	1	2.053680	-1.619487	1.638809
6	-3.943452	5.731507	-1.413944	6	3.611442	2.155874	-2.509734
6	-4.126347	2.882698	-0.447514	6	1.670593	2.228530	-4.088535
6	-4.053501	1.655157	-1.113078	6	3.764102	0.991494	-4.662585
6	-5.239613	0.985399	-1.529871	6	2.241494	0.928865	-4.646715
6	-6.479522	1.453119	-1.189956	1	0.634171	2.088569	-3.772143
6	-6.608940	2.597440	-0.358227	1	4.187363	0.046673	-5.014784
6	-5.423736	3.304346	0.033202	1	1.935370	0.085307	-4.020268
6	-5.579869	4.392897	0.938922	6	6.096206	2.999680	1.150742
6	-6.822663	4.772355	1.400544	6	8.414914	2.114837	1.455237
6	-7.989608	4.093177	0.978852	6	8.027060	4.189480	0.151007
6	-7.877125	3.023712	0.118015	6	8.753541	2.851949	0.168323
8	-2.911073	1.009963	-1.483802	1	8.903953	2.596844	2.315916

1	8.418454	4.852320	0.938703	6	-3.080720	2.187621	-3.368927
1	9.834554	3.004606	0.098899	6	-3.002179	3.447148	-2.760221
1	4.114150	1.784778	-5.342822	6	-3.739156	4.521451	-3.261231
1	1.852832	0.757998	-5.654709	6	-4.575250	4.344728	-4.367106
1	1.693498	3.015224	-4.856713	6	-4.663298	3.088772	-4.976378
1	8.178055	4.697246	-0.806337	6	-2.289479	0.994254	-2.864211
1	8.436230	2.256456	-0.695249	8	-2.155779	0.014090	-3.607254
1	8.777856	1.081806	1.413920	8	-1.818738	1.159335	-1.667061
7	6.591757	3.973058	0.324818	45	-0.737194	-0.111359	-0.354392
7	6.968409	2.076175	1.667126	6	0.873022	0.278470	-2.006263
7	2.429049	2.683700	-2.918524	6	0.227214	-0.998906	-2.063246
7	4.236701	1.221074	-3.300147	6	2.141863	0.522931	-1.442858
6	5.604472	0.845619	-2.964094	15	-2.498855	-1.624975	-0.276932
1	6.334526	1.593521	-3.308200	8	-2.219707	-3.064294	-0.630025
1	5.694287	0.726537	-1.885294	15	-1.185467	1.949732	1.145318
1	5.832459	-0.110362	-3.441264	6	0.069010	3.259964	0.744354
6	1.797823	3.678570	-2.048001	6	0.337715	3.462768	-0.622236
1	1.379210	3.205623	-1.159377	6	1.252694	4.431614	-1.031758
1	2.525301	4.442893	-1.762030	6	1.923409	5.211365	-0.083010
1	0.984341	4.149782	-2.601824	6	1.663199	5.018183	1.274324
6	5.694346	5.022908	-0.138372	6	0.736310	4.054256	1.686941
1	5.677123	5.876661	0.554892	8	-3.526137	-1.776290	1.113107
1	6.040273	5.378041	-1.113562	6	-4.633786	-1.024645	1.376308
1	4.690291	4.621441	-0.249809	6	-5.753359	-1.006323	0.541112
6	6.504513	1.118116	2.659002	6	-6.819618	-0.088266	0.850237
1	7.013634	1.288001	3.617790	6	-6.789720	0.658651	2.075258
1	5.432681	1.227899	2.802260	6	-5.684739	0.497427	2.950763
1	6.720807	0.095768	2.329389	6	-4.628470	-0.300585	2.596039
15	-1.575046	-2.269143	-1.724576	6	-7.832106	1.579358	2.365424
6	-3.225977	-2.991506	-1.345992	6	-8.860503	1.791449	1.474832
6	-3.595417	-4.308996	-1.661073	6	-8.878737	1.084413	0.248550
6	-4.179456	-2.134635	-0.785848	6	-7.891954	0.169957	-0.052458
6	-4.888869	-4.757798	-1.388101	6	-5.800501	-1.853742	-0.680982
1	-2.883125	-4.988308	-2.114369	6	-4.756799	-1.768877	-1.589017
6	-5.472682	-2.581220	-0.514935	6	-4.763420	-2.453570	-2.826075
1	-3.903313	-1.116288	-0.556051	6	-5.819435	-3.271439	-3.142293
6	-5.828097	-3.899000	-0.808787	6	-6.885046	-3.467838	-2.220115
1	-5.161105	-5.781849	-1.627738	6	-6.874829	-2.766305	-0.966342
1	-6.186637	-1.900083	-0.062264	6	-7.923640	-3.036152	-0.042271
1	-6.831005	-4.255631	-0.591596	6	-8.938037	-3.917296	-0.349676
6	-0.547299	-3.727469	-2.180402	6	-8.963612	-4.579812	-1.600439
6	0.232611	-3.737769	-3.344307	6	-7.953219	-4.359815	-2.510163
6	-0.424748	-4.785888	-1.262973	8	-3.679093	-0.968118	-1.298644
6	1.131204	-4.782593	-3.579184	6	-1.298481	1.967627	2.999720
1	0.160183	-2.926418	-4.060530	6	-2.549173	2.096535	3.628550
6	0.460058	-5.833092	-1.508962	6	-2.672964	1.970235	5.014161
1	-1.003358	-4.779917	-0.347630	6	-1.549115	1.725090	5.805088
6	1.248492	-5.829432	-2.664489	6	-0.297251	1.614201	5.196017
1	1.745652	-4.769388	-4.474238	6	-0.174103	1.729193	3.811201
1	0.543741	-6.641723	-0.788568	6	-2.746810	2.844912	0.713859
1	1.955883	-6.633391	-2.845184	6	-3.845339	2.138799	0.209188
6	-1.891071	-1.472428	-3.364963	6	-5.048711	2.797382	-0.052610
6	-2.935602	-1.930739	-4.185860	6	-5.164816	4.168471	0.178783
6	-1.058036	-0.447706	-3.835286	6	-4.070610	4.883541	0.674371
6	-3.146403	-1.367972	-5.444859	6	-2.869080	4.225559	0.942195
1	-3.592731	-2.724151	-3.847770	6	3.743602	0.431730	-2.963651
6	-1.272092	0.111550	-5.096978	6	3.761704	-0.989038	-3.394859
1	-0.271375	-0.050945	-3.209658	6	4.792786	-1.881585	-3.031552
6	-2.314972	-0.344018	-5.904328	6	4.810780	-3.193537	-3.501115
1	-3.963224	-1.729302	-6.063434	6	3.790494	-3.670186	-4.328230
1	-0.628007	0.914617	-5.440874	6	2.754223	-2.806558	-4.689071
1	-2.482547	0.098424	-6.882389	6	2.744889	-1.486254	-4.237525
				6	4.601285	0.921961	-1.946620
(4-7) _{re-aa} [*] ($\Phi_1 = -65.8^\circ$)				8	5.187478	0.254976	-1.049092
				6	3.253262	1.469117	-3.964095
Number of imaginary frequencies : 1				6	4.146957	1.591438	-5.206816
Electronic energy : HF=-5369.4974206				3	5.901389	0.324596	0.656362
Zero-point correction= 1.563343 (Hartree/Particle)				8	6.286171	-1.305690	1.410312
Thermal correction to Energy= 1.661668				8	6.797808	1.935255	1.063625
Thermal correction to Enthalpy= 1.662612				1	-9.674626	1.269318	-0.467664
Thermal correction to Gibbs Free Energy= 1.422669				1	-7.917380	-0.346287	-1.004458
Sum of electronic and zero-point Energies= -5367.934077				1	-7.788913	2.130468	3.301772
Sum of electronic and thermal Energies= -5367.835753				1	-9.646422	2.506378	1.701212
Sum of electronic and thermal Enthalpies= -5367.834809				1	-5.664823	1.049264	3.887023
Sum of electronic and thermal Free Energies= -5368.074752				1	-3.759750	-0.389741	3.231787
Standard State and RRHO Corrected G= -5368.04698				1	-7.914014	-2.544169	0.923577
				1	-3.925317	-2.292743	-3.495232
Cartesian Coordinates				1	-9.722721	-4.109008	0.377136
				1	-7.950533	-4.875765	-3.467320
6	-3.913354	2.020471	-4.484155	1	-5.844117	-3.797127	-4.093343

1	-9.771860	-5.267407	-1.833265
1	0.535617	3.937136	2.745654
1	-0.181586	2.859928	-1.359018
1	2.169022	5.626494	2.019475
1	1.439519	4.579804	-2.091953
1	2.633586	5.967924	-0.401847
1	-3.757028	1.086066	-0.013720
1	-2.027637	4.791014	1.331310
1	-5.888661	2.236494	-0.448877
1	-4.150831	5.952386	0.853974
1	-6.100610	4.678646	-0.032305
1	-3.438148	2.280578	3.039122
1	0.805643	1.629791	3.367833
1	-3.653513	2.067874	5.472359
1	0.590558	1.429028	5.794147
1	-1.646802	1.624976	6.882376
1	0.420553	1.100132	-2.551499
1	-0.533421	-1.146635	-2.819650
1	0.813677	-1.875547	-1.817785
1	-2.375645	3.573991	-1.886578
1	-3.960139	1.041536	-4.949973
1	-3.670297	5.492554	-2.778434
1	-5.314772	2.944188	-5.834357
1	-5.156741	5.178988	-4.750933
1	4.659345	2.024672	-1.882607
1	5.582261	-1.539975	-2.375700
1	1.930985	-0.837478	-4.539952
1	5.627110	-3.850657	-3.210290
1	1.948261	-3.157168	-5.328511
1	3.801677	-4.696584	-4.684533
1	2.227710	1.240892	-4.274836
1	3.196068	2.442501	-3.459850
1	4.204807	0.639248	-5.744353
1	3.760175	2.347146	-5.900359
1	5.168061	1.877602	-4.927113
1	2.626407	-0.246951	-0.855813
1	2.365387	1.545340	-1.162483
6	6.527316	2.987756	0.421831
6	5.588715	5.279472	0.343912
6	6.567646	4.296020	-1.708602
6	5.367971	5.036802	-1.140619
1	4.704114	5.733710	0.798803
1	6.354490	3.937161	-2.721659
1	4.459322	4.440564	-1.277153
6	6.643206	-2.482505	1.145779
6	6.548266	-4.932007	1.651320
6	8.172644	-4.034675	-0.009499
6	7.172781	-5.144664	0.279042
1	7.249961	-5.224515	2.445323
1	9.030520	-4.096043	0.677131
1	7.669183	-6.118746	0.249662
6	8.130039	-1.589074	-0.550512
1	7.371467	-0.878603	-0.879970
1	8.848688	-1.071629	0.099074
1	8.658156	-1.951554	-1.434658
6	5.231785	-3.307553	2.963134
1	5.056205	-2.242209	3.082847
1	4.275542	-3.804587	2.764175
1	5.652035	-3.713644	3.891712
6	5.690350	4.020581	2.471934
1	5.839213	3.018664	2.867270
1	6.429311	4.695854	2.925254
1	4.689694	4.372890	2.741132
6	7.769940	2.151752	-1.520669
1	8.125582	1.433500	-0.785747
1	7.240460	1.616321	-2.315651
1	8.631092	2.669977	-1.959290
1	8.557845	-4.121942	-1.028448
1	6.397959	-5.140295	-0.494331
1	5.653070	-5.553577	1.762255
1	6.434637	5.964406	0.506814
1	5.232203	5.985981	-1.666391
1	7.442116	4.959176	-1.772297
7	5.828181	4.003787	1.020303
7	6.897290	3.129772	-0.884131
7	6.151660	-3.535913	1.857772
7	7.509594	-2.732665	0.113795
15	0.513011	-1.397064	1.152335
6	1.798616	-0.478101	2.125538
6	2.324908	-1.009794	3.314783

6	2.278893	0.757347	1.677508
6	3.308615	-0.319760	4.025523
1	1.964764	-1.959220	3.696491
6	3.277256	1.440730	2.374283
1	1.845809	1.214745	0.802580
6	3.795871	0.904029	3.553918
1	3.696658	-0.740907	4.948515
1	3.619964	2.398450	1.999469
1	4.562913	1.437072	4.108074
6	-0.377494	-2.273504	2.515022
6	-0.097358	-3.598683	2.882865
6	-1.295743	-1.540184	3.278168
6	-0.727922	-4.173062	3.989248
1	0.613765	-4.188435	2.316831
6	-1.906821	-2.106956	4.395645
1	-1.533014	-0.523921	2.998230
6	-1.629060	-3.428207	4.752109
1	-0.506244	-5.202698	4.255960
1	-2.606279	-1.517071	4.980737
1	-2.112086	-3.874327	5.616986
6	1.503543	-2.748186	0.380889
6	0.817398	-3.811951	-0.234776
6	2.903603	-2.717406	0.335990
6	1.528255	-4.834061	-0.861812
1	-0.269335	-3.813406	-0.249686
6	3.605576	-3.733537	-0.317587
1	3.459760	-1.907446	0.794179
6	2.924664	-4.796186	-0.908711
1	0.987182	-5.650885	-1.331571
1	4.684292	-3.676693	-0.376214
1	3.476250	-5.580697	-1.418896

(4-7)_{re-aa}[‡] ($\Phi_1 = 50.0^\circ$)

Number of imaginary frequencies : 1
 Electronic energy : HF=-5369.5048683
 Zero-point correction= 1.562975 (Hartree/Particle)
 Thermal correction to Energy= 1.661246
 Thermal correction to Enthalpy= 1.662190
 Thermal correction to Gibbs Free Energy= 1.423105
 Sum of electronic and zero-point Energies= -5367.941893
 Sum of electronic and thermal Energies= -5367.843622
 Sum of electronic and thermal Enthalpies= -5367.842678
 Sum of electronic and thermal Free Energies= -5368.081763
 Standard State and RRHO Corrected G= -5368.054952

Cartesian Coordinates

6	-1.414947	-1.603170	4.958660
6	-1.568994	-0.667734	3.926656
6	-2.810252	-0.040212	3.755458
6	-3.880439	-0.347207	4.597932
6	-3.721350	-1.287960	5.619740
6	-2.483783	-1.914887	5.799552
6	-0.397846	-0.402828	2.996979
8	0.669105	-0.991864	3.188371
8	-0.671136	0.450105	2.061945
45	0.267040	1.084239	0.267302
6	-2.167977	1.070926	-0.250846
6	-1.339292	-0.046022	-0.598862
6	-2.743760	1.940303	-1.188537
15	1.487535	-0.862949	0.099880
8	0.745904	-2.111998	0.479354
15	1.197204	2.842788	1.814387
6	-0.092079	4.090414	2.281217
6	-1.433578	3.675032	2.261182
6	-2.458463	4.555575	2.608769
6	-2.158220	5.868280	2.983657
6	-0.825677	6.284320	3.030773
6	0.201552	5.399778	2.691940
8	2.121575	-1.244623	-1.470949
6	3.401541	-1.462803	-1.887878
6	4.392170	-2.119341	-1.153186
6	5.733148	-2.131918	-1.690386
6	5.981287	-1.667948	-3.024115
6	4.894519	-1.159887	-3.783833
6	3.654110	-1.036781	-3.221027
6	7.300436	-1.695682	-3.549309
6	8.359365	-2.138448	-2.787527
6	8.129671	-2.563675	-1.457943

6	6.856674	-2.563041	-0.927450
6	4.109892	-2.783109	0.149765
6	3.483107	-2.079250	1.163870
6	3.258655	-2.618845	2.450558
6	3.657935	-3.903242	2.723580
6	4.221163	-4.718300	1.702764
6	4.428636	-4.167811	0.392253
6	4.886179	-5.045066	-0.631511
6	5.152903	-6.372331	-0.371227
6	4.986694	-6.899965	0.931555
6	4.527364	-6.085490	1.942768
8	2.999390	-0.812001	0.896089
6	2.681838	3.874345	1.381398
6	3.974359	3.475795	1.763534
6	5.099001	4.182697	1.336004
6	4.958677	5.304875	0.517235
6	3.680228	5.719698	0.141696
6	2.554630	5.013407	0.568520
6	1.686532	2.170432	3.466959
6	2.554765	1.069219	3.510876
6	3.016017	0.580185	4.733516
6	2.584090	1.153957	5.930249
6	1.690734	2.227257	5.896896
6	1.251124	2.739405	4.673764
6	-4.699554	1.121637	-1.888349
6	-5.360836	0.817359	-0.603080
6	-4.974532	-0.279633	0.204189
6	-5.586335	-0.535215	1.430822
6	-6.604799	0.292994	1.908593
6	-6.987398	1.397095	1.140971
6	-6.375124	1.656886	-0.085303
6	-4.004443	0.138405	-2.652399
8	-3.639935	-1.009934	-2.306923
6	-5.188086	2.306220	-2.712408
6	-6.501257	2.037495	-3.467125
3	-3.439610	-2.749210	-1.763188
8	-2.003777	-3.560958	-1.010918
8	-5.087820	-3.640199	-1.933886
1	8.965697	-2.887990	-0.844156
1	6.709051	-2.880922	0.097814
1	7.458660	-1.345165	-4.566522
1	9.365875	-2.149458	-3.196153
1	5.069275	-0.828002	-4.803667
1	2.834242	-0.594244	-3.772415
1	5.008950	-4.662643	-1.637863
1	2.723664	-2.008290	3.166847
1	5.488750	-7.020694	-1.175888
1	4.372335	-6.481577	2.943517
1	3.498243	-4.331902	3.709724
1	5.207442	-7.945782	1.125778
1	1.230386	5.738698	2.746154
1	-1.669664	2.658470	1.969685
1	-0.581000	7.298482	3.334536
1	-3.490158	4.215070	2.582323
1	-2.955433	6.558869	3.244404
1	2.844260	0.571189	2.594299
1	0.568671	3.581960	4.670281
1	3.689805	-0.272131	4.745710
1	1.337699	2.674187	6.822433
1	2.931234	0.761939	6.882540
1	4.116068	2.608973	2.398124
1	1.575416	5.365625	0.273850
1	6.086440	3.851001	1.645167
1	3.549221	6.594561	-0.488829
1	5.834837	5.852022	0.180797
1	-2.565125	1.099421	0.756924
1	-1.389808	-0.938304	0.012809
1	-1.222975	-0.267444	-1.652106
1	-2.933348	0.676051	2.951712
1	-0.448021	-2.080327	5.077837
1	-4.839104	0.141427	4.447851
1	-2.354124	-2.645800	6.593463
1	-4.555778	-1.531151	6.272293
1	-3.701453	0.483623	-3.658567
1	-4.176609	-0.922289	-0.130196
1	-6.702390	2.524165	-0.647299
1	-5.249925	-1.381488	2.022639
1	-7.770053	2.062717	1.496275
1	-7.083998	0.088545	2.861987
1	-5.300755	3.191827	-2.076747

1	-4.411890	2.566552	-3.442529
1	-7.306695	1.748088	-2.784735
1	-6.829880	2.925699	-4.019794
1	-6.369322	1.222710	-4.187901
1	-2.310556	2.033145	-2.176959
1	-3.272717	2.819547	-0.839864
6	-6.206939	-3.089732	-1.739900
6	-8.104073	-1.695665	-2.546005
6	-8.177540	-2.680102	-0.267152
6	-8.397266	-1.414710	-1.080687
1	-8.108265	-0.764346	-3.121547
1	-8.216762	-2.453146	0.803082
1	-7.730477	-0.628818	-0.718173
6	-1.289410	-4.029267	-0.086720
6	0.828502	-5.101929	0.632323
6	-0.712835	-4.123416	2.312390
6	0.164087	-5.322430	1.981950
1	1.344198	-6.010032	0.300505
1	-1.287102	-4.305062	3.226496
1	-0.444664	-6.234605	1.962388
6	-2.800529	-3.033146	1.527862
1	-2.516764	-1.975195	1.524326
1	-3.606117	-3.184046	0.810668
1	-3.173892	-3.283227	2.524167
6	0.405650	-4.559008	-1.720847
1	-0.381970	-4.541017	-2.473147
1	0.970532	-3.618522	-1.762510
1	1.081353	-5.392406	-1.933932
6	-6.197389	-2.210954	-4.027131
1	-5.248390	-2.739965	-4.055334
1	-6.877098	-2.650732	-4.769190
1	-6.026859	-1.161601	-4.290096
6	-6.332269	-4.152351	0.462599
1	-5.411235	-4.609595	0.108399
1	-6.130607	-3.603854	1.390002
1	-7.062293	-4.942400	0.680156
1	-0.106487	-3.221451	2.450838
1	0.934953	-5.445416	2.748784
1	1.558787	-4.290951	0.702711
1	-8.869731	-2.355520	-2.981211
1	-9.428357	-1.068783	-0.964051
1	-8.959400	-3.425338	-0.476302
7	-6.780615	-2.302727	-2.697042
7	-6.860743	-3.252310	-0.551814
7	-0.164858	-4.749547	-0.390194
7	-1.673079	-3.905447	1.220726
15	0.940853	2.080886	-1.710404
6	0.561647	3.900813	-1.742891
6	1.323390	4.821057	-2.481443
6	-0.537161	4.377434	-1.013376
6	0.993387	6.177199	-2.483133
1	2.190794	4.495104	-3.041711
6	-0.864740	5.734485	-1.009039
1	-1.121442	3.690498	-0.419551
6	-0.098205	6.640735	-1.743685
1	1.600723	6.873565	-3.054527
1	-1.705615	6.077860	-0.413335
1	-0.343223	7.699078	-1.736046
6	2.725867	2.021013	-2.155120
6	3.158853	2.285293	-3.466409
6	3.679404	1.777908	-1.159375
6	4.520702	2.342589	-3.760938
1	2.433166	2.444659	-4.258276
6	5.041814	1.821530	-1.459901
1	3.361772	1.538230	-0.153374
6	5.465716	2.113385	-2.756731
1	4.842854	2.550226	-4.777499
1	5.767873	1.619613	-0.678406
1	6.526316	2.141991	-2.989479
6	0.108335	1.500988	-3.263305
6	0.148032	0.135042	-3.592483
6	-0.597751	2.376969	-4.102348
6	-0.508295	-0.340606	-4.728069
1	0.679062	-0.558619	-2.951835
6	-1.258744	1.896265	-5.236859
1	-0.644600	3.435806	-3.875281
6	-1.219510	0.536937	-5.551665
1	-0.470409	-1.401107	-4.960971
1	-1.803889	2.589340	-5.871608
1	-1.737152	0.163717	-6.430834

(4-7) _{re-aa} ⁺ ($\Phi_1 = 70.4^\circ$)			
Number of imaginary frequencies : 1			
Electronic energy : HF=-5369.5043512			
Zero-point correction= 1.563495			
(Hartree/Particle)			
Thermal correction to Energy= 1.661604			
Thermal correction to Enthalpy= 1.662548			
Thermal correction to Gibbs Free Energy= 1.425200			
Sum of electronic and zero-point Energies= -5367.940856			
Sum of electronic and thermal Energies= -5367.842747			
Sum of electronic and thermal Enthalpies= -5367.841803			
Sum of electronic and thermal Free Energies= -5368.079151			
Standard State and RRHO Corrected G= -5368.053109			
Cartesian Coordinates			
8	-1.745904	4.008592	0.274197
3	-1.343891	3.155944	-1.309991
8	1.054477	1.210073	2.734682
6	0.025514	0.602586	2.391573
8	-0.132374	-0.108837	1.323331
45	1.362091	-0.494070	-0.110206
15	2.675819	-1.637841	1.753635
6	1.896360	-1.691060	3.442764
6	0.551887	-2.075117	3.520918
6	-0.072304	-2.253392	4.755219
6	0.642444	-2.053226	5.937093
6	1.987659	-1.681853	5.870575
6	2.614038	-1.508430	4.634148
6	-1.197465	0.641316	3.279381
6	-2.351397	-0.084013	2.954875
6	-3.458721	-0.063085	3.804098
6	-3.411892	0.662922	4.998288
6	-2.252826	1.368206	5.339433
6	-1.152326	1.357392	4.481973
15	-0.180498	-1.875826	-1.143598
8	0.101638	-2.453473	-2.507618
6	0.426517	1.154685	-1.121452
6	1.273903	2.012513	-0.345290
6	2.409616	2.677034	-0.843630
8	-1.614495	-0.970218	-1.192571
6	-2.649107	-1.518607	-1.910792
6	-3.454786	-2.473447	-1.311922
6	-4.474378	-3.097793	-2.115764
6	-4.683695	-2.641871	-3.462955
6	-3.855621	-1.613841	-3.993347
6	-2.843847	-1.075734	-3.239693
6	-5.708297	-3.233988	-4.250281
6	-6.482807	-4.259390	-3.755561
6	-6.247859	-4.744963	-2.447129
6	-5.272469	-4.181927	-1.652114
6	-3.202615	-2.847614	0.107687
6	-1.931786	-3.251451	0.525373
6	-1.736157	-3.823099	1.810420
6	-2.760610	-3.883785	2.719480
6	-4.033938	-3.339551	2.403770
6	-4.254251	-2.804483	1.090988
6	-5.521660	-2.210693	0.824006
6	-6.511164	-2.167755	1.783335
6	-6.298095	-2.728342	3.065842
6	-5.080564	-3.300069	3.363913
8	-0.838074	-3.235354	-0.289613
6	4.306046	-0.855413	2.098402
6	4.295568	0.422147	2.691993
6	5.489307	1.110003	2.906281
6	6.709493	0.545306	2.518212
6	6.724459	-0.707710	1.905134
6	5.531198	-1.404231	1.693604
6	2.993039	-3.466726	1.694553
6	3.970399	-4.096804	2.484964
6	4.035667	-5.488013	2.555981
6	3.105530	-6.273719	1.867717
6	2.114686	-5.656258	1.105398
6	2.064478	-4.262648	1.013096
8	-0.114417	3.920245	-2.499837
6	1.119921	4.063211	-2.691738
6	2.089801	4.620015	-1.813075
6	1.718116	5.560050	-0.719387

6	2.650071	5.879199	0.291288
6	2.357212	6.811771	1.286072
6	1.121106	7.463893	1.300401
6	0.184783	7.160498	0.309674
6	0.474561	6.221394	-0.680632
6	3.487937	4.779743	-2.405246
6	3.721640	6.147744	-3.061968
8	-2.712746	2.114610	-2.030704
1	-7.463599	-1.698662	1.551606
1	-5.701803	-1.774894	-0.150834
1	-4.892905	-3.717745	4.349956
1	-7.087873	-2.696264	3.810876
1	-2.601052	-4.329641	3.697323
1	-0.753094	-4.217415	2.041407
1	-5.101558	-4.576373	-0.657629
1	-2.186131	-0.302829	-3.619728
1	-6.838071	-5.574159	-2.066753
1	-5.860139	-2.864824	-5.261716
1	-4.023227	-1.276362	-5.012626
1	-7.260155	-4.706300	-4.368829
1	5.562394	-2.371408	1.206457
1	3.345961	0.870985	2.969793
1	7.664665	-1.148033	1.584688
1	5.466326	2.091187	3.372874
1	7.638261	1.084006	2.683866
1	-0.021822	-2.193896	2.612962
1	3.661586	-1.230327	4.610454
1	-1.123427	-2.524773	4.783350
1	2.557276	-1.529284	6.783628
1	0.157159	-2.182781	6.900591
1	4.670906	-3.505789	3.065326
1	1.285320	-3.799731	0.422225
1	4.803565	-5.958545	3.164198
1	1.381050	-6.252571	0.569788
1	3.151222	-7.357294	1.933877
1	0.934328	2.302803	0.640585
1	-0.611979	1.060573	-0.823057
1	0.552403	1.132201	-2.199161
1	-2.362963	-0.669486	2.043898
1	-0.240440	1.886087	4.736662
1	-4.349941	-0.623701	3.540199
1	-2.207842	1.923562	6.272511
1	-4.270925	0.672138	5.664130
1	1.542657	3.628998	-3.618238
1	3.622316	5.395685	0.297844
1	-0.266162	5.995944	-1.435959
1	3.099128	7.031334	2.049617
1	-0.782461	7.656895	0.304698
1	0.892227	8.193655	2.072206
1	4.250735	4.612315	-1.635621
1	3.648147	3.989858	-3.149877
1	3.599746	6.959935	-2.337770
1	4.732870	6.216511	-3.479688
1	3.006030	6.316509	-3.875009
1	2.914302	2.289364	-1.714607
1	3.068395	3.168601	-0.136127
15	2.942994	-0.930425	-1.810802
6	-3.913504	1.749689	-2.048823
6	-5.988331	1.109993	-0.916593
6	-5.967165	1.216832	-3.398688
6	-6.407599	0.393745	-2.193365
1	-6.249361	0.524229	-0.033236
1	-5.929371	0.583207	-4.293344
1	-5.931255	-0.590023	-2.214677
6	-2.296492	4.305198	1.359235
6	-2.131644	4.768313	3.807266
6	-4.307113	4.989644	2.635384
6	-3.610773	4.420705	3.862321
1	-1.579916	4.198846	4.561702
1	-5.356451	4.679813	2.607589
1	-3.732774	3.332955	3.878272
1	-6.494153	2.083643	-0.831392
1	-7.491316	0.247371	-2.225373
1	-6.686877	2.022400	-3.599266
1	-1.973538	5.836331	4.018324
1	-4.054839	4.826709	4.775920
1	-4.289331	6.090764	2.650479
7	-1.563383	4.443781	2.498197
7	-3.659171	4.482697	1.426856
7	-4.538163	1.284623	-0.931038

7	-4.642507	1.819302	-3.205261	6	-0.156009	0.892741	-2.420358
6	-3.793272	1.088113	0.306098	6	-1.548776	2.611486	-1.104987
1	-2.749150	0.881134	0.083215	6	-3.345167	3.761736	-2.128622
1	-3.857333	1.956620	0.970129	6	-2.729311	4.142639	-3.465038
1	-4.211359	0.222432	0.822021	6	-3.703099	4.842061	-4.428453
6	-4.014845	2.336218	-4.411594	6	-3.533324	4.788777	-1.092910
1	-4.755157	2.903083	-4.986157	6	-4.102116	4.490539	0.172014
1	-3.184616	2.990774	-4.151333	6	-4.242239	5.468202	1.155281
1	-3.635664	1.521375	-5.043299	6	-3.828387	6.783110	0.924728
6	-0.107510	4.344008	2.445209	6	-3.257593	7.099049	-0.311082
1	0.238038	3.386739	2.845772	6	-3.106983	6.123837	-1.295993
1	0.230737	4.443632	1.417573	6	-3.979226	2.491956	-2.099525
1	0.323708	5.159588	3.034015	8	-4.617408	1.935113	-1.163440
6	-4.425287	4.584238	0.193092	15	2.053442	-1.218493	-1.005319
1	-4.569494	5.633233	-0.104118	8	2.991553	-1.643169	0.366336
1	-3.909980	4.058529	-0.606374	6	3.786383	-2.765490	0.249941
1	-5.409797	4.129163	0.340483	6	4.970196	-2.697431	-0.467027
6	3.701450	-2.619020	-1.771425	6	5.709466	-3.916931	-0.673441
6	5.063033	-2.785255	-1.467411	6	5.277980	-5.121795	-0.022509
6	2.918484	-3.762639	-2.005378	6	4.107831	-5.096829	0.783443
6	5.627567	-4.061181	-1.405289	6	3.363445	-3.949459	0.897194
1	5.691406	-1.925145	-1.272039	6	6.017208	-6.321668	-0.208901
6	3.495538	-5.032317	-1.972035	6	7.124498	-6.353557	-1.026447
1	1.858224	-3.655103	-2.206931	6	7.530761	-5.177647	-1.701658
6	4.848281	-5.189078	-1.665998	6	6.845454	-3.994440	-1.528549
1	6.680271	-4.167658	-1.157966	6	5.446502	-1.393960	-1.004553
1	2.875110	-5.903096	-2.163721	6	4.645905	-0.597062	-1.823277
1	5.289070	-6.181095	-1.623502	6	5.196552	0.508835	-2.519651
6	2.393288	-0.694260	-3.572031	6	6.484989	0.915969	-2.295620
6	2.183406	0.618704	-4.026034	6	7.285502	0.257404	-1.324995
6	2.196020	-1.747229	-4.473728	6	6.762328	-0.906630	-0.670567
6	1.751160	0.871573	-5.327784	6	8.574872	0.741978	-0.977777
1	2.371829	1.459242	-3.372255	6	9.324355	0.128064	0.000891
6	1.776899	-1.495196	-5.781455	6	8.802442	-1.002758	0.672970
1	2.362597	-2.770811	-4.168846	6	7.562982	-1.508660	0.342946
6	1.539995	-0.188451	-6.211640	8	3.332740	-0.850311	-2.093021
1	1.590107	1.897457	-5.647952	15	0.240765	0.036250	2.059002
1	1.631567	-2.328741	-6.463191	6	1.716364	0.281097	3.141531
1	1.206101	0.002438	-7.227773	6	2.086280	1.565691	3.574856
6	4.455302	0.144535	-1.834878	6	3.215774	1.749256	4.371890
6	4.838820	0.885930	-0.713446	6	4.013145	0.657486	4.722037
6	5.254164	0.206113	-2.992002	6	3.673086	-0.618366	4.268506
6	5.978331	1.694227	-0.747508	6	2.530923	-0.807572	3.488725
1	4.231944	0.859800	0.179688	8	1.475566	-2.479936	-1.588695
6	6.393638	1.008386	-3.025091	6	-1.108141	0.990750	2.910998
1	4.984915	-0.369431	-3.871543	6	-1.033825	1.473203	4.228167
6	6.756160	1.760609	-1.902815	6	-2.113874	2.158512	4.791150
1	6.248314	2.268592	0.132792	6	-3.288218	2.351602	4.058311
1	6.995570	1.049045	-3.928596	6	-3.377550	1.855872	2.755264
1	7.639462	2.392648	-1.932234	6	-2.291367	1.192184	2.183527
-----				6	-0.256117	-1.696064	2.521502
(4-7) _{re-aa} [‡] ($\Phi_1 = 165.1^\circ$)				6	-0.931771	-1.938748	3.730777
-----				6	-1.259441	-3.238435	4.118048
Number of imaginary frequencies : 1				6	-0.918462	-4.321474	3.303545
Electronic energy : HF=-5369.5024151				6	-0.245063	-4.090680	2.104481
Zero-point correction= 1.563636 (Hartree/Particle)				6	0.085405	-2.789707	1.714461
Thermal correction to Energy= 1.661801				8	-5.377829	-1.035300	-2.065757
Thermal correction to Enthalpy= 1.662745				1	9.381539	-1.475065	1.461750
Thermal correction to Gibbs Free Energy= 1.424874				1	7.177936	-2.366889	0.880724
Sum of electronic and zero-point Energies= -5367.938779				1	8.951998	1.622055	-1.493031
Sum of electronic and thermal Energies= -5367.840614				1	10.304855	0.513081	0.266131
Sum of electronic and thermal Enthalpies= -5367.839670				1	6.892902	1.769084	-2.831425
Sum of electronic and thermal Free Energies= -5368.077541				1	4.555011	1.023149	-3.224101
Standard State and RRHO Corrected G= -5368.051458				1	7.166245	-3.107884	-2.062528
-----				1	2.451732	-3.921860	1.480321
Cartesian Coordinates				1	8.388684	-5.208780	-2.367672
-----				1	5.680472	-7.220883	0.301229
8	-5.711970	-0.048527	1.021198	1	3.795050	-6.007318	1.287979
3	-4.700527	0.072373	-0.621344	1	7.678137	-7.277763	-1.165840
8	-2.978230	-0.730805	-0.149361	1	-1.212263	-1.114859	4.376965
6	-2.054423	-1.535759	-0.416215	1	0.578234	-2.639100	0.765684
6	-2.380725	-2.999511	-0.575624	1	-1.785765	-3.401057	5.054701
6	-1.428708	-3.886076	-1.100528	1	0.012495	-4.918705	1.451131
6	-1.730440	-5.245486	-1.205557	1	-1.180599	-5.333677	3.598931
6	-2.970085	-5.728853	-0.773062	1	1.492058	2.428914	3.296002
6	-3.917301	-4.843905	-0.248075	1	2.280750	-1.805507	3.148121
6	-3.628580	-3.481616	-0.160660	1	3.481535	2.749383	4.700995
8	-0.818147	-1.251739	-0.575043	1	4.293811	-1.472891	4.523722
45	0.457212	0.462273	-0.405860	1	4.899338	0.802575	5.333377
6	-1.261982	1.342334	-1.622613	1	-0.140483	1.318102	4.822312

1	-2.374499	0.806065	1.174563
1	-2.037168	2.532857	5.808453
1	-4.291578	1.962722	2.180800
1	-4.128005	2.879023	4.502564
1	-2.034164	0.618325	-1.417187
1	-0.291098	-0.045248	-2.952825
1	0.481845	1.592830	-2.944717
1	-0.457914	-3.495528	-1.394717
1	-4.360118	-2.788847	0.236134
1	-0.992856	-5.931137	-1.614389
1	-4.880996	-5.214409	0.091007
1	-3.196416	-6.789600	-0.843281
1	-3.818856	1.906514	-3.025739
1	-4.433979	3.479679	0.364151
1	-2.654700	6.411959	-2.238326
1	-4.677471	5.194973	2.113791
1	-2.920989	8.113357	-0.511687
1	-3.942270	7.543690	1.692370
1	-1.846704	4.775637	-3.309049
1	-2.351921	3.231452	-3.946433
1	-4.112329	5.758544	-3.990930
1	-3.210070	5.107812	-5.371526
1	-4.547957	4.183926	-4.661717
1	-0.920215	3.472892	-1.276954
1	-2.193409	2.671375	-0.239375
6	-6.334485	-1.027510	1.496013
6	-8.465220	-2.314150	1.753240
6	-6.442414	-2.970213	3.034777
6	-7.594532	-3.484487	2.185517
1	-9.042179	-1.925375	2.605685
1	-6.812449	-2.572276	3.992193
1	-8.192446	-4.204732	2.751304
6	-5.123298	-2.083162	-2.706626
6	-3.644370	-3.426542	-4.175870
6	-5.748100	-4.429272	-3.340653
6	-4.881958	-4.216756	-4.572312
1	-3.043513	-3.180120	-5.056487
1	-6.734534	-4.814497	-3.623908
1	-5.440408	-3.660534	-5.333686
1	-3.008680	-4.007444	-3.493227
1	-4.597870	-5.183695	-4.997557
1	-5.284848	-5.167482	-2.670912
1	-7.193388	-3.994507	1.303158
1	-9.186562	-2.632771	0.992621
1	-5.743622	-3.779667	3.265745
6	-8.380755	-0.251847	0.397831
1	-8.858821	-0.732050	-0.463832
1	-9.162294	0.218603	1.009259
1	-7.695952	0.514956	0.042657
6	-4.347206	-1.662466	2.765425
1	-3.823084	-2.610660	2.906320
1	-3.816107	-1.078426	2.020278
1	-4.348640	-1.117600	3.719512
6	-3.069144	-1.091106	-3.602721
1	-3.459186	-0.215532	-3.093476
1	-2.129353	-1.391495	-3.126704
1	-2.860494	-0.834752	-4.647955
6	-7.025000	-3.187112	-1.639097
1	-6.965324	-4.101107	-1.036117
1	-6.944614	-2.324673	-0.983438
1	-8.003618	-3.171117	-2.137220
7	-4.042782	-2.169282	-3.542638
7	-5.945588	-3.175987	-2.611588
7	-7.651668	-1.242003	1.177828
7	-5.704671	-1.939330	2.304357
15	1.811100	2.444761	-0.277737
6	3.360862	2.441203	0.736801
6	3.902003	3.644950	1.224354
6	4.075562	1.255660	0.932690
6	5.138862	3.655098	1.867893
1	3.371172	4.580923	1.098621
6	5.315127	1.268074	1.575779
1	3.667930	0.311166	0.611807
6	5.855420	2.467195	2.037268
1	5.542727	4.594984	2.234081
1	5.850642	0.335569	1.714737
1	6.821927	2.476111	2.533207
6	2.444346	3.168685	-1.873197
6	3.818704	3.296985	-2.112950
6	1.552705	3.700489	-2.825223

6	4.290178	3.905290	-3.280170
1	4.535459	2.922812	-1.394816
6	2.022627	4.305732	-3.989535
1	0.484960	3.682064	-2.652773
6	3.396500	4.404987	-4.225982
1	5.361496	3.986730	-3.441411
1	1.311554	4.710023	-4.704394
1	3.763503	4.878839	-5.131929
6	0.938039	3.936755	0.409828
6	1.222932	5.241726	-0.029726
6	-0.006385	3.769868	1.428222
6	0.576291	6.338298	0.544012
1	1.949209	5.414138	-0.815072
6	-0.653499	4.863495	2.002785
1	-0.270212	2.778741	1.755171
6	-0.362036	6.154492	1.561624
1	0.806231	7.338714	0.188219
1	-1.397610	4.696363	2.775070
1	-0.875140	7.008284	1.992514

(4-7)_{re-aa}[‡] ($\Phi_1 = -66.2^\circ$)

Number of imaginary frequencies : 1

Electronic energy : HF=-5369.4965101

Zero-point correction= 1.563547 (Hartree/Particle)

Thermal correction to Energy= 1.661944

Thermal correction to Enthalpy= 1.662888

Thermal correction to Gibbs Free Energy= 1.421662

Sum of electronic and zero-point Energies= -5367.932964

Sum of electronic and thermal Energies= -5367.834566

Sum of electronic and thermal Enthalpies= -5367.833622

Sum of electronic and thermal Free Energies= -5368.074848

Standard State and RRHO Corrected G= -5368.047349

Cartesian Coordinates

6	3.874788	4.108102	2.897345
6	3.015724	3.647270	1.890518
6	2.861597	4.408816	0.723541
6	3.555970	5.609305	0.566844
6	4.417971	6.058203	1.571570
6	4.576982	5.303116	2.738062
6	2.284045	2.333699	2.093558
8	2.285561	1.806013	3.213057
8	1.707868	1.900363	1.016181
45	0.705323	0.091982	0.566552
6	-0.910149	1.108313	1.979155
6	-0.137464	0.047028	2.547346
6	-2.224004	0.972682	1.494031
15	2.599895	-1.086029	1.200480
8	2.537413	-1.961369	2.427131
15	0.849892	1.258383	-1.762851
6	-0.373839	2.660972	-1.845095
6	-0.603182	3.367115	-0.650515
6	-1.463757	4.464645	-0.621134
6	-2.113502	4.879894	-1.786642
6	-1.887814	4.193216	-2.981023
6	-1.019384	3.097249	-3.013054
8	3.436610	-2.085445	0.076438
6	4.371502	-1.653524	-0.818504
6	5.602753	-1.134837	-0.413416
6	6.494791	-0.633275	-1.426310
6	6.164678	-0.801198	-2.813466
6	4.943217	-1.435647	-3.161583
6	4.058209	-1.825009	-2.188912
6	7.039804	-0.293037	-3.811409
6	8.188420	0.385323	-3.471342
6	8.502204	0.586265	-2.105592
6	7.682755	0.090410	-1.114362
6	5.927398	-1.023443	1.035410
6	5.027238	-0.376864	1.870167
6	5.293331	-0.126380	3.235823
6	6.470781	-0.565693	3.787692
6	7.402251	-1.308565	3.009595
6	7.126017	-1.559348	1.622031
6	8.045580	-2.366396	0.893988
6	9.185832	-2.863861	1.487389
6	9.473990	-2.582369	2.844498
6	8.594620	-1.825037	3.586131
8	3.832516	0.069621	1.358665

6	0.694844	0.415791	-3.410048
6	1.862638	-0.006451	-4.067761
6	1.794325	-0.740859	-5.252281
6	0.557253	-1.058909	-5.817179
6	-0.611800	-0.632722	-5.183002
6	-0.543588	0.090295	-3.990357
6	2.429883	2.186497	-2.033209
6	3.596705	1.770468	-1.383757
6	4.807893	2.426249	-1.616582
6	4.864448	3.506735	-2.497072
6	3.701978	3.931651	-3.147806
6	2.492145	3.275042	-2.919066
6	-3.689274	1.369553	3.106420
6	-3.416106	0.235199	4.018066
6	-4.148097	-0.971839	3.974592
6	-3.834036	-2.039699	4.813081
6	-2.776330	-1.948307	5.722073
6	-2.046685	-0.760274	5.789146
6	-2.362038	0.312962	4.954960
6	-4.693738	1.340066	2.101227
8	-5.299268	0.340316	1.617443
6	-3.268156	2.766044	3.543301
6	-4.055102	3.298504	4.749918
3	-6.280419	0.071373	0.038712
8	-6.974934	-1.522453	-0.577854
8	-6.924933	1.594203	-0.837003
1	9.394241	1.144377	-1.834628
1	7.933887	0.272074	-0.076517
1	6.771477	-0.437580	-4.855264
1	8.844695	0.777987	-4.242845
1	4.698457	-1.573073	-4.211647
1	3.099558	-2.263124	-2.434756
1	7.834954	-2.598405	-0.143756
1	4.544181	0.420949	3.798067
1	9.867259	-3.482223	0.909398
1	8.793417	-1.617405	4.634837
1	6.695788	-0.372984	4.833495
1	10.379205	-2.974901	3.299211
1	-0.842069	2.599017	-3.958974
1	-0.081664	3.065684	0.248814
1	-2.374120	4.516986	-3.897359
1	-1.618598	4.999039	0.312298
1	-2.777771	5.738030	-1.765235
1	3.561730	0.959577	-0.673335
1	1.598175	3.616822	-3.431254
1	5.702702	2.091357	-1.102989
1	3.735702	4.774035	-3.833720
1	5.806888	4.018099	-2.673051
1	2.834112	0.231130	-3.653181
1	-1.465662	0.393629	-3.516427
1	2.713926	-1.060197	-5.735022
1	-1.584274	-0.867491	-5.606988
1	0.505321	-1.627013	-6.741712
1	-0.519050	2.117244	2.060012
1	0.660052	0.305636	3.232651
1	-0.648964	-0.882958	2.764584
1	2.209886	4.046256	-0.061112
1	3.981072	3.511994	3.797733
1	3.431825	6.187237	-0.345084
1	5.247863	5.646229	3.521408
1	4.964621	6.989267	1.446174
1	-4.878326	2.321495	1.627935
1	-4.965231	-1.059110	3.273517
1	-1.767953	1.216175	5.028651
1	-4.417361	-2.954593	4.749315
1	-1.220196	-0.665531	6.488718
1	-2.525315	-2.787588	6.364629
1	-2.196358	2.786163	3.769150
1	-3.397983	3.451926	2.696223
1	-3.936000	2.643365	5.618966
1	-3.713630	4.300805	5.034002
1	-5.126363	3.356337	4.523433
1	-2.638874	-0.016969	1.342300
1	-2.598386	1.748650	0.835809
6	-6.608971	2.805338	-0.694004
6	-5.745779	4.925387	-1.620309
6	-6.467562	4.850375	0.747524
6	-5.361180	5.296600	-0.196387
1	-4.943774	5.172633	-2.319443
1	-6.129911	4.897980	1.789251

1	-4.418746	4.800238	0.058975
6	-6.725260	-2.735213	-0.805481
6	-6.641289	-4.662276	-2.392769
6	-5.814951	-4.912982	-0.064275
6	-6.667108	-5.546367	-1.154918
1	-7.398720	-4.988144	-3.113706
1	-5.896239	-5.481236	0.865920
1	-7.695935	-5.653080	-0.793816
6	-6.050318	-2.963295	1.511965
1	-5.106267	-2.413909	1.556057
1	-6.858691	-2.276993	1.767850
1	-6.027023	-3.766878	2.250543
6	-7.343857	-2.419007	-3.152686
1	-6.626349	-2.488566	-3.979280
1	-8.325107	-2.741111	-3.522876
1	-7.410919	-1.385585	-2.820473
6	-5.837432	2.875308	-3.015573
1	-6.032800	1.807198	-2.949531
1	-6.548962	3.321629	-3.723445
1	-4.822595	3.037781	-3.393333
6	-7.718355	2.862114	1.492803
1	-8.141093	1.928818	1.126510
1	-7.146524	2.661504	2.405991
1	-8.535936	3.549445	1.740590
1	-4.754517	-4.905002	-0.354253
1	-6.288127	-6.541889	-1.402563
1	-5.664595	-4.728861	-2.893422
1	-6.645347	5.472957	-1.939216
1	-5.210982	6.376099	-0.106516
1	-7.342853	5.509151	0.656915
7	-5.973094	3.482068	-1.697743
7	-6.873901	3.468369	0.471642
7	-6.917234	-3.265599	-2.049406
7	-6.286112	-3.550646	0.195964
15	-0.446170	-1.816710	-0.145560
6	-1.917384	-1.474181	-1.222731
6	-2.574802	-2.494134	-1.937243
6	-2.423538	-0.174368	-1.312349
6	-3.710515	-2.210553	-2.696838
1	-2.196600	-3.510658	-1.908275
6	-3.572781	0.110281	-2.051731
1	-1.900609	0.634660	-0.827673
6	-4.220946	-0.908385	-2.747760
1	-4.199846	-3.007884	-3.247271
1	-3.935090	1.131388	-2.094137
1	-5.107379	-0.690842	-3.333600
6	0.502009	-3.048564	-1.164834
6	1.261191	-4.057764	-0.553149
6	0.495077	-2.971705	-2.566539
6	1.975818	-4.975366	-1.322965
1	1.310663	-4.133746	0.525751
6	1.206553	-3.894793	-3.336142
1	-0.072603	-2.201764	-3.069805
6	1.948703	-4.901820	-2.717158
1	2.559146	-5.745911	-0.827013
1	1.181265	-3.813066	-4.418712
1	2.505382	-5.618912	-3.313994
6	-1.143433	-2.910685	1.187965
6	-0.304420	-3.261911	2.261848
6	-2.440929	-3.444516	1.146173
6	-0.740495	-4.155894	3.240129
1	0.690293	-2.831755	2.347201
6	-2.868788	-4.341451	2.128602
1	-3.131282	-3.169509	0.358586
6	-2.020413	-4.707613	3.172946
1	-0.075002	-4.411533	4.060017
1	-3.871974	-4.749322	2.076148
1	-2.360161	-5.403232	3.935254

(4-7)_{re-aa}⁺ ($\Phi_1 = -179.8^\circ$)

Number of imaginary frequencies : 1
 Electronic energy : HF=-5369.5054914
 Zero-point correction= 1.564338 (Hartree/Particle)
 Thermal correction to Energy= 1.662503
 Thermal correction to Enthalpy= 1.663447
 Thermal correction to Gibbs Free Energy= 1.425439
 Sum of electronic and zero-point Energies= -5367.941153
 Sum of electronic and thermal Energies= -5367.842988
 Sum of electronic and thermal Enthalpies= -5367.842044

Sum of electronic and thermal Free Energies=				-5368.080053	1	3.830266	2.359615	2.091092
Standard State and RRHO Corrected G=				-5368.054125	1	8.064332	0.317000	-0.207073
.....					1	3.581795	-1.637922	-3.606052
Cartesian Coordinates					1	10.205255	0.115994	-1.386870
.....					1	8.224823	-1.685625	-4.754300
6	2.032862	-4.533954	-1.385954		1	5.793715	-1.970323	-4.749112
6	1.211096	-3.629258	-0.702060		1	10.309220	-0.914498	-3.658168
6	0.711417	-3.977232	0.559316		1	-1.520838	-0.087984	4.504776
6	1.019462	-5.215727	1.123904		1	-1.561747	-1.466046	0.427239
6	1.847895	-6.111358	0.440699		1	-3.522224	-1.429193	4.979282
6	2.358453	-5.765318	-0.814924		1	-3.583387	-2.791291	0.897993
6	0.893005	-2.292917	-1.340344		1	-4.554375	-2.822861	3.191875
8	0.973283	-2.177910	-2.572574		1	2.684040	-1.044206	0.845964
8	0.549954	-1.394959	-0.476554		1	0.338377	-1.634159	4.405044
45	0.394132	0.714333	-0.493830		1	4.258952	-2.770304	1.598048
6	-1.529130	0.226179	-1.751522		1	1.906193	-3.373755	5.148664
6	-0.360525	0.607841	-2.485142		1	3.885597	-3.960440	3.748438
6	-2.628149	1.092867	-1.507932		1	2.549756	0.832611	3.683924
15	2.587503	0.919628	-1.275332		1	-1.546874	2.122532	3.421011
8	2.795113	1.559172	-2.627612		1	2.982669	2.561235	5.375647
15	0.236513	0.146157	2.013791		1	-1.118391	3.843387	5.111081
6	-1.388178	-0.670543	2.422403		1	1.157587	4.095725	6.101421
6	-2.000310	-1.438714	1.416518		1	-1.702271	-0.836672	-1.602170
6	-3.135300	-2.203527	1.690846		1	0.189377	-0.175121	-2.994725
6	-3.681806	-2.215134	2.975983		1	-0.364854	1.566211	-2.988651
6	-3.101586	-1.434918	3.977202		1	0.094378	-3.267498	1.095903
6	-1.964475	-0.669091	3.704133		1	2.408582	-4.254412	-2.364569
8	3.843614	1.640158	-0.340324		1	0.624355	-5.474734	2.102342
6	4.588259	1.007314	0.609626		1	3.008159	-6.454899	-1.347392
6	5.461693	-0.035590	0.297632		1	2.098022	-7.071084	0.885078
6	6.146205	-0.694522	1.379422		1	-3.603239	-0.460703	-3.849036
6	6.024997	-0.185078	2.716189		1	-6.080831	0.877115	-1.284726
6	5.208468	0.952580	2.951180		1	-3.995878	4.185450	-3.081155
6	4.491174	1.517394	1.928007		1	-7.380467	2.450884	0.080083
6	6.684439	-0.849882	3.785020		1	-5.283353	5.746933	-1.717786
6	7.417698	-1.994422	3.566193		1	-6.993048	4.909097	-0.103676
6	7.514616	-2.521368	2.255885		1	-2.563455	2.869633	-3.781902
6	6.901436	-1.889290	1.195502		1	-2.407428	1.258175	-4.419994
6	5.607680	-0.493853	-1.111725		1	-4.662848	3.204062	-5.205434
6	4.468464	-0.827402	-1.831005		1	-3.225093	2.842795	-6.175653
6	4.521848	-1.369348	-3.136045		1	-4.431073	1.579693	-5.862415
6	5.736648	-1.545786	-3.750134		1	-2.441160	2.159538	-1.519029
6	6.938509	-1.144357	-3.103392		1	-3.385805	0.775568	-0.797083
6	6.879139	-0.594794	-1.777172		6	-3.203039	-4.179655	-2.091912
6	8.093256	-0.136915	-1.190918		6	-1.303934	-5.802541	-2.001741
6	9.295356	-0.248471	-1.855885		6	-2.020286	-4.835271	-4.165824
6	9.354722	-0.826254	-3.146916		6	-0.822404	-5.141529	-3.282390
6	8.196975	-1.258271	-3.754809		1	-0.494949	-5.854036	-1.269419
8	3.229712	-0.655710	-1.262328		1	-1.712401	-4.272395	-5.052093
6	0.472616	1.352450	3.401271		1	-0.289896	-4.213110	-3.055060
6	1.743479	1.489858	3.984210		6	-6.508434	-1.894868	1.365196
6	1.988646	2.470956	4.945959		6	-7.490070	-3.462487	3.043996
6	0.966113	3.330529	5.354427		6	-7.022577	-1.102191	3.656622
6	-0.308316	3.189850	4.799678		6	-8.061608	-2.212428	3.696314
6	-0.551682	2.211774	3.833571		1	-8.278757	-4.205533	2.886469
6	1.401201	-1.195644	2.567971		1	-7.445529	-0.162083	4.024914
6	2.517976	-1.527411	1.795232		1	-8.959514	-1.890320	3.157377
6	3.405888	-2.519969	2.218910		6	-5.886110	0.373341	2.030985
6	3.193245	-3.189002	3.422732		1	-5.596434	0.438663	0.986038
6	2.082528	-2.860947	4.206670		1	-6.542066	1.216225	2.272775
6	1.193932	-1.873075	3.782414		1	-4.985542	0.436234	2.655431
6	-4.041135	1.463563	-3.057137		6	-6.779569	-4.257230	0.801116
6	-4.926321	2.389605	-2.305585		1	-6.528914	-5.162293	1.362881
6	-5.904299	1.938478	-1.389157		1	-7.720911	-4.433722	0.263849
6	-6.638824	2.837160	-0.614466		1	-5.987103	-4.069624	0.078072
6	-6.425130	4.213736	-0.715530		6	-2.678315	-5.328332	0.001660
6	-5.467490	4.680024	-1.618968		1	-1.988838	-4.789176	0.659085
6	-4.735455	3.785972	-2.399631		1	-3.701483	-5.054082	0.251889
6	-4.300030	0.065934	-3.172160		1	-2.548400	-6.402479	0.171108
8	-5.147373	-0.629264	-2.553301		6	-3.964858	-3.316930	-4.255884
6	-3.146499	2.023067	-4.156805		1	-4.569834	-2.642406	-3.655396
6	-3.910811	2.438386	-5.422226		1	-3.442486	-2.734228	-5.020491
3	-5.069149	-1.975335	-1.280432		1	-4.627354	-4.033436	-4.762575
8	-6.088513	-1.674700	0.201407		1	-6.162131	-1.347734	4.296076
8	-4.121126	-3.549144	-1.493999		1	-8.345620	-2.428898	4.729861
1	8.071786	-3.438301	2.084137		1	-6.729117	-3.924214	3.689012
1	6.974372	-2.320983	0.204664		1	-1.644328	-6.830207	-2.196193
1	6.581360	-0.442922	4.788108		1	-0.129174	-5.809192	-3.802186
1	7.908812	-2.499976	4.392808		1	-2.504641	-5.760813	-4.513492
1	5.130765	1.347880	3.960891		7	-2.405413	-5.039642	-1.401100

7	-2.984481	-4.010991	-3.431137	8	1.868534	2.287875	0.816044
7	-6.899050	-3.147153	1.739059	15	0.131358	-1.333087	-2.378617
7	-6.580278	-0.882310	2.281112	6	-1.638677	-1.658774	-2.817830
15	0.144587	3.024982	-0.301937	6	-2.080780	-2.694337	-3.652586
6	-1.227566	3.602067	0.800910	6	-3.444004	-2.850998	-3.925222
6	-1.286762	4.941064	1.229158	6	-4.377086	-1.963810	-3.386355
6	-2.286309	2.747590	1.130437	6	-3.940954	-0.906419	-2.580988
6	-2.381096	5.407726	1.956476	6	-2.584629	-0.757587	-2.296473
1	-0.482228	5.626562	0.985384	8	3.281135	0.340777	1.668711
6	-3.394785	3.220608	1.836674	6	4.550101	-0.141579	1.525235
1	-2.238071	1.702089	0.858281	6	5.524540	0.412601	0.689550
6	-3.445591	4.550815	2.251929	6	6.772947	-0.297730	0.546546
1	-2.406967	6.444070	2.280826	6	7.071660	-1.409536	1.401045
1	-4.209553	2.543470	2.067908	6	6.100549	-1.822335	2.351154
1	-4.306465	4.919154	2.802691	6	4.869190	-1.227046	2.386145
6	1.602136	3.960902	0.362712	6	8.306633	-2.096896	1.261150
6	2.607849	4.447694	-0.485032	6	9.217511	-1.732038	0.294246
6	1.735398	4.157520	1.746784	6	8.914538	-0.660113	-0.578232
6	3.710858	5.123690	0.036933	6	7.731365	0.037171	-0.453379
1	2.552482	4.292834	-1.554558	6	5.296267	1.683793	-0.053256
6	2.837319	4.839123	2.266085	6	4.170114	1.815370	-0.846712
1	0.975886	3.796683	2.426672	6	3.908111	2.962447	-1.630116
6	3.830210	5.324628	1.412978	6	4.794817	4.009397	-1.613309
1	4.479796	5.488564	-0.638084	6	5.939227	3.973044	-0.769433
1	2.914518	4.981174	3.339955	6	6.186792	2.812828	0.041957
1	4.689754	5.852223	1.816911	6	7.291097	2.854227	0.939691
6	-0.244565	3.939247	-1.878118	6	8.123185	3.951452	1.001864
6	0.577170	3.739647	-3.004163	6	7.900846	5.074098	0.169146
6	-1.337146	4.813568	-1.991505	6	6.826003	5.081474	-0.691537
6	0.323317	4.420667	-4.195483	8	3.241943	0.793699	-0.852810
1	1.402424	3.032256	-2.960456	6	0.602929	-0.134219	-3.711924
6	-1.582859	5.495413	-3.187291	6	1.829626	0.538548	-3.610898
1	-2.016294	4.965307	-1.162638	6	2.278490	1.359270	-4.646241
6	-0.754190	5.304651	-4.292595	6	1.494106	1.547036	-5.786713
1	0.969897	4.250642	-5.052104	6	0.256112	0.908029	-5.881083
1	-2.432505	6.169710	-3.249709	6	-0.184561	0.065811	-4.855618
1	-0.950237	5.831827	-5.222135	6	1.055443	-2.846273	-2.947143
				6	2.277774	-2.726601	-3.632096
(4-7) _{si-aa} [*] (Φ_1 = -36.7°)				6	3.040604	-3.852224	-3.946178
				6	2.601225	-5.127318	-3.586392
Number of imaginary frequencies : 1				6	1.383786	-5.263450	-2.918342
Electronic energy : HF=-5369.4889725				6	0.621104	-4.138095	-2.602057
Zero-point correction= 1.563529 (Hartree/Particle)				8	-1.505055	2.835217	-0.006653
Thermal correction to Energy= 1.661918				8	-5.645434	3.301707	0.467347
Thermal correction to Enthalpy= 1.662863				1	9.617980	-0.386539	-1.360004
Thermal correction to Gibbs Free Energy= 1.424530				1	7.516188	0.846267	-1.141356
Sum of electronic and zero-point Energies= -5367.925444				1	8.511373	-2.931639	1.927423
Sum of electronic and thermal Energies= -5367.827054				1	10.155886	-2.269478	0.190275
Sum of electronic and thermal Enthalpies= -5367.826110				1	6.328682	-2.650123	3.016831
Sum of electronic and thermal Free Energies= -5368.064442				1	4.100688	-1.577738	3.063626
Standard State and RRHO Corrected G= -5368.038401				1	7.471291	2.009298	1.593535
				1	2.996131	2.993491	-2.215241
Cartesian Coordinates				1	8.954297	3.956540	1.701848
				1	6.627915	5.946112	-1.320483
8	-6.528214	0.381338	-0.607187	1	4.606590	4.896063	-2.212657
3	-5.720592	1.475683	0.613116	1	8.567938	5.929928	0.222448
8	-5.028625	0.839230	2.204761	1	-1.370713	-3.384602	-4.094277
6	-4.750502	-0.258156	2.751807	1	-2.248371	0.062107	-1.670184
6	-3.633838	-0.576490	3.580794	1	-3.771379	-3.667371	-4.563574
6	-2.511071	-1.146479	1.808074	1	-4.655214	-0.209392	-2.154877
6	-1.862949	-0.036275	1.219294	1	-5.436342	-2.089694	-3.588767
6	-0.651524	0.511733	1.753153	1	2.423944	0.435381	-2.712522
45	0.225626	-0.381912	0.020397	1	-1.141294	-0.434064	-4.959387
8	-0.274263	1.332030	-1.175787	1	3.231113	1.871471	-4.545032
6	-0.644347	2.527059	-0.843574	1	-0.368769	1.054797	-6.758005
6	0.049370	3.623632	-1.617442	1	1.838673	2.193617	-6.589110
6	0.277229	3.513133	-2.993092	1	2.651175	-1.752355	-3.923579
6	0.919043	4.543188	-3.685895	1	-0.321830	-4.278905	-2.094107
6	1.362805	5.678960	-3.002764	1	3.982692	-3.726345	-4.472747
6	1.147518	5.787249	-1.624202	1	1.018882	-6.246600	-2.634708
6	0.482406	4.770653	-0.938518	1	3.197779	-6.002780	-3.826950
6	-2.779539	0.461525	4.200957	1	-2.424196	0.583392	0.527075
6	-2.748114	1.795657	3.732707	1	-0.485564	1.575423	1.642990
6	-1.882772	2.737037	4.290459	1	-0.291364	0.106183	2.693222
6	-1.012684	2.386640	5.324415	1	-0.041443	2.617132	-3.512216
6	-1.022967	1.071369	5.796008	1	0.312960	4.839937	0.130103
6	-1.888060	0.127882	5.243986	1	1.084631	4.448926	-4.755589
6	-3.749335	-1.937672	4.260333	1	1.501712	6.661903	-1.084917
6	-4.594530	-1.916072	5.543147	1	1.874589	6.473905	-3.539021
15	2.148014	0.853655	0.458907	1	-5.403008	-1.123019	2.528427

1	-3.396145	2.087263	2.920222
1	-1.847577	-0.886187	5.623094
1	-1.877291	3.748227	3.892925
1	-0.347692	0.771684	6.593125
1	-0.333887	3.120674	5.749897
1	-4.199040	-2.642492	3.549407
1	-2.754948	-2.339937	4.478753
1	-5.618267	-1.588902	5.327543
1	-4.646142	-2.911757	5.999354
1	-4.177566	-1.226479	6.283805
1	-1.928866	-1.811236	2.434852
1	-3.311745	-1.639937	1.267571
6	-4.756107	4.158604	0.736213
6	-2.901016	5.646646	-0.022834
6	-3.646121	5.665627	2.347594
6	-2.438127	5.611512	1.424029
1	-2.076335	5.362830	-0.678407
1	-4.168288	6.630677	2.254825
1	-1.888735	4.680747	1.588880
6	-7.216535	-0.476438	-1.215353
6	-7.723703	-2.860066	-1.731924
6	-9.207696	-1.050798	-2.567034
6	-8.482997	-2.335208	-2.941324
1	-7.055689	-3.677687	-2.021952
1	-10.008760	-1.253043	-1.840533
1	-7.785516	-2.132462	-3.761683
7	-8.253665	-0.086352	-2.014292
7	-6.901925	-1.804139	-1.134956
7	-4.551505	4.560531	2.028209
7	-3.996413	4.697609	-0.251954
6	-4.088511	4.162994	-1.603740
1	-3.285673	3.436044	-1.774528
1	-5.053982	3.682935	-1.754062
1	-3.982192	4.983327	-2.321037
6	-5.497932	4.146221	3.056985
1	-5.800861	3.113395	2.895340
1	-5.002307	4.209280	4.028680
1	-6.389940	4.788657	3.076915
6	-8.655589	1.315923	-2.007444
1	-9.380425	1.526256	-1.208840
1	-7.784697	1.954007	-1.865378
1	-9.118589	1.553940	-2.968764
6	-5.908534	-2.245857	-0.164827
1	-5.211883	-1.440157	0.048465
1	-6.384060	-2.566942	0.772114
1	-5.353747	-3.090738	-0.581239
1	-9.670670	-0.598029	-3.448188
1	-9.199086	-3.087156	-3.284375
1	-8.421350	-3.256559	-0.979714
1	-3.341060	5.556959	3.392101
1	-1.770326	6.455174	1.622639
1	-3.235895	6.654545	-0.307781
15	0.790874	-2.360578	1.044473
6	0.681104	-2.441269	2.891747
6	-0.070888	-3.413094	3.567722
6	1.402811	-1.498104	3.643228
6	-0.087787	-3.450714	4.965958
1	-0.644884	-4.147577	3.014281
6	1.388799	-1.542611	5.036681
1	1.972019	-0.725827	3.138942
6	0.645343	-2.520722	5.703779
1	-0.675174	-4.211095	5.473052
1	1.952379	-0.804352	5.599544
1	0.632099	-2.551399	6.789625
6	-0.292691	-3.780492	0.515355
6	0.115666	-5.120293	0.630090
6	-1.558286	-3.517828	-0.027861
6	-0.721632	-6.159010	0.220851
1	1.094790	-5.366705	1.021042
6	-2.397725	-4.555613	-0.438620
1	-1.874084	-2.496109	-0.171276
6	-1.982344	-5.881843	-0.315443
1	-0.381482	-7.186608	0.313180
1	-3.360013	-4.317392	-0.881910
1	-2.627164	-6.692564	-0.642910
6	2.490873	-3.012698	0.740666
6	3.051890	-4.000783	1.569338
6	3.215953	-2.571584	-0.372966
6	4.285532	-4.569582	1.255072
1	2.528914	-4.323980	2.464077

6	4.456912	-3.132889	-0.678454
1	2.822631	-1.777179	-0.992456
6	4.988021	-4.141630	0.125120
1	4.705061	-5.334768	1.902265
1	5.008791	-2.771518	-1.540542
1	5.956063	-4.573601	-0.111704

(4-7)_{si-aa}[‡] ($\Phi_1 = 70.5^\circ$)

Number of imaginary frequencies : 1
 Electronic energy : HF=-5369.4938172
 Zero-point correction= 1.563582 (Hartree/Particle)
 Thermal correction to Energy= 1.661866
 Thermal correction to Enthalpy= 1.662810
 Thermal correction to Gibbs Free Energy= 1.423519
 Sum of electronic and zero-point Energies= -5367.930236
 Sum of electronic and thermal Energies= -5367.831951
 Sum of electronic and thermal Enthalpies= -5367.831007
 Sum of electronic and thermal Free Energies= -5368.070298
 Standard State and RRHO Corrected G= -5368.043559

Cartesian Coordinates

8	-5.125766	3.888692	0.413271
3	-5.373628	2.102624	0.012544
8	-5.106574	1.387883	-1.672992
6	-4.354842	1.217327	-2.678294
6	-3.851789	0.003986	-3.210753
6	-2.264515	0.146610	-1.643299
6	-1.269057	-0.774302	-2.007100
6	-0.054920	-0.445419	-2.709798
45	0.708655	-0.791009	-0.747762
8	0.422641	-2.864480	-1.104809
6	0.324992	-3.596465	-2.169971
6	-0.347993	-4.935736	-1.910577
6	-0.680353	-5.363667	-0.617950
6	-1.338046	-6.579267	-0.422827
6	-1.678751	-7.377929	-1.518069
6	-1.348834	-6.958458	-2.811166
6	-0.684254	-5.746528	-3.003624
6	-4.370170	-1.336044	-2.842308
6	-5.411878	-1.522488	-1.906725
6	-5.838704	-2.798830	-1.540724
6	-5.227306	-3.938219	-2.072070
6	-4.185109	-3.777570	-2.987951
6	-3.771082	-2.501774	-3.373188
6	-3.062522	0.148721	-4.501388
6	-3.902113	-0.081466	-5.767472
15	2.974586	-1.021367	-1.127091
8	3.461599	-2.327207	-1.690408
15	0.540587	-1.790730	1.618091
6	-1.223839	-2.131456	2.078705
6	-1.732359	-2.071009	3.384974
6	-3.073803	-2.372585	3.638060
6	-3.921631	-2.745517	2.592983
6	-3.421359	-2.822113	1.290244
6	-2.084314	-2.517595	1.036424
8	3.743237	0.182601	-2.097871
6	4.642577	1.152961	-1.763321
6	5.679493	1.013536	-0.838173
6	6.407431	2.203699	-0.464047
6	6.226820	3.423710	-1.193343
6	5.303435	3.442783	-2.271380
6	4.519133	2.350313	-2.524064
6	6.940756	4.589448	-0.809386
6	7.789896	4.577175	0.275487
6	7.950639	3.384547	1.019685
6	7.284708	2.232689	0.657147
6	6.064406	-0.300445	-0.251663
6	5.117678	-1.101297	0.365240
6	5.454249	-2.304176	1.028227
6	6.757181	-2.732579	1.050602
6	7.765613	-2.007316	0.359512
6	7.418942	-0.792660	-0.324380
6	8.438423	-0.146630	-1.080451
6	9.723807	-0.642677	-1.122427
6	10.070172	-1.814330	-0.408311
6	9.104578	-2.482382	0.310567
8	3.792327	-0.728603	0.339669
6	1.263941	-3.493796	1.794422

6	2.237273	-3.962927	0.902117	1	-5.601371	1.162001	3.284280
6	2.788068	-5.237114	1.066497	1	-6.632616	0.490435	4.568482
6	2.371244	-6.060598	2.113036	1	-5.165439	-0.380461	4.057702
6	1.400679	-5.599980	3.006914	6	-8.301199	0.169341	-0.584941
6	0.854263	-4.325550	2.850473	1	-9.235455	0.711990	-0.383385
6	1.272275	-0.965841	3.101192	1	-7.547717	0.873072	-0.931609
6	2.574672	-1.312733	3.502657	1	-8.484853	-0.558138	-1.379939
6	3.223697	-0.603868	4.514341	6	-4.397366	5.179459	2.712320
6	2.581717	0.460553	5.151901	1	-5.151683	5.906344	3.044836
6	1.284318	0.807080	4.770064	1	-4.843790	4.188885	2.686304
6	0.636448	0.105432	3.752334	1	-3.572648	5.183286	3.429774
8	0.670247	-3.312746	-3.322981	6	-4.851776	4.897630	-2.105691
8	-6.467988	1.195080	1.181623	1	-5.028638	3.830080	-1.987882
1	8.599682	3.376915	1.891189	1	-5.818525	5.403894	-2.237472
1	7.408501	1.336657	1.253580	1	-4.251276	5.062370	-3.003888
1	6.789655	5.500675	-1.383318	1	-2.347501	6.724350	2.116612
1	8.324738	5.476722	0.566852	1	-2.062171	7.976031	-0.103319
1	5.198478	4.345094	-2.868055	1	-4.336057	7.530425	-1.020025
1	3.795779	2.362217	-3.330161	1	-8.824063	-2.292453	0.079993
1	8.193448	0.744906	-1.644764	1	-8.498952	-3.374081	2.354914
1	4.658948	-2.874851	1.492746	1	-8.362568	-1.362258	3.756027
1	10.476945	-0.131611	-1.715953	15	0.717237	1.472592	-0.133958
1	9.347544	-3.397787	0.844712	6	0.263779	2.622017	-1.503907
1	7.026610	-3.650924	1.565742	6	-0.826707	3.499194	-1.449304
1	11.088702	-2.190515	-0.443206	6	1.059638	2.594272	-2.659122
1	-1.089431	-1.792712	4.212629	6	-1.116270	4.325060	-2.539650
1	-1.697939	-2.589182	0.027373	1	-1.459286	3.539778	-0.569547
1	-3.451038	-2.321761	4.655988	6	0.781110	3.431509	-3.737777
1	-4.065429	-3.117613	0.468364	1	1.883809	1.893214	-2.712801
1	-4.960907	-2.985225	2.791489	6	-0.314857	4.297703	-3.681936
1	2.553378	-3.363323	0.059502	1	-1.971137	4.987599	-2.488624
1	0.099926	-3.987239	3.553293	1	1.409115	3.396528	-4.623505
1	3.538918	-5.583364	0.361468	1	-0.544980	4.942891	-4.525063
1	1.066546	-6.231325	3.825907	6	-0.544343	1.877203	1.165342
1	2.794270	-7.054613	2.230477	6	-0.407204	2.995983	2.004979
1	3.092361	-2.130746	3.016363	6	-1.667212	1.056410	1.321831
1	-0.365149	0.400670	3.469790	6	-1.364967	3.264731	2.983731
1	4.233327	-0.885247	4.800671	1	0.452233	3.650535	1.910902
1	0.771768	1.632490	5.256061	6	-2.630509	1.327063	2.295060
1	3.088235	1.014105	5.937475	1	-1.772469	0.175520	0.710374
1	-1.561304	-1.817138	-1.958721	6	-2.475249	2.427804	3.137905
1	0.373890	-1.209830	-3.348512	1	-1.236885	4.124617	3.635083
1	0.037619	0.566503	-3.085874	1	-3.478222	0.659098	2.402286
1	-0.419561	-4.741142	0.227298	1	-3.210321	2.633578	3.909764
1	-0.419458	-5.404814	-3.998841	6	2.206852	2.318590	0.566663
1	-1.584858	-6.900530	0.585842	6	2.568318	3.620614	0.182732
1	-1.608811	-7.576003	-3.667066	6	2.907656	1.705081	1.613802
1	-2.195633	-8.321999	-1.366340	6	3.602948	4.290288	0.839651
1	-3.959734	2.123664	-3.173031	1	2.045481	4.123727	-0.621815
1	-5.876048	-0.656324	-1.461315	6	3.941189	2.375624	2.266141
1	-2.956851	-2.418430	-4.083579	1	2.659734	0.699524	1.910773
1	-6.648262	-2.898080	-0.822528	6	4.289299	3.672728	1.885721
1	-3.681008	-4.647511	-3.400341	1	3.877357	5.292464	0.523767
1	-5.550256	-4.931606	-1.773124	1	4.475919	1.874182	3.066858
1	-2.628621	1.155672	-4.533500	1	5.104576	4.189551	2.382736
1	-2.205022	-0.533082	-4.498595	(4-7) _{si-aa} [‡] ($\Phi_1 = 71.3^\circ$)			
1	-4.722629	0.642795	-5.829135	Number of imaginary frequencies : 1			
1	-3.288157	0.023382	-6.669440	Electronic energy : HF=-5369.4949094			
1	-4.343172	-1.083429	-5.776024	Zero-point correction= 1.563988 (Hartree/Particle)			
1	-2.044758	1.206991	-1.685043	Thermal correction to Energy= 1.662132			
1	-3.028570	-0.141661	-0.930832	Thermal correction to Enthalpy= 1.663076			
6	-7.011279	0.103571	1.487159	Thermal correction to Gibbs Free Energy= 1.424265			
6	-7.476178	-1.663525	3.178296	Sum of electronic and zero-point Energies= -5367.930921			
6	-8.628218	-1.712068	0.986596	Sum of electronic and thermal Energies= -5367.832777			
6	-7.872407	-2.547984	2.007356	Sum of electronic and thermal Enthalpies= -5367.831833			
1	-6.809752	-2.197568	3.862879	Sum of electronic and thermal Free Energies= -5368.070645			
1	-9.601345	-1.393892	1.390207	Standard State and RRHO Corrected G= -5368.044018			
1	-6.975653	-2.971061	1.541929	Cartesian Coordinates			
6	-4.414910	4.916376	0.288705	8	-4.420179	3.640522	0.606545
6	-3.550254	6.763851	-1.097578	3	-5.092368	1.927003	0.585372
6	-3.117363	6.776445	1.339101	8	-5.122001	0.929050	-0.993266
6	-2.486204	6.970672	-0.030902	6	-4.482562	0.991566	-2.084553
1	-3.120267	6.839060	-2.099992	6	-3.964343	-0.081309	-2.853551
1	-3.773101	7.625179	1.584037	6	-2.292205	-0.084543	-1.409276
1	-1.677355	6.247035	-0.181284	6	-1.245427	-0.847316	-1.954379
7	-3.891521	5.533033	1.391722	6	-0.097245	-0.316930	-2.641463
7	-4.126907	5.423643	-0.952166				
7	-7.835638	-0.540241	0.602842				
7	-6.768211	-0.473495	2.701996				
6	-5.996196	0.242225	3.709004				

45	0.741635	-0.800097	-0.735213	1	0.415701	-4.425437	3.218806
8	0.620616	-2.850747	-1.269322	1	3.978109	-5.426622	-0.078314
6	0.531886	-3.484121	-2.396509	1	1.543392	-6.609047	3.269812
6	-0.002128	-4.900395	-2.243418	1	3.334901	-7.134630	1.619888
6	-0.262075	-5.466118	-0.987760	1	3.346980	-2.270695	2.765576
6	-0.787482	-6.755411	-0.887744	1	-0.261911	-0.086038	3.640360
6	-1.068268	-7.491298	-2.042310	1	4.488577	-1.116245	4.607494
6	-0.813161	-6.932933	-3.299233	1	0.875476	1.052829	5.485671
6	-0.280113	-5.647021	-3.396972	1	3.267388	0.562757	5.987748
6	-4.387416	-1.493903	-2.679439	1	-1.441371	-1.909943	-2.040372
6	-5.389571	-1.894053	-1.766744	1	0.379779	-0.957274	-3.374962
6	-5.719555	-3.240572	-1.603832	1	-0.105883	0.737385	-2.890332
6	-5.046049	-4.237289	-2.315937	1	-0.047566	-4.892468	-0.096383
6	-4.044042	-3.863478	-3.213741	1	-0.074678	-5.197627	-4.362995
6	-3.730514	-2.517069	-3.400685	1	-0.977284	-7.183308	0.093291
6	-3.296271	0.321361	-4.158289	1	-1.028425	-7.500404	-4.201004
6	-4.217789	0.221098	-5.383226	1	-1.481527	-8.493622	-1.964649
15	3.009846	-0.830894	-1.197302	1	-4.193906	1.994740	-2.450253
8	3.570183	-2.071742	-1.835529	1	-5.894823	-1.142657	-1.174933
15	0.711838	-2.008785	1.527636	1	-2.947729	-2.263840	-4.106128
6	-1.012062	-2.504349	2.002977	1	-6.505272	-3.513935	-0.904826
6	-1.486129	-2.582107	3.321225	1	-3.495248	-4.620364	-3.767865
6	-2.800116	-2.983595	3.580291	1	-5.295060	-5.284892	-2.171670
6	-3.652744	-3.325367	2.528563	1	-2.934067	1.351969	-4.059757
6	-3.184835	-3.268848	1.212186	1	-2.397094	-0.282789	-4.323587
6	-1.876157	-2.861359	0.952792	1	-5.089504	0.876455	-5.271587
8	3.665355	0.455951	-2.144650	1	-3.688467	0.513554	-6.297395
6	4.448644	1.509379	-1.776560	1	-4.586367	-0.800616	-5.520710
6	5.520106	1.441078	-0.882814	1	-2.156471	0.982204	-1.295805
6	6.123769	2.683241	-0.463445	1	-2.973800	-0.543938	-0.703362
6	5.779633	3.912361	-1.115205	6	-6.790314	0.164712	1.936349
6	4.827662	3.883656	-2.167806	6	-7.107470	-1.964708	3.151980
6	4.169068	2.721667	-2.467892	6	-8.167637	-1.665219	0.931797
6	6.371014	5.129849	-0.685301	6	-7.331396	-2.601911	1.789514
6	7.256212	5.155662	0.369955	1	-6.445752	-2.580866	3.767179
6	7.579755	3.950288	1.037068	1	-9.213297	-1.657047	1.271140
6	7.034775	2.751406	0.628883	1	-6.361897	-2.776810	1.312806
6	6.057438	0.144874	-0.382382	6	-4.435872	4.796772	0.112540
6	5.214257	-0.783608	0.205905	6	-5.545344	6.535206	-1.240417
6	5.686906	-1.990976	0.770950	6	-3.450093	7.093808	-0.025975
6	7.025356	-2.287878	0.731071	6	-4.192726	7.223835	-1.347545
6	7.936398	-1.418480	0.071548	1	-6.060395	6.545953	-2.204202
6	7.451339	-0.202089	-0.519111	1	-3.870811	7.778381	0.724149
6	8.379758	0.592116	-1.251075	1	-3.614057	6.759769	-2.153157
6	9.706588	0.232876	-1.353900	7	-3.510023	5.723512	0.490941
6	10.187877	-0.942446	-0.729731	7	-5.352078	5.135507	-0.848787
6	9.314030	-1.751290	-0.038648	7	-7.634236	-0.300237	0.971446
8	3.860327	-0.539556	0.249755	7	-6.468009	-0.660902	2.978664
6	1.549350	-3.668191	1.535324	6	-5.756920	-0.133862	4.135875
6	2.559065	-3.969880	0.611445	1	-5.361671	0.852278	3.903361
6	3.201418	-5.210632	0.650377	1	-6.432565	-0.052393	4.998096
6	2.841025	-6.166885	1.600864	1	-4.932074	-0.803320	4.402261
6	1.834918	-5.873252	2.525098	6	-8.130465	0.592229	-0.069836
6	1.197077	-4.632127	2.494914	1	-7.949857	1.628798	0.209217
6	1.450766	-1.270742	3.053873	1	-7.637122	0.395381	-1.026323
6	2.796516	-1.547968	3.355569	1	-9.209462	0.437588	-0.182158
6	3.445794	-0.891345	4.401348	6	-2.549660	5.412072	1.540539
6	2.761363	0.049385	5.175040	1	-2.607474	6.169171	2.331931
6	1.421950	0.323980	4.893800	1	-2.766679	4.435332	1.962633
6	0.773214	-0.324919	3.841866	1	-1.530423	5.405935	1.136946
8	0.786696	-3.061008	-3.530216	6	-6.447104	4.208297	-1.121429
8	-6.307103	1.329044	1.868491	1	-6.075393	3.189244	-1.232986
1	8.258761	3.969659	1.885250	1	-7.207393	4.225332	-0.328181
1	7.280733	1.843982	1.167414	1	-6.920960	4.501605	-2.060790
1	6.097460	6.047541	-1.200615	1	-2.394240	7.357671	-0.152030
1	7.696399	6.093434	0.696975	1	-4.323732	8.281352	-1.593568
1	4.603673	4.798823	-2.709605	1	-6.189293	7.053089	-0.513647
1	3.432608	2.687407	-3.262329	1	-8.164845	-1.994547	-0.112875
1	8.031674	1.489531	-1.747720	1	-7.840031	-3.564353	1.893944
1	4.965252	-2.668240	1.212601	1	-8.057603	-1.856323	3.696606
1	10.388154	0.855926	-1.926585	15	0.586894	1.398468	0.095127
1	9.661775	-2.671093	0.425452	6	-0.070150	2.617525	-1.127958
1	7.399537	-3.208346	1.171527	6	-1.297443	3.278120	-0.984307
1	11.237472	-1.210334	-0.811887	6	0.691400	2.840664	-2.285106
1	-0.837384	-2.334752	4.153955	6	-1.754757	4.132567	-1.994150
1	-1.514737	-2.827784	-0.067748	1	-1.916318	3.120077	-0.108235
1	-3.150970	-3.037307	4.607486	6	0.248363	3.712749	-3.277105
1	-3.832744	-3.540217	0.384381	1	1.625265	2.307982	-2.409867
1	-4.669343	-3.646023	2.732439	6	-0.984834	4.356384	-3.136255
1	2.831816	-3.266587	-0.163879	1	-2.716904	4.620030	-1.887591

1	0.854916	3.874041	-4.163764
1	-1.345510	5.022940	-3.914646
6	-0.610336	1.573873	1.503336
6	-0.472564	2.579809	2.474305
6	-1.691052	0.690384	1.607206
6	-1.390717	2.682845	3.521713
1	0.356712	3.276468	2.429641
6	-2.618892	0.800330	2.643488
1	-1.791313	-0.116948	0.901359
6	-2.469107	1.796417	3.610056
1	-1.261020	3.459400	4.270207
1	-3.432839	0.086567	2.699178
1	-3.178323	1.876206	4.428981
6	2.042467	2.305562	0.788709
6	2.289396	3.658027	0.502570
6	2.823582	1.668171	1.762927
6	3.289553	4.354235	1.185301
1	1.700966	4.181453	-0.241329
6	3.820884	2.365452	2.442223
1	2.660976	0.626375	1.986658
6	4.052995	3.713303	2.161437
1	3.474341	5.397256	0.946272
1	4.416239	1.847336	3.187723
1	4.837259	4.254367	2.681748

(4-7)_{si-aa}⁺ ($\Phi_1 = -167.7^\circ$)

Number of imaginary frequencies : 1
 Electronic energy : HF=-5369.4970585
 Zero-point correction= 1.561820 (Hartree/Particle)
 Thermal correction to Energy= 1.660678
 Thermal correction to Enthalpy= 1.661622
 Thermal correction to Gibbs Free Energy= 1.420088
 Sum of electronic and zero-point Energies= -5367.935239
 Sum of electronic and thermal Energies= -5367.836381
 Sum of electronic and thermal Enthalpies= -5367.835437
 Sum of electronic and thermal Free Energies= -5368.076970
 Standard State and RRHO Corrected G= -5368.049168

Cartesian Coordinates

8	1.514746	-3.827859	-0.143306
3	3.226326	-3.283765	0.127217
8	4.172325	-1.737775	-0.343527
6	4.397041	-0.981510	-1.317752
6	5.143574	0.234136	-1.350603
6	3.311499	1.339014	-0.749593
6	2.144439	0.953840	-1.440031
6	1.376106	-0.196538	-1.059213
45	-0.087237	1.242419	-0.533835
8	-0.721117	1.388323	-2.589399
6	-0.528961	0.580413	-3.588129
6	-1.760611	0.304661	-4.421394
6	-2.795083	1.238423	-4.539355
6	-3.930834	0.943205	-5.297763
6	-4.051983	-0.299514	-5.925843
6	-3.019349	-1.237339	-5.810678
6	-1.874238	-0.928603	-5.077009
6	6.059430	0.638687	-0.264543
6	5.997738	0.065848	1.029889
6	6.863166	0.473115	2.044143
6	7.819239	1.467532	1.817787
6	7.887925	2.055312	0.552559
6	7.025059	1.651981	-0.466546
6	5.370755	0.771975	-2.756707
6	6.545102	0.102819	-3.488783
15	-1.603092	-0.515284	-0.468031
8	-1.544506	-1.378110	-1.698451
15	-1.195538	3.539809	-0.577412
6	-0.035104	4.787609	-1.305846
6	-0.100657	6.164988	-1.044002
6	0.814228	7.042721	-1.631035
6	1.793590	6.560639	-2.502474
6	1.843866	5.195436	-2.797283
6	0.936325	4.316762	-2.204152
8	-1.545620	-1.650091	0.841555
6	-2.456279	-1.876569	1.834609
6	-3.831329	-2.019137	1.631393
6	-4.681209	-2.137982	2.790852
6	-4.104205	-2.297441	4.093450

6	-2.690216	-2.289614	4.220046
6	-1.896726	-2.054497	3.129685
6	-4.947666	-2.423453	5.229128
6	-6.318470	-2.368809	5.105078
6	-6.895365	-2.176902	3.827317
6	-6.101646	-2.067843	2.705041
6	-4.420387	-2.031078	0.264074
6	-4.131980	-0.997013	-0.609200
6	-4.668761	-0.921015	-1.915051
6	-5.499169	-1.916225	-2.363843
6	-5.778925	-3.047295	-1.547210
6	-5.227341	-3.120119	-0.222974
6	-5.445360	-4.312340	0.523935
6	-6.185964	-5.355014	0.008562
6	-6.758826	-5.263625	-1.282265
6	-6.554184	-4.131808	-2.040297
8	-3.227226	-0.030137	-0.214493
6	-2.649956	3.660511	-1.718061
6	-3.704237	2.747396	-1.560304
6	-4.864158	2.859416	-2.327830
6	-4.977695	3.866940	-3.288927
6	-3.919101	4.757578	-3.477654
6	-2.765289	4.661408	-2.693798
6	-1.870068	4.395823	0.933187
6	-3.226418	4.286508	1.286227
6	-3.707451	4.837278	2.474658
6	-2.845667	5.514283	3.339185
6	-1.499586	5.643158	2.995358
6	-1.017159	5.090426	1.807975
8	0.541702	0.055628	-3.926757
8	4.670371	-4.488735	0.386371
1	-7.975322	-2.107849	3.729003
1	-6.565361	-1.909575	1.738446
1	-4.484735	-2.549761	6.204973
1	-6.954817	-2.458398	5.980931
1	-2.245028	-2.423923	5.202001
1	-0.822316	-1.982389	3.232976
1	-5.007676	-4.404893	1.510614
1	-4.383874	-0.086005	-2.544849
1	-6.326897	-6.257030	0.597707
1	-6.970495	-4.055534	-3.041846
1	-5.910209	-1.874778	-3.368905
1	-7.345921	-6.088932	-1.675054
1	-0.860816	6.560692	-0.379364
1	0.975475	3.258058	-2.434072
1	0.757377	8.104533	-1.407465
1	2.591062	4.810785	-3.486161
1	2.506667	7.244647	-2.954257
1	-3.611225	1.932338	-0.854597
1	-1.961843	5.372302	-2.850634
1	-5.667062	2.140965	-2.188626
1	-3.988716	5.536096	-4.232552
1	-5.876666	3.949390	-3.893488
1	-3.923030	3.767772	0.639063
1	0.028294	5.218265	1.563152
1	-4.760385	4.733244	2.721789
1	-0.812877	6.172061	3.650014
1	-3.219834	5.940349	4.265843
1	2.002630	1.320723	-2.451099
1	0.939658	-0.782846	-1.854339
1	1.749902	-0.787826	-0.232637
1	-2.703936	2.188747	-4.029985
1	-1.060791	-1.640685	-4.988209
1	-4.723959	1.680601	-5.385779
1	-3.108671	-2.206628	-6.294704
1	-4.941987	-0.535872	-6.503458
1	3.896522	-1.219203	-2.273721
1	5.267641	-0.705297	1.226224
1	7.114602	2.130886	-1.435005
1	6.783057	0.009116	3.024098
1	8.619232	2.834639	0.352958
1	8.491495	1.781794	2.611316
1	4.453834	0.616072	-3.337867
1	5.518238	1.857578	-2.732288
1	6.363349	-0.972547	-3.600534
1	6.682517	0.526179	-4.490788
1	7.483932	0.224876	-2.938823
1	3.443227	1.023056	0.279946
1	3.809844	2.267613	-1.014089
6	5.797378	-4.073512	-0.008235

1	-8.920731	2.424238	0.047376
1	-6.547614	2.698904	0.575215
1	-7.913696	0.733239	-3.778203
1	-9.633938	1.468272	-2.146716
1	-5.558374	0.406525	-4.393733
1	-3.173484	0.432988	-3.747748
1	-5.401326	4.472793	-1.531938
1	-2.029976	2.456913	2.945967
1	-6.065164	6.795752	-1.131285
1	-4.099750	6.740575	2.694516
1	-2.854282	4.762154	3.413233
1	-5.452012	7.942110	0.999826
1	-0.847202	-4.966327	3.542886
1	2.066372	-2.566448	1.481118
1	0.903631	-6.592478	4.135655
1	3.827233	-4.201539	2.075087
1	3.251579	-6.235795	3.385954
1	-2.509740	-0.150542	2.627593
1	0.298520	-2.619902	4.758045
1	-3.139843	0.954752	4.734752
1	-0.261181	-1.449979	6.844451
1	-2.018409	0.313634	6.869118
1	-3.680086	-2.081906	2.813040
1	-1.325598	-5.123048	0.868479
1	-5.685130	-3.440911	2.503301
1	-3.340145	-6.467626	0.539892
1	-5.553291	-5.646734	1.349586
1	2.764223	-0.832381	0.242823
1	1.569251	0.989842	-0.877529
1	1.208568	-0.074180	-2.301028
1	0.090202	0.876422	4.086813
1	2.397489	3.708687	1.869292
1	-0.478177	2.619594	5.764879
1	1.772939	5.498759	3.484608
1	0.341922	4.953707	5.445955
1	5.744204	-1.768032	-0.738837
1	3.872736	1.213153	-2.156658
1	4.328642	-1.751933	-5.246544
1	2.858917	2.735561	-3.783311
1	3.382481	-0.206498	-6.874533
1	2.623050	2.068483	-6.179290
1	5.362316	-3.369326	-2.184943
1	4.517892	-3.182179	-3.701515
1	7.389660	-2.248588	-3.096691
1	6.937108	-3.630309	-4.113227
1	6.582245	-1.976527	-4.643000
1	2.404311	-2.311084	-2.450922
1	3.341358	-2.907182	-0.987718
6	4.340672	3.876343	-1.380540
6	2.888532	5.346448	-2.801463
6	5.219402	4.828477	-3.483854
6	4.193361	5.940507	-3.313463
1	2.354785	4.833366	-3.614695
1	6.186794	5.237802	-3.790588
1	4.018727	6.452186	-4.264362
6	4.805711	0.707301	3.193223
6	4.037563	-1.372470	4.323121
6	3.615887	0.826376	5.388056
6	2.992157	-0.507398	5.006102
1	3.582714	-2.288037	3.937438
1	4.323602	0.697046	6.221605
1	2.155275	-0.345966	4.320805
7	4.296346	1.427428	4.241161
7	4.620931	-0.650538	3.193424
7	5.405780	4.146763	-2.204633
7	3.121611	4.404759	-1.705522
6	1.928439	3.991655	-0.974119
1	2.148206	3.148248	-0.327481
1	1.534207	4.816100	-0.366674
1	1.150322	3.687748	-1.680460
6	6.635784	3.384797	-2.040872
1	7.490423	4.019390	-2.296523
1	6.729614	3.054534	-1.008009
1	6.646747	2.500899	-2.693311
6	4.637662	2.835892	4.369305
1	5.463201	2.979596	5.081746
1	4.933327	3.231410	3.399918
1	3.766306	3.389085	4.727669
6	5.213085	-1.465939	2.144273
1	5.742261	-0.826945	1.442229

1	5.908201	-2.195998	2.579945
1	4.434357	-2.009368	1.598783
1	2.840705	1.525312	5.719194
1	2.605245	-1.007632	5.898519
1	4.826446	-1.669024	5.032037
1	4.900055	4.115966	-4.259037
1	4.578775	6.675972	-2.598450
1	2.222929	6.136906	-2.433977
15	-0.979714	-2.164009	-1.647951
6	-0.413379	-1.825672	-3.374408
6	0.155701	-2.817368	-4.185028
6	-0.590936	-0.534273	-3.899899
6	0.524931	-2.526645	-5.502086
1	0.307837	-3.820041	-3.801998
6	-0.227056	-0.250356	-5.214471
1	-1.002731	0.250174	-3.275334
6	0.328620	-1.247620	-6.021275
1	0.965918	-3.305140	-6.118312
1	-0.364432	0.754370	-5.603164
1	0.617490	-1.023256	-7.043683
6	-0.642019	-3.983986	-1.486772
6	-1.526088	-4.963059	-1.969020
6	0.548859	-4.403064	-0.878487
6	-1.222671	-6.319014	-1.839893
1	-2.465345	-4.681459	-2.427996
6	0.849503	-5.759049	-0.739251
1	1.232945	-3.665850	-0.488546
6	-0.037767	-6.723648	-1.219199
1	-1.923407	-7.060041	-2.214077
1	1.767254	-6.053401	-0.238259
1	0.187547	-7.780459	-1.107175
6	-2.812939	-2.102201	-1.829755
6	-3.434876	-2.532092	-3.016101
6	-3.610906	-1.702394	-0.751960
6	-4.824860	-2.602212	-3.098037
1	-2.834643	-2.814948	-3.875297
6	-5.002751	-1.758866	-0.841628
1	-3.150230	-1.331419	0.152854
6	-5.612342	-2.220105	-2.008097
1	-5.292669	-2.940718	-4.018249
1	-5.606207	-1.432884	-0.000279
1	-6.695544	-2.258905	-2.077538

8

Number of imaginary frequencies : 0
Electronic energy : HF=-580.2611824
Zero-point correction= 0.256333 (Hartree/Particle)
Thermal correction to Energy= 0.270369
Thermal correction to Enthalpy= 0.271313
Thermal correction to Gibbs Free Energy= 0.214943
Sum of electronic and zero-point Energies= -580.004850
Sum of electronic and thermal Energies= -579.990813
Sum of electronic and thermal Enthalpies= -579.989869
Sum of electronic and thermal Free Energies= -580.046240
Standard State and RRHO Corrected G= -580.041209

Cartesian Coordinates

6	3.011176	0.332636	1.088563
6	1.639957	0.553939	0.940904
6	0.876779	-0.192097	0.028174
6	1.537897	-1.157047	-0.747817
6	2.909256	-1.376479	-0.607258
6	3.652123	-0.636715	0.315990
1	3.575775	0.923166	1.804830
1	1.168954	1.329636	1.538731
1	0.987067	-1.741607	-1.477359
1	3.397099	-2.128422	-1.221615
1	4.718616	-0.810907	0.427456
6	-0.618903	0.092494	-0.158014
6	-1.412103	-1.254411	-0.319845
1	-1.123486	-1.931640	0.491949
1	-1.090158	-1.719870	-1.258057
6	-0.863378	1.021356	-1.373996
1	-1.928254	1.273485	-1.400586
1	-0.647303	0.443966	-2.281181
6	-0.047667	2.317358	-1.387014
1	-0.317359	2.922332	-2.259666
1	-0.244106	2.913985	-0.492129

1	1.027470	2.120192	-1.436849
6	-2.909252	-1.093691	-0.341337
6	-3.730081	-1.563489	0.600011
6	-1.173611	0.699337	1.129406
8	-1.783108	1.745513	1.214061
1	-1.002354	0.069377	2.030108
1	-3.328846	-0.554588	-1.189791
1	-4.806545	-1.424606	0.540104
1	-3.354859	-2.107744	1.464956

Li-Obz.3DMPU

Number of imaginary frequencies : 0
 Electronic energy : HF=-1689.9128377
 Zero-point correction= 0.667517 (Hartree/Particle)
 Thermal correction to Energy= 0.708014
 Thermal correction to Enthalpy= 0.708959
 Thermal correction to Gibbs Free Energy= 0.591870
 Sum of electronic and zero-point Energies= -1689.245321
 Sum of electronic and thermal Energies= -1689.204823
 Sum of electronic and thermal Enthalpies= -1689.203879
 Sum of electronic and thermal Free Energies= -1689.320968
 Standard State and RRHO Corrected G= -1689.308706

Cartesian Coordinates

8	1.353654	-1.717472	-0.194342
3	0.568000	0.032964	-0.547265
8	-0.544535	0.691667	0.791372
6	-1.724343	0.805454	1.250181
8	-2.373472	1.870021	1.370567
6	-2.402825	-0.492864	1.684996
6	-3.713351	-0.470074	2.180333
6	-4.355881	-1.652094	2.554764
6	-3.687862	-2.875590	2.441383
6	-2.376829	-2.906492	1.954202
6	-1.738064	-1.722580	1.578291
8	2.064845	1.324114	-0.596824
1	-4.211572	0.490797	2.261053
1	-0.728087	-1.740629	1.181599
1	-5.374360	-1.621322	2.933782
1	-1.853516	-3.855364	1.864481
1	-4.185101	-3.797852	2.730720
6	1.735199	2.363652	0.033001
6	0.810967	4.662430	0.071503
6	1.285155	3.502369	2.209140
6	0.234851	4.276226	1.426314
1	1.649676	5.367939	0.185815
1	0.825076	3.032559	3.085426
1	-0.058075	5.171971	1.982910
6	2.599405	-1.874560	-0.186441
6	4.756561	-2.127286	-1.410897
6	4.686878	-2.399001	1.055704
6	5.434824	-1.753391	-0.101263
1	4.923558	-3.189921	-1.644036
1	5.085450	-2.052165	2.014291
1	6.476608	-2.086629	-0.110885
7	3.271146	-2.035294	1.000091
7	3.320748	-1.852577	-1.346977
7	1.240044	3.456367	-0.630743
7	1.878777	2.439673	1.389172
1	0.052006	5.155826	-0.544873
1	-0.647637	3.641026	1.285614
1	2.078808	4.170310	2.574193
1	4.802404	-3.493681	1.029597
1	5.426060	-0.664539	0.020885
1	5.174353	-1.544463	-2.238472
6	2.505945	-2.222991	2.225348
1	2.390941	-3.289405	2.467037
1	3.028783	-1.736035	3.054413
1	1.519735	-1.778174	2.115936
6	2.638016	-1.736652	-2.628516
1	2.733957	-2.669966	-3.200411
1	1.582617	-1.517747	-2.478158
1	3.086891	-0.926854	-3.215131
6	1.371566	3.542959	-2.075683
1	2.217382	4.185953	-2.360862
1	1.530748	2.548153	-2.487427
1	0.459586	3.969006	-2.505853
6	2.297135	1.251906	2.120383

1	1.422563	0.683889	2.457606
1	2.903486	0.612078	1.482230
1	2.889051	1.559721	2.989100
8	-0.538605	-0.213693	-2.159931
6	-1.778904	-0.297559	-1.959630
6	-3.963277	0.782995	-1.507007
6	-3.799032	-1.697473	-1.488429
6	-4.613810	-0.509363	-1.978621
1	-4.013611	0.885411	-0.415348
1	-4.128783	-2.617228	-1.984838
1	-5.636751	-0.580304	-1.597093
6	-1.561967	-2.722618	-1.739246
1	-0.517632	-2.470809	-1.565548
1	-1.907317	-3.359262	-0.918568
1	-1.652810	-3.287286	-2.677600
6	-1.930478	2.134480	-1.941700
1	-1.809317	2.499963	-0.915836
1	-0.956048	2.060770	-2.416821
1	-2.555990	2.832925	-2.508628
7	-2.374669	-1.514695	-1.775890
7	-2.567019	0.822038	-1.944162
1	-3.932981	-1.838736	-0.407767
1	-4.658831	-0.514483	-3.073825
1	-4.472873	1.648687	-1.942758

5 (X = NH₂)

Number of imaginary frequencies : 0
 Electronic energy : HF=-518.9111791
 Zero-point correction= 0.211427 (Hartree/Particle)
 Thermal correction to Energy= 0.223377
 Thermal correction to Enthalpy= 0.224322
 Thermal correction to Gibbs Free Energy= 0.172969
 Sum of electronic and zero-point Energies= -518.699752
 Sum of electronic and thermal Energies= -518.687802
 Sum of electronic and thermal Enthalpies= -518.686858
 Sum of electronic and thermal Free Energies= -518.738210
 Standard State and RRHO Corrected G= -518.733752

Cartesian Coordinates

6	-2.301676	-1.027697	0.625673
6	-0.924170	-1.147470	0.793193
6	-0.035011	-0.230670	0.216790
6	-0.579778	0.828074	-0.527410
6	-1.953920	0.960487	-0.702355
6	-2.843466	0.032152	-0.126631
1	-2.969849	-1.755757	1.079501
1	-0.532530	-1.977357	1.376807
1	-2.351120	1.789686	-1.282886
1	0.082836	1.562765	-0.978254
6	1.474799	-0.368833	0.381898
1	1.658165	-1.186556	1.093605
6	2.210981	-0.659079	-0.937646
1	1.694082	-1.483531	-1.442064
1	2.122399	0.216809	-1.589973
6	3.687873	-1.013197	-0.741447
1	3.800220	-1.897079	-0.101870
1	4.168398	-1.233829	-1.700890
1	4.232230	-0.186704	-0.275521
6	1.955550	0.901614	1.062914
8	2.651166	1.753933	0.544482
1	1.574956	1.033348	2.099687
7	-4.220799	0.193994	-0.246298
1	-4.524147	0.727122	-1.051848
1	-4.766462	-0.650628	-0.127940

(4-7)_{re}* (X = NH₂)

Number of imaginary frequencies : 1
 Electronic energy : HF=-5424.8810508
 Zero-point correction= 1.579822 (Hartree/Particle)
 Thermal correction to Energy= 1.679612
 Thermal correction to Enthalpy= 1.680556
 Thermal correction to Gibbs Free Energy= 1.436993
 Sum of electronic and zero-point Energies= -5423.301229
 Sum of electronic and thermal Energies= -5423.201439
 Sum of electronic and thermal Enthalpies= -5423.200495
 Sum of electronic and thermal Free Energies= -5423.444057
 Standard State and RRHO Corrected G= -5423.416033

..... Cartesian Coordinates							
8	4.567641	-3.197578	-1.298436	1	-1.986404	-3.120916	3.216287
3	3.675738	-2.192722	0.082635	1	-8.648542	-4.655119	0.980594
8	2.013395	-1.432722	-0.539398	1	-5.832647	-5.812048	4.019095
6	0.798377	-1.641088	-0.779487	1	-3.633971	-4.754170	4.124925
8	-0.161852	-0.823883	-0.582072	1	-8.071462	-6.036498	2.977926
45	-0.600180	1.030780	0.425021	1	1.606206	0.570276	-2.165794
15	-0.947302	1.825901	-2.013681	1	0.027120	4.359062	-3.481353
6	0.653627	2.428498	-2.729697	1	3.817632	1.191332	-3.040494
6	1.737436	1.537260	-2.639789	1	2.243365	4.979246	-4.337270
6	2.989198	1.884398	-3.141855	1	4.166482	3.409613	-4.118111
6	3.185313	3.131715	-3.744506	1	-2.250245	-0.831921	-1.796539
6	2.109291	4.012596	-3.858788	1	-0.441162	1.525036	-4.906937
6	0.848410	3.662695	-3.362723	1	-2.808423	-2.577230	-3.446332
6	0.399527	-2.973901	-1.371783	1	-1.003611	-0.215307	-6.556602
6	-0.922046	-3.432144	-1.282738	1	-2.192508	-2.285575	-5.834707
6	-1.269319	-4.683899	-1.791271	1	-1.212105	4.781187	-1.625565
6	-0.302706	-5.483442	-2.408444	1	-3.494310	1.658430	-3.518314
6	1.015961	-5.029147	-2.502335	1	-2.988936	6.385880	-2.120620
6	1.369800	-3.783800	-1.979011	1	-5.284876	3.267565	-3.998606
6	1.492033	1.469289	1.446067	1	-5.062245	5.647382	-3.296120
6	2.449534	1.391737	0.427927	1	-1.657019	-2.804554	-0.797908
6	4.651038	1.556316	1.236483	1	2.398552	-3.444488	-2.022124
6	5.298472	2.146284	0.050243	1	-2.296667	-5.028017	-1.714329
6	5.281184	3.542246	-0.174460	1	1.772614	-5.646711	-2.979188
6	5.810140	4.115993	-1.327915	1	-0.575009	-6.455595	-2.811295
6	6.400171	3.320786	-2.325004	1	4.049672	-0.102124	2.408903
6	6.447452	1.932741	-2.107985	1	4.834944	4.204202	0.560771
6	5.904994	1.364413	-0.960117	1	5.935036	0.292709	-0.827470
6	0.713647	0.386412	1.973221	1	5.762241	5.194331	-1.464868
15	-2.437605	-0.059208	1.381603	1	6.900294	1.290863	-2.861670
8	-2.660260	0.131949	2.861428	1	3.783921	3.323555	2.143540
8	-2.262536	-1.715904	1.056927	1	3.721267	1.889350	3.131997
6	-3.227616	-2.569036	1.547283	1	6.301159	3.457490	2.526219
6	-4.420615	-2.722120	0.855844	1	5.380391	3.531951	4.039140
6	-5.420806	-3.598024	1.411409	1	6.189377	2.027072	3.558410
6	-5.114389	-4.355540	2.592810	1	1.011125	-0.625870	1.719343
6	-3.853216	-4.184654	3.225558	1	0.305103	0.493773	2.972041
6	-2.938089	-3.291301	2.728533	1	1.438206	2.418666	1.966770
6	-6.088940	-5.239486	3.131027	1	2.773078	2.302608	-0.055320
6	-7.333602	-5.360478	2.555298	1	2.574973	0.471660	-0.121971
6	-7.656653	-4.582390	1.418114	6	2.839107	-2.904812	2.703408
6	-6.729244	-3.726471	0.863838	6	3.168978	-2.086242	5.014975
6	-4.660323	-1.925247	-0.377877	6	0.858448	-2.381948	4.146141
6	-4.512542	-0.538208	-0.347725	6	1.789781	-1.451127	4.909124
6	-4.942558	0.267672	-1.431574	6	3.134320	-2.993434	5.638258
6	-5.433352	-0.303687	-2.577275	1	-0.056313	-1.852059	3.859889
6	-5.461184	-1.715662	-2.721946	1	1.380373	-1.253075	5.904027
6	-5.053606	-2.537434	-1.618771	6	5.606098	-3.890209	-1.164153
6	-5.006918	-3.946554	-1.820602	6	8.069731	-4.163562	-1.451544
6	-5.350182	-4.506764	-3.032699	6	6.675733	-6.079830	-0.711394
6	-5.776691	-3.692187	-4.109491	6	7.960914	-5.306652	-0.453554
6	-5.830773	-2.325378	-3.950793	1	8.280400	-4.549380	-2.460664
8	-4.032565	0.111052	0.752528	1	6.523754	-6.841745	0.058991
6	-1.310924	0.471732	-3.226063	1	8.826363	-5.968956	-0.547759
6	-1.986403	-0.688193	-2.833432	7	5.530758	-5.169305	-0.676775
6	-2.298816	-1.677471	-3.771108	7	6.836907	-3.375511	-1.471145
6	-1.948496	-1.513518	-5.110032	7	3.665765	-2.398523	3.674888
6	-1.280226	-0.353281	-5.514770	7	1.489553	-2.881949	2.923469
6	-0.961914	0.630488	-4.580154	1	3.875618	-1.394220	5.482226
6	-2.208321	3.086632	-2.525597	1	1.875680	-0.495726	4.382081
6	-2.093015	4.435636	-2.145531	1	0.560346	-3.233113	4.776758
6	-3.107852	5.350566	-2.427236	1	6.725034	-6.599013	-1.681336
6	-4.267380	4.937341	-3.086239	1	7.946691	-4.907383	0.566856
6	-4.392562	3.602701	-3.476751	1	8.893308	-3.493713	-1.182235
6	-3.372147	2.688078	-3.205974	15	-1.192221	2.991212	1.550052
6	4.533878	0.162441	1.449771	6	-2.985426	3.376404	1.710051
8	4.857266	-0.790833	0.679535	6	-3.809388	3.177612	0.594381
6	4.366585	2.440260	2.437453	6	-3.536549	3.931740	2.875454
6	5.631466	2.893096	3.183666	1	-5.156115	3.535445	0.634320
8	3.313010	-3.349035	1.628539	6	-3.399577	2.737593	-0.303315
1	-5.288090	-5.583490	-3.163859	6	-4.889042	4.275832	2.917941
1	-4.677475	-4.583893	-1.008106	1	-2.918327	4.098649	3.750210
1	-6.135750	-1.684927	-4.774616	6	-5.700782	4.082363	1.797681
1	-6.047461	-4.146438	-5.058266	1	-5.778373	3.376460	-0.241351
1	-5.760775	0.319339	-3.405301	1	-5.305533	4.698600	3.827884
1	-4.867431	1.341923	-1.328406	1	-6.752140	4.353822	1.833164
1	-7.003612	-3.131343	0.001393	6	-0.555068	3.142184	3.286988
				6	0.394584	4.117075	3.634753
				6	-0.992935	2.237115	4.269528
				6	0.903361	4.179367	4.934104

1	0.751677	4.826483	2.897057	6	1.791661	3.304339	3.063275
6	-0.484603	2.309845	5.567769	8	1.480574	2.147630	0.467161
1	-1.714825	1.470642	4.002194	8	-2.120051	1.428225	0.629459
6	0.466595	3.276112	5.904539	6	-2.607158	2.703256	0.424893
1	1.640878	4.937231	5.183065	6	-3.823674	2.868898	-0.216117
1	-0.833045	1.603180	6.316278	6	-4.213916	4.211091	-0.568033
1	0.862938	3.325971	6.914990	6	-3.416070	5.317852	-0.117091
6	-0.518045	4.532853	0.783544	6	-2.235326	5.071905	0.636129
6	-1.163167	5.767611	0.965367	6	-1.818882	3.786225	0.873019
6	0.672702	4.492668	0.045122	6	-3.801421	6.642356	-0.460758
6	-0.630170	6.929952	0.407327	6	-4.911576	6.880094	-1.239961
1	-2.086740	5.825326	1.530932	6	-5.680968	5.791018	-1.714540
6	1.210772	5.658230	-0.504330	6	-5.343946	4.495544	-1.385703
1	1.165361	3.548949	-0.132779	6	-4.677257	1.684542	-0.521989
6	0.557790	6.879269	-0.328935	6	-4.198977	0.573552	-1.220287
1	-1.145639	7.876049	0.546451	6	-5.087285	-0.438467	-1.679828
1	2.127142	5.598025	-1.083586	6	-6.415017	-0.418835	-1.348912
1	0.967519	7.785930	-0.765034	6	-6.924940	0.595898	-0.495409
6	4.212720	-5.774708	-0.517753	6	-6.048175	1.647153	-0.065361
1	3.860145	-6.229852	-1.454272	6	-6.568329	2.596934	0.860459
1	4.278442	-6.557613	0.242966	6	-7.871158	2.526779	1.307073
1	3.493563	-5.028466	-0.189352	6	-8.739385	1.508296	0.848872
6	6.937418	-2.059225	-2.086013	6	-8.267448	0.561884	-0.033568
1	5.960166	-1.583732	-2.090774	8	-2.902828	0.380239	-1.593820
1	7.638593	-1.434124	-1.522179	6	-0.878858	-1.164652	3.694388
1	7.303359	-2.146034	-3.118295	6	-0.396034	-1.811561	4.838509
6	5.106721	-2.546650	3.509224	6	-0.248533	-1.107435	6.039126
1	5.462255	-3.521109	3.873970	6	-0.598707	0.240689	6.112049
1	5.367649	-2.433579	2.458796	6	-1.086579	0.889973	4.973517
1	5.606214	-1.759968	4.081604	6	-1.217044	0.198178	3.772120
6	0.589505	-3.520442	1.972300	3	3.193842	2.587045	-0.369439
1	-0.150319	-2.803353	1.606985	8	4.249928	0.958441	-0.528535
1	1.160273	-3.903318	1.131526	6	4.613902	0.270176	0.469590
1	0.058433	-4.351249	2.455696	6	5.092157	-1.061446	0.510332
7	6.848465	3.881457	-3.528217	6	5.335876	-1.876644	-0.684449
1	7.120303	4.855334	-3.460041	6	4.901860	-1.483069	-1.976011
1	7.564267	3.339883	-3.998748	6	5.065560	-2.301535	-3.089702
				6	5.666124	-3.566382	-2.984949
(4-7) _{st} [*] (X = NH ₂)				6	6.107259	-3.973274	-1.714706
				6	5.945294	-3.151360	-0.602457
Number of imaginary frequencies : 1				6	5.625782	-1.518117	1.857087
Electronic energy : HF=-5424.8765394				6	7.135777	-1.285825	2.039157
Zero-point correction= 1.578478 (Hartree/Particle)				8	4.450840	3.732536	0.638794
Thermal correction to Energy= 1.678490				8	2.738937	3.419482	-2.035172
Thermal correction to Enthalpy= 1.679434				1	-8.231116	3.258467	2.025096
Thermal correction to Gibbs Free Energy= 1.436294				1	-5.919286	3.376898	1.239696
Sum of electronic and zero-point Energies= -5423.298062				1	-8.912349	-0.241898	-0.380339
Sum of electronic and thermal Energies= -5423.198049				1	-9.765197	1.467603	1.203677
Sum of electronic and thermal Enthalpies= -5423.197105				1	-7.083035	-1.197054	-1.708228
Sum of electronic and thermal Free Energies= -5423.440245				1	-4.670432	-1.222805	-2.301422
Standard State and RRHO Corrected G= -5423.41273				1	-5.938914	3.674208	-1.767521
				1	-0.888409	3.562787	1.382434
Cartesian Coordinates				1	-6.542760	5.977357	-2.349412
				1	-3.189693	7.467355	-0.103934
6	0.639732	-3.957695	2.616436	1	-1.643713	5.915684	0.980257
6	-0.713477	-3.750000	2.290985	1	-5.191404	7.896604	-1.501522
6	-1.498344	-4.862854	1.948794	1	-2.532122	-4.734964	1.651135
6	-0.951272	-6.149308	1.962289	1	1.276766	-3.109178	2.843859
6	0.385486	-6.345817	2.311968	1	-1.575154	-6.994624	1.686219
6	1.181363	-5.241959	2.636337	1	2.227697	-5.379053	2.894514
15	-1.317328	-2.017670	2.106211	1	0.808148	-7.346400	2.320986
6	-3.136634	-2.084555	2.481269	1	-0.150690	-2.867680	4.814138
6	-3.697697	-3.030856	3.352906	1	-1.572624	0.712997	2.886105
6	-5.053194	-2.974807	3.681514	1	0.128308	-1.623124	6.918494
6	-5.859660	-1.953741	3.172059	1	-1.344244	1.944669	5.015501
6	-5.299141	-0.981662	2.340791	1	-0.486571	0.785260	7.045399
6	-3.947664	-1.048334	1.995829	1	-3.082470	-3.812854	3.784892
45	-0.200555	-1.038762	0.026712	1	-3.525498	-0.285680	1.351952
15	-1.440759	0.715188	-0.760168	1	-5.474679	-3.723771	4.346617
8	-0.772694	1.752030	-1.616774	1	-5.909494	-0.171309	1.957383
6	2.135051	-1.681499	-0.343460	1	-6.913836	-1.908057	3.431121
6	1.540172	-0.620486	-1.118508	1	2.264139	-2.633849	-0.839921
6	2.725108	-1.586479	0.910029	1	1.771598	0.409918	-0.889204
8	0.567429	0.343409	1.491682	1	1.473585	-0.819933	-2.185439
6	1.209990	1.451368	1.467354	1	1.964450	-0.041366	3.634701
6	1.692086	1.928011	2.818348	1	1.515272	3.998737	2.276981
6	2.077128	1.021960	3.813558	1	2.886330	0.775668	5.792923
6	2.578838	1.485827	5.030546	1	2.307752	4.836850	4.485758
6	2.656219	2.859334	5.278769	1	3.029948	3.220147	6.233173
6	2.249568	3.768466	4.296640	1	4.521631	0.736414	1.468371

1	4.427620	-0.517469	-2.085099
1	6.302112	-3.521709	0.353008
1	4.709562	-1.961177	-4.060384
1	6.576936	-4.948337	-1.600201
1	5.091463	-0.975903	2.647990
1	5.400299	-2.579082	2.025329
1	7.483959	-1.648192	3.014513
1	7.715635	-1.795643	1.262714
1	7.365389	-0.217376	1.971935
1	3.098475	-2.489774	1.379059
1	2.574471	-0.739456	1.557017
6	1.638043	3.660985	-2.589364
6	-0.059950	3.112843	-4.322741
6	-0.579697	4.761087	-2.545103
6	-0.667827	4.479010	-4.038011
1	0.027204	2.946976	-5.403066
1	-0.916050	5.778851	-0.323854
1	-0.130508	5.255004	-4.596268
6	5.676318	3.463645	0.663649
6	7.694911	2.741037	1.922856
6	7.914976	3.433558	-0.444255
6	8.296139	2.371641	0.575710
1	8.163895	3.654985	2.320146
1	8.450290	4.374260	-0.241626
1	9.384927	2.297028	0.651345
1	-1.205063	4.056915	-1.986591
1	-1.714008	4.491564	-4.359166
1	-0.692121	2.326469	-3.895550
1	8.195050	3.113229	-1.453578
1	7.906340	1.398070	0.258596
1	7.864910	1.945259	2.654761
7	6.471454	3.669400	-0.432353
7	6.251407	2.922613	1.787155
7	1.282398	3.013950	-3.745109
7	0.814091	4.640389	-2.104930
6	1.150962	5.224057	-0.811445
1	0.889136	4.550144	0.010959
1	2.221144	5.428706	-0.759766
1	0.602756	6.163360	-0.700587
6	2.054011	1.851829	-4.158990
1	3.053541	1.901134	-3.731560
1	1.579948	0.919216	-3.827434
1	2.127322	1.833765	-5.252153
6	5.933078	4.332926	-1.610791
1	6.382054	5.329393	-1.729922
1	6.164171	3.743566	-2.505724
1	4.853015	4.427593	-1.529306
6	5.464633	2.811790	3.006005
1	5.670012	3.644587	3.693753
1	4.406852	2.816060	2.760358
1	5.713319	1.875878	3.516111
15	-0.923167	-2.586911	-1.552230
6	-2.341619	-3.665300	-1.086273
6	-2.384325	-5.048391	-1.327311
6	-3.458635	-3.042046	-0.520642
6	-3.516530	-5.786206	-0.977828
1	-1.540677	-5.554873	-1.781290
6	-4.591639	-3.777369	-0.172857
1	-3.439076	-1.977011	-0.343548
6	-4.619465	-5.155388	-0.393740
1	-3.534339	-6.856845	-1.161208
1	-5.436504	-3.269292	0.281641
1	-5.494943	-5.735580	-0.116020
6	0.421133	-3.777493	-1.959845
6	1.165995	-3.662283	-3.141929
6	0.806816	-4.725611	-0.996466
6	2.285976	-4.471933	-3.347916
1	0.891756	-2.930786	-3.894301
6	1.915352	-5.541363	-1.213126
1	0.253773	-4.812851	-0.070095
6	2.665063	-5.408555	-2.385873
1	2.877934	-4.362040	-4.250985
1	2.200841	-6.265511	-0.455563
1	3.547285	-6.020086	-2.548515
6	-1.432752	-1.990007	-3.228015
6	-2.274411	-2.780316	-4.028347
6	-0.922233	-0.794963	-3.754043
6	-2.599964	-2.380384	-5.325105
1	-2.681629	-3.709933	-3.645978
6	-1.240299	-0.404511	-5.056386

1	-0.307551	-0.144975	-3.145507
6	-2.079888	-1.192962	-5.844728
1	-3.258419	-2.999762	-5.927728
1	-0.837095	0.523985	-5.447499
1	-2.331079	-0.882913	-6.855257
7	5.747248	-4.426527	-4.092406
1	5.778832	-3.944098	-4.983426
1	6.499403	-5.103614	-4.032580

5 (X = OH)

Number of imaginary frequencies : 0
 Electronic energy : HF=-538.771429
 Zero-point correction= 0.198943 (Hartree/Particle)
 Thermal correction to Energy= 0.210669
 Thermal correction to Enthalpy= 0.211613
 Thermal correction to Gibbs Free Energy= 0.160453
 Sum of electronic and zero-point Energies= -538.572486
 Sum of electronic and thermal Energies= -538.560760
 Sum of electronic and thermal Enthalpies= -538.559816
 Sum of electronic and thermal Free Energies= -538.610976
 Standard State and RRHO Corrected G= -538.606422

Cartesian Coordinates

6	-2.319562	-1.008292	0.627528
6	-0.940614	-1.130297	0.803121
6	-0.050763	-0.223777	0.215147
6	-0.584718	0.827687	-0.548463
6	-1.957533	0.963125	-0.732484
6	-2.832939	0.041117	-0.143937
1	-2.996355	-1.724996	1.087695
1	-0.553791	-1.950030	1.403078
1	-2.367024	1.776310	-1.323589
1	0.084090	1.553261	-1.003903
6	1.458180	-0.363655	0.388538
1	1.636528	-1.174917	1.108658
6	2.195426	-0.669786	-0.926993
1	1.673883	-1.494177	-1.426526
1	2.115511	0.201666	-1.586221
6	3.668785	-1.033784	-0.723198
1	3.772202	-1.914140	-0.077367
1	4.149963	-1.264640	-1.679817
1	4.218267	-0.208341	-0.261542
6	1.944308	0.911327	1.059139
8	2.653805	1.749042	0.536917
1	1.557657	1.058269	2.091469
8	-4.168019	0.218203	-0.355246
1	-4.660639	-0.478218	0.104309

(4-7)_{rr}[‡] (X = OH)

Number of imaginary frequencies : 1
 Electronic energy : HF=-5444.7477547
 Zero-point correction= 1.568225 (Hartree/Particle)
 Thermal correction to Energy= 1.667427
 Thermal correction to Enthalpy= 1.668371
 Thermal correction to Gibbs Free Energy= 1.427314
 Sum of electronic and zero-point Energies= -5443.179530
 Sum of electronic and thermal Energies= -5443.080328
 Sum of electronic and thermal Enthalpies= -5443.079383
 Sum of electronic and thermal Free Energies= -5443.320440
 Standard State and RRHO Corrected G= -5443.293264

Cartesian Coordinates

8	4.062083	-4.067169	-0.789575
3	3.194859	-2.968460	0.515382
8	1.751602	-1.926510	-0.250265
6	0.543744	-1.931974	-0.597832
8	-0.271308	-0.953751	-0.511381
45	-0.475002	0.966367	0.444111
15	-0.598003	1.748389	-2.017436
6	1.105037	2.094560	-2.666100
6	2.037930	1.053088	-2.519916
6	3.347709	1.202777	-2.967183
6	3.754274	2.397074	-3.571261
6	2.829186	3.427253	-3.742023
6	1.510134	3.276443	-3.299126
6	-0.025113	-3.197873	-1.194497

6	-1.406317	-3.435393	-1.194417
6	-1.915069	-4.626463	-1.712920
6	-1.050037	-5.583162	-2.252013
6	0.328302	-5.348677	-2.257164
6	0.841798	-4.165768	-1.722088
6	1.613217	1.111433	1.532701
6	2.595187	0.845095	0.570811
6	4.726937	0.647982	1.504370
6	5.516134	1.083315	0.337368
6	5.799884	2.452732	0.129204
6	6.450560	2.912926	-1.014961
6	6.855125	2.008881	-2.000674
6	6.614668	0.644591	-1.811922
6	5.950235	0.192944	-0.675433
6	0.658897	0.179780	2.062135
15	-2.501508	0.201646	1.326820
8	-2.762350	0.466871	2.788851
8	-2.578934	-1.468839	1.040507
6	-3.695434	-2.143198	1.488824
6	-4.857145	-2.122304	0.731010
6	-6.014426	-2.813242	1.240754
6	-5.900614	-3.576568	2.452236
6	-4.666491	-3.589545	3.157038
6	-3.593401	-2.867390	2.699392
6	-7.032845	-4.279695	2.946758
6	-8.246191	-4.217499	2.299359
6	-8.375705	-3.429864	1.130715
6	-7.293472	-2.747475	0.617845
6	-4.899188	-1.326247	-0.525346
6	-4.534792	0.020338	-0.504624
6	-4.775801	0.861264	-1.619559
6	-5.291539	0.350674	-2.782914
6	-5.534125	-1.042061	-2.911789
6	-5.318872	-1.894756	-1.778226
6	-5.484048	-3.297694	-1.960018
6	-5.847973	-3.821810	-3.182229
6	-6.084917	-2.972667	-4.290323
6	-5.931262	-1.611290	-4.151426
8	-4.014377	0.608597	0.611602
6	-1.095253	0.431631	-3.223900
6	-1.958351	-0.602594	-2.848292
6	-2.364375	-1.560663	-3.782557
6	-1.920495	-1.489520	-5.101729
6	-1.064186	-0.453968	-5.490107
6	-0.653517	0.497972	-4.558531
6	-1.629231	3.168981	-2.618501
6	-1.340722	4.491648	-2.238228
6	-2.184076	5.543087	-2.597851
6	-3.342459	5.296292	-3.337492
6	-3.638427	3.988902	-3.727887
6	-2.788724	2.936771	-3.378234
6	4.381773	-0.702241	1.757325
8	4.584840	-1.723914	1.039640
6	4.545500	1.600511	2.673066
6	5.824987	1.820855	3.495370
8	2.610168	-3.952853	2.076556
1	-5.949566	-4.897416	-3.296818
1	-5.301349	-3.962196	-1.123372
1	-6.088631	-0.947833	-4.998133
1	-6.374724	-3.398237	-5.246727
1	-5.474665	1.000523	-3.634449
1	-4.537176	1.912148	-1.525171
1	-7.419994	-2.140501	-0.270244
1	-2.656835	-2.835732	3.241435
1	-9.340014	-3.356228	0.635511
1	-6.922361	-4.860772	3.859059
1	-4.592790	-4.160219	4.079046
1	-9.105489	-4.755807	2.689074
1	1.740933	0.124439	-2.043496
1	0.808268	4.086127	-3.458072
1	4.057681	0.398134	-2.819302
1	3.126263	4.355467	-4.223025
1	4.781569	2.516386	-3.902547
1	-2.296992	-0.675499	-1.825793
1	0.011625	1.295879	-4.873031
1	-3.021232	-2.364247	-3.470192
1	-0.714007	-0.388200	-6.516756
1	-2.238444	-2.236828	-5.823654
1	-0.457975	4.709654	-1.656060
1	-3.041849	1.931740	-3.691550

1	-1.933699	6.553957	-2.288835
1	-4.532124	3.781509	-4.310263
1	-4.004696	6.113409	-3.609119
1	-2.062303	-2.687317	-0.771064
1	1.912081	-3.993479	-1.698611
1	-2.987206	-4.800477	-1.705160
1	1.005457	-6.090007	-2.673559
1	-1.447397	-6.507606	-2.663046
1	3.815978	-0.845959	2.697321
1	5.495364	3.188759	0.865149
1	5.739291	-0.862305	-0.568258
1	6.636745	3.977586	-1.143345
1	6.932586	-0.053092	-2.579978
1	4.159398	2.569766	2.331252
1	3.766090	1.198624	3.331200
1	6.632977	2.227038	2.877823
1	5.649518	2.518199	4.323539
1	6.178257	0.873222	3.918287
1	0.808302	-0.874786	1.855835
1	0.236029	0.386516	3.038701
1	1.690806	2.075647	2.022394
1	3.079870	1.677489	0.079897
1	2.597555	-0.102494	0.053858
6	2.149036	-3.368617	3.088796
6	2.461888	-2.487855	5.377693
6	0.195746	-2.439252	4.352571
6	1.219430	-1.639386	5.145950
1	2.233457	-3.345130	6.029872
1	-0.592022	-1.778338	3.975285
1	0.784046	-1.326027	6.099347
1	5.208685	-3.822194	-1.238872
6	6.625021	-2.966736	-3.077352
6	7.672172	-4.201014	-1.188768
6	7.786521	-2.981528	-2.092949
1	6.704322	-3.809221	-3.781854
1	8.385233	-4.130501	-0.360522
1	8.738089	-3.007218	-2.632083
7	6.327806	-4.305100	-0.619455
7	5.359084	-3.027269	-2.344974
7	2.985820	-2.944035	4.090108
7	0.812589	-3.106149	3.203914
1	3.242351	-1.900311	5.869507
1	1.500936	-0.738999	4.591231
1	-0.287065	-3.192262	4.993401
1	7.910524	-5.119892	-1.745943
1	7.761917	-2.069058	-1.488685
1	6.631161	-2.047298	-3.668835
15	-0.804743	3.019329	1.512933
6	-2.520717	3.680558	1.589889
6	-3.318095	3.593179	0.441136
6	-3.026338	4.335232	2.723908
6	-4.593938	4.154562	0.418500
1	-2.943296	3.081964	-0.433793
6	-4.309895	4.884223	2.703731
1	-2.426422	4.420135	3.622760
6	-5.095209	4.797868	1.551619
1	-5.196798	4.078098	-0.481563
1	-4.693227	5.381911	3.590045
1	-6.092809	5.227899	1.538857
6	-0.222895	3.101681	3.273780
6	0.865179	3.908147	3.646087
6	-0.845685	2.305105	4.250562
6	1.327966	3.910042	4.964057
1	1.364906	4.532056	2.913889
6	-0.381902	2.317564	5.567266
1	-1.675489	1.665415	3.964139
6	0.707342	3.114461	5.928498
1	2.174294	4.536280	5.232132
1	-0.873311	1.695698	6.310793
1	1.068589	3.116643	6.953201
6	0.131338	4.424675	0.758305
6	-0.323231	5.746879	0.897951
6	1.329877	4.189656	0.070169
6	0.402403	6.803659	0.347517
1	-1.248169	5.956077	1.424120
6	2.060675	5.249436	-0.471025
1	1.678965	3.178673	-0.076249
6	1.596180	6.558810	-0.338490
1	0.032543	7.819602	0.453229
1	2.978515	5.039585	-1.011747

1	2.156228	7.384068	-0.769053	6	-6.028348	1.694856	-0.064891
6	6.189487	-5.170882	0.542724	6	-6.540476	2.650974	0.858911
1	5.172375	-5.115902	0.925350	6	-7.844433	2.594025	1.304125
1	6.420671	-6.214531	0.287039	6	-8.721862	1.583175	0.846575
1	6.884474	-4.846147	1.324944	6	-8.257945	0.630842	-0.033760
6	4.148847	-2.577285	-3.026043	8	-2.893667	0.396004	-1.588848
1	3.686965	-3.375159	-3.623616	6	-0.875006	-1.167912	3.700105
1	3.416695	-2.220154	-2.300758	6	-0.395684	-1.819500	4.843028
1	4.414436	-1.755810	-3.694525	6	-0.243078	-1.118126	6.044665
6	4.392897	-3.321220	4.027655	6	-0.584701	0.232047	6.119855
1	4.570079	-4.316388	4.460082	6	-1.069079	0.886089	4.982546
1	4.729272	-3.311841	2.992467	6	-1.204434	0.196983	3.780174
1	4.975758	-2.588931	4.593596	3	3.210860	2.585087	-0.353196
6	-0.117663	-3.637090	2.215528	8	4.263016	0.950876	-0.507018
1	-0.703772	-2.827629	1.772752	6	4.626617	0.244326	0.475039
1	0.433173	-4.148983	1.431847	6	5.064503	-1.104468	0.491836
1	-0.808126	-4.346317	2.690770	6	5.270663	-1.904824	-0.721158
8	7.464806	2.396771	-3.165416	6	4.824526	-1.473624	-1.997403
1	7.563936	3.360378	-3.162637	6	4.933042	-2.279787	-3.126298
				6	5.483735	-3.560222	-3.031587
(4-7) _{cr} [±] (X = OH)				6	5.946987	-4.011822	-1.792029
				6	5.839955	-3.197852	-0.665042
Number of imaginary frequencies : 1				6	5.629640	-1.584026	1.817966
Electronic energy : HF=-5444.7377237				6	7.147701	-1.377484	1.956925
Zero-point correction= 1.566139 (Hartree/Particle)				8	4.476318	3.726783	0.649183
Thermal correction to Energy= 1.665778				8	2.768829	3.404649	-2.026230
Thermal correction to Enthalpy= 1.666722				1	-8.198194	3.330343	2.020498
Thermal correction to Gibbs Free Energy= 1.425432				1	-5.884482	3.425353	1.237641
Sum of electronic and zero-point Energies= -5443.171585				1	-8.910123	-0.167258	-0.380060
Sum of electronic and thermal Energies= -5443.071946				1	-9.748445	1.552921	1.200191
Sum of electronic and thermal Enthalpies= -5443.071002				1	-7.088540	-1.141416	-1.705128
Sum of electronic and thermal Free Energies= -5443.312292				1	-4.676107	-1.190653	-2.296180
Standard State and RRHO Corrected G= -5443.285608				1	-5.897982	3.717057	-1.772119
				1	-0.855062	3.566815	1.387807
Cartesian Coordinates				1	-6.480723	6.024469	-2.358854
				1	-3.120232	7.489014	-0.107753
6	0.618048	-3.974185	2.619577	1	-1.590085	5.925580	0.982311
6	-0.733187	-3.753194	2.294581	1	-5.114854	7.933304	-1.510742
6	-1.529279	-4.858299	1.953269	1	-2.561645	-4.720070	1.655239
6	-0.995308	-6.150259	1.968063	1	1.263569	-3.131667	2.845688
6	0.339307	-6.360013	2.318269	1	-1.627711	-6.989495	1.692844
6	1.146505	-5.263915	2.641102	1	2.191318	-5.411523	2.899737
15	-1.319878	-2.015006	2.110335	1	0.751541	-7.364929	2.328981
6	-3.140225	-2.065157	2.484646	1	-0.157308	-2.877172	4.817121
6	-3.710625	-3.005586	3.356606	1	-1.557308	0.715517	2.895198
6	-5.065845	-2.937022	3.684048	1	0.130778	-1.637576	6.923101
6	-5.862669	-1.909122	3.173130	1	-1.320089	1.942316	5.026239
6	-5.292647	-0.942772	2.341664	1	-0.468760	0.774472	7.053990
6	-3.941528	-1.021961	1.998005	1	-3.102893	-3.792784	3.789796
45	-0.196796	-1.041401	0.033487	1	-3.512082	-0.263422	1.354164
15	-1.428184	0.721437	-0.755157	1	-5.494624	-3.681611	4.349405
8	-0.753838	1.754011	-1.612361	1	-5.895237	-0.127226	1.956886
6	2.120564	-1.704693	-0.319573	1	-6.916621	-1.853791	3.431238
6	1.547278	-0.642479	-1.108614	1	2.235149	-2.664676	-0.805006
6	2.737138	-1.596707	0.923497	1	1.791935	0.386775	-0.887047
8	0.578571	0.335795	1.498269	1	1.481649	-0.850334	-2.173862
6	1.224802	1.441370	1.473308	1	1.972094	-0.052595	3.641960
6	1.708483	1.917288	2.824020	1	1.539871	3.988533	2.281455
6	2.089858	1.010372	3.819872	1	2.898155	0.762214	5.799413
6	2.593775	1.473042	5.036408	1	2.336623	4.824765	4.489184
6	2.677158	2.846390	5.283521	1	3.052640	3.206353	6.237550
6	2.273975	3.756501	4.300870	1	4.566640	0.700396	1.480660
6	1.813770	3.293396	3.067975	1	4.379363	-0.492342	-2.080957
8	1.498752	2.135636	0.472523	1	6.201853	-3.593459	0.277802
8	-2.102651	1.441903	0.633979	1	4.572556	-1.931206	-4.089999
6	-2.578937	2.720575	0.427876	1	6.383291	-5.005395	-1.705398
6	-3.792966	2.895943	-0.215290	1	5.126328	-1.042061	2.629059
6	-4.171078	4.240933	-0.569662	1	5.391712	-2.642715	1.981916
6	-3.364941	5.341486	-0.118338	1	7.393511	-0.312256	1.894274
6	-2.188025	5.086439	0.637788	1	7.518186	-1.756266	2.917566
6	-1.782707	3.797541	0.876511	1	7.695410	-1.888422	1.158166
6	-3.738168	6.668734	-0.464770	1	3.092470	-2.500454	1.406011
6	-4.844397	6.914830	-1.246968	1	2.593725	-0.742627	1.563153
6	-5.622042	5.831683	-1.721691	6	1.671146	3.653167	-2.583939
6	-5.296902	4.533867	-1.390156	6	-0.026723	3.109668	-4.317682
6	-4.656754	1.718843	-0.520497	6	-0.541056	4.764370	-2.544178
6	-4.188110	0.602597	-1.217061	6	-0.629036	4.479054	-4.036451
6	-5.085828	-0.401538	-1.675933	1	0.058925	2.940456	-5.397506
6	-6.413550	-0.369116	-1.346062	1	-0.872466	5.784343	-2.325698
6	-6.914679	0.651359	-0.494196	1	-0.088049	5.251387	-4.596233

6	5.698240	3.440740	0.668401
6	7.708289	2.669336	1.915603
6	7.934423	3.398377	-0.440133
6	8.302646	2.314756	0.561530
1	8.194798	3.566181	2.330293
1	8.476118	4.330991	-0.217955
1	9.390349	2.224192	0.635084
1	-1.170654	4.064728	-1.984710
1	-1.674945	4.495242	-4.358329
1	-0.661596	2.327170	-3.887483
1	8.215716	3.094527	-1.454036
1	7.900031	1.352028	0.227726
1	7.863543	1.856226	2.631800
7	6.492405	3.643188	-0.428802
7	6.268300	2.881869	1.785822
7	1.316078	3.008267	-3.740945
7	0.851612	4.637363	-2.101836
6	1.189479	5.220414	-0.808350
1	0.923272	4.548556	0.014395
1	2.260459	5.420637	-0.755405
1	0.645231	6.162138	-0.698800
6	2.084233	1.841084	-4.148246
1	3.096750	1.909260	-3.755105
1	1.630383	0.912967	-3.777977
1	2.122558	1.796736	-5.242095
6	5.960360	4.329384	-1.597431
1	6.399368	5.333288	-1.689141
1	6.208548	3.762735	-2.502115
1	4.878421	4.410522	-1.526694
6	5.484903	2.778842	3.007652
1	5.708314	3.604291	3.698610
1	4.426262	2.803102	2.766922
1	5.719168	1.836189	3.512159
15	-0.925875	-2.584830	-1.547241
6	-2.357958	-3.647980	-1.086117
6	-2.417040	-5.030273	-1.328752
6	-3.468135	-3.012313	-0.520932
6	-3.558103	-5.755033	-0.980866
1	-1.579359	-5.546446	-1.782810
6	-4.610018	-3.734586	-0.174722
1	-3.435915	-1.947742	-0.343047
6	-4.653943	-5.111923	-0.396839
1	-3.588409	-6.825179	-1.165526
1	-5.449149	-3.216934	0.279561
1	-5.536365	-5.682050	-0.120250
6	0.404326	-3.794598	-1.951643
6	1.150609	-3.696162	-3.134264
6	0.770857	-4.750520	-0.988448
6	2.250385	-4.532812	-3.344023
1	0.893276	-2.957703	-3.885786
6	1.857864	-5.593733	-1.208262
1	0.217577	-4.825254	-0.061246
6	2.606329	-5.480158	-2.383859
1	2.845693	-4.431421	-4.245608
1	2.126601	-6.325594	-0.451986
1	3.469101	-6.119025	-2.547092
6	-1.421244	-1.984102	-3.225856
6	-2.261009	-2.770842	-4.031786
6	-0.901563	-0.791550	-3.748531
6	-2.575538	-2.370121	-5.330915
1	-2.674963	-3.698492	-3.651784
6	-1.208762	-0.400362	-5.053320
1	-0.287775	-0.144230	-3.136322
6	-2.046237	-1.185316	-5.847277
1	-3.232450	-2.986778	-5.937997
1	-0.798310	0.525830	-5.442219
1	-2.288484	-0.874704	-6.859809
8	5.529834	-4.326065	-4.169092
1	5.917519	-5.186686	-3.952655

5 (X = OMe)			
Number of imaginary frequencies : 0			
Electronic energy :	HF=	-578.0765954	
Zero-point correction=		0.227582 (Hartree/Particle)	
Thermal correction to Energy=		0.240648	
Thermal correction to Enthalpy=		0.241592	
Thermal correction to Gibbs Free Energy=		0.187297	
Sum of electronic and zero-point Energies=		-577.849014	
Sum of electronic and thermal Energies=		-577.835947	

Sum of electronic and thermal Enthalpies=				-577.835003
Sum of electronic and thermal Free Energies=				-577.889298
Standard State and RRHO Corrected G=				-577.884549

Cartesian Coordinates				

6	-1.931297	-0.884081	0.564992	
6	-0.556467	-1.060688	0.749649	
6	0.377415	-0.182749	0.193132	
6	-0.104529	0.906118	-0.555499	
6	-1.466490	1.098016	-0.748928	
6	-2.393077	0.202051	-0.190183	
1	-2.622250	-1.590647	1.009260	
1	-0.210677	-1.907992	1.336632	
1	-1.838374	1.938547	-1.326732	
1	0.597412	1.613352	-0.989436	
6	1.876627	-0.388004	0.382354	
1	2.011669	-1.221617	1.086388	
6	2.619408	-0.695429	-0.929742	
1	2.069531	-1.483818	-1.456294	
1	2.588124	0.193918	-1.568909	
6	4.071892	-1.129831	-0.714207	
1	4.126116	-2.029386	-0.089147	
1	4.556907	-1.358832	-1.669351	
1	4.650336	-0.341261	-0.224450	
6	2.406071	0.849618	1.089272	
8	3.165323	1.663742	0.600772	
1	2.003993	0.993135	2.116249	
8	-3.703769	0.475688	-0.436290	
6	-4.689346	-0.396730	0.112868	
1	-5.654681	0.004235	-0.202038	
1	-4.583342	-1.419824	-0.269680	
1	-4.648436	-0.414994	1.209405	

(4-7) _{re} ² (X = OMe)				

Number of imaginary frequencies : 1				
Electronic energy :				HF=-5484.0534138
Zero-point correction=				1.596858 (Hartree/Particle)
Thermal correction to Energy=				1.697414
Thermal correction to Enthalpy=				1.698358
Thermal correction to Gibbs Free Energy=				1.454324
Sum of electronic and zero-point Energies=				-5482.456556
Sum of electronic and thermal Energies=				-5482.356000
Sum of electronic and thermal Enthalpies=				-5482.355056
Sum of electronic and thermal Free Energies=				-5482.599090
Standard State and RRHO Corrected G=				-5482.571586

Cartesian Coordinates				

8	3.792735	-4.277525	-0.857710	
3	2.948214	-3.201866	0.481533	
8	1.576255	-2.053311	-0.266572	
6	0.380307	-1.973789	-0.645201	
8	-0.378737	-0.953273	-0.538962	
45	-0.512802	0.926869	0.509916	
15	-0.521997	1.838719	-1.910820	
6	1.215578	2.109116	-2.502456	
6	2.079300	1.006885	-2.378570	
6	3.404414	1.090403	-2.796501	
6	3.896278	2.277796	-3.348799	
6	3.041157	3.370253	-3.494944	
6	1.706628	3.286556	-3.080915	
6	-0.242702	-3.179466	-1.309257	
6	-1.634864	-3.331043	-1.364330	
6	-2.196148	-4.468727	-1.944930	
6	-1.372229	-5.457566	-2.490246	
6	0.017104	-5.309244	-2.439767	
6	0.581952	-4.180398	-1.843261	
6	1.542256	0.898057	1.662814	
6	2.537496	0.626112	0.716286	
6	4.623746	0.277657	1.703548	
6	5.462249	0.742728	0.583872	
6	5.797964	2.107449	0.453743	
6	6.484747	2.613155	-0.652677	
6	6.875157	1.749398	-1.680965	
6	6.589708	0.382243	-1.561089	
6	5.890521	-0.108827	-0.466002	
6	0.522938	-0.003236	2.117565	
15	-2.602157	0.230326	1.302552	

8	-2.883414	0.439022	2.770007	1	5.547338	1.944323	4.646713
8	-2.757543	-1.418779	0.932792	1	6.015513	0.302478	4.161917
6	-3.919966	-2.056107	1.313143	1	0.619455	-1.053182	1.862379
6	-5.056206	-1.936469	0.526064	1	0.080937	0.179853	3.090363
6	-6.261555	-2.591890	0.966678	1	1.655682	1.831368	2.202646
6	-6.222219	-3.424216	2.136570	1	3.079010	1.453613	0.279538
6	-5.011919	-3.537858	2.872705	1	2.506075	-0.294812	0.153974
6	-3.891177	-2.847874	2.484844	6	1.816940	-3.670501	3.005453
6	-7.402417	-4.093420	2.561045	6	2.116464	-2.910098	5.340233
6	-8.591670	-3.933020	1.886374	6	-0.118696	-2.705270	4.267866
6	-8.647070	-3.076766	0.760916	6	0.922342	-1.992240	5.119048
6	-7.517063	-2.425316	0.315306	1	1.832077	-3.780915	5.951111
6	-5.022351	-1.075052	-0.686478	1	-0.867327	-1.991676	3.907579
6	-4.591958	0.247911	-0.583593	1	0.479644	-1.700161	6.075822
6	-4.759314	1.157888	-1.656934	6	4.956051	-4.056124	-1.275630
6	-5.267635	0.736844	-2.858874	6	6.438884	-3.159190	-3.042492
6	-5.576384	-0.632783	-3.068942	6	7.401547	-4.531003	-1.203684
6	-5.435755	-1.554128	-1.978172	6	7.578730	-3.270797	-2.039220
6	-5.667495	-2.934925	-2.239324	1	6.504839	-3.962192	-3.793005
6	-6.023648	-3.374332	-3.496678	1	8.101787	-4.532405	-0.361672
6	-6.186013	-2.456877	-4.562973	1	8.538989	-3.303973	-2.562292
6	-5.967425	-1.114560	-4.347005	7	6.044415	-4.610467	-0.661630
8	-4.075458	0.747998	0.576630	7	5.155549	-3.217189	-2.340615
6	-1.065908	0.618644	-3.196461	7	2.647605	-3.338966	4.046154
6	-1.984372	-0.390675	-2.891616	7	0.493236	-3.343052	3.100490
6	-2.416675	-1.277617	-3.882687	1	2.912946	-2.382072	5.872331
6	-1.945016	-1.157740	-5.188586	1	1.259596	-1.083191	4.611494
6	-1.033913	-0.145091	-5.506514	1	-0.649117	-3.465044	4.861404
6	-0.596136	0.734627	-4.518125	1	7.613910	-5.428137	-1.805043
6	-1.448188	3.349783	-2.459447	1	7.576998	-2.391935	-1.386775
6	-1.081607	4.633870	-2.018582	1	6.488669	-2.207780	-3.579054
6	-1.852381	5.751224	-2.340819	15	-0.759442	2.941652	1.668331
6	-3.014244	5.610749	-3.102370	6	-2.436407	3.699217	1.731013
6	-3.386916	4.342919	-3.552992	6	-3.204843	3.712530	0.559461
6	-2.609737	3.224971	-3.241050	6	-2.933921	4.331724	2.881206
6	4.208787	-1.066651	1.868404	6	-4.441890	4.354746	0.530152
8	4.384108	-2.054937	1.098687	1	-2.838563	3.217803	-0.328536
6	4.450533	1.170589	2.919489	6	-4.179334	4.962236	2.853191
6	5.715183	1.287028	3.784896	1	-2.356058	4.338434	3.798295
8	2.274359	-4.229097	1.977156	6	-4.934384	4.978379	1.678033
1	-6.176866	-4.435624	-3.671523	1	-5.022216	4.357465	-0.387787
1	-5.542778	-3.651046	-1.435229	1	-4.556310	5.443034	3.751465
1	-6.067562	-0.400137	-5.160334	1	-5.901799	5.472347	1.658656
1	-6.470476	-2.815766	-5.547915	6	-0.225944	2.909713	3.446145
1	-5.393926	1.439330	-3.678334	6	0.890761	3.639434	3.885942
1	-4.471453	2.188645	-1.499095	6	-0.918190	2.103461	4.366530
1	-7.586896	-1.764863	-0.540297	6	1.313628	3.556002	5.214595
1	-2.971584	-2.892987	3.054479	1	1.443817	4.268495	3.197858
1	-9.591695	-2.925613	0.245717	6	-0.493683	2.030593	5.694490
1	-7.348051	-4.728201	3.442094	1	-1.771385	1.523003	4.027485
1	-4.994312	-4.159893	3.763767	6	0.624161	2.750923	6.122790
1	-9.488042	-4.446404	2.222520	1	2.182958	4.123349	5.535041
1	1.715138	0.081746	-1.943995	1	-1.038652	1.402276	6.393962
1	1.059982	4.144186	-3.221661	1	0.954504	2.686621	7.155887
1	4.060094	0.238103	-2.666142	6	0.279585	4.320765	1.006274
1	3.405506	4.295071	-3.934479	6	-0.097334	5.660557	1.198527
1	4.934288	2.341559	-3.661360	6	1.481148	4.044084	0.339421
1	-2.346658	-0.499820	-1.880471	6	0.708321	6.694624	0.721025
1	0.112782	1.514533	-4.777658	1	-1.023212	5.901666	1.709220
1	-3.117292	-2.063577	-3.625373	6	2.292050	5.080179	-0.128647
1	-0.661826	-0.041665	-6.522303	1	1.770223	3.021345	0.151348
1	-2.284091	-1.849366	-5.955023	6	1.905171	6.408317	0.056547
1	-0.194067	4.771218	-1.419265	1	0.398749	7.725659	0.866806
1	-2.920926	2.252665	-3.601960	1	3.211241	4.838842	-0.653858
1	-1.542542	6.729956	-1.985682	1	2.527836	7.216575	-0.316466
1	-4.283851	4.218381	-4.153689	6	5.853435	-5.521669	0.457434
1	-3.619815	6.479323	-3.345104	1	4.829072	-5.453981	0.817977
1	-2.258942	-2.560525	-0.933377	1	6.061326	-6.559157	0.160253
1	1.659336	-4.075299	-1.779164	1	6.537778	-5.252641	1.269695
1	-3.276393	-4.575925	-1.979781	6	3.973939	-2.704983	-3.028411
1	0.662555	-6.075940	-2.860557	1	3.498387	-3.467397	-3.660441
1	-1.810138	-6.340212	-2.949178	1	3.239447	-2.347512	-2.305617
1	3.608541	-1.235317	2.782495	1	4.279150	-1.871526	-3.664246
1	5.503975	2.813134	1.223180	6	4.033897	-3.788771	4.000018
1	5.642683	-1.160582	-0.420148	1	4.146094	-4.810765	4.389439
1	6.696658	3.675122	-0.701540	1	4.398034	-3.750726	2.974918
1	6.900043	-0.281867	-2.361765	1	4.639716	-3.116129	4.613782
1	4.116745	2.173604	2.623449	6	-0.436816	-3.778591	2.066544
1	3.636295	0.768376	3.533747	1	-0.973087	-2.920611	1.652698
1	6.556436	1.690571	3.211621	1	0.108141	-4.276630	1.270011

1	-1.171416	-4.476377	2.489829	8	-4.127402	-1.281984	-0.419072
8	7.508747	2.135106	-2.831577	6	-4.507349	-0.659671	0.611217
6	7.765109	3.524370	-3.012454	6	-5.043156	0.650637	0.717069
1	8.244303	3.620016	-3.989027	6	-5.357359	1.493658	-0.443337
1	6.837502	4.111762	-3.008438	6	-4.902450	1.180418	-1.751990
1	8.441139	3.916937	-2.241658	6	-5.109504	2.039866	-2.822800
(4-7) _{st} ⁺ (X = OMe)							
Number of imaginary frequencies : 1							
Electronic energy : HF=-5484.0435317							
Zero-point correction= 1.594920 (Hartree/Particle)							
Thermal correction to Energy= 1.695759							
Thermal correction to Enthalpy= 1.696703							
Thermal correction to Gibbs Free Energy= 1.452599							
Sum of electronic and zero-point Energies= -5482.448612							
Sum of electronic and thermal Energies= -5482.347773							
Sum of electronic and thermal Enthalpies= -5482.346828							
Sum of electronic and thermal Free Energies= -5482.590933							
Standard State and RRHO Corrected G= -5482.563943							
Cartesian Coordinates							
6	-0.737078	3.730515	2.877387	1	2.157876	-5.903048	0.738013
6	0.616348	3.618752	2.508587	1	5.740141	-7.511301	-1.956546
6	1.327024	4.791318	2.206278	1	2.357761	4.738747	1.876935
6	0.708588	6.041543	2.301672	1	-1.319060	2.835718	3.072853
6	-0.626685	6.141935	2.695060	1	1.275627	6.934717	2.055200
6	-1.349549	4.978468	2.979852	1	-2.394207	5.041250	3.271488
15	1.311115	1.935727	2.218148	1	-1.104704	7.114529	2.768902
6	3.134676	2.089137	2.547977	1	0.175977	2.578169	4.998162
6	3.665616	3.019908	3.454543	1	1.743973	-0.809042	2.847400
6	5.031151	3.027609	3.744055	1	0.030541	1.213191	7.040645
6	5.880215	2.084591	3.159100	1	1.647349	-2.160584	4.913805
6	5.352883	1.126067	2.291167	1	0.785251	-1.158465	7.024274
6	3.990209	1.130144	1.985586	1	3.019134	3.740323	3.944226
45	0.186260	0.991229	0.127538	1	3.594724	0.379118	1.311448
15	1.483939	-0.661727	-0.783167	1	5.427796	3.764462	4.437375
8	0.826475	-1.702974	-1.642704	1	5.998016	0.374842	1.848747
6	-2.184903	1.519511	-0.137408	1	6.942439	2.088086	3.387479
6	-1.560470	0.535837	-0.986926	1	-2.376859	2.489481	-0.575743
6	-2.772315	1.309916	1.108423	1	-1.730486	-0.516451	-0.809431
8	-0.471583	-0.480221	1.552674	1	-1.535068	0.794738	-2.042883
6	-1.035747	-1.628964	1.495315	1	-1.822869	-0.277215	3.744017
6	-1.460745	-2.189732	2.832704	1	-1.177629	-4.220420	2.194278
6	-1.873762	-1.352069	3.875538	1	-2.654487	-1.240885	5.878415
6	-2.324476	-1.897579	5.078393	1	-1.880722	-5.200463	4.375265
6	-2.322815	-3.283232	5.263820	1	-2.657820	-3.706907	6.206696
6	-1.885379	-4.123105	4.234436	1	-4.376749	-1.162210	1.587885
6	-1.477851	-3.578993	3.016126	1	-4.372663	0.250920	-1.905299
8	-1.275450	-2.303338	0.473000	1	-6.422544	3.021175	0.667112
8	2.275140	-1.382438	0.544097	1	-4.741412	1.786341	-3.813085
6	2.847943	-2.606944	0.268635	1	-6.783369	4.520904	-1.200836
6	4.046991	-2.655572	-0.423464	1	-5.021856	0.476925	2.849047
6	4.524176	-3.949749	-0.840829	1	-5.457495	2.075366	2.294555
6	3.832525	-5.130793	-0.403213	1	-7.235073	-0.427960	2.154684
6	2.668514	-5.004220	0.403674	1	-7.458098	0.950527	3.248741
6	2.165113	-3.763947	0.705428	1	-7.709751	1.143561	1.504140
6	4.303325	-6.407884	-0.813480	1	-3.178690	2.164801	1.637896
6	5.394966	-6.529899	-1.643924	1	-2.545670	0.446144	1.709698
6	6.059089	-5.367749	-2.104019	6	-1.362638	-3.694939	-2.673910
6	5.638444	-4.115314	-1.711097	6	0.253809	-2.971143	-4.415345
6	4.793900	-1.398469	-0.716486	6	0.920751	-4.651791	-2.716654
6	4.199561	-0.310938	-1.359490	6	0.958445	-4.302896	-4.197499
6	4.981273	0.788156	-1.811204	1	0.142389	-2.765467	-5.486296
6	6.316743	0.871315	-1.523067	1	1.322970	-5.655484	-2.546567
6	6.940525	-0.124763	-0.724814	1	0.463211	-5.089643	-4.779143
6	6.172247	-1.262239	-0.306202	6	-5.361714	-3.916071	0.616005
6	6.804003	-2.197078	0.563656	6	-7.413810	-3.385662	1.913730
6	8.111019	-2.030445	0.970606	6	-7.600555	-3.934980	-0.494026
6	8.872136	-0.924313	0.524928	6	-8.037295	-2.964038	0.592153
6	8.290818	0.008332	-0.305380	1	-7.827800	-4.349797	2.248524
8	2.880165	-0.229409	-1.686215	1	-8.088971	-4.912362	-0.358376
6	0.969277	0.980682	3.772058	1	-9.128401	-2.954969	0.670494
6	0.482879	1.538563	4.960541	1	1.516235	-3.935117	-2.141838
6	0.410782	0.766252	6.125823	1	1.996640	-4.231545	-4.536535
6	0.838978	-0.561140	6.118412	1	0.834531	-2.161448	-3.959309
6	1.329288	-1.121849	4.934598	1	-7.893385	-3.561610	-1.481279
6	1.385810	-0.362459	3.768814	1	-7.703152	-1.951675	0.339600
3	-2.949089	-2.839564	-0.372308	1	-7.629164	-2.651073	2.695871

7	-6.147133	-4.101594	-0.489737
7	-5.962401	-3.472552	1.768922
7	-1.085421	-2.996679	-3.822108
7	-0.466442	-4.633794	-2.240937
6	-0.732399	-5.267765	-0.954019
1	-0.523752	-4.585963	-0.123272
1	-1.778444	-5.572365	-0.894461
1	-0.098623	-6.153920	-0.866699
6	-1.944921	-1.872704	-4.164327
1	-2.957143	-2.057718	-3.809030
1	-1.586524	-0.938272	-3.713551
1	-1.960808	-1.751312	-5.252454
6	-5.574858	-4.648866	-1.711075
1	-5.991098	-5.645542	-1.915073
1	-5.814653	-3.996516	-2.558999
1	-4.493399	-4.715925	-1.623660
6	-5.178888	-3.395442	2.992657
1	-5.325845	-4.284962	3.622045
1	-4.124019	-3.314296	2.747209
1	-5.485215	-2.514780	3.565746
15	0.771117	2.651081	-1.393574
6	2.141697	3.786820	-0.918223
6	2.101707	5.179611	-1.096799
6	3.307064	3.203633	-0.411054
6	3.201029	5.963802	-0.743572
1	1.218939	5.657739	-1.504712
6	4.407800	3.985177	-0.060233
1	3.350977	2.132558	-0.281979
6	4.353508	5.370886	-0.218224
1	3.154665	7.040795	-0.878313
1	5.292068	3.505550	0.347897
1	5.203351	5.986572	0.062721
6	-0.647582	3.786456	-1.700390
6	-1.426004	3.691910	-2.862387
6	-1.043831	4.668491	-0.680306
6	-2.586751	4.459318	-2.996125
1	-1.145239	3.008286	-3.656315
6	-2.190771	5.445591	-0.825092
1	-0.466066	4.735255	0.232369
6	-2.970165	5.336074	-1.980825
1	-3.206055	4.357903	-3.881547
1	-2.481196	6.122026	-0.026392
1	-3.876259	5.924801	-2.085895
6	1.253742	2.167474	-3.113461
6	2.012103	3.048759	-3.902063
6	0.802420	0.967396	-3.680330
6	2.314439	2.733140	-5.227396
1	2.371547	3.984572	-3.487979
6	1.096353	0.660869	-5.010384
1	0.253273	0.249925	-3.084964
6	1.853209	1.539567	-5.786994
1	2.908503	3.422638	-5.820711
1	0.739386	-0.272723	-5.433059
1	2.085778	1.294831	-6.819653
8	-5.889030	4.051888	-3.759947
6	-6.591077	5.282889	-3.631224
1	-6.568849	5.750262	-4.618010
1	-7.635936	5.124993	-3.332587
1	-6.112530	5.955413	-2.907396

5 (X = Me)			

Number of imaginary frequencies : 0			
Electronic energy : HF=-502.8705853			
Zero-point correction= 0.222082 (Hartree/Particle)			
Thermal correction to Energy= 0.234543			
Thermal correction to Enthalpy= 0.235487			
Thermal correction to Gibbs Free Energy= 0.181792			
Sum of electronic and zero-point Energies= -502.648503			
Sum of electronic and thermal Energies= -502.636042			
Sum of electronic and thermal Enthalpies= -502.635098			
Sum of electronic and thermal Free Energies= -502.688793			
Standard State and RRHO Corrected G= -502.683415			

Cartesian Coordinates			

6	-2.279819	-1.027883	0.632582
6	-0.900051	-1.141124	0.813105
6	-0.022484	-0.221316	0.227284
6	-0.566902	0.823921	-0.534864

6	-1.945172	0.934660	-0.712594
6	-2.827383	0.011698	-0.131098
1	-2.941154	-1.759048	1.091539
1	-0.500705	-1.959056	1.407820
1	-2.343985	1.751043	-1.310257
1	0.093958	1.555298	-0.993256
6	1.488340	-0.348070	0.394967
1	1.676225	-1.143616	1.130111
6	2.215272	-0.678838	-0.920702
1	1.689755	-1.512077	-1.400962
1	2.130316	0.180542	-1.594922
6	3.689740	-1.040488	-0.720996
1	3.796888	-1.909381	-0.060472
1	4.163529	-1.288803	-1.676917
1	4.243252	-0.207558	-0.278077
6	1.976103	0.942000	1.035089
8	2.687225	1.765475	0.493191
1	1.592402	1.112862	2.064719
6	-4.320302	0.155160	-0.300259
1	-4.835239	-0.798320	-0.147823
1	-4.730710	0.868989	0.425669
1	-4.576388	0.526999	-1.297785

(4-7)_{re}⁺ (X = Me)			

Number of imaginary frequencies : 1			
Electronic energy : HF=-5408.8411169			
Zero-point correction= 1.590466 (Hartree/Particle)			
Thermal correction to Energy= 1.690723			
Thermal correction to Enthalpy= 1.691667			
Thermal correction to Gibbs Free Energy= 1.446021			
Sum of electronic and zero-point Energies= -5407.250651			
Sum of electronic and thermal Energies= -5407.150394			
Sum of electronic and thermal Enthalpies= -5407.149450			
Sum of electronic and thermal Free Energies= -5407.395096			
Standard State and RRHO Corrected G= -5407.366266			

Cartesian Coordinates			

8	4.561387	-3.176903	-1.396006
3	3.647903	-2.246421	0.026515
8	1.994037	-1.435845	-0.547249
6	0.774642	-1.652805	-0.760122
8	-0.184144	-0.837544	-0.552761
45	-0.622769	1.037799	0.418094
15	-0.946712	1.782623	-2.038198
6	0.664191	2.361949	-2.752240
6	1.742772	1.468782	-2.626273
6	3.003199	1.798408	-3.118402
6	3.211275	3.029390	-3.748648
6	2.141693	3.912356	-3.899851
6	0.872652	3.579412	-3.412807
6	0.370056	-2.993896	-1.328951
6	-0.947713	-3.455459	-1.207818
6	-1.300297	-4.714759	-1.693392
6	-0.343139	-5.518965	-2.319232
6	0.971361	-5.060783	-2.446786
6	1.330324	-3.807027	-1.947674
6	1.460299	1.490002	1.445693
6	2.441257	1.388520	0.448703
6	4.573165	1.483003	1.323120
6	5.256544	2.121686	0.182697
6	5.279851	3.529747	0.045056
6	5.839440	4.148219	-1.071100
6	6.420001	3.403726	-2.107818
6	6.414286	2.008778	-1.972953
6	5.845342	1.380530	-0.866872
6	0.678701	0.415953	1.983951
15	-2.461928	-0.032689	1.392415
8	-2.682797	0.184712	2.868920
8	-2.284814	-1.695340	1.099097
6	-3.247866	-2.540401	1.606270
6	-4.443174	-2.705257	0.921513
6	-5.442090	-3.569908	1.496268
6	-5.132128	-4.306585	2.689866
6	-3.867719	-4.127283	3.313878
6	-2.953514	-3.243911	2.797599
6	-6.106091	-5.178974	3.247672
6	-7.353148	-5.308171	2.678916
6	-7.679206	-4.550592	1.528789

6	-6.752537	-3.706438	0.955585
6	-4.684592	-1.933256	-0.327710
6	-4.535807	-0.546070	-0.326377
6	-4.962886	0.237482	-1.427592
6	-5.452411	-0.357201	-2.561903
6	-5.482739	-1.771877	-2.676560
6	-5.078074	-2.570933	-1.555699
6	-5.034563	-3.984120	-1.727618
6	-5.378162	-4.569094	-2.927849
6	-5.801633	-3.776618	-4.022176
6	-5.852527	-2.406621	-3.892613
8	-4.056773	0.125404	0.760962
6	-1.307448	0.403102	-3.222656
6	-1.998942	-0.740675	-2.810464
6	-2.312071	-1.748003	-3.728487
6	-1.945364	-1.618922	-5.066877
6	-1.260711	-0.475356	-5.491002
6	-0.942826	0.527041	-4.576153
6	-2.201004	3.034255	-2.586782
6	-2.080258	4.393895	-2.248999
6	-3.094254	5.302475	-2.553787
6	-4.258047	4.872410	-3.194106
6	-4.388576	3.526712	-3.542962
6	-3.369331	2.618105	-3.249074
6	4.464774	0.076249	1.480740
8	4.796911	-0.841620	0.680395
6	4.289023	2.305006	2.568218
6	5.550238	2.665993	3.367936
8	3.295635	-3.470350	1.531151
1	-5.318684	-5.648531	-3.035916
1	-4.707565	-4.605050	-0.901581
1	-6.155372	-1.782968	-4.730009
1	-6.072711	-4.250364	-4.961281
1	-5.777504	0.248573	-3.403548
1	-4.886274	1.313491	-1.346599
1	-7.028814	-3.126748	0.083249
1	-1.998520	-3.067574	3.277291
1	-8.672810	-4.629805	1.096318
1	-5.847442	-5.735949	4.144919
1	-3.645121	-4.682266	4.221463
1	-8.090545	-5.975054	3.116597
1	1.601596	0.514201	-2.131295
1	0.056071	4.275779	-3.560043
1	3.826565	1.103795	-2.989258
1	2.286741	4.865970	-4.400584
1	4.198004	3.293200	-4.116685
1	-2.274131	-0.858386	-1.773134
1	-0.410065	1.408748	-4.918141
1	-2.833777	-2.635091	-3.388507
1	-0.971351	-0.364631	-6.532621
1	-2.189227	-2.405320	-5.776009
1	-1.195972	4.752922	-1.744114
1	-3.495922	1.579596	-3.528677
1	-2.971159	6.346383	-2.279722
1	-5.284284	3.178140	-4.049987
1	-5.052139	5.577798	-3.421810
1	-1.675140	-2.823231	-0.717604
1	2.355881	-3.463279	-2.021648
1	-2.324642	-5.061396	-1.591831
1	1.720747	-5.681353	-2.931124
1	-0.619639	-6.497504	-2.703287
1	3.964174	-0.225052	2.420392
1	4.839421	4.157312	0.812853
1	5.832262	0.302496	-0.803098
1	5.821708	5.234309	-1.139724
1	6.851472	1.395727	-2.759469
1	3.743006	3.222660	2.315077
1	3.608460	1.736203	3.212980
1	6.254792	3.244438	2.761025
1	5.301000	3.260607	4.255118
1	6.068627	1.759244	3.701158
1	0.978767	-0.599278	1.744254
1	0.263345	0.535460	2.978806
1	1.404974	2.446834	1.952010
1	2.768944	2.290427	-0.049494
1	2.555523	0.461883	-0.093353
6	2.913117	-2.982430	2.624548
6	3.430324	-2.016712	4.862465
6	1.065072	-2.311378	4.164815
6	2.066341	-1.347574	4.783177

1	3.425200	-2.829119	5.604941
1	0.124927	-1.794926	3.944754
1	1.731535	-1.047855	5.780466
6	5.630960	-3.819470	-1.251097
6	8.107376	-3.976146	-1.513590
6	6.806137	-5.945021	-0.748494
6	8.046158	-5.101550	-0.492032
1	8.344620	-4.372323	-2.512644
1	6.682229	-6.697644	0.036206
1	8.945742	-5.719882	-0.561587
7	5.614690	-5.095373	-0.748556
7	6.837379	-3.250259	-1.557157
7	3.818269	-2.535238	3.550869
7	1.580148	-2.853949	2.907891
1	4.193003	-1.295407	5.174213
1	2.138040	-0.446956	4.164970
1	0.834216	-3.132207	4.860978
1	6.894677	-6.481362	-1.706201
1	7.998588	-4.681561	0.519124
1	8.894648	-3.261005	-1.252821
15	-1.220249	3.020606	1.496840
6	-3.014102	3.408082	1.642501
6	-3.829458	3.199736	0.522109
6	-3.573683	3.973282	2.798993
6	-5.176717	3.556523	0.549413
1	-3.411668	2.754532	-0.369462
6	-4.926908	4.316145	2.828705
1	-2.962023	4.148758	3.676608
6	-5.730377	4.112201	1.704447
1	-5.792297	3.390850	-0.329738
1	-5.350320	4.746477	3.731883
1	-6.782216	4.382872	1.730045
6	-0.588083	3.214263	3.231256
6	0.351210	4.205715	3.560112
6	-1.022293	2.328488	4.232818
6	0.853656	4.303013	4.859710
1	0.704555	4.901418	2.807750
6	-0.520992	2.436916	5.531391
1	-1.737623	1.550546	3.981056
6	0.420201	3.419192	5.849366
1	1.583049	5.073318	5.094005
1	-0.867549	1.745965	6.295293
1	0.811092	3.496715	6.860198
6	-0.546181	4.543902	0.695009
6	-1.200699	5.779248	0.833521
6	0.655203	4.490202	-0.025225
6	-0.666314	6.928898	0.250958
1	-2.132350	5.846889	1.384493
6	1.194514	5.643352	-0.599017
1	1.155751	3.544677	-0.169201
6	0.532168	6.864903	-0.466898
1	-1.188902	7.875399	0.356586
1	2.119837	5.573121	-1.162685
1	0.943140	7.761579	-0.922050
6	4.332275	-5.776649	-0.609153
1	4.062225	-6.314684	-1.529398
1	4.406916	-6.502748	0.205463
1	3.550454	-5.062050	-0.367822
6	6.880866	-1.937020	-2.185428
1	7.257996	-2.017847	-3.214041
1	5.882408	-1.507909	-2.202956
1	7.547874	-1.274234	-1.623556
6	5.243155	-2.741461	3.341485
1	5.648268	-3.400737	4.120915
1	5.407139	-3.191697	2.366089
1	5.774320	-1.783924	3.384334
6	0.591065	-3.468935	2.032395
1	-0.144404	-2.728509	1.706890
1	1.086862	-3.884817	1.160521
1	0.063957	-4.273363	2.562925
6	7.036084	4.080448	-3.308084
1	7.065231	3.411686	-4.174541
1	6.477994	4.979474	-3.591734
1	8.069007	4.394652	-3.106244

(4-7)_{sr}⁺ (X = Me)

Number of imaginary frequencies : 1

Electronic energy : HF=-5408.8348683

Zero-point correction= 1.589013 (Hartree/Particle)

Thermal correction to Energy=	1.689563	8	-2.791589	-3.496834	-1.925160		
Thermal correction to Enthalpy=	1.690507	1	8.369155	-3.393352	2.064149		
Thermal correction to Gibbs Free Energy=	1.445810	1	6.054928	-3.445475	1.279327		
Sum of electronic and zero-point Energies=	-5407.245855	1	9.119542	0.149380	-0.257210		
Sum of electronic and thermal Energies=	-5407.145305	1	9.940067	-1.616767	1.281799		
Sum of electronic and thermal Enthalpies=	-5407.144361	1	7.304459	1.174279	-1.557372		
Sum of electronic and thermal Free Energies=	-5407.389058	1	4.895089	1.262238	-2.141288		
Standard State and RRHO Corrected G=	-5407.361089	1	6.135194	-3.637958	-1.735351		
.....			1	1.011073	-3.642005	1.298169	
Cartesian Coordinates			1	6.749242	-5.915429	-2.393414	
.....			1	3.340538	-7.486174	-0.291865	
6	-0.685421	3.897260	2.611862	1.765147	-5.976746	0.805567	
6	0.659280	3.723770	2.236246	5.378016	-7.865186	-1.651820	
6	1.391448	4.852651	1.834171	2.418423	4.751763	1.505192	
6	0.800777	6.119472	1.830088	1	-1.281310	3.037363	2.897432
6	-0.528871	6.281340	2.222009	1	1.385032	6.976450	1.507291
6	-1.271697	5.162128	2.612114	1	-2.310957	5.271496	2.909275
15	1.322025	2.011111	2.064094	1	-0.986028	7.266655	2.216467
6	3.142743	2.156139	2.405434	1	0.189988	2.854555	4.790829
6	3.688357	3.147495	3.235608	1	1.691792	-0.700165	2.873117
6	5.051122	3.145485	3.538099	1	0.004551	1.628888	6.915086
6	5.881433	2.136068	3.043651	1	1.558043	-1.909331	5.021306
6	5.337355	1.120341	2.254797	1	0.706787	-0.755014	7.056980
6	3.978122	1.132338	1.937094	1	3.056398	3.922750	3.655172
45	0.242813	0.933363	0.013297	1	3.568360	0.335091	1.329327
15	1.612309	-0.754901	-0.724578	1	5.460356	3.928314	4.171086
8	1.039255	-1.809984	-1.628234	1	5.965911	0.319042	1.882001
6	-2.069110	1.467547	-0.357524	1	6.941428	2.133550	3.282145
6	-1.479842	0.387672	-1.106401	1	-2.260645	2.381918	-0.901410
6	-2.576283	1.452824	0.944056	1	-1.660452	-0.639788	-0.826122
8	-0.447592	-0.470536	1.504165	1	-1.435621	0.541796	-2.182686
6	-1.060632	-1.594399	1.510491	1	-1.815627	-0.079965	3.663800
6	-1.508749	-2.057618	2.877800	1	-1.282995	-4.133257	2.374316
6	-1.899639	-1.142205	3.862630	1	-2.681707	-0.877665	5.850117
6	-2.369384	-1.594680	5.096232	1	-2.021736	-4.947913	4.610534
6	-2.408601	-2.964845	5.371369	1	-2.757501	-3.316326	6.338537
6	-1.994805	-3.882335	4.400300	1	-4.200969	-0.913940	1.752799
6	-1.568375	-3.430834	3.150687	1	-4.551103	0.384084	-1.769552
8	-1.330236	-2.317153	0.526233	1	-6.113208	3.347506	0.923233
8	2.268913	-1.479357	0.671252	1	-5.114327	1.834605	-3.676258
6	2.762712	-2.748234	0.434694	1	-6.664386	4.779271	-0.967769
6	3.989429	-2.888995	-0.191654	1	-4.586997	0.798012	3.008046
6	4.383356	-4.216367	-0.594377	1	-5.002481	2.399412	2.447018
6	3.570761	-5.338616	-0.212777	1	-6.911161	-0.001509	2.626908
6	2.371399	-5.121293	0.519693	1	-6.924746	1.421538	3.685399
6	1.957902	-3.845831	0.811072	1	-7.382591	1.572262	1.978931
6	3.963005	-6.649366	-0.599207	1	-2.901035	2.396273	1.366451
6	5.092491	-6.859061	-1.358053	1	-2.334980	0.675834	1.648721
6	5.873260	-5.753320	-1.771361	6	-2.063409	-3.235957	-2.914409
6	5.530165	-4.471368	-1.398840	6	-1.684819	-1.969511	-5.040414
6	4.847065	-1.695211	-0.447339	6	0.070634	-3.472180	-4.124319
6	4.386236	-0.555499	-1.112164	6	-0.689664	-3.070229	-5.380588
6	5.295391	0.452934	-1.541631	1	-2.388713	-1.819316	-5.868051
6	6.622980	0.399899	-1.215418	1	0.736298	-4.315389	-4.334131
6	7.115326	-0.645012	-0.388625	1	-1.222023	-3.941267	-5.779960
6	6.217808	-1.688584	0.015226	6	-5.600994	-3.567513	0.826078
6	6.719387	-2.669778	0.918312	6	-7.533386	-2.852256	2.210461
6	8.023944	-2.637414	1.364202	6	-7.865941	-3.303200	-0.200127
6	8.912919	-1.627118	0.928656	6	-8.157074	-2.325104	0.927639
6	8.458969	-0.649408	0.071183	1	-8.027958	-3.783213	2.529198
8	3.094076	-0.303582	-1.469074	1	-8.458893	-4.222552	-0.076192
6	0.947802	1.162848	3.672432	1	-9.237659	-2.204435	1.048320
6	0.470899	1.807565	4.820632	1	0.682204	-2.647481	-3.739588
6	0.377530	1.114716	6.033188	1	0.003607	-2.718937	-6.150895
6	0.776953	-0.219256	6.114489	1	-1.167905	-1.013555	-4.878558
6	1.260818	-0.865400	4.972632	1	-8.144204	-2.867114	-1.165779
6	1.337870	-0.185549	3.759699	1	-7.726866	-1.345676	0.691229
3	-3.098644	-2.776219	-0.201393	1	-7.648050	-2.129961	3.024082
8	-4.167233	-1.115106	-0.261078	7	-6.441966	-3.636449	-0.251970
6	-4.411919	-0.439739	0.775668	7	-6.103471	-3.074063	2.005062
6	-4.865721	0.901754	0.888845	7	-2.455754	-2.310708	-3.845461
6	-5.285251	1.722050	-0.254603	7	-0.883593	-3.899074	-3.098235
6	-5.023673	1.338417	-1.594169	6	-0.347092	-4.624624	-1.945125
6	-5.343807	2.167645	-2.665208	1	0.499819	-5.226998	-2.283202
6	-5.939500	3.423233	-2.476106	1	-0.009127	-3.925937	-1.176826
6	-6.205339	3.810604	-1.156515	1	-1.109740	-5.287238	-1.531504
6	-5.889984	2.987554	-0.075570	6	-3.664711	-1.529829	-3.633259
6	-5.229473	1.336108	2.299284	1	-4.445287	-1.810623	-4.353870
6	-6.697769	1.071223	2.670949	1	-4.033338	-1.678552	-2.621585
8	-4.397059	-3.913718	0.739343	1	-3.439463	-0.465557	-3.771682

6	-5.987676	-4.235236	-1.498388
1	-4.911774	-4.385344	-1.475250
1	-6.492744	-5.196528	-1.670543
1	-6.225737	-3.568806	-2.335545
6	-5.265725	-3.083857	3.194675
1	-4.219273	-3.104766	2.905725
1	-5.459006	-2.180819	3.781810
1	-5.472830	-3.958785	3.827578
15	0.876488	2.483803	-1.599575
6	2.251321	3.629411	-1.164934
6	2.229716	5.010573	-1.417410
6	3.404597	3.057469	-0.617611
6	3.337202	5.798208	-1.097946
1	1.355805	5.477450	-1.856340
6	4.512069	3.843090	-0.299243
1	3.429859	1.993670	-0.434080
6	4.477366	5.219207	-0.532209
1	3.306326	6.867067	-1.289814
1	5.386649	3.375300	0.142043
1	5.333257	5.837912	-0.277555
6	-0.516401	3.610306	-2.023767
6	-1.239539	3.462675	-3.215009
6	-0.953047	4.543560	-1.067378
6	-2.385946	4.230396	-3.440279
1	-0.924284	2.741691	-3.961744
6	-2.088497	5.315383	-1.301932
1	-0.418031	4.650065	-0.132150
6	-2.813357	5.155577	-2.487620
1	-2.946045	4.098281	-4.361353
1	-2.414064	6.028908	-0.550620
1	-3.710340	5.741464	-2.662940
6	1.416144	1.878569	-3.264185
6	2.198430	2.708468	-4.085832
6	1.020198	0.624072	-3.748027
6	2.588421	2.285565	-5.356585
1	2.513496	3.685994	-3.737409
6	1.420124	0.201946	-5.018506
1	0.442297	-0.050092	-3.129550
6	2.203223	1.027534	-5.825684
1	3.198480	2.937856	-5.975182
1	1.127521	-0.782910	-5.368197
1	2.515777	0.692277	-6.810728
6	-6.278895	4.310172	-3.649164
1	-5.444199	4.373891	-4.357037
1	-7.141217	3.925555	-4.209723
1	-6.525978	5.326900	-3.327194

5 (X = F)			

Number of imaginary frequencies : 0			
Electronic energy : HF=-562.778454			
Zero-point correction= 0.186499 (Hartree/Particle)			
Thermal correction to Energy= 0.197908			
Thermal correction to Enthalpy= 0.198852			
Thermal correction to Gibbs Free Energy= 0.148024			
Sum of electronic and zero-point Energies= -562.591955			
Sum of electronic and thermal Energies= -562.580546			
Sum of electronic and thermal Enthalpies= -562.579602			
Sum of electronic and thermal Free Energies= -562.630430			
Standard State and RRHO Corrected G= -562.625794			

Cartesian Coordinates			

6	-2.325709	-1.019268	0.635664
6	-0.945557	-1.132495	0.811512
6	-0.063832	-0.217531	0.220875
6	-0.594908	0.831572	-0.546575
6	-1.970855	0.961614	-0.733390
6	-2.811034	0.028804	-0.136506
1	-3.018121	-1.723822	1.084275
1	-0.551360	-1.947682	1.411946
1	-2.393463	1.767674	-1.323854
1	0.072929	1.557249	-1.002279
6	1.445508	-0.352122	0.394359
1	1.626296	-1.153232	1.124946
6	2.176075	-0.677838	-0.920550
1	1.647454	-1.503936	-1.409539
1	2.100219	0.187238	-1.588582
6	3.647064	-1.050642	-0.716328
1	3.745202	-1.925441	-0.062311

1	4.123354	-1.294468	-1.672079
1	4.204025	-0.224935	-0.264411
6	1.938213	0.931229	1.046101
8	2.658455	1.751955	0.512813
1	1.550066	1.098245	2.074517
9	-4.149337	0.147503	-0.311789

(4-7) _{re} [‡] (X = F)			

Number of imaginary frequencies : 1			
Electronic energy : HF=-5468.7561673			
Zero-point correction= 1.555954 (Hartree/Particle)			
Thermal correction to Energy= 1.654767			
Thermal correction to Enthalpy= 1.655711			
Thermal correction to Gibbs Free Energy= 1.415581			
Sum of electronic and zero-point Energies= -5467.200213			
Sum of electronic and thermal Energies= -5467.101400			
Sum of electronic and thermal Enthalpies= -5467.100456			
Sum of electronic and thermal Free Energies= -5467.340586			
Standard State and RRHO Corrected G= -5467.313608			

Cartesian Coordinates			

8	4.086355	-4.064429	-0.769996
3	3.205923	-2.967837	0.524705
8	1.767877	-1.926580	-0.246377
6	0.560737	-1.933766	-0.598130
8	-0.253869	-0.954786	-0.519510
45	-0.468594	0.964473	0.440740
15	-0.604142	1.753418	-2.016399
6	1.096400	2.099752	-2.672280
6	2.023794	1.050365	-2.548706
6	3.330587	1.198221	-3.005117
6	3.741052	2.399096	-3.593414
6	2.821831	3.438215	-3.739321
6	1.504955	3.288790	-3.289352
6	-0.006127	-3.203080	-1.189828
6	-1.387738	-3.438239	-1.196885
6	-1.895565	-4.631869	-1.710428
6	-1.029082	-5.594088	-2.237129
6	0.349750	-5.362410	-2.234774
6	0.862079	-4.176709	-1.704847
6	1.620217	1.121393	1.506750
6	2.607678	0.859301	0.544440
6	4.696659	0.672011	1.473498
6	5.487011	1.100980	0.303945
6	5.760089	2.473932	0.090674
6	6.401809	2.932800	-1.058807
6	6.796513	2.007782	-2.014620
6	6.581146	0.647583	-1.843650
6	5.922967	0.200680	-0.698701
6	0.681546	0.182642	2.049614
15	-2.492948	0.188361	1.324301
8	-2.749591	0.445902	2.788656
8	-2.569222	-1.481715	1.031741
6	-3.683704	-2.158799	1.481087
6	-4.846973	-2.138145	0.725654
6	-6.002018	-2.832723	1.235453
6	-5.884877	-3.598353	2.445161
6	-4.649890	-3.609610	3.148412
6	-3.578881	-2.884509	2.690521
6	-7.014800	-4.305194	2.939684
6	-8.229138	-4.244462	2.294015
6	-8.362035	-3.454565	1.127271
6	-7.282096	-2.768502	0.614471
6	-4.892976	-1.337560	-0.527604
6	-4.531448	0.009772	-0.501759
6	-4.775949	0.854479	-1.613108
6	-5.292429	0.347391	-2.777696
6	-5.532212	-1.045329	-2.911794
6	-5.313395	-1.902014	-1.781945
6	-5.475546	-3.304639	-1.969008
6	-5.840006	-3.824753	-3.192773
6	-6.080508	-2.971754	-4.297162
6	-5.929809	-1.610580	-4.153095
8	-4.010412	0.594221	0.616048
6	-1.105280	0.439560	-3.224574
6	-1.957556	-0.602291	-2.845824
6	-2.365004	-1.559343	-3.780611
6	-1.934055	-1.478871	-5.103495

6	-1.089187	-0.435102	-5.495185
6	-0.676516	0.515296	-4.563015
6	-1.638840	3.174860	-2.610437
6	-1.352960	4.496969	-2.226172
6	-2.199483	5.547656	-2.580630
6	-3.358764	5.300747	-3.318722
6	-3.652508	3.993949	-3.712732
6	-2.799624	2.942683	-3.368382
6	4.380982	-0.685147	1.746876
8	4.596572	-1.707364	1.039152
6	4.525662	1.627306	2.642611
6	5.811170	1.843710	3.455827
8	2.630078	-3.926673	2.098682
1	-5.939336	-4.900125	-3.311505
1	-5.290166	-3.971965	-1.135180
1	-6.089933	-0.944140	-4.996944
1	-6.370744	-3.394187	-5.254827
1	-5.478189	1.000235	-3.626367
1	-4.539391	1.905472	-1.515008
1	-7.411262	-2.159901	-0.272112
1	-2.642153	-2.851408	3.232013
1	-9.327174	-3.382097	0.633512
1	-6.901745	-4.887954	3.850600
1	-4.573841	-4.181357	4.069572
1	-9.086657	-4.785642	2.683676
1	1.724305	0.116994	-2.083012
1	0.807323	4.105290	-3.430810
1	4.034725	0.384979	-2.877287
1	3.122241	4.372290	-4.206498
1	4.766842	2.519332	-3.928732
1	-2.287042	-0.681343	-1.820821
1	-0.020231	1.319656	-4.879838
1	-3.013584	-2.368807	-3.466089
1	-0.749535	-0.361848	-6.524859
1	-2.253634	-2.224960	-5.825960
1	-0.470134	4.715404	-1.644431
1	-3.051355	1.938210	-3.684463
1	-1.950740	6.558014	-2.268664
1	-4.547009	3.786314	-4.293785
1	-4.023435	6.117233	-3.586255
1	-2.044931	-2.686767	-0.781796
1	1.932520	-4.006498	-1.676496
1	-2.968122	-4.803661	-1.708108
1	1.028140	-6.108005	-2.641420
1	-1.425612	-6.520612	-2.644234
1	3.821655	-0.827297	2.690817
1	5.450432	3.209905	0.823767
1	5.718353	-0.854386	-0.581442
1	6.587028	3.990016	-1.219815
1	6.903918	-0.045359	-2.613009
1	4.139212	2.596396	2.302130
1	3.749242	1.227618	3.305413
1	6.165453	0.895012	3.875483
1	6.615781	2.249423	2.833527
1	5.642340	2.540450	4.285678
1	0.836126	-0.871167	1.844214
1	0.264244	0.389276	3.028401
1	1.695580	2.086218	1.995355
1	3.065692	1.697623	0.037647
1	2.609249	-0.087644	0.025499
6	2.161483	-3.340928	3.106694
6	2.459166	-2.454757	5.394685
6	0.197646	-2.416520	4.358146
6	1.213942	-1.612185	5.156735
1	2.231520	-3.314231	6.044185
1	-0.589051	-1.758503	3.973489
1	0.772129	-1.300876	6.107808
6	5.228305	-3.814852	-1.228548
6	6.626407	-2.966412	-3.083419
6	7.695399	-4.173303	-1.189981
6	7.794092	-2.961651	-2.106321
1	6.706995	-3.816533	-3.778417
1	8.411834	-4.088544	-0.365988
1	8.742634	-2.984555	-2.650819
7	6.354756	-4.284754	-0.612954
7	5.365811	-3.026760	-2.341635
7	2.992251	-2.906569	4.109171
7	0.823511	-3.086356	3.215771
1	3.234142	-1.864191	5.891480
1	1.494550	-0.710382	4.603990

1	-0.287789	-3.168870	4.997636
1	7.939174	-5.095170	-1.739623
1	7.765408	-2.043751	-1.510354
1	6.622180	-2.054203	-3.686136
15	-0.806233	3.010348	1.518460
6	-2.525384	3.661996	1.604685
6	-3.324087	3.580172	0.456449
6	-3.032476	4.304617	2.744886
6	-4.602726	4.135321	0.440362
1	-2.948122	3.078110	-0.423291
6	-4.318871	4.847146	2.731238
1	-2.431635	4.385105	3.643511
6	-5.105510	4.766538	1.579607
1	-5.206559	4.063331	-0.459414
1	-4.703334	5.335468	3.622258
1	-6.105261	5.191661	1.571951
6	-0.217756	3.085983	3.277521
6	0.871012	3.891968	3.648765
6	-0.834955	2.283748	4.253313
6	1.340123	3.887819	4.964541
1	1.366314	4.520427	2.917437
6	-0.365223	2.290561	5.567943
1	-1.664626	1.643637	3.967383
6	0.724902	3.086859	5.927964
1	2.186944	4.513780	5.231711
1	-0.852375	1.664404	6.310666
1	1.090894	3.084457	6.950984
6	0.119410	4.425470	0.768714
6	-0.340849	5.744231	0.921475
6	1.314961	4.202309	0.071370
6	0.376352	6.809120	0.375585
1	-1.263812	5.944594	1.454503
6	2.037487	5.270080	-0.465187
1	1.667230	3.194334	-0.087260
6	1.567477	6.576041	-0.318991
1	0.001918	7.822257	0.491570
1	2.952829	5.069472	-1.013607
1	2.121051	7.407498	-0.745925
6	6.231464	-5.143227	0.556404
1	5.213010	-5.104634	0.937212
1	6.482674	-6.184035	0.308685
1	6.919254	-4.799459	1.336929
6	4.147758	-2.596010	-3.021633
1	3.688854	-3.405769	-3.605161
1	3.416952	-2.234521	-2.297128
1	4.402966	-1.782119	-3.703353
6	4.401130	-3.278330	4.055945
1	4.740487	-3.282682	3.021739
1	4.979419	-2.535975	4.613568
1	4.581140	-4.266759	4.502417
6	-0.099556	-3.625708	2.225037
1	-0.687330	-2.820824	1.776225
1	0.456991	-4.138566	1.446037
1	-0.788714	-4.336116	2.700205
9	7.382686	2.447959	-3.162949

(4-7)_{st}[±] (X = F)

Number of imaginary frequencies : 1
 Electronic energy : HF=-5468.7470991
 Zero-point correction= 1.554559 (Hartree/Particle)
 Thermal correction to Energy= 1.653517
 Thermal correction to Enthalpy= 1.654462
 Thermal correction to Gibbs Free Energy= 1.415038
 Sum of electronic and zero-point Energies= -5467.192540
 Sum of electronic and thermal Energies= -5467.093582
 Sum of electronic and thermal Enthalpies= -5467.092637
 Sum of electronic and thermal Free Energies= -5467.332061
 Standard State and RRHO Corrected G= -5467.305812

Cartesian Coordinates

6	0.637272	-3.963252	2.591046
6	-0.717040	-3.739453	2.281058
6	-1.517861	-4.842449	1.944164
6	-0.984930	-6.134948	1.947306
6	0.353327	-6.347410	2.281422
6	1.164864	-5.253475	2.600761
15	-1.303455	-1.999715	2.107247
6	-3.119116	-2.048892	2.504464

6	-3.677538	-2.990517	3.382889	1	-1.516142	0.731608	2.896418
6	-5.028418	-2.923392	3.728003	1	0.199756	-1.634953	6.904625
6	-5.832519	-1.895655	3.228377	1	-1.248240	1.955575	5.025797
6	-5.274067	-0.928221	2.390342	1	-0.382378	0.780858	7.043430
6	-3.927437	-1.005915	2.028884	1	-3.063675	-3.777816	3.807173
45	-0.198700	-1.032087	0.019709	1	-3.507228	-0.246921	1.379417
15	-1.428424	0.744074	-0.746212	1	-5.447957	-3.668998	4.398091
8	-0.745023	1.783027	-1.588456	1	-5.882430	-0.112940	2.014208
6	2.102343	-1.709131	-0.352769	1	-6.883086	-1.841294	3.500123
6	1.531255	-0.648232	-1.145325	1	2.204694	-2.673925	-0.831396
6	2.745312	-1.593357	0.879227	1	1.784082	0.381261	-0.934423
8	0.598452	0.345138	1.475278	1	1.452267	-0.863933	-2.208305
6	1.272237	1.434014	1.442764	1	1.984650	-0.069807	3.615251
6	1.776532	1.903003	2.788267	1	1.666576	3.975704	2.236500
6	2.137879	0.989761	3.785892	1	2.956187	0.726527	5.759331
6	2.667579	1.442648	4.995178	1	2.509796	4.797833	4.432125
6	2.796654	2.813902	5.233771	1	3.192405	3.166949	6.182179
6	2.412262	3.731084	4.250081	1	4.540978	0.760365	1.340531
6	1.926342	3.276377	3.024012	1	4.410576	-0.611013	-2.150467
8	1.560327	2.115457	0.437351	1	6.132303	-3.611325	0.413479
8	-2.100040	1.451248	0.651659	1	4.568667	-2.190300	-4.070590
6	-2.582657	2.729781	0.460672	1	6.266868	-5.163809	-1.497247
6	-3.801861	2.906719	-0.172534	1	5.080030	-0.908574	2.589889
6	-4.188968	4.253324	-0.509896	1	5.355042	-2.545761	2.047546
6	-3.384113	5.352964	-0.054122	1	7.345236	-0.216906	1.797405
6	-2.200780	5.095622	0.691206	1	7.472807	-1.571817	2.937243
6	-1.788879	3.806166	0.915613	1	7.659629	-1.846789	1.195438
6	-3.766060	6.681826	-0.384468	1	3.093443	-2.498451	1.364793
6	-4.879773	6.930460	-1.155163	1	2.606337	-0.739483	1.520236
6	-5.656594	5.848546	-1.634057	6	1.643786	3.675551	-2.601280
6	-5.322909	4.549025	-1.318108	6	-0.087357	3.144636	-4.304376
6	-4.660878	1.728283	-0.485505	6	-0.566859	4.787753	-2.510031
6	-4.187812	0.625914	-1.200322	6	-0.682972	4.512404	-4.002136
6	-5.078455	-0.382149	-1.663304	1	-0.024968	2.982041	-5.386751
6	-6.403325	-0.367395	-1.320350	1	-0.890639	5.807562	-2.279398
6	-6.907056	0.638418	-0.452673	1	-0.152035	5.287903	-4.567137
6	-6.028040	1.686604	-0.019449	6	5.765483	3.389824	0.601773
6	-6.541910	2.627905	0.918444	6	7.816382	2.700651	1.828141
6	-7.841170	2.552362	1.374455	6	7.992292	3.446160	-0.526743
6	-8.711696	1.536692	0.914191	6	8.418107	2.378644	0.469335
6	-8.245823	0.598831	0.019496	1	8.258538	3.620949	2.240902
8	-2.894495	0.443649	-1.587697	1	8.494587	4.401283	-0.308015
6	-0.837167	-1.156383	3.692770	1	9.509373	2.340662	0.535167
6	-0.349954	-1.811951	4.830130	1	-1.188493	4.086680	-1.943619
6	-0.179961	-1.112457	6.030524	1	-1.734852	4.531786	-4.303692
6	-0.511856	0.239926	6.110208	1	-0.712579	2.359444	-3.865100
6	-1.004070	0.897882	4.978576	1	8.276519	3.156842	-1.544107
6	-1.156977	0.210487	3.777271	1	8.060349	1.398084	0.136013
3	3.238521	2.566150	-0.433515	1	8.017555	1.895568	2.541792
8	4.279816	0.911913	-0.659577	7	6.540947	3.629742	-0.501390
6	4.616254	0.253135	0.361825	7	6.366171	2.839709	1.708143
6	5.031232	-1.102429	0.461193	7	1.267902	3.041269	-3.757494
6	5.247062	-1.970329	-0.702304	7	0.832908	4.653079	-2.092518
6	4.825373	-1.598305	-2.004857	6	1.189128	5.213502	-0.793873
6	4.912875	-2.478089	-3.082173	1	0.940131	4.523667	0.019378
6	5.418650	-3.752777	-2.873223	1	2.259497	5.420185	-0.754890
6	5.870603	-4.161448	-1.625846	1	0.641394	6.149547	-0.657165
6	5.786196	-3.271211	-0.556091	6	2.026955	1.874487	-4.183414
6	5.589818	-1.499019	1.817821	1	1.594631	0.947143	-3.786122
6	7.105584	-1.274706	1.947234	1	2.021648	1.820518	-5.277282
8	4.534246	3.630883	0.597191	1	3.054235	1.952083	-3.832260
8	2.752987	3.422532	-2.068183	6	5.975230	4.313125	-1.656105
1	-8.196567	3.277454	2.101379	1	6.385533	5.329560	-1.741475
1	-5.890628	3.405326	1.299124	1	6.228160	3.763697	-2.570069
1	-8.892759	-0.202341	-0.329530	1	4.892475	4.365760	-1.572415
1	-9.734656	1.491626	1.276630	6	5.600834	2.698371	2.938169
1	-7.073645	-1.142854	-1.681362	1	5.818208	3.515754	3.640284
1	-4.665777	-1.159520	-2.296415	1	4.538563	2.707503	2.712235
1	-5.923498	3.733202	-1.702980	1	5.860508	1.751152	3.421861
1	-0.858158	3.575292	1.421695	15	-0.958266	-2.565497	-1.555684
1	-6.521501	6.043762	-2.261990	6	-2.386491	-3.626677	-1.078798
1	-3.149091	7.501450	-0.024318	6	-2.451535	-5.008110	-1.324895
1	-1.604493	5.933958	1.040569	6	-3.487650	-2.990633	-0.496811
1	-5.156964	7.950222	-1.406666	6	-3.589397	-5.731617	-0.964226
1	-2.553535	-4.702081	1.658887	1	-1.621056	-5.524686	-1.791473
1	1.285834	-3.122505	2.814915	6	-4.626393	-3.711601	-0.137888
1	-1.621124	-6.972402	1.675452	1	-3.451097	-1.926754	-0.315614
1	2.212226	-5.403232	2.847622	6	-4.676141	-5.088098	-0.363857
1	0.764913	-7.352634	2.282622	1	-3.624296	-6.801110	-1.151790
1	-0.118675	-2.871120	4.800923	1	-5.458333	-3.193707	0.329154

1	-5.556061	-5.657296	-0.077568	8	-3.903304	3.831022	-0.891180
6	0.358042	-3.780443	-1.990096	3	-2.998921	2.870776	0.493865
6	1.072253	-3.692383	-3.193086	8	-1.564276	1.811182	-0.229705
6	0.743043	-4.736524	-1.034123	6	-0.380451	1.803386	-0.650288
6	2.158947	-4.538948	-3.428642	8	0.452722	0.843469	-0.537822
1	0.798767	-2.956421	-3.941371	45	0.732290	-1.000385	0.544685
6	1.817896	-5.588376	-1.279520	15	0.703395	-1.956616	-1.860454
1	0.213611	-4.803880	-0.092388	6	-1.048138	-2.316732	-2.359825
6	2.535716	-5.484799	-2.474929	6	-1.942041	-1.234218	-2.272611
1	2.726536	-4.446878	-4.349229	6	-3.281392	-1.385107	-2.622538
1	2.102397	-6.318675	-0.527557	6	-3.757480	-2.624829	-3.061884
1	3.393881	-6.123511	-2.659751	6	-2.875578	-3.700615	-3.165857
6	-1.478041	-1.949526	-3.221366	6	-1.526487	-3.547642	-2.825892
6	-2.345890	-2.718480	-4.014371	6	0.137331	3.025420	-1.374607
6	-0.951847	-0.761282	-3.747655	6	1.514069	3.267345	-1.478809
6	-2.681600	-2.304624	-5.304199	6	1.980884	4.421455	-2.108220
1	-2.765787	-3.642273	-3.631630	6	1.076939	5.337541	-2.654192
6	-1.279816	-0.357357	-5.043340	6	-0.296916	5.098352	-2.556131
1	-0.316839	-0.126396	-3.143975	6	-0.767288	3.952569	-1.911312
6	-2.145408	-1.124698	-5.824391	6	-1.285720	-1.103932	1.733413
1	-3.360387	-2.907483	-5.900966	6	-2.346824	-0.919092	0.829633
1	-0.864184	0.565381	-5.434915	6	-4.327122	-0.671016	1.895373
1	-2.404156	-0.803977	-6.829658	6	-5.224087	-1.144621	0.825439
9	5.442096	-4.638433	-3.910518	6	-5.533994	-2.518949	0.697563
				6	-6.314851	-3.008454	-0.349301
5 (X = Br)				6	-6.811071	-2.112790	-1.289943
				6	-6.545777	-0.750309	-1.206457
Number of imaginary frequencies : 0				6	-5.753993	-0.279786	-0.160549
Electronic energy : HF=-476.3236332				6	-0.335630	-0.115506	2.153989
Zero-point correction= 0.184354 (Hartree/Particle)				15	2.797351	-0.142341	1.239522
Thermal correction to Energy= 0.196487				8	3.135877	-0.273467	2.704173
Thermal correction to Enthalpy= 0.197431				8	2.846716	1.498574	0.806589
Thermal correction to Gibbs Free Energy= 0.143456				6	3.982009	2.212717	1.126100
Sum of electronic and zero-point Energies= -476.139279				6	5.097928	2.125596	0.306499
Sum of electronic and thermal Energies= -476.127146				6	6.278572	2.860240	0.683189
Sum of electronic and thermal Enthalpies= -476.126202				6	6.230952	3.730723	1.824653
Sum of electronic and thermal Free Energies= -476.180177				6	5.039193	3.807805	2.595180
Standard State and RRHO Corrected G= -476.175078				6	3.945508	3.046155	2.268519
				6	7.386217	4.476037	2.186342
Cartesian Coordinates				6	8.560111	4.355466	1.477274
				6	8.625692	3.465028	0.379135
6	-1.135621	-1.114927	0.755122	6	7.519215	2.738653	-0.005489
6	0.254184	-1.196530	0.871215	6	5.069842	1.222780	-0.875617
6	1.088304	-0.246245	0.270464	6	4.715817	-0.117022	-0.714974
6	0.501714	0.807461	-0.445827	6	4.884080	-1.049423	-1.768952
6	-0.884144	0.909741	-0.574573	6	5.321277	-0.640128	-3.002628
6	-1.678873	-0.059347	0.030351	6	5.550725	0.735910	-3.264846
1	-1.770681	-1.859928	1.221359	6	5.405264	1.682300	-2.196505
1	0.689427	-2.017809	1.433848	6	5.550905	3.064622	-2.507593
1	-1.325444	1.728943	-1.130907	6	5.832092	3.482378	-3.791052
1	1.129620	1.562802	-0.909925	6	6.001177	2.541568	-4.835768
6	2.605506	-0.349383	0.375732	6	5.863904	1.197129	-4.571586
1	2.836337	-1.161878	1.078819	8	4.274741	-0.604308	0.481798
6	3.280611	-0.630720	-0.979053	6	1.122628	-0.736768	-3.191872
1	2.744548	-1.454324	-1.463994	6	1.995643	0.327895	-2.949332
1	3.160920	0.248584	-1.621597	6	2.338237	1.210946	-3.978383
6	4.764937	-0.982748	-0.848263	6	1.822027	1.031839	-5.260310
1	4.905785	-1.871525	-0.221577	6	0.955765	-0.036375	-5.516104
1	5.202106	-1.194738	-1.829863	6	0.607035	-0.912228	-4.489833
1	5.327974	-0.158913	-0.400568	6	1.684684	-3.425568	-2.431125
6	3.101660	0.931437	1.032384	6	1.421645	-4.719704	-1.947830
8	3.779002	1.776938	0.482703	6	2.240767	-5.796013	-2.290320
1	2.761624	1.068086	2.081757	6	3.350915	-5.603251	-3.114659
35	-3.636683	0.070936	-0.143551	6	3.623029	-4.324804	-3.605508
				6	2.796855	-3.248829	-3.273231
(4-7) _{re} ⁺ (X = Br)				6	-4.005316	0.703653	2.079093
				8	-4.283075	1.681932	1.336468
Number of imaginary frequencies : 1				6	-4.076206	-1.565471	3.098468
Electronic energy : HF=-5382.2975292				6	-5.296463	-1.717104	4.019213
Zero-point correction= 1.553243 (Hartree/Particle)				8	-2.315362	4.013448	1.932287
Thermal correction to Energy= 1.653121				1	5.920279	4.544255	-4.003321
Thermal correction to Enthalpy= 1.654065				1	5.419626	3.798155	-1.720417
Thermal correction to Gibbs Free Energy= 1.409463				1	5.969207	0.463804	-5.367229
Sum of electronic and zero-point Energies= -5380.744286				1	6.225888	2.883598	-5.841920
Sum of electronic and thermal Energies= -5380.644408				1	5.448661	-1.360201	-3.806484
Sum of electronic and thermal Enthalpies= -5380.643464				1	4.654119	-2.087673	-1.572203
Sum of electronic and thermal Free Energies= -5380.888066				1	7.596527	2.053615	-0.840957
Standard State and RRHO Corrected G= -5380.8597				1	3.041495	3.065792	2.864230
				1	9.559931	3.347110	-0.162948
Cartesian Coordinates							

1	7.325887	5.137757	3.046955
1	5.015366	4.461061	3.463496
1	9.437706	4.927130	1.765501
1	-1.591402	-0.270411	-1.919158
1	-0.859217	-4.393505	-2.937381
1	-3.956632	-0.540440	-2.533356
1	-3.230335	-4.665513	-3.518378
1	-4.804553	-2.746659	-3.319608
1	2.392793	0.481989	-1.957328
1	-0.067391	-1.736222	-4.700795
1	3.005017	2.039535	-3.769202
1	0.549498	-0.186047	-6.512837
1	2.091652	1.720317	-6.056585
1	0.579530	-4.896583	-1.296160
1	3.031586	-2.267762	-3.666329
1	2.009449	-6.783317	-1.900835
1	4.479202	-4.159111	-4.253861
1	3.994463	-6.439249	-3.373495
1	2.200496	2.552880	-1.046504
1	-1.832908	3.781068	-1.808404
1	3.050310	4.597989	-2.180330
1	-1.004815	5.806930	-2.978334
1	1.440856	6.233014	-3.151347
1	-3.378102	0.900048	2.969102
1	-5.155139	-3.234244	1.419023
1	-5.530970	0.774816	-0.096344
1	-6.525283	-4.069964	-0.421964
1	-6.934266	-0.057405	-1.945457
1	-3.729575	-2.556867	2.780426
1	-3.245457	-1.143999	3.676309
1	-6.151238	-2.145890	3.485602
1	-5.069512	-2.368432	4.871645
1	-5.607583	-0.741540	4.410501
1	-0.518179	0.918707	1.881484
1	0.141691	-0.245486	3.118368
1	-1.313943	-2.032866	2.292003
1	-2.815906	-1.797784	0.406728
1	-2.391116	-0.013916	0.242092
6	-1.782124	3.519231	2.957461
6	-1.927578	2.832760	5.328377
6	0.260692	2.698447	4.157014
6	-0.700546	1.966785	5.082604
1	-1.658655	3.742762	5.886962
1	1.022920	2.008678	3.778632
1	-0.198136	1.733231	6.025842
6	-4.837271	4.669740	-0.885119
6	-7.224891	5.244293	-1.342375
6	-5.612600	7.012920	-0.684961
6	-7.003082	6.446600	-0.437259
1	-7.346043	5.563540	-2.388365
1	-5.393208	7.819582	0.020729
1	-7.763116	7.207863	-0.635213
7	-4.608105	5.965096	-0.497157
7	-6.106034	4.305577	-1.242312
7	-2.544124	3.177457	4.046824
7	-0.438236	3.273297	3.005208
1	-2.668803	2.290554	5.922425
1	-1.015192	1.023617	4.625426
1	0.784234	3.499692	4.699894
1	-5.541968	7.435281	-1.699567
1	-7.090317	6.143219	0.612093
1	-8.138272	4.710753	-1.058126
15	1.179090	-2.951716	1.745637
6	2.914586	-3.564657	1.762055
6	3.604668	-3.615340	0.543294
6	3.540241	-4.047644	2.921107
6	4.890565	-4.148913	0.477549
1	3.137614	-3.234510	-0.354021
6	4.835217	-4.566138	2.856000
1	3.025582	-4.023927	3.874733
6	5.511707	-4.621609	1.635331
1	5.408045	-4.183528	-0.476591
1	5.311809	-4.930433	3.761715
1	6.517678	-5.029087	1.587760
6	0.697284	-2.906507	3.538075
6	-0.344506	-3.708913	4.032159
6	1.341077	-2.013388	4.412775
6	-0.741836	-3.612833	5.367865
1	-0.859273	-4.406245	3.381212
6	0.943923	-1.928972	5.748521

1	2.134006	-1.376090	4.031894
6	-0.100360	-2.722279	6.230173
1	-1.553442	-4.237755	5.729928
1	1.451337	-1.233473	6.411740
1	-0.410607	-2.648349	7.268851
6	0.241945	-4.433683	1.159953
6	0.743659	-5.728066	1.374695
6	-1.003176	-4.284485	0.533265
6	0.016101	-6.843935	0.959672
1	1.705346	-5.869700	1.855853
6	-1.735388	-5.402544	0.128377
1	-1.387667	-3.297587	0.324055
6	-1.225436	-6.685212	0.336172
1	0.421645	-7.838586	1.121769
1	-2.690013	-5.261187	-0.369197
1	-1.787427	-7.556314	0.011537
6	-3.227312	6.407722	-0.328407
1	-3.214126	7.249882	0.369270
1	-2.619000	5.605392	0.082461
1	-2.790294	6.739853	-1.280844
6	-6.365390	2.960697	-1.737946
1	-6.761878	3.007402	-2.760501
1	-5.442032	2.386713	-1.739065
1	-7.103342	2.456374	-1.103387
6	-3.951801	3.555477	4.063331
1	-4.356117	3.501352	3.055015
1	-4.496471	2.851070	4.698793
1	-4.097173	4.569034	4.463953
6	0.422409	3.739904	1.926245
1	0.999357	2.907941	1.514931
1	-0.183346	4.178301	1.138923
1	1.123845	4.495801	2.303932
35	-7.903919	-2.793183	-2.788003

(4-7)_v[±] (X = Br)

Number of imaginary frequencies : 1
 Electronic energy : HF=-5382.2940508
 Zero-point correction= 1.551819 (Hartree/Particle)
 Thermal correction to Energy= 1.651824
 Thermal correction to Enthalpy= 1.652769
 Thermal correction to Gibbs Free Energy= 1.409177
 Sum of electronic and zero-point Energies= -5380.742232
 Sum of electronic and thermal Energies= -5380.642226
 Sum of electronic and thermal Enthalpies= -5380.641282
 Sum of electronic and thermal Free Energies= -5380.884873
 Standard State and RRHO Corrected G= -5380.857342

Cartesian Coordinates

6	0.850022	-3.305362	3.266556
6	-0.484123	-3.379403	2.825458
6	-1.040762	-4.646063	2.586337
6	-0.292632	-5.805244	2.812253
6	1.021269	-5.720159	3.275012
6	1.591836	-4.462584	3.498706
15	-1.347681	-1.816459	2.364543
6	-3.156251	-2.159687	2.628279
6	-3.620977	-3.070223	3.590150
6	-4.989444	-3.218970	3.821807
6	-5.911443	-2.436780	3.121338
6	-5.455425	-1.495829	2.195791
6	-4.087529	-1.360177	1.949552
45	-0.236239	-0.910738	0.248833
15	-1.686567	0.492152	-0.840028
8	-1.115647	1.538732	-1.753503
6	2.167303	-1.178323	0.136717
6	1.497206	-0.345813	-0.831128
6	2.653196	-0.806997	1.392746
8	0.162923	0.753600	1.558393
6	0.618752	1.943417	1.424435
6	0.896357	2.662676	2.724316
6	1.315503	1.966570	3.864440
6	1.634795	2.659612	5.033083
6	1.493440	4.049426	5.084450
6	1.048043	4.746394	3.956443
6	0.772505	4.057819	2.774805
8	0.866728	2.542194	0.357846
8	-2.618734	1.212085	0.392452
6	-3.307424	2.340185	-0.003622

6	-4.463954	2.201010	-0.753135	1	4.506819	0.519337	3.218170
6	-5.054824	3.398206	-1.295779	1	5.220109	-1.048148	2.930533
6	-4.521921	4.679113	-0.921557	1	6.632661	1.659897	2.588766
6	-3.399400	4.745543	-0.051259	1	6.918303	0.501417	3.902242
6	-2.781605	3.596072	0.372690	1	7.396850	0.106292	2.241202
6	-5.105156	5.860849	-1.454812	1	3.102717	-1.576003	2.011662
6	-6.155189	5.796645	-2.343287	1	2.280017	0.056056	1.917675
6	-6.661452	4.535895	-2.740243	6	0.918350	3.711430	-2.860423
6	-6.129575	3.371610	-2.228855	6	-0.529850	2.661854	-4.586448
6	-5.054137	0.849500	-0.975389	6	-1.457092	4.380936	-3.058142
6	-4.314177	-0.213439	-1.497079	6	-1.391416	3.914107	-4.504873
6	-4.949976	-1.423681	-1.890343	1	-0.345709	2.388803	-5.632036
6	-6.283027	-1.629637	-1.658509	1	-1.981356	5.338973	-2.985035
6	-7.051231	-0.648666	-0.975825	1	-0.966078	4.705487	-5.133576
6	-6.430848	0.594818	-0.618137	6	4.745506	4.600881	0.581269
6	-7.204514	1.519789	0.140592	6	6.755725	4.494215	2.033273
6	-8.507932	1.244498	0.496910	6	7.033867	4.803834	-0.407637
6	-9.123226	0.031147	0.109059	6	7.519826	4.024788	0.804966
6	-8.401598	-0.894883	-0.611278	1	7.003586	5.541015	2.269000
8	-2.976573	-0.179873	-1.753095	1	7.388537	5.845047	-0.365332
6	-1.199227	-0.708292	3.845564	1	8.594468	4.177326	0.941063
6	-0.708637	-1.106345	5.095139	1	-1.986376	3.645435	-2.443776
6	-0.783587	-0.240343	6.192417	1	-2.399034	3.693501	-4.870742
6	-1.364809	1.020186	6.056061	1	-1.034548	1.827110	-4.087452
6	-1.862213	1.419961	4.811629	1	7.430557	4.364390	-1.329287
6	-1.772035	0.569310	3.712980	1	7.341782	2.954128	0.654862
3	2.491987	3.213114	-0.461701	1	7.019552	3.893133	2.908710
8	3.831671	1.765444	-0.331236	7	5.572984	4.783861	-0.493259
6	4.147415	1.322236	0.803081	7	5.319770	4.345668	1.803347
6	4.790428	0.096419	1.140882	7	0.769128	2.888535	-3.947395
6	5.343712	-0.819779	0.138771	7	-0.098300	4.568801	-2.538495
6	5.013781	-0.718829	-1.236845	6	0.029412	5.329665	-1.300599
6	5.474370	-1.642625	-2.174289	1	-0.181562	4.705026	-0.426412
6	6.276811	-2.694198	-1.747796	1	1.041395	5.725400	-1.206434
6	6.632442	-2.841575	-0.411351	1	-0.676978	6.163644	-1.330220
6	6.166223	-1.908742	0.514102	6	1.761301	1.844965	-4.161713
6	5.238205	-0.005586	2.590569	1	1.476323	0.911562	-3.659656
6	6.628824	0.596731	2.848621	1	1.852450	1.649812	-5.235394
8	3.497129	4.631999	0.456396	1	2.726195	2.164251	-3.771967
8	2.003334	3.738069	-2.227399	6	5.020007	5.138394	-1.792466
1	-9.064845	1.965621	1.088806	1	5.347158	6.146638	-2.082463
1	-6.751319	2.448977	0.464213	1	5.371503	4.431522	-2.553360
1	-8.849935	-1.842316	-0.900334	1	3.933824	5.102931	-1.763844
1	-10.152564	-0.171077	0.390901	6	4.473816	4.281546	2.986189
1	-6.757540	-2.558227	-1.964425	1	4.467818	5.237383	3.529295
1	-4.337336	-2.173254	-2.378570	1	3.455097	4.041908	2.695514
1	-6.523249	2.415364	-2.552983	1	4.850141	3.505111	3.659665
1	-1.884563	3.611559	0.981699	15	-0.544092	-2.741983	-1.145640
1	-7.474078	4.484669	-3.459634	6	-1.800193	-3.989256	-0.638029
1	-4.693537	6.821237	-1.154128	6	-1.590744	-5.377179	-0.690018
1	-3.010645	5.718750	0.235295	6	-3.051389	-3.507712	-0.240303
1	-6.587429	6.706731	-2.749364	6	-2.612134	-6.254154	-0.321239
1	-2.050940	-4.738656	2.206109	1	-0.637035	-5.779269	-1.011061
1	1.315732	-2.337151	3.418178	6	-4.073997	-4.382585	0.125828
1	-0.741627	-6.774131	2.613104	1	-3.222884	-2.442055	-0.209223
1	2.618535	-4.381679	3.844618	6	-3.852948	-5.760449	0.093825
1	1.600185	-6.622452	3.449955	1	-2.435380	-7.325466	-0.356603
1	-0.284457	-2.094858	5.233099	1	-5.029128	-3.979255	0.447607
1	-2.137036	0.894556	2.744760	1	-4.641838	-6.447064	0.387688
1	-0.397625	-0.563551	7.155640	6	1.009366	-3.721686	-1.295401
1	-2.300748	2.406731	4.690995	6	1.825108	-3.632165	-2.431556
1	-1.424856	1.690169	6.909163	1	1.459394	-4.458603	-0.186048
1	-2.920805	-3.664471	4.167511	6	3.074785	-4.257988	-2.450490
1	-3.747894	-0.624010	1.230525	1	1.501659	-3.063438	-3.296569
1	-5.332953	-3.938894	4.559793	6	2.700101	-5.091310	-0.214178
1	-6.159793	-0.866838	1.662192	1	0.849264	-4.520201	0.705815
1	-6.976357	-2.550224	3.304700	6	3.516839	-4.984157	-1.344406
1	2.496280	-2.150192	-0.205047	1	3.708140	-4.166788	-3.327254
1	1.536816	0.730723	-0.745535	1	3.032238	-5.653532	0.653766
1	1.560572	-0.698146	-1.858200	1	4.494715	-5.455266	-1.360855
1	1.371014	0.884316	3.834165	6	-0.986110	-2.451226	-2.918960
1	0.468297	4.590476	1.879959	6	-1.586735	-3.477586	-3.666985
1	1.970265	2.112714	5.909665	6	-0.653635	-1.249683	-3.560274
1	0.934314	5.826330	3.993056	6	-1.851043	-3.302834	-5.026058
1	1.725904	4.587086	5.999682	1	-1.852978	-4.416984	-3.194619
1	3.851181	1.919185	1.685275	6	-0.908699	-1.083167	-4.922873
1	4.384825	0.097654	-1.562050	1	-0.229574	-0.426386	-3.000934
1	6.452896	-2.045095	1.550768	6	-1.508212	-2.106079	-5.659281
1	5.196901	-1.539384	-3.217806	1	-2.323089	-4.104039	-5.587770
1	7.258446	-3.665877	-0.087026	1	-0.645620	-0.146261	-5.403198

1	-1.711364	-1.970739	-6.717953
35	6.916185	-4.019972	-3.066905

5 (X = COCH₃)

Number of imaginary frequencies : 0
 Electronic energy : HF=-616.2055374
 Zero-point correction= 0.232229 (Hartree/Particle)
 Thermal correction to Energy= 0.246334
 Thermal correction to Enthalpy= 0.247278
 Thermal correction to Gibbs Free Energy= 0.189723
 Sum of electronic and zero-point Energies= -615.973309
 Sum of electronic and thermal Energies= -615.959203
 Sum of electronic and thermal Enthalpies= -615.958259
 Sum of electronic and thermal Free Energies= -616.015814
 Standard State and RRHO Corrected G= -616.010277

Cartesian Coordinates

6	-1.569931	-1.163780	0.458849
6	-0.188259	-1.308692	0.577293
6	0.676423	-0.274443	0.197602
6	0.123825	0.919968	-0.296077
6	-1.252922	1.067040	-0.414284
6	-2.120180	0.027436	-0.038993
1	-2.212005	-1.985510	0.757973
1	0.224230	-2.236985	0.963092
1	-1.681133	1.988473	-0.795016
1	0.779357	1.736542	-0.586048
6	2.187756	-0.433139	0.303335
1	2.388755	-1.375746	0.832014
6	2.881672	-0.453598	-1.071341
1	2.333603	-1.145437	-1.720829
1	2.797012	0.540906	-1.522944
6	4.353211	-0.869558	-0.994613
1	4.457779	-1.871411	-0.561189
1	4.803346	-0.890112	-1.992925
1	4.929195	-0.171765	-0.380372
6	2.702442	0.674576	1.212801
8	3.430147	1.581673	0.862005
1	2.330145	0.615642	2.258447
6	-3.596721	0.237909	-0.184036
8	-4.035101	1.293420	-0.626406
6	-4.533605	-0.878404	0.227626
1	-4.397078	-1.128867	1.285664
1	-5.563780	-0.561220	0.058975
1	-4.332060	-1.787140	-0.350612

(4-7)_{re}[‡] (X = COCH₃)

Number of imaginary frequencies : 1
 Electronic energy : HF=-5522.1810502
 Zero-point correction= 1.601036 (Hartree/Particle)
 Thermal correction to Energy= 1.702962
 Thermal correction to Enthalpy= 1.703906
 Thermal correction to Gibbs Free Energy= 1.454246
 Sum of electronic and zero-point Energies= -5520.580015
 Sum of electronic and thermal Energies= -5520.478088
 Sum of electronic and thermal Enthalpies= -5520.477144
 Sum of electronic and thermal Free Energies= -5520.726804
 Standard State and RRHO Corrected G= -5520.697323

Cartesian Coordinates

8	-4.120566	3.675749	-1.046555
3	-3.233879	2.731101	0.350918
8	-1.737065	1.732704	-0.321404
6	-0.532319	1.786553	-0.675720
8	0.332416	0.858347	-0.544611
45	0.631776	-1.008966	0.495467
15	0.716068	-1.892454	-1.923828
6	-0.998055	-2.275215	-2.525873
6	-1.921914	-1.217824	-2.441180
6	-3.229610	-1.375389	-2.892499
6	-3.645663	-2.597168	-3.431600
6	-2.735604	-3.650283	-3.524521
6	-1.416732	-3.490120	-3.082937
6	-0.026975	3.050359	-1.333985
6	1.343839	3.341121	-1.365046
6	1.799006	4.532255	-1.930707

6	0.889824	5.438144	-2.484998
6	-0.478009	5.150354	-2.460277
6	-0.937519	3.966206	-1.880223
6	-1.415804	-1.209431	1.597763
6	-2.470687	-1.039118	0.675268
6	-4.424694	-0.891703	1.698000
6	-5.270060	-1.442299	0.627227
6	-5.520693	-2.834714	0.550612
6	-6.206937	-3.396743	-0.518857
6	-6.691774	-2.596505	-1.568071
6	-6.476897	-1.208680	-1.485834
6	-5.784677	-0.644742	-0.426359
6	-0.527176	-0.196937	2.084857
15	2.644378	-0.108630	1.295009
8	2.932071	-0.268519	2.768140
8	2.651853	1.546279	0.909248
6	3.742581	2.292391	1.299519
6	4.898616	2.269304	0.532822
6	6.030743	3.036735	0.985659
6	5.895076	3.873495	2.145310
6	4.665358	3.886184	2.857955
6	3.618984	3.093425	2.458777
6	7.002252	4.650987	2.581918
6	8.212579	4.593509	1.928312
6	8.364827	3.736520	0.812324
6	7.306725	2.980404	0.355574
6	4.960274	1.401004	-0.673968
6	4.649038	0.044996	-0.569083
6	4.902172	-0.848619	-1.639770
6	5.379089	-0.387043	-2.839641
6	5.567617	1.003947	-3.051469
6	5.338923	1.911696	-1.964153
6	5.446356	3.307145	-2.228876
6	5.768858	3.773375	-3.485696
6	6.019655	2.871377	-4.548049
6	5.921546	1.515438	-4.328751
8	4.169679	-0.495585	0.588346
6	1.171973	-0.624050	-3.198407
6	2.002170	0.455453	-2.881860
6	2.369642	1.378820	-3.866154
6	1.923098	1.224733	-5.177171
6	1.102297	0.141138	-5.507192
6	0.727632	-0.774215	-4.525473
6	1.762375	-3.319058	-2.487698
6	1.502110	-4.637586	-2.073807
6	2.371883	-5.678819	-2.399834
6	3.529549	-5.426592	-3.138162
6	3.798482	-4.123657	-3.561863
6	2.922755	-3.082546	-3.246233
6	-4.201790	0.512284	1.869826
8	-4.514360	1.456157	1.105160
6	-4.164344	-1.730468	2.940320
6	-5.394860	-1.880401	3.846828
8	-2.664306	3.861418	1.841817
1	5.826301	4.843674	-3.663415
1	5.252270	4.011510	-1.428157
1	6.089643	0.810637	-5.139249
1	6.276184	3.251654	-5.532631
1	5.570965	-1.077253	-3.656842
1	4.702891	-1.899872	-1.481242
1	7.450147	2.321882	-0.492408
1	2.686183	3.063028	3.007950
1	9.327731	3.668329	0.313607
1	6.875361	5.286328	3.455102
1	4.574501	4.515066	3.739745
1	9.052713	5.189294	2.273681
1	-1.618732	-0.266966	-2.016566
1	-0.724025	-4.315614	-3.192722
1	-3.927647	-0.548929	-2.809715
1	-3.042771	-4.601508	-3.951201
1	-4.666865	-2.717889	-3.779250
1	2.344703	0.590703	-1.867072
1	0.087876	-1.608848	-4.794360
1	2.999816	2.219430	-3.599756
1	0.750668	0.010476	-6.527112
1	2.211760	1.944464	-5.938365
1	0.622555	-4.861726	-1.489716
1	3.155855	-2.081195	-3.585509
1	2.141788	-6.686258	-2.064989
1	4.691206	-3.911401	-4.144015

1	4.211875	-6.235587	-3.383045
1	2.033741	2.634578	-0.925525
1	-2.000149	3.755353	-1.836773
1	2.864019	4.746068	-1.946313
1	-1.190030	5.850487	-2.889620
1	1.244870	6.363142	-2.931966
1	-3.615649	0.757958	2.775191
1	-5.157526	-3.494768	1.330189
1	-5.611937	0.420507	-0.397247
1	-6.354933	-4.472041	-0.534255
1	-6.847601	-0.580274	-2.290323
1	-3.782862	-2.721035	2.665978
1	-3.355886	-1.261108	3.512408
1	-6.227060	-2.356804	3.318051
1	-5.162659	-2.487997	4.729455
1	-5.741641	-0.899326	4.191997
1	-0.736005	0.836569	1.828716
1	-0.082066	-0.333770	3.063787
1	-1.429656	-2.151228	2.134308
1	-2.871046	-1.925187	0.199706
1	-2.524393	-0.124512	0.102591
6	-2.169288	3.373936	2.889476
6	-2.423813	2.626646	5.235700
6	-0.168133	2.615638	4.193008
6	-1.148502	1.819299	5.041479
1	-2.227821	3.528387	5.836233
1	0.649154	1.971424	3.851432
1	-0.693022	1.581643	6.007193
6	-5.116716	4.439783	-1.063577
6	-7.519935	4.840964	-1.609729
6	-6.072576	6.714690	-0.862792
6	-7.425921	6.042768	-0.681734
1	-7.621501	5.165919	-2.656002
1	-5.943694	7.524245	-0.138237
1	-8.231945	6.748290	-0.902994
7	-5.001710	5.740829	-0.645296
7	-6.339096	3.986139	-1.474199
7	-2.977176	2.988114	3.930151
7	-0.822062	3.177782	3.009096
1	-3.176259	2.036365	5.766781
1	-1.392874	0.876392	4.542407
1	0.280391	3.429785	4.781739
1	-5.991396	7.156689	-1.868134
1	-7.533973	5.718054	0.359275
1	-8.401815	4.237117	-1.370435
15	1.084385	-2.983728	1.650998
6	2.832228	-3.556687	1.719918
6	3.576588	-3.543420	0.532429
6	3.417223	-4.071577	2.886608
6	4.876448	-4.045823	0.504358
1	3.140916	-3.138126	-0.369916
6	4.725691	-4.558763	2.859957
1	2.860299	-4.096842	3.816176
6	5.456638	-4.550855	1.669771
1	5.436003	-4.031479	-0.426277
1	5.170244	-4.948337	3.771433
1	6.472983	-4.934253	1.651928
6	0.534456	-3.006319	3.424264
6	-0.496663	-3.856006	3.857897
6	1.115347	-2.116510	4.345089
6	-0.946022	-3.808936	5.179683
1	-0.963288	-4.551677	3.169932
6	0.666229	-2.080850	5.666554
1	1.900604	-1.443776	4.011390
6	-0.367600	-2.920809	6.087921
1	-1.748771	-4.469660	5.494910
1	1.124948	-1.387180	6.366165
1	-0.718475	-2.884782	7.115607
6	0.207446	-4.468705	0.982831
6	0.729757	-5.757985	1.177444
6	-1.014758	-4.327457	0.310717
6	0.045181	-6.875625	0.698510
1	1.674552	-5.894410	1.692400
6	-1.704984	-5.447217	-0.157787
1	-1.410767	-3.342517	0.115438
6	-1.174080	-6.724495	0.030757
1	0.466946	-7.865833	0.845804
1	-2.643060	-5.310239	-0.687287
1	-1.702239	-7.597083	-0.343036
6	-3.665632	6.279301	-0.408751

1	-3.019327	5.516089	0.018982
1	-3.211537	6.656649	-1.336146
1	-3.744946	7.109330	0.298900
6	-6.475197	2.634584	-2.001024
1	-6.816594	2.669184	-3.043700
1	-5.515371	2.126098	-1.956293
1	-7.209935	2.070493	-1.415298
6	-4.396372	3.316065	3.878514
1	-4.601738	4.302179	4.319072
1	-4.738126	3.301832	2.846115
1	-4.952468	2.562147	4.443772
6	0.079668	3.685866	1.983588
1	0.699040	2.876904	1.587453
1	-0.496724	4.123493	1.174119
1	0.740486	4.452122	2.410106
6	-7.371097	-3.155741	-2.765503
8	-7.730936	-2.428385	-3.689618
6	-7.593777	-4.654978	-2.842065
1	-6.635979	-5.187318	-2.819958
1	-8.183512	-5.010212	-1.989891
1	-8.116263	-4.891451	-3.770440

(4-7)_{st}[‡] (X = COCH₃)

Number of imaginary frequencies : 1
 Electronic energy : HF=-5522.1785825
 Zero-point correction= 1.599971 (Hartree/Particle)
 Thermal correction to Energy= 1.701864
 Thermal correction to Enthalpy= 1.702809
 Thermal correction to Gibbs Free Energy= 1.455484
 Sum of electronic and zero-point Energies= -5520.578611
 Sum of electronic and thermal Energies= -5520.476718
 Sum of electronic and thermal Enthalpies= -5520.475774
 Sum of electronic and thermal Free Energies= -5520.723099
 Standard State and RRHO Corrected G= -5520.695131

Cartesian Coordinates

6	0.891924	-3.558456	3.041231
6	-0.454697	-3.539092	2.632939
6	-1.084934	-4.760739	2.347058
6	-0.394855	-5.967798	2.492844
6	0.933125	-5.976028	2.921678
6	1.576031	-4.763519	3.193446
15	-1.242701	-1.912160	2.269226
6	-3.059578	-2.170873	2.571577
6	-3.551136	-3.107339	3.494395
6	-4.919829	-3.193099	3.755480
6	-5.813685	-2.323817	3.124520
6	-5.328204	-1.358791	2.239593
6	-3.961342	-1.284829	1.964727
45	-0.163323	-0.963064	0.165321
15	-1.603590	0.559195	-0.783421
8	-1.041248	1.614840	-1.693785
6	2.184338	-1.355402	-0.056826
6	1.551965	-0.430166	-0.960330
6	2.748286	-1.082011	1.199205
8	0.368445	0.616146	1.533668
6	0.888212	1.782363	1.438505
6	1.249554	2.422847	2.758696
6	1.661015	1.650741	3.851798
6	2.057370	2.268446	5.038896
6	2.002079	3.660287	5.157061
6	1.564814	4.434202	4.077092
6	1.211768	3.818944	2.875730
8	1.136921	2.416181	0.391681
8	-2.426410	1.287853	0.523259
6	-3.039551	2.481423	0.204436
6	-4.223244	2.465096	-0.514708
6	-4.728933	3.726996	-0.993489
6	-4.088875	4.945460	-0.580760
6	-2.945744	4.886732	0.262604
6	-2.409056	3.675368	0.619494
6	-4.587854	6.190725	-1.051313
6	-5.657534	6.246472	-1.916647
6	-6.269949	5.046966	-2.352110
6	-5.821721	3.824190	-1.900639
6	-4.932296	1.176851	-0.766357
6	-4.307952	0.068687	-1.343767
6	-5.066962	-1.062171	-1.757934

6	-6.406937	-1.151936	-1.496296
6	-7.062143	-0.130049	-0.758268
6	-6.317470	1.035079	-0.375431
6	-6.980941	1.996865	0.439904
6	-8.295138	1.831126	0.823663
6	-9.032949	0.697883	0.408879
6	-8.420206	-0.262827	-0.364924
8	-2.979661	-0.030828	-1.629599
6	-0.993595	-0.887446	3.797024
6	-0.496636	-1.374851	5.012142
6	-0.493301	-0.561914	6.151761
6	-1.001792	0.735569	6.092790
6	-1.505796	1.224497	4.883325
6	-1.494170	0.425646	3.742918
3	2.773187	3.041484	-0.436569
8	4.033593	1.505166	-0.391832
6	4.342139	0.969460	0.698277
6	4.873775	-0.339023	0.941714
6	5.321026	-1.233590	-0.127555
6	5.065144	-0.966607	-1.497313
6	5.404561	-1.877637	-2.490024
6	5.988914	-3.116262	-2.175842
6	6.249463	-3.392185	-0.820411
6	5.941416	-2.475435	0.171160
6	5.366282	-0.556222	2.365954
6	6.828803	-0.135212	2.576507
8	3.904388	4.352012	0.490289
8	2.267182	3.655372	-2.166509
1	-8.765316	2.577221	1.458354
1	-6.434271	2.865841	0.785284
1	-8.962801	-1.152356	-0.675662
1	-10.069528	0.582417	0.712277
1	-6.973622	-2.020427	-1.821200
1	-4.541164	-1.847886	-2.288404
1	-6.296461	2.916081	-2.253401
1	-1.498316	3.595823	1.202585
1	-7.098526	5.089793	-3.053639
1	-4.095178	7.102253	-0.721767
1	-2.475463	5.813399	0.579590
1	-6.024546	7.203927	-2.275213
1	-2.107884	-4.780421	1.991092
1	1.412087	-2.625034	3.229585
1	-0.900251	-6.900117	2.257536
1	2.613897	-4.754932	3.514392
1	1.467180	-6.915234	3.033490
1	-0.128181	-2.391804	5.090841
1	-1.864319	0.819067	2.802502
1	-0.103499	-0.954672	7.087193
1	-1.888379	2.239660	4.822465
1	-1.000886	1.364482	6.978656
1	-2.872178	-3.771399	4.018460
1	-3.598991	-0.528656	1.279302
1	-5.284966	-3.933525	4.462163
1	-6.008203	-0.663724	1.758615
1	-6.878454	-2.389474	3.330654
1	2.443804	-2.324432	-0.461163
1	1.656492	0.635942	-0.818432
1	1.556930	-0.731322	-2.005384
1	1.650102	0.569709	3.771479
1	0.912251	4.409920	2.016706
1	2.386103	1.662424	5.878368
1	1.517790	5.516057	4.165836
1	2.294557	4.140072	6.087099
1	4.126299	1.531642	1.625538
1	4.586420	-0.034912	-1.762110
1	6.166915	-2.733636	1.199939
1	5.183700	-1.623209	-3.522216
1	6.697916	-4.347245	-0.564777
1	4.728201	0.021876	3.046091
1	5.240759	-1.602551	2.667135
1	6.954956	0.929694	2.355650
1	7.149577	-0.309134	3.610595
1	7.501322	-0.692189	1.915519
1	3.138243	-1.922137	1.763905
1	2.433699	-0.236106	1.787962
6	1.161057	3.725802	-2.759040
6	-0.408360	2.849857	-4.476405
6	-1.172912	4.548868	-2.840403
6	-1.183858	4.148758	-4.308366
1	-0.276242	2.614678	-5.538864

1	-1.632510	5.532942	-2.704738
1	-0.728697	4.940850	-4.914938
6	5.148377	4.199741	0.568482
6	7.184724	3.831415	1.940838
6	7.411564	4.224218	-0.494273
6	7.856956	3.346777	0.665486
1	7.547257	4.834487	2.214728
1	7.867070	5.223502	-0.420368
1	8.945275	3.386261	0.768251
1	-1.727983	3.818731	-2.242670
1	-2.214827	4.009667	-4.648264
1	-0.950005	2.027346	-3.996715
1	7.733759	3.791632	-1.447630
1	7.568637	2.306760	0.476285
1	7.412698	3.163693	2.777204
7	5.953602	4.347977	-0.527474
7	5.734341	3.841223	1.758251
7	0.922925	2.964423	-3.874409
7	0.211685	4.626865	-2.361457
6	0.429455	5.325596	-1.099822
1	0.195122	4.683047	-0.244834
1	1.470386	5.641397	-1.020933
1	-0.213157	6.209766	-1.075965
6	1.841924	1.875118	-4.172124
1	2.841122	2.125475	-3.820091
1	1.528497	0.940805	-3.689062
1	1.870451	1.715171	-5.254967
6	5.393682	4.791173	-1.796044
1	4.311869	4.870619	-1.724739
1	5.816024	5.765848	-2.076859
1	5.638212	4.070458	-2.585475
6	4.924584	3.813733	2.967654
1	5.019336	4.748832	3.537983
1	3.879941	3.671788	2.706224
1	5.253449	2.987105	3.605037
15	-0.623427	-2.708537	-1.299101
6	-1.938898	-3.899778	-0.806850
6	-1.811170	-5.294365	-0.912544
6	-3.151300	-3.361692	-0.363578
6	-2.874177	-6.124316	-0.552177
1	-0.888797	-5.738262	-1.268039
6	-4.214665	-4.189541	-0.004566
1	-3.257855	-2.289498	-0.291720
6	-4.074854	-5.575816	-0.090867
1	-2.760870	-7.201982	-0.629775
1	-5.137358	-3.744574	0.354643
1	-4.896028	-6.226366	0.196659
6	0.850311	-3.785290	-1.560075
6	1.584181	-3.756910	-2.753268
6	1.316766	-4.568397	-0.489641
6	2.768022	-4.491597	-2.867433
1	1.246411	-3.157019	-3.591317
6	2.494012	-5.303266	-0.610498
1	0.769102	-4.587299	0.443535
6	3.230316	-5.260232	-1.798891
1	3.333049	-4.455134	-3.793636
1	2.841403	-5.896348	0.230509
1	4.165478	-5.804343	-1.889177
6	-1.111331	-2.301474	-3.037496
6	-1.780346	-3.261372	-3.815452
6	-0.752646	-1.081000	-3.626325
6	-2.086900	-3.002757	-5.151842
1	-2.065911	-4.214588	-3.383605
6	-1.052368	-0.829796	-4.967044
1	-0.274485	-0.306686	-3.041373
6	-1.719920	-1.786651	-5.732879
1	-2.610691	-3.753508	-5.736949
1	-0.770282	0.121268	-5.406911
1	-1.956755	-1.585490	-6.773960
6	6.291627	-4.148459	-3.197151
6	6.178413	-3.777454	-4.664993
1	6.828554	-2.928131	-4.902615
1	6.462780	-4.637688	-5.273343
1	5.155116	-3.480048	-4.918272
8	6.626784	-5.288028	-2.872721

5 (X = CF₃)

Number of imaginary frequencies : 0
Electronic energy : HF=800.5845365

Zero-point correction= 0.199295 (Hartree/Particle)
 Thermal correction to Energy= 0.213545
 Thermal correction to Enthalpy= 0.214489
 Thermal correction to Gibbs Free Energy= 0.155192
 Sum of electronic and zero-point Energies= -800.385242
 Sum of electronic and thermal Energies= -800.370992
 Sum of electronic and thermal Enthalpies= -800.370047
 Sum of electronic and thermal Free Energies= -800.429345
 Standard State and RRHO Corrected G= -800.423079

Cartesian Coordinates

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6      1.209718 -1.124284 -0.716341
6      -0.174837 -1.207925 -0.852984
6      -1.012453 -0.254335 -0.260019
6      -0.433030 0.796634 0.467836
6      0.949289 0.887999 0.609064
6      1.770589 -0.075986 0.017531
1      1.850548 -1.871736 -1.172331
1      -0.609735 -2.026518 -1.419409
1      1.388245 1.701363 1.177250
1      -1.067953 1.548768 0.927081
6      -2.528319 -0.352284 -0.384203
1      -2.753769 -1.162793 -1.091226
6      -3.218970 -0.633273 0.963101
1      -2.691115 -1.459294 1.452848
1      -3.103601 0.244909 1.607800
6      -4.702821 -0.980282 0.814973
1      -4.839488 -1.868001 0.185919
1      -5.151611 -1.191627 1.791441
1      -5.258064 -0.154144 0.361787
6      -3.013122 0.932026 -1.043466
8      -3.691737 1.779042 -0.498041
1      -2.664272 1.068663 -2.089822
6      3.262804 0.052155 0.116243
9      3.883452 -1.150225 0.072754
9      3.775951 0.786925 -0.904281
9      3.649666 0.662790 1.260702

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(4-7)_{re}[‡] (X = CF₃)

Number of imaginary frequencies : 1
 Electronic energy : HF=-5706.5669122
 Zero-point correction= 1.568733 (Hartree/Particle)
 Thermal correction to Energy= 1.670376
 Thermal correction to Enthalpy= 1.671320
 Thermal correction to Gibbs Free Energy= 1.424271
 Sum of electronic and zero-point Energies= -5704.998179
 Sum of electronic and thermal Energies= -5704.896536
 Sum of electronic and thermal Enthalpies= -5704.895592
 Sum of electronic and thermal Free Energies= -5705.142641
 Standard State and RRHO Corrected G= -5705.114285

Cartesian Coordinates

```

8      3.624336 -4.320730 -0.721261
3      2.695715 -3.285021 0.581386
8      1.410866 -2.071366 -0.194823
6      0.249295 -1.956571 -0.662789
8      -0.499812 -0.927005 -0.576662
45     -0.682844 0.905944 0.555113
15     -0.632704 1.922347 -1.824009
6      1.132107 2.200490 -2.326770
6      1.967107 1.069912 -2.276936
6      3.312326 1.162583 -2.623980
6      3.853886 2.388641 -3.024324
6      3.028577 3.510897 -3.094185
6      1.673437 3.418076 -2.756740
6      -0.337841 -3.125239 -1.419075
6      -1.725013 -3.264866 -1.561971
6      -2.256402 -4.369345 -2.228367
6      -1.406116 -5.335813 -2.773257
6      -0.021385 -5.199179 -2.635772
6      0.512352 -4.104517 -1.953127
6      1.350570 0.862102 1.711092
6      2.395309 0.614453 0.802985
6      4.330658 0.181636 1.888925
6      5.278381 0.594303 0.842538
6      5.807772 1.907945 0.826766
6      6.657421 2.348792 -0.182944

```

```

6      7.020015 1.485068 -1.218634
6      6.506624 0.182753 -1.234075
6      5.649999 -0.254668 -0.232571
6      0.342355 -0.066892 2.136487
15     -2.797951 0.158174 1.232877
8      -3.128539 0.268071 2.701106
8      -2.959229 -1.462433 0.753662
6      -4.143598 -2.102233 1.058379
6      -5.246536 -1.923035 0.236562
6      -6.476477 -2.584251 0.591832
6      -6.495000 -3.476657 1.717047
6      -5.317756 -3.643653 2.495273
6      -4.173184 -2.951642 2.188900
6      -7.699257 -4.151144 2.057353
6      -8.857457 -3.940222 1.343705
6      -8.856306 -3.026708 0.262747
6      -7.701736 -2.367550 -0.101116
6      -5.153592 -0.993025 -0.920356
6      -4.713259 0.315773 -0.721144
6      -4.824763 1.288146 -1.746000
6      -5.289749 0.944545 -2.989598
6      -5.603840 -0.406192 -3.292601
6      -5.516685 -1.391245 -2.253455
6      -5.746484 -2.752319 -2.604677
6      -6.053080 -3.113693 -3.899376
6      -6.165002 -2.133401 -4.915173
6      -5.945636 -0.808274 -4.611657
8      -4.238753 0.738735 0.487313
6      -1.125253 0.763783 -3.183550
6      -2.045732 -0.263720 -2.958453
6      -2.440589 -1.102411 -4.005613
6      -1.928294 -0.915183 -5.287968
6      -1.013740 0.116395 -5.526123
6      -0.613460 0.947891 -4.481877
6      -1.526935 3.462708 -2.347782
6      -1.194989 4.720018 -1.812140
6      -1.942402 5.855593 -2.125629
6      -3.047856 5.760368 -2.973198
6      -3.387984 4.519513 -3.515177
6      -2.633344 3.384053 -3.211508
6      3.897434 -1.167222 2.052592
8      4.109797 -2.157711 1.308918
6      4.141825 1.063415 3.113387
6      5.330966 1.031798 4.085849
8      1.974461 -4.317352 2.040528
1      -6.205933 -4.161396 -4.142976
1      -5.659422 -3.515383 -1.839627
1      -6.006275 -0.046708 -5.385090
1      -6.410846 -2.430974 -5.930469
1      -5.374454 1.695236 -3.770704
1      -4.529548 2.303593 -1.518967
1      -7.728536 -1.663296 -0.923575
1      -3.280233 -3.038037 2.793915
1      -9.776814 -2.837069 -0.282499
1      -7.688649 -4.831107 2.905712
1      -5.344441 -4.309334 3.353983
1      -9.772699 -4.458465 1.615398
1      1.562727 0.116531 -1.952946
1      1.051491 4.301121 -2.838048
1      3.942975 0.282694 -2.560530
1      3.432762 4.466776 -3.416801
1      4.906115 2.461520 -3.276710
1      -2.439538 -0.423329 -1.965905
1      0.097700 1.744088 -4.678647
1      -3.145628 -1.902302 -3.810779
1      -0.610534 0.271948 -6.523207
1      -2.239050 -1.568689 -6.098591
1      -0.354469 4.821261 -1.142271
1      -2.920096 2.433822 -3.643757
1      -1.659257 6.812297 -1.696055
1      -4.241646 4.429864 -4.181562
1      -3.635637 6.642618 -3.210277
1      -2.370027 -2.512540 -1.130176
1      1.584635 -4.010418 -1.821970
1      -3.333591 -4.467249 -2.329889
1      0.644364 -5.948508 -3.056181
1      -1.819935 -6.192269 -3.299214
1      3.244401 -1.318458 2.933025
1      5.554374 2.604747 1.616933
1      5.257380 -1.260453 -0.270602

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1	7.043804	3.362472	-0.160784
1	6.778272	-0.491025	-2.040119
1	3.929609	2.098211	2.817314
1	3.244263	0.728149	3.645811
1	6.257031	1.360795	3.603073
1	5.151350	1.681697	4.950578
1	5.496455	0.013214	4.455878
1	0.455681	-1.108720	1.857399
1	-0.111574	0.086661	3.108374
1	1.447582	1.779714	2.279914
1	2.928031	1.462760	0.392634
1	2.377383	-0.284999	0.204944
6	1.445978	-3.764988	3.038385
6	1.564442	-3.070921	5.405264
6	-0.570673	-2.782602	4.157035
6	0.408015	-2.123202	5.119468
1	1.215823	-3.960947	5.951623
1	-1.261318	-2.036919	3.747596
1	-0.110112	-1.858328	6.045691
6	4.830121	-4.150036	-1.027221
6	6.504693	-3.339299	-2.654374
6	7.236717	-4.726083	-0.725282
6	7.543149	-3.483918	-1.550611
1	6.593639	-4.161605	-3.380876
1	7.852567	-4.744901	0.179966
1	8.545605	-3.563335	-1.981229
7	5.831084	-4.749628	-0.315801
7	5.165108	-3.317640	-2.063860
7	2.198300	-3.456119	4.143749
7	0.124289	-3.420005	3.035387
1	2.319590	-2.579871	6.025363
1	0.803846	-1.202645	4.680276
1	-1.176037	-3.537402	4.680885
1	7.470255	-5.637227	-1.296722
1	7.516076	-2.595927	-0.910490
1	6.649846	-2.404879	-3.202959
15	-0.991328	2.852069	1.813640
6	-2.678147	3.587634	1.864026
6	-3.389054	3.693453	0.661026
6	-3.239247	4.116109	3.036789
6	-4.632163	4.323232	0.624116
1	-2.971285	3.282515	-0.246841
6	-4.491276	4.733230	3.000203
1	-2.706728	4.052799	3.978662
6	-5.189069	4.841055	1.795054
1	-5.166770	4.397772	-0.318257
1	-4.917758	5.132779	3.915962
1	-6.161584	5.324596	1.769785
6	-0.510948	2.714510	3.600959
6	0.603428	3.400311	4.111106
6	-1.237341	1.865524	4.454651
6	0.989907	3.234060	5.443205
1	1.182333	4.060561	3.475311
6	-0.851202	1.712363	5.787366
1	-2.084391	1.312359	4.059377
6	0.264472	2.390119	6.285557
1	1.858263	3.768522	5.818174
1	-1.423569	1.053712	6.435042
1	0.565201	2.262518	7.321816
6	0.045475	4.284085	1.269590
6	-0.358579	5.601506	1.543969
6	1.264717	4.073216	0.610486
6	0.437472	6.679141	1.154988
1	-1.298180	5.792219	2.050933
6	2.065600	5.152623	0.231287
1	1.574514	3.070736	0.355653
6	1.651951	6.458554	0.498019
1	0.106603	7.692512	1.363949
1	2.997718	4.964483	-0.292614
1	2.267512	7.300187	0.193393
6	5.494634	-5.662865	0.767756
1	4.456552	-5.523087	1.062915
1	5.643777	-6.708662	0.464260
1	6.141380	-5.458627	1.627947
6	4.078428	-2.730448	-2.841558
1	3.630182	-3.449815	-3.540411
1	3.296243	-2.360949	-2.177609
1	4.478656	-1.893414	-3.417844
6	3.582091	-3.912584	4.193916
1	3.662039	-4.938156	4.581839

1	4.017662	-3.870493	3.197352
1	4.145752	-3.247609	4.854652
6	-0.727706	-3.834297	1.927772
1	-1.235741	-2.967632	1.498252
1	-0.126579	-4.312621	1.160185
1	-1.487495	-4.543893	2.280990
6	7.908201	1.931357	-2.332313
9	7.227794	2.094051	-3.507278
9	8.518749	3.111226	-2.080189
9	8.882991	1.025912	-2.605489

(4-7)_{sr}⁺ (X = CF₃)

Number of imaginary frequencies : 1
 Electronic energy : HF=-5706.5587044
 Zero-point correction= 1.567168 (Hartree/Particle)
 Thermal correction to Energy= 1.669109
 Thermal correction to Enthalpy= 1.670053
 Thermal correction to Gibbs Free Energy= 1.421835
 Sum of electronic and zero-point Energies= -5704.991537
 Sum of electronic and thermal Energies= -5704.889596
 Sum of electronic and thermal Enthalpies= -5704.888651
 Sum of electronic and thermal Free Energies= -5705.136870
 Standard State and RRHO Corrected G= -5705.108448

Cartesian Coordinates

6	0.832040	-3.421000	3.164643
6	-0.507321	-3.461297	2.735244
6	-1.090713	-4.712404	2.478557
6	-0.363714	-5.889794	2.677674
6	0.955344	-5.838522	3.130747
6	1.552639	-4.596462	3.370574
15	-1.346119	-1.874048	2.313636
6	-3.158293	-2.193952	2.585854
6	-3.628780	-3.112785	3.537169
6	-4.997307	-3.245212	3.778004
6	-5.913531	-2.438858	3.097577
6	-5.451215	-1.490022	2.183370
6	-4.083431	-1.370203	1.928325
45	-0.237841	-0.937340	0.212006
15	-1.686966	0.504733	-0.827358
8	-1.116875	1.567446	-1.722883
6	2.161562	-1.226288	0.066030
6	1.490158	-0.363259	-0.872718
6	2.669940	-0.892049	1.326471
8	0.198256	0.689623	1.558680
6	0.662671	1.878505	1.450035
6	0.964715	2.561344	2.764065
6	1.387690	1.831631	3.881683
6	1.729431	2.491127	5.063313
6	1.606835	3.880940	5.150849
6	1.157128	4.611410	4.046013
6	0.859214	3.956171	2.850884
8	0.902014	2.502805	0.395980
8	-2.600282	1.206597	0.430073
6	-3.276471	2.353213	0.067831
6	-4.437558	2.249179	-0.680376
6	-5.013363	3.468057	-1.190045
6	-4.463827	4.731490	-0.782256
6	-3.339063	4.759861	0.087070
6	-2.733771	3.591577	0.476362
6	-5.031525	5.934501	-1.283754
6	-6.082244	5.907526	-2.173356
6	-6.605198	4.664429	-2.603124
6	-6.088871	3.480185	-2.122570
6	-5.049681	0.912850	-0.933077
6	-4.329958	-0.150267	-1.482176
6	-4.988403	-1.339950	-1.900728
6	-6.323999	-1.528212	-1.668984
6	-7.072779	-0.550409	-0.960681
6	-6.429466	0.673209	-0.576215
6	-7.184270	1.592786	0.207710
6	-8.491111	1.331778	0.562302
6	-9.129088	0.139279	0.147537
6	-8.426072	-0.781663	-0.597294
8	-2.992648	-0.136920	-1.741118
6	-1.168132	-0.801858	3.818214
6	-0.669536	-1.234199	5.053117
6	-0.720683	-0.391952	6.170129

6	-1.285738	0.879115	6.068364
6	-1.791315	1.313162	4.838773
6	-1.724949	0.485978	3.720706
3	2.509864	3.187427	-0.440046
8	3.840983	1.711689	-0.355728
6	4.136783	1.254886	0.775592
6	4.768317	0.017436	1.110720
6	5.360630	-0.869972	0.106691
6	5.053049	-0.756537	-1.275181
6	5.584706	-1.635182	-2.211499
6	6.441594	-2.666984	-1.813172
6	6.748158	-2.814348	-0.455947
6	6.218898	-1.934000	0.480316
6	5.196464	-0.091990	2.567190
6	6.564083	0.546841	2.856179
8	3.563782	4.547252	0.502516
8	1.985698	3.775675	-2.171488
1	-9.033151	2.048052	1.173588
1	-6.713945	2.505805	0.552135
1	-8.891890	-1.713870	-0.907436
1	-10.160953	-0.051542	0.428090
1	-6.815509	-2.441080	-1.994753
1	-4.390537	-2.088805	-2.407953
1	-6.495190	2.537980	-2.471309
1	-1.833940	3.579480	1.081285
1	-7.418465	4.642909	-3.323291
1	-4.607062	6.881065	-0.958187
1	-2.937670	5.719840	0.399441
1	-6.502257	6.833605	-2.555372
1	-2.105463	-4.778357	2.104900
1	1.318670	-2.464967	3.327866
1	-0.833229	-6.846075	2.465330
1	2.583786	-4.541718	3.708232
1	1.517737	-6.754907	3.285087
1	-0.257372	-2.231110	5.164527
1	-2.096497	0.837689	2.764266
1	-0.328762	-0.741768	7.121579
1	-2.217474	2.308233	4.744873
1	-1.326972	1.530682	6.936713
1	-2.932885	-3.726347	4.099303
1	-3.738861	-0.626767	1.219634
1	-5.345232	-3.971610	4.507533
1	-6.150368	-0.842326	1.665412
1	-6.978460	-2.539818	3.288028
1	2.480064	-2.190792	-0.304918
1	1.538502	0.710505	-0.760396
1	1.537240	-0.690245	-1.909007
1	1.427717	0.749829	3.824526
1	0.550735	4.514981	1.973611
1	2.067673	1.918247	5.922039
1	1.057479	5.691407	4.110902
1	1.856643	4.392672	6.076308
1	3.830203	1.842513	1.660892
1	4.397998	0.039768	-1.596904
1	6.485557	-2.076234	1.521197
1	5.336923	-1.514826	-3.261934
1	7.410744	-3.611815	-0.134481
1	4.440114	0.402993	3.189569
1	5.201906	-1.139265	2.891384
1	6.539946	1.612772	2.610788
1	6.838424	0.445581	3.913218
1	7.356212	0.087545	2.255471
1	3.111325	-1.686375	1.919179
1	2.296233	-0.049957	1.884495
6	0.896091	3.761233	-2.797307
6	-0.565168	2.747738	-4.533040
6	-1.480507	4.434130	-2.960773
6	-1.426082	3.997872	-4.417558
1	-0.389420	2.497535	-5.585752
1	-2.004762	5.389890	-2.863460
1	-1.005961	4.802589	-5.032693
6	4.813059	4.500897	0.611951
6	6.837141	4.394639	2.038756
6	7.092944	4.653960	-0.411181
6	7.583868	3.894194	0.811697
1	7.089545	5.446363	2.246019
1	7.472932	5.686825	-0.402531
1	8.661414	4.038979	0.932442
1	-2.004460	3.685317	-2.358197
1	-2.436611	3.784798	-4.779857

1	-1.066125	1.902485	-4.048270
1	7.461707	4.181697	-1.328380
1	7.394221	2.822483	0.685964
1	7.110516	3.814155	2.924818
7	5.630397	4.671577	-0.471400
7	5.398605	4.242169	1.828286
7	0.738929	2.960825	-3.899614
7	-0.117180	4.611579	-2.449060
6	0.028201	5.347695	-1.197902
1	-0.710205	6.153267	-1.181348
1	-0.125612	4.695616	-0.331832
1	1.026823	5.782063	-1.131415
6	1.728119	1.919550	-4.137859
1	2.700156	2.238041	-3.765305
1	1.454260	0.983052	-3.635417
1	1.799022	1.730819	-5.214081
6	5.067250	5.006591	-1.771162
1	5.458100	5.975178	-2.111338
1	5.344394	4.245228	-2.510326
1	3.982706	5.052392	-1.714004
6	4.563441	4.191188	3.019531
1	4.550733	5.156143	3.546236
1	3.544796	3.935744	2.742065
1	4.954078	3.430556	3.702549
15	-0.580149	-2.734314	-1.218563
6	-1.854227	-3.972999	-0.735476
6	-1.666708	-5.362397	-0.822990
6	-3.094869	-3.482427	-0.316612
6	-2.698576	-6.232452	-0.467410
1	-0.721647	-5.770895	-1.161154
6	-4.127921	-4.350340	0.036721
1	-3.249311	-2.415397	-0.259173
6	-3.928286	-5.730185	-0.030138
1	-2.538602	-7.305141	-0.530239
1	-5.074348	-3.940432	0.375507
1	-4.725294	-6.411682	0.253572
6	0.961000	-3.729983	-1.383060
6	1.793646	-3.608578	-2.504240
6	1.393531	-4.499517	-0.289300
6	3.046566	-4.227892	-2.519088
1	1.482181	-3.015579	-3.357449
6	2.636430	-5.127755	-0.314941
1	0.769113	-4.588803	0.589908
6	3.473256	-4.982518	-1.425589
1	3.697909	-4.110282	-3.378465
1	2.955163	-5.714402	0.541839
1	4.455763	-5.441665	-1.439179
6	-1.013368	-2.402374	-2.986923
6	-1.601225	-3.416148	-3.761903
6	-0.686882	-1.183791	-3.598435
6	-1.858797	-3.212751	-5.118136
1	-1.862539	-4.368164	-3.312484
6	-0.935828	-0.988225	-4.958429
1	-0.271781	-0.370149	-3.018506
6	-1.522350	-1.998858	-5.721629
1	-2.320611	-4.004792	-5.700960
1	-0.677781	-0.038471	-5.415693
1	-1.720302	-1.841005	-6.778168
6	6.976891	-3.628256	-2.821621
9	7.207535	-3.043742	-4.022789
9	8.137082	-4.206064	-2.427037
9	6.116642	-4.663344	-3.078000

5 (X = CN)

Number of imaginary frequencies : 0
Electronic energy : HF=-555.7917854
Zero-point correction= 0.193393 (Hartree/Particle)
Thermal correction to Energy= 0.205793
Thermal correction to Enthalpy= 0.206737
Thermal correction to Gibbs Free Energy= 0.153384
Sum of electronic and zero-point Energies= -555.598392
Sum of electronic and thermal Energies= -555.585992
Sum of electronic and thermal Enthalpies= -555.585048
Sum of electronic and thermal Free Energies= -555.638402
Standard State and RRHO Corrected G= -555.633466

Cartesian Coordinates

6	-2.008261	-1.070619	0.695401
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6	-0.627881	-1.170560	0.840118
6	0.228338	-0.237113	0.239893
6	-0.328072	0.815757	-0.504888
6	-1.704774	0.931141	-0.659768
6	-2.551906	-0.016296	-0.058176
1	-2.664838	-1.798963	1.159822
1	-0.209396	-1.986533	1.421956
1	-2.127938	1.746806	-1.236614
1	0.323022	1.552998	-0.965163
6	1.740434	-0.355079	0.378896
1	1.949211	-1.173817	1.081185
6	2.440203	-0.632324	-0.964883
1	1.906494	-1.446337	-1.468041
1	2.343827	0.253721	-1.601626
6	3.917497	-1.000790	-0.804255
1	4.035424	-1.897121	-0.183801
1	4.373493	-1.207276	-1.778350
1	4.478988	-0.187195	-0.336301
6	2.234587	0.919511	1.053001
8	2.921047	1.765110	0.516054
1	1.885912	1.048316	2.100126
6	-3.971481	0.095318	-0.211164
7	-5.124954	0.185835	-0.335240
(4-7) _{re} * (X = CN)			
Number of imaginary frequencies : 1			
Electronic energy : HF=-5461.7738829			
Zero-point correction= 1.563121 (Hartree/Particle)			
Thermal correction to Energy= 1.662860			
Thermal correction to Enthalpy= 1.663804			
Thermal correction to Gibbs Free Energy= 1.421977			
Sum of electronic and zero-point Energies= -5460.210762			
Sum of electronic and thermal Energies= -5460.111023			
Sum of electronic and thermal Enthalpies= -5460.110079			
Sum of electronic and thermal Free Energies= -5460.351906			
Standard State and RRHO Corrected G= -5460.324875			
Cartesian Coordinates			
8	3.967876	-4.180764	-0.755777
3	3.067031	-3.120632	0.546530
8	1.696908	-1.991443	-0.221236
6	0.503951	-1.950030	-0.620171
8	-0.277394	-0.944024	-0.555886
45	-0.484348	0.952733	0.459703
15	-0.578967	1.815153	-1.965399
6	1.135184	2.155831	-2.589159
6	2.039129	1.081414	-2.511579
6	3.351430	1.222348	-2.955068
6	3.790720	2.441941	-3.480618
6	2.896854	3.508490	-3.575696
6	1.574154	3.365605	-3.141109
6	-0.083715	-3.189798	-1.253977
6	-1.471426	-3.378730	-1.308580
6	-2.002008	-4.546274	-1.857873
6	-1.151832	-5.528943	-2.373058
6	0.233099	-5.343931	-2.323288
6	0.767137	-4.184642	-1.757486
6	1.590427	1.050577	1.514869
6	2.615326	0.780520	0.580851
6	4.555464	0.502046	1.576567
6	5.431086	0.933499	0.477586
6	5.845168	2.287209	0.382251
6	6.580800	2.758672	-0.694108
6	6.950339	1.883139	-1.731714
6	6.563906	0.531918	-1.654381
6	5.816670	0.070621	-0.580955
6	0.647306	0.114741	2.052012
15	-2.538466	0.179550	1.295210
8	-2.802115	0.386236	2.767053
8	-2.653517	-1.478891	0.944052
6	-3.791691	-2.141941	1.353499
6	-4.941170	-2.068793	0.580303
6	-6.121517	-2.750738	1.046824
6	-6.044866	-3.557433	2.232694
6	-4.823805	-3.619925	2.956953
6	-3.727624	-2.906793	2.541480
6	-7.200130	-4.252053	2.684082
6	-8.400699	-4.140790	2.019642

6	-8.493467	-3.310284	0.877422
6	-7.388235	-2.634829	0.406176
6	-4.946719	-1.224056	-0.643935
6	-4.555737	0.112788	-0.560813
6	-4.758291	1.001575	-1.646034
6	-5.263421	0.548411	-2.837718
6	-5.533412	-0.832201	-3.026723
6	-5.356399	-1.733459	-1.924677
6	-5.548159	-3.124296	-2.164689
6	-5.901145	-3.591721	-3.412807
6	-6.099719	-2.694489	-4.490266
6	-5.919877	-1.343335	-4.294733
8	-4.044124	0.641243	0.588756
6	-1.081251	0.547003	-3.220721
6	-1.958084	-0.489349	-2.885947
6	-2.367218	-1.411603	-3.854247
6	-1.913322	-1.301270	-5.167288
6	-1.043780	-0.262328	-5.515237
6	-0.629593	0.653364	-4.549573
6	-1.583874	3.270266	-2.530055
6	-1.295611	4.572592	-2.084805
6	-2.119376	5.646882	-2.421714
6	-3.258968	5.443504	-3.202437
6	-3.555489	4.156884	-3.656019
6	-2.724640	3.082517	-3.329480
6	4.237241	-0.874771	1.818303
8	4.483991	-1.872858	1.102924
6	4.389483	1.403586	2.791803
6	5.633554	1.456753	3.690714
8	2.459001	-4.036690	2.121633
1	-6.023906	-4.659447	-3.571859
1	-5.395299	-3.824895	-1.351762
1	-6.047828	-0.643643	-5.116923
1	-6.381201	-3.075566	-5.467695
1	-5.416023	1.235540	-3.665661
1	-4.499026	2.042575	-1.508266
1	-7.486607	-1.994647	-0.461936
1	-2.802363	-2.912120	3.102639
1	-9.447538	-3.198058	0.369751
1	-7.117648	-4.866551	3.577257
1	-4.778571	-4.221119	3.861292
1	-9.277882	-4.673159	2.376290
1	1.714146	0.133257	-2.094868
1	0.895337	4.203331	-3.244644
1	4.036077	0.386622	-2.870630
1	3.221061	4.457614	-3.993948
1	4.817798	2.554643	-3.814800
1	-2.306695	-0.590379	-1.869178
1	0.045201	1.454786	-4.833088
1	-3.036594	-2.216796	-3.574072
1	-0.686485	-0.165504	-6.536957
1	-2.234722	-2.020078	-5.916113
1	-0.428547	4.757200	-1.468517
1	-2.978725	2.094709	-3.692441
1	-1.868769	6.641015	-2.062642
1	-4.434885	3.983114	-4.270281
1	-3.906324	6.277954	-3.456712
1	-2.116372	-2.613800	-0.899603
1	1.841258	-4.051732	-1.695173
1	-3.079238	-4.681653	-1.891597
1	0.899238	-6.105210	-2.721000
1	-1.565746	-6.435003	-2.807941
1	3.640094	-1.032466	2.735832
1	5.576964	2.991876	1.160214
1	5.509633	-0.965230	-0.556673
1	6.870297	3.803833	-0.740462
1	6.840247	-0.148047	-2.452854
1	4.104599	2.417183	2.486649
1	3.542444	1.034146	3.380932
1	6.509204	1.826737	3.147213
1	5.468544	2.113464	4.552900
1	5.878368	0.456927	4.067956
1	0.785110	-0.938221	1.832065
1	0.229860	0.315583	3.031550
1	1.680130	2.005117	2.020625
1	3.063762	1.624713	0.072748
1	2.594248	-0.151540	0.034104
6	1.955816	-3.453702	3.114936
6	2.162617	-2.614627	5.428537
6	-0.045278	-2.498988	4.284351

1	8.394733	-2.967398	1.918971
1	6.090343	-3.198424	1.135569
1	8.873631	0.612775	-0.416868
1	9.823851	-1.077125	1.131816
1	6.991067	1.491426	-1.722066
1	4.579823	1.392331	-2.317921
1	6.091730	-3.450315	-1.872070
1	1.076500	-3.616576	1.331708
1	6.794007	-5.714812	-2.494993
1	3.532362	-7.389664	-0.244845
1	1.931682	-5.924993	0.883219
1	5.537767	-7.706095	-1.666889
1	2.386582	4.718921	1.812493
1	-1.367714	2.944035	2.963314
1	1.364004	6.946948	1.923826
1	-2.383951	5.182624	3.094440
1	-1.025340	7.208162	2.578831
1	0.063039	2.665548	4.912789
1	1.597934	-0.792655	2.852467
1	-0.172946	1.335234	6.969038
1	1.411892	-2.109776	4.934395
1	0.519657	-1.055110	7.006329
1	2.961072	3.740944	3.916592
1	3.516612	0.317886	1.360953
1	5.353879	3.706521	4.480229
1	5.901952	0.256126	1.968239
1	6.850110	1.969777	3.504550
1	-2.278625	2.577454	-0.695632
1	-1.749960	-0.453879	-0.923763
1	-1.487447	0.852549	-2.152122
1	-1.925637	-0.186262	3.661820
1	-1.456651	-4.152678	2.106187
1	-2.844292	-1.113016	5.775609
1	-2.245249	-5.101921	4.270312
1	-2.978532	-3.576929	6.093983
1	-4.330984	-1.108000	1.372667
1	-4.377532	0.549335	-2.002016
1	-6.267104	3.185554	0.837137
1	-4.764466	2.203361	-3.783398
1	-6.651132	4.824908	-0.928612
1	-4.832663	0.483395	2.773581
1	-5.308425	2.109355	2.353612
1	-7.045757	-0.405881	2.024468
1	-7.259186	0.839146	3.270979
1	-7.568139	1.217882	1.566536
1	-3.122583	2.303792	1.502529
1	-2.553809	0.573191	1.611807
6	-1.420082	-3.713932	-2.699515
6	0.261842	-3.027267	-4.392605
6	0.851453	-4.698874	-2.656058
6	0.939874	-4.366321	-4.138418
1	0.186139	-2.832462	-5.468642
1	1.232190	-5.706799	-2.463707
1	0.452013	-5.152449	-4.727057
6	-5.588261	-3.671463	0.506850
6	-7.665258	-3.195178	1.776304
6	-7.809676	-3.699792	-0.644513
6	-8.282770	-2.762060	0.455641
1	-8.046558	-4.182890	2.079014
1	-8.293058	-4.683769	-0.547515
1	-9.374656	-2.781937	0.518477
1	1.438854	-3.984938	-2.069721
1	1.989022	-4.313107	-4.445313
1	0.839234	-2.220902	-3.927031
1	-8.079749	-3.302500	-1.629052
1	-7.971928	-1.735979	0.229969
1	-7.918441	-2.490574	2.574007
7	-6.355131	-3.863130	-0.609353
7	-6.208847	-3.224166	1.649177
7	-1.095787	-3.027534	-3.841097
7	-0.549826	-4.655143	-2.223825
6	-0.864286	-5.265869	-0.936760
1	-0.689001	-4.567549	-0.111774
1	-1.910392	-5.575431	-0.912189
1	-0.231216	-6.147059	-0.807322
6	-1.927436	-1.892938	-4.216696
1	-1.886732	-1.763540	-5.302977
1	-2.958466	-2.071815	-3.916148
1	-1.583506	-0.965599	-3.740253
6	-5.762023	-4.402401	-1.824990

1	-6.230593	-5.363272	-2.077634
1	-5.922963	-3.710883	-2.660751
1	-4.692054	-4.543796	-1.695276
6	-5.446919	-3.151431	2.887975
1	-5.600997	-4.045967	3.507952
1	-4.387700	-3.065480	2.662903
1	-5.768785	-2.275569	3.460000
15	0.843828	2.633113	-1.453645
6	2.236079	3.731769	-0.953958
6	2.241572	5.123626	-1.142468
6	3.372209	3.117419	-0.417454
6	3.356342	5.877150	-0.771096
1	1.382893	5.625255	-1.572733
6	4.487719	3.868517	-0.047631
1	3.381870	2.046359	-0.280532
6	4.478688	5.254048	-0.216548
1	3.345294	6.953928	-0.914642
1	5.348112	3.365907	0.383214
1	5.340583	5.845999	0.078326
6	-0.517685	3.817289	-1.835904
6	-1.210295	3.782216	-3.053888
6	-0.937965	4.711689	-0.836080
6	-2.301882	4.629714	-3.267154
1	-0.909261	3.094805	-3.836963
6	-2.019550	5.561508	-1.056217
1	-0.426111	4.734775	0.117275
6	-2.707732	5.520724	-2.273203
1	-2.838435	4.590538	-4.210494
1	-2.327507	6.247311	-0.272233
1	-3.558790	6.172542	-2.445695
6	1.369745	2.099906	-3.146315
6	2.185360	2.940183	-3.922643
6	0.896995	0.905652	-3.708357
6	2.522836	2.590075	-5.230675
1	2.562051	3.870894	-3.512508
6	1.226369	0.565102	-5.021811
1	0.303238	0.217888	-3.120646
6	2.040151	1.402948	-5.785850
1	3.160812	3.247886	-5.814259
1	0.853201	-0.363736	-5.440821
1	2.300190	1.131426	-6.805173
6	-5.893863	4.616770	-3.498764
7	-5.997955	5.429851	-4.328251

-----End of Electronic Supplementary Informtion-----