

Hydrogen Bonding and Non-Covalent Interactions Assisted Nickel (0) Catalysed Reversible Alkenyl Functional Group Swapping: A Computational Study

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1. Different Possibilities studied for the Identification of Potential Catalytic Active Species

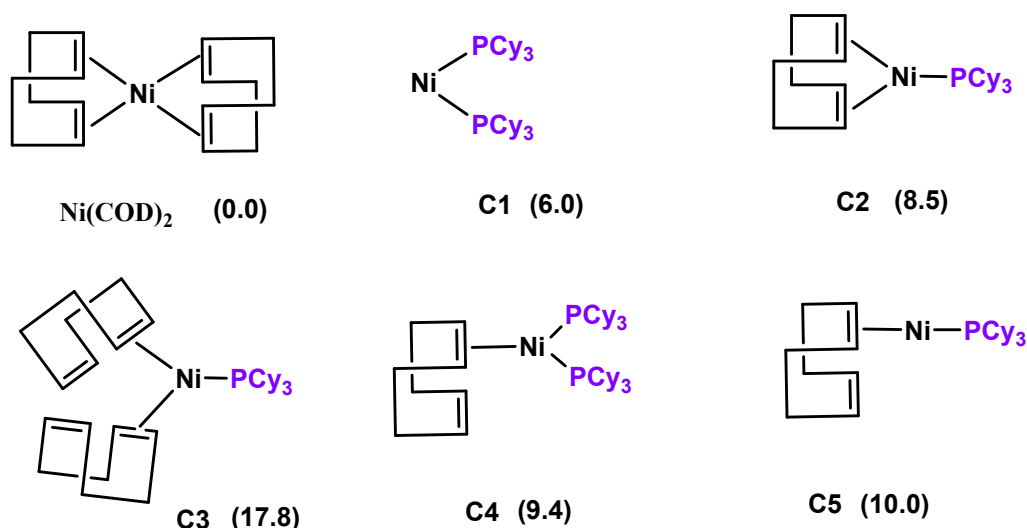


Fig. S1 Various ligand combinations around Ni considered for the identification of potential active catalyst and the corresponding relative Gibbs free energies obtained at the SMD(hexane)/ B3LYP-D3/SDD(Ni),6-31G** level of theory. The energies are calculated with Ni(COD)₂ as the reference.

2. Energetic span model

We have calculated the energy span using the energetic span model developed by Shaik and Kozuch which convey the turnover frequency (TOF) of a catalytic cycle using energetic of various stationary points. In the catalytic cycle, two states can be identified such as transition state and intermediate. The TOF of the catalytic cycle can be determined by these states. Therefore, the TOF of the catalytic cycle depends on the TOF-determining intermediate (TDI) and TOF-determining transition state (TDTS). The energy span δE can be calculated using the following equations:

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

Table S1. The Calculation of Energetic Span (δE , in kcal/mol) using Different Combination of TDI and TDTS (highlighted ones give the maximum energetic span)

TDI	TDTS	δE
-----	------	------------

6	[3-4]‡	18.0
	[5-6]‡	10.2
	[8a-9a]‡	17.7
	[10a-11a]‡	19.0
	[12-13]‡	5.2
	[14-15]‡	31.6
12	[3-4]‡	19.6
	[5-6]‡	11.8
	[8a-9a]‡	2.3
	[10a-11a]‡	2.9
	[12-13]‡	6.8
	[14-15]‡	33.2
13	[3-4]‡	18.7
	[5-6]‡	10.9
	[8a-9a]‡	1.0
	[10a-11a]‡	2.3
	[12-13]‡	11.5
	[14-15]‡	32.3
15	[3-4]‡	13.1
	[5-6]‡	5.3
	[8a-9a]‡	-4.6
	[10a-11a]‡	-3.6
	[12-13]‡	-17.1
	[14-15]‡	9.3

3. Activation Strain Analysis

Following literature precedence, the activation barrier (ΔE^\ddagger) is splitting into (a) destabilizing distortion energy in the reactants (ΔE_d^\ddagger) and (b) stabilizing interaction energy between parallel distorted reactants (ΔE_i^\ddagger). The activation barrier can therefore be written as sum of the distortion and interaction energies, $\Delta E^\ddagger = \Delta E_d^\ddagger + \Delta E_i^\ddagger$. Distortion energy is calculated as the difference between the energies of the ground state geometries of undistorted reactants and the corresponding distorted structure in the transition state.

For this analysis, first we have access the reaction profile by performing the IRC calculations. After this single-point computations are done along the reaction coordinate. We have taken seven different points on the reaction coordinate to perform these calculations (**Figure S3**).

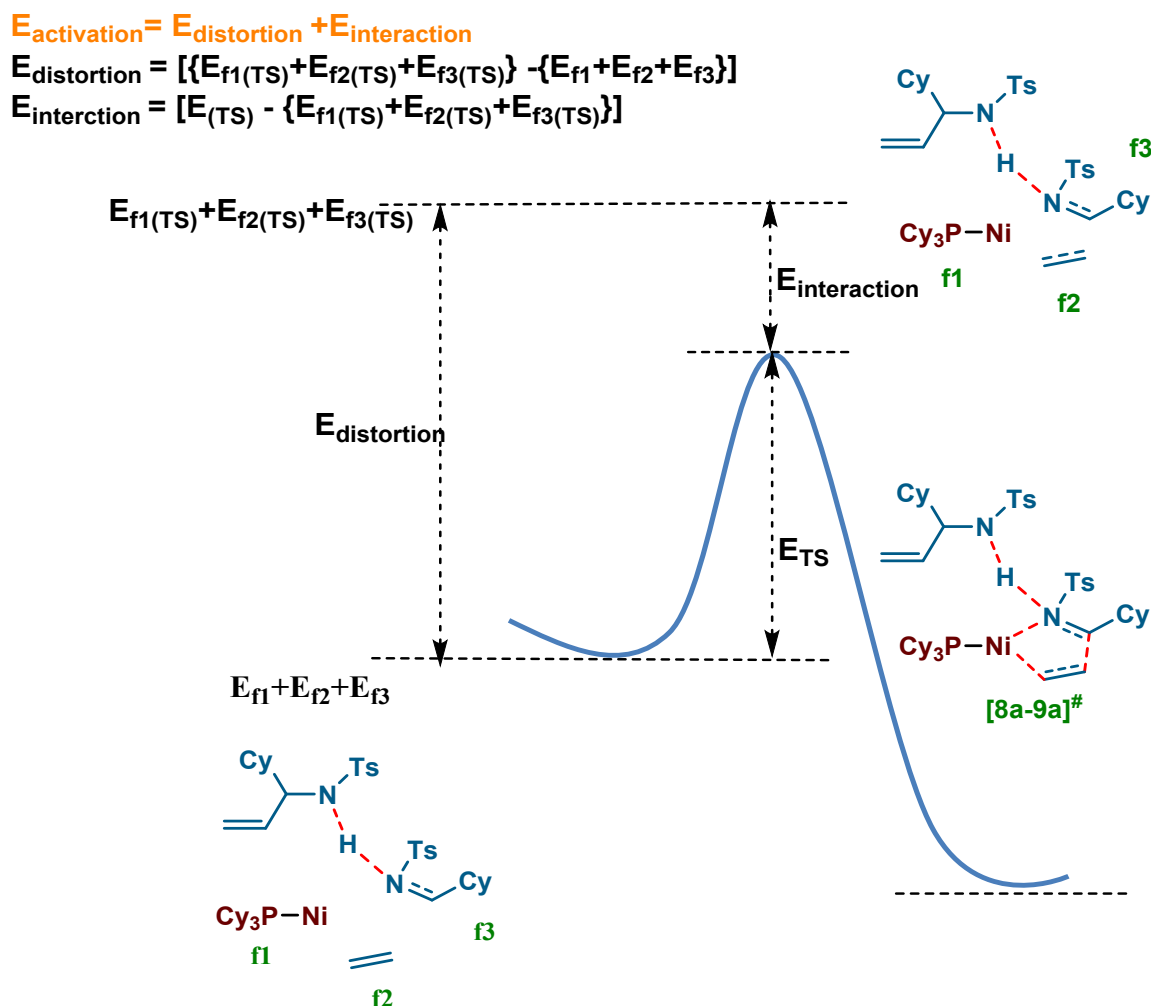


Fig. S2 Illustration of interaction and distortion energies in the Activation Strain Analysis for C-C bond cleavage step leading to the formation of nickel complex coordinated by an alkene and imine via the five member transition state.

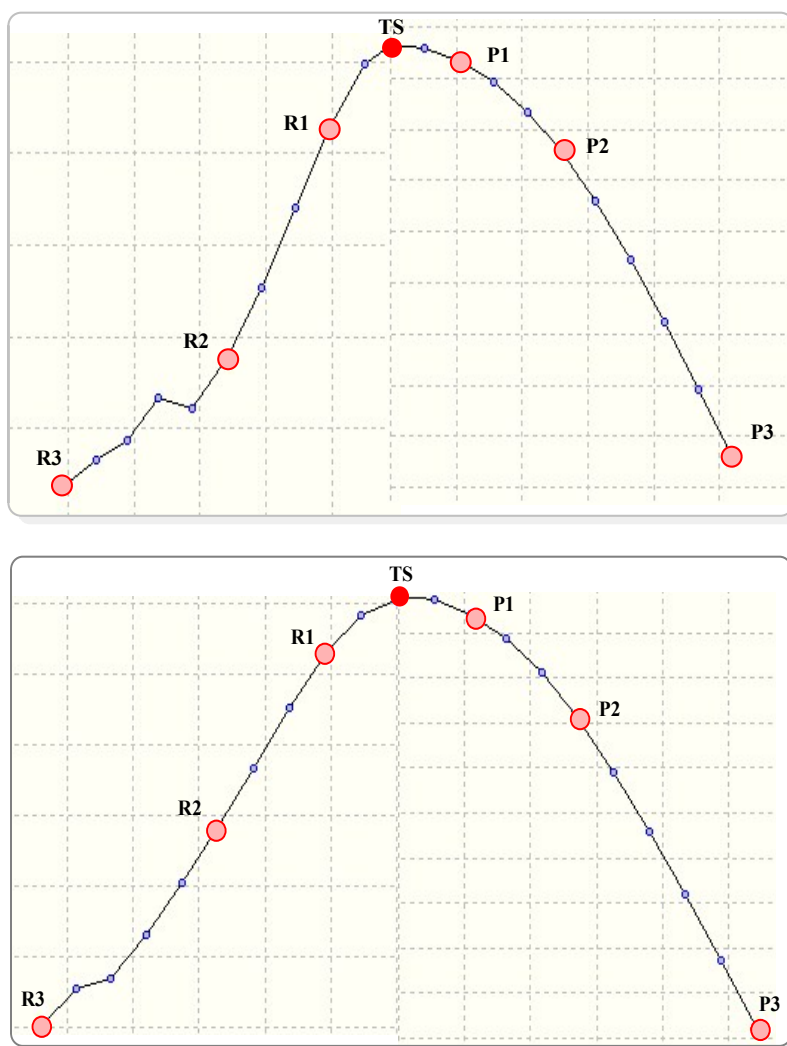


Fig. S3 The reaction profile along the intrinsic reaction coordinate (IRC) trajectory starting from **[8a-9a]‡** (shown above) and **[8-9]‡**(shown below) as obtained at the SMD(Hexane)/B3LYP-D3/SDD(Ni),6-31G** level of theory for the C-C bond cleavage step.

Table S2. Relative Distortion and Interaction Energies (in kcal/mol) for the C-C bond cleavage Step at the SMD(Hexane)/B3LYP-D3/SDD(Ni),6-31G** Level of Theory. The IRC points toward the product side (**P1, P2,...**) and the reactant side (**R1, R2, ...**) along the reaction coordinate are shown in Figure S3

Transition states (RE)	Distortion Energy ($E_{\text{distortion}}$)			Total Distortion Energy	Interaction Energy ($E_{\text{interaction}}$)	Activation Strain Energy (E_{act})
	f1	f2	f3			
	f1	f2	f3	f1+f2+f3		

[8a-9a]‡	3.15	38.63	42.60	84.39	-157.41	-73.02
P1	3.33	33.29	38.82	75.46	-148.58	-73.11
P2	3.67	26.09	33.54	63.31	-136.99	-73.67
P3	4.44	17.35	27.45	49.25	-124.80	-75.55
R1	3.01	44.08	46.31	93.41	-166.50	-73.08
R2	2.91	50.19	49.94	103.05	-176.29	-73.24
R3	2.86	54.31	52.44	109.61	-182.94	-73.32
[8-9]‡	1.88	36.41	40.05	78.34	-141.02	-62.67
P1	2.08	31.02	35.97	69.09	-131.90	-62.80
P2	2.49	23.95	30.48	56.92	-120.45	-63.52
P3	3.35	15.99	24.47	43.82	-109.51	-65.68
R1	1.69	42.02	44.21	87.93	-150.70	-62.77
R2	1.51	48.94	48.87	99.33	-162.42	-63.08
R3	1.40	56.26	53.69	111.36	-174.79	-63.43

It is evident from the data given in Table S4 that the interaction energy is more stabilizing for the transition state **[8a-9a]‡** as compared to that in **[8-9]‡**. This can be mainly attributed to the larger number and more effective non-covalent interactions and hydrogen bonding present (O...H-C, C-H... π and N...H) in **[8a-9a]‡** as shown in (AIM analysis).

For calculating the distortion energy, the overall system is divided into three fragments, f1, f2 and f3. In both the transition states f1 and f2 are same fragment, but f3 is different. In the transition state **[8a-9a]‡** the one extra tosylamine molecule stabilized the transition state. Here we explain on the basis of strain model, out of three fragments which is more destabilized the distortion energy. It can be noted from Table S2 that there is not much difference in the distortion energy of fragment f1 and f2 for both the transition states. Therefore, it is the fragment f3 that is contributing appreciably to the destabilizing distortion energy. A closer look at the transition state structures reveals that the distortion originates mainly from the five membered nickelacycle (tosylamine molecule).

Table S3. Gibbs free energies (ΔG in kcal/mol) of intermediates and transition states at (i) SMD(hexane)/M06/SDD(Ni),6-311++G**//SMD(hexane)/B3LYP-D3/SDD(Ni),6-31G** and (ii) SMD(hexane)/M06/LANL2DZ(Ni),6-311++G**//SMD(hexane)/B3LYP-D3/SDD(Ni),6-31G** level of theory.

Name	M06/SDD(Ni),6-	M06/LANL2DZ(Ni),6-
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	311++G**(SMD model)	311++G*** (SMD model)
C1	0	0
3	3.3	2.9
[3-4]‡	26.5	26.5
4	18.1	20.2
5	1.5	4.3
[5-6]‡	22.7	25.6
6	-2.6	0.1
7	3.9	6.2
8a	8.5	12.6
[8a-9a]‡	8.6	12.4
9a	-5.2	-2.4
10a	-2.9	0.1
[10a-11a]‡	10.8	13.9
11a	11.0	14.4
12	-2.9	-0.6
[12-13]‡	5.7	7.9
13	0.3	2.8
14	4.8	6.7
[14-15]‡	31.1	33.0
15	4.4	7.0

The single point calculation at the level of theory M06/SDD(Ni),6-311++G** and (ii) M06/LANL2DZ (Ni),6-311++G** with the SMD solvation model, obtained the most of transition states have the higher relative free energy then compare to the optimization at SMD(hexane)/B3LYP-D3/SDD(Ni),6-31G** level of theory.

Table S4. Gibbs Free Energies of Various Species (in hartree) Involved in the Computation of the Overall Free Energy Change of the Reaction Obtained at the SMD(hexane)/B3LYPD3/SDD(Ni),6-31G** Level of Theory

Species	Gibbs free energy
R1(Styrene)	-309.570076
R2(tosylamine)	-1226.625072
Alkene	-78.565223
1,5-Cyclooctadiene (COD)	-311.913603
PCy ₃	-1046.843131
P1(Product)	-1457.629202

Optimized Cartesian Coordinates of Various Reactants, Products, Intermediates and Transition States

The Optimized Coordinates of all the Stationary Points obtained at the SMD(hexane)/B3LYPD3/

6-31G** Level of Theory

Ni (COD)₂

Number of imaginary frequencies : 0
 The smallest frequencies are : 80.2690 100.7381 114.4623 cm(-1)

Electronic energy : HF=-795.1503473
 Zero-point correction= 0.364853
 (Hartree/Particle)
 Thermal correction to Energy= 0.381205
 Thermal correction to Enthalpy= 0.382149
 Thermal correction to Gibbs Free Energy= 0.323461
 Sum of electronic and zero-point Energies= -794.785494
 Sum of electronic and thermal Energies= -794.769142
 Sum of electronic and thermal Enthalpies= -794.768198
 Sum of electronic and thermal Free Energies= -794.826886

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 Cartesian Coordinates

6	-2.609679	-0.584859	1.419489
6	-2.210865	-1.837537	0.606821
1	-2.863509	-0.891974	2.440254
1	-1.626262	-2.500999	1.255455
1	-3.111021	-2.406151	0.324133
6	-2.211543	1.837157	-0.606283
1	-1.626899	2.500745	-1.254727
1	-3.111892	2.405547	-0.323780
6	-2.609695	0.584341	-1.419009
1	-3.520862	0.139367	-1.009063
1	-2.863748	0.891472	-2.439720
6	-1.359571	1.532748	0.609393
1	-0.752809	2.367488	0.956491
6	-1.504346	0.462845	1.476483
1	-0.975886	0.530520	2.423998
6	-1.503672	-0.462750	-1.476024
1	-0.976438	-0.531192	-2.424198
6	-1.358565	-1.532790	-0.608559
1	-0.752749	-2.368011	-0.956291
1	-3.521057	-0.140376	1.009496
6	2.609219	0.584680	1.419798
6	2.210367	1.837573	0.607462
1	2.862973	0.891537	2.440662
1	1.625547	2.500770	1.256171
1	3.110517	2.406402	0.325168
6	2.211995	-1.836779	-0.606529
1	1.627638	-2.500266	-1.255343
1	3.112412	-2.405073	-0.324044
6	2.610111	-0.583593	-1.418702
1	3.521010	-0.138499	-1.008261
1	2.864621	-0.890332	-2.439418
6	1.359611	-1.532943	0.609010

1	0.753157	-2.368039	0.955811
6	1.503989	-0.463117	1.476357
1	0.975120	-0.531074	2.423621
6	1.503858	0.463269	-1.475812
1	0.976769	0.531759	-2.424062
6	1.358432	1.533102	-0.608216
1	0.752327	2.368179	-0.955744
1	3.520658	0.140396	1.009703
28	0.000090	-0.000367	-0.001442

C1

Number of imaginary frequencies : 0
The smallest frequencies are : 18.0690 18.9994 29.5530 cm(-1)

Electronic energy : HF=-2265.5754782
Zero-point correction= 0.973830
(Hartree/Particle)
Thermal correction to Energy= 1.015544
Thermal correction to Enthalpy= 1.016488
Thermal correction to Gibbs Free Energy= 0.899245
Sum of electronic and zero-point Energies= -2264.601648
Sum of electronic and thermal Energies= -2264.559934
Sum of electronic and thermal Enthalpies= -2264.558990
Sum of electronic and thermal Free Energies= -2264.676234

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Cartesian Coordinates
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28	-0.000012	-0.258778	-0.000518
15	2.126491	-0.138749	-0.139418
6	2.827270	-1.210295	-1.515289
6	4.349839	-1.191054	-1.735336
6	2.313264	-2.657838	-1.371169
1	2.345483	-0.795001	-2.411019
6	4.744995	-2.044738	-2.953005
1	4.851192	-1.593619	-0.845317
1	4.711488	-0.164252	-1.865375
6	2.712991	-3.514217	-2.582789
1	2.731575	-3.110687	-0.460755
1	1.223760	-2.643453	-1.242119
6	4.230672	-3.485324	-2.817057
1	5.834765	-2.038097	-3.079450
1	4.320013	-1.592925	-3.860732
1	2.367963	-4.546245	-2.444616
1	2.201854	-3.128654	-3.476616
1	4.491654	-4.069230	-3.708223
1	4.734636	-3.967002	-1.966415
6	3.124085	-0.650550	1.384183
6	4.484534	0.040802	1.605761
6	2.257307	-0.552590	2.658821
1	3.319204	-1.718940	1.210735
6	5.214286	-0.548829	2.825194
1	4.327681	1.112876	1.779081
1	5.117677	-0.041188	0.717397
6	2.986670	-1.128997	3.882105
1	2.005231	0.500026	2.847581
1	1.302744	-1.065388	2.491293

6	4.351798	-0.458081	4.092095
1	6.169824	-0.030954	2.975174
1	5.455787	-1.602927	2.625912
1	2.363884	-1.017526	4.778171
1	3.135193	-2.208681	3.734757
1	4.874707	-0.910760	4.943398
1	4.196874	0.600802	4.345036
6	2.716602	1.595780	-0.561121
6	2.253061	1.989482	-1.979525
6	2.150989	2.590575	0.476884
1	3.813311	1.631748	-0.528497
6	2.596967	3.449709	-2.313003
1	1.165688	1.838559	-2.044638
1	2.706539	1.331120	-2.728711
6	2.500257	4.047060	0.138194
1	1.059348	2.469586	0.504371
1	2.509643	2.345264	1.482384
6	2.023160	4.419456	-1.271798
1	2.226284	3.698456	-3.315103
1	3.690299	3.563479	-2.345421
1	2.055933	4.718590	0.883492
1	3.589372	4.185795	0.200376
1	2.304551	5.451812	-1.513173
1	0.925070	4.374638	-1.304215
15	-2.126462	-0.138769	0.139134
6	-2.826538	-1.209774	1.515768
6	-4.348976	-1.190272	1.736596
6	-2.312760	-2.657428	1.371976
1	-2.344217	-0.794146	2.411056
6	-4.743590	-2.043397	2.954831
1	-4.850843	-1.593130	0.846990
1	-4.710437	-0.163372	1.866410
6	-2.711940	-3.513255	2.584164
1	-2.731594	-3.110635	0.461981
1	-1.223324	-2.643203	1.242340
6	-4.229500	-3.484095	2.819238
1	-5.833294	-2.036570	3.081843
1	-4.318079	-1.591241	3.862143
1	-2.367100	-4.545378	2.446237
1	-2.200293	-3.127376	3.477563
1	-4.490068	-4.067584	3.710796
1	-4.733971	-3.966098	1.969080
6	-3.124466	-0.651455	-1.383927
6	-4.485044	0.039624	-1.605527
6	-2.258007	-0.554118	-2.658831
1	-3.319426	-1.719772	-1.209860
6	-5.215038	-0.550677	-2.824496
1	-4.328372	1.111631	-1.779439
1	-5.117943	-0.042011	-0.716953
6	-2.987620	-1.131199	-3.881639
1	-2.006001	0.498406	-2.848213
1	-1.303382	-1.066797	-2.491268
6	-4.352847	-0.460491	-4.091644
1	-6.170647	-0.032944	-2.974507
1	-5.456422	-1.604690	-2.624633
1	-2.365059	-1.020136	-4.777912
1	-3.136025	-2.210821	-3.733710

1	-4.875924	-0.913626	-4.942601
1	-4.198057	0.598278	-4.345140
6	-2.716781	1.595818	0.560371
6	-2.253144	1.990016	1.978589
6	-2.151446	2.590296	-0.478104
1	-3.813496	1.631607	0.527892
6	-2.597055	3.450352	2.311600
1	-1.165762	1.839160	2.043708
1	-2.706565	1.331891	2.728027
6	-2.500642	4.046884	-0.139814
1	-1.059813	2.469279	-0.505878
1	-2.510416	2.344654	-1.483409
6	-2.023357	4.419734	1.269995
1	-2.226271	3.699463	3.313568
1	-3.690388	3.564116	2.344091
1	-2.056382	4.718162	-0.885378
1	-3.589759	4.185632	-0.201895
1	-2.304727	5.452172	1.511050
1	-0.925265	4.374937	1.302308

C2

Number of imaginary frequencies : 0
 The smallest frequencies are : 33.1014 37.4770 44.1851 cm(-1)

Electronic energy : HF=-1530.3499779
 Zero-point correction= 0.666799
 (Hartree/Particle)
 Thermal correction to Energy= 0.696553
 Thermal correction to Enthalpy= 0.697497
 Thermal correction to Gibbs Free Energy= 0.607124
 Sum of electronic and zero-point Energies= -1529.683179
 Sum of electronic and thermal Energies= -1529.653425
 Sum of electronic and thermal Enthalpies= -1529.652481
 Sum of electronic and thermal Free Energies= -1529.742853

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 Cartesian Coordinates

28	1.527850	0.418333	0.344701
15	-0.571828	0.010001	-0.084995
6	-1.353464	1.487340	-0.948012
6	-2.848483	1.415661	-1.304583
6	-1.042934	2.779251	-0.162763
1	-0.781273	1.545801	-1.884360
6	-3.285966	2.660903	-2.095828
1	-3.441459	1.356734	-0.382710
1	-3.067205	0.509013	-1.880982
6	-1.486072	4.026881	-0.942951
1	-1.564730	2.759765	0.804678
1	0.031393	2.825617	0.058425
6	-2.971849	3.952086	-1.325644
1	-4.357055	2.604395	-2.325972
1	-2.756947	2.676221	-3.059504
1	-1.288979	4.930208	-0.352768
1	-0.880504	4.109123	-1.856857
1	-3.257782	4.829051	-1.918887
1	-3.580154	3.980028	-0.410096

6	-1.746134	-0.277252	1.382552
6	-2.990052	-1.157475	1.145859
6	-0.966870	-0.779052	2.615394
1	-2.102050	0.735662	1.622373
6	-3.887456	-1.198171	2.395017
1	-2.675468	-2.182300	0.909076
1	-3.566796	-0.802240	0.286477
6	-1.857901	-0.833551	3.865234
1	-0.565346	-1.781620	2.410040
1	-0.096490	-0.135615	2.783932
6	-3.112629	-1.686205	3.627151
1	-4.756590	-1.841978	2.210245
1	-4.279477	-0.189260	2.588960
1	-1.287625	-1.222228	4.717930
1	-2.162969	0.189140	4.131223
1	-3.758298	-1.675518	4.513647
1	-2.811828	-2.732067	3.469597
6	-0.918280	-1.432429	-1.238165
6	-0.437924	-1.152346	-2.676557
6	-0.228512	-2.696811	-0.682760
1	-2.000003	-1.611196	-1.273230
6	-0.643167	-2.372859	-3.588798
1	0.627954	-0.890799	-2.654133
1	-0.965449	-0.289975	-3.098127
6	-0.435747	-3.914091	-1.595691
1	0.845367	-2.488436	-0.584616
1	-0.590829	-2.919888	0.327045
6	0.042793	-3.624388	-3.024908
1	-0.267424	-2.150682	-4.595092
1	-1.720233	-2.567945	-3.692304
1	0.090273	-4.783954	-1.183440
1	-1.504190	-4.173167	-1.617433
1	-0.143504	-4.487958	-3.674678
1	1.130728	-3.465398	-3.014821
6	4.064596	-0.618388	-0.652300
6	3.588377	-1.494370	0.549851
1	4.320823	-1.291035	-1.478555
1	3.010420	-2.339397	0.158105
1	4.474309	-1.933707	1.034314
6	3.704375	2.362292	0.412749
1	3.113914	3.212946	0.775816
1	4.635585	2.792392	0.010266
6	4.034467	1.442950	1.619031
1	4.932893	0.855797	1.410042
1	4.284622	2.074982	2.479472
6	2.895679	1.687621	-0.676450
1	2.278204	2.360839	-1.273317
6	3.034417	0.390314	-1.135250
1	2.519195	0.134405	-2.059677
6	2.878905	0.527121	1.983299
1	2.257326	0.862693	2.815766
6	2.710839	-0.782064	1.561360
1	2.037580	-1.427238	2.124426
1	4.991632	-0.102355	-0.388048

C3

Number of imaginary frequencies : 0
The smallest frequencies are : 19.4733 21.9885 32.2841 cm(-1)

Electronic energy : HF=-1842.4254601
Zero-point correction= 0.853133
(Hartree/Particle)
Thermal correction to Energy= 0.891129
Thermal correction to Enthalpy= 0.892073
Thermal correction to Gibbs Free Energy= 0.783847
Sum of electronic and zero-point Energies= -1841.572327
Sum of electronic and thermal Energies= -1841.534331
Sum of electronic and thermal Enthalpies= -1841.533387
Sum of electronic and thermal Free Energies= -1841.641613

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

28	-0.818749	0.532489	-0.760077
15	1.213099	-0.364182	-0.117371
6	1.723555	-1.864394	-1.174230
6	2.846231	-2.765105	-0.625849
6	0.520463	-2.713206	-1.612721
1	2.098288	-1.385310	-2.087537
6	3.249812	-3.853396	-1.635161
1	2.494874	-3.259217	0.288351
1	3.726986	-2.174348	-0.353854
6	0.918133	-3.834518	-2.587142
1	0.023696	-3.148913	-0.733514
1	-0.200746	-2.056384	-2.101708
6	2.043551	-4.713822	-2.030060
1	4.045792	-4.476561	-1.209360
1	3.667863	-3.378344	-2.534261
1	0.037264	-4.441195	-2.830630
1	1.255330	-3.378885	-3.529235
1	2.335406	-5.474944	-2.763745
1	1.679501	-5.252629	-1.143278
6	1.139700	-1.018618	1.663961
6	2.439739	-1.371826	2.420610
6	0.304157	-0.074521	2.558473
1	0.565183	-1.950643	1.546026
6	2.111731	-2.053248	3.762949
1	3.008011	-0.453916	2.617142
1	3.093499	-2.021145	1.838172
6	-0.060473	-0.748555	3.887902
1	0.891022	0.827171	2.773515
1	-0.584584	0.267909	2.027602
6	1.202971	-1.185142	4.644980
1	3.040837	-2.291503	4.295422
1	1.612474	-3.011904	3.560440
1	-0.659045	-0.067573	4.505687
1	-0.690561	-1.627025	3.685994
1	0.937426	-1.722511	5.563361
1	1.757803	-0.288086	4.954900
6	2.869207	0.560765	-0.133938
6	3.338858	0.928234	-1.558832
6	2.852562	1.805528	0.773789
1	3.608655	-0.135980	0.282234

6	4.674634	1.690694	-1.545917
1	2.571951	1.535340	-2.053673
1	3.460755	0.027999	-2.168723
6	4.201488	2.540350	0.778520
1	2.079296	2.490921	0.426114
1	2.585003	1.527694	1.796736
6	4.623559	2.929102	-0.643380
1	4.947241	1.971726	-2.570498
1	5.465762	1.017752	-1.184389
1	4.134700	3.429295	1.417694
1	4.970827	1.890913	1.220803
1	5.596674	3.434730	-0.632897
1	3.898461	3.647092	-1.052338
6	0.345825	3.344597	-1.499124
6	0.089713	4.064719	-0.143430
1	1.386646	3.011016	-1.509471
1	1.035987	4.510183	0.186274
1	-0.584929	4.909056	-0.320137
6	-3.030619	2.642973	-1.171496
1	-3.794867	1.903843	-0.911057
1	-3.508818	3.282364	-1.931253
6	-2.795621	3.515779	0.085711
1	-2.474555	4.513134	-0.233291
1	-3.764141	3.655744	0.580951
6	-1.882217	1.876375	-1.824008
1	-2.276510	1.300777	-2.666019
6	-0.491247	2.144189	-1.929305
1	-0.042969	1.715539	-2.832893
6	-1.793800	2.959839	1.059320
1	-2.155755	2.318513	1.858473
6	-0.481428	3.206204	0.953459
1	0.203583	2.759647	1.667502
1	0.286902	4.111842	-2.288041
6	-5.623914	-1.107267	1.025148
6	-4.323143	-1.314128	1.769803
6	-3.770161	-0.777338	-1.666498
6	-3.189524	-0.313218	1.369335
6	-2.469387	-1.071343	-0.957213
6	-2.217622	-0.922096	0.383821
1	-3.956631	-2.337964	1.612671
1	-3.637131	0.594943	0.957502
1	-4.155330	0.212211	-1.423553
1	-6.447500	-0.707857	1.616683
1	-4.518526	-1.221677	2.843574
1	-3.590108	-0.789294	-2.746930
1	-2.648022	-0.014200	2.272062
1	-1.851857	-1.782505	-1.491954
1	-1.457623	-1.561382	0.825261
6	-5.855877	-1.332339	-0.273965
1	-6.851361	-1.098874	-0.651124
6	-4.866470	-1.832676	-1.303283
1	-4.376121	-2.748470	-0.946266
1	-5.413808	-2.110653	-2.210169

C4

Number of imaginary frequencies : 0

The smallest frequencies are : 12.1514 30.5775 35.8390 cm(-1)

Electronic energy : HF=-2577.661602
Zero-point correction= 1.158117
(Hartree/Particle)
Thermal correction to Energy= 1.207852
Thermal correction to Enthalpy= 1.208796
Thermal correction to Gibbs Free Energy= 1.077104
Sum of electronic and zero-point Energies= -2576.503485
Sum of electronic and thermal Energies= -2576.453750
Sum of electronic and thermal Enthalpies= -2576.452806
Sum of electronic and thermal Free Energies= -2576.584498

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Cartesian Coordinates
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28	0.027870	-0.859891	-0.534015
15	1.795929	0.486055	0.108448
6	2.581247	-0.383585	1.595653
6	3.692780	0.249173	2.458268
6	1.505063	-0.971712	2.533288
1	3.042374	-1.232524	1.082323
6	4.335916	-0.828331	3.350915
1	3.261821	1.017199	3.110227
1	4.455285	0.742644	1.848322
6	2.105688	-2.039064	3.461150
1	1.073745	-0.163792	3.139791
1	0.681674	-1.396821	1.948698
6	3.292278	-1.487134	4.265464
1	5.140165	-0.385507	3.951228
1	4.802653	-1.593600	2.714466
1	1.333201	-2.424137	4.138371
1	2.438758	-2.890064	2.851349
1	3.754108	-2.283842	4.860987
1	2.923165	-0.735621	4.978690
6	1.488036	2.296624	0.601981
6	2.619646	3.119655	1.254392
6	0.961017	3.070664	-0.624905
1	0.676643	2.225165	1.331389
6	2.145573	4.539850	1.619055
1	3.471369	3.196399	0.565927
1	2.988464	2.636890	2.156896
6	0.460677	4.474524	-0.256871
1	1.773190	3.178399	-1.355432
1	0.175457	2.498863	-1.117921
6	1.571327	5.292816	0.413230
1	2.978648	5.102001	2.059121
1	1.374001	4.467612	2.398997
1	0.089677	4.986527	-1.153368
1	-0.390208	4.389366	0.432523
1	1.196081	6.276871	0.719543
1	2.373664	5.474405	-0.316245
6	3.238175	0.758966	-1.106722
6	4.439698	-0.199920	-0.985902
6	2.716944	0.758949	-2.560677
1	3.620113	1.765352	-0.893613
6	5.546046	0.163934	-1.992039
1	4.114165	-1.227715	-1.169713

1	4.858852	-0.179300	0.023187
6	3.820320	1.141221	-3.557976
1	2.344782	-0.240766	-2.798423
1	1.860322	1.431167	-2.668314
6	5.023586	0.197184	-3.434363
1	6.375153	-0.548866	-1.901438
1	5.953039	1.152385	-1.733947
1	3.422518	1.122631	-4.580132
1	4.146486	2.174223	-3.366172
1	5.822845	0.496404	-4.123396
1	4.714356	-0.815722	-3.729357
15	-1.998693	0.095326	-0.082300
6	-2.074348	1.654036	0.993951
6	-3.416286	2.408382	1.067307
6	-1.564076	1.357985	2.419370
1	-1.349551	2.324136	0.522870
6	-3.289506	3.698422	1.896049
1	-4.173937	1.767813	1.535234
1	-3.782953	2.654247	0.065486
6	-1.439768	2.640138	3.258044
1	-2.258167	0.676829	2.929990
1	-0.606105	0.834650	2.370439
6	-2.766850	3.408932	3.309619
1	-4.260201	4.207131	1.944332
1	-2.600010	4.387551	1.388152
1	-1.099538	2.392348	4.271101
1	-0.669235	3.287692	2.817921
1	-2.646463	4.342468	3.872426
1	-3.511063	2.807637	3.851409
6	-3.426219	-0.882084	0.728774
6	-4.856409	-0.656160	0.191475
6	-3.135158	-2.386558	0.789977
1	-3.414920	-0.515598	1.763725
6	-5.892225	-1.389880	1.062470
1	-4.929540	-1.034365	-0.835961
1	-5.107566	0.406900	0.151543
6	-4.158673	-3.132983	1.656967
1	-3.161843	-2.789938	-0.228167
1	-2.120485	-2.553790	1.158733
6	-5.590734	-2.891383	1.161421
1	-6.898801	-1.227733	0.657276
1	-5.886529	-0.951270	2.071060
1	-3.932300	-4.206513	1.664281
1	-4.071086	-2.786585	2.697199
1	-6.316232	-3.384774	1.819654
1	-5.707100	-3.346628	0.167251
6	-2.775448	0.710434	-1.697478
6	-2.050437	1.926629	-2.302766
6	-2.860031	-0.402810	-2.759235
1	-3.797979	1.024574	-1.459910
6	-2.759907	2.426305	-3.572747
1	-1.021435	1.637449	-2.552933
1	-1.987549	2.747241	-1.581269
6	-3.590899	0.080785	-4.021814
1	-1.840290	-0.702670	-3.027884
1	-3.350759	-1.295236	-2.356111
6	-2.899516	1.313387	-4.619484

1	-2.213119	3.280392	-3.991225
1	-3.759312	2.795543	-3.300963
1	-3.634186	-0.728813	-4.760564
1	-4.630805	0.332336	-3.767544
1	-3.449907	1.678103	-5.495140
1	-1.899096	1.024795	-4.972269
6	2.628127	-3.431161	-0.363642
6	2.095288	-3.005084	-1.763894
1	2.212944	-2.727391	0.359313
1	2.880332	-2.428421	-2.264475
1	1.964088	-3.910958	-2.376385
6	-0.077678	-4.256191	0.628346
1	0.222388	-3.290579	1.052458
1	-0.831218	-4.673022	1.305096
6	-0.716559	-3.992711	-0.769793
1	-0.349908	-4.770044	-1.457316
1	-1.793756	-4.158678	-0.699814
6	1.100945	-5.191958	0.554366
1	0.933016	-6.231049	0.836672
6	2.297456	-4.832823	0.076327
1	3.079675	-5.585773	-0.016906
6	-0.475937	-2.634263	-1.430216
1	-1.290027	-2.404531	-2.114213
6	0.811129	-2.176398	-1.824924
1	0.796704	-1.562598	-2.734053
1	3.716557	-3.303668	-0.339381

C5

Number of imaginary frequencies : 0
 The smallest frequencies are : 14.3059 23.0985 29.7134 cm(-1)

Electronic energy : HF=-1530.3455085
 Zero-point correction= 0.667536
 (Hartree/Particle)
 Thermal correction to Energy= 0.697565
 Thermal correction to Enthalpy= 0.698510
 Thermal correction to Gibbs Free Energy= 0.605141
 Sum of electronic and zero-point Energies= -1529.677973
 Sum of electronic and thermal Energies= -1529.647943
 Sum of electronic and thermal Enthalpies= -1529.646999
 Sum of electronic and thermal Free Energies= -1529.740368

.....
 Cartesian Coordinates

28	-1.066789	-0.161614	-1.212551
15	0.776480	0.092595	-0.089710
6	2.284668	0.307002	-1.185859
6	3.641545	0.507990	-0.488203
6	2.363003	-0.839728	-2.215342
1	2.048222	1.219601	-1.749916
6	4.759251	0.760360	-1.514646
1	3.889556	-0.392148	0.089334
1	3.594685	1.339649	0.224822
6	3.484597	-0.593778	-3.236711
1	2.555595	-1.790154	-1.697418

1	1.392913	-0.943592	-2.717266
6	4.838596	-0.375101	-2.545463
1	5.720713	0.878947	-1.000093
1	4.561143	1.708355	-2.034799
1	3.544497	-1.435316	-3.937554
1	3.235178	0.295217	-3.833382
1	5.616946	-0.162103	-3.287964
1	5.136216	-1.302693	-2.035156
6	1.252482	-1.322461	1.068871
6	2.048840	-0.945910	2.334791
6	0.013998	-2.165584	1.440149
1	1.899658	-1.956956	0.446431
6	2.444124	-2.200072	3.132350
1	1.434298	-0.303475	2.977242
1	2.941969	-0.368531	2.079082
6	0.401547	-3.410051	2.252766
1	-0.684008	-1.548897	2.021302
1	-0.525576	-2.446013	0.528334
6	1.212315	-3.038045	3.502580
1	2.995351	-1.909590	4.035127
1	3.129773	-2.811030	2.527799
1	-0.499119	-3.970258	2.532438
1	1.003124	-4.077933	1.619407
1	1.513384	-3.941231	4.046865
1	0.575306	-2.456580	4.184593
6	0.751994	1.634267	0.982274
6	0.722377	2.910233	0.115602
6	-0.479302	1.596114	1.911948
1	1.661002	1.654327	1.597399
6	0.602563	4.179421	0.975044
1	-0.131075	2.849007	-0.574864
1	1.623632	2.975589	-0.503364
6	-0.588021	2.862599	2.773427
1	-1.376352	1.494734	1.287966
1	-0.453564	0.708313	2.552888
6	-0.618961	4.125226	1.902242
1	0.552054	5.061652	0.325398
1	1.512171	4.289109	1.583248
1	-1.485834	2.807720	3.401382
1	0.271351	2.913569	3.457632
1	-0.663467	5.024136	2.528928
1	-1.534298	4.119298	1.293303
6	-3.544215	1.437505	-1.203736
6	-4.488755	0.814205	-0.157532
1	-2.856978	2.123576	-0.686287
1	-4.952907	1.638089	0.398829
1	-5.302729	0.303104	-0.683927
6	-3.148140	-2.112562	-1.853867
1	-2.303575	-2.764207	-1.577704
1	-3.630762	-2.617619	-2.705047
6	-4.158069	-2.110752	-0.690315
1	-5.084981	-1.637507	-1.032977
1	-4.410113	-3.155970	-0.471532
6	-2.534454	-0.814537	-2.364056
1	-2.029018	-1.009937	-3.317485
6	-2.676514	0.563681	-2.100949
1	-2.257689	1.185355	-2.900656

6	-3.661326	-1.437032	0.560056
1	-3.115217	-2.051981	1.273470
6	-3.813684	-0.129709	0.800442
1	-3.393959	0.298570	1.708937
1	-4.157380	2.082394	-1.852870

3

Number of imaginary frequencies : 0
 The smallest frequencies are : 17.0780 20.5021 27.9226 cm(-1)

Electronic energy : HF=-3492.5575923
 Zero-point correction= 1.346105
 (Hartree/Particle)
 Thermal correction to Energy= 1.408945
 Thermal correction to Enthalpy= 1.409889
 Thermal correction to Gibbs Free Energy= 1.247684
 Sum of electronic and zero-point Energies= -3491.211487
 Sum of electronic and thermal Energies= -3491.148648
 Sum of electronic and thermal Enthalpies= -3491.147704
 Sum of electronic and thermal Free Energies= -3491.309908

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 Cartesian Coordinates

28	1.077467	-0.391644	-0.176568
15	2.290223	1.287441	0.407067
6	2.236484	2.767640	-0.752052
6	3.078389	4.002525	-0.382644
6	2.547312	2.334286	-2.200263
1	1.177475	3.058768	-0.725035
6	2.809690	5.158601	-1.362321
1	4.143739	3.739920	-0.424624
1	2.872044	4.326766	0.643368
6	2.269475	3.477403	-3.187985
1	3.605513	2.048486	-2.279761
1	1.968758	1.440967	-2.458128
6	3.065640	4.738002	-2.817426
1	3.431089	6.024698	-1.102492
1	1.763838	5.478293	-1.256124
1	2.511597	3.160878	-4.210342
1	1.194899	3.706509	-3.173983
1	2.819049	5.560556	-3.499881
1	4.138311	4.533157	-2.946894
6	4.143795	0.877159	0.462987
6	4.997510	1.637065	1.498349
6	4.389103	-0.639685	0.592005
1	4.496409	1.173093	-0.534957
6	6.489634	1.297991	1.339891
1	4.677670	1.358251	2.510752
1	4.854700	2.718274	1.412169
6	5.876296	-0.986665	0.435585
1	4.035846	-0.982980	1.573131
1	3.782299	-1.169513	-0.148543
6	6.740511	-0.213501	1.442096
1	7.076093	1.834042	2.096420
1	6.837519	1.657118	0.360365

1	6.024715	-2.067365	0.554151
1	6.197482	-0.735409	-0.586047
1	7.803694	-0.435621	1.288354
1	6.492167	-0.549669	2.459196
6	1.914226	2.010179	2.098830
6	0.618866	2.842032	2.078929
6	1.788500	0.852903	3.113816
1	2.739557	2.663695	2.406892
6	0.230718	3.335721	3.482207
1	-0.186405	2.224548	1.673238
1	0.725955	3.703512	1.410818
6	1.431808	1.364072	4.517059
1	1.000840	0.174927	2.760525
1	2.715737	0.267753	3.147970
6	0.132649	2.180388	4.488584
1	-0.724881	3.870261	3.426771
1	0.982925	4.059333	3.830594
1	1.335319	0.516613	5.207727
1	2.253421	1.988973	4.898472
1	-0.099095	2.567725	5.488726
1	-0.694035	1.523794	4.193466
15	0.603893	-2.437596	-0.604092
6	2.041932	-3.166425	-1.577956
6	1.982098	-4.659848	-1.943186
6	2.324896	-2.309044	-2.828300
1	2.891911	-3.022329	-0.898586
6	3.278465	-5.107725	-2.641838
1	1.137379	-4.836696	-2.621922
1	1.807308	-5.272277	-1.050760
6	3.612224	-2.759208	-3.535855
1	1.481693	-2.388284	-3.530181
1	2.389047	-1.254178	-2.533788
6	3.569432	-4.254260	-3.884571
1	3.211067	-6.168341	-2.914184
1	4.115951	-5.017085	-1.935308
1	3.774708	-2.159971	-4.440359
1	4.468456	-2.566880	-2.872935
1	4.512275	-4.566785	-4.349522
1	2.779019	-4.426095	-4.629573
6	-0.912075	-3.017164	-1.588226
6	-1.458212	-4.426231	-1.276593
6	-2.040324	-1.972053	-1.497724
1	-0.555147	-3.021455	-2.628871
6	-2.641117	-4.781172	-2.193677
1	-1.803094	-4.464469	-0.235908
1	-0.673622	-5.182059	-1.371586
6	-3.243390	-2.332023	-2.381249
1	-2.373026	-1.887055	-0.456606
1	-1.651463	-0.992096	-1.782863
6	-3.766003	-3.743056	-2.079679
1	-3.016461	-5.782083	-1.946439
1	-2.291533	-4.825162	-3.235288
1	-4.040962	-1.591400	-2.241362
1	-2.942534	-2.276304	-3.437665
1	-4.595239	-3.998955	-2.750883
1	-4.167626	-3.761942	-1.057022
6	0.571987	-3.455660	0.979016

6	1.912902	-3.321962	1.729895
6	-0.580982	-2.950745	1.870919
1	0.405350	-4.513969	0.739619
6	1.880240	-4.018050	3.098959
1	2.121232	-2.252300	1.864063
1	2.734427	-3.730648	1.130753
6	-0.612316	-3.645297	3.239985
1	-0.470774	-1.867973	2.008742
1	-1.539775	-3.097842	1.362964
6	0.729052	-3.496287	3.968779
1	2.841301	-3.874290	3.608778
1	1.760829	-5.101929	2.953953
1	-1.424961	-3.228079	3.847583
1	-0.833320	-4.714444	3.104452
1	0.705519	-4.023703	4.930300
1	0.898658	-2.434082	4.193287
7	-2.090523	1.334467	0.144885
6	-2.869440	1.904200	-0.977446
6	-3.309630	3.375353	-0.673203
6	-2.155976	4.322925	-0.278258
6	-4.205066	3.983737	-1.779655
1	-3.939314	3.284205	0.214842
6	-1.429640	4.982189	-1.459755
1	-1.452770	3.781852	0.358332
1	-2.586252	5.116729	0.347006
6	-3.459692	4.687008	-2.928972
1	-4.884246	3.217409	-2.178217
1	-4.846942	4.732558	-1.296922
6	-2.419364	5.682998	-2.399799
1	-0.870138	4.226940	-2.021984
1	-0.694465	5.701240	-1.076985
1	-4.189630	5.199171	-3.568257
1	-2.951052	3.955504	-3.566578
1	-1.889459	6.156250	-3.235459
1	-2.930887	6.488937	-1.852881
16	-2.784512	1.000370	1.630148
8	-1.778018	0.207271	2.348834
8	-3.292874	2.255621	2.195771
6	-4.202436	-0.058120	1.328291
6	-5.393023	0.488762	0.842603
6	-4.084662	-1.431256	1.550751
6	-6.455140	-0.360883	0.535160
1	-5.495170	1.562162	0.726141
6	-5.161401	-2.263156	1.254313
1	-3.165222	-1.827965	1.962527
6	-6.353284	-1.746677	0.722831
1	-7.379488	0.060489	0.149636
1	-5.075025	-3.331049	1.436367
6	-2.123054	1.732211	-2.277281
6	-0.835732	1.431950	-2.449865
1	-2.756158	1.868256	-3.150605
1	-0.421391	1.319783	-3.447535
1	-0.148724	1.256916	-1.624051
1	-3.804511	1.332859	-1.097863
1	-1.441635	0.579315	-0.093658
6	-7.483574	-2.668733	0.341157
1	-7.292373	-3.126885	-0.637472

1	-7.597249	-3.484477	1.062286
1	-8.436377	-2.135839	0.274720

TS [3-4]

Number of imaginary frequencies : 1
 The smallest frequencies are : -1041.7203 16.9155 23.1904 cm(-1)

Electronic energy : HF=-3492.5250306
 Zero-point correction= 1.341270
 (Hartree/Particle)
 Thermal correction to Energy= 1.403700
 Thermal correction to Enthalpy= 1.404645
 Thermal correction to Gibbs Free Energy= 1.244608
 Sum of electronic and zero-point Energies= -3491.183760
 Sum of electronic and thermal Energies= -3491.121330
 Sum of electronic and thermal Enthalpies= -3491.120386
 Sum of electronic and thermal Free Energies= -3491.280423

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 Cartesian Coordinates

28	0.317560	-0.137885	0.053648
15	2.020745	1.310776	0.570492
6	2.097338	2.763244	-0.638986
6	2.780938	4.086129	-0.219166
6	2.637461	2.328042	-2.018013
1	1.030107	2.982613	-0.775914
6	2.503210	5.182513	-1.261861
1	3.863186	3.948405	-0.142981
1	2.446862	4.418730	0.765970
6	2.383376	3.413009	-3.076500
1	3.716357	2.135916	-1.949446
1	2.174521	1.390662	-2.334944
6	2.984614	4.762619	-2.657984
1	2.989338	6.117739	-0.958023
1	1.424265	5.384069	-1.292526
1	2.793902	3.096200	-4.043523
1	1.299211	3.522582	-3.213622
1	2.737092	5.534975	-3.396324
1	4.081069	4.678064	-2.646883
6	3.780241	0.622193	0.578120
6	4.965032	1.597836	0.716769
6	3.953685	-0.524788	1.591443
1	3.837555	0.176009	-0.424668
6	6.310446	0.868827	0.537051
1	4.932445	2.079780	1.703416
1	4.903336	2.393415	-0.025999
6	5.272858	-1.277411	1.371039
1	3.967592	-0.110098	2.605889
1	3.100730	-1.201563	1.544245
6	6.467004	-0.321876	1.491820
1	7.135982	1.578536	0.670544
1	6.374606	0.507046	-0.499643
1	5.361817	-2.098234	2.093457
1	5.272242	-1.734384	0.371843
1	7.407651	-0.849606	1.292243

1	6.525643	0.048228	2.525318
6	1.729249	2.115902	2.247324
6	0.527560	3.086046	2.168509
6	1.427669	1.037152	3.315336
1	2.630606	2.675984	2.535639
6	0.183787	3.702285	3.532285
1	-0.343982	2.539068	1.804975
1	0.707214	3.890218	1.451805
6	1.089060	1.653872	4.681790
1	0.574868	0.440694	2.970616
1	2.270570	0.353185	3.428934
6	-0.096344	2.620656	4.580254
1	-0.688072	4.357190	3.418783
1	1.018623	4.336058	3.868521
1	0.868683	0.851054	5.396407
1	1.968604	2.189764	5.070345
1	-0.306842	3.075885	5.556265
1	-0.992271	2.065501	4.277805
15	0.571492	-2.192306	-0.518853
6	2.310767	-2.508122	-1.195047
6	2.782461	-3.950380	-1.458080
6	2.578061	-1.636348	-2.437194
1	2.934763	-2.103544	-0.389744
6	4.277346	-3.975609	-1.823711
1	2.217007	-4.375874	-2.295179
1	2.601163	-4.593100	-0.589821
6	4.064208	-1.656587	-2.828313
1	1.985358	-2.007708	-3.284460
1	2.244104	-0.612850	-2.243553
6	4.569266	-3.090650	-3.044537
1	4.597611	-5.006919	-2.016156
1	4.863905	-3.619983	-0.965205
1	4.224122	-1.053537	-3.730653
1	4.652243	-1.185436	-2.028640
1	5.643210	-3.087860	-3.267000
1	4.067204	-3.519167	-3.923906
6	-0.547783	-2.894803	-1.887748
6	-0.641328	-4.433657	-1.992367
6	-1.972945	-2.309679	-1.871287
1	-0.066461	-2.523303	-2.803728
6	-1.421103	-4.856870	-3.249818
1	-1.162291	-4.825183	-1.109370
1	0.345011	-4.900861	-2.000379
6	-2.767048	-2.719711	-3.119791
1	-2.506102	-2.661376	-0.981500
1	-1.928819	-1.223711	-1.802574
6	-2.828350	-4.245366	-3.274277
1	-1.479039	-5.951362	-3.300416
1	-0.867324	-4.530250	-4.141940
1	-3.778690	-2.297983	-3.068664
1	-2.287933	-2.281849	-4.007452
1	-3.350241	-4.519956	-4.199098
1	-3.415260	-4.665494	-2.444512
6	0.422411	-3.458144	0.866215
6	1.468402	-3.213865	1.970388
6	-0.992781	-3.452486	1.475025
1	0.609390	-4.446771	0.428303

6	1.333807	-4.220524	3.123612
1	1.333386	-2.196964	2.360195
1	2.482236	-3.269796	1.559695
6	-1.127440	-4.461123	2.626492
1	-1.207633	-2.443681	1.843515
1	-1.736575	-3.683786	0.705951
6	-0.080423	-4.205935	3.717408
1	2.078301	-3.995609	3.897278
1	1.561859	-5.230142	2.751455
1	-2.139052	-4.404901	3.046889
1	-1.003544	-5.482146	2.235840
1	-0.168417	-4.951377	4.517286
1	-0.269732	-3.224181	4.173114
7	-1.687004	0.883241	0.141919
6	-2.525875	1.398850	-0.976032
6	-3.041107	2.861429	-0.731709
6	-1.925055	3.924531	-0.643055
6	-4.184581	3.284401	-1.688102
1	-3.491164	2.819840	0.259401
6	-1.529994	4.571580	-1.980055
1	-1.054006	3.475925	-0.159824
1	-2.272231	4.716848	0.033513
6	-3.752222	3.957329	-3.001922
1	-4.835339	2.423909	-1.893448
1	-4.807295	4.007004	-1.143103
6	-2.755352	5.093706	-2.741667
1	-1.004542	3.842089	-2.605492
1	-0.826101	5.391591	-1.792043
1	-4.640995	4.338204	-3.520568
1	-3.289904	3.229682	-3.679160
1	-2.450383	5.557165	-3.688001
1	-3.246594	5.879856	-2.149273
16	-2.423833	0.723541	1.614969
8	-1.606629	-0.241470	2.380686
8	-2.702671	2.031400	2.247242
6	-4.029673	-0.038237	1.316198
6	-5.189365	0.735264	1.320952
6	-4.085965	-1.403399	1.025128
6	-6.412636	0.133228	1.019316
1	-5.132610	1.788101	1.573094
6	-5.311078	-1.989490	0.725851
1	-3.180145	-1.993741	1.046107
6	-6.493535	-1.230938	0.713189
1	-7.317669	0.734789	1.024762
1	-5.354578	-3.052468	0.501276
6	-1.855137	1.247357	-2.318617
6	-0.571385	1.017333	-2.587444
1	-2.551157	1.351810	-3.147691
1	-0.216147	0.927081	-3.610342
1	0.165505	0.877225	-1.796963
1	-3.438460	0.782278	-1.040404
1	-1.129815	-0.397559	-0.146749
6	-7.814230	-1.887449	0.394002
1	-8.627228	-1.157940	0.343492
1	-7.773406	-2.415192	-0.565610
1	-8.078627	-2.629861	1.156445

Number of imaginary frequencies : 0
 The smallest frequencies are : 16.0422 19.9586 23.9579 cm(-1)

Electronic energy : HF=-3492.5515888
 Zero-point correction= 1.345517
 (Hartree/Particle)
 Thermal correction to Energy= 1.407409
 Thermal correction to Enthalpy= 1.408354
 Thermal correction to Gibbs Free Energy= 1.250534
 Sum of electronic and zero-point Energies= -3491.206072
 Sum of electronic and thermal Energies= -3491.144179
 Sum of electronic and thermal Enthalpies= -3491.143235
 Sum of electronic and thermal Free Energies= -3491.301055

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 Cartesian Coordinates

28	-0.052437	0.166528	-0.076993
15	-1.307541	-1.775485	0.435609
6	-1.059733	-2.888676	-1.065144
6	-1.346093	-4.405658	-0.983883
6	-1.744556	-2.289806	-2.312534
1	0.018249	-2.768014	-1.222074
6	-0.861332	-5.113917	-2.261047
1	-2.418180	-4.586943	-0.876920
1	-0.873489	-4.854266	-0.107629
6	-1.287405	-3.006686	-3.593048
1	-2.835532	-2.374628	-2.217785
1	-1.517055	-1.221381	-2.386452
6	-1.523839	-4.520824	-3.512198
1	-1.071804	-6.187994	-2.189782
1	0.228623	-5.010681	-2.344654
1	-1.804686	-2.582316	-4.462631
1	-0.215627	-2.816381	-3.735778
1	-1.144531	-5.012974	-4.415826
1	-2.605294	-4.718097	-3.475929
6	-3.185538	-1.650103	0.650410
6	-4.006844	-2.949095	0.513043
6	-3.586047	-0.939979	1.961594
1	-3.470895	-1.000248	-0.183355
6	-5.520685	-2.683194	0.609232
1	-3.709554	-3.660486	1.294911
1	-3.809731	-3.429416	-0.445275
6	-5.090679	-0.640252	2.020272
1	-3.349771	-1.599486	2.802736
1	-3.000790	-0.027881	2.107218
6	-5.906341	-1.932603	1.888103
1	-6.061926	-3.635095	0.543844
1	-5.830233	-2.089694	-0.262591
1	-5.328315	-0.127190	2.960044
1	-5.364097	0.045775	1.209025
1	-6.981007	-1.714764	1.894421
1	-5.707767	-2.572782	2.759232
6	-0.728422	-2.783527	1.925391
6	0.637642	-3.462741	1.687525

6	-0.623953	-1.916980	3.205345
1	-1.488025	-3.564325	2.080650
6	1.079409	-4.301164	2.895690
1	1.376722	-2.684188	1.499688
1	0.622088	-4.095611	0.800636
6	-0.177202	-2.747373	4.419774
1	0.101594	-1.120131	3.025717
1	-1.569648	-1.429160	3.441107
6	1.164535	-3.442619	4.161970
1	2.050553	-4.763159	2.678694
1	0.365932	-5.124208	3.054492
1	-0.106708	-2.092138	5.296766
1	-0.942238	-3.504194	4.651804
1	1.456144	-4.053586	5.025459
1	1.944243	-2.682689	4.021256
15	-1.271532	1.953679	-0.421859
6	-3.157446	1.795414	-0.562546
6	-4.007012	3.065981	-0.347680
6	-3.574556	1.108836	-1.880210
1	-3.394183	1.108356	0.255362
6	-5.509886	2.736493	-0.352474
1	-3.811363	3.781322	-1.153815
1	-3.744103	3.562595	0.591109
6	-5.076168	0.780936	-1.901184
1	-3.358515	1.775125	-2.725370
1	-2.987272	0.200404	-2.041754
6	-5.927943	2.032478	-1.650721
1	-6.088851	3.657760	-0.214644
1	-5.740762	2.091288	0.505552
1	-5.341087	0.321617	-2.861116
1	-5.295170	0.035348	-1.126597
1	-6.991853	1.769273	-1.617367
1	-5.802006	2.728417	-2.492507
6	-0.846356	2.997768	-1.947731
6	-1.131541	4.511492	-1.808353
6	0.584896	2.798462	-2.482088
1	-1.525393	2.603376	-2.714250
6	-0.943850	5.233807	-3.153097
1	-0.440324	4.943767	-1.075462
1	-2.138269	4.698415	-1.430900
6	0.784285	3.517077	-3.825300
1	1.301193	3.194502	-1.753631
1	0.808827	1.734970	-2.588568
6	0.465250	5.014053	-3.718587
1	-1.144052	6.304865	-3.027556
1	-1.686890	4.857404	-3.870960
1	1.814139	3.367886	-4.172125
1	0.129804	3.058577	-4.581000
1	0.566562	5.501560	-4.695800
1	1.197158	5.489966	-3.050265
6	-1.035496	3.079258	1.058399
6	-1.552102	2.382818	2.336191
6	0.435713	3.502901	1.240158
1	-1.637873	3.978114	0.877017
6	-1.344897	3.257787	3.582625
1	-1.006808	1.439415	2.459215
1	-2.616107	2.139009	2.236468

6	0.617559	4.393685	2.477346
1	1.039686	2.604479	1.367729
1	0.809211	4.017611	0.349950
6	0.123371	3.675272	3.739487
1	-1.687364	2.713713	4.471327
1	-1.972082	4.158217	3.502237
1	1.676795	4.658528	2.576649
1	0.063733	5.335979	2.347873
1	0.245289	4.315239	4.622018
1	0.736535	2.778630	3.897797
7	1.867296	-0.703606	0.156666
6	2.937323	-1.189016	-0.762766
6	3.465314	-2.634448	-0.393401
6	2.746320	-3.821474	-1.068871
6	4.996556	-2.779979	-0.548024
1	3.273441	-2.699506	0.677028
6	3.245182	-4.183082	-2.479463
1	1.671992	-3.633470	-1.097240
1	2.885529	-4.700033	-0.423587
6	5.473412	-3.084391	-1.975944
1	5.493508	-1.887170	-0.150282
1	5.313752	-3.614064	0.093940
6	4.772666	-4.334402	-2.528616
1	2.933760	-3.413222	-3.193544
1	2.764157	-5.114853	-2.804419
1	6.561213	-3.227561	-1.979527
1	5.277862	-2.229453	-2.636861
1	5.102351	-4.540951	-3.554450
1	5.070034	-5.202846	-1.922704
16	2.477041	-0.035168	1.496581
8	1.336999	0.466801	2.312570
8	3.452977	-0.901189	2.203895
6	3.424986	1.449582	1.043311
6	4.175053	2.074772	2.043364
6	3.346268	2.013020	-0.229222
6	4.822950	3.276711	1.768453
1	4.243806	1.623188	3.027676
6	4.010854	3.210988	-0.496144
1	2.755726	1.529432	-0.996661
6	4.750374	3.866225	0.495786
1	5.396526	3.766370	2.551932
1	3.943115	3.645783	-1.490554
6	2.587186	-1.037419	-2.219586
6	1.408631	-0.749950	-2.771784
1	3.435662	-1.201731	-2.880100
1	1.294316	-0.672266	-3.849516
1	0.524908	-0.567117	-2.167614
1	3.826188	-0.551943	-0.636434
1	0.715267	1.329359	-0.422325
6	5.479521	5.154527	0.202385
1	5.407187	5.856142	1.040086
1	6.547171	4.971012	0.027076
1	5.081461	5.648958	-0.688924

3a

Number of imaginary frequencies : 0
The smallest frequencies are : 12.9481 17.9434 28.7109 cm(-1)

Electronic energy : HF=-2445.2231071
Zero-point correction= 0.856451
(Hartree/Particle)
Thermal correction to Energy= 0.898726
Thermal correction to Enthalpy= 0.899670
Thermal correction to Gibbs Free Energy= 0.779993
Sum of electronic and zero-point Energies= -2444.366656
Sum of electronic and thermal Energies= -2444.324381
Sum of electronic and thermal Enthalpies= -2444.323437
Sum of electronic and thermal Free Energies= -2444.443114

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

28	-0.286485	0.205891	0.357345
15	1.777359	0.149726	0.088682
6	2.490209	1.834353	-0.358389
6	4.021100	1.987849	-0.392622
6	1.871645	2.350192	-1.673640
1	2.101644	2.475207	0.445428
6	4.419009	3.452637	-0.645909
1	4.430152	1.366936	-1.200166
1	4.472454	1.632592	0.540662
6	2.263865	3.812376	-1.935330
1	2.225925	1.736315	-2.513830
1	0.783247	2.235037	-1.639502
6	3.789986	3.989663	-1.940105
1	5.511454	3.544331	-0.686534
1	4.083167	4.066523	0.202089
1	1.837246	4.153454	-2.886747
1	1.828568	4.446282	-1.149658
1	4.052939	5.045000	-2.082410
1	4.210916	3.442604	-2.796225
6	2.523796	-0.995830	-1.224633
6	3.946937	-1.535351	-0.976901
6	1.566397	-2.161889	-1.539298
1	2.560043	-0.360585	-2.120971
6	4.444379	-2.355727	-2.179844
1	3.943410	-2.180968	-0.089485
1	4.647274	-0.721886	-0.767481
6	2.056669	-2.992067	-2.733948
1	1.490703	-2.810561	-0.656422
1	0.557579	-1.775071	-1.715713
6	3.485262	-3.508527	-2.510073
1	5.450850	-2.742885	-1.978084
1	4.531113	-1.695385	-3.054688
1	1.371909	-3.830129	-2.917518
1	2.034645	-2.366643	-3.637986
1	3.837829	-4.059266	-3.390547
1	3.482005	-4.221948	-1.673066
6	2.662624	-0.310463	1.685235
6	2.431851	0.763503	2.768012
6	2.139841	-1.676626	2.179289
1	3.741440	-0.389775	1.498621
6	3.044007	0.355638	4.118311

1	1.347775	0.911508	2.880081
1	2.850489	1.725889	2.452220
6	2.762096	-2.083773	3.522978
1	1.048604	-1.604002	2.288611
1	2.328724	-2.454289	1.430585
6	2.520649	-1.007588	4.589735
1	2.833103	1.127180	4.869316
1	4.138270	0.306842	4.017932
1	2.346814	-3.045551	3.848573
1	3.844300	-2.233793	3.395279
1	2.994350	-1.291797	5.537343
1	1.441492	-0.932545	4.783756
7	-2.141039	0.427364	1.018661
6	-3.140370	1.350890	0.365253
6	-2.761515	2.827273	0.711741
6	-1.441616	3.354560	0.106719
6	-3.921772	3.820790	0.455443
1	-2.627373	2.802070	1.803618
6	-1.564728	3.872849	-1.333583
1	-0.672097	2.570404	0.166925
1	-1.096167	4.180243	0.744556
6	-4.019916	4.356168	-0.983161
1	-4.875312	3.375051	0.765938
1	-3.756377	4.680323	1.118800
6	-2.676427	4.922635	-1.461679
1	-1.771395	3.036126	-2.009155
1	-0.604678	4.299178	-1.645382
1	-4.798181	5.128056	-1.025184
1	-4.336665	3.562540	-1.669495
1	-2.758423	5.270357	-2.498631
1	-2.417186	5.802026	-0.853807
16	-2.859835	-1.070911	1.673002
8	-1.979008	-1.415146	2.796250
8	-4.294699	-0.839361	1.902352
6	-2.695519	-2.291760	0.383287
6	-3.811382	-2.623306	-0.381725
6	-1.455918	-2.901851	0.178897
6	-3.673871	-3.581238	-1.386670
1	-4.763222	-2.140820	-0.192993
6	-1.342989	-3.859179	-0.823719
1	-0.602226	-2.610333	0.780975
6	-2.443910	-4.208157	-1.623785
1	-4.536183	-3.844676	-1.992533
1	-0.384735	-4.340667	-0.994703
6	-3.360234	1.023549	-1.091113
6	-2.606706	0.262657	-1.884468
1	-4.272141	1.460162	-1.491994
1	-2.887754	0.092087	-2.920216
1	-1.686413	-0.206946	-1.535722
1	-4.100465	1.187126	0.869668
1	-1.818377	0.869298	1.891755
6	-2.287726	-5.239177	-2.713238
1	-1.533370	-4.925041	-3.443821
1	-1.955334	-6.199322	-2.302094
1	-3.225227	-5.408045	-3.249728

TS [3a-4a]

Number of imaginary frequencies : 1
The smallest frequencies are : -1120.9202 11.5526 21.4870 cm(-1)

Electronic energy : HF=-2445.2057761
Zero-point correction= 0.850692
(Hartree/Particle)
Thermal correction to Energy= 0.892844
Thermal correction to Enthalpy= 0.893788
Thermal correction to Gibbs Free Energy= 0.773748
Sum of electronic and zero-point Energies= -2444.355084
Sum of electronic and thermal Energies= -2444.312932
Sum of electronic and thermal Enthalpies= -2444.311988
Sum of electronic and thermal Free Energies= -2444.432028

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

28	-0.266402	0.240823	0.157517
15	1.829464	-0.146898	0.050816
6	2.829780	1.376510	-0.373321
6	4.362605	1.248603	-0.320402
6	2.384869	1.971582	-1.725735
1	2.516940	2.087150	0.404215
6	5.029525	2.614507	-0.553444
1	4.696040	0.551714	-1.100458
1	4.687979	0.830920	0.638786
6	3.047416	3.336990	-1.966329
1	2.669482	1.290460	-2.539904
1	1.293334	2.061472	-1.757666
6	4.578687	3.241162	-1.881766
1	6.120889	2.508002	-0.532985
1	4.762848	3.286552	0.274443
1	2.743518	3.734121	-2.942248
1	2.684500	4.047515	-1.210192
1	5.030493	4.232298	-2.007484
1	4.945004	2.621118	-2.712644
6	2.369249	-1.448259	-1.201698
6	3.638043	-2.255513	-0.861455
6	1.199989	-2.399565	-1.537974
1	2.576882	-0.862039	-2.108468
6	4.004018	-3.217900	-2.004574
1	3.465821	-2.840856	0.050409
1	4.480287	-1.590015	-0.650031
6	1.565727	-3.365931	-2.673816
1	0.935169	-2.979650	-0.644433
1	0.306066	-1.820627	-1.797933
6	2.838922	-4.158183	-2.344636
1	4.894931	-3.796847	-1.732303
1	4.269712	-2.632747	-2.896591
1	0.728208	-4.047190	-2.869025
1	1.723978	-2.791833	-3.597989
1	3.109731	-4.812893	-3.181617
1	2.642635	-4.812789	-1.483241
6	2.472162	-0.715761	1.714001
6	2.394743	0.423270	2.752384
6	1.645675	-1.928775	2.196712
1	3.521343	-1.018975	1.603453

6	2.831244	-0.053408	4.146709
1	1.358748	0.786648	2.793334
1	3.018033	1.270145	2.444458
6	2.095161	-2.404738	3.585798
1	0.588376	-1.634851	2.238744
1	1.719698	-2.753360	1.478794
6	2.013899	-1.266389	4.611366
1	2.735905	0.770805	4.863987
1	3.896965	-0.323941	4.117900
1	1.473504	-3.250057	3.903961
1	3.129745	-2.774294	3.530494
1	2.363283	-1.608292	5.593235
1	0.963228	-0.969278	4.731460
7	-1.999703	0.697531	0.745514
6	-2.774032	1.849837	0.220583
6	-2.094995	3.194762	0.648245
6	-0.752422	3.526880	-0.039290
6	-3.044268	4.417734	0.589204
1	-1.880886	3.023395	1.710606
6	-0.891694	4.173099	-1.424861
1	-0.134596	2.622412	-0.099532
1	-0.209745	4.224312	0.615074
6	-3.150157	5.114424	-0.779265
1	-4.041192	4.137536	0.951878
1	-2.656200	5.155097	1.304993
6	-1.765641	5.433222	-1.361935
1	-1.330627	3.453880	-2.126033
1	0.104407	4.420848	-1.811969
1	-3.736308	6.034877	-0.667855
1	-3.702335	4.488800	-1.490090
1	-1.866331	5.884146	-2.356718
1	-1.270059	6.181191	-0.725715
16	-2.822460	-0.488700	1.606797
8	-1.902047	-0.980412	2.646241
8	-4.157101	0.008735	1.985560
6	-3.065737	-1.837346	0.445123
6	-4.291188	-1.992836	-0.197260
6	-1.986755	-2.673716	0.151346
6	-4.430793	-2.998833	-1.155361
1	-5.116821	-1.335457	0.051680
6	-2.140098	-3.666754	-0.810348
1	-1.041108	-2.528122	0.663001
6	-3.361849	-3.843677	-1.481225
1	-5.384566	-3.123226	-1.661245
1	-1.300987	-4.316270	-1.046085
6	-3.095869	1.699028	-1.250974
6	-2.726608	0.710262	-2.066058
1	-3.743609	2.479177	-1.644171
1	-3.043602	0.695310	-3.105104
1	-2.112872	-0.119472	-1.727672
1	-3.735074	1.850494	0.748993
1	-0.787926	0.944467	1.359218
6	-3.519258	-4.944297	-2.501069
1	-3.695119	-5.909359	-2.009215
1	-4.364291	-4.757962	-3.170169
1	-2.617753	-5.054078	-3.112873

4a

 Number of imaginary frequencies : 0
 The smallest frequencies are : 13.7045 17.9257 24.0946 cm(-1)

Electronic energy : HF=-2445.237033
 Zero-point correction= 0.852843
 (Hartree/Particle)
 Thermal correction to Energy= 0.895307
 Thermal correction to Enthalpy= 0.896251
 Thermal correction to Gibbs Free Energy= 0.775626
 Sum of electronic and zero-point Energies= -2444.384190
 Sum of electronic and thermal Energies= -2444.341726
 Sum of electronic and thermal Enthalpies= -2444.340782
 Sum of electronic and thermal Free Energies= -2444.461407

.....
 Cartesian Coordinates

28	0.125910	-0.526811	0.779218
15	-1.865686	-0.352418	0.042130
6	-2.387801	-1.963305	-0.732565
6	-3.797430	-1.996408	-1.348924
6	-1.332322	-2.458424	-1.744616
1	-2.360428	-2.654953	0.119971
6	-4.140210	-3.411117	-1.846033
1	-3.836401	-1.303292	-2.199097
1	-4.548093	-1.657395	-0.625793
6	-1.678373	-3.868611	-2.246176
1	-1.291704	-1.772900	-2.602688
1	-0.336584	-2.447109	-1.288919
6	-3.091640	-3.923615	-2.844288
1	-5.137048	-3.413404	-2.302651
1	-4.186264	-4.092432	-0.984809
1	-0.934944	-4.192442	-2.983853
1	-1.612784	-4.571672	-1.403969
1	-3.334069	-4.945775	-3.157752
1	-3.123730	-3.300733	-3.749934
6	-2.003509	0.959597	-1.297839
6	-3.403194	1.580007	-1.492700
6	-0.948145	2.074194	-1.117065
1	-1.744980	0.409491	-2.214236
6	-3.410305	2.541013	-2.693847
1	-3.680583	2.141005	-0.591136
1	-4.164787	0.806479	-1.628668
6	-0.958653	3.046200	-2.305610
1	-1.151381	2.628007	-0.192509
1	0.051841	1.648356	-0.993768
6	-2.353538	3.643039	-2.536475
1	-4.408671	2.979529	-2.809934
1	-3.207874	1.970230	-3.611377
1	-0.223436	3.838446	-2.132064
1	-0.636670	2.508951	-3.209453
1	-2.349867	4.295899	-3.417478
1	-2.620046	4.275473	-1.677436
6	-3.131446	0.066472	1.342741
6	-3.421445	-1.118885	2.286349
6	-2.647310	1.298450	2.141274

1	-4.063935	0.322049	0.823737
6	-4.416727	-0.721804	3.388539
1	-2.483220	-1.448791	2.750442
1	-3.818225	-1.971209	1.723835
6	-3.638731	1.678287	3.251353
1	-1.665822	1.071110	2.578440
1	-2.497846	2.152817	1.472197
6	-3.918613	0.492444	4.183229
1	-4.583523	-1.575989	4.055290
1	-5.388459	-0.484209	2.931842
1	-3.243574	2.528112	3.819873
1	-4.582208	2.013092	2.795967
1	-4.649999	0.773003	4.950431
1	-2.992317	0.223470	4.709478
7	1.953942	-0.199772	0.731180
6	3.031680	-1.015111	0.136922
6	3.194821	-2.352633	0.942334
6	2.052081	-3.374303	0.763147
6	4.571795	-3.038014	0.766267
1	3.156565	-1.997958	1.977810
6	2.188080	-4.274882	-0.475198
1	1.086924	-2.854119	0.751156
1	2.034881	-4.016705	1.654519
6	4.701175	-3.977124	-0.445674
1	5.365962	-2.280946	0.750093
1	4.746306	-3.639893	1.668828
6	3.547223	-4.988515	-0.500220
1	2.072125	-3.676494	-1.386510
1	1.374240	-5.011078	-0.480590
1	5.663520	-4.501548	-0.394555
1	4.720198	-3.403807	-1.380420
1	3.635061	-5.620223	-1.392814
1	3.616017	-5.659695	0.368494
16	2.417368	1.080389	1.667501
8	1.359679	1.322200	2.672048
8	3.813890	0.929151	2.128041
6	2.371471	2.503371	0.557415
6	3.073035	2.471340	-0.651494
6	1.632746	3.628422	0.917651
6	3.022866	3.572958	-1.499744
1	3.631230	1.588122	-0.940360
6	1.596132	4.728754	0.058336
1	1.088192	3.629185	1.855277
6	2.287674	4.720626	-1.158894
1	3.559592	3.543803	-2.444739
1	1.016116	5.604429	0.338030
6	2.873367	-1.175728	-1.357582
6	1.923229	-0.664715	-2.141591
1	3.665746	-1.757540	-1.822218
1	1.928530	-0.836975	-3.214490
1	1.117091	-0.059710	-1.742023
1	3.987443	-0.495085	0.288079
1	-0.581353	-1.403246	1.654917
6	2.257054	5.911153	-2.085348
1	1.477605	6.624362	-1.801102
1	3.215567	6.445062	-2.070370
1	2.075608	5.606394	-3.122092

3b

Number of imaginary frequencies : 0
The smallest frequencies are : 21.3217 22.6519 29.1559 cm(-1)

Electronic energy : HF=-2445.2442805
Zero-point correction= 0.856426
(Hartree/Particle)
Thermal correction to Energy= 0.898212
Thermal correction to Enthalpy= 0.899156
Thermal correction to Gibbs Free Energy= 0.781437
Sum of electronic and zero-point Energies= -2444.387855
Sum of electronic and thermal Energies= -2444.346069
Sum of electronic and thermal Enthalpies= -2444.345125
Sum of electronic and thermal Free Energies= -2444.462844

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Cartesian Coordinates
.....

28	-0.324979	0.984654	-0.987378
15	-1.962850	-0.102486	-0.020982
6	-1.487024	-0.242760	1.793963
6	-2.503534	-0.869401	2.764501
6	-0.111510	-0.926098	1.950395
1	-1.348900	0.809333	2.080088
6	-2.006238	-0.764021	4.217014
1	-2.637605	-1.929116	2.512439
1	-3.485396	-0.393185	2.667135
6	0.392914	-0.826971	3.397262
1	-0.190182	-1.985903	1.673375
1	0.611984	-0.485201	1.257039
6	-0.624909	-1.414110	4.385852
1	-2.731753	-1.227386	4.896605
1	-1.944510	0.297060	4.498006
1	1.358825	-1.337407	3.492020
1	0.572566	0.229334	3.642615
1	-0.270905	-1.294528	5.416582
1	-0.714649	-2.495535	4.207276
6	-2.246330	-1.886289	-0.556859
6	-3.617971	-2.507450	-0.221112
6	-1.915656	-2.103604	-2.048229
1	-1.483850	-2.432398	0.016541
6	-3.638420	-4.005325	-0.571447
1	-4.400635	-1.998628	-0.798365
1	-3.869588	-2.369638	0.834080
6	-1.940169	-3.597402	-2.406365
1	-2.646078	-1.567610	-2.669395
1	-0.939773	-1.668648	-2.274732
6	-3.284952	-4.244944	-2.046180
1	-4.623598	-4.428597	-0.340880
1	-2.913691	-4.532119	0.066409
1	-1.724536	-3.730703	-3.473349
1	-1.134465	-4.107201	-1.857704
1	-3.264834	-5.319681	-2.263936
1	-4.072816	-3.810356	-2.677970
6	-3.659648	0.694632	0.004119
6	-3.621732	2.047961	0.744410

6	-4.164711	0.900342	-1.441103
1	-4.360238	0.032998	0.529711
6	-4.988768	2.749454	0.713745
1	-2.874569	2.692994	0.262913
1	-3.302634	1.917689	1.784502
6	-5.530096	1.605433	-1.474054
1	-3.425586	1.503395	-1.987463
1	-4.229155	-0.058229	-1.966539
6	-5.488685	2.943202	-0.723570
1	-4.921373	3.714804	1.229927
1	-5.716638	2.144016	1.272674
1	-5.843348	1.758373	-2.513802
1	-6.284736	0.953606	-1.010758
1	-6.479137	3.413824	-0.724165
1	-4.811978	3.630972	-1.250578
7	3.803497	1.124913	-1.120708
6	2.443651	1.451771	-0.593063
6	2.449881	2.737369	0.279270
6	2.587378	4.068398	-0.498916
6	1.254530	2.792620	1.257900
1	3.346917	2.633819	0.898051
6	1.272593	4.654974	-1.049477
1	3.313562	3.955737	-1.315230
1	3.024158	4.806911	0.186711
6	-0.043206	3.337714	0.652081
1	1.085590	1.798884	1.688353
1	1.528135	3.450325	2.094613
6	0.176245	4.716594	0.022135
1	0.904230	4.051807	-1.884744
1	1.465608	5.658188	-1.448673
1	-0.830814	3.370965	1.412190
1	-0.430107	2.663475	-0.147830
1	-0.757455	5.095891	-0.409769
1	0.469447	5.421289	0.813934
16	4.852709	0.262052	-0.141541
8	6.101884	0.143015	-0.907835
8	4.904464	0.766741	1.244149
6	3.985686	-1.309244	-0.085331
6	3.475297	-1.770347	1.129030
6	3.782932	-2.020861	-1.268224
6	2.739847	-2.953751	1.149785
1	3.643894	-1.195729	2.032979
6	3.042393	-3.200900	-1.230195
1	4.175010	-1.641747	-2.205640
6	2.502711	-3.679839	-0.026923
1	2.332723	-3.312420	2.091633
1	2.871246	-3.752680	-2.150393
6	1.440209	1.380177	-1.727187
6	0.948227	0.127072	-2.175876
1	1.477742	2.203578	-2.441243
1	0.588599	0.029156	-3.202089
1	1.327560	-0.803393	-1.750984
1	2.214485	0.622983	0.085280
1	4.299938	1.879916	-1.588870
6	1.688117	-4.949078	0.014547
1	2.187423	-5.717228	0.617050
1	0.705967	-4.775155	0.469053

1 1.529160 -5.361082 -0.985650

4b

Number of imaginary frequencies : 0
The smallest frequencies are : 2.4670 18.5910 21.9960 cm(-1)

Electronic energy : HF=-2445.2284492
Zero-point correction= 0.853695
(Hartree/Particle)
Thermal correction to Energy= 0.894585
Thermal correction to Enthalpy= 0.895529
Thermal correction to Gibbs Free Energy= 0.780963
Sum of electronic and zero-point Energies= -2444.374754
Sum of electronic and thermal Energies= -2444.333865
Sum of electronic and thermal Enthalpies= -2444.332920
Sum of electronic and thermal Free Energies= -2444.447486

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Cartesian Coordinates
.....

28	-0.058402	0.799769	0.271477
15	-1.931001	-0.278580	-0.050120
6	-2.988814	-0.299573	1.491721
6	-4.399665	-0.898031	1.349655
6	-2.229509	-0.955108	2.663946
1	-3.081564	0.766594	1.734441
6	-5.190411	-0.756148	2.662108
1	-4.322503	-1.964083	1.098084
1	-4.948494	-0.418126	0.530758
6	-3.021262	-0.815112	3.973309
1	-2.076037	-2.023677	2.456943
1	-1.236048	-0.506844	2.755985
6	-4.438890	-1.390877	3.841305
1	-6.183564	-1.208753	2.551750
1	-5.351762	0.311471	2.868172
1	-2.482064	-1.311215	4.789218
1	-3.084840	0.249539	4.240013
1	-5.000548	-1.245302	4.772223
1	-4.372237	-2.476818	3.680740
6	-1.922687	-2.093190	-0.575319
6	-3.053294	-2.536955	-1.526803
6	-0.552422	-2.540151	-1.117192
1	-2.072691	-2.621219	0.376250
6	-3.013304	-4.058533	-1.749677
1	-2.938563	-2.033662	-2.494931
1	-4.033307	-2.246760	-1.136495
6	-0.513112	-4.057178	-1.353401
1	-0.344552	-2.018801	-2.060603
1	0.228143	-2.239143	-0.415163
6	-1.647394	-4.515726	-2.280694
1	-3.811807	-4.354583	-2.441000
1	-3.219172	-4.565040	-0.795808
1	0.460562	-4.344016	-1.769667
1	-0.605701	-4.572856	-0.386336
1	-1.630308	-5.605789	-2.400365
1	-1.489678	-4.086256	-3.280550
6	-2.957316	0.640309	-1.320115

6	-3.361767	2.038078	-0.804397
6	-2.171905	0.778617	-2.641816
1	-3.871228	0.064664	-1.513396
6	-4.155458	2.819906	-1.863249
1	-2.450386	2.590543	-0.538769
1	-3.956948	1.957054	0.111074
6	-2.977766	1.544107	-3.701228
1	-1.240958	1.320884	-2.433756
1	-1.877424	-0.205150	-3.023807
6	-3.384263	2.931449	-3.185469
1	-4.402279	3.816989	-1.478760
1	-5.111388	2.308261	-2.045877
1	-2.390722	1.634195	-4.623441
1	-3.880986	0.971621	-3.956482
1	-3.985418	3.459678	-3.935315
1	-2.478504	3.533807	-3.024077
7	2.628482	1.005775	1.385782
6	1.698061	1.809393	0.583890
6	1.728372	3.248766	1.120663
6	3.114746	3.928636	0.940989
6	0.608830	4.191948	0.613848
1	1.551074	3.138690	2.198586
6	3.334777	4.463800	-0.480068
1	3.920467	3.237025	1.213077
1	3.175750	4.770368	1.644783
6	0.850078	4.879821	-0.743114
1	-0.335137	3.637965	0.605393
1	0.506982	4.983310	1.368512
6	2.254931	5.491245	-0.847150
1	3.315604	3.631380	-1.196220
1	4.331040	4.916175	-0.554589
1	0.088400	5.656777	-0.884276
1	0.706245	4.173441	-1.569235
1	2.422677	5.886072	-1.856621
1	2.332051	6.345545	-0.158860
16	2.485159	-0.609897	1.853012
8	3.170658	-0.665625	3.154487
8	1.104683	-1.113602	1.732775
6	3.461127	-1.493350	0.638313
6	3.075747	-2.793856	0.306663
6	4.600558	-0.914156	0.077323
6	3.840213	-3.513858	-0.609113
1	2.181501	-3.223764	0.743736
6	5.350134	-1.648563	-0.837874
1	4.871453	0.104234	0.332577
6	4.984881	-2.955675	-1.195242
1	3.538765	-4.522901	-0.877135
1	6.229187	-1.196965	-1.290016
6	1.459549	1.526295	-0.789601
6	1.222224	0.243900	-1.308222
1	1.110959	2.363468	-1.384719
1	0.865827	0.168740	-2.329886
1	1.739210	-0.635392	-0.945716
1	-0.658040	1.440965	1.463672
1	2.893851	1.488011	2.240171
6	5.820327	-3.748161	-2.169344
1	6.650393	-4.246484	-1.652756

1	5.231417	-4.524684	-2.666332
1	6.257016	-3.104691	-2.939395

TS [3b-4b]

Number of imaginary frequencies : 1
 The smallest frequencies are : -776.3819 11.9648 14.1683 cm(-1)

Electronic energy : HF=-2445.2083261
 Zero-point correction= 0.851908
 (Hartree/Particle)
 Thermal correction to Energy= 0.893531
 Thermal correction to Enthalpy= 0.894476
 Thermal correction to Gibbs Free Energy= 0.776171
 Sum of electronic and zero-point Energies= -2444.356418
 Sum of electronic and thermal Energies= -2444.314795
 Sum of electronic and thermal Enthalpies= -2444.313850
 Sum of electronic and thermal Free Energies= -2444.432155

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 Cartesian Coordinates

28	-0.036163	0.726659	-0.113321
15	-1.914149	-0.323004	-0.065981
6	-2.894724	-0.065250	1.512593
6	-4.302796	-0.683325	1.579937
6	-2.064153	-0.475591	2.745620
1	-2.995170	1.028582	1.551395
6	-5.019134	-0.278785	2.880216
1	-4.218303	-1.777473	1.549458
1	-4.905920	-0.387260	0.713618
6	-2.776617	-0.072398	4.045639
1	-1.915320	-1.564313	2.746771
1	-1.066913	-0.029356	2.686536
6	-4.193584	-0.660844	4.117694
1	-6.011022	-0.745891	2.922354
1	-5.183163	0.808484	2.874949
1	-2.184964	-0.394397	4.911172
1	-2.837200	1.024501	4.096196
1	-4.701962	-0.329609	5.031415
1	-4.123485	-1.756668	4.176408
6	-1.844807	-2.198883	-0.251078
6	-3.046411	-2.873989	-0.943882
6	-0.521245	-2.650278	-0.901518
1	-1.823522	-2.549064	0.790264
6	-2.907056	-4.405797	-0.913281
1	-3.100091	-2.547729	-1.990093
1	-3.989490	-2.577278	-0.475555
6	-0.385016	-4.179972	-0.887909
1	-0.478494	-2.287403	-1.937096
1	0.314139	-2.184389	-0.374898
6	-1.588573	-4.863373	-1.552963
1	-3.760775	-4.868182	-1.424009
1	-2.941487	-4.748713	0.130631
1	0.545217	-4.476608	-1.388469
1	-0.305772	-4.521951	0.154348
1	-1.493896	-5.954451	-1.493038

1	-1.601209	-4.606119	-2.622100
6	-3.055446	0.289721	-1.422504
6	-3.469042	1.755756	-1.173983
6	-2.357380	0.164881	-2.793296
1	-3.962166	-0.328690	-1.431059
6	-4.340912	2.301429	-2.316279
1	-2.559307	2.366602	-1.081087
1	-4.010297	1.850658	-0.226587
6	-3.234411	0.704166	-3.932917
1	-1.414284	0.725799	-2.750563
1	-2.082230	-0.876179	-2.992334
6	-3.645798	2.160177	-3.676779
1	-4.593326	3.350943	-2.121383
1	-5.291311	1.748657	-2.337246
1	-2.698709	0.619771	-4.886510
1	-4.137066	0.082562	-4.023227
1	-4.298995	2.522472	-4.479877
1	-2.747711	2.794264	-3.689009
7	2.530169	1.100681	1.390660
6	1.566540	1.835403	0.549806
6	1.594322	3.312735	1.030044
6	2.948899	4.023193	0.772902
6	0.407499	4.184248	0.548371
1	1.471693	3.237086	2.119544
6	3.088647	4.613575	-0.637932
1	3.778234	3.338270	0.981797
1	3.034163	4.845411	1.496832
6	0.572969	4.872926	-0.817864
1	-0.505771	3.577446	0.562397
1	0.273885	4.972706	1.300697
6	1.932415	5.574058	-0.950133
1	3.115625	3.807996	-1.381504
1	4.048222	5.139093	-0.716382
1	-0.240129	5.597845	-0.946668
1	0.456216	4.148777	-1.631948
1	2.044120	5.997034	-1.955750
1	1.973335	6.419537	-0.247844
16	2.490224	-0.519557	1.862304
8	3.204254	-0.509353	3.150082
8	1.145349	-1.112909	1.786818
6	3.500465	-1.351023	0.643087
6	3.161275	-2.656708	0.284149
6	4.633369	-0.728652	0.115783
6	3.965926	-3.338634	-0.626664
1	2.272416	-3.119552	0.697259
6	5.423366	-1.425189	-0.794375
1	4.868886	0.292941	0.392336
6	5.105173	-2.737011	-1.179161
1	3.700795	-4.351893	-0.916330
1	6.298077	-0.941117	-1.220288
6	1.535472	1.584389	-0.888542
6	1.439977	0.332342	-1.522549
1	1.256654	2.441203	-1.492689
1	1.283855	0.329263	-2.598150
1	1.912242	-0.564476	-1.136448
1	0.211916	1.522931	1.166384
1	2.732034	1.602102	2.251837

6	5.985826	-3.488837	-2.145562
1	6.810334	-3.982334	-1.615573
1	5.428758	-4.265319	-2.678085
1	6.431641	-2.818415	-2.886799

5

Number of imaginary frequencies : 0
 The smallest frequencies are : 12.9488 15.5875 17.6573 cm(-1)

Electronic energy : HF=-3672.236785
 Zero-point correction= 1.226640
 (Hartree/Particle)
 Thermal correction to Energy= 1.289615
 Thermal correction to Enthalpy= 1.290559
 Thermal correction to Gibbs Free Energy= 1.124993
 Sum of electronic and zero-point Energies= -3671.010145
 Sum of electronic and thermal Energies= -3670.947170
 Sum of electronic and thermal Enthalpies= -3670.946226
 Sum of electronic and thermal Free Energies= -3671.111792

Cartesian Coordinates

28	1.383241	0.481928	0.536461
15	2.912681	-0.022335	-0.906387
6	3.366827	-1.830185	-0.780209
6	4.449633	-2.331419	-1.754672
6	3.708138	-2.240123	0.667233
1	2.424077	-2.327597	-1.039165
6	4.607710	-3.857883	-1.648900
1	5.408259	-1.857009	-1.507673
1	4.209171	-2.050834	-2.785938
6	3.875169	-3.763418	0.776316
1	4.640091	-1.749733	0.980947
1	2.928723	-1.886884	1.347545
6	4.927366	-4.289657	-0.210543
1	5.392325	-4.199192	-2.334706
1	3.673994	-4.337247	-1.974520
1	4.144575	-4.034870	1.803991
1	2.908473	-4.242892	0.566669
1	4.996216	-5.382093	-0.148079
1	5.914112	-3.894954	0.071904
6	4.516116	0.926380	-0.660743
6	5.392154	1.089377	-1.921108
6	4.299464	2.297687	0.016060
1	5.064227	0.298833	0.056358
6	6.737868	1.746449	-1.572590
1	4.868868	1.724528	-2.646918
1	5.565194	0.128318	-2.413322
6	5.640823	2.966090	0.354650
1	3.726099	2.952165	-0.654238
1	3.697673	2.171311	0.919789
6	6.537780	3.103173	-0.883666
1	7.337986	1.863969	-2.482902
1	7.303291	1.078768	-0.906861
1	5.461418	3.947619	0.809631
1	6.158870	2.359687	1.111434

1	7.505923	3.538804	-0.609335
1	6.068510	3.799625	-1.593520
6	2.410777	0.245618	-2.684617
6	1.338783	-0.755532	-3.159549
6	1.898910	1.691569	-2.867996
1	3.307117	0.109598	-3.303047
6	0.950985	-0.488250	-4.622728
1	0.445513	-0.659238	-2.534671
1	1.693935	-1.787114	-3.061033
6	1.513852	1.965231	-4.329372
1	1.018405	1.822521	-2.226433
1	2.650044	2.416661	-2.535907
6	0.471859	0.955054	-4.825405
1	0.161787	-1.185447	-4.916709
1	1.821955	-0.681292	-5.267001
1	1.134104	2.990160	-4.425581
1	2.415849	1.904412	-4.955531
1	0.240639	1.133082	-5.882570
1	-0.463144	1.087128	-4.269009
7	0.036909	1.017467	1.818454
6	-0.174661	1.160053	3.261465
6	-0.331945	-0.249597	3.922440
6	0.909095	-1.156492	3.804518
6	-0.864918	-0.229516	5.375912
1	-1.118566	-0.699807	3.306884
6	1.972779	-0.904989	4.881911
1	1.340887	-1.046722	2.807201
1	0.572570	-2.200172	3.890154
6	0.197832	-0.067354	6.478975
1	-1.640566	0.540848	5.480808
1	-1.370212	-1.190507	5.544848
6	1.371540	-1.038977	6.288151
1	2.397488	0.098227	4.754686
1	2.800397	-1.614263	4.753139
1	-0.273393	-0.227451	7.456855
1	0.585550	0.957770	6.496170
1	2.135400	-0.865626	7.056111
1	1.013627	-2.069913	6.427109
16	-1.192180	1.157861	0.819349
8	-0.529851	0.705167	-0.481933
8	-2.447906	0.498152	1.218835
6	0.845701	2.094083	3.869789
6	1.724702	2.841760	3.201873
1	0.796520	2.177779	4.951967
1	2.398174	3.516477	3.723728
1	1.794953	2.795880	2.120952
1	-1.150025	1.648657	3.426302
7	-1.933355	-1.838463	-1.341006
1	-1.296533	-1.063686	-1.129257
6	-2.484482	-2.392321	-0.075570
6	-3.327102	-3.684979	-0.303842
6	-2.627124	-4.788016	-1.129996
6	-3.929094	-4.244517	1.008702
1	-4.173607	-3.347819	-0.905924
6	-1.737512	-5.741068	-0.316547
1	-2.059428	-4.324580	-1.941092
1	-3.415370	-5.382236	-1.611781

Thermal correction to Energy=	1.288310
Thermal correction to Enthalpy=	1.289254
Thermal correction to Gibbs Free Energy=	1.126826
Sum of electronic and zero-point Energies=	-3670.975697
Sum of electronic and thermal Energies=	-3670.913344
Sum of electronic and thermal Enthalpies=	-3670.912400
Sum of electronic and thermal Free Energies=	-3671.074829

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 Cartesian Coordinates

28	0.291222	-0.746133	0.793717
15	2.419153	-1.242621	-0.258470
6	2.802863	-2.994714	0.312873
6	4.076594	-3.678000	-0.218796
6	2.760215	-3.089539	1.853781
1	1.948983	-3.566820	-0.067658
6	4.127973	-5.148588	0.231690
1	4.961918	-3.160550	0.170266
1	4.126399	-3.622550	-1.311701
6	2.819432	-4.552926	2.320812
1	3.616357	-2.547794	2.278431
1	1.860082	-2.600897	2.243743
6	4.056175	-5.270732	1.760693
1	5.042271	-5.621898	-0.145942
1	3.284520	-5.691653	-0.218001
1	2.815090	-4.596520	3.416542
1	1.913099	-5.074773	1.981152
1	4.052889	-6.325609	2.059845
1	4.959299	-4.821967	2.198952
6	3.963813	-0.289332	0.265987
6	5.194188	-0.403390	-0.662843
6	3.687487	1.194688	0.567612
1	4.224294	-0.768089	1.220771
6	6.425081	0.262415	-0.022517
1	4.977522	0.098352	-1.613121
1	5.423729	-1.443113	-0.905443
6	4.907901	1.858513	1.220626
1	3.456653	1.718962	-0.365705
1	2.808856	1.301187	1.203869
6	6.153769	1.730468	0.334710
1	7.282503	0.184165	-0.702222
1	6.696753	-0.288179	0.889828
1	4.687548	2.912554	1.421875
1	5.099081	1.382819	2.193804
1	7.029007	2.170944	0.827894
1	5.990953	2.301195	-0.591067
6	2.521776	-1.346611	-2.126973
6	1.496458	-2.331461	-2.726006
6	2.356535	0.038363	-2.787245
1	3.526835	-1.721351	-2.359284
6	1.658936	-2.432448	-4.252024
1	0.481771	-1.980342	-2.505452
1	1.601243	-3.326530	-2.278709
6	2.522863	-0.055744	-4.311823
1	1.362047	0.422985	-2.549064
1	3.073710	0.756406	-2.377419
6	1.529988	-1.056312	-4.919480

1	0.906768	-3.121283	-4.654085
1	2.643610	-2.865500	-4.482499
1	2.385053	0.937001	-4.758302
1	3.551608	-0.366953	-4.547959
1	1.689258	-1.143345	-6.001333
1	0.507749	-0.687890	-4.771714
7	0.309706	1.155120	1.340242
6	-0.136177	1.666132	2.659219
6	-1.617011	1.209666	3.009426
6	-1.773685	0.086056	4.061416
6	-2.524975	2.402313	3.369486
1	-1.979652	0.811063	2.059512
6	-1.705102	0.544182	5.529950
1	-1.028803	-0.700290	3.890060
1	-2.756885	-0.375970	3.893419
6	-2.326924	2.891689	4.810067
1	-2.367243	3.207116	2.644667
1	-3.571438	2.083652	3.256197
6	-2.606212	1.756868	5.806111
1	-0.672710	0.798920	5.791890
1	-1.985908	-0.292616	6.181676
1	-2.982701	3.747477	5.011316
1	-1.296955	3.254260	4.944203
1	-2.468870	2.101416	6.838432
1	-3.660213	1.457252	5.712002
16	-0.138291	2.039840	0.070670
8	-0.202499	1.103310	-1.096090
8	-1.336414	2.873881	0.325264
6	0.884536	1.361356	3.727273
6	1.891229	0.488273	3.668671
1	0.746485	1.936760	4.641053
1	2.561671	0.350389	4.512863
1	2.077550	-0.114193	2.786840
1	-0.185101	2.760178	2.599489
7	-1.937403	-1.126775	-1.518979
1	-1.174442	-0.442514	-1.499509
6	-2.539012	-1.211626	-0.165347
6	-3.885466	-1.998509	-0.141591
6	-3.775716	-3.492084	-0.525386
6	-4.697045	-1.786059	1.162391
1	-4.480481	-1.521610	-0.922300
6	-3.490955	-4.445686	0.646930
1	-3.029035	-3.606612	-1.315468
1	-4.733760	-3.782919	-0.974844
6	-4.423356	-2.781132	2.303341
1	-4.574702	-0.753730	1.514461
1	-5.756813	-1.886481	0.893260
6	-4.475879	-4.231094	1.804018
1	-2.468587	-4.303709	1.015081
1	-3.548048	-5.480639	0.287662
1	-5.161690	-2.623061	3.099219
1	-3.444204	-2.594552	2.761938
1	-4.260953	-4.924376	2.626344
1	-5.495452	-4.457617	1.459396
16	-2.810667	-0.787014	-2.914437
8	-1.785179	-0.335264	-3.865573
8	-3.665525	-1.933619	-3.246037

6	-3.889628	0.591571	-2.517035
6	-5.268180	0.469065	-2.688812
6	-3.325548	1.763986	-2.007160
6	-6.089527	1.542792	-2.342334
1	-5.682152	-0.453291	-3.081287
6	-4.161060	2.817130	-1.652244
1	-2.255453	1.847130	-1.871014
6	-5.552798	2.725559	-1.815852
1	-7.164342	1.455891	-2.477223
1	-3.720432	3.715854	-1.230140
6	-1.505893	-1.811769	0.774101
6	-0.426948	-2.601904	0.366806
1	-1.884572	-1.921926	1.782186
1	-0.002200	-3.307066	1.076282
1	-0.308420	-2.844862	-0.681929
1	-2.770027	-0.194195	0.183865
1	-0.268606	-0.868765	2.067085
6	1.181800	3.190047	-0.354432
6	1.538652	3.350771	-1.692426
6	1.828992	3.919972	0.645940
6	2.571019	4.229515	-2.025328
1	1.026575	2.781269	-2.458795
6	2.851776	4.796346	0.297520
1	1.568668	3.781746	1.689401
6	3.247970	4.958522	-1.040077
1	2.856209	4.343088	-3.067970
1	3.362381	5.356365	1.076852
6	-6.439944	3.880466	-1.421832
1	-6.163357	4.792707	-1.962823
1	-7.493252	3.672296	-1.629712
1	-6.344944	4.102295	-0.352401
6	4.395520	5.872956	-1.390195
1	4.321871	6.828533	-0.860140
1	5.354312	5.421145	-1.106632
1	4.432857	6.082051	-2.463025

6

Number of imaginary frequencies : 0
The smallest frequencies are : 18.7983 20.2939 25.2825 cm(-1)

Electronic energy : HF=-3672.2533301
Zero-point correction= 1.231627
(Hartree/Particle)
Thermal correction to Energy= 1.293652
Thermal correction to Enthalpy= 1.294596
Thermal correction to Gibbs Free Energy= 1.134544
Sum of electronic and zero-point Energies= -3671.021703
Sum of electronic and thermal Energies= -3670.959678
Sum of electronic and thermal Enthalpies= -3670.958734
Sum of electronic and thermal Free Energies= -3671.118786

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Cartesian Coordinates
.....

28	-0.890899	0.521830	0.338424
15	-2.076793	-0.082172	-1.392197
6	-2.668922	1.418706	-2.334529

6	-3.570426	1.154219	-3.555253
6	-3.322470	2.457632	-1.398314
1	-1.731565	1.858042	-2.698322
6	-3.850335	2.462762	-4.313937
1	-4.524848	0.730821	-3.217797
1	-3.114779	0.421662	-4.229802
6	-3.611282	3.765468	-2.151668
1	-4.266195	2.057312	-1.003381
1	-2.680429	2.649615	-0.533114
6	-4.478771	3.519728	-3.394662
1	-4.505046	2.262571	-5.170509
1	-2.906057	2.849134	-4.722576
1	-4.098600	4.481281	-1.479290
1	-2.657554	4.218388	-2.457482
1	-4.634592	4.456535	-3.942454
1	-5.472267	3.172255	-3.076127
6	-3.634025	-0.967161	-0.803090
6	-4.325273	-1.881066	-1.839267
6	-3.419141	-1.744770	0.514385
1	-4.317413	-0.134659	-0.583132
6	-5.663301	-2.407666	-1.291907
1	-3.674582	-2.735867	-2.058323
1	-4.492709	-1.360619	-2.786185
6	-4.753741	-2.266600	1.063545
1	-2.748287	-2.592559	0.339215
1	-2.929164	-1.120426	1.263705
6	-5.474556	-3.150559	0.037904
1	-6.132513	-3.062748	-2.035840
1	-6.348403	-1.561049	-1.140856
1	-4.572040	-2.822856	1.989200
1	-5.393880	-1.412411	1.327561
1	-6.443245	-3.484949	0.428373
1	-4.874527	-4.055295	-0.137960
6	-1.323929	-1.211537	-2.672411
6	-0.237333	-0.557779	-3.547206
6	-0.750217	-2.483206	-2.017208
1	-2.156133	-1.498279	-3.328847
6	0.219370	-1.534279	-4.643743
1	0.619340	-0.311276	-2.913111
1	-0.593163	0.373206	-4.003280
6	-0.271098	-3.479170	-3.085268
1	0.094401	-2.198111	-1.383061
1	-1.486413	-2.964588	-1.367521
6	0.746755	-2.845316	-4.043792
1	0.997692	-1.059814	-5.252871
1	-0.626443	-1.743398	-5.315570
1	0.171862	-4.353801	-2.594908
1	-1.141306	-3.839761	-3.654361
1	1.001129	-3.550885	-4.844265
1	1.671849	-2.638001	-3.497067
7	-0.773289	0.387540	2.240320
6	-1.294950	1.276766	3.309064
6	-0.379381	2.547683	3.449947
6	-0.548377	3.582932	2.316935
6	-0.427372	3.221173	4.841919
1	0.626665	2.124850	3.356025
6	-1.658897	4.623500	2.543065

1	-0.721876	3.056862	1.374618
1	0.404931	4.116421	2.200612
6	-1.548111	4.254434	5.037625
1	-0.468428	2.452363	5.623694
1	0.529184	3.743675	4.981447
6	-1.535914	5.300493	3.914478
1	-2.638749	4.140175	2.467788
1	-1.617155	5.373678	1.742733
1	-1.427469	4.740345	6.013708
1	-2.528690	3.762906	5.059912
1	-2.345350	6.026929	4.057021
1	-0.593551	5.866141	3.959830
16	0.296176	-0.753761	2.773059
8	1.508184	-0.724581	1.906551
8	0.520531	-0.660981	4.231022
6	-2.764109	1.593356	3.180630
6	-3.573613	1.438930	2.133575
1	-3.181681	2.022000	4.090079
1	-4.619896	1.728392	2.181837
1	-3.220845	1.040012	1.192001
1	-1.188215	0.752231	4.265145
7	2.224386	-0.228591	-0.798870
1	1.709397	-0.546780	0.028762
6	2.735285	1.146725	-0.537973
6	3.540583	1.718568	-1.734856
6	2.791115	1.882905	-3.075359
6	4.327606	3.004870	-1.369514
1	4.307002	0.960144	-1.916887
6	2.043985	3.215723	-3.240510
1	2.124448	1.032076	-3.227492
1	3.539609	1.819385	-3.876733
6	3.586967	4.335375	-1.590943
1	4.689762	2.939384	-0.335534
1	5.225226	3.023433	-2.002407
6	2.975945	4.409955	-2.996297
1	1.202582	3.275456	-2.540796
1	1.613325	3.266972	-4.248677
1	4.286126	5.165908	-1.432766
1	2.789437	4.464235	-0.849097
1	2.434402	5.354956	-3.127049
1	3.782059	4.401339	-3.744679
16	3.226254	-1.491280	-1.239562
8	2.466420	-2.704672	-0.885075
8	3.665516	-1.296260	-2.628984
6	4.682523	-1.406719	-0.194604
6	5.931052	-1.166163	-0.766268
6	4.535110	-1.563178	1.187828
6	7.051328	-1.087083	0.061983
1	6.016459	-1.052944	-1.841361
6	5.663732	-1.474269	1.996235
1	3.556548	-1.734433	1.623235
6	6.935830	-1.235077	1.450099
1	8.028057	-0.906772	-0.378854
1	5.556156	-1.590069	3.071527
6	1.520785	1.942739	-0.003870
6	0.183702	1.703282	-0.727209
1	1.770893	3.006711	-0.029569

1	-0.415660	2.622609	-0.759101
1	0.342604	1.372279	-1.751236
1	3.458090	1.095155	0.290185
1	1.416122	1.694954	1.056567
6	-0.479054	-2.344230	2.455399
6	-0.025833	-3.147140	1.410169
6	-1.542733	-2.748980	3.265390
6	-0.671217	-4.359644	1.160898
1	0.815178	-2.837014	0.800717
6	-2.170505	-3.963626	3.005207
1	-1.873268	-2.120890	4.086253
6	-1.752662	-4.783529	1.943922
1	-0.323632	-4.982809	0.341204
1	-2.999692	-4.281045	3.632181
6	8.139214	-1.117807	2.352123
1	8.118972	-0.171627	2.906972
1	8.159980	-1.923730	3.093492
1	9.074827	-1.150915	1.786638
6	-2.436230	-6.100785	1.671109
1	-1.951990	-6.916451	2.222799
1	-3.486864	-6.078888	1.977028
1	-2.396500	-6.359269	0.608406

5a.log

Number of imaginary frequencies : 0
The smallest frequencies are : 11.3684 18.8344 21.9178 cm(-1)

Electronic energy :	HF=-2445.231159	
Zero-point correction=		0.855579
(Hartree/Particle)		
Thermal correction to Energy=		0.896988
Thermal correction to Enthalpy=		0.897933
Thermal correction to Gibbs Free Energy=		0.780594
Sum of electronic and zero-point Energies=		-2444.375580
Sum of electronic and thermal Energies=		-2444.334171
Sum of electronic and thermal Enthalpies=		-2444.333226
Sum of electronic and thermal Free Energies=		-2444.450565

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Cartesian Coordinates
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28	0.473290	0.811711	-0.955735
15	2.237717	-0.058779	0.045961
6	2.829452	1.381830	1.132000
6	3.700843	1.033682	2.358355
6	3.509236	2.496898	0.308836
1	1.879895	1.787893	1.509126
6	3.976459	2.284281	3.212434
1	4.655023	0.605679	2.026556
1	3.217153	0.280273	2.984916
6	3.768765	3.746094	1.164873
1	4.470186	2.128589	-0.074631
1	2.897432	2.756889	-0.559854
6	4.621206	3.409978	2.394251
1	4.613198	2.013677	4.063263
1	3.026045	2.642210	3.633371
1	4.258259	4.515674	0.556039

1	2.806540	4.166427	1.490691
1	4.767285	4.300414	3.017272
1	5.619235	3.089209	2.062577
6	3.606395	-0.416495	-1.170376
6	4.915077	-0.985910	-0.591330
6	3.077983	-1.260574	-2.352255
1	3.828232	0.579011	-1.576369
6	5.973278	-1.156931	-1.695094
1	4.728569	-1.956634	-0.117909
1	5.302675	-0.325505	0.191504
6	4.153659	-1.417561	-3.436580
1	2.772502	-2.252222	-2.002597
1	2.179553	-0.786834	-2.766141
6	5.447272	-2.009458	-2.858949
1	6.881532	-1.602319	-1.271214
1	6.257040	-0.165058	-2.075348
1	3.772208	-2.048156	-4.248062
1	4.371046	-0.433688	-3.876952
1	6.211307	-2.095797	-3.640762
1	5.247709	-3.028943	-2.498812
6	2.133848	-1.486985	1.251163
6	0.933189	-1.240470	2.194807
6	2.076160	-2.880734	0.590642
1	3.059625	-1.446551	1.840663
6	0.771935	-2.372097	3.220624
1	0.027650	-1.166456	1.587918
1	1.049758	-0.282224	2.716853
6	1.897715	-3.985213	1.645936
1	1.245256	-2.917581	-0.114411
1	2.997824	-3.070206	0.032888
6	0.666479	-3.736355	2.526523
1	-0.116278	-2.182193	3.836355
1	1.633446	-2.377226	3.905187
1	1.818536	-4.956078	1.142196
1	2.794077	-4.032716	2.282867
1	0.560438	-4.536323	3.269731
1	-0.230492	-3.750306	1.895503
7	-1.300140	0.083013	-0.426484
6	-2.161955	1.133808	-1.059261
6	-3.266020	1.657046	-0.094649
6	-2.846380	2.639501	1.022755
6	-4.505436	2.191574	-0.847804
1	-3.583577	0.740795	0.410496
6	-2.810509	4.126757	0.617774
1	-1.887482	2.325207	1.452512
1	-3.582234	2.536280	1.832027
6	-4.363170	3.646866	-1.311871
1	-4.737294	1.533004	-1.693720
1	-5.368213	2.131362	-0.169683
6	-4.089918	4.561758	-0.110215
1	-1.962958	4.324918	-0.045115
1	-2.653732	4.740859	1.513724
1	-5.271173	3.964304	-1.838820
1	-3.536422	3.732526	-2.031615
1	-4.004109	5.607750	-0.429328
1	-4.945225	4.511714	0.579317
16	-1.683952	-1.426473	-0.950067

8	-1.804458	-1.514540	-2.425981
8	-0.794635	-2.394452	-0.276019
6	-3.337762	-1.723297	-0.297471
6	-3.498125	-1.945983	1.073354
6	-4.442473	-1.672765	-1.144325
6	-4.779034	-2.107187	1.591328
1	-2.627319	-1.984789	1.719391
6	-5.722468	-1.834801	-0.609759
1	-4.293134	-1.510954	-2.206223
6	-5.911427	-2.050415	0.760528
1	-4.908018	-2.279311	2.657152
1	-6.585423	-1.792644	-1.269266
6	-1.118681	2.066755	-1.660348
6	-0.203185	2.804346	-0.955034
1	-1.093386	2.126328	-2.747397
1	-2.693035	0.708048	-1.917002
1	1.625707	1.445660	-1.542070
1	-0.251237	2.926202	0.122635
1	0.469191	3.477361	-1.476546
6	-7.291366	-2.250862	1.337616
1	-7.481548	-3.312850	1.537604
1	-7.408519	-1.718920	2.287812
1	-8.070505	-1.900100	0.654457

TS [5a-8]

Number of imaginary frequencies : 1
 The smallest frequencies are : -626.0827 14.7313 22.1141 cm(-1)

Electronic energy : HF=-2445.1998594
 Zero-point correction= 0.852225
 (Hartree/Particle)
 Thermal correction to Energy= 0.893664
 Thermal correction to Enthalpy= 0.894608
 Thermal correction to Gibbs Free Energy= 0.776936
 Sum of electronic and zero-point Energies= -2444.347634
 Sum of electronic and thermal Energies= -2444.306195
 Sum of electronic and thermal Enthalpies= -2444.305251
 Sum of electronic and thermal Free Energies= -2444.422923

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 Cartesian Coordinates

28	0.064899	0.229954	-0.771836
15	2.233476	-0.176711	-0.083052
6	3.270625	1.385146	-0.182710
6	4.585607	1.454434	0.618708
6	3.516612	1.801312	-1.647609
1	2.591752	2.132340	0.249233
6	5.184700	2.870511	0.544818
1	5.309630	0.738175	0.211940
1	4.423339	1.180266	1.665977
6	4.106373	3.218150	-1.725190
1	4.225226	1.101554	-2.110037
1	2.586558	1.737950	-2.224354
6	5.401619	3.323808	-0.906280
1	6.130283	2.903310	1.099264

1	4.502740	3.572135	1.046171
1	4.292136	3.489811	-2.771194
1	3.370269	3.936994	-1.338212
1	5.786437	4.350237	-0.930716
1	6.170278	2.688817	-1.369918
6	3.076405	-1.449663	-1.167711
6	4.393185	-2.038805	-0.622373
6	2.091077	-2.563006	-1.592763
1	3.313992	-0.879738	-2.076625
6	5.026663	-3.009851	-1.633057
1	4.197935	-2.575112	0.314137
1	5.102628	-1.240939	-0.383303
6	2.744414	-3.525730	-2.595632
1	1.757545	-3.124769	-0.714118
1	1.188385	-2.115730	-2.021873
6	4.047222	-4.118632	-2.041128
1	5.941233	-3.441342	-1.208179
1	5.330591	-2.448655	-2.528538
1	2.039069	-4.324466	-2.854146
1	2.962921	-2.984060	-3.527716
1	4.511669	-4.782536	-2.780123
1	3.816386	-4.737626	-1.162444
6	2.373725	-0.718012	1.698062
6	1.647981	0.330677	2.574312
6	1.785709	-2.126794	1.927766
1	3.437793	-0.735946	1.969203
6	1.654264	-0.064228	4.058753
1	0.608213	0.419274	2.231775
1	2.110840	1.317973	2.452482
6	1.788224	-2.499867	3.418913
1	0.759830	-2.161757	1.553401
1	2.359400	-2.871016	1.367206
6	1.042772	-1.456410	4.260975
1	1.103406	0.686454	4.638150
1	2.688736	-0.058106	4.433534
1	1.329540	-3.487985	3.543340
1	2.826402	-2.584395	3.774608
1	1.067945	-1.733104	5.322285
1	-0.008001	-1.437019	3.948292
7	-1.848243	0.463526	0.883647
6	-2.390452	1.246939	-0.254387
6	-3.354675	2.332461	0.310476
6	-2.725854	3.331900	1.306814
6	-4.174613	3.059266	-0.780015
1	-4.059079	1.719237	0.887268
6	-2.070175	4.567319	0.666338
1	-2.015408	2.797944	1.946510
1	-3.529438	3.685692	1.967759
6	-3.472807	4.274684	-1.407817
1	-4.475821	2.345179	-1.557919
1	-5.105254	3.415088	-0.316933
6	-3.012498	5.261398	-0.326285
1	-1.156202	4.280770	0.135482
1	-1.765298	5.265655	1.455974
1	-4.153430	4.766994	-2.113392
1	-2.600254	3.954078	-1.991239
1	-2.518114	6.128192	-0.782325

1	-3.892397	5.645828	0.210436
16	-1.829527	-1.106731	0.707629
8	-0.838494	-1.535873	-0.403304
8	-1.572567	-1.780226	1.994247
6	-3.416947	-1.698756	0.092194
6	-4.513522	-1.645773	0.959416
6	-3.569508	-2.131100	-1.223933
6	-5.765322	-2.038309	0.498283
1	-4.379474	-1.309765	1.982686
6	-4.834023	-2.521235	-1.671841
1	-2.704866	-2.166083	-1.877379
6	-5.946911	-2.479504	-0.823599
1	-6.618533	-2.005067	1.171377
1	-4.954585	-2.861595	-2.697044
6	-1.259218	1.706190	-1.166725
6	0.001861	2.180941	-0.716987
1	-1.548816	1.939661	-2.188533
1	-3.032221	0.621973	-0.892750
1	-0.407486	0.240853	-2.117664
1	0.161086	2.398947	0.336665
1	0.620357	2.749211	-1.406969
6	-7.314021	-2.906285	-1.299211
1	-7.314405	-3.147870	-2.365806
1	-7.660341	-3.793331	-0.755527
1	-8.056758	-2.117866	-1.131587

7

Number of imaginary frequencies : 0
The smallest frequencies are : 14.4109 20.2805 24.0845 cm(-1)

Electronic energy : HF=-3672.239434
Zero-point correction= 1.229572
(Hartree/Particle)
Thermal correction to Energy= 1.291173
Thermal correction to Enthalpy= 1.292117
Thermal correction to Gibbs Free Energy= 1.132378
Sum of electronic and zero-point Energies= -3671.009862
Sum of electronic and thermal Energies= -3670.948261
Sum of electronic and thermal Enthalpies= -3670.947317
Sum of electronic and thermal Free Energies= -3671.107056

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Cartesian Coordinates
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28	1.461017	-0.159653	0.226047
15	3.541076	0.375245	-0.229124
6	3.974633	2.090622	0.359924
6	5.417481	2.578065	0.137671
6	2.962010	3.116168	-0.190129
1	3.807921	2.031710	1.441991
6	5.623701	3.950086	0.803393
1	5.611609	2.672664	-0.937988
1	6.140918	1.855593	0.532893
6	3.166553	4.490431	0.463442
1	3.088108	3.215605	-1.277399
1	1.943984	2.755293	-0.024373

6	4.610681	4.984474	0.289517
1	6.648137	4.298639	0.626860
1	5.511546	3.840270	1.891391
1	2.460301	5.213536	0.038501
1	2.931217	4.413395	1.534098
1	4.751524	5.941581	0.805232
1	4.799799	5.170931	-0.777379
6	3.994578	0.360300	-2.057306
6	5.487745	0.102394	-2.360108
6	3.119310	-0.585688	-2.907689
1	3.762156	1.387992	-2.371427
6	5.780402	0.298958	-3.857030
1	5.738289	-0.929789	-2.085321
1	6.134868	0.752846	-1.765880
6	3.412031	-0.402021	-4.404750
1	3.313187	-1.625697	-2.621418
1	2.061355	-0.418319	-2.709848
6	4.898454	-0.609773	-4.723799
1	6.841911	0.105510	-4.053301
1	5.596766	1.349578	-4.124447
1	2.793620	-1.094629	-4.987213
1	3.114572	0.613060	-4.706186
1	5.092199	-0.427168	-5.787395
1	5.165411	-1.658580	-4.529861
6	4.729268	-0.802465	0.601381
6	4.764011	-0.642134	2.134592
6	4.362249	-2.256240	0.226901
1	5.731496	-0.578559	0.215065
6	5.744614	-1.641623	2.768563
1	3.761995	-0.826448	2.537250
1	5.042004	0.380359	2.413703
6	5.324227	-3.263482	0.874755
1	3.335979	-2.459214	0.556846
1	4.367775	-2.389190	-0.859411
6	5.382756	-3.086339	2.397534
1	5.746684	-1.513898	3.857594
1	6.764465	-1.419354	2.422866
1	5.012035	-4.282727	0.619404
1	6.331352	-3.126419	0.454876
1	6.103748	-3.785709	2.837165
1	4.400565	-3.331344	2.825199
7	-2.242445	0.575190	-0.327409
6	-2.001692	1.979347	-0.717790
6	-2.533215	2.934863	0.398116
6	-1.738943	2.919403	1.720732
6	-2.801895	4.388964	-0.063321
1	-3.514207	2.503073	0.618390
6	-0.527502	3.865403	1.753545
1	-1.432191	1.893409	1.940313
1	-2.420000	3.216170	2.530836
6	-1.595072	5.340283	-0.004318
1	-3.237181	4.383973	-1.070624
1	-3.577002	4.801339	0.597995
6	-0.922999	5.300037	1.375807
1	0.244153	3.513155	1.060949
1	-0.072806	3.846716	2.752317
1	-1.924060	6.361263	-0.235550

1	-0.858761	5.080002	-0.774777
1	-0.045287	5.957975	1.395371
1	-1.624725	5.689177	2.127926
16	-3.321456	-0.186132	-1.240458
8	-2.940216	-0.265491	-2.680311
8	-3.649472	-1.467794	-0.571927
6	-0.584660	2.206850	-1.196908
6	0.170178	1.286147	-1.804036
1	-0.195546	3.216016	-1.102403
1	1.143639	1.544978	-2.206409
1	-0.200892	0.282288	-1.980428
1	-2.612789	2.240371	-1.598019
7	-0.324380	-1.024792	0.754734
1	-1.115490	-0.488062	0.201565
6	-0.555973	-0.883352	2.240782
6	-1.284902	-2.059169	2.925935
6	-1.385937	-1.853862	4.455525
6	-2.704112	-2.274620	2.357084
1	-0.686651	-2.960232	2.756564
6	-2.317876	-0.693397	4.838327
1	-0.394728	-1.722463	4.901469
1	-1.791506	-2.780408	4.884402
6	-3.675191	-1.145688	2.736843
1	-2.693067	-2.366984	1.271067
1	-3.084092	-3.226151	2.755152
6	-3.723121	-0.905318	4.253237
1	-1.906421	0.256723	4.470311
1	-2.369107	-0.602566	5.930383
1	-4.672873	-1.396912	2.359667
1	-3.378963	-0.227280	2.215431
1	-4.366324	-0.047419	4.486008
1	-4.177607	-1.779809	4.741886
16	0.216269	-2.478895	0.028527
8	0.960128	-1.893016	-1.134843
8	0.955470	-3.265380	1.026827
6	-1.078329	-3.481463	-0.645812
6	-1.486266	-4.615542	0.061513
6	-1.652757	-3.127894	-1.868299
6	-2.492444	-5.409364	-0.478756
1	-1.014998	-4.871828	1.003315
6	-2.652395	-3.940214	-2.389089
1	-1.354749	-2.226924	-2.389531
6	-3.090222	-5.083103	-1.706069
1	-2.818428	-6.295212	0.058857
1	-3.119742	-3.660851	-3.328304
6	0.783611	-0.466038	2.855836
6	1.452911	0.598753	1.980019
1	0.619931	-0.073556	3.868632
1	0.818901	1.487786	1.881032
1	2.405477	0.911651	2.412473
1	-1.216963	-0.013705	2.259506
6	-4.840557	0.801226	-1.222498
6	-5.192403	1.575118	-2.328652
6	-5.620630	0.831758	-0.064137
6	-6.321119	2.393378	-2.266730
1	-4.581069	1.524698	-3.223233
6	-6.748549	1.648292	-0.016432

1	-5.339137	0.222148	0.787121
6	-7.114908	2.444161	-1.112956
1	-6.590420	3.000497	-3.127930
1	-7.354554	1.672274	0.886175
1	1.425508	-1.349716	2.953783
6	-8.348743	3.312718	-1.062180
1	-8.215310	4.233548	-1.639044
1	-9.217314	2.790201	-1.483188
1	-8.603826	3.590453	-0.034776
6	-4.209097	-5.920412	-2.271144
1	-5.169894	-5.405198	-2.150592
1	-4.071562	-6.097796	-3.342934
1	-4.285369	-6.889614	-1.770258

8

Number of imaginary frequencies : 0
The smallest frequencies are : 10.6226 17.7570 29.4359 cm(-1)

Electronic energy : HF=-2445.2851124
Zero-point correction= 0.859671
(Hartree/Particle)
Thermal correction to Energy= 0.900203
Thermal correction to Enthalpy= 0.901147
Thermal correction to Gibbs Free Energy= 0.786156
Sum of electronic and zero-point Energies= -2444.425442
Sum of electronic and thermal Energies= -2444.384910
Sum of electronic and thermal Enthalpies= -2444.383965
Sum of electronic and thermal Free Energies= -2444.498956

.....
Cartesian Coordinates
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28	0.140626	-0.463128	-0.194199
15	2.288112	-0.056301	0.168250
6	2.820797	-0.165778	1.954498
6	4.336789	-0.102158	2.218073
6	2.076789	0.879818	2.812773
1	2.461902	-1.152775	2.269296
6	4.638540	-0.306245	3.712640
1	4.720559	0.878785	1.909696
1	4.868456	-0.853417	1.623398
6	2.378061	0.678445	4.305961
1	2.392709	1.890882	2.520813
1	0.999955	0.819799	2.627545
6	3.888353	0.713385	4.581853
1	5.718847	-0.236006	3.887444
1	4.337892	-1.322799	4.003310
1	1.863800	1.445567	4.897174
1	1.970986	-0.291304	4.625048
1	4.086836	0.527195	5.643943
1	4.269164	1.721148	4.362191
6	3.003067	1.587477	-0.413076
6	4.439545	1.529691	-0.975885
6	2.061204	2.321227	-1.389271
1	3.037902	2.184429	0.508966
6	4.959163	2.940773	-1.298234

1	4.450921	0.934652	-1.896952
1	5.118486	1.036328	-0.273689
6	2.591222	3.723459	-1.722339
1	1.954123	1.737778	-2.311623
1	1.054921	2.382320	-0.967595
6	4.023987	3.673696	-2.269757
1	5.971343	2.874097	-1.715275
1	5.041407	3.517831	-0.365694
1	1.921563	4.209109	-2.441693
1	2.575188	4.339890	-0.811339
1	4.396022	4.686243	-2.467026
1	4.022001	3.144521	-3.233313
6	3.227497	-1.396770	-0.735060
6	2.990929	-2.780157	-0.093341
6	2.791519	-1.421321	-2.217732
1	4.299001	-1.168102	-0.684400
6	3.716363	-3.887148	-0.875325
1	1.912261	-2.984165	-0.082989
1	3.326866	-2.787690	0.949726
6	3.523973	-2.523198	-2.997022
1	1.708412	-1.600119	-2.262592
1	2.960170	-0.448481	-2.691245
6	3.302900	-3.898658	-2.353381
1	3.512795	-4.859867	-0.411774
1	4.801614	-3.725170	-0.804073
1	3.182323	-2.528054	-4.038715
1	4.600494	-2.298957	-3.017886
1	3.858730	-4.670859	-2.898528
1	2.238457	-4.161647	-2.427680
7	-1.603422	-0.994549	-0.749287
6	-2.473472	-1.581736	0.295081
6	-3.646945	-2.426699	-0.260350
6	-4.246603	-3.391068	0.789845
6	-4.801466	-1.571581	-0.834053
1	-3.219691	-3.025596	-1.075054
6	-4.997320	-2.650570	1.908973
1	-3.475284	-4.044113	1.209395
1	-4.956698	-4.051215	0.272509
6	-5.575876	-0.811196	0.255466
1	-4.438871	-0.885108	-1.600377
1	-5.496876	-2.250205	-1.347782
6	-6.113783	-1.765409	1.332301
1	-4.293585	-2.026601	2.476727
1	-5.415077	-3.372395	2.621684
1	-6.400611	-0.250387	-0.201105
1	-4.924069	-0.061282	0.721158
1	-6.608575	-1.201915	2.133249
1	-6.881070	-2.412915	0.883708
16	-1.914779	0.241232	-1.740048
8	-0.496356	0.739603	-1.957326
8	-2.693028	-0.039103	-2.957729
6	-2.805454	1.519765	-0.837808
6	-3.989839	2.035437	-1.361924
6	-2.328576	1.951303	0.404445
6	-4.696711	2.995574	-0.637340
1	-4.348464	1.680167	-2.321451
6	-3.046439	2.907598	1.116229

1	-1.411178	1.533443	0.809780
6	-4.240050	3.446005	0.607915
1	-5.620241	3.396930	-1.045988
1	-2.678802	3.240205	2.083783
6	-1.441815	-2.377084	1.112996
6	-0.215634	-1.497419	1.394214
1	-0.455573	-0.749913	2.167290
1	-1.144556	-3.252531	0.520765
1	-1.885231	-2.749169	2.045717
1	-2.862376	-0.777480	0.937459
1	0.619460	-2.100006	1.769072
6	-4.994413	4.498342	1.381705
1	-4.516066	5.479926	1.273440
1	-6.025992	4.594571	1.031286
1	-5.018195	4.267863	2.451887

9

Number of imaginary frequencies : 0
The smallest frequencies are : 18.2673 22.4961 33.5385 cm(-1)

Electronic energy : HF=-2445.2487986
Zero-point correction= 0.856804
(Hartree/Particle)
Thermal correction to Energy= 0.898562
Thermal correction to Enthalpy= 0.899506
Thermal correction to Gibbs Free Energy= 0.783483
Sum of electronic and zero-point Energies= -2444.391995
Sum of electronic and thermal Energies= -2444.350237
Sum of electronic and thermal Enthalpies= -2444.349293
Sum of electronic and thermal Free Energies= -2444.465316

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

28	0.334069	1.288273	0.311384
15	2.123292	-0.115664	-0.023970
6	3.603407	0.839756	-0.694465
6	4.931422	0.062748	-0.808094
6	3.255745	1.509492	-2.040654
1	3.762522	1.641477	0.034309
6	6.066768	0.989475	-1.277606
1	4.827196	-0.758571	-1.528203
1	5.201572	-0.394454	0.149325
6	4.388705	2.436522	-2.507818
1	3.093249	0.737195	-2.803673
1	2.313726	2.064146	-1.954102
6	5.721621	1.680284	-2.604465
1	6.997575	0.417615	-1.375292
1	6.246833	1.753337	-0.507661
1	4.132199	2.885334	-3.474989
1	4.493742	3.265057	-1.792712
1	6.527670	2.362738	-2.899453
1	5.646889	0.921159	-3.396343
6	2.013216	-1.483959	-1.334942
6	1.973346	-2.943121	-0.839641
6	0.862734	-1.218933	-2.327945

1	2.951595	-1.378119	-1.893496
6	2.039752	-3.915000	-2.030604
1	1.046393	-3.115360	-0.290254
1	2.806454	-3.146997	-0.158453
6	0.924984	-2.195661	-3.512069
1	-0.085913	-1.326022	-1.800229
1	0.895730	-0.183893	-2.688015
6	0.905032	-3.653112	-3.030472
1	1.996727	-4.948298	-1.664883
1	3.006853	-3.802082	-2.542934
1	0.086590	-2.006346	-4.194036
1	1.844925	-2.018541	-4.089432
1	0.977581	-4.341567	-3.881545
1	-0.056354	-3.853814	-2.537684
6	2.814685	-0.908168	1.536711
6	3.517438	0.106233	2.466210
6	1.723980	-1.648124	2.339608
1	3.565785	-1.638610	1.207124
6	4.137322	-0.600010	3.682803
1	2.775417	0.830545	2.824672
1	4.292139	0.673795	1.942073
6	2.318955	-2.350420	3.569997
1	0.962015	-0.923510	2.654371
1	1.196801	-2.369506	1.717825
6	3.077972	-1.373577	4.477522
1	4.636394	0.137801	4.323076
1	4.916495	-1.294734	3.336755
1	1.518327	-2.848722	4.129273
1	3.006748	-3.140847	3.234385
1	3.542115	-1.905862	5.316881
1	2.364591	-0.659071	4.912379
7	-1.189804	0.244308	-0.297121
6	-1.598770	1.562256	-0.150510
6	-2.867081	1.997355	0.593166
6	-2.915634	3.457372	1.091528
6	-4.089797	1.782617	-0.354137
1	-2.984834	1.352768	1.465979
6	-2.951793	4.493276	-0.042034
1	-2.101282	3.661068	1.785592
1	-3.841306	3.562995	1.674898
6	-4.179656	2.820083	-1.485442
1	-4.073398	0.778026	-0.779489
1	-4.998446	1.845894	0.260220
6	-4.164998	4.259642	-0.953720
1	-2.033018	4.430869	-0.641014
1	-2.978651	5.505438	0.379496
1	-5.090599	2.639035	-2.069085
1	-3.341528	2.683969	-2.182092
1	-4.168857	4.975749	-1.784503
1	-5.083512	4.440399	-0.376690
16	-1.625820	-0.946153	0.813692
8	-0.796749	-2.115107	0.467865
8	-1.642955	-0.492868	2.223698
6	-3.305009	-1.384732	0.359983
6	-4.332567	-1.243445	1.289397
6	-3.552966	-1.884645	-0.921238
6	-5.631829	-1.594493	0.922169

1	-4.110546	-0.858707	2.278752
6	-4.856604	-2.219490	-1.274525
1	-2.738687	-1.995969	-1.629450
6	-5.914738	-2.081627	-0.360619
1	-6.438000	-1.484717	1.642768
1	-5.059842	-2.597883	-2.273010
6	0.274517	3.164165	1.130884
6	1.587835	2.778796	0.901775
1	2.124534	3.174370	0.042556
1	-0.158424	3.060709	2.122401
1	-0.213104	3.875805	0.474382
1	-1.474915	2.090079	-1.101566
1	2.212009	2.439409	1.721751
6	-7.316449	-2.484914	-0.746029
1	-7.517827	-2.276118	-1.801507
1	-7.466983	-3.561089	-0.593210
1	-8.066558	-1.961823	-0.145528

TS [8-9]

Number of imaginary frequencies : 1
 The smallest frequencies are : -182.1527 14.6377 18.1233 cm(-1)

Electronic energy : HF=-2445.2285914
 Zero-point correction= 0.856313
 (Hartree/Particle)
 Thermal correction to Energy= 0.897342
 Thermal correction to Enthalpy= 0.898287
 Thermal correction to Gibbs Free Energy= 0.781856
 Sum of electronic and zero-point Energies= -2444.372279
 Sum of electronic and thermal Energies= -2444.331249
 Sum of electronic and thermal Enthalpies= -2444.330305
 Sum of electronic and thermal Free Energies= -2444.446735

.....
 Cartesian Coordinates

28	0.414259	0.890979	0.452577
15	2.263737	-0.084847	-0.054461
6	3.604216	1.196342	-0.300209
6	5.005452	0.643454	-0.620470
6	3.186250	2.255810	-1.341251
1	3.643499	1.702770	0.672303
6	6.040020	1.778797	-0.694022
1	4.978263	0.121876	-1.585821
1	5.314369	-0.093546	0.129048
6	4.220199	3.390364	-1.415386
1	3.096895	1.789161	-2.331962
1	2.196261	2.653214	-1.090332
6	5.627064	2.851062	-1.712535
1	7.025467	1.370213	-0.947857
1	6.136884	2.239633	0.299292
1	3.921248	4.119277	-2.178067
1	4.232149	3.925723	-0.455301
1	6.355819	3.670358	-1.719983
1	5.637415	2.411499	-2.720220
6	2.297271	-1.069545	-1.664308

6	3.227415	-2.300925	-1.674569
6	0.885905	-1.451434	-2.153854
1	2.706675	-0.345190	-2.382883
6	3.278298	-2.935828	-3.074729
1	2.854036	-3.045958	-0.961682
1	4.240377	-2.035080	-1.355514
6	0.942513	-2.088950	-3.549679
1	0.427653	-2.145987	-1.443221
1	0.235341	-0.572052	-2.152578
6	1.875970	-3.307069	-3.575835
1	3.927080	-3.820028	-3.055678
1	3.737851	-2.223587	-3.775500
1	-0.067945	-2.376264	-3.865431
1	1.299528	-1.345695	-4.278274
1	1.932515	-3.729136	-4.586640
1	1.459848	-4.091257	-2.927725
6	2.909304	-1.210220	1.292750
6	3.390771	-0.434522	2.535683
6	1.829348	-2.235269	1.694912
1	3.770329	-1.748004	0.876309
6	3.913512	-1.396433	3.615008
1	2.552903	0.143236	2.943620
1	4.177204	0.281613	2.274801
6	2.350165	-3.197825	2.770926
1	0.951116	-1.697151	2.068894
1	1.470383	-2.791589	0.825713
6	2.854837	-2.437381	4.004699
1	4.232280	-0.824247	4.494834
1	4.807316	-1.911569	3.234595
1	1.554177	-3.897141	3.051993
1	3.170457	-3.801811	2.355504
1	3.261055	-3.133984	4.748154
1	2.006232	-1.925532	4.479877
7	-1.320356	0.270662	-0.205525
6	-1.593911	1.631837	0.214215
6	-3.049713	1.954458	0.654988
6	-3.331345	3.358906	1.235669
6	-3.983401	1.757357	-0.573134
1	-3.317112	1.228850	1.426160
6	-3.173750	4.492221	0.210023
1	-2.739253	3.555648	2.132303
1	-4.377245	3.347936	1.572384
6	-3.870414	2.883874	-1.613543
1	-3.786094	0.798604	-1.052019
1	-5.015499	1.716145	-0.200326
6	-4.099274	4.269116	-0.994539
1	-2.132371	4.546643	-0.138272
1	-3.390051	5.456101	0.686190
1	-4.591549	2.704069	-2.420093
1	-2.878477	2.856036	-2.084536
1	-3.953087	5.055305	-1.745236
1	-5.143270	4.344639	-0.657582
16	-1.802088	-0.987058	0.774162
8	-0.988925	-2.159704	0.396576
8	-1.864860	-0.615412	2.211457
6	-3.477146	-1.403422	0.262745
6	-4.534135	-1.288953	1.162054

1	2.202869	-5.592368	-1.689299
6	0.116988	-2.092256	1.412347
6	0.680283	-2.715190	2.710286
6	-1.172677	-1.314921	1.746443
1	-0.161813	-2.913326	0.733454
6	-0.357273	-3.637750	3.373627
1	0.932583	-1.910175	3.410878
1	1.601109	-3.269698	2.529672
6	-2.216238	-2.226836	2.407104
1	-0.927274	-0.502193	2.440672
1	-1.573480	-0.835782	0.853366
6	-1.665267	-2.893621	3.673901
1	0.062556	-4.063695	4.293397
1	-0.565035	-4.484155	2.702801
1	-3.120900	-1.650112	2.633899
1	-2.517811	-3.004770	1.691814
1	-2.405359	-3.578723	4.105218
1	-1.471381	-2.120932	4.431689
6	2.464499	-0.119087	1.458823
6	1.661679	0.819149	2.385773
6	3.597672	-0.823428	2.228671
1	2.950027	0.534069	0.723569
6	2.583798	1.850955	3.051285
1	1.157274	0.233833	3.164031
1	0.875475	1.324567	1.814747
6	4.511514	0.214160	2.907199
1	3.184723	-1.495450	2.989125
1	4.194333	-1.440694	1.548457
6	3.719401	1.160678	3.820451
1	2.002311	2.495623	3.721427
1	3.012293	2.501253	2.275831
1	5.297501	-0.298430	3.475249
1	5.014824	0.806181	2.130478
1	4.388704	1.906947	4.264901
1	3.291383	0.584873	4.653813
7	-1.317668	0.751147	-0.792638
6	-1.948257	2.065537	-0.454234
6	-3.056018	1.898978	0.633530
6	-2.588445	2.028523	2.102523
6	-4.280757	2.806707	0.382255
1	-3.405281	0.870008	0.512254
6	-2.464456	3.471879	2.626136
1	-1.641794	1.496669	2.238731
1	-3.323529	1.504707	2.729462
6	-4.075134	4.256475	0.841082
1	-4.552147	2.773466	-0.679775
1	-5.137308	2.389654	0.930871
6	-3.722690	4.302337	2.334534
1	-1.602749	3.970542	2.170187
1	-2.267803	3.448239	3.705678
1	-4.979741	4.844702	0.643008
1	-3.267416	4.722011	0.259474
1	-3.579164	5.337688	2.667294
1	-4.568184	3.900392	2.911954
16	-1.931249	-0.012306	-2.109991
8	-2.263654	0.904301	-3.226715
8	-1.023209	-1.152739	-2.390871

6	-3.498044	-0.728047	-1.587354
6	-3.502198	-1.942843	-0.899471
6	-4.689138	-0.042286	-1.826691
6	-4.708478	-2.459129	-0.432577
1	-2.568766	-2.470449	-0.740295
6	-5.888679	-0.567943	-1.348173
1	-4.668021	0.888283	-2.382731
6	-5.918304	-1.779555	-0.643527
1	-4.713067	-3.404063	0.104900
1	-6.816049	-0.030134	-1.528145
6	-0.746904	2.956772	-0.139992
6	0.293289	2.694536	-1.217965
1	-0.084521	2.988035	-2.203014
1	-0.337205	2.700598	0.842431
1	-1.027127	4.019119	-0.096734
1	-2.422355	2.478215	-1.354897
1	1.249571	3.192417	-1.024251
6	2.638538	0.715113	-2.112547
6	1.542785	0.923401	-2.932623
1	1.358005	1.879052	-3.410092
1	1.024947	0.078972	-3.382188
1	2.934551	-0.310841	-1.932926
6	3.651554	1.705173	-1.704533
6	3.604631	3.064304	-2.069661
6	4.743076	1.272013	-0.926753
6	4.587790	3.953664	-1.641229
1	2.799910	3.427188	-2.699566
6	5.727812	2.161027	-0.498976
1	4.818974	0.221361	-0.658791
6	5.649562	3.511197	-0.846562
1	4.528247	4.997993	-1.934873
1	6.556348	1.797326	0.102261
1	6.412664	4.208642	-0.513877
6	-7.222162	-2.357937	-0.151436
1	-7.959817	-1.574975	0.049467
1	-7.658358	-3.033382	-0.898377
1	-7.082501	-2.936741	0.766992

TS [A-B]

Normal termination of Gaussian 09 at Fri Apr 19 22:04:20 2019.

Number of imaginary frequencies : 1

The smallest frequencies are : -287.7869 17.5455 23.1443 cm(-1)

Electronic energy : HF=-2754.9293157

Zero-point correction= 0.997103
 (Hartree/Particle)

Thermal correction to Energy= 1.044737

Thermal correction to Enthalpy= 1.045681

Thermal correction to Gibbs Free Energy= 0.916866

Sum of electronic and zero-point Energies= -2753.932213

Sum of electronic and thermal Energies= -2753.884579

Sum of electronic and thermal Enthalpies= -2753.883634

Sum of electronic and thermal Free Energies= -2754.012450

.....
 Cartesian Coordinates

28	0.496187	0.499884	-1.228813
15	1.433839	-0.840680	0.365609
6	2.494334	-2.163036	-0.453755
6	3.129474	-3.276391	0.407077
6	1.726512	-2.823447	-1.623082
1	3.319285	-1.570452	-0.872146
6	4.085570	-4.132727	-0.442554
1	2.338008	-3.921712	0.807597
1	3.673731	-2.867744	1.260795
6	2.662367	-3.683789	-2.484421
1	0.922412	-3.446279	-1.215741
1	1.216473	-2.076224	-2.234597
6	3.370503	-4.757494	-1.647144
1	4.535614	-4.912660	0.183635
1	4.912133	-3.499481	-0.796630
1	2.093333	-4.146965	-3.298978
1	3.415959	-3.035577	-2.956428
1	4.081349	-5.321235	-2.263420
1	2.624086	-5.479239	-1.285868
6	0.391183	-1.783274	1.622066
6	1.146916	-2.260586	2.884852
6	-0.893792	-1.058588	2.068207
1	0.081201	-2.659597	1.035734
6	0.269258	-3.194438	3.735918
1	1.411699	-1.384004	3.488247
1	2.080299	-2.765342	2.641647
6	-1.781036	-1.981254	2.917736
1	-0.623836	-0.183290	2.671523
1	-1.429221	-0.686295	1.196693
6	-1.040867	-2.513399	4.150507
1	0.830405	-3.520803	4.620207
1	0.042242	-4.100378	3.155569
1	-2.692772	-1.446502	3.211101
1	-2.102611	-2.835701	2.305426
1	-1.674191	-3.209511	4.714075
1	-0.812529	-1.675914	4.825437
6	2.609106	0.311317	1.266954
6	1.821055	1.346749	2.097186
6	3.809754	-0.252115	2.052058
1	3.036861	0.860769	0.424902
6	2.741130	2.475438	2.586182
1	1.353320	0.860774	2.962093
1	1.007972	1.762130	1.489955
6	4.715080	0.894638	2.536183
1	3.475128	-0.836542	2.914732
1	4.394604	-0.922233	1.414901
6	3.936535	1.918984	3.372789
1	2.169986	3.182005	3.200819
1	3.111414	3.032345	1.715069
1	5.551955	0.484134	3.114485
1	5.147854	1.398630	1.661410
1	4.598444	2.735147	3.686920
1	3.572535	1.436929	4.291895
7	-1.420300	0.289823	-0.745715
6	-2.161427	1.577054	-0.773353
6	-3.015090	1.760117	0.516126

6	-2.231119	2.228934	1.764122
6	-4.278951	2.625837	0.304955
1	-3.374332	0.750321	0.733887
6	-2.044541	3.752498	1.890539
1	-1.259564	1.728820	1.792404
1	-2.776954	1.881849	2.652278
6	-4.033231	4.139376	0.381951
1	-4.753175	2.357524	-0.646860
1	-5.002660	2.361434	1.088891
6	-3.366164	4.512193	1.713335
1	-1.331574	4.114192	1.141296
1	-1.602019	3.980921	2.868375
1	-4.982867	4.676631	0.266007
1	-3.391447	4.462156	-0.448918
1	-3.194202	5.594000	1.771040
1	-4.047117	4.256368	2.538163
16	-2.027018	-0.890326	-1.695975
8	-2.138936	-0.505020	-3.128047
8	-1.281330	-2.130829	-1.377010
6	-3.722706	-1.139450	-1.136994
6	-3.954005	-1.915732	-0.001088
6	-4.781996	-0.521283	-1.802014
6	-5.252325	-2.051598	0.484550
1	-3.121008	-2.406652	0.486428
6	-6.077452	-0.665467	-1.305530
1	-4.586449	0.055119	-2.699685
6	-6.332854	-1.424236	-0.154296
1	-5.430584	-2.653251	1.372388
1	-6.903759	-0.181647	-1.820482
6	-1.081698	2.611256	-1.067830
6	-0.308229	2.204082	-2.329989
1	-1.007506	1.909064	-3.112944
1	-0.413955	2.721760	-0.205066
1	-1.510340	3.607253	-1.250732
1	-2.856299	1.602130	-1.624381
1	0.261792	3.070521	-2.653099
6	2.218423	0.591122	-2.259107
6	1.165209	1.022761	-3.139697
1	1.336747	1.900014	-3.750422
1	0.626374	0.244241	-3.679782
1	2.552906	-0.429453	-2.417408
6	3.303614	1.503439	-1.836670
6	3.071458	2.849419	-1.490706
6	4.618425	1.015242	-1.712141
6	4.107027	3.666197	-1.039425
1	2.064034	3.246174	-1.546508
6	5.655304	1.831393	-1.259441
1	4.824564	-0.019317	-1.975802
6	5.405773	3.162835	-0.917792
1	3.897526	4.698746	-0.773020
1	6.660032	1.426421	-1.174282
1	6.210497	3.799087	-0.561545
6	-7.741664	-1.594580	0.358856
1	-8.346360	-0.700940	0.174962
1	-8.242094	-2.433307	-0.141707
1	-7.756854	-1.800633	1.433452

6	4.104022	-0.003961	2.019693
1	3.108916	1.159937	0.540887
6	2.551653	2.362779	2.947020
1	1.487130	0.483152	3.035261
1	0.973767	1.525443	1.711909
6	4.785251	1.204287	2.686426
1	3.890109	-0.762489	2.779516
1	4.794039	-0.453519	1.299388
6	3.839727	1.924556	3.657791
1	1.864729	2.843703	3.653686
1	2.798639	3.109669	2.181876
1	5.692795	0.875861	3.207206
1	5.103111	1.906855	1.903932
1	4.341304	2.791592	4.104305
1	3.585578	1.246985	4.486112
7	-1.690135	0.513641	-1.059512
6	-2.411252	1.786490	-0.814880
6	-3.186068	1.682413	0.535405
6	-2.278763	1.548320	1.781306
6	-4.281996	2.758508	0.739071
1	-3.718993	0.731890	0.447437
6	-1.850289	2.870407	2.439979
1	-1.398754	0.955726	1.514659
1	-2.823590	0.962001	2.534549
6	-3.828905	4.062108	1.419714
1	-4.764794	2.979935	-0.221697
1	-5.062026	2.313724	1.372651
6	-3.056626	3.777374	2.715294
1	-1.139861	3.406441	1.800054
1	-1.317734	2.651634	3.374585
1	-4.708222	4.683842	1.629909
1	-3.193964	4.650676	0.746544
1	-2.733800	4.715680	3.182805
1	-3.725730	3.280708	3.433541
16	-2.375183	-0.561770	-2.094107
8	-2.915658	0.082601	-3.312571
8	-1.400066	-1.667434	-2.246584
6	-3.794407	-1.241745	-1.220822
6	-3.588663	-2.221291	-0.245418
6	-5.069768	-0.734082	-1.461981
6	-4.669225	-2.676576	0.502555
1	-2.593766	-2.621779	-0.089596
6	-6.145008	-1.200477	-0.703056
1	-5.210461	0.015140	-2.233373
6	-5.962819	-2.169665	0.291410
1	-4.511915	-3.440393	1.260223
1	-7.139973	-0.804217	-0.888196
6	-1.400236	2.937260	-0.893643
6	-0.798840	3.223805	-2.276199
1	-1.601937	3.560833	-2.944886
1	-0.598554	2.720055	-0.177912
1	-1.883309	3.854170	-0.544904
1	-3.156309	1.940356	-1.608066
1	-0.122796	4.081219	-2.171609
6	0.966491	1.227611	-2.210791
6	-0.059969	2.074667	-2.990217
1	0.467445	2.518060	-3.850695

1	-0.799337	1.390207	-3.406599
1	1.244872	0.394532	-2.868808
6	2.216387	1.929348	-1.786738
6	2.222460	3.058780	-0.942825
6	3.467319	1.458201	-2.233763
6	3.414220	3.678062	-0.565955
1	1.287207	3.438607	-0.552587
6	4.663012	2.062718	-1.844063
1	3.494442	0.604046	-2.905422
6	4.644146	3.179734	-1.005506
1	3.382654	4.546986	0.085959
1	5.608903	1.667543	-2.205276
1	5.571370	3.658379	-0.704097
6	-7.123209	-2.684068	1.107246
1	-8.028679	-2.093934	0.940112
1	-7.352807	-3.725526	0.850489
1	-6.897161	-2.661029	2.179203

8a

Number of imaginary frequencies : 0
The smallest frequencies are : 15.5467 23.4031 23.8716 cm(-1)

Electronic energy : HF=-3672.2221557
Zero-point correction= 1.228408
(Hartree/Particle)
Thermal correction to Energy= 1.291019
Thermal correction to Enthalpy= 1.291963
Thermal correction to Gibbs Free Energy= 1.129828
Sum of electronic and zero-point Energies= -3670.993748
Sum of electronic and thermal Energies= -3670.931136
Sum of electronic and thermal Enthalpies= -3670.930192
Sum of electronic and thermal Free Energies= -3671.092328

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Cartesian Coordinates
.....

28	3.196184	-0.241676	-0.062250
15	2.231244	-2.120039	-0.396309
6	1.231980	-2.622672	1.102859
6	0.846288	-4.114056	1.171316
6	1.863210	-2.145207	2.427460
1	0.320563	-2.029563	0.972891
6	-0.101925	-4.373297	2.354087
1	1.747016	-4.726047	1.299798
1	0.377834	-4.443546	0.237454
6	0.912056	-2.418056	3.602747
1	2.817402	-2.659386	2.600781
1	2.076866	-1.074176	2.368016
6	0.508744	-3.896996	3.679447
1	-0.350056	-5.440453	2.405543
1	-1.044709	-3.837971	2.179701
1	1.379369	-2.097034	4.541177
1	0.009998	-1.803608	3.475983
1	-0.197958	-4.058876	4.502313
1	1.398319	-4.503205	3.904687
6	3.358346	-3.542945	-0.840067

6	4.154512	-3.209073	-2.120945
6	4.326405	-3.946843	0.289833
1	2.695983	-4.394981	-1.053450
6	5.055431	-4.379453	-2.545764
1	4.769672	-2.320119	-1.923866
1	3.482038	-2.948497	-2.945003
6	5.210850	-5.130314	-0.134977
1	4.964428	-3.090957	0.533691
1	3.779978	-4.200531	1.202640
6	5.997313	-4.808808	-1.412883
1	5.629930	-4.099629	-3.437022
1	4.423573	-5.231685	-2.833743
1	5.896052	-5.390905	0.680517
1	4.578444	-6.012789	-0.308503
1	6.597143	-5.673197	-1.721970
1	6.703958	-3.993148	-1.203164
6	1.036449	-2.100509	-1.864051
6	-0.461529	-2.166574	-1.507801
6	1.307338	-0.868036	-2.756212
1	1.280178	-3.006536	-2.437377
6	-1.322148	-2.202902	-2.779670
1	-0.729932	-1.286487	-0.918644
1	-0.683701	-3.046374	-0.898267
6	0.433237	-0.881631	-4.018862
1	1.106471	0.033248	-2.167945
1	2.368807	-0.821602	-3.029901
6	-1.058875	-0.980282	-3.668337
1	-2.379933	-2.257923	-2.496802
1	-1.102388	-3.121567	-3.344044
1	0.627908	0.021657	-4.609434
1	0.715271	-1.738492	-4.648971
1	-1.660881	-1.034909	-4.584084
1	-1.371736	-0.072149	-3.136266
7	2.231770	1.427623	-0.334764
6	3.590923	1.950545	-0.042099
6	3.607897	3.412697	0.500130
6	4.988168	3.966939	0.915285
6	2.999901	4.366225	-0.559975
1	2.974055	3.422470	1.391531
6	5.939838	4.174834	-0.273587
1	5.455453	3.350594	1.688375
1	4.807182	4.942902	1.386404
6	3.934853	4.620395	-1.754546
1	2.045371	3.978554	-0.916268
1	2.785706	5.322117	-0.063901
6	5.316456	5.120566	-1.310585
1	6.163431	3.209467	-0.750099
1	6.898119	4.573073	0.081323
1	3.467514	5.344618	-2.432509
1	4.053484	3.695925	-2.336192
1	5.980384	5.234623	-2.176118
1	5.210565	6.118275	-0.860805
16	1.076729	1.473688	0.832179
8	0.087895	0.421266	0.452881
8	1.601263	1.430633	2.222482
6	0.185716	3.020610	0.656655
6	0.160004	3.937558	1.703814

6	-0.526026	3.254449	-0.522187
6	-0.604220	5.098365	1.570128
1	0.712501	3.729716	2.613322
6	-1.288257	4.410781	-0.636231
1	-0.515773	2.531067	-1.328715
6	-1.346533	5.346102	0.408817
1	-0.636946	5.812143	2.389363
1	-1.873885	4.568509	-1.536327
6	4.604549	1.019026	0.962155
6	4.814771	-0.501369	0.779828
1	5.682237	-0.759742	0.163842
1	4.276502	1.253182	1.975095
1	5.550031	1.510751	0.737718
1	4.082495	1.950078	-1.020340
7	-2.752491	0.583913	0.042893
1	-1.743188	0.762000	-0.015067
6	-3.212370	0.302850	1.429686
6	-2.772412	-1.137014	1.797331
6	-3.228229	-1.561503	3.212271
6	-3.275868	-2.175881	0.769045
1	-1.676062	-1.138878	1.768583
6	-4.743213	-1.805173	3.306020
1	-2.920240	-0.823622	3.956652
1	-2.708735	-2.496952	3.462983
6	-4.786248	-2.444715	0.858995
1	-3.014224	-1.852749	-0.240380
1	-2.741930	-3.118179	0.952220
6	-5.205297	-2.848654	2.279104
1	-5.282606	-0.862764	3.137390
1	-5.002306	-2.127695	4.321840
1	-5.060731	-3.227997	0.141844
1	-5.342564	-1.550535	0.554825
1	-6.292154	-2.988126	2.334222
1	-4.749633	-3.818408	2.527990
16	-3.634072	1.611260	-0.921473
8	-4.178157	2.767069	-0.185828
8	-2.809802	1.830658	-2.123394
6	-5.030873	0.575144	-1.354713
6	-4.846178	-0.459811	-2.274463
6	-6.266420	0.785591	-0.746194
6	-5.913185	-1.301538	-2.567952
1	-3.882183	-0.591167	-2.752270
6	-7.326787	-0.070327	-1.050517
1	-6.388967	1.608113	-0.050206
6	-7.165834	-1.127511	-1.954672
1	-5.776103	-2.108822	-3.282702
1	-8.291303	0.086125	-0.575119
6	-2.732976	1.410641	2.350276
6	-1.663101	1.372881	3.143449
1	-3.290126	2.339281	2.245633
1	-1.358827	2.248610	3.708294
1	-1.030302	0.497732	3.244353
1	-4.306945	0.334736	1.398647
6	-2.233930	6.558810	0.286094
1	-2.064557	7.086348	-0.659225
1	-3.288958	6.259449	0.301815
1	-2.072391	7.266831	1.104100

6	-8.294753	-2.083864	-2.247428
1	-8.146621	-3.030501	-1.712813
1	-9.261550	-1.677486	-1.937068
1	-8.351008	-2.321696	-3.314759
1	4.822728	-1.049955	1.723418

TS[8a-9a]

Number of imaginary frequencies : 1
 The smallest frequencies are : -158.5784 14.8449 24.2358 cm(-1)

Electronic energy : HF=-3672.2216749
 Zero-point correction= 1.228374
 (Hartree/Particle)
 Thermal correction to Energy= 1.290300
 Thermal correction to Enthalpy= 1.291244
 Thermal correction to Gibbs Free Energy= 1.131157
 Sum of electronic and zero-point Energies= -3670.993301
 Sum of electronic and thermal Energies= -3670.931375
 Sum of electronic and thermal Enthalpies= -3670.930431
 Sum of electronic and thermal Free Energies= -3671.090517

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 Cartesian Coordinates

28	-3.247571	-0.207027	0.017867
15	-2.236025	-2.075409	0.388318
6	-1.227098	-2.609498	-1.094887
6	-0.831236	-4.099239	-1.136414
6	-1.859425	-2.161433	-2.429524
1	-0.318814	-2.009597	-0.975467
6	0.119877	-4.373985	-2.313394
1	-1.726818	-4.720172	-1.254828
1	-0.361939	-4.409024	-0.196429
6	-0.904870	-2.448337	-3.598593
1	-2.809214	-2.686501	-2.594918
1	-2.083371	-1.091492	-2.389664
6	-0.492002	-3.925821	-3.648054
1	0.375010	-5.440312	-2.345523
1	1.059080	-3.829596	-2.148259
1	-1.372224	-2.147294	-4.543695
1	-0.006520	-1.826432	-3.480952
1	0.216673	-4.098260	-4.467177
1	-1.377536	-4.541509	-3.863321
6	-3.356293	-3.502276	0.851313
6	-4.177903	-3.136539	2.107378
6	-4.299585	-3.959376	-0.279558
1	-2.688506	-4.339152	1.104178
6	-5.075590	-4.300079	2.556718
1	-4.797120	-2.259914	1.871533
1	-3.521259	-2.843221	2.933193
6	-5.178125	-5.137037	0.173152
1	-4.942790	-3.122920	-0.568711
1	-3.733643	-4.241515	-1.171633
6	-5.992785	-4.777252	1.422819
1	-5.668541	-3.995252	3.427570
1	-4.441988	-5.136324	2.884804

1	-5.844140	-5.437133	-0.644779
1	-4.538947	-6.004251	0.393202
1	-6.591798	-5.635190	1.751016
1	-6.701489	-3.975553	1.170293
6	-1.049247	-2.051243	1.865652
6	0.451803	-2.129462	1.524291
6	-1.319343	-0.814068	2.750780
1	-1.301293	-2.952417	2.443181
6	1.301634	-2.165605	2.803420
1	0.732349	-1.255041	0.933085
1	0.673759	-3.013451	0.921102
6	-0.456104	-0.827949	4.020997
1	-1.110836	0.083872	2.160961
1	-2.382659	-0.759924	3.015934
6	1.038594	-0.937592	3.684603
1	2.361564	-2.228546	2.529756
1	1.071662	-3.080275	3.370217
1	-0.650013	0.078631	4.607005
1	-0.748578	-1.680616	4.652084
1	1.632140	-0.991946	4.605942
1	1.362390	-0.033978	3.151208
7	-2.216100	1.404288	0.349892
6	-3.542351	1.937702	0.103959
6	-3.616149	3.363700	-0.508729
6	-5.016636	3.898465	-0.882552
6	-2.981404	4.364550	0.497781
1	-3.015350	3.351543	-1.422269
6	-5.924032	4.133084	0.335514
1	-5.511182	3.265038	-1.622325
1	-4.857204	4.864161	-1.381622
6	-3.870453	4.647791	1.720345
1	-2.006818	4.007209	0.829367
1	-2.804394	5.304773	-0.041072
6	-5.274299	5.118671	1.317352
1	-6.117180	3.181782	0.851517
1	-6.899943	4.508398	0.004745
1	-3.383306	5.398954	2.353395
1	-3.954117	3.742311	2.336705
1	-5.904834	5.251603	2.204847
1	-5.199181	6.102978	0.833197
16	-1.069822	1.452347	-0.843273
8	-0.080243	0.402652	-0.469269
8	-1.617786	1.402433	-2.222376
6	-0.186074	3.001910	-0.677587
6	-0.170595	3.912153	-1.730839
6	0.536663	3.240499	0.493551
6	0.596035	5.072569	-1.610748
1	-0.732205	3.699751	-2.633642
6	1.299500	4.397622	0.594158
1	0.533734	2.521724	1.304172
6	1.348722	5.326421	-0.457197
1	0.622145	5.781502	-2.434307
1	1.893386	4.560095	1.487854
6	-4.744392	0.930676	-0.925795
6	-4.885354	-0.557925	-0.807579
1	-5.714835	-0.898780	-0.182902
1	-4.479711	1.267546	-1.926163

1	-5.610707	1.449065	-0.525343
1	-4.036038	1.942371	1.079251
7	2.765310	0.579976	-0.046638
1	1.756775	0.757179	0.011923
6	3.223457	0.288088	-1.431541
6	2.785739	-1.155295	-1.787711
6	3.246258	-1.590381	-3.197925
6	3.286751	-2.185199	-0.749260
1	1.689408	-1.158580	-1.762414
6	4.761623	-1.834109	-3.285088
1	2.940261	-0.858364	-3.948964
1	2.727923	-2.527813	-3.443228
6	4.797537	-2.453798	-0.832846
1	3.021327	-1.854417	0.256820
1	2.753774	-3.129074	-0.926228
6	5.220843	-2.869174	-2.248435
1	5.300305	-0.890236	-3.122333
1	5.023894	-2.164534	-4.297535
1	5.070444	-3.231071	-0.108624
1	5.352647	-1.556852	-0.534585
1	6.307890	-3.008809	-2.299192
1	4.766108	-3.840959	-2.490866
16	3.646739	1.614804	0.910097
8	4.192474	2.763377	0.164321
8	2.819672	1.846854	2.107817
6	5.040945	0.581104	1.355399
6	4.851319	-0.449189	2.279489
6	6.279376	0.788452	0.751733
6	5.916846	-1.289353	2.582449
1	3.884834	-0.578579	2.752923
6	7.338153	-0.065876	1.065812
1	6.405318	1.607147	0.051858
6	7.172580	-1.118460	1.974504
1	5.776109	-2.093246	3.300266
1	8.304996	0.088097	0.594371
6	2.740148	1.388374	-2.359219
6	1.671892	1.341747	-3.154188
1	3.293391	2.319891	-2.259047
1	1.364927	2.213174	-3.724325
1	1.043964	0.462696	-3.252528
1	4.318010	0.322720	-1.402102
6	2.238651	6.538547	-0.349868
1	2.080153	7.070369	0.594840
1	3.292861	6.237086	-0.375284
1	2.069351	7.242785	-1.169459
6	8.299890	-2.073359	2.277770
1	8.153030	-3.023481	1.749042
1	9.268029	-1.669686	1.968107
1	8.352125	-2.304002	3.346882
1	-4.821372	-1.107419	-1.748035

9a

Number of imaginary frequencies : 0
The smallest frequencies are : 13.2904 16.9571 29.2701 cm(-1)

Electronic energy :	HF=-3672.2375879	
Zero-point correction=		1.227890
(Hartree/Particle)		
Thermal correction to Energy=		1.290983
Thermal correction to Enthalpy=		1.291927
Thermal correction to Gibbs Free Energy=		1.128991
Sum of electronic and zero-point Energies=		-3671.009698
Sum of electronic and thermal Energies=		-3670.946605
Sum of electronic and thermal Enthalpies=		-3670.945661
Sum of electronic and thermal Free Energies=		-3671.108597

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

28	3.453187	0.168899	0.054718
15	2.457959	-1.865618	-0.293599
6	1.446084	-2.402099	1.190627
6	0.997357	-3.875314	1.248747
6	2.110980	-1.969371	2.515347
1	0.553294	-1.778850	1.088644
6	0.043762	-4.096438	2.435954
1	1.864781	-4.534629	1.368424
1	0.507230	-4.173314	0.315257
6	1.153585	-2.199414	3.694379
1	3.036073	-2.537643	2.682800
1	2.387163	-0.911557	2.462849
6	0.681383	-3.658740	3.762167
1	-0.257516	-5.150256	2.483054
1	-0.870997	-3.513036	2.271262
1	1.637910	-1.907329	4.633898
1	0.283080	-1.540526	3.570084
1	-0.029816	-3.793148	4.586381
1	1.542615	-4.307231	3.980122
6	3.496465	-3.379100	-0.739535
6	4.295639	-3.166988	-2.044275
6	4.424440	-3.925419	0.366111
1	2.746013	-4.158313	-0.940039
6	5.000405	-4.460846	-2.486124
1	5.040208	-2.375733	-1.888764
1	3.643661	-2.822399	-2.852753
6	5.092188	-5.236627	-0.080698
1	5.208841	-3.200121	0.592463
1	3.873167	-4.089048	1.295412
6	5.889717	-5.037656	-1.376684
1	5.590265	-4.270793	-3.391038
1	4.237547	-5.203971	-2.759258
1	5.745368	-5.609926	0.717238
1	4.320259	-6.002992	-0.240809
1	6.338573	-5.984093	-1.701122
1	6.721223	-4.344523	-1.183415
6	1.277114	-1.895765	-1.781806
6	-0.227622	-1.875269	-1.453791
6	1.610259	-0.753805	-2.768214
1	1.480315	-2.851990	-2.284516
6	-1.064003	-1.994886	-2.736368
1	-0.476485	-0.943036	-0.943245
1	-0.492622	-2.689231	-0.774453
6	0.760868	-0.844124	-4.045479

1	1.425513	0.198199	-2.260566
1	2.677369	-0.764401	-3.023504
6	-0.740909	-0.865407	-3.722768
1	-2.128318	-1.989262	-2.475471
1	-0.864759	-2.966008	-3.213814
1	0.997630	-0.001244	-4.706389
1	1.024393	-1.759379	-4.596815
1	-1.325419	-0.980963	-4.644410
1	-1.038891	0.092953	-3.277010
7	1.969996	1.387366	-0.298946
6	3.160778	2.105012	-0.353385
6	3.398104	3.440969	0.360490
6	4.870029	3.877598	0.532680
6	2.674777	4.567648	-0.441996
1	2.951776	3.380152	1.355784
6	5.581382	4.166513	-0.797769
1	5.432855	3.159956	1.127077
1	4.856786	4.807089	1.119109
6	3.365692	4.909918	-1.772388
1	1.634788	4.300275	-0.628744
1	2.656749	5.464170	0.193126
6	4.846740	5.264521	-1.580718
1	5.630354	3.252615	-1.405937
1	6.619234	4.464966	-0.605782
1	2.834897	5.741555	-2.251528
1	3.282173	4.060145	-2.463102
1	5.328925	5.436982	-2.550643
1	4.920384	6.207568	-1.019818
16	0.967966	1.479733	1.049262
8	-0.006881	0.375689	0.863928
8	1.674799	1.539350	2.348779
6	0.035389	2.988841	0.847764
6	-0.032383	3.903645	1.894520
6	-0.690952	3.175662	-0.330472
6	-0.856485	5.021952	1.757269
1	0.539884	3.731784	2.799350
6	-1.507186	4.293537	-0.448625
1	-0.638671	2.454109	-1.136842
6	-1.609600	5.228356	0.594415
1	-0.923099	5.737532	2.572517
1	-2.097486	4.419643	-1.350294
6	5.315163	0.720956	0.689782
6	5.211042	-0.660991	0.606546
1	5.668424	-1.193878	-0.222568
1	5.192255	1.217003	1.648149
1	5.846273	1.282942	-0.071982
1	3.526248	2.115232	-1.385045
7	-2.839528	0.468434	0.075711
1	-1.841076	0.691228	0.081950
6	-3.369458	0.162101	1.431225
6	-2.868609	-1.245163	1.843638
6	-3.460415	-1.707253	3.196099
6	-3.169560	-2.311787	0.765981
1	-1.779219	-1.170304	1.943769
6	-4.953131	-2.066189	3.107283
1	-3.303222	-0.948398	3.966964
1	-2.904439	-2.599960	3.515170

6	-4.657222	-2.682046	0.670638
1	-2.802572	-1.970871	-0.203764
1	-2.602732	-3.216615	1.022029
6	-5.212502	-3.129347	2.030061
1	-5.540206	-1.165888	2.878180
1	-5.305008	-2.418335	4.084641
1	-4.790203	-3.474129	-0.076496
1	-5.233346	-1.824403	0.306435
1	-6.285686	-3.345247	1.954832
1	-4.722465	-4.067402	2.329572
16	-3.699160	1.462580	-0.946325
8	-4.332055	2.595917	-0.247506
8	-2.805755	1.716218	-2.090799
6	-5.026645	0.379687	-1.466654
6	-4.771392	-0.588300	-2.440129
6	-6.280002	0.485072	-0.865383
6	-5.783340	-1.474884	-2.792576
1	-3.798513	-0.630744	-2.916013
6	-7.282850	-0.415001	-1.228364
1	-6.460352	1.262451	-0.131166
6	-7.048522	-1.411531	-2.184843
1	-5.592197	-2.230943	-3.549540
1	-8.260246	-0.341715	-0.759369
6	-3.024174	1.303384	2.371507
6	-2.040418	1.324508	3.270103
1	-3.606823	2.205259	2.195950
1	-1.834286	2.222188	3.845700
1	-1.391168	0.475246	3.455496
1	-4.458982	0.124998	1.326193
6	-2.549874	6.399124	0.464099
1	-2.379649	6.946956	-0.469371
1	-3.589080	6.049345	0.445344
1	-2.444546	7.102348	1.295101
6	-8.115151	-2.416943	-2.538978
1	-7.941464	-3.363707	-2.012138
1	-9.112632	-2.064411	-2.261472
1	-8.116715	-2.639013	-3.610960
1	5.041098	-1.247688	1.505510

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Number of imaginary frequencies : 0
The smallest frequencies are : 12.9225 16.2535 26.5119 cm(-1)

Electronic energy : HF=-2676.3238494
Zero-point correction= 0.938018
(Hartree/Particle)
Thermal correction to Energy= 0.984477
Thermal correction to Enthalpy= 0.985421
Thermal correction to Gibbs Free Energy= 0.857416
Sum of electronic and zero-point Energies= -2675.385832
Sum of electronic and thermal Energies= -2675.339372
Sum of electronic and thermal Enthalpies= -2675.338428
Sum of electronic and thermal Free Energies= -2675.466433

.....
Cartesian Coordinates

28	0.142713	-0.932534	0.438385
15	1.755631	0.732446	0.352366
6	3.114364	0.187239	1.535906
6	4.330790	1.113911	1.722410
6	2.536296	-0.188574	2.917610
1	3.476060	-0.738322	1.070794
6	5.406274	0.425972	2.581717
1	4.013779	2.037055	2.224051
1	4.759371	1.404980	0.757899
6	3.596974	-0.880527	3.788488
1	2.194443	0.720564	3.430504
1	1.653990	-0.828871	2.804201
6	4.848766	-0.004586	3.946141
1	6.263251	1.097193	2.715771
1	5.780622	-0.457553	2.045227
1	3.176207	-1.125842	4.771143
1	3.877410	-1.834681	3.319180
1	5.616296	-0.535159	4.522273
1	4.586091	0.893023	4.524258
6	1.260845	2.418450	1.086940
6	2.129637	3.620276	0.652649
6	-0.230470	2.771471	0.919508
1	1.432869	2.262944	2.161449
6	1.770960	4.883272	1.453397
1	1.959181	3.822988	-0.411692
1	3.195390	3.407715	0.766099
6	-0.594321	4.044516	1.700054
1	-0.457011	2.905315	-0.145465
1	-0.852331	1.935762	1.239402
6	0.285861	5.236048	1.303750
1	2.400865	5.719046	1.124421
1	2.000641	4.715605	2.515840
1	-1.654104	4.283621	1.545205
1	-0.473516	3.852665	2.776836
1	0.038372	6.119054	1.905789
1	0.084628	5.500279	0.255823
6	2.711335	1.190837	-1.203558
6	3.657255	0.091947	-1.719948
6	1.768386	1.638776	-2.336723
1	3.334593	2.047070	-0.921204
6	4.468065	0.592798	-2.926415
1	3.071017	-0.774085	-2.029436
1	4.341120	-0.249392	-0.936501
6	2.567121	2.138948	-3.550258
1	1.136079	0.795881	-2.632374
1	1.077116	2.412978	-1.993219
6	3.545874	1.070701	-4.056206
1	5.124440	-0.210654	-3.282131
1	5.121295	1.420512	-2.612304
1	1.876301	2.434720	-4.348945
1	3.130254	3.041696	-3.269867
1	4.136091	1.455295	-4.897131
1	2.974840	0.211465	-4.434241
7	-1.534329	0.058866	0.238838
6	-1.793242	-1.036933	1.033102
6	-2.984431	-1.982789	0.867719

6	-2.911207	-3.323778	1.634083
6	-4.259704	-1.235812	1.375173
1	-3.105029	-2.203223	-0.195243
6	-2.889483	-3.152760	3.160375
1	-2.073702	-3.934537	1.301204
1	-3.816128	-3.887675	1.367342
6	-4.299921	-1.062690	2.902779
1	-4.350700	-0.260590	0.896251
1	-5.131507	-1.824274	1.058460
6	-4.137242	-2.397814	3.642544
1	-1.986433	-2.605870	3.464912
1	-2.831009	-4.136384	3.642194
1	-5.245790	-0.585126	3.185638
1	-3.506632	-0.372079	3.218419
1	-4.095945	-2.233226	4.726108
1	-5.021644	-3.022676	3.451982
16	-1.966411	0.087754	-1.396299
8	-1.218198	1.216345	-1.973189
8	-1.874658	-1.234868	-2.060077
6	-3.692032	0.571012	-1.382615
6	-4.659771	-0.286718	-1.899891
6	-4.038494	1.814806	-0.847362
6	-5.998960	0.102175	-1.861682
1	-4.362392	-1.243842	-2.313929
6	-5.379625	2.183204	-0.810304
1	-3.268413	2.472508	-0.458597
6	-6.379699	1.334131	-1.313747
1	-6.759549	-0.564193	-2.259849
1	-5.659609	3.144019	-0.386043
6	0.145362	-2.919853	0.838602
6	1.443442	-2.531939	0.495076
1	2.163404	-2.419929	1.301898
6	2.036669	-2.825086	-0.830619
6	1.287485	-2.740900	-2.020118
6	3.386328	-3.204413	-0.915048
6	1.880365	-3.020914	-3.250113
1	0.252955	-2.409465	-1.983479
6	3.976446	-3.488671	-2.147125
1	3.977536	-3.269621	-0.004508
6	3.226539	-3.395044	-3.321659
1	1.291055	-2.931554	-4.158624
1	5.023363	-3.776928	-2.190249
1	3.686314	-3.605653	-4.283035
1	-0.467248	-3.449942	0.115392
1	-0.101275	-3.093404	1.881955
1	-1.611935	-0.779301	2.081600
6	-7.826360	1.760675	-1.292663
1	-8.046940	2.430912	-2.133016
1	-8.501258	0.903441	-1.371383
1	-8.070703	2.303854	-0.374096

TS[10-11]

Number of imaginary frequencies : 1

The smallest frequencies are : -178.4605 20.4007 25.5438 cm(-1)

Electronic energy :	HF=-2676.3119415	
Zero-point correction=		0.938591
(Hartree/Particle)		
Thermal correction to Energy=		0.983923
Thermal correction to Enthalpy=		0.984867
Thermal correction to Gibbs Free Energy=		0.860507
Sum of electronic and zero-point Energies=		-2675.373351
Sum of electronic and thermal Energies=		-2675.328019
Sum of electronic and thermal Enthalpies=		-2675.327074
Sum of electronic and thermal Free Energies=		-2675.451434

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

28	0.258088	-0.667165	0.337281
15	1.911308	0.753065	0.369136
6	3.255382	0.040580	1.459232
6	4.551696	0.860953	1.602016
6	2.717008	-0.331944	2.856672
1	3.496576	-0.898988	0.943840
6	5.609888	0.068502	2.389046
1	4.332986	1.792283	2.139732
1	4.951431	1.145244	0.623123
6	3.763839	-1.128412	3.651604
1	2.471911	0.583729	3.411892
1	1.786408	-0.902783	2.766081
6	5.085139	-0.354120	3.768975
1	6.523030	0.666599	2.495029
1	5.884875	-0.827047	1.814006
1	3.374171	-1.371817	4.647438
1	3.947035	-2.085317	3.142173
1	5.835377	-0.957037	4.294349
1	4.919457	0.544798	4.380146
6	1.496015	2.415618	1.166799
6	2.394604	3.598569	0.747038
6	0.008208	2.793863	1.014039
1	1.673970	2.226079	2.235137
6	2.059549	4.860362	1.559840
1	2.234784	3.815009	-0.316444
1	3.454616	3.354661	0.864518
6	-0.325068	4.064863	1.809292
1	-0.225936	2.940392	-0.046418
1	-0.626310	1.963248	1.330068
6	0.579812	5.240281	1.416989
1	2.702954	5.688226	1.237420
1	2.288132	4.678684	2.620104
1	-1.379692	4.327979	1.660071
1	-0.203342	3.861559	2.883845
1	0.351813	6.124305	2.025019
1	0.379974	5.514603	0.371448
6	2.776685	1.171591	-1.238179
6	3.625053	0.016772	-1.803872
6	1.758653	1.645335	-2.294656
1	3.454881	2.002533	-1.008174
6	4.336912	0.443028	-3.097602
1	2.976961	-0.832893	-2.022913
1	4.366574	-0.328268	-1.076988
6	2.462582	2.065848	-3.593242

1	1.056170	0.831669	-2.501339
1	1.146393	2.466916	-1.913203
6	3.334118	0.932164	-4.150813
1	4.919283	-0.401251	-3.485236
1	5.052990	1.247772	-2.874255
1	1.713092	2.372728	-4.332399
1	3.092701	2.946608	-3.398587
1	3.858449	1.259451	-5.056991
1	2.687527	0.092861	-4.441396
7	-1.573807	0.033804	0.329083
6	-1.722171	-1.251209	0.950505
6	-3.081873	-1.984366	0.800767
6	-3.187282	-3.409271	1.391791
6	-4.176289	-1.115166	1.485258
1	-3.296997	-2.052624	-0.268300
6	-3.060823	-3.445461	2.923089
1	-2.482135	-4.099021	0.923861
1	-4.184709	-3.782782	1.122964
6	-4.105201	-1.141162	3.021028
1	-4.122783	-0.084854	1.135695
1	-5.151818	-1.504471	1.165497
6	-4.138467	-2.570511	3.579299
1	-2.066811	-3.090041	3.230066
1	-3.140148	-4.479998	3.277354
1	-4.936437	-0.554108	3.429774
1	-3.187876	-0.639801	3.358019
1	-4.017252	-2.560534	4.669295
1	-5.124145	-3.013129	3.375793
16	-2.019144	0.244473	-1.263328
8	-1.299486	1.440928	-1.738682
8	-1.920744	-1.004146	-2.063880
6	-3.755724	0.711634	-1.239690
6	-4.715046	-0.124749	-1.805456
6	-4.119285	1.929069	-0.657443
6	-6.057801	0.253140	-1.765180
1	-4.406306	-1.052726	-2.274070
6	-5.462931	2.289405	-0.620744
1	-3.357772	2.579782	-0.240858
6	-6.453582	1.455728	-1.165441
1	-6.808334	-0.396545	-2.208061
1	-5.751136	3.233741	-0.165996
6	-0.441124	-2.632582	0.537536
6	1.024802	-2.406294	0.392124
1	1.602755	-2.639071	1.288426
6	1.713366	-2.804287	-0.857211
6	1.105625	-2.667324	-2.123364
6	3.032585	-3.290732	-0.806565
6	1.801962	-2.994460	-3.285315
1	0.099835	-2.262164	-2.194796
6	3.728780	-3.612809	-1.971875
1	3.516700	-3.407719	0.160663
6	3.117954	-3.465214	-3.219361
1	1.317304	-2.868124	-4.249843
1	4.749673	-3.979943	-1.905393
1	3.658857	-3.712555	-4.128236
1	-0.920022	-3.077653	-0.331103
1	-0.662760	-3.163937	1.457017

1	-1.511183	-1.097887	2.011800
6	-7.910785	1.838588	-1.083518
1	-8.348736	1.507311	-0.133309
1	-8.045216	2.923321	-1.140520
1	-8.493711	1.380271	-1.888081

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Number of imaginary frequencies : 0
 The smallest frequencies are : 13.4238 16.7483 25.7968 cm(-1)

Electronic energy : HF=-2676.353401
 Zero-point correction= 0.940265
 (Hartree/Particle)
 Thermal correction to Energy= 0.986002
 Thermal correction to Enthalpy= 0.986947
 Thermal correction to Gibbs Free Energy= 0.859939
 Sum of electronic and zero-point Energies= -2675.413136
 Sum of electronic and thermal Energies= -2675.367399
 Sum of electronic and thermal Enthalpies= -2675.366454
 Sum of electronic and thermal Free Energies= -2675.493462

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 Cartesian Coordinates

28	-0.124432	-0.257544	-0.004782
15	-2.115107	0.708979	-0.365135
6	-3.327421	-0.151865	-1.488401
6	-4.607583	0.640188	-1.817514
6	-2.650916	-0.641227	-2.786032
1	-3.611918	-1.041579	-0.914089
6	-5.579708	-0.217494	-2.645053
1	-4.342885	1.536462	-2.393721
1	-5.100356	0.985632	-0.902603
6	-3.619291	-1.499399	-3.615517
1	-2.335872	0.222215	-3.388179
1	-1.742744	-1.204421	-2.552909
6	-4.916582	-0.739838	-3.927594
1	-6.477128	0.364103	-2.887965
1	-5.912000	-1.068947	-2.034265
1	-3.131844	-1.822827	-4.542870
1	-3.860772	-2.412018	-3.051836
1	-5.611802	-1.382639	-4.480547
1	-4.684750	0.111091	-4.584225
6	-1.722083	2.327816	-1.269138
6	-2.622668	3.526706	-0.911845
6	-0.229569	2.709814	-1.142014
1	-1.902731	2.078959	-2.323789
6	-2.277323	4.756215	-1.768097
1	-2.484698	3.785768	0.145023
1	-3.678691	3.269199	-1.039195
6	0.108496	3.953538	-1.978192
1	0.017837	2.887204	-0.089211
1	0.399857	1.871074	-1.464337
6	-0.798347	5.139354	-1.624506
1	-2.922061	5.596659	-1.483988
1	-2.494391	4.535147	-2.823043

1	1.162776	4.220409	-1.834250
1	-0.011513	3.713506	-3.044673
1	-0.563910	6.003847	-2.257124
1	-0.604697	5.444505	-0.586371
6	-3.086933	1.184984	1.161477
6	-3.900647	0.000239	1.718512
6	-2.106100	1.722837	2.226854
1	-3.788590	1.983414	0.889835
6	-4.613285	0.374138	3.027483
1	-3.231548	-0.842746	1.905218
1	-4.641484	-0.340071	0.988010
6	-2.831392	2.093714	3.528003
1	-1.348368	0.957995	2.431220
1	-1.553843	2.587589	1.842372
6	-3.626618	0.901549	4.077163
1	-5.148911	-0.502739	3.410399
1	-5.371489	1.144536	2.824282
1	-2.101596	2.442976	4.267931
1	-3.517589	2.932566	3.339793
1	-4.157850	1.182838	4.994525
1	-2.927209	0.098140	4.346646
7	1.748828	-0.539910	-0.113671
6	2.108271	-1.929758	-0.508220
6	3.575635	-2.327976	-0.236477
6	3.851800	-3.822266	-0.518826
6	4.563756	-1.471198	-1.063948
1	3.764922	-2.154303	0.829152
6	3.777281	-4.165428	-2.014905
1	3.172670	-4.457276	0.059071
1	4.864797	-4.051170	-0.159368
6	4.538621	-1.806473	-2.564895
1	4.358890	-0.408031	-0.921275
1	5.576785	-1.648416	-0.677627
6	4.760293	-3.304574	-2.823638
1	2.755413	-4.000921	-2.383294
1	3.992321	-5.230343	-2.165805
1	5.301939	-1.215124	-3.085536
1	3.574674	-1.502750	-2.994532
1	4.673422	-3.524764	-3.894998
1	5.786494	-3.571119	-2.530873
16	2.132406	0.132561	1.316055
8	1.020039	1.140868	1.463201
8	2.382416	-0.782874	2.452255
6	3.625409	1.096049	1.079855
6	4.785230	0.779933	1.781559
6	3.607266	2.140817	0.149679
6	5.946729	1.517340	1.541522
1	4.771184	-0.030908	2.501535
6	4.771644	2.864615	-0.077530
1	2.692135	2.371615	-0.385448
6	5.959668	2.564141	0.612535
1	6.854566	1.274578	2.087393
1	4.765187	3.678056	-0.798940
6	1.027858	-2.818829	0.103687
6	-0.358420	-2.186735	-0.177394
1	-0.643243	-2.387687	-1.217676
6	-1.428553	-2.655932	0.749533

6	-1.261719	-2.583582	2.149012
6	-2.633951	-3.195417	0.264767
6	-2.251245	-3.039194	3.017559
1	-0.351800	-2.144409	2.548694
6	-3.632243	-3.641534	1.133314
1	-2.778665	-3.278303	-0.809689
6	-3.445208	-3.569060	2.515112
1	-2.096471	-2.970081	4.091008
1	-4.552867	-4.054483	0.729020
1	-4.218122	-3.919125	3.193250
1	1.210463	-2.884076	1.180180
1	1.055641	-3.842316	-0.295934
1	1.946505	-1.919903	-1.592539
6	7.218438	3.347289	0.332390
1	7.028207	4.426043	0.350991
1	8.001847	3.129175	1.063521
1	7.615097	3.108241	-0.661947

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Number of imaginary frequencies : 0
 The smallest frequencies are : 15.2974 20.4714 24.9707 cm(-1)

Electronic energy : HF=-3903.318498
 Zero-point correction= 1.310186
 (Hartree/Particle)
 Thermal correction to Energy= 1.377836
 Thermal correction to Enthalpy= 1.378781
 Thermal correction to Gibbs Free Energy= 1.205543
 Sum of electronic and zero-point Energies= -3902.008312
 Sum of electronic and thermal Energies= -3901.940662
 Sum of electronic and thermal Enthalpies= -3901.939717
 Sum of electronic and thermal Free Energies= -3902.112955

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 Cartesian Coordinates

28	-2.949721	0.321615	0.745083
15	-1.970697	-1.777550	0.771490
6	-1.189193	-2.300178	-0.849938
6	-0.767633	-3.776311	-0.996140
6	-2.052280	-1.844826	-2.046330
1	-0.284754	-1.685973	-0.874774
6	-0.021255	-3.988718	-2.324626
1	-1.646519	-4.430222	-0.983126
1	-0.136414	-4.091811	-0.158760
6	-1.315198	-2.082719	-3.371975
1	-3.008332	-2.382779	-2.058524
1	-2.289694	-0.783650	-1.947439
6	-0.870114	-3.543646	-3.524183
1	0.268026	-5.042076	-2.426627
1	0.908448	-3.405061	-2.309146
1	-1.957776	-1.785030	-4.209189
1	-0.432025	-1.429844	-3.405158
1	-0.307910	-3.678552	-4.456519
1	-1.758759	-4.187807	-3.595719

6	-2.975888	-3.282291	1.322554
6	-3.616064	-3.061243	2.711730
6	-4.022451	-3.799462	0.315249
1	-2.221356	-4.075027	1.434058
6	-4.327001	-4.327838	3.216204
1	-4.342571	-2.240068	2.659642
1	-2.860415	-2.754204	3.441409
6	-4.716339	-5.069784	0.833448
1	-4.779690	-3.036613	0.128183
1	-3.562149	-4.003229	-0.653279
6	-5.362453	-4.835727	2.204820
1	-4.801516	-4.125101	4.183892
1	-3.578157	-5.113314	3.391491
1	-5.467001	-5.402009	0.106093
1	-3.977193	-5.879703	0.914700
1	-5.834047	-5.755733	2.570046
1	-6.164312	-4.089852	2.103250
6	-0.610243	-1.868806	2.098397
6	0.842685	-1.927181	1.589561
6	-0.760396	-0.713599	3.112742
1	-0.799660	-2.812524	2.629387
6	1.822899	-2.089477	2.762029
1	1.074264	-1.008787	1.048334
1	0.983029	-2.752610	0.887829
6	0.231651	-0.851060	4.278212
1	-0.589247	0.229707	2.584998
1	-1.789222	-0.668290	3.493002
6	1.679388	-0.945165	3.773069
1	2.846129	-2.137540	2.372636
1	1.635490	-3.048933	3.266993
1	0.119722	-0.000204	4.961404
1	-0.007591	-1.754770	4.859016
1	2.366998	-1.088447	4.616518
1	1.964961	-0.001742	3.288752
7	-1.411072	1.493590	0.764381
6	-2.550192	2.273810	0.953986
6	-2.897225	3.508712	0.108680
6	-4.392699	3.875742	-0.001430
6	-2.141196	4.746808	0.683295
1	-2.539991	3.331662	-0.907463
6	-5.004873	4.372731	1.317423
1	-4.965443	3.045343	-0.420724
1	-4.468943	4.688736	-0.737273
6	-2.746741	5.282028	1.990500
1	-1.085706	4.514154	0.834795
1	-2.178861	5.539176	-0.077204
6	-4.241781	5.595490	1.845495
1	-4.972977	3.577955	2.074441
1	-6.063605	4.616369	1.166278
1	-2.196821	6.177704	2.303561
1	-2.608498	4.544886	2.793022
1	-4.659769	5.926088	2.804156
1	-4.369910	6.429409	1.140358
16	-0.560333	1.504969	-0.675748
8	0.412810	0.391067	-0.552472
8	-1.386441	1.533131	-1.904944
6	0.405166	3.005707	-0.619688

6	0.342909	3.908441	-1.677130
6	1.280878	3.196920	0.451334
6	1.188516	5.018846	-1.663456
1	-0.345397	3.731803	-2.495940
6	2.122652	4.302259	0.442774
1	1.328231	2.484330	1.266142
6	2.096818	5.223442	-0.616927
1	1.152973	5.725912	-2.487976
1	2.832219	4.429449	1.253900
6	-4.870606	0.773139	1.301231
6	-4.899252	-0.357235	0.493479
1	-5.006470	-1.315923	0.984219
6	-5.256070	-0.352362	-0.948273
6	-4.712939	0.576284	-1.854541
6	-6.145096	-1.321158	-1.445432
6	-5.047236	0.534345	-3.207262
1	-3.982749	1.300285	-1.511162
6	-6.483243	-1.360253	-2.798205
1	-6.585022	-2.043136	-0.762290
6	-5.933417	-0.433183	-3.686561
1	-4.597354	1.250379	-3.889225
1	-7.175203	-2.116803	-3.158166
1	-6.188831	-0.468137	-4.741818
1	-5.213801	1.724177	0.928533
1	-4.875642	0.661657	2.384691
1	-2.704301	2.444032	2.022221
7	3.302099	0.426503	-0.212029
1	2.315501	0.669776	-0.088795
6	3.653062	0.126389	-1.625292
6	3.055477	-1.256271	-1.991401
6	3.441128	-1.707902	-3.419007
6	3.464255	-2.354642	-0.983121
1	1.965783	-1.146249	-1.940776
6	4.919286	-2.113521	-3.541645
1	3.204463	-0.929402	-4.148556
1	2.818551	-2.576926	-3.673567
6	4.939321	-2.769379	-1.097483
1	3.243557	-2.023467	0.033327
1	2.837856	-3.236203	-1.174998
6	5.290195	-3.204722	-2.526868
1	5.560652	-1.235793	-3.381904
1	5.123034	-2.456916	-4.563262
1	5.148442	-3.579767	-0.388539
1	5.585550	-1.934990	-0.801374
1	6.356380	-3.452485	-2.602947
1	4.735229	-4.122405	-2.771080
16	4.306869	1.380234	0.708682
8	4.902441	2.490879	-0.056421
8	3.556317	1.663684	1.945048
6	5.636824	0.240909	1.081794
6	5.436986	-0.735294	2.061271
6	6.828176	0.307448	0.362689
6	6.440318	-1.667384	2.299374
1	4.512227	-0.750340	2.626360
6	7.824215	-0.638837	0.612636
1	6.967522	1.088700	-0.376391
6	7.643757	-1.641513	1.573169

1	6.291879	-2.430769	3.058792
1	8.753734	-0.595530	0.051791
6	3.237033	1.293821	-2.503347
6	2.139933	1.369567	-3.256074
1	3.879706	2.166031	-2.404783
1	1.897804	2.280856	-3.794737
1	1.434259	0.551475	-3.354718
1	4.745383	0.051076	-1.654569
6	3.051312	6.390412	-0.619534
1	2.881850	7.053523	-1.472389
1	2.955097	6.983249	0.296996
1	4.087705	6.035671	-0.664963
6	8.705736	-2.681619	1.829321
1	8.977598	-2.718273	2.890184
1	8.347881	-3.681133	1.554859
1	9.614312	-2.483050	1.254272

TS[10a-11a]

Number of imaginary frequencies : 1
 The smallest frequencies are : -167.2310 14.7866 21.6184 cm(-1)

Electronic energy : HF=-3903.3005153
 Zero-point correction= 1.310214
 (Hartree/Particle)
 Thermal correction to Energy= 1.376874
 Thermal correction to Enthalpy= 1.377818
 Thermal correction to Gibbs Free Energy= 1.206593
 Sum of electronic and zero-point Energies= -3901.990301
 Sum of electronic and thermal Energies= -3901.923642
 Sum of electronic and thermal Enthalpies= -3901.922697
 Sum of electronic and thermal Free Energies= -3902.093922

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 Cartesian Coordinates

28	-2.865364	0.295484	0.450853
15	-1.995472	-1.639268	0.983453
6	-1.135455	-2.496533	-0.444711
6	-0.895378	-4.009148	-0.265554
6	-1.814831	-2.183080	-1.791037
1	-0.167023	-1.988292	-0.471197
6	-0.100900	-4.582022	-1.451387
1	-1.854388	-4.535991	-0.203243
1	-0.366672	-4.214370	0.672537
6	-1.018608	-2.777186	-2.961615
1	-2.838154	-2.574189	-1.809945
1	-1.890470	-1.100271	-1.910075
6	-0.794115	-4.285242	-2.788411
1	0.037367	-5.662079	-1.318449
1	0.900948	-4.133877	-1.463283
1	-1.540457	-2.569666	-3.903288
1	-0.043069	-2.274252	-3.023132
1	-0.200630	-4.684231	-3.620154
1	-1.764462	-4.801772	-2.816400
6	-3.181456	-2.886516	1.724668
6	-3.853075	-2.308009	2.989175

6	-4.254223	-3.366076	0.731897
1	-2.565664	-3.747446	2.022925
6	-4.819311	-3.317222	3.630253
1	-4.402038	-1.398964	2.706554
1	-3.103351	-2.005831	3.727649
6	-5.210674	-4.382648	1.373051
1	-4.827755	-2.503083	0.390795
1	-3.799243	-3.798947	-0.162796
6	-5.874820	-3.806537	2.630221
1	-5.299581	-2.863644	4.505909
1	-4.243982	-4.178580	3.998900
1	-5.970197	-4.682248	0.640842
1	-4.653793	-5.292290	1.640295
1	-6.527777	-4.552919	3.098346
1	-6.517250	-2.961558	2.343169
6	-0.703273	-1.526968	2.368249
6	0.760877	-1.716589	1.924516
6	-0.843074	-0.204339	3.154848
1	-0.949165	-2.358222	3.044624
6	1.707594	-1.684968	3.133199
1	1.036245	-0.919401	1.229548
1	0.892045	-2.663528	1.394821
6	0.118211	-0.153384	4.352313
1	-0.636136	0.624501	2.470987
1	-1.878007	-0.067888	3.492882
6	1.573974	-0.371528	3.913732
1	2.737577	-1.830258	2.787230
1	1.478936	-2.530940	3.798247
1	0.014853	0.810227	4.866250
1	-0.160035	-0.929779	5.080644
1	2.239009	-0.372808	4.786426
1	1.895434	0.459995	3.272353
7	-1.510975	1.695999	0.571702
6	-2.724517	2.455123	0.604972
6	-2.718996	3.866260	-0.037928
6	-4.068444	4.616054	-0.133522
6	-1.743778	4.762499	0.779476
1	-2.331411	3.754523	-1.054993
6	-4.653669	5.002478	1.233822
1	-4.801642	4.067685	-0.728020
1	-3.868288	5.540280	-0.692671
6	-2.304522	5.194923	2.144446
1	-0.790561	4.256717	0.924482
1	-1.535947	5.656320	0.176876
6	-3.670915	5.881242	2.019616
1	-4.880094	4.099223	1.817964
1	-5.607375	5.524809	1.092559
1	-1.584533	5.862659	2.632265
1	-2.397095	4.319696	2.801834
1	-4.073148	6.120294	3.011469
1	-3.548385	6.836846	1.489812
16	-0.620622	1.555753	-0.823541
8	0.297117	0.414922	-0.564225
8	-1.438900	1.503341	-2.061724
6	0.441402	2.991140	-0.953436
6	0.393216	3.790422	-2.091812
6	1.375067	3.228015	0.057493

6	1.309331	4.836459	-2.221493
1	-0.335608	3.579276	-2.866233
6	2.287249	4.264515	-0.092915
1	1.409893	2.601644	0.940884
6	2.274839	5.079234	-1.236634
1	1.285401	5.457612	-3.112960
1	3.038898	4.416278	0.674493
6	-4.337756	1.657100	-0.106498
6	-4.707607	0.210758	-0.061285
1	-5.385448	-0.045176	0.756563
6	-5.079398	-0.447901	-1.342052
6	-4.380553	-0.200394	-2.540666
6	-6.163824	-1.343091	-1.391789
6	-4.735280	-0.844708	-3.723811
1	-3.530652	0.475253	-2.530702
6	-6.513339	-1.995982	-2.574532
1	-6.740496	-1.528273	-0.488490
6	-5.798654	-1.752505	-3.748946
1	-4.169914	-0.643932	-4.630234
1	-7.351742	-2.687900	-2.578865
1	-6.068599	-2.257939	-4.671914
1	-4.295574	2.059320	-1.114271
1	-4.956715	2.254844	0.555635
1	-3.004716	2.527652	1.657967
7	3.222979	0.316826	-0.254052
1	2.254059	0.632301	-0.153438
6	3.511056	-0.216977	-1.612997
6	2.880417	-1.628840	-1.713440
6	3.162318	-2.314977	-3.069710
6	3.351019	-2.552632	-0.566044
1	1.797727	-1.489304	-1.611125
6	4.623817	-2.766564	-3.223806
1	2.882925	-1.661144	-3.899465
1	2.514642	-3.200140	-3.136010
6	4.808768	-3.016036	-0.712686
1	3.209862	-2.050904	0.393577
1	2.704005	-3.439624	-0.559465
6	5.051147	-3.687036	-2.071596
1	5.284120	-1.888593	-3.253206
1	4.751126	-3.276155	-4.186762
1	5.057213	-3.704704	0.103996
1	5.486148	-2.161463	-0.601716
1	6.105608	-3.970903	-2.177678
1	4.466869	-4.617507	-2.123553
16	4.305242	1.355237	0.468097
8	4.897305	2.315946	-0.480524
8	3.630978	1.847533	1.683333
6	5.615536	0.233787	0.947620
6	5.418859	-0.605908	2.046723
6	6.796227	0.190770	0.209276
6	6.415423	-1.511452	2.391601
1	4.503137	-0.535640	2.622516
6	7.786737	-0.725172	0.569121
1	6.932480	0.868088	-0.626494
6	7.610003	-1.591238	1.655025
1	6.269780	-2.167788	3.245680
1	8.709061	-0.765405	-0.003822

1	-4.358795	-1.483997	2.650353
1	-3.082223	-2.167963	3.650224
6	-5.247334	-4.375693	1.182801
1	-4.794464	-2.470834	0.276283
1	-3.801158	-3.780973	-0.314144
6	-5.899321	-3.836820	2.462773
1	-5.305932	-2.998069	4.381898
1	-4.287828	-4.320522	3.820972
1	-6.012673	-4.614319	0.434678
1	-4.723203	-5.315281	1.409839
1	-6.577384	-4.583440	2.893172
1	-6.513631	-2.960236	2.211863
6	-0.666166	-1.646283	2.310667
6	0.790760	-1.845542	1.849420
6	-0.783048	-0.333046	3.117319
1	-0.920869	-2.485709	2.973575
6	1.745783	-1.848876	3.051970
1	1.069084	-1.036192	1.168476
1	0.906283	-2.783563	1.300508
6	0.189860	-0.311895	4.306451
1	-0.571235	0.504376	2.444473
1	-1.813373	-0.190613	3.466777
6	1.638707	-0.544905	3.852168
1	2.770391	-2.007940	2.697375
1	1.505918	-2.700669	3.705588
1	0.104388	0.646468	4.832822
1	-0.093565	-1.093870	5.026656
1	2.310326	-0.569007	4.719474
1	1.965867	0.292032	3.220809
7	-1.483580	1.706074	0.556433
6	-2.749606	2.482522	0.578611
6	-2.610234	3.949786	0.068686
6	-3.927461	4.746119	-0.058534
6	-1.651272	4.734319	0.999141
1	-2.169077	3.894282	-0.931340
6	-4.578552	5.059465	1.297610
1	-4.635760	4.250479	-0.728488
1	-3.676023	5.697262	-0.547464
6	-2.279935	5.094934	2.355678
1	-0.734717	4.167030	1.160301
1	-1.362424	5.658024	0.480470
6	-3.611247	5.842328	2.197139
1	-4.867132	4.126484	1.802941
1	-5.504406	5.626717	1.143903
1	-1.570214	5.698570	2.933807
1	-2.446031	4.180958	2.942462
1	-4.064504	6.031780	3.177723
1	-3.421477	6.825079	1.742266
16	-0.615446	1.570766	-0.828818
8	0.315482	0.429498	-0.592529
8	-1.442372	1.519026	-2.065691
6	0.454189	3.002793	-0.981790
6	0.422840	3.779616	-2.136373
6	1.386097	3.251172	0.027957
6	1.351906	4.812382	-2.283131
1	-0.303827	3.560100	-2.910587
6	2.313533	4.271533	-0.139734

1	1.409477	2.641212	0.923419
6	2.316850	5.062730	-1.299822
1	1.339441	5.415586	-3.187227
1	3.063610	4.430200	0.628015
6	-4.071820	1.795381	-0.169785
6	-4.581748	0.320797	0.036226
1	-5.250386	0.247502	0.900545
6	-5.180039	-0.314524	-1.164076
6	-4.565640	-0.245142	-2.431235
6	-6.384962	-1.034479	-1.058203
6	-5.122660	-0.890395	-3.532689
1	-3.633314	0.301023	-2.540540
6	-6.938670	-1.687390	-2.159597
1	-6.888397	-1.083889	-0.095314
6	-6.308291	-1.621407	-3.403761
1	-4.624108	-0.828054	-4.496448
1	-7.867459	-2.240423	-2.046520
1	-6.738602	-2.125278	-4.264605
1	-3.960321	2.014992	-1.230500
1	-4.864167	2.410581	0.253867
1	-3.003739	2.521491	1.642538
7	3.224148	0.329163	-0.262474
1	2.253003	0.645133	-0.175252
6	3.541194	-0.178781	-1.624917
6	2.903174	-1.583201	-1.770017
6	3.200877	-2.238160	-3.138264
6	3.350543	-2.537919	-0.638778
1	1.820009	-1.438318	-1.680476
6	4.661847	-2.694702	-3.281943
1	2.937202	-1.562322	-3.955398
1	2.549573	-3.117843	-3.236128
6	4.806553	-3.009869	-0.775240
1	3.201753	-2.057185	0.330098
1	2.695544	-3.418814	-0.661805
6	5.065934	-3.646954	-2.147272
1	5.327453	-1.820335	-3.279270
1	4.800883	-3.180716	-4.255402
1	5.036341	-3.721944	0.026775
1	5.488275	-2.163836	-0.630371
1	6.120183	-3.934867	-2.244413
1	4.477060	-4.572176	-2.232100
16	4.297016	1.345446	0.502306
8	4.928606	2.308800	-0.417582
8	3.595840	1.831610	1.704549
6	5.580342	0.202219	1.005103
6	5.341473	-0.646436	2.088669
6	6.781191	0.151356	0.300784
6	6.315257	-1.569395	2.452236
1	4.410293	-0.569690	2.637980
6	7.748567	-0.782022	0.678789
1	6.950494	0.835438	-0.523391
6	7.529459	-1.657324	1.749433
1	6.136021	-2.232294	3.294842
1	8.686438	-0.828799	0.132167
6	3.132152	0.862057	-2.652237
6	2.001819	0.874940	-3.357777
1	3.811776	1.709269	-2.714302

1	1.766069	1.707107	-4.014374
1	1.257812	0.087561	-3.294392
1	4.630413	-0.286780	-1.662718
6	3.367295	6.129743	-1.479091
1	3.233672	6.679726	-2.415167
1	3.347482	6.853445	-0.655912
1	4.368015	5.682402	-1.488363
6	8.559777	-2.686691	2.141141
1	8.739498	-2.678930	3.221615
1	8.221067	-3.696307	1.878170
1	9.514890	-2.515591	1.636973

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Number of imaginary frequencies : 0
The smallest frequencies are : 18.7461 22.0949 25.0725 cm(-1)

Electronic energy : HF=-3903.3381908
Zero-point correction= 1.313187
(Hartree/Particle)
Thermal correction to Energy= 1.379551
Thermal correction to Enthalpy= 1.380496
Thermal correction to Gibbs Free Energy= 1.211882
Sum of electronic and zero-point Energies= -3902.025004
Sum of electronic and thermal Energies= -3901.958639
Sum of electronic and thermal Enthalpies= -3901.957695
Sum of electronic and thermal Free Energies= -3902.126309

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Cartesian Coordinates
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28	-0.937166	-0.065032	-0.645827
15	-3.039617	0.713862	-0.197706
6	-3.183455	2.188069	-1.369170
6	-4.508934	2.978195	-1.344244
6	-1.968868	3.140905	-1.302260
1	-3.116678	1.678947	-2.342041
6	-4.543334	4.041918	-2.456636
1	-4.629270	3.470316	-0.371168
1	-5.368450	2.312244	-1.465254
6	-2.024440	4.189458	-2.422299
1	-1.963256	3.654918	-0.335317
1	-1.030099	2.587704	-1.369001
6	-3.335150	4.984365	-2.386073
1	-5.480842	4.608072	-2.393844
1	-4.546920	3.534777	-3.432098
1	-1.160584	4.859512	-2.336462
1	-1.928330	3.682843	-3.392691
1	-3.371447	5.710789	-3.207024
1	-3.382577	5.562044	-1.451168
6	-3.350376	1.239150	1.591449
6	-2.694084	0.219953	2.553482
6	-2.958153	2.674991	1.989481
1	-4.440341	1.165518	1.713154
6	-3.069531	0.507566	4.015743
1	-1.609963	0.287623	2.439489
1	-2.972806	-0.804343	2.287348

6	-3.348437	2.956934	3.450793
1	-1.881193	2.805339	1.874031
1	-3.446882	3.403197	1.336735
6	-2.709777	1.945855	4.412681
1	-2.559542	-0.208379	4.672426
1	-4.149112	0.346743	4.153282
1	-3.048973	3.977924	3.717821
1	-4.443450	2.914311	3.547643
1	-3.028122	2.147906	5.442864
1	-1.620560	2.061506	4.378229
6	-4.696371	-0.151707	-0.523946
6	-4.952413	-0.564739	-1.987824
6	-5.039778	-1.319986	0.425120
1	-5.409749	0.650859	-0.288899
6	-6.410899	-1.010330	-2.184759
1	-4.298870	-1.401332	-2.247661
1	-4.719646	0.251238	-2.679271
6	-6.492447	-1.782985	0.218189
1	-4.364710	-2.157915	0.244795
1	-4.911064	-1.025776	1.469815
6	-6.767495	-2.166170	-1.241025
1	-6.567683	-1.304468	-3.229668
1	-7.081772	-0.160337	-1.992543
1	-6.700660	-2.630771	0.881763
1	-7.176448	-0.974168	0.514706
1	-7.817197	-2.456820	-1.369871
1	-6.158899	-3.042805	-1.501131
7	0.905742	-0.477826	-1.262151
6	0.935501	-1.800846	-1.985569
6	1.330143	-2.909534	-0.981397
6	0.997061	-4.343670	-1.441610
6	2.834733	-2.832261	-0.645159
1	0.761649	-2.717545	-0.066678
6	1.870079	-4.803631	-2.618980
1	-0.064764	-4.438382	-1.680932
1	1.175161	-5.017123	-0.591145
6	3.745416	-3.315414	-1.786248
1	3.099734	-1.806242	-0.379696
1	3.024780	-3.458958	0.235758
6	3.361845	-4.725039	-2.259026
1	1.672327	-4.172168	-3.496072
1	1.602377	-5.827717	-2.907140
1	4.790294	-3.294292	-1.453164
1	3.686330	-2.617309	-2.628657
1	3.981658	-5.022687	-3.113937
1	3.569588	-5.445230	-1.453898
6	-0.420051	-1.936217	-2.675640
6	-1.567998	-1.536625	-1.727028
1	-0.413713	-1.228199	-3.506959
1	-2.386029	-1.183040	-2.362831
1	1.705181	-1.775406	-2.764878
1	-0.575305	-2.936388	-3.102148
6	-2.094204	-2.696082	-0.905212
6	-1.841998	-2.850101	0.465958
6	-2.876576	-3.685319	-1.530088
6	-2.341564	-3.936432	1.187000
1	-1.264175	-2.090402	0.978807

6	-3.387714	-4.770926	-0.816642
1	-3.089652	-3.595212	-2.592872
6	-3.122155	-4.902099	0.549462
1	-2.126702	-4.018856	2.249329
1	-3.995166	-5.513935	-1.326972
1	-3.519809	-5.745053	1.107502
7	1.765884	0.295404	1.569969
1	1.633651	-0.235007	0.693709
6	2.437203	-0.238396	2.785241
6	1.472611	-1.112157	3.641294
6	0.852940	-2.322153	2.915738
6	2.081672	-1.513253	5.004758
1	0.653177	-0.418025	3.853369
6	1.704534	-3.600309	2.929501
1	0.602853	-2.041220	1.889261
1	-0.104266	-2.546251	3.405904
6	2.928740	-2.796184	4.979650
1	2.666709	-0.677518	5.410318
1	1.248659	-1.669362	5.703432
6	2.151341	-3.961109	4.351864
1	2.595290	-3.468744	2.306070
1	1.132250	-4.420476	2.479530
1	3.237279	-3.047855	6.001700
1	3.847792	-2.625786	4.406777
1	2.765097	-4.869796	4.340355
1	1.267291	-4.184814	4.967045
16	0.819715	1.624540	1.657499
8	-0.298613	1.453267	0.692954
8	0.456115	1.869885	3.062375
6	1.799925	3.022123	1.129222
6	3.178532	3.016841	1.327470
6	1.146794	4.133758	0.599114
6	3.913721	4.147494	0.975441
1	3.679090	2.141551	1.727524
6	1.897386	5.252748	0.254953
1	0.077841	4.107632	0.428124
6	3.289340	5.277531	0.431740
1	4.991108	4.146009	1.116837
1	1.397428	6.117518	-0.173072
6	3.749006	-0.843762	2.356692
6	4.936856	-0.389093	2.759480
1	3.701426	-1.680973	1.668183
1	5.862907	-0.850749	2.428012
1	5.026850	0.446089	3.451152
1	2.669402	0.632002	3.407246
16	1.502818	0.726423	-2.231970
8	1.004686	0.666109	-3.627145
8	1.363288	2.012982	-1.521346
6	3.275653	0.392262	-2.332250
6	4.058076	0.503704	-1.179484
6	3.855992	0.048600	-3.550649
6	5.422514	0.247483	-1.250747
1	3.603131	0.782085	-0.237425
6	5.230035	-0.199478	-3.609902
1	3.232579	-0.020130	-4.435407
6	6.031687	-0.108600	-2.466130
1	6.024789	0.322713	-0.348389

1	5.682247	-0.471357	-4.560211
6	4.095534	6.479769	0.008757
1	5.044736	6.539538	0.549586
1	4.329364	6.431800	-1.062122
1	3.546257	7.411174	0.178795
6	7.517102	-0.366426	-2.525343
1	7.814360	-0.800967	-3.483861
1	8.083455	0.563768	-2.392657
1	7.834163	-1.051163	-1.730912

TS[12-13]

Number of imaginary frequencies : 1
 The smallest frequencies are : -1466.6435 16.1821 24.5859 cm(-1)

Electronic energy : HF=-3903.3252777
 Zero-point correction= 1.309654
 (Hartree/Particle)
 Thermal correction to Energy= 1.375255
 Thermal correction to Enthalpy= 1.376199
 Thermal correction to Gibbs Free Energy= 1.209891
 Sum of electronic and zero-point Energies= -3902.015624
 Sum of electronic and thermal Energies= -3901.950023
 Sum of electronic and thermal Enthalpies= -3901.949079
 Sum of electronic and thermal Free Energies= -3902.115386

.....
 Cartesian Coordinates

28	-0.982601	-0.143483	-0.553527
15	-3.126723	0.519577	-0.257904
6	-3.323948	1.920576	-1.504761
6	-4.690714	2.636821	-1.529679
6	-2.164036	2.941515	-1.483471
1	-3.221929	1.365302	-2.448781
6	-4.776590	3.627415	-2.704130
1	-4.842640	3.179746	-0.588543
1	-5.511792	1.918562	-1.612850
6	-2.268711	3.916447	-2.664582
1	-2.189106	3.509242	-0.548231
1	-1.196597	2.437551	-1.508219
6	-3.622124	4.637640	-2.686411
1	-5.743890	4.144130	-2.678593
1	-4.746571	3.063168	-3.647323
1	-1.444986	4.638101	-2.611058
1	-2.135093	3.359522	-3.602835
1	-3.690386	5.308056	-3.551740
1	-3.709705	5.269337	-1.790259
6	-3.510841	1.101859	1.495887
6	-2.829200	0.155464	2.512759
6	-3.187053	2.568694	1.839444
1	-4.599451	0.981469	1.592645
6	-3.251198	0.485681	3.952374
1	-1.747554	0.274507	2.422261
1	-3.051224	-0.890860	2.284587
6	-3.617893	2.895521	3.279788

1	-2.112909	2.729279	1.740817
1	-3.687483	3.249334	1.145216
6	-2.956394	1.952577	4.294203
1	-2.726557	-0.180599	4.648183
1	-4.326512	0.286575	4.074820
1	-3.364013	3.938228	3.507691
1	-4.712100	2.813281	3.359653
1	-3.299844	2.185214	5.309820
1	-1.871874	2.108931	4.269305
6	-4.700569	-0.481177	-0.588667
6	-4.857963	-0.990573	-2.036071
6	-4.984302	-1.618472	0.417605
1	-5.483968	0.272439	-0.425143
6	-6.253178	-1.594658	-2.263379
1	-4.111842	-1.765349	-2.230549
1	-4.681824	-0.188290	-2.759864
6	-6.369841	-2.240364	0.172538
1	-4.220763	-2.393184	0.330995
1	-4.946144	-1.246159	1.444119
6	-6.529922	-2.731395	-1.271142
1	-6.332800	-1.955738	-3.295876
1	-7.015597	-0.811039	-2.144277
1	-6.523093	-3.066633	0.876975
1	-7.147421	-1.492986	0.388499
1	-7.534352	-3.143010	-1.427791
1	-5.817308	-3.547893	-1.451731
7	0.996846	-0.443192	-1.042282
6	1.137962	-1.815869	-1.687438
6	1.692097	-2.831329	-0.654844
6	1.286655	-4.303709	-0.886393
6	3.236567	-2.741582	-0.617649
1	1.298412	-2.543426	0.323985
6	1.955629	-4.939682	-2.114570
1	0.201068	-4.403001	-0.940667
1	1.595989	-4.867015	0.005121
6	3.920900	-3.385774	-1.835342
1	3.547106	-1.697175	-0.542785
1	3.597378	-3.253118	0.284029
6	3.484448	-4.843669	-2.023840
1	1.618614	-4.433191	-3.029357
1	1.641652	-5.986613	-2.206113
1	5.008988	-3.318686	-1.716136
1	3.683277	-2.815820	-2.742552
1	3.953258	-5.272465	-2.918173
1	3.831783	-5.440451	-1.167802
6	-0.196219	-2.118457	-2.372269
6	-1.422264	-1.753712	-1.513101
1	-0.230215	-1.494731	-3.266716
1	-2.234306	-1.565226	-2.221931
1	1.887229	-1.744316	-2.482286
1	-0.240401	-3.161811	-2.708385
6	-1.867511	-2.873258	-0.597692
6	-1.587925	-2.896875	0.776610
6	-2.585390	-3.960116	-1.130505
6	-2.008243	-3.950989	1.590392
1	-1.050477	-2.064801	1.217008
6	-3.012755	-5.016680	-0.324511

1	-2.813498	-3.970084	-2.193991
6	-2.727086	-5.015632	1.043787
1	-1.777593	-3.933755	2.652245
1	-3.572365	-5.838663	-0.763492
1	-3.061196	-5.834620	1.674499
7	1.661880	0.400160	1.355368
1	1.486665	-0.139945	0.167848
6	2.560851	0.113992	2.520135
6	1.861760	-0.760308	3.614437
6	1.196379	-2.054767	3.115181
6	2.765768	-1.020899	4.842196
1	1.050437	-0.110125	3.949902
6	2.123083	-3.274037	3.020677
1	0.720513	-1.853818	2.152989
1	0.382955	-2.299790	3.812722
6	3.671877	-2.258870	4.729917
1	3.369530	-0.129302	5.055925
1	2.108886	-1.159195	5.711782
6	2.869674	-3.508292	4.340319
1	2.858241	-3.126799	2.222482
1	1.537314	-4.158383	2.741065
1	4.189182	-2.418519	5.684283
1	4.450342	-2.085190	3.978080
1	3.533048	-4.377928	4.257029
1	2.143520	-3.739483	5.133491
16	0.646822	1.625961	1.573198
8	-0.482905	1.454607	0.595205
8	0.218571	1.803699	2.977173
6	1.428645	3.181815	1.123591
6	2.814542	3.296605	1.090888
6	0.612809	4.283545	0.861554
6	3.389361	4.529698	0.782092
1	3.443155	2.436263	1.287179
6	1.200741	5.504392	0.548337
1	-0.465938	4.180675	0.882396
6	2.596552	5.648118	0.499588
1	4.472100	4.617691	0.748929
1	0.567551	6.360776	0.330278
6	3.876634	-0.394188	2.001343
6	5.046149	0.212841	2.214550
1	3.851501	-1.310628	1.424812
1	5.976854	-0.198822	1.833337
1	5.119452	1.130527	2.794902
1	2.776054	1.062217	3.029529
16	1.472525	0.763806	-2.155872
8	0.820072	0.554404	-3.462276
8	1.331721	2.069724	-1.499397
6	3.232215	0.483732	-2.402845
6	4.108645	0.743870	-1.347254
6	3.704622	0.042384	-3.636618
6	5.471435	0.543635	-1.532875
1	3.724633	1.079363	-0.392907
6	5.077775	-0.146067	-3.809295
1	3.005047	-0.143166	-4.444234
6	5.978663	0.096672	-2.764972
1	6.152342	0.733016	-0.707027
1	5.450986	-0.491172	-4.769689

1	-2.937798	-0.910363	2.405999
6	-3.376103	2.877776	3.461151
1	-1.943990	2.682378	1.855546
1	-3.532121	3.256401	1.337341
6	-2.696641	1.908987	4.438520
1	-2.491028	-0.231626	4.756393
1	-4.107051	0.270806	4.262452
1	-3.085178	3.911152	3.686694
1	-4.468044	2.823320	3.586586
1	-2.997514	2.136237	5.468919
1	-1.611844	2.043000	4.372151
6	-4.755796	-0.431620	-0.355124
6	-5.032241	-0.912149	-1.794528
6	-4.999394	-1.579717	0.649216
1	-5.507410	0.336935	-0.124466
6	-6.462720	-1.459366	-1.928210
1	-4.334781	-1.714256	-2.049086
1	-4.875008	-0.106953	-2.519375
6	-6.420083	-2.150522	0.498183
1	-4.269878	-2.375568	0.490297
1	-4.872422	-1.231707	1.677104
6	-6.707248	-2.605050	-0.937712
1	-6.632588	-1.796757	-2.957893
1	-7.183480	-0.650638	-1.738642
1	-6.548831	-2.985470	1.197193
1	-7.151875	-1.381766	0.786699
1	-7.735780	-2.975640	-1.024526
1	-6.042678	-3.443518	-1.187338
7	0.844431	-0.468999	-1.303619
6	0.923809	-1.842510	-1.948383
6	1.404873	-2.865147	-0.896025
6	1.126849	-4.332861	-1.280791
6	2.913278	-2.705063	-0.607551
1	0.851367	-2.657360	0.023367
6	1.987948	-4.808212	-2.460343
1	0.064491	-4.490363	-1.480195
1	1.361522	-4.947978	-0.401348
6	3.810725	-3.192550	-1.756263
1	3.148457	-1.664951	-0.372346
1	3.145066	-3.286277	0.291651
6	3.484149	-4.639148	-2.154212
1	1.731376	-4.234889	-3.362293
1	1.762550	-5.857136	-2.687262
1	4.862259	-3.105508	-1.457504
1	3.692726	-2.537436	-2.627704
1	4.090653	-4.944601	-3.015610
1	3.753643	-5.309667	-1.325446
6	-0.457737	-2.062497	-2.561360
6	-1.600790	-1.712346	-1.583497
1	-0.535282	-1.390370	-3.417750
1	-2.463871	-1.482576	-2.214807
1	1.664601	-1.804615	-2.753080
1	-0.550426	-3.084491	-2.949146
6	-1.997077	-2.860543	-0.676016
6	-1.647863	-2.929219	0.682808
6	-2.761975	-3.918652	-1.200468
6	-2.048210	-4.000190	1.484968

1	-1.071650	-2.122822	1.126568
6	-3.169283	-4.991023	-0.404829
1	-3.047078	-3.891654	-2.249881
6	-2.815439	-5.034603	0.946304
1	-1.766463	-4.018233	2.534314
1	-3.766868	-5.788884	-0.838102
1	-3.134246	-5.864512	1.570570
7	1.807465	0.328018	1.362504
1	1.409718	-0.365416	-0.427316
6	2.671984	0.088166	2.557512
6	1.994380	-0.916591	3.544491
6	1.715881	-2.319349	2.967128
6	2.696606	-1.002246	4.920064
1	1.023206	-0.443580	3.718471
6	2.886524	-3.310634	3.075618
1	1.387142	-2.217050	1.929079
1	0.865858	-2.746725	3.517969
6	3.861163	-2.002990	4.993242
1	3.033218	-0.003261	5.226050
1	1.942709	-1.307618	5.659135
6	3.424217	-3.392650	4.510213
1	3.708143	-3.004345	2.418119
1	2.562112	-4.299368	2.726165
1	4.235520	-2.055480	6.023379
1	4.693176	-1.652785	4.371667
1	4.260755	-4.100373	4.565413
1	2.638042	-3.781083	5.174491
16	0.780614	1.512768	1.551297
8	-0.368775	1.338309	0.574297
8	0.318818	1.757972	2.942533
6	1.516255	3.082712	1.038732
6	2.901368	3.228444	1.013718
6	0.686466	4.155265	0.712357
6	3.455057	4.456238	0.650635
1	3.546245	2.391770	1.258888
6	1.251795	5.373018	0.345056
1	-0.388834	4.026900	0.718868
6	2.643606	5.545463	0.308972
1	4.536556	4.565588	0.623320
1	0.602802	6.202200	0.074035
6	4.042113	-0.285057	2.053610
6	5.165091	0.371378	2.356892
1	4.089750	-1.135243	1.379737
1	6.132497	0.060753	1.969820
1	5.160916	1.229262	3.026236
1	2.789692	1.012025	3.141271
16	1.379947	0.795123	-2.400481
8	0.747640	0.536722	-3.699400
8	1.186206	2.077523	-1.728805
6	3.135261	0.482340	-2.547595
6	3.942532	0.654251	-1.419737
6	3.668002	0.098239	-3.776460
6	5.307568	0.421000	-1.534406
1	3.504607	0.935045	-0.468260
6	5.043496	-0.119419	-3.872085
1	3.017171	-0.023982	-4.635305
6	5.880051	0.036217	-2.759095

1	5.935668	0.537756	-0.655542
1	5.469498	-0.418629	-4.825642
6	3.251267	6.876847	-0.059367
1	3.433037	7.486497	0.835128
1	4.212581	6.752686	-0.568078
1	2.592175	7.452525	-0.716559
6	7.366892	-0.194030	-2.859597
1	7.648729	-0.609443	-3.830790
1	7.917328	0.744843	-2.724586
1	7.713127	-0.883350	-2.081628

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Number of imaginary frequencies : 0
The smallest frequencies are : 15.5547 20.1590 21.5084 cm(-1)

Electronic energy : HF=-3903.3210725
Zero-point correction= 1.313060
(Hartree/Particle)
Thermal correction to Energy= 1.379647
Thermal correction to Enthalpy= 1.380591
Thermal correction to Gibbs Free Energy= 1.210956
Sum of electronic and zero-point Energies= -3902.008012
Sum of electronic and thermal Energies= -3901.941426
Sum of electronic and thermal Enthalpies= -3901.940482
Sum of electronic and thermal Free Energies= -3902.110117

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

28	0.798040	-0.051186	0.348474
15	2.298784	0.511905	-1.191047
6	3.925678	-0.292226	-0.747122
6	5.113283	-0.066869	-1.700009
6	4.326734	0.036299	0.706333
1	3.680564	-1.359052	-0.771769
6	6.314004	-0.926443	-1.269797
1	5.412069	0.988230	-1.674804
1	4.834820	-0.297925	-2.733971
6	5.548114	-0.788967	1.140556
1	4.563134	1.105646	0.793763
1	3.483469	-0.158096	1.378685
6	6.728310	-0.611833	0.174679
1	7.154330	-0.761647	-1.954947
1	6.042960	-1.988528	-1.347811
1	5.841377	-0.508155	2.159624
1	5.261938	-1.846678	1.174108
1	7.565993	-1.250973	0.478527
1	7.089593	0.425791	0.225352
6	2.713111	2.347891	-1.374130
6	3.386552	2.767379	-2.701561
6	1.521298	3.283177	-1.096718
1	3.446937	2.505312	-0.571056
6	3.871913	4.224949	-2.617326
1	2.657161	2.687979	-3.516852
1	4.224486	2.117603	-2.961865
6	1.978960	4.746921	-1.020626

1	0.773129	3.175423	-1.890193
1	1.031152	2.984743	-0.173881
6	2.717625	5.182197	-2.292774
1	4.351547	4.507903	-3.562206
1	4.642915	4.302646	-1.837095
1	1.110983	5.392048	-0.846481
1	2.641517	4.868366	-0.150592
1	3.089218	6.209299	-2.191994
1	2.009660	5.183860	-3.133590
6	1.940979	-0.019807	-2.954735
6	2.041038	-1.530067	-3.232765
6	0.581853	0.523918	-3.440103
1	2.733875	0.458483	-3.542494
6	1.850870	-1.813495	-4.732109
1	1.254362	-2.055928	-2.685848
1	3.001868	-1.929762	-2.891784
6	0.361809	0.223447	-4.930613
1	-0.221718	0.061170	-2.864771
1	0.505096	1.599814	-3.261951
6	0.503022	-1.274423	-5.230104
1	1.923494	-2.893023	-4.912383
1	2.669050	-1.342950	-5.297163
1	-0.634210	0.572592	-5.222849
1	1.092758	0.787067	-5.529935
1	0.393544	-1.460806	-6.305394
1	-0.313866	-1.808261	-4.728977
7	-0.074427	1.575255	1.253722
6	-0.070143	1.955042	2.694258
6	-0.441996	0.759125	3.637037
6	0.701800	-0.256386	3.825728
6	-1.059725	1.176996	4.992502
1	-1.247213	0.263357	3.087503
6	1.678185	0.047782	4.974538
1	1.266450	-0.330320	2.888719
1	0.256450	-1.244803	4.003927
6	-0.053217	1.486521	6.111976
1	-1.741916	2.022814	4.840672
1	-1.686384	0.341591	5.334814
6	0.941331	0.331667	6.289604
1	2.295213	0.914111	4.713582
1	2.365775	-0.799146	5.095359
1	-0.595677	1.671769	7.047129
1	0.500031	2.408055	5.891093
1	1.658718	0.560835	7.086732
1	0.395051	-0.568993	6.606185
16	-1.505880	1.763011	0.536613
8	-1.355312	1.284478	-0.871372
8	-2.648626	1.158901	1.274873
6	1.219432	2.646448	3.061597
6	2.332440	2.680606	2.328735
1	1.205889	3.142319	4.029989
1	3.226895	3.190229	2.676183
1	2.379633	2.181518	1.371408
1	-0.866166	2.695178	2.860714
7	-1.662197	-1.619502	-1.167741
1	-1.455282	-0.612486	-1.172264
6	-1.774612	-2.113879	0.230663

6	-2.311523	-3.563693	0.330561
6	-1.422869	-4.669626	-0.288020
6	-2.788059	-3.923943	1.764305
1	-3.226660	-3.542615	-0.265539
6	-0.415979	-5.316245	0.675717
1	-0.918643	-4.273910	-1.173899
1	-2.093722	-5.455767	-0.657397
6	-1.745136	-4.587542	2.679403
1	-3.214330	-3.035355	2.247512
1	-3.618173	-4.634593	1.656516
6	-1.080563	-5.777433	1.977938
1	0.382504	-4.614025	0.924913
1	0.070713	-6.160876	0.172470
1	-2.234328	-4.906603	3.608000
1	-0.968047	-3.871058	2.976594
1	-0.341635	-6.247780	2.637836
1	-1.842374	-6.539640	1.758133
16	-2.817169	-1.872007	-2.352573
8	-2.496909	-0.878055	-3.387847
8	-2.856888	-3.297356	-2.704550
6	-4.397420	-1.455347	-1.610654
6	-5.451682	-2.366620	-1.664939
6	-4.535165	-0.226242	-0.961102
6	-6.665763	-2.032353	-1.065359
1	-5.311348	-3.321256	-2.160143
6	-5.749484	0.083249	-0.356466
1	-3.701265	0.462519	-0.902472
6	-6.833607	-0.807473	-0.404526
1	-7.491768	-2.737636	-1.104558
1	-5.851342	1.025737	0.174803
6	-0.397831	-1.848273	0.906463
6	0.846813	-1.977172	0.064156
1	-0.328638	-2.389881	1.848679
1	0.599811	-2.218380	-0.964235
1	-2.505578	-1.483310	0.754575
1	-0.485146	-0.779508	1.299328
6	-1.894770	3.523418	0.432255
6	-3.144887	3.866718	-0.095224
6	-1.003819	4.515315	0.836094
6	-3.488497	5.207018	-0.228095
1	-3.837302	3.090639	-0.404016
6	-1.370350	5.858004	0.710191
1	-0.033489	4.252814	1.239995
6	-2.608907	6.226107	0.174481
1	-4.455556	5.471312	-0.648641
1	-0.673918	6.628450	1.030712
6	1.987381	-2.797265	0.554286
6	2.677366	-3.630785	-0.348815
6	2.399713	-2.824214	1.899473
6	3.729347	-4.444878	0.068905
1	2.361908	-3.658199	-1.386275
6	3.446785	-3.642107	2.321934
1	1.886584	-2.208887	2.626206
6	4.122852	-4.455564	1.409117
1	4.233197	-5.082245	-0.652726
1	3.736211	-3.641266	3.369378
1	4.938562	-5.092413	1.738427

6	4.384003	5.890828	0.005071
1	4.711439	6.289241	-2.109713
1	5.724324	5.012294	-1.445119
1	4.048478	5.023966	1.976308
1	5.318749	4.236986	1.044318
1	5.125438	6.622764	0.346951
1	3.410965	6.402529	0.007289
6	0.965844	2.455747	-2.152083
6	0.056157	1.285196	-2.589882
6	0.217673	3.393975	-1.189375
1	1.246707	3.041578	-3.035787
6	-1.249712	1.787711	-3.218304
1	-0.197948	0.706176	-1.698748
1	0.574762	0.611611	-3.281536
6	-1.108800	3.877314	-1.799366
1	0.008783	2.861268	-0.263390
1	0.835775	4.259715	-0.934865
6	-1.990438	2.703013	-2.238640
1	-1.887426	0.939033	-3.481571
1	-1.028662	2.333870	-4.148243
1	-1.634624	4.498749	-1.063635
1	-0.897137	4.522480	-2.665354
1	-2.926916	3.060233	-2.678663
1	-2.253633	2.110102	-1.356801
7	1.205772	0.870228	1.779992
6	1.781021	0.631514	3.148234
6	1.699451	-0.877721	3.584566
6	2.989437	-1.708776	3.414838
6	1.147945	-1.042558	5.014256
1	0.958593	-1.305324	2.909713
6	4.029231	-1.533201	4.535544
1	3.446867	-1.498733	2.445673
1	2.690886	-2.767307	3.386113
6	2.197258	-0.770044	6.100392
1	0.266329	-0.404652	5.136652
1	0.797540	-2.079034	5.126520
6	3.404922	-1.703525	5.927823
1	4.477294	-0.536226	4.472829
1	4.846010	-2.250311	4.387398
1	1.752575	-0.897835	7.095119
1	2.535191	0.273113	6.036772
1	4.155385	-1.515263	6.705654
1	3.072054	-2.744590	6.056702
16	-0.417381	0.976991	1.818831
8	-0.946319	0.703611	0.458505
8	-1.040977	0.213437	2.931207
6	3.156379	1.240513	3.165811
6	3.529514	2.256791	3.945570
1	3.873689	0.805948	2.472950
1	4.538967	2.658385	3.912102
1	2.843107	2.718919	4.651907
1	1.174867	1.199654	3.863834
7	0.341112	-2.079735	-1.589828
1	0.342432	-1.167376	-1.134975
6	1.612310	-2.831225	-1.487684
6	2.295573	-2.910486	-2.886758
6	3.632045	-3.691591	-2.879799

6	1.368010	-3.504847	-3.969968
1	2.502265	-1.874406	-3.179219
6	3.446466	-5.210893	-2.743458
1	4.308230	-3.325927	-2.101989
1	4.134049	-3.489803	-3.836263
6	1.197526	-5.028902	-3.870186
1	0.392555	-3.015194	-3.936314
1	1.813832	-3.262267	-4.944772
6	2.546614	-5.757894	-3.859353
1	3.000505	-5.448231	-1.766701
1	4.427089	-5.701989	-2.760001
1	0.577516	-5.376699	-4.704683
1	0.639699	-5.273596	-2.960677
1	2.399222	-6.838040	-3.739132
1	3.052017	-5.614560	-4.825652
16	-1.114065	-2.844803	-1.259365
8	-2.103564	-1.760922	-1.315395
8	-1.215366	-4.013310	-2.138540
6	-1.010453	-3.454117	0.416511
6	-1.219595	-2.559189	1.463812
6	-0.683588	-4.791533	0.656381
6	-1.090458	-3.009163	2.774559
1	-1.479842	-1.530955	1.262061
6	-0.552964	-5.222931	1.976025
1	-0.559900	-5.477887	-0.174206
6	-0.744772	-4.340026	3.051003
1	-1.250605	-2.299651	3.579402
1	-0.305535	-6.262533	2.174429
6	2.538662	-2.265936	-0.391755
6	3.598736	-1.395764	-0.650487
1	2.591547	-2.859245	0.516644
1	3.746872	-1.057671	-1.664936
1	1.366262	-3.849488	-1.169393
1	1.549823	-1.236516	0.724344
6	-0.813035	2.698618	2.196292
6	0.187829	3.641538	2.408815
6	-2.162739	3.059247	2.278822
6	-0.163247	4.966583	2.679156
1	1.226180	3.339087	2.353133
6	-2.495586	4.381532	2.554683
1	-2.939298	2.314790	2.131911
6	-1.504138	5.359352	2.748058
1	0.621050	5.702793	2.836495
1	-3.542918	4.664114	2.628579
6	-0.555710	-4.803897	4.473876
1	0.485084	-4.663690	4.792458
1	-1.185545	-4.237585	5.166020
1	-0.790734	-5.866688	4.587781
6	-1.894177	6.788968	3.031558
1	-1.017871	7.436176	3.127454
1	-2.523843	7.192654	2.230149
1	-2.470583	6.865193	3.961222
6	4.784841	-1.322806	0.247974
6	5.338863	-2.502225	0.776736
6	5.390328	-0.098812	0.579939
6	6.451252	-2.456369	1.616579
1	4.896771	-3.460354	0.519593

6	6.501047	-0.051332	1.422018
1	4.954563	0.821211	0.209473
6	7.035333	-1.230485	1.944835
1	6.863544	-3.379600	2.013272
1	6.939731	0.908843	1.678189
1	7.897588	-1.195197	2.603924
7	-4.804034	-0.578385	-0.968981
1	-3.915044	-1.031482	-1.178436
6	-5.687638	-1.148576	0.056242
6	-6.116006	-2.608097	-0.304936
6	-4.955320	-3.623019	-0.388281
6	-7.269692	-3.162576	0.565667
1	-6.516831	-2.489385	-1.317625
6	-4.528172	-4.204111	0.967838
1	-4.099356	-3.176344	-0.899864
1	-5.287747	-4.451354	-1.029147
6	-6.849934	-3.822291	1.893045
1	-8.012320	-2.375200	0.751465
1	-7.783798	-3.926304	-0.033658
6	-5.721310	-4.843518	1.690604
1	-4.100945	-3.412285	1.592510
1	-3.732307	-4.942595	0.815913
1	-7.725573	-4.305051	2.345337
1	-6.515173	-3.066553	2.612556
1	-5.410040	-5.258941	2.657307
1	-6.097413	-5.686081	1.091627
16	-5.431864	0.247716	-2.249895
8	-4.330860	0.406542	-3.211363
8	-6.710861	-0.327342	-2.703605
6	-5.831272	1.843740	-1.528996
6	-6.941776	2.538799	-2.007679
6	-4.988879	2.415348	-0.571752
6	-7.202683	3.822439	-1.527030
1	-7.594534	2.071935	-2.737309
6	-5.259231	3.698452	-0.108112
1	-4.146471	1.853551	-0.189298
6	-6.364607	4.423804	-0.579183
1	-8.070560	4.363152	-1.895008
1	-4.595527	4.146083	0.625699
6	-5.102553	-0.929505	1.431040
6	-3.917432	-0.384440	1.705878
1	-5.748625	-1.240229	2.248054
1	-3.231820	-0.062335	0.929813
1	-3.570108	-0.262943	2.726508
1	-6.614782	-0.558754	0.017996
6	-6.626123	5.821456	-0.074161
1	-6.591160	5.862348	1.020333
1	-5.867228	6.520675	-0.446505
1	-7.603935	6.192435	-0.394386

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Normal termination of Gaussian 09 at Sat Apr 20 09:24:28 2019.

Number of imaginary frequencies : 0

The smallest frequencies are : 37.1983 8.5783 8.2273 cm(-1)

S108

Electronic energy :	HF=-3903.3191442	
Zero-point correction=		1.307903
(Hartree/Particle)		
Thermal correction to Energy=		1.374083
Thermal correction to Enthalpy=		1.375027
Thermal correction to Gibbs Free Energy=		1.203265
Sum of electronic and zero-point Energies=		-3902.011241
Sum of electronic and thermal Energies=		-3901.945061
Sum of electronic and thermal Enthalpies=		-3901.944117
Sum of electronic and thermal Free Energies=		-3902.115879

.....
 Cartesian Coordinates

28	0.793697	0.831612	0.614179
15	2.428571	1.430470	-0.676355
6	3.993982	0.428025	-0.394942
6	5.102348	0.580278	-1.458908
6	4.582219	0.651109	1.015410
1	3.624879	-0.605972	-0.434822
6	6.266840	-0.385010	-1.182463
1	5.486845	1.607172	-1.443718
1	4.711344	0.401837	-2.465035
6	5.753713	-0.303438	1.291301
1	4.946954	1.683886	1.101318
1	3.804838	0.522328	1.775052
6	6.847963	-0.179708	0.222791
1	7.045260	-0.248682	-1.943381
1	5.903173	-1.415282	-1.277419
1	6.164649	-0.099525	2.287574
1	5.377719	-1.332762	1.304191
1	7.649474	-0.904002	0.412318
1	7.304510	0.819005	0.283875
6	2.877774	3.223760	-0.332522
6	3.697618	3.940221	-1.425633
6	1.644743	4.070236	0.051142
1	3.499262	3.151777	0.569493
6	4.105520	5.351832	-0.969776
1	3.097886	4.021001	-2.341072
1	4.589722	3.366259	-1.688390
6	2.053823	5.478649	0.505231
1	0.974853	4.156666	-0.812102
1	1.074339	3.566833	0.836886
6	2.885433	6.192784	-0.569427
1	4.669008	5.849729	-1.767892
1	4.785175	5.268178	-0.109830
1	1.157973	6.061487	0.751331
1	2.642745	5.400621	1.430186
1	3.202907	7.181008	-0.215993
1	2.258280	6.361551	-1.456839
6	2.092354	1.303033	-2.508586
6	1.884981	-0.169860	-2.915566
6	0.865848	2.139414	-2.931742
1	2.976277	1.695259	-3.028604
6	1.628623	-0.302017	-4.423886
1	1.026430	-0.563353	-2.360411
1	2.741693	-0.785667	-2.625513
6	0.613110	2.017832	-4.443017

1	-0.011992	1.783344	-2.379019
1	1.006014	3.192824	-2.670064
6	0.437729	0.555342	-4.871812
1	1.451200	-1.353987	-4.677020
1	2.533387	0.006781	-4.967927
1	-0.273662	2.603066	-4.715773
1	1.461973	2.462086	-4.983472
1	0.313834	0.491540	-5.959434
1	-0.480872	0.150276	-4.432523
7	-0.676820	0.534924	1.829256
6	-0.983392	0.270642	3.237039
6	-0.633642	-1.218547	3.566769
6	0.849422	-1.593364	3.384528
6	-1.160335	-1.722048	4.931815
1	-1.197078	-1.758151	2.795967
6	1.737681	-1.231766	4.582232
1	1.234232	-1.138849	2.467149
1	0.895897	-2.683758	3.245750
6	-0.242842	-1.457947	6.141064
1	-2.162842	-1.315812	5.120556
1	-1.287324	-2.809738	4.842599
6	1.207504	-1.883174	5.867254
1	1.768078	-0.142313	4.702484
1	2.767720	-1.556197	4.386696
1	-0.637577	-1.992341	7.014079
1	-0.251998	-0.395033	6.407455
1	1.843323	-1.627523	6.723659
1	1.251164	-2.977034	5.758240
16	-1.859132	0.754398	0.783008
8	-1.077850	0.646877	-0.522856
8	-3.042765	-0.097583	0.991647
6	-0.419219	1.323908	4.162522
6	0.225592	2.433610	3.802587
1	-0.622494	1.150829	5.216467
1	0.561748	3.152763	4.544781
1	0.440578	2.646951	2.762026
1	-2.076150	0.315595	3.367141
7	-1.572100	-2.093170	-1.974119
1	-1.069319	-1.205531	-1.982514
6	-1.561551	-2.620427	-0.581490
6	-2.393949	-3.924743	-0.400383
6	-1.952192	-5.127290	-1.264349
6	-2.547712	-4.307987	1.091790
1	-3.394864	-3.650065	-0.740749
6	-0.854457	-6.013908	-0.649492
1	-1.652826	-4.769165	-2.253075
1	-2.841777	-5.749901	-1.428461
6	-1.421495	-5.182909	1.665689
1	-2.682581	-3.402417	1.697486
1	-3.483387	-4.876015	1.185336
6	-1.188880	-6.422585	0.791397
1	0.104693	-5.487372	-0.654133
1	-0.724093	-6.906002	-1.275123
1	-1.679938	-5.477216	2.690875
1	-0.485725	-4.615470	1.734222
1	-0.384743	-7.039904	1.210480
1	-2.098066	-7.041922	0.795687

16	-2.945225	-1.863958	-2.916276
8	-2.439879	-1.133857	-4.088979
8	-3.623711	-3.154606	-3.076161
6	-4.064911	-0.760600	-2.055705
6	-5.107191	-1.280638	-1.290603
6	-3.868803	0.618765	-2.162715
6	-5.956595	-0.403892	-0.617551
1	-5.261368	-2.352609	-1.240380
6	-4.728193	1.478445	-1.487822
1	-3.057806	1.005705	-2.768149
6	-5.781139	0.982221	-0.703970
1	-6.768526	-0.804457	-0.016446
1	-4.574455	2.551615	-1.558655
6	-0.112829	-2.751739	-0.173929
6	0.905573	-2.965696	-1.021979
1	0.059168	-2.698042	0.895930
1	0.675879	-3.006155	-2.084180
1	-2.033202	-1.885935	0.075896
1	1.803185	0.998790	1.605551
6	-2.460205	2.445465	0.825959
6	-1.844899	3.423716	0.045392
6	-3.500959	2.774817	1.695820
6	-2.276194	4.744978	0.142727
1	-1.053707	3.142019	-0.638009
6	-3.914110	4.102741	1.789372
1	-3.997207	1.997627	2.266453
6	-3.308100	5.108136	1.020762
1	-1.806706	5.506461	-0.474875
1	-4.725968	4.361606	2.464105
6	2.308689	-3.235104	-0.680208
6	3.219167	-3.491295	-1.723132
6	2.787510	-3.307778	0.642431
6	4.547780	-3.824953	-1.459293
1	2.869921	-3.444152	-2.751363
6	4.112035	-3.645565	0.906433
1	2.117903	-3.106913	1.469075
6	5.000797	-3.909582	-0.141227
1	5.226795	-4.025084	-2.283436
1	4.452969	-3.705356	1.936333
1	6.033011	-4.173573	0.069156
6	-6.708071	1.933303	0.010241
1	-6.152675	2.772814	0.439574
1	-7.449662	2.353188	-0.681099
1	-7.254914	1.435757	0.816521
6	-3.740084	6.547166	1.153542
1	-4.805365	6.627579	1.390622
1	-3.188899	7.045994	1.960668
1	-3.551937	7.110128	0.234412