

Electronic Supplementary Information

for

Two Chiral Catalysts in Action: Insights on Cooperativity and Stereoselectivity in Proline and Cinchona-Thiourea Dual Organo Catalysis

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-----PART-B-----

Cartesian Coordinates of optimized geometries at the SMD/M06-2X/6-31G** Level of Theory

Scheme 1(a) Details

Cartesian Coordinates of optimized geometries at the SMD_(benzene)/M06-2X/6-31G** Level of Theory

Stationary points relevant to Schemes 1(a), 2, 3, Figures 1

butanone

Number of imaginary frequencies : 0

Electronic energy : =-232.367908
Zero-point correction= 0.113679
Thermal correction to Energy= 0.120194
Thermal correction to Enthalpy= 0.121138
Thermal correction to Gibbs Free Energy= 0.083370
Sum of electronic and zero-point Energies= -232.254229
Sum of electronic and thermal Energies= -232.247714
Sum of electronic and thermal Enthalpies= -232.246770
Sum of electronic and thermal Free Energies= -232.284538

Cartesian Coordinates

6	0.523164	0.166044	-0.015648
6	-0.677154	-0.761487	-0.043520
6	-2.002428	-0.021254	0.035991
8	0.397402	1.371751	-0.016923
1	-0.566491	-1.482831	0.776363
1	-0.608629	-1.356030	-0.964295
1	-2.105966	0.677512	-0.797069
1	-2.067894	0.559254	0.959366
1	-2.841016	-0.721084	0.007613
6	1.883287	-0.492585	0.025301
1	2.664444	0.255334	-0.112042
1	2.019845	-0.982890	0.995273
1	1.965268	-1.267578	-0.742569

(RR)-Cinchona-Thiourea

Number of imaginary frequencies : 0

Electronic energy : =-2412.6836597
Zero-point correction= 0.544871
Thermal correction to Energy= 0.580324
Thermal correction to Enthalpy= 0.581268
Thermal correction to Gibbs Free Energy= 0.473734
Sum of electronic and zero-point Energies= -2412.138789
Sum of electronic and thermal Energies= -2412.103336
Sum of electronic and thermal Enthalpies= -2412.102392
Sum of electronic and thermal Free Energies= -2412.209926

Cartesian Coordinates

7	-1.813167	0.684814	0.689402
6	-3.096156	0.237679	0.335994
6	-3.434233	-1.109448	0.172685

6	-4.748281	-1.447103	-0.129174
6	-5.747631	-0.488164	-0.253537
6	-5.400594	0.843532	-0.066443
6	-4.092373	1.210985	0.219657
6	-5.093509	-2.892257	-0.362872
9	-4.276688	-3.718601	0.302456
6	-6.435557	1.919394	-0.235455
9	-7.671547	1.466413	0.009255
6	-0.575735	0.173396	0.389052
16	-0.287153	-1.215815	-0.501997
7	0.423289	0.937788	0.886567
6	1.832714	0.700691	0.614614
6	2.587446	1.981633	1.035814
6	4.062557	1.983932	0.557608
6	4.281717	3.222794	-0.325376
6	4.006180	4.474101	0.523045
6	2.562193	4.369068	1.088837
7	1.869479	3.182338	0.566516
6	1.853518	3.249368	-0.900921
6	3.293676	3.225337	-1.505574
6	3.459350	2.106506	-2.502663
6	4.500031	1.285627	-2.629562
6	2.373953	-0.491642	1.390894
6	3.277005	-1.442707	0.817863
6	3.783237	-2.459239	1.680907
7	3.439580	-2.572050	2.995631
6	2.591788	-1.696026	3.473610
6	2.038223	-0.639794	2.712483
6	4.692257	-3.411001	1.158030
6	5.085896	-3.379228	-0.154807
6	4.567020	-2.378500	-1.015390
6	3.680451	-1.437368	-0.537323
9	-6.348960	-3.167145	0.022794
9	-5.006723	-3.213827	-1.662621
9	-6.437435	2.414066	-1.483310
9	-6.212874	2.954934	0.589523
1	2.548092	2.027260	2.131488
1	4.740730	2.020066	1.415959
1	4.294515	1.070162	0.006535
1	1.966831	5.247878	0.823284
1	2.570259	4.296531	2.181002
1	4.119295	5.373811	-0.091102
1	4.736613	4.542546	1.335321
1	5.310884	3.242024	-0.697008
1	3.442063	4.165001	-2.056181
1	1.328425	4.169319	-1.175694
1	1.256254	2.415701	-1.285863
1	2.624898	1.991315	-3.196866
1	4.516508	0.517048	-3.396015
1	5.370837	1.338820	-1.981245
1	1.962938	0.528794	-0.459306
1	1.338899	0.048149	3.178669
1	3.306076	-0.703153	-1.240941
1	2.317108	-1.801371	4.521761
1	5.065870	-4.169809	1.837718
1	5.783038	-4.121078	-0.525642
1	0.232084	1.909304	1.127727
1	-1.811391	1.588330	1.147880
1	-2.684862	-1.879518	0.288731
1	-3.844294	2.259763	0.357840
1	-6.770567	-0.771628	-0.473868
8	4.897268	-2.279923	-2.329254
6	5.750600	-3.266016	-2.877303
1	5.849742	-3.023794	-3.935771
1	6.743148	-3.245393	-2.411691

1 5.321624 -4.269755 -2.778569

trans- β -nitrostyrene

Number of imaginary frequencies : 0

Electronic energy : =-513.9498892
Zero-point correction= 0.138632
Thermal correction to Energy= 0.147644
Thermal correction to Enthalpy= 0.148588
Thermal correction to Gibbs Free Energy= 0.103120
Sum of electronic and zero-point Energies= -513.811257
Sum of electronic and thermal Energies= -513.802245
Sum of electronic and thermal Enthalpies= -513.801301
Sum of electronic and thermal Free Energies= -513.846770

Cartesian Coordinates

8	-3.811942	-0.926959	0.000043
8	-3.243065	1.158698	-0.000075
6	-0.617948	0.452956	-0.000017
1	-0.921834	1.497229	-0.000052
1	-1.500983	-1.535464	0.000073
6	0.819366	0.178356	-0.000011
6	1.344469	-1.122620	-0.000098
6	1.701503	1.265944	0.000085
6	2.716913	-1.323850	-0.000083
1	0.677355	-1.978894	-0.000182
6	3.077098	1.062656	0.000102
1	1.300297	2.275616	0.000147
6	3.586642	-0.232276	0.000018
1	3.112864	-2.334139	-0.000155
1	3.749196	1.914426	0.000177
1	4.659701	-0.394976	0.000027
7	-2.978998	-0.033192	0.000014
6	-1.591969	-0.458727	0.000025

(S)-Proline

Number of imaginary frequencies : 0

Electronic energy : =-401.0032749
Zero-point correction= 0.146575
Thermal correction to Energy= 0.154022
Thermal correction to Enthalpy= 0.154966
Thermal correction to Gibbs Free Energy= 0.113878
Sum of electronic and zero-point Energies= -400.856700
Sum of electronic and thermal Energies= -400.849253
Sum of electronic and thermal Enthalpies= -400.848309
Sum of electronic and thermal Free Energies= -400.889397

Cartesian Coordinates

6	-0.724841	-0.711330	1.075508
6	-1.741866	-0.903502	-0.053334
6	-2.011431	0.534529	-0.480638
7	-0.675193	1.137519	-0.450348
6	0.127360	0.485430	0.595634

6	1.452753	0.039031	0.003837
8	2.537184	0.452536	0.337418
8	1.299907	-0.892790	-0.952247
1	0.382883	1.158187	1.420091
1	-0.126462	-1.602183	1.279557
1	-1.240133	-0.431195	1.999198
1	-1.287438	-1.456353	-0.879761
1	-2.644137	-1.426402	0.271022
1	-2.441422	0.608677	-1.483883
1	-2.710513	1.009013	0.226516
1	2.187390	-1.107601	-1.280540
1	-0.702397	2.142306	-0.327174

(RR)-Cinchona-(S)-Proline-complex

Number of imaginary frequencies : 0

Electronic energy : =-2813.7282562
Zero-point correction= 0.692940
Thermal correction to Energy= 0.736791
Thermal correction to Enthalpy= 0.737735
Thermal correction to Gibbs Free Energy= 0.610946
Sum of electronic and zero-point Energies= -2813.035316
Sum of electronic and thermal Energies= -2812.991465
Sum of electronic and thermal Enthalpies= -2812.990521
Sum of electronic and thermal Free Energies= -2813.117310

Cartesian Coordinates

6	-3.609969	3.983893	-0.128581
6	-4.443912	4.002041	1.173716
6	-3.899741	2.809684	2.001715
7	-2.615494	2.422649	1.392366
6	-2.842473	2.646581	-0.042974
6	-1.551654	2.636816	-0.837421
8	-0.511117	3.068214	-0.138139
8	-1.495561	2.292461	-1.999315
1	-3.468173	1.831590	-0.425109
1	-2.890461	4.809349	-0.140117
1	-4.214609	4.051733	-1.034505
1	-5.511091	3.883039	0.973914
1	-4.313631	4.947539	1.705332
1	-4.582578	1.957046	1.927586
1	-3.760270	3.037876	3.060271
1	0.391118	2.831095	-0.670936
1	-1.908742	3.101860	1.678084
7	-1.339028	-0.094839	0.653459
6	-2.507262	-0.798584	0.323193
6	-2.695665	-1.449865	-0.900168
6	-3.923400	-2.038256	-1.174470
6	-4.987654	-1.971574	-0.279143
6	-4.791840	-1.301792	0.920616
6	-3.563576	-0.729652	1.233749
6	-4.096979	-2.793181	-2.462684
9	-3.337210	-2.290419	-3.444885
6	-5.921774	-1.132415	1.893319
9	-5.525884	-1.333252	3.158611
6	-0.043539	-0.390123	0.343995
16	0.477095	-1.846798	-0.322922
7	0.798589	0.625249	0.646629
6	2.224876	0.634042	0.372706
6	2.657513	2.001912	-0.206201

6	4.094984	1.924616	-0.786491
6	4.039213	2.227688	-2.293070
6	3.546414	3.669232	-2.472382
6	2.190814	3.804703	-1.740679
7	1.717875	2.490452	-1.246886
6	1.630904	1.545218	-2.380016
6	3.037394	1.299001	-3.006759
6	3.395248	-0.166606	-3.013334
6	4.587473	-0.699460	-2.754419
6	3.041700	0.329979	1.625283
6	4.054815	-0.679804	1.664541
6	4.789121	-0.817094	2.880929
7	4.552239	-0.063727	3.991857
6	3.597104	0.829225	3.924540
6	2.823477	1.064615	2.763694
6	5.820352	-1.784473	2.952938
6	6.121598	-2.588018	1.883643
6	5.379790	-2.460432	0.681258
6	4.365594	-1.531570	0.580113
9	-3.759075	-4.084807	-2.328086
9	-5.370975	-2.766684	-2.884500
9	-6.935374	-1.970539	1.646236
9	-6.424835	0.117381	1.847177
1	2.609557	2.743276	0.602312
1	4.747148	2.651077	-0.291931
1	4.523444	0.935340	-0.607634
1	1.409570	4.199860	-2.396449
1	2.262338	4.469645	-0.874360
1	3.435093	3.896952	-3.537021
1	4.276619	4.372665	-2.061712
1	5.034020	2.114759	-2.733795
1	2.992128	1.617112	-4.057600
1	0.925951	1.976133	-3.093888
1	1.183356	0.613168	-2.020897
1	2.575055	-0.834190	-3.281401
1	4.742583	-1.772868	-2.799438
1	5.450321	-0.097466	-2.480118
1	2.398638	-0.141262	-0.375004
1	2.055162	1.833024	2.790904
1	3.812380	-1.493057	-0.350764
1	3.410367	1.417391	4.821218
1	6.363305	-1.866833	3.888808
1	6.915882	-3.319880	1.968880
1	0.377826	1.497809	0.947768
1	-1.548101	0.753919	1.197686
1	-1.895913	-1.482476	-1.628371
1	-3.417723	-0.223721	2.183688
1	-5.944064	-2.423056	-0.515745
8	5.606430	-3.222096	-0.418600
6	6.624136	-4.202528	-0.354953
1	6.626621	-4.695906	-1.327249
1	7.608113	-3.751604	-0.180239
1	6.419638	-4.947298	0.422823

water

Number of imaginary frequencies : 0

Electronic energy : =-76.3880687

Zero-point correction= 0.021603

Thermal correction to Energy=	0.024438
Thermal correction to Enthalpy=	0.025382
Thermal correction to Gibbs Free Energy=	0.003954
Sum of electronic and zero-point Energies=	-76.366466
Sum of electronic and thermal Energies=	-76.363631
Sum of electronic and thermal Enthalpies=	-76.362686
Sum of electronic and thermal Free Energies=	-76.384115

Cartesian Coordinates

8	0.000000	-0.000000	0.118449
1	0.000000	0.759279	-0.473797
1	-0.000000	-0.759279	-0.473797

(1) Enamine formation between proline and butanone (Scheme S2 and Fig. S1)

2_re

Number of imaginary frequencies : 0

Electronic energy :	=-633.3877366
Zero-point correction=	0.262362
Thermal correction to Energy=	0.277308
Thermal correction to Enthalpy=	0.278252
Thermal correction to Gibbs Free Energy=	0.219460
Sum of electronic and zero-point Energies=	-633.125375
Sum of electronic and thermal Energies=	-633.110429
Sum of electronic and thermal Enthalpies=	-633.109484
Sum of electronic and thermal Free Energies=	-633.168277

Cartesian Coordinates

6	-2.657678	-0.644506	-0.462676
6	-2.520341	-1.778721	0.572365
6	-1.001800	-1.917629	0.731801
7	-0.468011	-0.551812	0.625361
6	-1.280224	0.058491	-0.454683
6	2.129054	-0.424877	-0.547901
6	2.705973	-0.163626	0.822824
6	2.530358	1.266515	1.303641
6	-1.350281	1.569918	-0.243697
8	-0.192281	2.218837	-0.363523
8	1.700705	0.467856	-1.263215
8	-2.362545	2.157856	0.047603
1	3.769511	-0.437013	0.769789
1	-0.746914	-0.119366	-1.398233
1	-3.443697	0.064818	-0.199166
1	-2.875845	-1.036899	-1.458831
1	-3.005152	-2.705758	0.257325
1	-2.960576	-1.477954	1.528721
1	-0.588445	-2.511335	-0.093782
1	-0.686780	-2.376059	1.672851
1	0.539092	1.623871	-0.641856
1	-0.695693	-0.073235	1.498302
1	2.245059	-0.878208	1.513049
1	1.471563	1.502013	1.435210
1	2.944298	1.977965	0.584683
1	3.033780	1.414876	2.261674
6	2.186639	-1.844323	-1.048202
1	1.578302	-1.950886	-1.947257
1	3.225024	-2.095770	-1.292566
1	1.855329	-2.542218	-0.275205

[2-3]TS *re*

Number of imaginary frequencies : 1

The smallest frequency is : -187.5266 cm(-1)

Electronic energy : =-633.3779472
Zero-point correction= 0.263167
Thermal correction to Energy= 0.275882
Thermal correction to Enthalpy= 0.276826
Thermal correction to Gibbs Free Energy= 0.224565
Sum of electronic and zero-point Energies= -633.114780
Sum of electronic and thermal Energies= -633.102065
Sum of electronic and thermal Enthalpies= -633.101121
Sum of electronic and thermal Free Energies= -633.153382

Cartesian Coordinates

6	-2.368214	-0.916102	-0.378172
6	-2.038593	-1.696241	0.900363
6	-0.524724	-1.858076	0.791097
7	-0.067079	-0.535292	0.297027
6	-1.160135	0.005411	-0.579601
6	1.569459	-0.290870	-0.539732
6	2.490748	-0.233577	0.682763
6	2.451106	1.100061	1.418413
6	-1.400430	1.473576	-0.187712
8	-0.309630	2.206821	-0.174090
8	1.414410	0.783647	-1.221354
8	-2.497690	1.886876	0.112495
1	3.502519	-0.395741	0.289039
1	-0.777642	0.002909	-1.605995
1	-3.281490	-0.325451	-0.299491
1	-2.463042	-1.601337	-1.224865
1	-2.559646	-2.653097	0.970946
1	-2.287761	-1.100278	1.784923
1	-0.274584	-2.611109	0.038296
1	-0.014311	-2.102487	1.724590
1	0.501038	1.692701	-0.612037
1	0.029125	0.081594	1.105241
1	2.283530	-1.076882	1.352338
1	1.485106	1.297201	1.896893
1	2.640446	1.917672	0.719796
1	3.210585	1.129039	2.203435
6	1.705015	-1.569125	-1.347934
1	0.842635	-1.707240	-2.007129
1	2.587810	-1.452630	-1.982935
1	1.843120	-2.456910	-0.725547

3_ *re*

Number of imaginary frequencies : 0

Electronic energy : =-633.3990232
Zero-point correction= 0.264739
Thermal correction to Energy= 0.278082
Thermal correction to Enthalpy= 0.279026
Thermal correction to Gibbs Free Energy= 0.225405
Sum of electronic and zero-point Energies= -633.134284

Sum of electronic and thermal Energies= -633.120941
 Sum of electronic and thermal Enthalpies= -633.119997
 Sum of electronic and thermal Free Energies= -633.173618

Cartesian Coordinates

6	-1.944232	-1.431396	-0.287074
6	-1.361210	-1.900305	1.047270
6	0.128582	-1.629542	0.853455
7	0.148929	-0.340808	0.140320
6	-1.126441	-0.165248	-0.583978
6	1.365899	0.004679	-0.619342
6	2.572474	0.011014	0.331212
6	2.418495	0.928590	1.539525
6	-1.837093	1.092221	-0.060759
8	-1.198711	1.686251	0.949604
8	1.158004	1.282778	-1.183319
8	-2.877641	1.496449	-0.514414
1	3.436141	0.322847	-0.265210
1	-0.981344	-0.004142	-1.655050
1	-3.016207	-1.227845	-0.265517
1	-1.750072	-2.179276	-1.062713
1	-1.571692	-2.947628	1.271282
1	-1.749686	-1.288260	1.869182
1	0.582085	-2.431984	0.253202
1	0.679631	-1.557277	1.796325
1	0.962211	1.905015	-0.468835
1	-0.425096	1.083899	1.106101
1	2.773646	-1.014276	0.662739
1	1.615138	0.597624	2.205127
1	2.211321	1.963226	1.243460
1	3.341872	0.949716	2.123525
6	1.630207	-0.921688	-1.803011
1	0.771413	-0.954661	-2.478422
1	2.487672	-0.548286	-2.367765
1	1.857164	-1.936793	-1.468425

2_si

Number of imaginary frequencies : 0

Electronic energy : =-633.3861067
 Zero-point correction= 0.262562
 Thermal correction to Energy= 0.277697
 Thermal correction to Enthalpy= 0.278641
 Thermal correction to Gibbs Free Energy= 0.218050
 Sum of electronic and zero-point Energies= -633.123545
 Sum of electronic and thermal Energies= -633.108410
 Sum of electronic and thermal Enthalpies= -633.107466
 Sum of electronic and thermal Free Energies= -633.168056

Cartesian Coordinates

6	2.676485	0.941471	-0.520754
6	2.205792	2.312273	0.021184
6	0.724766	2.082706	0.386999
7	0.570578	0.641874	0.632150
6	1.435741	0.038444	-0.400846
6	-1.916755	-0.452207	-0.210438
6	-1.972250	-1.148997	1.122829
6	1.746776	-1.407413	-0.015413
8	0.809614	-2.306042	-0.311364

8	-1.346392	-0.949365	-1.173320
8	2.758487	-1.727390	0.560112
1	-2.911933	-1.711500	1.180822
1	0.861069	0.042109	-1.335415
1	3.478592	0.522838	0.090814
1	3.032625	0.993988	-1.551930
1	2.323648	3.116214	-0.708956
1	2.778422	2.590041	0.910258
1	0.080189	2.346564	-0.460546
1	0.390420	2.654303	1.256350
1	0.016969	-1.883839	-0.723846
1	0.989459	0.432900	1.540285
1	-1.956730	-0.428878	1.943449
6	-2.662000	0.851747	-0.348971
1	-2.538840	1.200768	-1.377133
1	-1.143079	-1.850103	1.221516
1	-2.172377	1.568816	0.321428
6	-4.143218	0.726862	0.020372
1	-4.650534	1.681476	-0.136065
1	-4.642254	-0.024161	-0.598676
1	-4.275386	0.448423	1.069411

[2-3]TS_si

Number of imaginary frequencies : 1

The smallest frequency is : -160.2234 cm(-1)

Electronic energy : =-633.3767543

Zero-point correction= 0.263340

Thermal correction to Energy= 0.276038

Thermal correction to Enthalpy= 0.276982

Thermal correction to Gibbs Free Energy= 0.224191

Sum of electronic and zero-point Energies= -633.113415

Sum of electronic and thermal Energies= -633.100716

Sum of electronic and thermal Enthalpies= -633.099772

Sum of electronic and thermal Free Energies= -633.152563

Cartesian Coordinates

6	2.062637	1.230680	-0.850194
6	1.833946	2.140328	0.363440
6	0.351844	1.920521	0.652174
7	0.179376	0.456405	0.475372
6	1.120709	0.042210	-0.619521
6	-1.470751	-0.326589	0.218648
6	-1.873512	-0.513394	1.675321
6	1.818763	-1.256840	-0.174827
8	0.992871	-2.200927	0.211705
8	-1.224063	-1.391612	-0.457015
8	3.025468	-1.358767	-0.154710
1	-2.892711	-0.910160	1.699178
1	0.501961	-0.199105	-1.490262
1	3.091182	0.879217	-0.936589
1	1.790093	1.753089	-1.770985
1	2.072934	3.187840	0.169973
1	2.433826	1.800760	1.214658
1	-0.262453	2.428575	-0.096109
1	0.020168	2.216276	1.649418
1	-0.012783	-1.962085	-0.045963
1	0.481015	0.004542	1.340934
1	-1.852748	0.420280	2.245223

6	-2.241537	0.752878	-0.533556
1	-1.651372	1.047028	-1.410304
1	-1.223128	-1.255300	2.148348
1	-2.384704	1.638661	0.094973
6	-3.590576	0.205090	-0.997247
1	-4.127875	0.950242	-1.589210
1	-3.437352	-0.686879	-1.608056
1	-4.225033	-0.066678	-0.148087

3_si

Number of imaginary frequencies : 0

Electronic energy : =-633.3971501
Zero-point correction= 0.264865
Thermal correction to Energy= 0.278266
Thermal correction to Enthalpy= 0.279210
Thermal correction to Gibbs Free Energy= 0.225183
Sum of electronic and zero-point Energies= -633.132285
Sum of electronic and thermal Energies= -633.118884
Sum of electronic and thermal Enthalpies= -633.117940
Sum of electronic and thermal Free Energies= -633.171967

Cartesian Coordinates

6	1.699116	1.276543	-1.061103
6	1.587911	2.116839	0.212408
6	0.173825	1.790562	0.686652
7	0.045991	0.347748	0.408236
6	0.994561	-0.027813	-0.660610
6	-1.314877	-0.214352	0.285123
6	-2.081598	0.090816	1.569017
6	1.998482	-1.052138	-0.110228
8	1.842298	-1.310662	1.187918
8	-1.171261	-1.608626	0.109405
8	2.854867	-1.560110	-0.789372
1	-3.004172	-0.492254	1.589840
1	0.502225	-0.514310	-1.505386
1	2.722316	1.099670	-1.397347
1	1.145470	1.755288	-1.875383
1	1.737754	3.185047	0.045191
1	2.319779	1.778540	0.954598
1	-0.559218	2.379992	0.116422
1	0.017700	1.991705	1.749975
1	-0.782688	-1.979715	0.913628
1	1.092366	-0.710496	1.440087
1	-2.340062	1.150878	1.646755
6	-2.060588	0.282772	-0.961358
1	-1.472091	0.002754	-1.841228
1	-2.102027	1.376779	-0.934738
6	-3.470087	-0.287161	-1.099877
1	-4.143648	0.101034	-0.330532
1	-3.895135	-0.020915	-2.071207
1	-3.450911	-1.377023	-1.022956
1	-1.477298	-0.182435	2.440869

3_re

Number of imaginary frequencies : 0

Electronic energy : =-633.3851652

Zero-point correction= 0.266163
 Thermal correction to Energy= 0.279150
 Thermal correction to Enthalpy= 0.280094
 Thermal correction to Gibbs Free Energy= 0.227086
 Sum of electronic and zero-point Energies= -633.119002
 Sum of electronic and thermal Energies= -633.106015
 Sum of electronic and thermal Enthalpies= -633.105071
 Sum of electronic and thermal Free Energies= -633.158079

Cartesian Coordinates

6	-2.152799	1.204876	-0.180072
6	-1.192523	2.365541	-0.440303
6	0.029744	1.666529	-1.031119
7	0.092320	0.348546	-0.306295
6	-1.245754	0.109016	0.370530
6	1.317609	0.094281	0.596745
6	2.551556	-0.033716	-0.309627
6	2.446802	-1.126454	-1.370018
6	-1.682786	-1.351828	0.048579
8	-0.730674	-2.090754	-0.367558
8	1.061837	-1.076759	1.284197
8	-2.867442	-1.609213	0.225027
1	3.375981	-0.263030	0.372671
1	-1.096905	0.206994	1.447944
1	-2.619375	0.867009	-1.111315
1	-2.950780	1.445961	0.522299
1	-0.922737	2.858362	0.499805
1	-1.589309	3.120128	-1.122017
1	0.967454	2.205913	-0.904790
1	-0.111662	1.449474	-2.092242
1	0.532533	-1.687669	0.700776
1	0.124597	-0.442792	-0.971420
1	2.785924	0.931825	-0.772608
1	3.426866	-1.313563	-1.814352
1	1.776466	-0.852972	-2.192687
1	2.088821	-2.064722	-0.937961
6	1.473107	1.217041	1.607624
1	2.285373	0.936521	2.281755
1	1.731511	2.170400	1.141072
1	0.569480	1.334444	2.209776

[3-4]TS_{re}

Number of imaginary frequencies : 1
 The smallest frequency is : -440.0071 cm(-1)

Electronic energy : =-633.3842825
 Zero-point correction= 0.262532
 Thermal correction to Energy= 0.275221
 Thermal correction to Enthalpy= 0.276165
 Thermal correction to Gibbs Free Energy= 0.224165
 Sum of electronic and zero-point Energies= -633.121750
 Sum of electronic and thermal Energies= -633.109062
 Sum of electronic and thermal Enthalpies= -633.108118
 Sum of electronic and thermal Free Energies= -633.160117

Cartesian Coordinates

6	-2.125642	1.261205	-0.162317
6	-1.120569	2.355213	-0.526202
6	0.054558	1.555385	-1.083938

7	0.083918	0.313242	-0.253963
6	-1.245860	0.154526	0.427793
6	1.293085	0.080057	0.625954
6	2.531567	-0.087378	-0.266818
6	2.385626	-1.126583	-1.375166
6	-1.691558	-1.285931	0.040697
8	-0.829525	-1.841880	-0.742796
8	1.031177	-1.082909	1.356262
8	-2.748520	-1.718682	0.465242
1	3.339071	-0.378069	0.412625
1	-1.137804	0.232304	1.510133
1	-2.632462	0.896541	-1.062414
1	-2.889966	1.585920	0.544389
1	-0.807823	2.898062	0.372398
1	-1.504937	3.078147	-1.248640
1	1.012583	2.072698	-1.029023
1	-0.123842	1.263027	-2.122908
1	0.725781	-1.778104	0.748929
1	-0.061105	-0.677405	-0.828300
1	2.815373	0.881117	-0.692878
1	3.350858	-1.297254	-1.857244
1	1.685528	-0.806449	-2.153346
1	2.038859	-2.089936	-0.989237
6	1.479112	1.202777	1.631171
1	2.338406	0.962144	2.261327
1	1.672973	2.158238	1.137605
1	0.604102	1.298470	2.277615

4_re

Number of imaginary frequencies : 0

Electronic energy : =-633.3968661
Zero-point correction= 0.265259
Thermal correction to Energy= 0.278519
Thermal correction to Enthalpy= 0.279463
Thermal correction to Gibbs Free Energy= 0.226160
Sum of electronic and zero-point Energies= -633.131607
Sum of electronic and thermal Energies= -633.118347
Sum of electronic and thermal Enthalpies= -633.117403
Sum of electronic and thermal Free Energies= -633.170706

Cartesian Coordinates

6	-2.070961	1.285694	-0.283350
6	-1.088047	2.447820	-0.407645
6	0.201014	1.745332	-0.840496
7	0.127317	0.396847	-0.232479
6	-1.200688	0.199730	0.367933
6	1.261482	-0.024350	0.619177
6	2.538348	-0.107417	-0.231224
6	2.414812	-0.982046	-1.475117
6	-1.729634	-1.193359	0.043981
8	-1.106376	-1.772050	-0.993183
8	0.935835	-1.287638	1.159034
8	-2.649513	-1.711086	0.621337
1	3.323302	-0.497989	0.424827
1	-1.204587	0.302662	1.458725
1	-2.394772	0.955743	-1.277635
1	-2.958930	1.505737	0.310655
1	-0.944458	2.915976	0.572603
1	-1.409884	3.217186	-1.112731

1	1.094188	2.283620	-0.512684
1	0.253537	1.656876	-1.932566
1	0.841071	-1.921638	0.434411
1	-0.412557	-1.119495	-1.249244
1	2.845371	0.903272	-0.521894
1	3.382184	-1.069022	-1.976148
1	1.705484	-0.563682	-2.195109
1	2.096113	-2.003160	-1.234643
6	1.479241	0.881781	1.828349
1	2.310295	0.499093	2.425788
1	1.718714	1.903488	1.522064
1	0.590730	0.900493	2.463786

3_si

Number of imaginary frequencies : 0

Electronic energy : =-633.3837609
Zero-point correction= 0.266295
Thermal correction to Energy= 0.279371
Thermal correction to Enthalpy= 0.280315
Thermal correction to Gibbs Free Energy= 0.227009
Sum of electronic and zero-point Energies= -633.117466
Sum of electronic and thermal Energies= -633.104390
Sum of electronic and thermal Enthalpies= -633.103445
Sum of electronic and thermal Free Energies= -633.156752

Cartesian Coordinates

6	1.917040	1.471690	-0.482606
6	0.856771	2.485956	-0.053824
6	0.099621	1.737366	1.040740
7	0.100105	0.303412	0.579030
6	1.158579	0.148488	-0.497506
6	-1.261465	-0.352403	0.239899
6	-1.982633	-0.550922	1.568953
6	1.998523	-1.117448	-0.146187
8	1.434931	-1.887051	0.699433
8	-0.973341	-1.559095	-0.367073
8	3.082141	-1.216732	-0.709862
1	-2.917994	-1.081560	1.383459
1	0.645993	-0.018440	-1.447140
1	2.730788	1.424569	0.248520
1	2.357918	1.684375	-1.456617
1	0.182825	2.713077	-0.886729
1	1.270796	3.425099	0.318068
1	-0.920562	2.080614	1.207162
1	0.640617	1.772229	1.988621
1	-0.185780	-1.960846	0.088359
1	0.472317	-0.322307	1.314270
1	-2.210512	0.392767	2.072661
6	-2.027225	0.518184	-0.754487
1	-2.280111	1.478848	-0.294102
1	-1.371220	0.720891	-1.607889
1	-1.375020	-1.174888	2.232708
6	-3.297668	-0.166013	-1.254151
1	-4.033482	-0.290483	-0.455175
1	-3.762125	0.435752	-2.038833
1	-3.064271	-1.149951	-1.665522

[3-4]TS_si

Number of imaginary frequencies : 0
The smallest frequency is : 52.8380 cm(-1)

Electronic energy : =-633.3837609
Zero-point correction= 0.266295
Thermal correction to Energy= 0.279371
Thermal correction to Enthalpy= 0.280315
Thermal correction to Gibbs Free Energy= 0.227009
Sum of electronic and zero-point Energies= -633.117466
Sum of electronic and thermal Energies= -633.104390
Sum of electronic and thermal Enthalpies= -633.103445
Sum of electronic and thermal Free Energies= -633.156752

Cartesian Coordinates

6	1.917040	1.471690	-0.482606
6	0.856771	2.485956	-0.053824
6	0.099621	1.737366	1.040740
7	0.100105	0.303412	0.579030
6	1.158579	0.148488	-0.497506
6	-1.261465	-0.352403	0.239899
6	-1.982633	-0.550922	1.568953
6	1.998523	-1.117448	-0.146187
8	1.434931	-1.887051	0.699433
8	-0.973341	-1.559095	-0.367073
8	3.082141	-1.216732	-0.709862
1	-2.917994	-1.081560	1.383459
1	0.645993	-0.018440	-1.447140
1	2.730788	1.424569	0.248520
1	2.357918	1.684375	-1.456617
1	0.182825	2.713077	-0.886729
1	1.270796	3.425099	0.318068
1	-0.920562	2.080614	1.207162
1	0.640617	1.772229	1.988621
1	-0.185780	-1.960846	0.088359
1	0.472317	-0.322307	1.314270
1	-2.210512	0.392767	2.072661
6	-2.027225	0.518184	-0.754487
1	-2.280111	1.478848	-0.294102
1	-1.371220	0.720891	-1.607889
1	-1.375020	-1.174888	2.232708
6	-3.297668	-0.166013	-1.254151
1	-4.033482	-0.290483	-0.455175
1	-3.762125	0.435752	-2.038833
1	-3.064271	-1.149951	-1.665522

4_si

Number of imaginary frequencies : 0

Electronic energy : =-633.3952599
Zero-point correction= 0.265009
Thermal correction to Energy= 0.278371
Thermal correction to Enthalpy= 0.279315
Thermal correction to Gibbs Free Energy= 0.225630
Sum of electronic and zero-point Energies= -633.130251
Sum of electronic and thermal Energies= -633.116889
Sum of electronic and thermal Enthalpies= -633.115945
Sum of electronic and thermal Free Energies= -633.169630

Cartesian Coordinates

6	1.993337	1.389916	-0.515785
6	0.979224	2.498023	-0.237706
6	0.063731	1.854619	0.805984
7	0.086486	0.405728	0.497012
6	1.103133	0.136486	-0.531407
6	-1.215643	-0.267622	0.281020
6	-2.015709	-0.203111	1.579180
6	1.906513	-1.108282	-0.168483
8	1.818822	-1.436950	1.128025
8	-0.937885	-1.610559	-0.057063
8	2.598897	-1.708440	-0.948248
1	-2.890838	-0.852138	1.508401
1	0.683580	-0.027295	-1.529505
1	2.715341	1.322090	0.306830
1	2.546359	1.506129	-1.448708
1	0.410455	2.715601	-1.148740
1	1.434167	3.426788	0.113236
1	-0.952192	2.256706	0.767726
1	0.445384	2.022365	1.819827
1	-0.548603	-2.049867	0.712172
1	1.182247	-0.778128	1.494158
1	-2.355762	0.811812	1.803242
6	-1.991396	0.301797	-0.915841
1	-2.120786	1.380577	-0.774087
1	-1.373861	0.164132	-1.809256
1	-1.393000	-0.545227	2.412804
6	-3.347631	-0.361248	-1.141903
1	-4.058623	-0.117660	-0.347362
1	-3.783389	-0.024211	-2.086147
1	-3.237908	-1.447644	-1.185732

4_anti

Number of imaginary frequencies : 0

Electronic energy : =-633.3944292
Zero-point correction= 0.265093
Thermal correction to Energy= 0.278444
Thermal correction to Enthalpy= 0.279388
Thermal correction to Gibbs Free Energy= 0.225817
Sum of electronic and zero-point Energies= -633.129336
Sum of electronic and thermal Energies= -633.115985
Sum of electronic and thermal Enthalpies= -633.115041
Sum of electronic and thermal Free Energies= -633.168612

Cartesian Coordinates

6	-1.200153	0.036582	0.782642
6	-2.093701	1.283679	0.808188
6	-1.697826	1.972629	-0.499296
6	-0.181261	1.745035	-0.575189
7	0.057024	0.579190	0.285754
6	1.259495	-0.190223	0.116044
6	2.482627	0.732809	0.225021
6	3.827924	0.025323	0.094832
6	-1.906727	-1.052594	-0.053397
8	-3.005688	-1.440705	0.264945
8	-1.291108	-1.538396	-1.126856
8	1.294495	-0.838946	-1.190977
1	-1.081613	-0.386804	1.784871
1	-3.150342	1.023058	0.870853

1	-1.821850	1.901086	1.669092
1	-2.195912	1.475728	-1.338781
1	-1.961466	3.031444	-0.531653
1	0.137919	1.570533	-1.613436
1	0.371846	2.616830	-0.204339
1	2.412700	1.261224	1.181289
1	-0.366386	-1.211250	-1.228507
1	4.635662	0.757672	0.018759
1	3.856967	-0.605026	-0.798601
1	1.531898	-0.177454	-1.855588
1	2.399641	1.497788	-0.557995
1	4.039885	-0.606578	0.960995
6	1.313047	-1.344091	1.106022
1	2.226199	-1.918768	0.948416
1	1.293677	-0.970817	2.132789
1	0.469854	-2.023509	0.955454

[4-5]TS_anti

Number of imaginary frequencies : 1
The smallest frequency is : -327.3938 cm(-1)

Electronic energy : =-633.3669709
Zero-point correction= 0.261330
Thermal correction to Energy= 0.274487
Thermal correction to Enthalpy= 0.275432
Thermal correction to Gibbs Free Energy= 0.222177
Sum of electronic and zero-point Energies= -633.105641
Sum of electronic and thermal Energies= -633.092483
Sum of electronic and thermal Enthalpies= -633.091539
Sum of electronic and thermal Free Energies= -633.144794

Cartesian Coordinates

6	-1.251978	0.057371	0.768110
6	-2.180280	1.267514	0.700309
6	-1.758255	1.920506	-0.616470
6	-0.233044	1.785171	-0.605767
7	0.016524	0.605728	0.246281
6	1.199553	0.022557	0.348401
6	2.413561	0.863381	0.012854
6	3.748407	0.131195	0.061250
6	-1.817825	-1.138083	-0.065307
8	-3.002715	-1.391983	0.123800
8	-1.014048	-1.766269	-0.832144
8	1.324507	-1.210886	-1.193871
1	-1.105834	-0.292312	1.793624
1	-3.219732	0.943107	0.716358
1	-1.992522	1.941797	1.542308
1	-2.178277	1.356004	-1.454852
1	-2.072750	2.960980	-0.712583
1	0.181950	1.627227	-1.606094
1	0.252029	2.662996	-0.164756
1	2.413958	1.695411	0.730608
1	0.276469	-1.474984	-1.073563
1	4.540926	0.788564	-0.304059
1	3.722717	-0.762545	-0.566265
1	1.387683	-0.700959	-2.012275
1	2.271987	1.313998	-0.973449
1	4.012263	-0.164848	1.079543
6	1.344121	-1.090642	1.347328
1	2.280695	-1.619982	1.186952

1	1.337917	-0.669017	2.358654
1	0.527350	-1.806249	1.249355

5_anti

Number of imaginary frequencies : 0

Electronic energy : =-633.3757213
Zero-point correction= 0.261752
Thermal correction to Energy= 0.276708
Thermal correction to Enthalpy= 0.277653
Thermal correction to Gibbs Free Energy= 0.219485
Sum of electronic and zero-point Energies= -633.113970
Sum of electronic and thermal Energies= -633.099013
Sum of electronic and thermal Enthalpies= -633.098069
Sum of electronic and thermal Free Energies= -633.156236

Cartesian Coordinates

6	-1.276040	0.086145	0.822498
6	-2.200893	1.282257	0.635074
6	-1.714840	1.853432	-0.698215
6	-0.192768	1.730007	-0.605777
7	0.020097	0.597095	0.328334
6	1.180842	0.114362	0.622216
6	2.411618	0.822159	0.123863
6	3.702364	0.018548	0.200722
6	-1.774146	-1.174247	-0.001570
8	-2.975850	-1.403541	0.130440
8	-0.893557	-1.807068	-0.638191
8	1.236878	-0.863122	-1.899999
1	-1.165576	-0.217641	1.866006
1	-3.234808	0.940034	0.613474
1	-2.071249	2.013299	1.440434
1	-2.088401	1.235917	-1.520384
1	-2.023429	2.885001	-0.873872
1	0.288204	1.480950	-1.554128
1	0.271282	2.624605	-0.178421
1	2.497129	1.748940	0.711082
1	0.423055	-1.229101	-1.468412
1	4.517197	0.600167	-0.236105
1	3.600091	-0.905681	-0.373056
1	1.388459	-1.426318	-2.665090
1	2.232726	1.109809	-0.913055
1	3.983556	-0.225052	1.228529
6	1.268046	-1.081460	1.512442
1	2.224112	-1.585143	1.383896
1	1.186438	-0.766475	2.560387
1	0.465675	-1.780348	1.274860

4_syn

Number of imaginary frequencies : 0

Electronic energy : =-633.3943103
Zero-point correction= 0.265125
Thermal correction to Energy= 0.278445
Thermal correction to Enthalpy= 0.279389
Thermal correction to Gibbs Free Energy= 0.225919

Sum of electronic and zero-point Energies= -633.129185
 Sum of electronic and thermal Energies= -633.115865
 Sum of electronic and thermal Enthalpies= -633.114921
 Sum of electronic and thermal Free Energies= -633.168391

Cartesian Coordinates

6	1.039245	-0.203394	-0.789055
6	2.227693	0.727833	-1.054423
6	2.189911	1.632479	0.180143
6	0.687626	1.838349	0.430443
7	0.039739	0.732101	-0.287311
6	-1.308700	0.370422	0.053164
6	-1.792264	-0.783685	-0.831536
6	-3.255908	-1.157706	-0.626529
6	1.512308	-1.339508	0.144526
8	2.444770	-2.037647	-0.177311
8	0.887902	-1.519413	1.303532
8	-1.394016	-0.151125	1.414276
1	0.700653	-0.689512	-1.709076
1	3.159596	0.174124	-1.168086
1	2.033555	1.303350	-1.963971
1	2.645028	1.110327	1.028372
1	2.720680	2.576420	0.044202
1	0.464597	1.825494	1.507815
1	0.344350	2.801695	0.034860
1	-1.169036	-1.657321	-0.607449
1	0.088128	-0.950234	1.408131
1	-3.482725	-2.085357	-1.157854
1	-3.932535	-0.388426	-1.007949
1	-1.428149	0.591790	2.031698
1	-1.607534	-0.510447	-1.875650
1	-3.469008	-1.314360	0.434026
6	-2.219363	1.591282	-0.032537
1	-3.231944	1.331963	0.281926
1	-1.860191	2.394580	0.618237
1	-2.246175	1.970251	-1.057210

[4-5]TS_{syn}

Number of imaginary frequencies : 1
 The smallest frequency is : -323.4003 cm(-1)

Electronic energy : =-633.367024
 Zero-point correction= 0.261439
 Thermal correction to Energy= 0.274571
 Thermal correction to Enthalpy= 0.275515
 Thermal correction to Gibbs Free Energy= 0.222386
 Sum of electronic and zero-point Energies= -633.105585
 Sum of electronic and thermal Energies= -633.092453
 Sum of electronic and thermal Enthalpies= -633.091509
 Sum of electronic and thermal Free Energies= -633.144638

Cartesian Coordinates

6	1.083896	-0.193109	-0.788250
6	2.294382	0.714566	-0.984562
6	2.242113	1.588975	0.269571
6	0.747927	1.877328	0.439585
7	0.083444	0.736251	-0.222998
6	-1.214280	0.495813	-0.133257
6	-1.767908	-0.620757	-0.994138

6	-3.256339	-0.894447	-0.825660
6	1.428402	-1.399763	0.144585
8	2.480286	-1.975587	-0.112264
8	0.590150	-1.710225	1.055087
8	-1.460228	-0.507228	1.555451
1	0.714623	-0.600468	-1.732933
1	3.201215	0.116714	-1.063667
1	2.175730	1.324377	-1.886393
1	2.612357	1.018202	1.126878
1	2.825930	2.507493	0.191386
1	0.448317	1.934103	1.490567
1	0.452571	2.807347	-0.057837
1	-1.194505	-1.524786	-0.771854
1	-0.539122	-1.054191	1.379848
1	-3.534745	-1.764079	-1.425315
1	-3.870312	-0.053843	-1.160794
1	-1.299903	0.080316	2.305228
1	-1.549982	-0.347099	-2.035200
1	-3.487852	-1.110683	0.219209
6	-2.119496	1.641008	0.223116
1	-3.088271	1.269554	0.551080
1	-1.702265	2.270231	1.009692
1	-2.261738	2.259688	-0.671032

5_syn

Number of imaginary frequencies : 0

Electronic energy : =-633.3797595
 Zero-point correction= 0.262179
 Thermal correction to Energy= 0.276902
 Thermal correction to Enthalpy= 0.277846
 Thermal correction to Gibbs Free Energy= 0.220961
 Sum of electronic and zero-point Energies= -633.117581
 Sum of electronic and thermal Energies= -633.102858
 Sum of electronic and thermal Enthalpies= -633.101913
 Sum of electronic and thermal Free Energies= -633.158798

Cartesian Coordinates

6	1.127975	-0.269727	-0.864561
6	2.411109	0.551576	-0.780930
6	2.111816	1.500534	0.379251
6	0.668227	1.917548	0.116435
7	0.075223	0.718767	-0.533251
6	-1.195170	0.556171	-0.683413
6	-1.783328	-0.707981	-1.229067
6	-2.811348	-1.287260	-0.246879
6	1.149920	-1.483415	0.152475
8	2.164552	-2.173482	0.064790
8	0.134995	-1.620253	0.884392
8	-0.942389	0.379075	2.235072
1	0.942723	-0.672994	-1.862232
1	3.253288	-0.116216	-0.602919
1	2.582393	1.115320	-1.704396
1	2.167604	0.960497	1.329810
1	2.778045	2.363176	0.427971
1	0.099893	2.138677	1.020289
1	0.608980	2.752536	-0.590366
1	-1.011948	-1.451340	-1.417659
1	-0.510849	-0.383207	1.770137
1	-3.187346	-2.234881	-0.638078

1	-3.663173	-0.617568	-0.104597
1	-1.020322	0.100842	3.152831
1	-2.274416	-0.454612	-2.177773
1	-2.332973	-1.468543	0.716299
6	-2.132485	1.645277	-0.276150
1	-2.279984	1.551448	0.807182
1	-1.724816	2.635499	-0.487695
1	-3.091222	1.530936	-0.783041

6_anti

Number of imaginary frequencies : 0

Electronic energy : =-633.3763478
Zero-point correction= 0.261644
Thermal correction to Energy= 0.276526
Thermal correction to Enthalpy= 0.277470
Thermal correction to Gibbs Free Energy= 0.220188
Sum of electronic and zero-point Energies= -633.114704
Sum of electronic and thermal Energies= -633.099822
Sum of electronic and thermal Enthalpies= -633.098878
Sum of electronic and thermal Free Energies= -633.156160

Cartesian Coordinates

6	1.569644	1.979490	0.140770
6	0.053529	1.819365	0.067675
7	-0.123204	0.455655	-0.495977
6	1.174847	-0.105305	-0.921992
6	2.066810	1.127123	-1.027491
6	-1.252659	-0.169425	-0.538656
6	-2.474740	0.514440	0.007653
6	-3.812114	-0.128742	-0.339397
6	1.753514	-1.140182	0.136620
8	2.931316	-1.429155	-0.068775
8	0.952591	-1.559810	1.010848
1	1.047384	-0.636949	-1.867939
1	3.110240	0.825338	-0.944216
1	1.913472	1.648765	-1.978555
1	1.931506	1.564974	1.087031
1	1.867867	3.027318	0.081827
1	-0.439787	1.865415	1.038331
1	-0.398473	2.531901	-0.631329
1	-2.322865	0.539378	1.096929
1	0.005012	-0.541591	1.951754
8	-0.554304	0.099111	2.457250
1	-4.620554	0.503967	0.033459
1	-3.947009	-0.238078	-1.419338
1	-0.323059	-0.041568	3.380349
1	-2.462187	1.557573	-0.328590
1	-3.926264	-1.110509	0.125837
6	-1.298438	-1.546235	-1.117209
1	-0.556768	-2.164993	-0.605050
1	-2.284153	-1.991830	-1.006559
1	-1.051117	-1.513047	-2.184521

[6-7]TS_anti

Number of imaginary frequencies : 1

The smallest frequency is : -1426.0659 cm(-1)

Electronic energy : =-633.349542
Zero-point correction= 0.255482
Thermal correction to Energy= 0.269060
Thermal correction to Enthalpy= 0.270004
Thermal correction to Gibbs Free Energy= 0.215741
Sum of electronic and zero-point Energies= -633.094060
Sum of electronic and thermal Energies= -633.080482
Sum of electronic and thermal Enthalpies= -633.079538
Sum of electronic and thermal Free Energies= -633.133801

Cartesian Coordinates

6 1.702794 1.909460 0.497340
6 0.184914 1.838628 0.310640
7 -0.018279 0.619606 -0.496321
6 1.264988 -0.000600 -0.851197
6 2.250819 1.160897 -0.718574
6 -1.205416 0.063870 -0.690557
6 -2.347060 0.534590 0.007473
6 -3.739914 0.031812 -0.320246
6 1.664033 -1.168659 0.102767
8 2.737446 -1.698305 -0.145543
8 0.858271 -1.493170 1.047648
1 1.235931 -0.403617 -1.865289
1 3.266354 0.786948 -0.589005
1 2.212482 1.792959 -1.611499
1 1.984490 1.382398 1.414202
1 2.056169 2.939020 0.572519
1 -0.347885 1.751856 1.260877
1 -0.210145 2.700422 -0.239891
1 -1.816715 -0.027435 1.151739
1 -0.131970 -0.879145 1.567861
8 -1.033264 -0.418646 2.078591
1 -4.454522 0.460609 0.386525
1 -4.072891 0.312656 -1.326287
1 -1.439813 -1.085045 2.646387
1 -2.310520 1.587765 0.284054
1 -3.823668 -1.055028 -0.231082
6 -1.241804 -1.217793 -1.469957
1 -0.723130 -2.000520 -0.905767
1 -2.264693 -1.533412 -1.663664
1 -0.731270 -1.099918 -2.429126

7_anti

Number of imaginary frequencies : 0

Electronic energy : =-633.3799301
Zero-point correction= 0.261236
Thermal correction to Energy= 0.276559
Thermal correction to Enthalpy= 0.277503
Thermal correction to Gibbs Free Energy= 0.219248
Sum of electronic and zero-point Energies= -633.118694
Sum of electronic and thermal Energies= -633.103371
Sum of electronic and thermal Enthalpies= -633.102427
Sum of electronic and thermal Free Energies= -633.160682

Cartesian Coordinates

6 1.499703 2.091685 0.268307

6	-0.005255	1.854911	0.162127
7	-0.094661	0.481857	-0.324334
6	1.171926	0.002739	-0.859857
6	2.049056	1.268380	-0.897387
6	-1.318724	-0.128123	-0.554648
6	-2.493135	0.474942	-0.250802
6	-3.855136	-0.141651	-0.449660
6	1.851701	-1.073722	0.001557
8	2.824025	-1.659721	-0.410362
8	1.354474	-1.311401	1.209278
1	1.071502	-0.433639	-1.857594
1	3.110108	1.026027	-0.819283
1	1.880263	1.792549	-1.842987
1	1.870856	1.695211	1.219621
1	1.761625	3.149782	0.212260
1	-0.515463	1.953354	1.126657
1	-0.478408	2.550068	-0.548539
1	-1.532925	-0.100318	1.767728
1	0.571493	-0.756849	1.437815
8	-0.812468	-0.186210	2.415346
1	-4.614867	0.449239	0.067667
1	-4.149180	-0.181497	-1.505800
1	-1.110382	-0.832737	3.065587
1	-2.475465	1.504718	0.093099
1	-3.924621	-1.161231	-0.056449
6	-1.244012	-1.529884	-1.098694
1	-0.578233	-2.152374	-0.491343
1	-2.227854	-1.997271	-1.113897
1	-0.860800	-1.535035	-2.123963

6_syn

Number of imaginary frequencies : 0

Electronic energy : =-633.3728043
Zero-point correction= 0.262273
Thermal correction to Energy= 0.277320
Thermal correction to Enthalpy= 0.278264
Thermal correction to Gibbs Free Energy= 0.220093
Sum of electronic and zero-point Energies= -633.110531
Sum of electronic and thermal Energies= -633.095484
Sum of electronic and thermal Enthalpies= -633.094540
Sum of electronic and thermal Free Energies= -633.152711

Cartesian Coordinates

6	-2.779504	-0.669229	0.377222
6	-1.618436	-1.657854	0.489681
7	-0.501760	-0.981298	-0.215638
6	-0.965629	0.273945	-0.832926
6	-2.477961	0.084786	-0.919720
6	0.740711	-1.312587	-0.110889
6	1.792021	-0.440208	-0.735673
6	3.231192	-0.912630	-0.568128
6	-0.602247	1.474913	0.124981
8	-0.719088	2.586378	-0.412578
8	-0.242821	1.155325	1.279271
1	-0.481759	0.426663	-1.797910
1	-2.976792	1.052348	-0.988331
1	-2.749802	-0.515812	-1.794370
1	-2.745610	0.022511	1.221717
1	-3.742364	-1.182092	0.372741

1	-1.324839	-1.862209	1.519930
1	-1.829576	-2.600680	-0.025585
1	1.689500	0.561992	-0.291642
1	1.431297	2.240281	1.237447
8	1.993609	2.697682	0.590748
1	3.898840	-0.158485	-0.989167
1	3.495442	-1.029254	0.486164
1	1.553338	-0.324546	-1.800368
1	3.425611	-1.857190	-1.083946
6	1.118562	-2.519176	0.682046
1	0.321047	-3.260478	0.724180
1	2.018756	-2.981074	0.277587
1	1.343911	-2.194146	1.706318
1	1.299457	3.084409	0.035617

[6-7]TS_{syn}

Number of imaginary frequencies : 1
The smallest frequency is : -1340.5506 cm(-1)

Electronic energy : =-633.3470607
Zero-point correction= 0.256179
Thermal correction to Energy= 0.269875
Thermal correction to Enthalpy= 0.270820
Thermal correction to Gibbs Free Energy= 0.216226
Sum of electronic and zero-point Energies= -633.090881
Sum of electronic and thermal Energies= -633.077185
Sum of electronic and thermal Enthalpies= -633.076241
Sum of electronic and thermal Free Energies= -633.130834

Cartesian Coordinates

6	-2.720257	-0.793316	0.487960
6	-1.483360	-1.691918	0.474146
7	-0.485437	-0.913091	-0.285559
6	-1.086056	0.278597	-0.903120
6	-2.590724	0.005281	-0.810151
6	0.827695	-1.086656	-0.189832
6	1.761818	-0.130994	-0.658972
6	3.221005	-0.510802	-0.855503
6	-0.651370	1.536278	-0.110938
8	-0.333782	2.540955	-0.736353
8	-0.592564	1.364060	1.164288
1	-0.737976	0.386824	-1.933225
1	-3.168802	0.931540	-0.807477
1	-2.909714	-0.596113	-1.667672
1	-2.666182	-0.116765	1.342743
1	-3.643025	-1.373786	0.544545
1	-1.113758	-1.904637	1.479041
1	-1.677796	-2.640696	-0.040352
1	1.802078	0.754556	0.439376
1	0.677279	1.619062	1.425799
8	1.785785	1.604459	1.342922
1	3.783288	0.371037	-1.173147
1	3.685382	-0.862150	0.070748
1	1.374935	0.563593	-1.405320
1	3.368466	-1.281922	-1.621277
6	1.299369	-2.300898	0.560380
1	0.609919	-3.138232	0.444624
1	2.284351	-2.612409	0.215050
1	1.373112	-2.066324	1.628907
1	2.012269	2.448842	0.925856

7_syn

Number of imaginary frequencies : 0

Electronic energy : =-633.3762072
Zero-point correction= 0.261292
Thermal correction to Energy= 0.276914
Thermal correction to Enthalpy= 0.277858
Thermal correction to Gibbs Free Energy= 0.218205
Sum of electronic and zero-point Energies= -633.114915
Sum of electronic and thermal Energies= -633.099293
Sum of electronic and thermal Enthalpies= -633.098349
Sum of electronic and thermal Free Energies= -633.158002

Cartesian Coordinates

6	2.096508	1.695407	0.056003
6	0.592150	1.961522	0.016277
7	0.039037	0.649592	-0.328127
6	1.046905	-0.256037	-0.845275
6	2.278242	0.645908	-1.042125
6	-1.323917	0.389455	-0.460546
6	-1.783834	-0.860094	-0.700780
6	-3.210376	-1.281180	-0.911154
6	1.401763	-1.411546	0.102356
8	2.060479	-2.348579	-0.278828
8	1.003863	-1.308862	1.367731
1	0.725048	-0.719629	-1.784819
1	3.212504	0.085558	-0.979179
1	2.220041	1.116755	-2.028240
1	2.375346	1.273714	1.027822
1	2.683628	2.600946	-0.107538
1	0.205042	2.307770	0.979375
1	0.353186	2.716985	-0.746299
1	-1.622740	-0.228444	1.757558
1	0.418320	-0.535141	1.517197
8	-1.049817	0.211322	2.405748
1	-3.456333	-2.147786	-0.287588
1	-3.933421	-0.497594	-0.677754
1	-1.175796	-0.270310	3.232200
1	-1.055463	-1.661203	-0.808649
1	-3.385880	-1.587063	-1.949777
6	-2.207582	1.590832	-0.251205
1	-1.954844	2.386507	-0.958784
1	-3.258996	1.344869	-0.386855
1	-2.078243	1.990270	0.759709

(2) Proline-enamine formation in the presence of cinchona-thiourea (Scheme S3 and Fig. S2)

2_re

Number of imaginary frequencies : 0

Electronic energy : =-3046.1135112
Zero-point correction= 0.811859
Thermal correction to Energy= 0.862950
Thermal correction to Enthalpy= 0.863894

Thermal correction to Gibbs Free Energy=	0.722369
Sum of electronic and zero-point Energies=	-3045.301652
Sum of electronic and thermal Energies=	-3045.250562
Sum of electronic and thermal Enthalpies=	-3045.249617
Sum of electronic and thermal Free Energies=	-3045.391142

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

6	-2.818495	-4.502526	-0.935401
6	-4.179434	-3.874855	-1.299100
6	-4.492238	-2.985113	-0.089852
7	-3.193065	-2.471302	0.355551
6	-2.259743	-3.605798	0.207694
6	-2.127224	-0.830862	2.245002
6	-3.385078	0.010625	2.212911
6	-3.144022	1.342557	2.930112
6	-0.858143	-3.045022	-0.068910
8	-0.730926	-2.421283	-1.168399
8	-1.134801	-0.462522	1.630111
8	0.041515	-3.203318	0.782661
1	-4.220319	-0.533678	2.660824
1	-2.233637	-4.158527	1.152617
1	-2.139115	-4.506531	-1.790044
1	-2.934449	-5.532392	-0.587436
1	-4.954889	-4.619139	-1.497851
1	-4.083691	-3.246457	-2.190716
1	-4.928425	-3.578979	0.723770
1	-5.176433	-2.160319	-0.308104
1	0.616791	-1.373118	1.618613
1	-2.893692	-1.768398	-0.321952
1	-3.627222	0.197310	1.162352
1	-2.948397	1.192968	3.997225
1	-4.017767	1.992525	2.837407
7	-0.940536	0.390121	-1.223350
6	-2.162710	1.043729	-1.087394
6	-2.384939	2.223935	-0.370206
6	-3.685429	2.696044	-0.221891
6	-4.782268	2.040842	-0.767116
6	-4.545318	0.880939	-1.500160
6	-3.261329	0.389102	-1.670324
6	-3.924000	3.962046	0.553346
9	-5.010402	3.855600	1.340344
6	-5.719999	0.155627	-2.090830
9	-6.365781	0.904074	-2.995746
6	0.300410	0.696071	-0.730972
16	0.864885	2.254704	-0.403226
7	1.037884	-0.420040	-0.570378
6	2.425344	-0.460420	-0.174064
6	2.596966	-1.480673	0.969596
6	3.992823	-1.411137	1.625214
6	3.849113	-1.026255	3.105054
6	3.055614	-2.131300	3.815121
6	1.710442	-2.327496	3.087546
7	1.560155	-1.265262	2.041539
6	1.647045	0.088207	2.667750
6	3.067916	0.294895	3.255497
6	3.732375	1.517145	2.666777
6	5.019380	1.646415	2.354880
6	3.334217	-0.869838	-1.328383
6	4.513172	-0.136504	-1.670031
6	5.321055	-0.660064	-2.722734
7	5.006621	-1.788762	-3.418893
6	3.900635	-2.412597	-3.095583
6	3.036076	-1.996048	-2.054188
6	6.512852	0.020199	-3.072791

6	6.898409	1.166584	-2.426750
6	6.083865	1.693744	-1.392247
6	4.916161	1.057359	-1.029113
9	-2.890141	4.277790	1.343999
9	-4.139855	5.009940	-0.255695
9	-6.620256	-0.161642	-1.143247
9	-5.364113	-0.987738	-2.694648
1	2.359193	-2.475323	0.583806
1	4.494573	-2.379225	1.543678
1	4.609232	-0.680137	1.096927
1	0.852669	-2.226814	3.755357
1	1.623707	-3.280373	2.565524
1	2.887452	-1.860164	4.861379
1	3.621841	-3.065974	3.805458
1	4.836601	-0.926129	3.562721
1	2.949826	0.481429	4.331132
1	0.866876	0.116753	3.431081
1	1.390261	0.827038	1.904006
1	3.068624	2.368336	2.511095
1	5.403804	2.575381	1.945922
1	5.737829	0.840170	2.480611
1	2.693480	0.536411	0.179250
1	2.136968	-2.573550	-1.847795
1	4.320513	1.516845	-0.249527
1	3.655515	-3.305509	-3.667088
1	7.110515	-0.400376	-3.874965
1	7.815965	1.664101	-2.717514
1	0.567546	-1.319898	-0.797409
1	-1.050583	-0.606493	-1.434402
1	-1.557927	2.747873	0.086887
1	-3.097648	-0.518523	-2.246233
1	-5.790115	2.417079	-0.624008
8	6.387175	2.826374	-0.707953
6	7.533519	3.556914	-1.100911
1	7.562565	4.438058	-0.459865
1	8.452585	2.977273	-0.954036
1	7.466897	3.877441	-2.146878
1	-2.284342	1.856849	2.492498
6	-2.071305	-2.025196	3.160843
1	-3.028854	-2.547673	3.186082
1	-1.281280	-2.702372	2.826024
1	-1.851680	-1.670207	4.177140

[2-3]TS_re

Number of imaginary frequencies : 1

The smallest frequency is : -119.2088 cm(-1)

Electronic energy : =-3046.1069319

Zero-point correction= 0.812340

Thermal correction to Energy= 0.861624

Thermal correction to Enthalpy= 0.862568

Thermal correction to Gibbs Free Energy= 0.728606

Sum of electronic and zero-point Energies= -3045.294592

Sum of electronic and thermal Energies= -3045.245308

Sum of electronic and thermal Enthalpies= -3045.244364

Sum of electronic and thermal Free Energies= -3045.378326

Cartesian Coordinates

6	-3.032013	-4.062841	-0.991022
6	-4.479426	-3.565771	-0.751751

6	-4.358605	-2.537916	0.391622
7	-2.927858	-2.183506	0.455268
6	-2.201648	-3.435486	0.138612
6	-2.179174	-1.137990	1.891605
6	-3.341516	-0.155668	2.049661
6	-2.914956	1.043765	2.892239
6	-0.752168	-3.069813	-0.234424
8	-0.637105	-2.400348	-1.307715
8	-1.104572	-0.668848	1.410214
8	0.163791	-3.412398	0.530860
1	-4.209188	-0.656482	2.493413
1	-2.209360	-4.060347	1.035856
1	-2.645748	-3.689524	-1.942698
1	-2.950139	-5.151496	-0.993298
1	-5.157301	-4.376529	-0.477001
1	-4.884291	-3.091202	-1.649168
1	-4.630086	-2.981726	1.355797
1	-4.962314	-1.641317	0.241233
1	0.442474	-1.216983	1.569033
1	-2.704806	-1.521815	-0.293759
1	-3.634553	0.198920	1.055926
1	-2.654936	0.748542	3.914843
1	-3.721170	1.779914	2.952849
7	-0.918525	0.438672	-1.372083
6	-2.151860	1.054960	-1.184470
6	-2.384528	2.182377	-0.387370
6	-3.687642	2.625216	-0.194745
6	-4.782767	1.996340	-0.776877
6	-4.537960	0.889784	-1.584206
6	-3.248916	0.421439	-1.793296
6	-3.935644	3.819256	0.685282
9	-4.993397	3.615488	1.491567
6	-5.707313	0.172582	-2.195036
9	-6.535408	1.015204	-2.824461
6	0.312854	0.744900	-0.840996
16	0.858996	2.308476	-0.504837
7	1.048985	-0.364200	-0.674350
6	2.410770	-0.417047	-0.198803
6	2.498973	-1.425842	0.963951
6	3.871328	-1.382594	1.672961
6	3.681788	-0.989178	3.144303
6	2.834323	-2.073205	3.822759
6	1.510377	-2.231003	3.046550
7	1.424789	-1.176533	1.987816
6	1.528918	0.174713	2.614676
6	2.927973	0.350988	3.259891
6	3.643691	1.554450	2.693559
6	4.942738	1.652755	2.422833
6	3.364717	-0.864229	-1.301263
6	4.567611	-0.156152	-1.610361
6	5.404722	-0.711038	-2.623479
7	5.098628	-1.847731	-3.310387
6	3.973715	-2.451030	-3.013916
6	3.077531	-2.002223	-2.013541
6	6.619755	-0.056232	-2.940300
6	7.000974	1.093921	-2.298278
6	6.158262	1.651678	-1.302867
6	4.967682	1.040415	-0.972456
9	-2.887404	4.100513	1.468843
9	-4.205744	4.921601	-0.029915
9	-6.442949	-0.454830	-1.255616
9	-5.328747	-0.761791	-3.078545
1	2.258307	-2.418780	0.575724
1	4.354592	-2.361774	1.612895
1	4.524761	-0.668341	1.166627

1	0.637573	-2.094363	3.687283
1	1.410155	-3.186903	2.530937
1	2.636513	-1.799962	4.863393
1	3.376616	-3.022219	3.830772
1	4.653355	-0.912342	3.639936
1	2.772071	0.546425	4.329317
1	0.716105	0.228024	3.341975
1	1.323588	0.916889	1.839034
1	3.007670	2.422689	2.516546
1	5.360756	2.573143	2.027597
1	5.638103	0.830488	2.570936
1	2.675847	0.581723	0.151891
1	2.164194	-2.564370	-1.825143
1	4.353238	1.518320	-0.218796
1	3.737301	-3.352396	-3.575849
1	7.239642	-0.500106	-3.712535
1	7.937511	1.570888	-2.561654
1	0.587944	-1.266250	-0.909696
1	-1.007818	-0.551276	-1.614115
1	-1.559583	2.684792	0.096664
1	-3.081757	-0.444295	-2.429825
1	-5.793280	2.353267	-0.606367
8	6.455383	2.791840	-0.627875
6	7.647670	3.474128	-0.965298
1	7.673973	4.365463	-0.338404
1	8.534603	2.864488	-0.756680
1	7.653305	3.779395	-2.017778
1	-2.041146	1.520733	2.440365
6	-2.081580	-2.213515	2.959649
1	-3.023560	-2.749907	3.105376
1	-1.287697	-2.918063	2.698870
1	-1.826617	-1.724866	3.908086

3_re

Number of imaginary frequencies : 0

Electronic energy : =-3046.1190251
Zero-point correction= 0.814188
Thermal correction to Energy= 0.863498
Thermal correction to Enthalpy= 0.864442
Thermal correction to Gibbs Free Energy= 0.730203
Sum of electronic and zero-point Energies= -3045.304837
Sum of electronic and thermal Energies= -3045.255527
Sum of electronic and thermal Enthalpies= -3045.254583
Sum of electronic and thermal Free Energies= -3045.388822

Cartesian Coordinates

6	-3.336764	-3.853656	-1.098171
6	-4.651554	-3.676005	-0.325487
6	-4.421546	-2.454188	0.580412
7	-2.976915	-2.073111	0.389014
6	-2.267359	-3.278650	-0.175974
6	-2.278201	-1.330598	1.570705
6	-3.223253	-0.187342	1.967716
6	-2.546837	0.841448	2.866590
6	-1.001642	-2.773652	-0.912426
8	-1.257102	-1.945410	-1.829186
8	-1.135661	-0.794673	1.034328
8	0.102987	-3.183455	-0.527429
1	-4.114791	-0.593010	2.457269

1	-2.022053	-3.952597	0.646187
1	-3.339345	-3.261727	-2.017948
1	-3.127572	-4.893172	-1.355109
1	-4.863190	-4.554850	0.287654
1	-5.499279	-3.517363	-0.993451
1	-4.573258	-2.688485	1.634411
1	-5.038058	-1.592841	0.321996
1	-0.268639	-1.249023	1.291847
1	-2.918267	-1.387630	-0.382283
1	-3.550924	0.310057	1.047696
1	-2.288853	0.424326	3.845202
1	-3.220670	1.685265	3.033010
7	-0.785518	0.751843	-1.432642
6	-2.034350	1.300735	-1.170566
6	-2.299726	2.417882	-0.362947
6	-3.618537	2.777764	-0.114605
6	-4.702765	2.075175	-0.635542
6	-4.426652	0.983520	-1.449839
6	-3.120188	0.607007	-1.732404
6	-3.920477	3.927205	0.806119
9	-4.630170	3.509496	1.873961
6	-5.546015	0.161938	-2.020034
9	-5.918194	0.558639	-3.241033
6	0.402252	0.910865	-0.752535
16	0.965993	2.372990	-0.130705
7	1.070350	-0.251229	-0.679601
6	2.408239	-0.449758	-0.160873
6	2.425267	-1.597045	0.871123
6	3.821546	-1.678051	1.546785
6	3.654316	-1.483145	3.059632
6	2.790331	-2.636482	3.582721
6	1.456452	-2.636865	2.790829
7	1.354644	-1.470478	1.891014
6	1.514740	-0.239562	2.685441
6	2.919647	-0.162593	3.361969
6	3.653977	1.096285	2.971575
6	4.946369	1.209613	2.672058
6	3.360763	-0.791414	-1.302966
6	4.551295	-0.046498	-1.570413
6	5.357700	-0.479120	-2.664728
7	5.041695	-1.544836	-3.454685
6	3.937129	-2.194265	-3.179962
6	3.067134	-1.859405	-2.114754
6	6.550745	0.226035	-2.954013
6	6.945312	1.303146	-2.201889
6	6.141689	1.729663	-1.113916
6	4.967698	1.072760	-0.813396
9	-2.819813	4.523349	1.270616
9	-4.667098	4.863432	0.201091
9	-6.636283	0.201682	-1.238145
9	-5.188672	-1.137570	-2.124751
1	2.193205	-2.522797	0.338131
1	4.284148	-2.651254	1.353134
1	4.491481	-0.919238	1.133618
1	0.607789	-2.601755	3.479356
1	1.346860	-3.531655	2.170021
1	2.604022	-2.511278	4.654686
1	3.316047	-3.587311	3.452305
1	4.630984	-1.489920	3.553621
1	2.765593	-0.114537	4.449487
1	0.715074	-0.237684	3.434980
1	1.338701	0.619769	2.029882
1	3.037461	1.996279	2.954645
1	5.378515	2.170642	2.410550
1	5.620840	0.357201	2.665753

1	2.705367	0.482612	0.320367
1	2.168227	-2.452177	-1.950547
1	4.382033	1.449116	0.017492
1	3.695111	-3.041579	-3.818970
1	7.144544	-0.118431	-3.794448
1	7.864334	1.821247	-2.448559
1	0.603932	-1.097674	-1.009615
1	-0.880886	-0.191818	-1.824085
1	-1.484977	2.976307	0.076730
1	-2.923703	-0.263002	-2.354453
1	-5.722273	2.359860	-0.398652
8	6.461428	2.782911	-0.317979
6	7.632028	3.515937	-0.620120
1	7.686578	4.314599	0.120217
1	8.531865	2.894250	-0.541060
1	7.582316	3.959848	-1.621284
1	-1.634434	1.215953	2.396815
6	-2.013926	-2.312474	2.697941
1	-2.922266	-2.824807	3.025263
1	-1.268778	-3.052551	2.399582
1	-1.618640	-1.753826	3.550303

2_si

Number of imaginary frequencies : 0

Electronic energy : =-3046.1117751
Zero-point correction= 0.811126
Thermal correction to Energy= 0.862584
Thermal correction to Enthalpy= 0.863528
Thermal correction to Gibbs Free Energy= 0.721737
Sum of electronic and zero-point Energies= -3045.300649
Sum of electronic and thermal Energies= -3045.249191
Sum of electronic and thermal Enthalpies= -3045.248247
Sum of electronic and thermal Free Energies= -3045.390038

Cartesian Coordinates

6	2.652668	-4.414242	1.675574
6	4.177077	-4.488193	1.561954
6	4.566139	-3.112762	0.975062
7	3.339282	-2.543498	0.368561
6	2.285661	-3.567608	0.448918
6	2.304444	-1.009857	-1.976119
6	3.562567	-0.186118	-1.960506
6	0.920053	-2.879424	0.560503
8	0.813025	-2.026631	1.495634
8	1.267184	-0.590687	-1.481708
8	0.018787	-3.186111	-0.248320
1	4.292462	-0.671905	-1.304960
1	2.298923	-4.187193	-0.456797
1	2.354266	-3.860137	2.572463
1	2.167767	-5.393841	1.688719
1	4.459499	-5.287319	0.868453
1	4.670501	-4.688221	2.516133
1	5.354453	-3.212528	0.220198
1	4.946321	-2.436512	1.746052
1	-0.514751	-1.542330	-1.385349
1	3.009467	-1.781383	0.954463
1	3.344982	0.818202	-1.593717
7	0.895690	0.796355	1.113177
6	2.081917	1.495105	0.900141

6	2.227235	2.690358	0.188351
6	3.502659	3.215266	-0.011964
6	4.649652	2.591631	0.458773
6	4.488607	1.414082	1.182982
6	3.233121	0.883321	1.423017
6	3.610447	4.520587	-0.750165
9	4.865034	4.767575	-1.154707
6	5.694406	0.635169	1.618505
9	6.756821	1.420734	1.831518
6	-0.354488	0.962524	0.579482
16	-1.006603	2.421113	0.033762
7	-1.021536	-0.209263	0.560287
6	-2.402770	-0.384789	0.177302
6	-2.512628	-1.574519	-0.797855
6	-3.881477	-1.652826	-1.506138
6	-3.689779	-1.459814	-3.019005
6	-2.848234	-2.628553	-3.551079
6	-1.543524	-2.714249	-2.734529
7	-1.439915	-1.505803	-1.855512
6	-1.517351	-0.261381	-2.677015
6	-2.927149	-0.152574	-3.315694
6	-3.627902	1.119867	-2.900937
6	-4.929855	1.263190	-2.666699
6	-3.285862	-0.675976	1.387227
6	-4.525497	-0.002940	1.616950
6	-5.280941	-0.404531	2.758582
7	-4.869903	-1.371173	3.627165
6	-3.717909	-1.949102	3.390907
6	-2.892469	-1.638711	2.283123
6	-6.522686	0.227325	3.011909
6	-7.007746	1.208875	2.185885
6	-6.249305	1.611482	1.056683
6	-5.033117	1.021898	0.786462
9	2.827092	4.539714	-1.839204
9	3.231386	5.554665	0.016361
9	6.055506	-0.263654	0.681741
9	5.467445	-0.058778	2.745233
1	-2.269521	-2.489163	-0.252611
1	-4.346677	-2.624662	-1.318714
1	-4.550451	-0.890130	-1.100592
1	-0.649478	-2.718495	-3.361110
1	-1.493673	-3.576122	-2.069576
1	-2.627870	-2.478271	-4.611925
1	-3.402048	-3.566179	-3.460348
1	-4.661044	-1.444431	-3.520119
1	-2.785375	-0.098445	-4.403181
1	-0.723253	-0.343233	-3.421897
1	-1.278595	0.583576	-2.025957
1	-2.981539	1.994180	-2.819010
1	-5.344803	2.227778	-2.391902
1	-5.631648	0.434930	-2.727329
1	-2.723814	0.533931	-0.316783
1	-1.946444	-2.163201	2.161499
1	-4.482366	1.383431	-0.074165
1	-3.397769	-2.713226	4.096586
1	-7.078035	-0.093803	3.887103
1	-7.961868	1.672891	2.405713
1	-0.510256	-1.036639	0.926920
1	1.065908	-0.167141	1.415670
1	1.359994	3.193261	-0.216629
1	3.134674	-0.018585	2.022109
1	5.632829	3.007630	0.274330
8	-6.654420	2.574983	0.190216
6	-7.866404	3.251835	0.464761
1	-7.983141	3.992877	-0.326156

1	-8.723972	2.569167	0.444545
1	-7.830167	3.764485	1.432842
6	2.303460	-2.340736	-2.701167
1	1.575386	-2.973485	-2.180503
1	1.884880	-2.124937	-3.696706
6	3.651883	-3.035675	-2.852427
1	4.102443	-3.203046	-1.871119
1	3.524976	-4.001699	-3.348251
1	4.348089	-2.445272	-3.455185
1	3.995446	-0.131275	-2.964714

[2-3]TS_{si}

Number of imaginary frequencies : 1
The smallest frequency is : -149.7731 cm(-1)

Electronic energy : =-3046.1013885
Zero-point correction= 0.813375
Thermal correction to Energy= 0.862351
Thermal correction to Enthalpy= 0.863295
Thermal correction to Gibbs Free Energy= 0.729340
Sum of electronic and zero-point Energies= -3045.288013
Sum of electronic and thermal Energies= -3045.239038
Sum of electronic and thermal Enthalpies= -3045.238094
Sum of electronic and thermal Free Energies= -3045.372049

Cartesian Coordinates

6	3.196942	-3.254754	2.258520
6	4.576596	-3.243271	1.588676
6	4.372453	-2.400724	0.312794
7	2.897114	-2.259154	0.139691
6	2.234169	-3.209242	1.072874
6	2.008086	-2.070491	-1.523363
6	3.061426	-1.257236	-2.259178
6	0.823150	-2.676368	1.394054
8	0.810689	-1.570466	2.019714
8	0.946805	-1.438534	-1.213259
8	-0.160841	-3.330230	1.015238
1	4.033028	-1.748618	-2.335151
1	2.159844	-4.185407	0.585542
1	3.040079	-2.351481	2.857210
1	3.033844	-4.125645	2.897155
1	4.876336	-4.261389	1.322297
1	5.354362	-2.822318	2.229067
1	4.799199	-2.881984	-0.568867
1	4.812899	-1.405060	0.390927
1	-0.554153	-1.923349	-1.006327
1	2.619535	-1.328619	0.460007
1	3.174473	-0.285162	-1.770118
7	0.987061	0.939545	0.761176
6	2.192701	1.559984	0.459835
6	2.398475	2.582437	-0.471823
6	3.689683	3.068968	-0.673769
6	4.791249	2.575176	0.008984
6	4.572168	1.559866	0.938484
6	3.302211	1.065040	1.172321
6	3.868215	4.207788	-1.639893
9	5.140715	4.319841	-2.050853
6	5.750795	0.971605	1.659038
9	6.476034	1.903506	2.289280
6	-0.256454	0.992172	0.190025

16	-0.821925	2.197431	-0.848725
7	-0.994711	-0.058449	0.592717
6	-2.387361	-0.294709	0.303950
6	-2.558197	-1.740678	-0.198011
6	-3.989175	-2.015495	-0.712029
6	-3.940104	-2.392522	-2.199285
6	-3.138830	-3.694153	-2.334257
6	-1.754159	-3.495627	-1.684933
7	-1.584012	-2.061380	-1.297947
6	-1.766485	-1.186651	-2.493876
6	-3.221970	-1.301253	-3.018008
6	-3.904802	0.045405	-3.048195
6	-5.176749	0.297277	-2.748970
6	-3.241626	-0.118746	1.556564
6	-4.412772	0.700512	1.583358
6	-5.149832	0.738295	2.804714
7	-4.781547	0.054762	3.925114
6	-3.689567	-0.666561	3.863552
6	-2.889338	-0.788379	2.702298
6	-6.327053	1.522542	2.867941
6	-6.768029	2.239006	1.785093
6	-6.028022	2.206100	0.575170
6	-4.873589	1.458640	0.482492
9	3.104830	4.061302	-2.731148
9	3.531280	5.381306	-1.083446
9	6.582572	0.353738	0.799257
9	5.386000	0.056014	2.570439
1	-2.267656	-2.418530	0.608509
1	-4.443771	-2.830451	-0.141662
1	-4.610406	-1.129338	-0.560918
1	-0.938863	-3.728950	-2.371849
1	-1.605745	-4.073556	-0.771278
1	-3.031070	-3.960580	-3.389928
1	-3.667634	-4.513504	-1.840611
1	-4.952985	-2.539016	-2.583696
1	-3.167869	-1.655572	-4.056139
1	-1.027920	-1.523370	-3.224286
1	-1.497019	-0.167954	-2.201636
1	-3.271626	0.872917	-3.370517
1	-5.577114	1.304009	-2.815164
1	-5.865658	-0.476152	-2.418377
1	-2.693567	0.412232	-0.468764
1	-1.996694	-1.410898	2.734358
1	-4.333495	1.485809	-0.456422
1	-3.403353	-1.201956	4.766701
1	-6.869604	1.535043	3.807591
1	-7.674084	2.828057	1.863247
1	-0.523000	-0.741840	1.209158
1	1.102021	0.127670	1.375784
1	1.565616	2.984736	-1.032281
1	3.151932	0.290627	1.921003
1	5.786683	2.964183	-0.174520
8	-6.394898	2.886103	-0.541591
6	-7.519573	3.740754	-0.461536
1	-7.609194	4.212905	-1.440091
1	-8.438487	3.181501	-0.249830
1	-7.381230	4.517071	0.299596
6	1.831373	-3.519908	-1.971421
1	1.101327	-3.972189	-1.290319
1	1.339736	-3.439843	-2.951789
6	3.070552	-4.396766	-2.105460
1	3.536794	-4.598344	-1.136610
1	2.801453	-5.364098	-2.538853
1	3.823787	-3.946011	-2.758397
1	2.686471	-1.076311	-3.272374

3_si

Number of imaginary frequencies : 0

Electronic energy : =-3046.1129281
Zero-point correction= 0.814976
Thermal correction to Energy= 0.864161
Thermal correction to Enthalpy= 0.865106
Thermal correction to Gibbs Free Energy= 0.730162
Sum of electronic and zero-point Energies= -3045.297952
Sum of electronic and thermal Energies= -3045.248767
Sum of electronic and thermal Enthalpies= -3045.247822
Sum of electronic and thermal Free Energies= -3045.382766

Cartesian Coordinates

6	3.453607	-3.359643	1.901726
6	4.743923	-3.338035	1.075356
6	4.487136	-2.297178	-0.023668
7	2.998840	-2.031245	0.015590
6	2.356752	-3.092513	0.878132
6	2.269602	-1.681091	-1.318257
6	3.164516	-0.710106	-2.077214
6	1.063677	-2.473108	1.465116
8	1.280376	-1.437338	2.154684
8	1.140981	-0.994343	-0.932798
8	-0.021284	-2.998270	1.181164
1	4.090125	-1.159553	-2.440576
1	2.145266	-3.966187	0.260488
1	3.441124	-2.546393	2.633824
1	3.294025	-4.303364	2.425612
1	4.923029	-4.317642	0.623143
1	5.618942	-3.075268	1.671770
1	4.757827	-2.659242	-1.012094
1	4.996582	-1.349410	0.148846
1	0.273768	-1.504329	-1.008817
1	2.849187	-1.173790	0.571402
1	3.403621	0.151511	-1.445301
7	0.811826	1.096328	1.150770
6	2.037493	1.629996	0.773650
6	2.256689	2.616348	-0.194758
6	3.563452	2.988963	-0.505835
6	4.672281	2.416852	0.103193
6	4.440378	1.449498	1.079610
6	3.154366	1.069988	1.425685
6	3.754106	4.075656	-1.528579
9	5.021045	4.135359	-1.967135
6	5.608192	0.806807	1.770445
9	6.139947	1.581460	2.720992
6	-0.392207	1.084389	0.484491
16	-0.994115	2.353152	-0.449246
7	-1.044752	-0.070176	0.700289
6	-2.393914	-0.384061	0.280609
6	-2.437158	-1.756210	-0.422754
6	-3.854938	-1.997951	-1.012796
6	-3.733077	-2.214860	-2.525576
6	-2.877995	-3.468074	-2.745133
6	-1.515101	-3.254056	-2.035441
7	-1.397278	-1.894228	-1.472474
6	-1.595641	-0.911595	-2.551891
6	-3.016063	-1.022787	-3.188672

6	-3.750485	0.293902	-3.130862
6	-5.037814	0.483387	-2.848997
6	-3.327944	-0.410474	1.486428
6	-4.525954	0.367384	1.553155
6	-5.327111	0.227346	2.725645
7	-4.995681	-0.584556	3.769517
6	-3.882541	-1.268898	3.673097
6	-3.020256	-1.220811	2.551503
6	-6.533494	0.961950	2.821892
6	-6.944904	1.796283	1.814292
6	-6.143059	1.938221	0.652974
6	-4.957766	1.244929	0.531809
9	2.968383	3.893807	-2.599211
9	3.452645	5.281412	-1.025868
9	6.593424	0.524685	0.898227
9	5.264136	-0.358541	2.354768
1	-2.185546	-2.517181	0.321722
1	-4.315774	-2.877464	-0.551634
1	-4.507559	-1.147245	-0.799677
1	-0.695775	-3.393990	-2.745475
1	-1.364317	-3.956013	-1.209241
1	-2.732366	-3.643060	-3.816503
1	-3.391238	-4.345189	-2.338972
1	-4.723148	-2.352222	-2.971096
1	-2.888162	-1.267859	-4.252855
1	-0.815254	-1.094417	-3.299108
1	-1.415227	0.088927	-2.145512
1	-3.137410	1.167044	-3.360068
1	-5.467772	1.480239	-2.837681
1	-5.710249	-0.336165	-2.608337
1	-2.698505	0.396982	-0.416967
1	-2.117567	-1.829520	2.544437
1	-4.375163	1.403401	-0.368347
1	-3.627576	-1.910177	4.514742
1	-7.122963	0.837322	3.724566
1	-7.875531	2.341771	1.915266
1	-0.559145	-0.809151	1.210561
1	0.935540	0.262692	1.735622
1	1.418322	3.074015	-0.703189
1	2.992088	0.315539	2.191755
1	5.678655	2.710216	-0.171955
8	-6.477129	2.743373	-0.389146
6	-7.647633	3.527889	-0.275266
1	-7.703627	4.119016	-1.189725
1	-8.546917	2.905277	-0.197022
1	-7.597080	4.204928	0.585439
6	1.920930	-2.947846	-2.097218
1	1.155060	-3.484333	-1.526447
1	1.430286	-2.584795	-3.007756
6	3.054585	-3.895277	-2.477595
1	3.503217	-4.379867	-1.604366
1	2.663279	-4.689530	-3.117828
1	3.847037	-3.387349	-3.035363
1	2.592496	-0.343756	-2.932155

3_re

Number of imaginary frequencies : 0

Electronic energy : =-3046.1198482

Zero-point correction= 0.813770

Thermal correction to Energy= 0.863174

Thermal correction to Enthalpy=	0.864118
Thermal correction to Gibbs Free Energy=	0.729589
Sum of electronic and zero-point Energies=	-3045.306079
Sum of electronic and thermal Energies=	-3045.256674
Sum of electronic and thermal Enthalpies=	-3045.255730
Sum of electronic and thermal Free Energies=	-3045.390259

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Cartesian Coordinates

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6	-2.698206	4.486243	1.090301
6	-3.807831	4.680493	0.056620
6	-4.133204	3.250916	-0.377058
7	-2.844259	2.484677	-0.183801
6	-1.832066	3.399663	0.460300
6	-2.280521	1.682752	-1.390815
6	-3.313829	0.600261	-1.725291
6	-2.794246	-0.378218	-2.773628
6	-1.016698	2.565351	1.467462
8	-1.682713	1.676953	2.063123
8	-1.150620	1.068270	-0.912068
8	0.189929	2.838021	1.577715
1	-4.244711	1.065839	-2.066426
1	-1.172532	3.803638	-0.309299
1	-3.109579	4.110988	2.033871
1	-2.123385	5.390295	1.295286
1	-3.432472	5.255432	-0.796291
1	-4.688228	5.189910	0.451948
1	-4.457245	3.171657	-1.413696
1	-4.885991	2.786868	0.261216
1	-0.267303	1.543490	-1.056728
1	-2.971794	1.769397	0.557116
1	-3.537075	0.054363	-0.802068
1	-2.667621	0.099016	-3.750314
1	-3.497668	-1.204375	-2.895511
7	-0.910690	-0.917510	1.278721
6	-2.134297	-1.505213	0.967024
6	-2.345702	-2.559213	0.064617
6	-3.644132	-2.975932	-0.205339
6	-4.759403	-2.385381	0.381734
6	-4.533178	-1.363698	1.294257
6	-3.249403	-0.936599	1.603353
6	-3.872116	-4.060898	-1.220204
9	-2.780220	-4.799854	-1.437061
6	-5.674827	-0.598244	1.891261
9	-5.562556	-0.462482	3.217741
6	0.298267	-0.979682	0.633389
16	0.865557	-2.300336	-0.257083
7	1.007919	0.147305	0.813047
6	2.349913	0.399871	0.330842
6	2.410466	1.753255	-0.410038
6	3.823590	1.960401	-1.024152
6	3.689760	2.148818	-2.539913
6	2.848456	3.407330	-2.783598
6	1.491027	3.227533	-2.055235
7	1.363341	1.883013	-1.457901
6	1.539265	0.871766	-2.517499
6	2.953432	0.950751	-3.169474
6	3.672067	-0.373367	-3.086698
6	4.961067	-0.570725	-2.819425
6	3.339863	0.417248	1.492062
6	4.504793	-0.411858	1.522830
6	5.377815	-0.267961	2.642020
7	5.141382	0.594724	3.671352
6	4.050547	1.318571	3.614517
6	3.122326	1.269509	2.546473

6	6.553636	-1.054798	2.697413
6	6.866376	-1.944534	1.701397
6	5.991624	-2.091289	0.594993
6	4.835512	-1.345403	0.513818
9	-4.857155	-4.890726	-0.841938
9	-4.245885	-3.550568	-2.410525
9	-6.861723	-1.159135	1.636287
9	-5.716925	0.657297	1.383985
1	2.178676	2.537619	0.316619
1	4.304934	2.839559	-0.583916
1	4.463769	1.102327	-0.804239
1	0.662437	3.358607	-2.757352
1	1.366837	3.955136	-1.246447
1	2.694512	3.557220	-3.857472
1	3.375746	4.287857	-2.404109
1	4.677464	2.264436	-2.996381
1	2.817744	1.173213	-4.237511
1	0.753623	1.047723	-3.260767
1	1.348888	-0.115734	-2.084782
1	3.044337	-1.244809	-3.280834
1	5.378334	-1.572425	-2.784198
1	5.646841	0.246832	-2.611633
1	2.596407	-0.406142	-0.360446
1	2.241011	1.908144	2.571748
1	4.191630	-1.512796	-0.341472
1	3.870482	1.998289	4.445535
1	7.200995	-0.926883	3.559076
1	7.774887	-2.531045	1.770788
1	0.590969	0.930183	1.320377
1	-1.053807	-0.038369	1.789570
1	-1.506009	-3.038307	-0.418110
1	-3.101353	-0.124425	2.309823
1	-5.763760	-2.716561	0.144099
8	6.224750	-2.952002	-0.430644
6	7.359813	-3.791031	-0.350194
1	7.335561	-4.417153	-1.242342
1	8.291554	-3.212887	-0.345723
1	7.324906	-4.432499	0.537969
1	-1.832788	-0.792036	-2.458429
6	-2.034739	2.627815	-2.559536
1	-2.969841	2.982155	-3.000381
1	-1.431506	3.492328	-2.276529
1	-1.492519	2.076091	-3.331150

[3-4]TS_re

Number of imaginary frequencies : 1
The smallest frequency is : -1053.4478 cm(-1)

Electronic energy : =-3046.1100388
Zero-point correction= 0.808167
Thermal correction to Energy= 0.857765
Thermal correction to Enthalpy= 0.858709
Thermal correction to Gibbs Free Energy= 0.721602
Sum of electronic and zero-point Energies= -3045.301872
Sum of electronic and thermal Energies= -3045.252274
Sum of electronic and thermal Enthalpies= -3045.251330
Sum of electronic and thermal Free Energies= -3045.388437

Cartesian Coordinates

6	-2.024119	4.888714	1.186994

6	-3.151712	5.204784	0.203917
6	-3.728283	3.822117	-0.100365
7	-2.561051	2.896206	-0.022504
6	-1.410377	3.617173	0.587053
6	-2.189351	2.098895	-1.257861
6	-3.339871	1.128231	-1.546725
6	-3.022230	0.170714	-2.691095
6	-0.886736	2.628738	1.637352
8	-1.797971	1.744155	1.914800
8	-1.091990	1.328387	-0.897038
8	0.241355	2.694292	2.103180
1	-4.256070	1.687950	-1.763596
1	-0.620549	3.841888	-0.134863
1	-2.438054	4.669545	2.177723
1	-1.286474	5.685143	1.292360
1	-2.740036	5.646298	-0.710542
1	-3.899504	5.889375	0.608815
1	-4.203918	3.759863	-1.079693
1	-4.461250	3.519028	0.653132
1	-0.199833	1.766423	-1.000745
1	-2.518191	2.069008	0.981762
1	-3.517191	0.558437	-0.626811
1	-3.006837	0.684698	-3.657374
1	-3.773709	-0.619877	-2.749546
7	-1.033434	-0.918098	0.995488
6	-2.251477	-1.527475	0.692091
6	-2.493243	-2.408560	-0.369877
6	-3.785544	-2.874667	-0.584678
6	-4.858829	-2.498800	0.214949
6	-4.603181	-1.631070	1.269503
6	-3.324391	-1.153982	1.516377
6	-4.057941	-3.752328	-1.773509
9	-2.962179	-4.382357	-2.208468
6	-5.731611	-1.120617	2.116913
9	-5.380686	-1.005912	3.405403
6	0.192399	-0.973431	0.392378
16	0.732365	-2.212805	-0.619364
7	0.951798	0.088521	0.724693
6	2.331354	0.312985	0.343049
6	2.510803	1.745726	-0.202735
6	3.960415	1.939485	-0.729261
6	3.907183	2.311803	-2.217481
6	3.159350	3.645101	-2.344943
6	1.770866	3.480946	-1.674014
7	1.525426	2.085685	-1.260140
6	1.676174	1.207353	-2.436076
6	3.123928	1.252286	-3.015683
6	3.747328	-0.120621	-3.065256
6	5.006325	-0.438036	-2.771595
6	3.256099	0.104836	1.540576
6	4.361898	-0.803655	1.518406
6	5.173948	-0.868608	2.690092
7	4.932085	-0.136409	3.814556
6	3.896330	0.664745	3.801030
6	3.034915	0.824550	2.689169
6	6.293304	-1.735193	2.700458
6	6.608256	-2.509344	1.613200
6	5.793152	-2.451655	0.454168
6	4.693136	-1.621193	0.413283
9	-4.982144	-4.685494	-1.499343
9	-4.536573	-3.036064	-2.809935
9	-6.808057	-1.915108	2.057309
9	-6.124845	0.103726	1.716521
1	2.298766	2.439804	0.618476
1	4.467845	2.732200	-0.170320

1	4.541458	1.024687	-0.585923
1	0.971342	3.768622	-2.364145
1	1.685441	4.107647	-0.779842
1	3.050491	3.915373	-3.400467
1	3.728987	4.443512	-1.859837
1	4.920437	2.411244	-2.618291
1	3.057007	1.608066	-4.053598
1	0.946366	1.546373	-3.179242
1	1.386791	0.191143	-2.148766
1	3.074574	-0.915266	-3.392434
1	5.357899	-1.462562	-2.844879
1	5.730810	0.299373	-2.435149
1	2.564039	-0.407918	-0.440733
1	2.200575	1.518807	2.763389
1	4.092252	-1.629332	-0.487982
1	3.708423	1.238543	4.706803
1	6.894626	-1.763157	3.603308
1	7.472529	-3.161642	1.649874
1	0.569028	0.788114	1.356430
1	-1.176108	-0.088137	1.570912
1	-1.684794	-2.720494	-1.015446
1	-3.150606	-0.471630	2.344355
1	-5.857615	-2.877043	0.029090
8	6.032722	-3.186480	-0.662859
6	7.105105	-4.108124	-0.636247
1	7.094866	-4.609164	-1.604622
1	8.069592	-3.603479	-0.505589
1	6.974190	-4.855793	0.154534
1	-2.046356	-0.296639	-2.531512
6	-1.895823	3.025080	-2.434159
1	-2.799163	3.529901	-2.787693
1	-1.156900	3.785984	-2.168721
1	-1.494649	2.435268	-3.261846

4_re

Number of imaginary frequencies : 0

Electronic energy : =-3046.1163832
Zero-point correction= 0.812561
Thermal correction to Energy= 0.862210
Thermal correction to Enthalpy= 0.863154
Thermal correction to Gibbs Free Energy= 0.726585
Sum of electronic and zero-point Energies= -3045.303822
Sum of electronic and thermal Energies= -3045.254173
Sum of electronic and thermal Enthalpies= -3045.253229
Sum of electronic and thermal Free Energies= -3045.389799

Cartesian Coordinates

6	-2.526044	4.624569	1.277037
6	-3.583499	4.973718	0.229703
6	-4.013021	3.600676	-0.299087
7	-2.840634	2.720693	-0.085524
6	-1.780413	3.470271	0.589592
6	-2.358892	1.896352	-1.228587
6	-3.445948	0.869576	-1.564281
6	-3.074518	-0.042748	-2.727843
6	-1.099454	2.552464	1.587760
8	-1.902042	1.596461	2.055947
8	-1.243764	1.184019	-0.756426
8	0.048409	2.669241	1.960800

1	-4.383106	1.395101	-1.781408
1	-1.000194	3.855969	-0.081835
1	-3.002518	4.259713	2.194062
1	-1.860518	5.449226	1.536014
1	-3.123251	5.556463	-0.575673
1	-4.416871	5.551281	0.634658
1	-4.296201	3.642315	-1.354522
1	-4.871686	3.208344	0.256801
1	-0.371268	1.611754	-0.961596
1	-2.673653	1.620182	1.426261
1	-3.612638	0.276424	-0.656747
1	-3.040650	0.502775	-3.676189
1	-3.812811	-0.841112	-2.839028
7	-0.868049	-1.058300	1.181376
6	-2.101701	-1.603918	0.822592
6	-2.352524	-2.355070	-0.332283
6	-3.653894	-2.744755	-0.619398
6	-4.730212	-2.418347	0.200049
6	-4.462817	-1.695661	1.354788
6	-3.171217	-1.299374	1.675097
6	-3.919811	-3.556373	-1.856274
9	-2.921248	-3.472168	-2.743686
6	-5.583446	-1.239860	2.242868
9	-5.268506	-1.352674	3.541331
6	0.329248	-1.047578	0.508226
16	0.899957	-2.304200	-0.458537
7	1.020931	0.078530	0.753192
6	2.372931	0.370208	0.321979
6	2.439114	1.777548	-0.307269
6	3.854862	2.024792	-0.900463
6	3.722824	2.293025	-2.405342
6	2.893157	3.570200	-2.582707
6	1.541836	3.370158	-1.847567
7	1.392961	1.993185	-1.336577
6	1.552010	1.052031	-2.460861
6	2.973289	1.139549	-3.099560
6	3.674846	-0.195825	-3.084558
6	4.962315	-0.420529	-2.830915
6	3.337144	0.288219	1.502727
6	4.487159	-0.562576	1.504153
6	5.326866	-0.520183	2.657416
7	5.074339	0.266971	3.741777
6	3.999500	1.014753	3.708477
6	3.104846	1.062243	2.612586
6	6.483739	-1.335677	2.690576
6	6.808282	-2.158773	1.642645
6	5.967107	-2.204346	0.501605
6	4.830523	-1.426744	0.439625
9	-4.092930	-4.856115	-1.572541
9	-5.041432	-3.145372	-2.475913
9	-6.708920	-1.933945	2.035679
9	-5.875178	0.057549	2.031371
1	2.218063	2.504156	0.483601
1	4.329427	2.883140	-0.414237
1	4.499063	1.159846	-0.720520
1	0.704713	3.566020	-2.523175
1	1.448381	4.049868	-0.993693
1	2.729196	3.767754	-3.647242
1	3.433239	4.428506	-2.171292
1	4.712197	2.422763	-2.854240
1	2.847956	1.419223	-4.155304
1	0.779213	1.300349	-3.196070
1	1.333508	0.040614	-2.101866
1	3.037859	-1.048819	-3.324332
1	5.370005	-1.426604	-2.851925

1	5.656992	0.378616	-2.584500
1	2.632897	-0.376868	-0.428053
1	2.235043	1.713336	2.667273
1	4.212332	-1.513397	-0.445891
1	3.804530	1.632855	4.583052
1	7.105014	-1.287136	3.578944
1	7.701007	-2.770519	1.696299
1	0.578739	0.814361	1.298131
1	-0.986021	-0.283573	1.827928
1	-1.545383	-2.612972	-1.002823
1	-2.989742	-0.738116	2.588123
1	-5.740537	-2.718157	-0.053581
8	6.214873	-2.992392	-0.576119
6	7.320983	-3.871877	-0.517945
1	7.308591	-4.432986	-1.452546
1	8.268886	-3.326213	-0.441859
1	7.234671	-4.572040	0.321101
1	-2.095548	-0.500774	-2.556743
6	-2.001090	2.758157	-2.444008
1	-2.897333	3.122899	-2.953830
1	-1.399922	3.624802	-2.155064
1	-1.428205	2.166408	-3.162656

4_si

Number of imaginary frequencies : 0

Electronic energy : =-3046.1158272
 Zero-point correction= 0.814336
 Thermal correction to Energy= 0.863773
 Thermal correction to Enthalpy= 0.864718
 Thermal correction to Gibbs Free Energy= 0.729827
 Sum of electronic and zero-point Energies= -3045.301491
 Sum of electronic and thermal Energies= -3045.252054
 Sum of electronic and thermal Enthalpies= -3045.251110
 Sum of electronic and thermal Free Energies= -3045.386000

Cartesian Coordinates

6	-2.775693	4.290373	1.329598
6	-3.983270	4.424435	0.403073
6	-4.281350	2.976820	0.022350
7	-2.933359	2.290553	0.037776
6	-1.918328	3.239358	0.625709
6	-2.476785	1.568425	-1.259982
6	-3.550714	0.530652	-1.573821
6	-1.021238	2.423465	1.576217
8	-1.620368	1.490298	2.176511
8	-1.320211	0.896014	-0.929837
8	0.173167	2.752644	1.644744
1	-4.442172	0.977800	-2.020301
1	-1.322537	3.678669	-0.174628
1	-3.084452	3.904690	2.307395
1	-2.226787	5.221003	1.478442
1	-3.715866	5.002882	-0.487464
1	-4.844153	4.900400	0.875532
1	-4.746940	2.861932	-0.954944
1	-4.904322	2.477888	0.766599
1	-0.456312	1.390239	-1.055325
1	-2.940141	1.538336	0.754784
1	-3.840680	-0.007822	-0.667671
7	-0.867429	-1.052505	1.314397

6	-2.091739	-1.603915	0.951678
6	-2.318840	-2.461094	-0.133073
6	-3.616966	-2.859268	-0.429574
6	-4.716641	-2.441781	0.312099
6	-4.476630	-1.597290	1.389956
6	-3.192821	-1.183361	1.716733
6	-3.844302	-3.659435	-1.679715
9	-2.820753	-4.474254	-1.957391
6	-5.623486	-0.994965	2.144163
9	-5.388686	-0.918777	3.459484
6	0.338939	-1.082681	0.657403
16	0.932757	-2.403357	-0.212490
7	1.016715	0.063432	0.828360
6	2.345544	0.359088	0.334265
6	2.337713	1.694651	-0.440991
6	3.738230	1.956916	-1.062730
6	3.596764	2.079274	-2.584530
6	2.691568	3.281775	-2.876193
6	1.342392	3.057497	-2.143517
7	1.281629	1.735918	-1.488690
6	1.512953	0.697878	-2.510781
6	2.923652	0.821904	-3.165403
6	3.710220	-0.458899	-3.036842
6	5.008546	-0.578778	-2.768823
6	3.340168	0.441306	1.488970
6	4.534625	-0.345472	1.530932
6	5.411464	-0.139665	2.637617
7	5.151476	0.737803	3.648463
6	4.033987	1.418478	3.583792
6	3.100326	1.310846	2.524521
6	6.618667	-0.876205	2.701567
6	6.959185	-1.777275	1.725291
6	6.080598	-1.987834	0.632552
6	4.893478	-1.292643	0.544394
9	-4.953586	-4.409399	-1.605112
9	-3.997332	-2.848539	-2.746059
9	-6.763289	-1.672946	1.970228
9	-5.855130	0.271159	1.724672
1	2.067842	2.484647	0.266380
1	4.167539	2.878729	-0.657312
1	4.425890	1.145726	-0.810035
1	0.511316	3.109510	-2.855126
1	1.173868	3.815269	-1.370730
1	2.533738	3.383601	-3.955090
1	3.170419	4.202245	-2.528367
1	4.577827	2.228535	-3.045778
1	2.776789	0.996498	-4.240949
1	0.731225	0.814462	-3.266706
1	1.366435	-0.283773	-2.050434
1	3.128546	-1.368597	-3.196676
1	5.477707	-1.555401	-2.698282
1	5.650544	0.280451	-2.591663
1	2.622221	-0.452530	-0.338623
1	2.197669	1.918730	2.542259
1	4.250360	-1.508025	-0.300312
1	3.834974	2.110545	4.400160
1	7.267083	-0.698330	3.553501
1	7.891602	-2.324028	1.800407
1	0.583534	0.829893	1.344740
1	-1.004609	-0.205025	1.876784
1	-1.491791	-2.796317	-0.743853
1	-3.032824	-0.504488	2.549941
1	-5.721488	-2.757006	0.057228
8	6.339865	-2.864015	-0.373783
6	7.509944	-3.652588	-0.284815

1	7.505171	-4.298396	-1.163162
1	8.416599	-3.036121	-0.300378
1	7.508534	-4.275442	0.617172
6	-2.303828	2.596780	-2.379063
1	-3.192042	3.235588	-2.438562
1	-1.459742	3.247556	-2.133693
6	-2.058155	1.930863	-3.731544
1	-2.965467	1.461975	-4.120404
1	-1.724353	2.668928	-4.464928
1	-1.291106	1.156654	-3.649465
1	-3.136709	-0.195288	-2.275142

[3-4]TS_si

Number of imaginary frequencies : 1
The smallest frequency is : -1065.0736 cm(-1)

Electronic energy : =-3046.108147
Zero-point correction= 0.809376
Thermal correction to Energy= 0.858674
Thermal correction to Enthalpy= 0.859618
Thermal correction to Gibbs Free Energy= 0.723859
Sum of electronic and zero-point Energies= -3045.298771
Sum of electronic and thermal Energies= -3045.249473
Sum of electronic and thermal Enthalpies= -3045.248529
Sum of electronic and thermal Free Energies= -3045.384288

Cartesian Coordinates

6	-2.027480	4.654552	1.447537
6	-3.265226	4.944061	0.598922
6	-3.860794	3.551966	0.397935
7	-2.681169	2.641320	0.312141
6	-1.481322	3.366787	0.814395
6	-2.471522	1.869619	-0.974866
6	-3.672219	0.948570	-1.155217
6	-0.876713	2.399010	1.842645
8	-1.728280	1.468247	2.146193
8	-1.355465	1.055490	-0.776135
8	0.259755	2.527345	2.275490
1	-4.566928	1.501209	-1.453918
1	-0.752771	3.574427	0.027634
1	-2.319177	4.464364	2.486430
1	-1.285247	5.453732	1.442819
1	-2.968215	5.366176	-0.367802
1	-3.965874	5.632855	1.074993
1	-4.477580	3.470181	-0.497234
1	-4.466058	3.252217	1.258569
1	-0.498772	1.549431	-0.803563
1	-2.530751	1.793578	1.273779
1	-3.881815	0.413867	-0.223710
7	-0.955400	-1.159726	1.141070
6	-2.175092	-1.687854	0.711222
6	-2.419765	-2.218350	-0.559109
6	-3.708461	-2.615732	-0.895966
6	-4.777138	-2.499869	-0.015678
6	-4.518849	-1.972648	1.244853
6	-3.241346	-1.575244	1.614202
6	-3.956229	-3.069373	-2.305808
9	-2.944329	-3.799273	-2.788647
6	-5.654301	-1.720911	2.193067
9	-5.292858	-1.887682	3.472488

6	0.253490	-1.118625	0.495277
16	0.817616	-2.298362	-0.569614
7	0.967574	-0.033968	0.845623
6	2.318764	0.271996	0.419775
6	2.407034	1.740537	-0.044193
6	3.816994	2.033589	-0.629910
6	3.668276	2.480462	-2.089859
6	2.856252	3.780622	-2.106619
6	1.522246	3.522231	-1.358225
7	1.346931	2.094824	-1.022905
6	1.475142	1.300080	-2.259936
6	2.891516	1.426676	-2.901229
6	3.567077	0.084951	-3.043931
6	4.855127	-0.184786	-2.843423
6	3.308312	0.032411	1.556870
6	4.447253	-0.823787	1.423607
6	5.327638	-0.913664	2.542860
7	5.117483	-0.258899	3.719900
6	4.047420	0.490344	3.810093
6	3.119733	0.674435	2.756212
6	6.486203	-1.720533	2.440691
6	6.775614	-2.414158	1.293602
6	5.890904	-2.335712	0.188264
6	4.750137	-1.564170	0.257734
9	-5.073886	-3.800922	-2.413231
9	-4.101473	-2.015358	-3.134754
9	-6.697913	-2.526525	1.957276
9	-6.103345	-0.455901	2.081208
1	2.212129	2.373357	0.827977
1	4.313693	2.820676	-0.053481
1	4.448690	1.143790	-0.566918
1	0.671430	3.834229	-1.973769
1	1.477755	4.084912	-0.419393
1	2.667677	4.092123	-3.139549
1	3.419582	4.583436	-1.621344
1	4.653339	2.647659	-2.536324
1	2.762104	1.825094	-3.917558
1	0.705500	1.664927	-2.948956
1	1.229279	0.257469	-2.028986
1	2.909723	-0.726909	-3.360129
1	5.246627	-1.188285	-2.979476
1	5.565931	0.573262	-2.523929
1	2.542353	-0.388381	-0.418211
1	2.263342	1.327003	2.912873
1	4.097463	-1.556725	-0.606577
1	3.885944	1.001347	4.757559
1	7.138667	-1.767614	3.306439
1	7.671642	-3.021169	1.245185
1	0.573883	0.622673	1.515036
1	-1.099874	-0.400643	1.805739
1	-1.617777	-2.301107	-1.279878
1	-3.065695	-1.157852	2.601940
1	-5.775894	-2.810085	-0.299413
8	6.097891	-2.995697	-0.980970
6	7.231259	-3.835337	-1.081867
1	7.189541	-4.277825	-2.077514
1	8.165196	-3.269632	-0.980590
1	7.206963	-4.636225	-0.333661
6	-2.277871	2.816657	-2.164629
1	-3.101612	3.538762	-2.203950
1	-1.359689	3.391628	-1.996914
6	-2.180287	2.068090	-3.492790
1	-3.153182	1.681585	-3.807502
1	-1.815563	2.729845	-4.282621
1	-1.494653	1.220415	-3.407911

1 -3.448756 0.211672 -1.927911

4_si

Number of imaginary frequencies : 0

Electronic energy : =-3046.1119114
Zero-point correction= 0.812644
Thermal correction to Energy= 0.862614
Thermal correction to Enthalpy= 0.863559
Thermal correction to Gibbs Free Energy= 0.724795
Sum of electronic and zero-point Energies= -3045.299267
Sum of electronic and thermal Energies= -3045.249297
Sum of electronic and thermal Enthalpies= -3045.248353
Sum of electronic and thermal Free Energies= -3045.387116

Cartesian Coordinates

6	1.720189	-5.108218	1.811286
6	2.697064	-5.782850	0.847806
6	3.434051	-4.593146	0.226929
7	2.453771	-3.483194	0.250839
6	1.256054	-3.895368	0.988660
6	2.191111	-2.742042	-1.014547
6	3.484315	-2.052494	-1.431678
6	0.814465	-2.739117	1.876487
8	1.791792	-1.864118	2.114131
8	1.264315	-1.728609	-0.705859
8	-0.296107	-2.617910	2.344442
1	4.217415	-2.770812	-1.809672
1	0.405836	-4.162414	0.348993
1	2.247479	-4.768081	2.710060
1	0.883168	-5.736210	2.119398
1	2.138890	-6.320649	0.073296
1	3.369377	-6.489204	1.338825
1	3.775810	-4.800265	-0.790438
1	4.314121	-4.319330	0.819107
1	0.338024	-2.067383	-0.689821
1	2.506271	-2.186267	1.487663
1	3.923779	-1.528672	-0.579660
7	1.229270	0.896814	0.682914
6	2.361957	1.654161	0.375672
6	2.349642	2.955323	-0.137894
6	3.557250	3.599260	-0.389236
6	4.786364	3.001968	-0.137342
6	4.783224	1.720867	0.401077
6	3.594989	1.056498	0.662698
6	3.515709	5.015273	-0.893293
9	4.647010	5.349248	-1.532868
6	6.076546	1.037698	0.737808
9	6.410662	1.199747	2.027554
6	-0.033987	0.912327	0.155308
16	-0.602225	2.005153	-0.992647
7	-0.785699	-0.094734	0.647682
6	-2.202198	-0.285434	0.396695
6	-2.522608	-1.780840	0.220656
6	-4.005620	-1.959308	-0.212433
6	-4.044115	-2.674170	-1.569446
6	-3.413914	-4.060922	-1.390476
6	-2.000116	-3.873015	-0.781545
7	-1.607026	-2.450539	-0.734480
6	-1.734967	-1.875812	-2.085472
6	-3.205408	-1.904486	-2.607270
6	-3.702087	-0.523015	-2.955740

6	-4.919327	-0.031023	-2.735614
6	-3.034107	0.279481	1.546394
6	-4.064217	1.253394	1.353814
6	-4.804953	1.654159	2.506260
7	-4.560624	1.177796	3.760040
6	-3.592058	0.306730	3.896638
6	-2.807473	-0.175873	2.822030
6	-5.851321	2.595367	2.353414
6	-6.164178	3.123507	1.127160
6	-5.419357	2.730972	-0.014412
6	-4.390036	1.821259	0.101137
9	2.497979	5.216594	-1.739471
9	3.363618	5.891146	0.113939
9	7.095541	1.505146	0.006144
9	6.002856	-0.289388	0.526190
1	-2.343152	-2.275368	1.180177
1	-4.552070	-2.549159	0.530502
1	-4.503632	-0.988389	-0.278875
1	-1.254883	-4.416441	-1.371705
1	-1.951478	-4.255461	0.243643
1	-3.354591	-4.572531	-2.357177
1	-4.037089	-4.676297	-0.734455
1	-5.076899	-2.772484	-1.917824
1	-3.216528	-2.489398	-3.537922
1	-1.083352	-2.462650	-2.741185
1	-1.335884	-0.854645	-2.067423
1	-2.968069	0.114213	-3.452324
1	-5.176989	0.980749	-3.033402
1	-5.700525	-0.604435	-2.242829
1	-2.431814	0.244287	-0.527942
1	-2.032118	-0.912172	3.022621
1	-3.836115	1.572841	-0.795895
1	-3.403364	-0.062712	4.903051
1	-6.399005	2.882962	3.244930
1	-6.971188	3.841423	1.041985
1	-0.403763	-0.667693	1.395093
1	1.453963	0.037791	1.179045
1	1.413004	3.451217	-0.349211
1	3.622826	0.055492	1.083536
1	5.715013	3.515107	-0.357949
8	-5.660335	3.209740	-1.262518
6	-6.661860	4.196341	-1.416181
1	-6.662845	4.462050	-2.473509
1	-7.652602	3.813493	-1.143334
1	-6.439861	5.090906	-0.822977
6	1.640574	-3.650077	-2.126391
1	2.270660	-4.541062	-2.224646
1	0.651242	-4.000853	-1.810417
6	1.531384	-2.947038	-3.478812
1	2.514630	-2.808419	-3.936341
1	0.925272	-3.534801	-4.173946
1	1.070945	-1.960795	-3.370043
1	3.275656	-1.320234	-2.213444

4_anti

Number of imaginary frequencies : 0

Electronic energy : =-3046.1098318

Zero-point correction= 0.811940

Thermal correction to Energy= 0.861551

Thermal correction to Enthalpy= 0.862495

Thermal correction to Gibbs Free Energy=	0.724486
Sum of electronic and zero-point Energies=	-3045.297892
Sum of electronic and thermal Energies=	-3045.248281
Sum of electronic and thermal Enthalpies=	-3045.247337
Sum of electronic and thermal Free Energies=	-3045.385346

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Cartesian Coordinates
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6	2.312825	3.584435	-0.986909
6	3.457985	3.198818	-0.047198
6	2.718708	2.540852	1.130546
6	1.291439	3.132170	1.089391
7	1.314528	4.069314	-0.039344
6	0.079301	4.699548	-0.440917
6	-0.509197	5.464657	0.754829
6	-1.683413	6.375221	0.405560
6	1.910002	2.355629	-1.828566
8	2.728157	1.552367	-2.226926
8	0.622591	2.180768	-2.111821
8	-0.905990	3.729874	-0.894145
1	2.607529	4.371546	-1.687953
1	4.175478	2.533991	-0.528110
1	3.966582	4.111484	0.270928
1	2.681423	1.457916	0.995825
1	3.213621	2.734710	2.083762
1	0.543694	2.331482	0.942588
1	1.037285	3.657439	2.013525
1	0.300162	6.044200	1.210411
1	-0.014738	2.852158	-1.662369
1	-2.407044	5.862325	-0.234839
1	-1.351092	7.276791	-0.115584
1	-1.282014	3.171976	-0.147617
1	-0.825226	4.726047	1.501953
7	1.402103	-0.422590	-0.450039
6	2.637532	-0.988991	-0.085341
6	3.004863	-1.233585	1.238373
6	4.268482	-1.748287	1.513616
6	5.187234	-2.009317	0.507194
6	4.816972	-1.730272	-0.804949
6	3.560546	-1.227316	-1.109500
6	4.612866	-2.017791	2.950842
9	4.419091	-0.928826	3.712967
6	5.817271	-1.931692	-1.907223
9	6.640629	-2.957926	-1.645416
6	0.164512	-0.630083	0.099115
16	-0.158467	-1.733552	1.327024
7	-0.784499	0.169821	-0.450785
6	-2.212592	-0.086558	-0.337590
6	-3.055950	1.201913	-0.217926
6	-4.496303	0.809683	0.221232
6	-4.771280	1.403633	1.612209
6	-4.775579	2.927715	1.467246
6	-3.437045	3.336381	0.807741
7	-2.487332	2.200782	0.718427
6	-2.313819	1.619073	2.060747
6	-3.656087	1.036717	2.611383
6	-3.541918	-0.428062	2.952432
6	-4.463720	-1.367167	2.750458
6	-2.704428	-0.892514	-1.540561
6	-3.332098	-2.172790	-1.416731
6	-3.782437	-2.795808	-2.619892
7	-3.617406	-2.249747	-3.857849
6	-3.013620	-1.090557	-3.931374
6	-2.548918	-0.374605	-2.802606
6	-4.436852	-4.048390	-2.538862

6	-4.645736	-4.668412	-1.333921
6	-4.187392	-4.052378	-0.141164
6	-3.538056	-2.836776	-0.186243
9	3.849454	-2.989561	3.471270
9	5.891222	-2.389218	3.102970
9	6.591664	-0.848395	-2.078307
9	5.223866	-2.178701	-3.083055
1	-3.076032	1.697616	-1.196598
1	-5.233985	1.197075	-0.488565
1	-4.607882	-0.278026	0.235712
1	-2.945665	4.131037	1.376953
1	-3.587711	3.711736	-0.209535
1	-4.886928	3.400680	2.448450
1	-5.621253	3.248928	0.851791
1	-5.738399	1.054667	1.985895
1	-3.881159	1.559273	3.551764
1	-1.936525	2.416219	2.709884
1	-1.539234	0.846658	2.011093
1	-2.605186	-0.714947	3.432017
1	-4.289035	-2.396398	3.048835
1	-5.419190	-1.157398	2.276072
1	-2.341924	-0.666673	0.575982
1	-2.070702	0.589400	-2.958179
1	-3.177630	-2.423113	0.748114
1	-2.880865	-0.666749	-4.924905
1	-4.768735	-4.499403	-3.468341
1	-5.151160	-5.626211	-1.303102
1	-0.482688	0.764830	-1.217811
1	1.432952	0.053052	-1.349072
1	2.313506	-1.026742	2.045130
1	3.293244	-1.009539	-2.138215
1	6.165902	-2.415400	0.735041
8	-4.349238	-4.600071	1.089831
6	-4.982572	-5.861756	1.179637
1	-4.994575	-6.117345	2.239346
1	-6.013672	-5.822965	0.808863
1	-4.426411	-6.631719	0.632606
1	-2.202071	6.695792	1.313367
6	0.311340	5.602324	-1.645044
1	-0.622690	6.086915	-1.929932
1	1.058888	6.365583	-1.413355
1	0.650190	5.021037	-2.506673

[4-5]TS_anti

Number of imaginary frequencies : 1

The smallest frequency is : -208.7831 cm⁻¹)

Electronic energy : =-3046.0944552

Zero-point correction= 0.811443

Thermal correction to Energy= 0.860489

Thermal correction to Enthalpy= 0.861434

Thermal correction to Gibbs Free Energy= 0.726467

Sum of electronic and zero-point Energies= -3045.283012

Sum of electronic and thermal Energies= -3045.233966

Sum of electronic and thermal Enthalpies= -3045.233022

Sum of electronic and thermal Free Energies= -3045.367988

Cartesian Coordinates

6	2.370903	3.488571	-1.236056
6	3.611466	3.125827	-0.425627

6	2.995793	2.511407	0.835329
6	1.747891	3.365925	1.098860
7	1.478037	4.028736	-0.193166
6	0.441626	4.831952	-0.389038
6	-0.155809	5.480137	0.844013
6	-1.357088	6.379586	0.584965
6	1.760262	2.231264	-1.918874
8	2.542439	1.350498	-2.287158
8	0.490238	2.180241	-2.036265
8	-1.083758	3.683925	-0.789944
1	2.566477	4.248577	-1.995664
1	4.243762	2.429015	-0.974096
1	4.178210	4.030792	-0.185882
1	2.703449	1.478928	0.626833
1	3.672402	2.505247	1.690939
1	0.880799	2.761959	1.395265
1	1.923574	4.124471	1.866814
1	0.651312	6.057764	1.314293
1	-0.505371	3.084146	-1.376988
1	-2.126805	5.849701	0.018818
1	-1.076604	7.279761	0.031756
1	-1.335570	3.107421	-0.012240
1	-0.422757	4.688842	1.552004
7	1.362673	-0.504464	-0.426893
6	2.588968	-1.087741	-0.067113
6	2.937758	-1.406176	1.246072
6	4.201641	-1.925962	1.513374
6	5.140646	-2.119890	0.511328
6	4.788485	-1.767900	-0.789340
6	3.534114	-1.259163	-1.087944
6	4.520257	-2.280836	2.937299
9	4.300487	-1.242819	3.763145
6	5.813690	-1.905635	-1.877955
9	6.569029	-3.001870	-1.707451
6	0.126271	-0.672846	0.132424
16	-0.233140	-1.834606	1.304331
7	-0.788859	0.200050	-0.356154
6	-2.224769	-0.021343	-0.251645
6	-3.038866	1.267524	0.002621
6	-4.478298	0.881844	0.448925
6	-4.700963	1.375174	1.889199
6	-4.651801	2.906303	1.873455
6	-3.318091	3.322694	1.208564
7	-2.417674	2.164911	1.003407
6	-2.229653	1.469476	2.287152
6	-3.577453	0.885617	2.823895
6	-3.508455	-0.607096	3.030475
6	-4.472864	-1.491105	2.783389
6	-2.748248	-0.689976	-1.522551
6	-3.431521	-1.946689	-1.515265
6	-3.901907	-2.439570	-2.769537
7	-3.715100	-1.787386	-3.951645
6	-3.058036	-0.654650	-3.919498
6	-2.558287	-0.068180	-2.732330
6	-4.593011	-3.674791	-2.802660
6	-4.818995	-4.398243	-1.659962
6	-4.345654	-3.908070	-0.415752
6	-3.664687	-2.711300	-0.349568
9	3.757076	-3.289426	3.382213
9	5.799563	-2.648763	3.093670
9	6.656713	-0.858761	-1.899648
9	5.255658	-1.983454	-3.092468
1	-3.068881	1.848205	-0.927240
1	-5.221677	1.339968	-0.211447
1	-4.622171	-0.200224	0.387073

1	-2.778441	4.056158	1.819022
1	-3.484206	3.777875	0.227333
1	-4.717938	3.295615	2.894741
1	-5.501965	3.309900	1.315187
1	-5.672019	1.031465	2.257812
1	-3.760423	1.330940	3.812013
1	-1.812874	2.198445	2.989818
1	-1.484556	0.678731	2.154406
1	-2.565335	-0.970653	3.439684
1	-4.326111	-2.547940	2.983647
1	-5.435978	-1.206052	2.367159
1	-2.360316	-0.686427	0.601371
1	-2.019101	0.874358	-2.799344
1	-3.294665	-2.395093	0.618532
1	-2.904577	-0.148687	-4.870761
1	-4.937452	-4.029334	-3.768623
1	-5.349918	-5.340907	-1.718193
1	-0.455532	0.846961	-1.076788
1	1.418009	0.021470	-1.301983
1	2.230761	-1.255036	2.051035
1	3.281627	-0.977514	-2.104329
1	6.118355	-2.532232	0.732661
8	-4.524836	-4.562958	0.759969
6	-5.137113	-5.837164	0.726664
1	-5.147108	-6.192987	1.757096
1	-6.168632	-5.782271	0.358881
1	-4.566484	-6.541402	0.110479
1	-1.788308	6.702421	1.535831
6	0.366596	5.560796	-1.702371
1	-0.611466	6.020953	-1.823460
1	1.134835	6.342024	-1.720985
1	0.528180	4.878958	-2.538077

5_anti

Number of imaginary frequencies : 0

Electronic energy : =-3046.1074555
Zero-point correction= 0.809941
Thermal correction to Energy= 0.861149
Thermal correction to Enthalpy= 0.862093
Thermal correction to Gibbs Free Energy= 0.721087
Sum of electronic and zero-point Energies= -3045.297515
Sum of electronic and thermal Energies= -3045.246306
Sum of electronic and thermal Enthalpies= -3045.245362
Sum of electronic and thermal Free Energies= -3045.386369

Cartesian Coordinates

6	2.735375	3.169516	-1.690751
6	4.124682	2.547083	-1.713743
6	4.272901	2.042011	-0.279254
6	3.664829	3.163268	0.561208
7	2.690113	3.821253	-0.356998
6	1.898417	4.774391	0.006854
6	2.036975	5.384413	1.373979
6	0.744342	5.955917	1.948611
6	1.595884	2.101438	-1.782286
8	1.872444	1.042294	-2.364913
8	0.496665	2.423477	-1.254051
8	0.631730	2.759723	1.486471
1	2.583649	3.919518	-2.469090

1	4.174719	1.752954	-2.457207
1	4.879451	3.306973	-1.940457
1	3.689679	1.124800	-0.151748
1	5.304061	1.830901	0.005204
1	3.110833	2.804421	1.430977
1	4.405859	3.908840	0.863049
1	2.791705	6.178802	1.266329
1	0.571761	2.674737	0.518632
1	0.012112	5.151906	2.047209
1	0.329270	6.759734	1.336129
1	-0.110848	2.192543	1.783089
1	2.438307	4.647151	2.067352
7	1.169166	-0.941082	-0.434633
6	2.340330	-1.649854	-0.168975
6	2.537072	-2.527902	0.904277
6	3.789084	-3.103713	1.095509
6	4.871814	-2.827407	0.268851
6	4.663310	-1.948079	-0.786572
6	3.421669	-1.376678	-1.020711
6	3.980061	-3.992609	2.291871
9	4.160939	-3.275075	3.414952
6	5.785466	-1.564609	-1.704843
9	6.960018	-2.078816	-1.319114
6	-0.100405	-1.058045	0.070960
16	-0.706614	-2.421877	0.864034
7	-0.825611	0.049416	-0.172268
6	-2.266969	0.154030	-0.044415
6	-2.662767	1.454349	0.687178
6	-4.198545	1.500584	0.932157
6	-4.454295	1.633293	2.441128
6	-3.829659	2.951833	2.916910
6	-2.327225	2.933456	2.530393
7	-1.930018	1.636718	1.954726
6	-2.241012	0.571438	2.917061
6	-3.773725	0.484052	3.209481
6	-4.312706	-0.896599	2.932223
6	-5.469472	-1.205857	2.349910
6	-2.918794	0.128800	-1.425675
6	-3.989993	-0.758168	-1.764019
6	-4.553760	-0.631247	-3.069050
7	-4.105622	0.260102	-3.998632
6	-3.099572	1.027306	-3.660513
6	-2.478049	1.002673	-2.389445
6	-5.633530	-1.470941	-3.433047
6	-6.138957	-2.403180	-2.563527
6	-5.565235	-2.540118	-1.273626
6	-4.512700	-1.737279	-0.887864
9	2.919343	-4.781606	2.506094
9	5.053854	-4.786155	2.161386
9	5.935365	-0.223914	-1.752454
9	5.568877	-1.962369	-2.966556
1	-2.354182	2.293285	0.048712
1	-4.646750	2.350057	0.406421
1	-4.677037	0.597335	0.545159
1	-1.687705	3.120476	3.399478
1	-2.096537	3.704565	1.787567
1	-3.952865	3.056360	4.000141
1	-4.340849	3.798770	2.448009
1	-5.530390	1.634334	2.641124
1	-3.923163	0.673728	4.282043
1	-1.681302	0.793411	3.830926
1	-1.855653	-0.376199	2.528472
1	-3.667186	-1.711505	3.264534
1	-5.761669	-2.240558	2.199428
1	-6.162754	-0.450445	1.988267

1	-2.595724	-0.704616	0.541586
1	-1.643385	1.673533	-2.195526
1	-4.099645	-1.893703	0.101569
1	-2.740395	1.724732	-4.415338
1	-6.046213	-1.350626	-4.429378
1	-6.966662	-3.031085	-2.870732
1	-0.352891	0.847568	-0.611400
1	1.278391	-0.249255	-1.185887
1	1.722587	-2.760792	1.576269
1	3.282454	-0.686183	-1.849722
1	5.841262	-3.278472	0.441966
8	-6.000152	-3.443870	-0.357523
6	-7.034523	-4.330148	-0.736611
1	-7.203221	-4.980852	0.121916
1	-7.963200	-3.794018	-0.965964
1	-6.744959	-4.942717	-1.598233
1	0.944050	6.365183	2.941228
6	0.869721	5.340504	-0.909443
1	-0.108925	5.099037	-0.480947
1	0.963771	6.430346	-0.930277
1	0.898534	4.931113	-1.914587

4_syn

Number of imaginary frequencies : 0

Electronic energy : =-3046.1103554
Zero-point correction= 0.811988
Thermal correction to Energy= 0.861639
Thermal correction to Enthalpy= 0.862583
Thermal correction to Gibbs Free Energy= 0.724085
Sum of electronic and zero-point Energies= -3045.298368
Sum of electronic and thermal Energies= -3045.248716
Sum of electronic and thermal Enthalpies= -3045.247772
Sum of electronic and thermal Free Energies= -3045.386270

Cartesian Coordinates

6	-2.306067	3.671485	0.750487
6	-3.485750	3.288715	-0.145039
6	-2.796098	2.507602	-1.275866
6	-1.351778	3.056989	-1.315336
7	-1.309239	4.060105	-0.243946
6	-0.036947	4.654142	0.095416
6	-0.218372	5.663418	1.237137
6	1.038169	6.458187	1.576018
6	-1.937207	2.464584	1.640073
8	-2.775135	1.694944	2.062966
8	-0.655604	2.271924	1.935774
8	0.903064	3.673201	0.607255
1	-2.547222	4.505109	1.417167
1	-4.232828	2.701573	0.388492
1	-3.944422	4.204843	-0.523800
1	-2.788930	1.440205	-1.043858
1	-3.305862	2.631012	-2.232920
1	-0.619443	2.246632	-1.147554
1	-1.119488	3.520527	-2.277449
1	-0.530223	5.106265	2.128360
1	0.000418	2.888776	1.431271
1	1.284858	7.187095	0.799619
1	1.892132	5.787848	1.707974
1	1.316630	3.094330	-0.111267

1	-1.041027	6.334797	0.968707
7	-1.381386	-0.374141	0.403839
6	-2.613116	-0.980658	0.093075
6	-2.998003	-1.308976	-1.206878
6	-4.255384	-1.865023	-1.427428
6	-5.149670	-2.084728	-0.390189
6	-4.761943	-1.722820	0.896819
6	-3.511847	-1.177606	1.147508
6	-4.635551	-2.191822	-2.843481
9	-3.713830	-2.959888	-3.441111
6	-5.741078	-1.886547	2.023946
9	-6.493325	-2.986387	1.867522
6	-0.147663	-0.599849	-0.144492
16	0.172752	-1.749459	-1.329530
7	0.802691	0.227864	0.365146
6	2.230743	-0.043358	0.275454
6	3.083074	1.230555	0.087344
6	4.525181	0.808991	-0.314647
6	4.818946	1.331414	-1.730084
6	4.822565	2.861040	-1.661692
6	3.469351	3.306878	-1.058390
7	2.525182	2.172094	-0.912657
6	2.366047	1.513185	-2.220695
6	3.718135	0.910302	-2.723935
6	3.612020	-0.570807	-2.988804
6	4.524669	-1.498866	-2.708591
6	2.711056	-0.782617	1.524642
6	3.326041	-2.073909	1.474850
6	3.771204	-2.630464	2.711873
7	3.610399	-2.012952	3.916370
6	3.016971	-0.846037	3.923174
6	2.560450	-0.190950	2.754701
6	4.415364	-3.890763	2.702524
6	4.616115	-4.581648	1.535206
6	4.160159	-4.032673	0.309142
6	3.523549	-2.809703	0.284654
9	-5.807401	-2.837724	-2.915107
9	-4.748205	-1.079707	-3.589773
9	-6.588428	-0.847312	2.097825
9	-5.129911	-1.978894	3.212403
1	3.096397	1.785723	1.033621
1	5.256999	1.226397	0.384076
1	4.629826	-0.278631	-0.273431
1	2.984545	4.053069	-1.693241
1	3.594265	3.753775	-0.066953
1	4.959879	3.284547	-2.661903
1	5.654324	3.209927	-1.042290
1	5.791192	0.964860	-2.072530
1	3.953139	1.385049	-3.686944
1	1.989654	2.269077	-2.917535
1	1.596020	0.739913	-2.133166
1	2.688088	-0.882760	-3.477659
1	4.354605	-2.542886	-2.953400
1	5.466735	-1.264706	-2.219006
1	2.361554	-0.675098	-0.602913
1	2.093845	0.786273	2.854831
1	3.165648	-2.447355	-0.671718
1	2.886889	-0.366121	4.891218
1	4.746154	-4.289862	3.655738
1	5.114213	-5.543360	1.560481
1	0.502312	0.834379	1.123215
1	-1.408343	0.158486	1.270256
1	-2.324093	-1.138248	-2.036401
1	-3.230116	-0.895918	2.156665
1	-6.122167	-2.526140	-0.574953

8	4.313002	-4.653257	-0.887864
6	4.917520	-5.932295	-0.903262
1	4.919790	-6.250819	-1.945820
1	5.950614	-5.895393	-0.538006
1	4.345511	-6.654659	-0.309605
1	0.893943	7.009473	2.508568
6	0.570266	5.300289	-1.145151
1	1.533520	5.752124	-0.902400
1	0.735950	4.560384	-1.933279
1	-0.102484	6.070814	-1.530411

[4-5]TS_{syn}

Number of imaginary frequencies : 1
The smallest frequency is : -199.5653 cm(-1)

Electronic energy : =-3046.0936276
Zero-point correction= 0.810580
Thermal correction to Energy= 0.860044
Thermal correction to Enthalpy= 0.860989
Thermal correction to Gibbs Free Energy= 0.723946
Sum of electronic and zero-point Energies= -3045.283048
Sum of electronic and thermal Energies= -3045.233583
Sum of electronic and thermal Enthalpies= -3045.232639
Sum of electronic and thermal Free Energies= -3045.369682

Cartesian Coordinates

6	-2.626000	3.263468	1.180750
6	-3.969914	2.745348	0.678641
6	-3.567487	2.018423	-0.607663
6	-2.446390	2.884246	-1.200739
7	-1.992203	3.722370	-0.071675
6	-1.011010	4.611506	-0.172996
6	-0.811837	5.544225	1.007089
6	0.322163	6.549820	0.861389
6	-1.791447	2.131234	1.844827
8	-2.403574	1.189123	2.355289
8	-0.519423	2.239577	1.801585
8	0.650004	3.664689	0.114522
1	-2.722973	4.094448	1.883002
1	-4.435578	2.082570	1.407415
1	-4.635147	3.587474	0.464516
1	-3.180456	1.029696	-0.352143
1	-4.392350	1.886701	-1.309297
1	-1.611166	2.283144	-1.581657
1	-2.808568	3.529826	-2.005576
1	-0.650694	4.930123	1.897773
1	0.242383	3.101613	0.860749
1	0.128046	7.275732	0.067340
1	1.264678	6.038854	0.653619
1	0.924538	3.011688	-0.592652
1	-1.764859	6.070796	1.148738
7	-1.277674	-0.705806	0.464650
6	-2.472562	-1.373433	0.159535
6	-2.785651	-1.881253	-1.104968
6	-4.044119	-2.429736	-1.329927
6	-5.020024	-2.467950	-0.342086
6	-4.699637	-1.941403	0.903626
6	-3.445041	-1.409851	1.166628
6	-4.355894	-2.919572	-2.715213
9	-3.358519	-3.657017	-3.221431

6	-5.737411	-1.867534	1.985953
9	-6.780317	-2.673928	1.743054
6	-0.032788	-0.839334	-0.091667
16	0.426732	-2.118684	-1.091341
7	0.793926	0.172649	0.258973
6	2.242432	0.105186	0.136692
6	2.879260	1.427256	-0.359404
6	4.348330	1.162318	-0.796147
6	4.478810	1.443175	-2.302202
6	4.226686	2.938431	-2.522114
6	2.853128	3.276531	-1.893461
7	2.124696	2.059728	-1.466085
6	2.010123	1.145056	-2.613325
6	3.415890	0.671599	-3.108374
6	3.546841	-0.830491	-3.091269
6	4.618456	-1.534677	-2.733027
6	2.864195	-0.268044	1.482106
6	3.775248	-1.359212	1.642958
6	4.334745	-1.555090	2.941170
7	4.018806	-0.784552	4.020202
6	3.150146	0.179073	3.839979
6	2.553068	0.478763	2.592410
6	5.264702	-2.605216	3.133653
6	5.628361	-3.435922	2.104991
6	5.055602	-3.250866	0.820242
6	4.145075	-2.239371	0.600709
9	-5.468779	-3.665657	-2.749371
9	-4.544526	-1.894672	-3.567002
9	-6.224935	-0.619403	2.107351
9	-5.237713	-2.201906	3.183441
1	2.849516	2.153048	0.462754
1	5.036033	1.812731	-0.245916
1	4.637544	0.132452	-0.572032
1	2.210095	3.807591	-2.603807
1	2.960802	3.914742	-1.011228
1	4.234466	3.169151	-3.592506
1	5.019767	3.529641	-2.054149
1	5.481164	1.174480	-2.648963
1	3.518679	0.980976	-4.158188
1	1.479449	1.684979	-3.403981
1	1.389346	0.291220	-2.325746
1	2.661866	-1.370216	-3.430374
1	4.613946	-2.619357	-2.775012
1	5.534115	-1.069215	-2.376352
1	2.443284	-0.674059	-0.599189
1	1.838436	1.297731	2.536578
1	3.715479	-2.155186	-0.390836
1	2.893012	0.777720	4.711649
1	5.678651	-2.729878	4.128951
1	6.343471	-4.229959	2.283480
1	0.406480	0.877643	0.893643
1	-1.355612	-0.113770	1.295663
1	-2.057146	-1.850422	-1.904352
1	-3.221091	-0.989123	2.141623
1	-5.997160	-2.894063	-0.534813
8	5.356379	-4.030745	-0.249799
6	6.230433	-5.124690	-0.051797
1	6.311869	-5.623226	-1.018007
1	7.227098	-4.794308	0.264043
1	5.830418	-5.831883	0.683901
1	0.433770	7.107049	1.794443
6	-0.677446	5.112843	-1.551142
1	0.270707	5.647500	-1.537555
1	-0.607778	4.295455	-2.270286
1	-1.467290	5.799030	-1.878351

5_syn

Number of imaginary frequencies : 0

Electronic energy : =-3046.11087
Zero-point correction= 0.810814
Thermal correction to Energy= 0.861621
Thermal correction to Enthalpy= 0.862565
Thermal correction to Gibbs Free Energy= 0.723149
Sum of electronic and zero-point Energies= -3045.300056
Sum of electronic and thermal Energies= -3045.249249
Sum of electronic and thermal Enthalpies= -3045.248305
Sum of electronic and thermal Free Energies= -3045.387721

Cartesian Coordinates

6	-2.857541	3.168493	1.352508
6	-4.198821	2.442175	1.301866
6	-4.208095	1.896264	-0.125283
6	-3.679681	3.068790	-0.944497
7	-2.760061	3.769845	-0.002914
6	-1.961282	4.712548	-0.376868
6	-0.956790	5.334561	0.541718
6	0.457895	5.169787	-0.036933
6	-1.672510	2.175792	1.592656
8	-1.902784	1.227929	2.356711
8	-0.593176	2.431348	0.990945
8	-0.741456	2.348319	-1.782919
1	-2.816496	3.957160	2.106966
1	-4.242475	1.670339	2.069788
1	-5.023576	3.146180	1.452129
1	-3.515865	1.051196	-0.208700
1	-5.191003	1.567784	-0.463365
1	-3.107376	2.772708	-1.825007
1	-4.477635	3.765924	-1.220462
1	-0.995464	4.887493	1.532923
1	-0.735546	2.368557	-0.810771
1	0.588618	5.738985	-0.960601
1	0.648908	4.114308	-0.238838
1	0.060299	1.818246	-1.988213
1	-1.204093	6.400585	0.620874
7	-1.157206	-0.912647	0.578855
6	-2.351091	-1.592085	0.340926
6	-2.584944	-2.485804	-0.708547
6	-3.862578	-3.013931	-0.885049
6	-4.930773	-2.668605	-0.069872
6	-4.683325	-1.771407	0.966091
6	-3.419354	-1.253620	1.189139
6	-4.058919	-3.975217	-2.023319
9	-3.308769	-5.076916	-1.880187
6	-5.819196	-1.254875	1.797226
9	-6.820629	-2.138232	1.899611
6	0.098333	-1.070512	0.045038
16	0.672311	-2.491800	-0.663419
7	0.830691	0.047620	0.191747
6	2.264217	0.153106	0.001850
6	2.615289	1.371062	-0.878702
6	4.147566	1.441444	-1.138282
6	4.393145	1.420971	-2.654248
6	3.713554	2.652896	-3.267142
6	2.211991	2.614219	-2.879767

7	1.872236	1.377726	-2.154287
6	2.225066	0.223078	-2.992012
6	3.758957	0.166427	-3.284767
6	4.356170	-1.150452	-2.855486
6	5.529546	-1.341546	-2.255989
6	2.959728	0.280992	1.355164
6	4.031860	-0.577184	1.756717
6	4.635921	-0.319247	3.023435
7	4.226288	0.674833	3.861845
6	3.219793	1.416636	3.470971
6	2.558237	1.261520	2.228931
6	5.714762	-1.133409	3.444932
6	6.182308	-2.160915	2.665947
6	5.569826	-2.424237	1.414343
6	4.516413	-1.650783	0.975371
9	-5.334727	-4.373473	-2.136510
9	-3.710202	-3.423394	-3.197357
9	-6.345873	-0.135000	1.255174
9	-5.433696	-0.926416	3.038014
1	2.281339	2.269183	-0.339891
1	4.568832	2.355772	-0.707666
1	4.656624	0.599742	-0.661751
1	1.568786	2.662533	-3.764136
1	1.940098	3.458391	-2.237606
1	3.836078	2.645823	-4.355409
1	4.187772	3.566041	-2.893073
1	5.467653	1.444040	-2.861154
1	3.897472	0.239633	-4.372965
1	1.652882	0.315486	-3.920291
1	1.880198	-0.688984	-2.495575
1	3.741669	-2.023961	-3.080835
1	5.865680	-2.337807	-1.985515
1	6.191836	-0.519060	-1.997316
1	2.587795	-0.757311	-0.502714
1	1.724038	1.917820	1.987924
1	4.074068	-1.905379	0.019719
1	2.892766	2.197805	4.155085
1	6.158020	-0.916234	4.411388
1	7.009814	-2.766358	3.016140
1	0.361327	0.877721	0.574012
1	-1.243503	-0.181881	1.293487
1	-1.783743	-2.763428	-1.380469
1	-3.247504	-0.553803	2.002185
1	-5.919428	-3.079799	-0.234002
8	5.965961	-3.425836	0.586561
6	6.996785	-4.287311	1.028112
1	7.129108	-5.027624	0.238877
1	7.940487	-3.748363	1.174300
1	6.722451	-4.800665	1.957115
1	1.188078	5.530565	0.690311
6	-1.989250	5.175666	-1.795185
1	-1.412902	4.441088	-2.374411
1	-3.004653	5.214165	-2.193873
1	-1.524642	6.157625	-1.885673

6_anti

Number of imaginary frequencies : 0

Electronic energy : =-3046.1083269

Zero-point correction= 0.810369

Thermal correction to Energy= 0.861415

Thermal correction to Enthalpy=	0.862360
Thermal correction to Gibbs Free Energy=	0.721307
Sum of electronic and zero-point Energies=	-3045.297958
Sum of electronic and thermal Energies=	-3045.246911
Sum of electronic and thermal Enthalpies=	-3045.245967
Sum of electronic and thermal Free Energies=	-3045.387020

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

6	-4.096106	1.871934	-0.083338
6	-3.584981	3.126626	-0.782769
7	-2.703902	3.761509	0.240351
6	-2.829112	3.048951	1.535728
6	-4.145018	2.293136	1.384092
6	-1.884946	4.724810	-0.023853
6	-1.813420	5.248181	-1.430287
6	-1.066089	6.565094	-1.609804
6	-1.614520	2.075820	1.718903
8	-1.831722	1.067201	2.407340
8	-0.535750	2.405735	1.155774
1	-2.833657	3.768888	2.356783
1	-4.189908	1.460947	2.085603
1	-4.994345	2.959496	1.566476
1	-3.368097	1.064151	-0.220624
1	-5.056721	1.541299	-0.478691
1	-2.992276	2.914753	-1.672849
1	-4.392206	3.830817	-1.011188
1	-1.323055	4.437277	-1.992453
1	-0.696429	2.371343	-0.658240
8	-0.807896	2.247950	-1.616277
1	-1.057163	6.828058	-2.669477
1	-1.546310	7.385200	-1.069161
1	0.009163	1.759080	-1.858212
1	-2.828750	5.330647	-1.831556
7	-1.148945	-1.003137	0.547930
6	-2.338481	-1.680385	0.285697
6	-3.416033	-1.342755	1.120136
6	-4.677770	-1.861730	0.882425
6	-4.910899	-2.756542	-0.156789
6	-3.831419	-3.102248	-0.960408
6	-2.557107	-2.575436	-0.768068
6	-5.822562	-1.349057	1.703809
9	-6.341496	-0.224423	1.165378
6	-4.032378	-4.113706	-2.053760
9	-3.218561	-3.897563	-3.096442
6	0.110500	-1.130261	0.019968
16	0.701772	-2.509827	-0.755053
7	0.835454	-0.016545	0.229645
6	2.267549	0.112840	0.044467
6	2.594204	1.375890	-0.780703
6	4.122140	1.496263	-1.044161
6	4.356310	1.579723	-2.559874
6	3.633426	2.826031	-3.090146
6	2.134388	2.710791	-2.708284
7	1.843492	1.425690	-2.050824
6	2.227515	0.331001	-2.952313
6	3.758358	0.346302	-3.263339
6	4.404549	-0.973381	-2.923271
6	5.589647	-1.160580	-2.346158
6	2.965986	0.190370	1.400427
6	4.084356	-0.633938	1.744743
6	4.680497	-0.424019	3.024257
7	4.226065	0.494693	3.923576
6	3.182335	1.207726	3.580545
6	2.522303	1.095436	2.333421

6	5.801311	-1.206219	3.393633
6	6.318078	-2.157723	2.552101
6	5.716337	-2.372813	1.285965
6	4.621948	-1.629841	0.897252
9	-6.826106	-2.231773	1.789089
9	-5.449594	-1.031237	2.951611
9	-5.292451	-4.098732	-2.519242
9	-3.793253	-5.363032	-1.625432
1	2.241305	2.238523	-0.198363
1	4.526644	2.389510	-0.556954
1	4.653264	0.637147	-0.626679
1	1.490106	2.781171	-3.590400
1	1.828536	3.508023	-2.022286
1	3.754422	2.895678	-4.176374
1	4.077857	3.727457	-2.655708
1	5.427861	1.650935	-2.771133
1	3.881379	0.492806	-4.345953
1	1.640994	0.451142	-3.868475
1	1.920583	-0.617671	-2.501691
1	3.818028	-1.851645	-3.198535
1	5.963365	-2.159278	-2.142081
1	6.225241	-0.333088	-2.040562
1	2.598914	-0.771832	-0.499753
1	1.655415	1.723175	2.135752
1	4.193084	-1.843341	-0.074554
1	2.820000	1.928412	4.311577
1	6.236443	-1.026627	4.371378
1	7.177111	-2.740262	2.862829
1	0.359135	0.794957	0.638475
1	-1.244231	-0.292005	1.281751
1	-3.251801	-0.646955	1.938385
1	-1.747602	-2.850385	-1.429604
1	-5.898411	-3.165845	-0.335318
8	6.163594	-3.296660	0.396191
6	7.229537	-4.138413	0.790040
1	7.398128	-4.820818	-0.043425
1	8.147975	-3.569215	0.976927
1	6.973485	-4.720601	1.682775
1	-0.027104	6.495071	-1.278930
6	-0.971994	5.292156	1.007033
1	-1.124612	6.373635	1.068402
1	-1.077717	4.836856	1.987035
1	0.055166	5.121722	0.668405

[6-7]TS_anti

Number of imaginary frequencies : 1
The smallest frequency is : -1268.8807 cm(-1)

Electronic energy : =-3046.0829463
Zero-point correction= 0.805222
Thermal correction to Energy= 0.855029
Thermal correction to Enthalpy= 0.855973
Thermal correction to Gibbs Free Energy= 0.719372
Sum of electronic and zero-point Energies= -3045.277724
Sum of electronic and thermal Energies= -3045.227918
Sum of electronic and thermal Enthalpies= -3045.226973
Sum of electronic and thermal Free Energies= -3045.363574

Cartesian Coordinates

6	-4.470058	1.813186	0.240072

6	-3.768952	2.892911	-0.592682
7	-2.942111	3.630568	0.384121
6	-3.035546	3.002036	1.711264
6	-4.411672	2.346748	1.674099
6	-2.093577	4.590899	0.040230
6	-1.784810	4.833806	-1.321852
6	-1.015920	6.068331	-1.754267
6	-1.899348	1.945175	1.874740
8	-2.139632	0.934005	2.543039
8	-0.796258	2.208318	1.291957
1	-2.930611	3.748584	2.502706
1	-4.494592	1.560964	2.424043
1	-5.189058	3.097605	1.844812
1	-3.909139	0.875576	0.179122
1	-5.484630	1.618004	-0.109514
1	-3.135119	2.467773	-1.376801
1	-4.472567	3.594263	-1.054242
1	-1.013028	3.666188	-1.376965
1	-0.763346	2.304701	-0.314775
8	-0.597759	2.479986	-1.284874
1	-0.815171	6.012500	-2.827172
1	-1.565848	7.000078	-1.577449
1	0.412264	2.273266	-1.405792
1	-2.558495	4.529221	-2.026415
7	-1.094580	-0.876513	0.474198
6	-2.245553	-1.592722	0.132137
6	-3.307501	-1.527964	1.044805
6	-4.529262	-2.111014	0.739153
6	-4.729445	-2.800215	-0.449929
6	-3.662590	-2.872144	-1.338981
6	-2.436558	-2.270543	-1.078421
6	-5.664755	-1.887970	1.693791
9	-6.124249	-0.621972	1.609650
6	-3.823282	-3.652606	-2.612908
9	-3.076885	-3.151612	-3.607792
6	0.175386	-0.924967	-0.039647
16	0.790174	-2.180966	-0.987073
7	0.894508	0.157643	0.321373
6	2.331929	0.285238	0.183423
6	2.725177	1.676947	-0.356406
6	4.250353	1.735754	-0.651858
6	4.461456	2.052636	-2.140659
6	3.863986	3.437006	-2.424496
6	2.381816	3.416073	-1.977655
7	1.962215	2.058231	-1.569438
6	2.205578	1.119501	-2.680935
6	3.724181	1.028733	-3.025943
6	4.229662	-0.390660	-2.943376
6	5.399879	-0.795906	-2.455294
6	3.016973	0.049352	1.528246
6	4.047459	-0.927214	1.708138
6	4.631098	-1.027503	3.006586
7	4.244095	-0.261110	4.065235
6	3.280857	0.603386	3.865471
6	2.640690	0.795792	2.617423
6	5.663836	-1.971864	3.222252
6	6.113115	-2.782807	2.211781
6	5.527385	-2.684456	0.923689
6	4.512687	-1.782549	0.683267
9	-6.703781	-2.697085	1.449756
9	-5.297255	-2.072051	2.968848
9	-5.098377	-3.661191	-3.033974
9	-3.457626	-4.934888	-2.459475
1	2.453501	2.420629	0.404019
1	4.730801	2.505514	-0.039755

1	4.722528	0.783555	-0.396609
1	1.712571	3.737877	-2.782933
1	2.209285	4.078110	-1.122712
1	3.943782	3.669268	-3.491167
1	4.419207	4.206920	-1.880403
1	5.530038	2.051844	-2.376047
1	3.848713	1.349806	-4.069664
1	1.624416	1.481784	-3.534251
1	1.795424	0.142714	-2.404992
1	3.548024	-1.140759	-3.347335
1	5.669391	-1.847466	-2.448641
1	6.127282	-0.106507	-2.033956
1	2.647791	-0.475964	-0.530000
1	1.842294	1.530714	2.543701
1	4.084280	-1.765801	-0.311572
1	2.974101	1.202012	4.720988
1	6.087198	-2.030248	4.219755
1	6.904973	-3.496178	2.407015
1	0.403020	0.879085	0.863396
1	-1.229605	-0.263824	1.284803
1	-3.178798	-0.982114	1.975843
1	-1.641330	-2.323995	-1.808221
1	-5.684341	-3.257335	-0.680458
8	5.913673	-3.447630	-0.130747
6	6.905322	-4.432615	0.085819
1	7.041802	-4.937349	-0.870798
1	7.858559	-3.986655	0.393241
1	6.586726	-5.166449	0.835161
1	-0.046118	6.156021	-1.256399
6	-1.352133	5.284283	1.146769
1	-2.064019	5.692600	1.870238
1	-0.705427	4.570154	1.663305
1	-0.752219	6.106346	0.762441

7_anti

Number of imaginary frequencies : 0

Electronic energy : =-3046.1024635
Zero-point correction= 0.809980
Thermal correction to Energy= 0.861142
Thermal correction to Enthalpy= 0.862086
Thermal correction to Gibbs Free Energy= 0.720450
Sum of electronic and zero-point Energies= -3045.292483
Sum of electronic and thermal Energies= -3045.241322
Sum of electronic and thermal Enthalpies= -3045.240378
Sum of electronic and thermal Free Energies= -3045.382014

Cartesian Coordinates

6	-4.277869	2.225942	0.284875
6	-3.620861	3.337164	-0.540761
7	-2.609340	3.893869	0.351153
6	-2.601858	3.213501	1.644222
6	-4.023485	2.657851	1.730998
6	-1.766593	4.902820	-0.050500
6	-1.769517	5.386826	-1.321670
6	-0.924633	6.540387	-1.804532
6	-1.546046	2.079203	1.692953
8	-1.812417	1.028560	2.299613
8	-0.446423	2.300629	1.078264
1	-2.376706	3.912535	2.456978

1	-4.097708	1.840345	2.447958
1	-4.712972	3.457410	2.020083
1	-3.770393	1.272588	0.096167
1	-5.334486	2.095102	0.046276
1	-3.164680	2.948105	-1.460421
1	-4.335011	4.122872	-0.827646
1	-0.803406	3.330009	-1.769771
1	-0.697669	2.414879	-0.544732
8	-0.610429	2.405947	-1.534139
1	-0.992098	6.623961	-2.892526
1	-1.243743	7.507541	-1.394860
1	0.894599	1.863295	-1.633598
1	-2.496714	4.995788	-2.026721
7	-1.173518	-0.959142	0.367033
6	-2.357929	-1.655233	0.107024
6	-3.429756	-1.347649	0.957126
6	-4.676238	-1.918235	0.746992
6	-4.897016	-2.816596	-0.289200
6	-3.823657	-3.119605	-1.119526
6	-2.564677	-2.554026	-0.946105
6	-5.795934	-1.493651	1.651746
9	-6.106253	-0.195512	1.473484
6	-4.016559	-4.128355	-2.216531
9	-3.195397	-3.909808	-3.253479
6	0.080284	-1.060617	-0.155399
16	0.684895	-2.362394	-1.047974
7	0.815180	0.039120	0.138691
6	2.257840	0.116985	0.076446
6	2.681527	1.471240	-0.527637
6	4.197527	1.537160	-0.823747
6	4.423792	1.739996	-2.329874
6	3.828871	3.097408	-2.728069
6	2.346983	3.123503	-2.307015
7	1.944070	1.770294	-1.805231
6	2.186853	0.739231	-2.857075
6	3.709239	0.647675	-3.150741
6	4.219994	-0.759776	-2.955660
6	5.387826	-1.114860	-2.426274
6	2.878271	-0.001563	1.468100
6	3.963565	-0.887419	1.757608
6	4.487468	-0.856287	3.084705
7	3.993211	-0.054752	4.069806
6	2.978623	0.716948	3.770432
6	2.390001	0.782338	2.484493
6	5.576366	-1.700072	3.411120
6	6.130304	-2.544038	2.483451
6	5.597970	-2.584778	1.169291
6	4.535795	-1.777646	0.819743
9	-6.914816	-2.199230	1.441157
9	-5.469826	-1.629639	2.945228
9	-5.273106	-4.112900	-2.689882
9	-3.780152	-5.379101	-1.789718
1	2.368104	2.264122	0.160752
1	4.655049	2.361378	-0.269727
1	4.676117	0.615624	-0.485268
1	1.674645	3.359492	-3.134456
1	2.147022	3.827230	-1.495352
1	3.920646	3.247986	-3.807231
1	4.370984	3.907535	-2.234414
1	5.494252	1.727989	-2.550084
1	3.851487	0.894739	-4.211058
1	1.609743	1.052089	-3.729741
1	1.768545	-0.205372	-2.497754
1	3.551401	-1.541382	-3.317836
1	5.668192	-2.160182	-2.345536

1	6.104211	-0.392312	-2.043493
1	2.604308	-0.696624	-0.563232
1	1.544774	1.449098	2.322730
1	4.152891	-1.866626	-0.189999
1	2.584061	1.341671	4.569344
1	5.955515	-1.654463	4.426750
1	6.963257	-3.177432	2.763743
1	0.340272	0.813907	0.638946
1	-1.280524	-0.261605	1.118740
1	-3.279283	-0.636408	1.766748
1	-1.758718	-2.803385	-1.621377
1	-5.872892	-3.259888	-0.447894
8	6.082802	-3.394641	0.193742
6	7.113039	-4.303751	0.533356
1	7.316435	-4.878831	-0.370244
1	8.027918	-3.781996	0.837725
1	6.798844	-4.987207	1.330302
1	0.138539	6.427494	-1.562034
6	-0.857366	5.458683	1.013583
1	-1.446046	5.942041	1.801168
1	-0.267881	4.659638	1.470277
1	-0.181589	6.207360	0.601099

6_syn

Number of imaginary frequencies : 0

Electronic energy : =-3046.105234
Zero-point correction= 0.809457
Thermal correction to Energy= 0.861073
Thermal correction to Enthalpy= 0.862017
Thermal correction to Gibbs Free Energy= 0.718308
Sum of electronic and zero-point Energies= -3045.295777
Sum of electronic and thermal Energies= -3045.244161
Sum of electronic and thermal Enthalpies= -3045.243217
Sum of electronic and thermal Free Energies= -3045.386926

Cartesian Coordinates

6	4.332713	-1.606328	2.625678
6	5.000459	-2.465786	1.552023
7	3.924724	-3.386766	1.099323
6	2.697929	-3.188995	1.898814
6	3.220591	-2.508623	3.166695
6	3.985804	-4.128886	0.044097
6	2.771460	-4.896293	-0.389111
6	2.934939	-5.747134	-1.641839
6	1.750081	-2.231258	1.127026
8	2.300308	-1.524845	0.236861
8	0.565735	-2.222130	1.492768
1	2.198452	-4.139652	2.083592
1	2.422477	-1.963455	3.672343
1	3.623881	-3.257354	3.855580
1	3.904629	-0.712440	2.166903
1	5.047127	-1.298036	3.389899
1	5.360794	-1.885547	0.701678
1	5.818169	-3.069210	1.958030
1	1.976834	-4.156788	-0.584918
8	0.866921	-2.821320	-1.849324
1	1.970579	-6.197280	-1.885480
1	3.233251	-5.139212	-2.499384
1	2.433156	-5.511375	0.453958

7	0.977121	0.895802	-0.281307
6	1.951862	1.883390	-0.397469
6	3.272257	1.429130	-0.217607
6	4.335432	2.311913	-0.254868
6	4.142648	3.672029	-0.488472
6	2.839731	4.107458	-0.676799
6	1.743242	3.246442	-0.632463
6	5.725856	1.775274	-0.086692
9	6.542750	2.666416	0.490706
6	2.567557	5.556583	-0.969461
9	3.652728	6.322687	-0.781219
6	-0.386795	0.913541	-0.387848
16	-1.324602	2.212471	-0.918516
7	-0.920696	-0.274974	-0.041249
6	-2.344485	-0.534073	0.048288
6	-2.595027	-2.046143	-0.133228
6	-4.110968	-2.351082	-0.291745
6	-4.340491	-3.000273	-1.666839
6	-3.576821	-4.332554	-1.700511
6	-2.091853	-4.036799	-1.362731
7	-1.841251	-2.589804	-1.276823
6	-2.245577	-1.954413	-2.537066
6	-3.778770	-2.107687	-2.791775
6	-4.457224	-0.771469	-2.963036
6	-5.648262	-0.410515	-2.489975
6	-2.904484	-0.088586	1.398454
6	-4.096115	0.691369	1.534730
6	-4.549267	0.964954	2.859719
7	-3.895255	0.545793	3.980361
6	-2.791816	-0.139657	3.810615
6	-2.261054	-0.484969	2.545379
6	-5.739683	1.710593	3.035641
6	-6.458114	2.174982	1.963873
6	-5.996266	1.915629	0.648142
6	-4.838084	1.197599	0.442938
9	5.746796	0.662960	0.677758
9	6.285723	1.437509	-1.259703
9	1.591520	6.047126	-0.191858
9	2.174641	5.736368	-2.240390
1	-2.190845	-2.552574	0.751906
1	-4.449680	-3.033808	0.494342
1	-4.702305	-1.436722	-0.197054
1	-1.414706	-4.442532	-2.121422
1	-1.803970	-4.473957	-0.400875
1	-3.669024	-4.791016	-2.690939
1	-4.008445	-5.031192	-0.976748
1	-5.408821	-3.177051	-1.825979
1	-3.908947	-2.651292	-3.738407
1	-1.659344	-2.425255	-3.332022
1	-1.948598	-0.900851	-2.507087
1	-3.894450	-0.047105	-3.554753
1	-6.050151	0.580445	-2.677025
1	-6.263605	-1.074834	-1.888276
1	-2.834904	0.019058	-0.754757
1	-1.342295	-1.065118	2.491551
1	-4.511482	1.049611	-0.579309
1	-2.273158	-0.461395	4.712395
1	-6.062901	1.902228	4.053722
1	-7.366757	2.740869	2.131784
1	-0.321099	-0.984125	0.399935
1	1.382261	-0.027534	-0.067964
1	3.444286	0.372200	-0.036179
1	0.741849	3.629977	-0.772427
1	4.976252	4.363503	-0.512455
8	-6.643941	2.345663	-0.467306

6	-7.794600	3.148606	-0.298578
1	-8.131046	3.407630	-1.302920
1	-8.596010	2.606305	0.217168
1	-7.566416	4.069625	0.250420
1	3.659363	-6.556023	-1.511311
6	5.233028	-4.145274	-0.772330
1	5.116020	-3.406569	-1.576567
1	6.120295	-3.885977	-0.196170
1	5.373567	-5.118924	-1.240816
1	-0.029984	-2.641070	-1.484788
1	1.428257	-2.168782	-1.406700

[6-7]TS_{syn}

Number of imaginary frequencies : 1
The smallest frequency is : -1164.7849 cm(-1)

Electronic energy : =-3046.0873217
Zero-point correction= 0.803543
Thermal correction to Energy= 0.854203
Thermal correction to Enthalpy= 0.855147
Thermal correction to Gibbs Free Energy= 0.713569
Sum of electronic and zero-point Energies= -3045.283779
Sum of electronic and thermal Energies= -3045.233119
Sum of electronic and thermal Enthalpies= -3045.232175
Sum of electronic and thermal Free Energies= -3045.373753

Cartesian Coordinates

6	4.414030	-2.563904	2.515973
6	4.678188	-3.326538	1.214928
7	3.364207	-3.893532	0.849293
6	2.349315	-3.613502	1.869494
6	3.184425	-3.259807	3.105675
6	3.060934	-4.376299	-0.348893
6	1.729402	-4.656500	-0.741125
6	1.459968	-5.547366	-1.945705
6	1.482425	-2.421052	1.414938
8	2.106009	-1.504396	0.791102
8	0.269821	-2.439362	1.679640
1	1.709922	-4.484020	2.030448
1	2.626906	-2.633710	3.805264
1	3.470954	-4.180921	3.622524
1	4.181679	-1.521967	2.289930
1	5.277593	-2.594282	3.182487
1	5.043801	-2.670984	0.420840
1	5.397761	-4.140265	1.359791
1	1.333220	-3.375584	-1.172569
8	0.947695	-2.262240	-1.540576
1	0.384414	-5.715481	-2.039147
1	1.792407	-5.090776	-2.883532
1	1.026339	-4.789405	0.081426
7	1.074386	1.003020	0.257402
6	2.108571	1.908443	0.014244
6	3.402610	1.367461	0.122284
6	4.513976	2.170116	-0.049906
6	4.388123	3.527115	-0.346296
6	3.108100	4.048389	-0.448806
6	1.965751	3.268614	-0.264844
6	5.890507	1.582758	0.060430
9	6.650165	2.263656	0.932408
6	2.915140	5.495468	-0.805237

9	4.040879	6.207567	-0.647190
6	-0.246426	1.004293	-0.084276
16	-1.054681	2.248399	-0.890853
7	-0.841212	-0.158750	0.265859
6	-2.257243	-0.438766	0.134627
6	-2.460162	-1.889203	-0.346736
6	-3.952029	-2.156600	-0.686342
6	-4.070491	-2.517518	-2.175044
6	-3.295076	-3.820124	-2.413235
6	-1.846288	-3.611736	-1.911050
7	-1.612418	-2.202692	-1.524075
6	-1.929523	-1.327047	-2.671226
6	-3.436122	-1.423378	-3.056494
6	-4.113799	-0.076282	-3.011668
6	-5.345547	0.183226	-2.578939
6	-2.989136	-0.232313	1.459319
6	-4.133834	0.617920	1.582892
6	-4.764130	0.680124	2.861871
7	-4.315901	-0.001164	3.954397
6	-3.248340	-0.745040	3.804360
6	-2.554422	-0.897098	2.579612
6	-5.915933	1.487899	3.019234
6	-6.434709	2.206137	1.972460
6	-5.799137	2.152165	0.705935
6	-4.670858	1.381967	0.521669
9	5.869596	0.302037	0.466678
9	6.538947	1.611570	-1.115397
9	1.966903	6.071283	-0.051963
9	2.534434	5.641922	-2.084087
1	-2.109587	-2.558069	0.447800
1	-4.340584	-2.979842	-0.078567
1	-4.556596	-1.275335	-0.455411
1	-1.110290	-3.862375	-2.682558
1	-1.628035	-4.227117	-1.031617
1	-3.303351	-4.072910	-3.478344
1	-3.772387	-4.645987	-1.877601
1	-5.121518	-2.654871	-2.445935
1	-3.490078	-1.771179	-4.097629
1	-1.284330	-1.643687	-3.496088
1	-1.642331	-0.302391	-2.414126
1	-3.512825	0.750976	-3.393057
1	-5.742439	1.193669	-2.592725
1	-6.000765	-0.587712	-2.180790
1	-2.653283	0.247913	-0.613262
1	-1.677639	-1.539558	2.540623
1	-4.205885	1.401159	-0.456178
1	-2.895996	-1.277734	4.686044
1	-6.374301	1.518118	4.002380
1	-7.318352	2.814406	2.125214
1	-0.320695	-0.851539	0.819792
1	1.420040	0.098366	0.613007
1	3.515642	0.309742	0.341306
1	0.982635	3.713337	-0.334996
1	5.261809	4.154861	-0.483388
8	-6.242317	2.836733	-0.381225
6	-7.362601	3.684802	-0.223770
1	-7.525845	4.150793	-1.195864
1	-8.260423	3.121816	0.057780
1	-7.174829	4.467508	0.520362
1	1.931152	-6.534157	-1.865977
6	4.188379	-4.487184	-1.334296
1	4.384813	-3.502027	-1.773716
1	5.106583	-4.826056	-0.850580
1	3.942200	-5.175667	-2.140461
1	-0.101864	-2.167562	-1.406278

1 1.383594 -1.698097 -0.865019

7_syn

Number of imaginary frequencies : 0

Electronic energy : =-3046.1068668
Zero-point correction= 0.810574
Thermal correction to Energy= 0.862190
Thermal correction to Enthalpy= 0.863134
Thermal correction to Gibbs Free Energy= 0.720598
Sum of electronic and zero-point Energies= -3045.296293
Sum of electronic and thermal Energies= -3045.244677
Sum of electronic and thermal Enthalpies= -3045.243733
Sum of electronic and thermal Free Energies= -3045.386269

Cartesian Coordinates

6	4.273730	-2.595560	2.528134
6	4.510685	-3.320853	1.192282
7	3.249834	-4.019790	0.920083
6	2.202192	-3.625820	1.843912
6	2.996035	-3.227961	3.094848
6	2.957030	-4.604706	-0.291961
6	1.693026	-4.922537	-0.680406
6	1.356813	-5.720664	-1.919934
6	1.388438	-2.438198	1.301136
8	2.065316	-1.462649	0.850089
8	0.136875	-2.495591	1.328865
1	1.519691	-4.460739	2.029920
1	2.437171	-2.551377	3.746098
1	3.230307	-4.133651	3.661950
1	4.110484	-1.533254	2.342016
1	5.123165	-2.701644	3.206188
1	4.751674	-2.600122	0.401656
1	5.334933	-4.040965	1.257269
1	1.459861	-2.962714	-1.537444
8	1.146937	-2.049234	-1.683240
1	0.308493	-6.031053	-1.892426
1	1.501010	-5.164701	-2.856599
1	0.867265	-4.669168	-0.021077
7	1.088712	1.045083	0.239719
6	2.134768	1.942471	0.012390
6	3.421264	1.390640	0.150750
6	4.541464	2.183118	-0.008930
6	4.431553	3.538870	-0.318419
6	3.158690	4.070154	-0.448596
6	2.006759	3.300395	-0.281057
6	5.911947	1.587249	0.133656
9	6.652775	2.263822	1.025673
6	2.982607	5.516291	-0.816609
9	4.116347	6.216692	-0.666277
6	-0.233079	1.078371	-0.075968
16	-1.047750	2.333848	-0.857013
7	-0.841866	-0.081381	0.275078
6	-2.258622	-0.347258	0.158178
6	-2.448808	-1.813065	-0.275206
6	-3.893657	-2.125797	-0.722708
6	-3.902418	-2.507621	-2.211911
6	-3.094122	-3.801859	-2.385442
6	-1.693086	-3.593838	-1.777518
7	-1.526075	-2.152009	-1.413853

6	-1.755421	-1.286790	-2.613358
6	-3.233092	-1.412317	-3.066634
6	-3.929028	-0.072032	-3.069649
6	-5.193574	0.163574	-2.729133
6	-2.998897	-0.130979	1.475237
6	-4.186851	0.659207	1.568630
6	-4.817682	0.730442	2.846765
7	-4.333429	0.109351	3.958850
6	-3.230351	-0.585893	3.833228
6	-2.530497	-0.741310	2.612383
6	-6.011032	1.480597	2.979892
6	-6.567718	2.134299	1.910901
6	-5.931872	2.071685	0.644332
6	-4.764802	1.355872	0.482548
9	5.873572	0.307496	0.534402
9	6.587898	1.619627	-1.026669
9	2.042113	6.109101	-0.066247
9	2.600215	5.656865	-2.095781
1	-2.118608	-2.461307	0.540768
1	-4.299994	-2.950916	-0.131319
1	-4.529337	-1.255177	-0.543177
1	-0.884054	-3.834595	-2.470846
1	-1.539549	-4.162176	-0.857057
1	-3.014877	-4.055451	-3.446335
1	-3.596573	-4.632429	-1.883930
1	-4.929236	-2.666706	-2.550626
1	-3.222692	-1.770324	-4.104352
1	-1.045498	-1.629328	-3.367673
1	-1.483165	-0.263920	-2.338324
1	-3.316299	0.762605	-3.412110
1	-5.607465	1.165531	-2.782077
1	-5.863275	-0.617746	-2.378035
1	-2.659551	0.318916	-0.607026
1	-1.627153	-1.347818	2.586022
1	-4.304214	1.365732	-0.498012
1	-2.851951	-1.070842	4.731096
1	-6.469887	1.519069	3.962435
1	-7.483547	2.697680	2.044419
1	-0.313297	-0.816348	0.770304
1	1.418944	0.130759	0.596142
1	3.521528	0.334818	0.386441
1	1.028984	3.752613	-0.374278
1	5.313084	4.157938	-0.444137
8	-6.412262	2.694011	-0.462770
6	-7.560732	3.508666	-0.323814
1	-7.740341	3.944970	-1.306650
1	-8.438431	2.922753	-0.026581
1	-7.396896	4.314509	0.400619
1	1.948819	-6.638919	-2.003518
6	4.155863	-4.916316	-1.148641
1	4.688687	-4.001516	-1.426681
1	4.861087	-5.553989	-0.605704
1	3.866040	-5.427242	-2.066068
1	-0.515318	-2.031505	-1.158266
1	1.587397	-1.578500	-0.949221

(3) Comparison of two possibilities (denoted here as path-A and path-B) for the first Michael Addition [8-9][‡] [Figs. 2 and S3 and Table S2]

si-si-PathA_TS

Number of imaginary frequencies : 1

The smallest frequency is : -223.9531 cm(-1)

Electronic energy : =-3483.6643243
Zero-point correction= 0.924658
Thermal correction to Energy= 0.982520
Thermal correction to Enthalpy= 0.983464
Thermal correction to Gibbs Free Energy= 0.829719
Sum of electronic and zero-point Energies= -3482.739666
Sum of electronic and thermal Energies= -3482.681804
Sum of electronic and thermal Enthalpies= -3482.680860
Sum of electronic and thermal Free Energies= -3482.834605

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 Cartesian Coordinates
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6	1.242934	5.006577	-1.585225
6	2.305101	4.557665	-2.590142
6	3.497044	4.200407	-1.699512
7	2.878793	3.795012	-0.430244
6	1.430933	3.997700	-0.441031
6	3.577720	3.403761	0.658133
6	2.966234	2.895283	1.790778
8	0.376583	-0.288710	3.441236
8	0.299502	1.090829	1.762723
1	1.095387	4.396098	0.520003
1	0.225346	4.983022	-1.979475
1	1.455638	6.018380	-1.224330
1	4.098305	3.388168	-2.119818
1	4.153597	5.066243	-1.540960
1	1.880812	2.915815	1.829398
6	3.677700	2.716801	3.103688
1	4.572893	2.088870	3.016635
1	3.010872	2.227256	3.819073
6	2.831013	0.669334	1.130719
1	2.147413	1.045470	0.378734
1	2.759625	-0.579629	2.956527
6	4.173799	0.343416	0.645069
6	4.453918	0.610652	-0.704803
6	5.152521	-0.266250	1.440688
6	5.683434	0.261432	-1.249703
1	3.675715	1.077072	-1.309435
6	6.382712	-0.613016	0.891090
1	4.950289	-0.480762	2.485727
6	6.647413	-0.356169	-0.452770
1	5.884110	0.448153	-2.299875
1	7.133039	-1.093550	1.510965
1	7.602636	-0.642745	-0.881822
7	0.939675	0.290814	2.499348
6	2.274398	0.072864	2.246734
7	0.306254	-0.734203	-0.860014
6	1.393112	-1.623540	-0.853358
6	1.702613	-2.411341	0.259904
6	2.897394	-3.116750	0.285135
6	3.795227	-3.073157	-0.779622
6	3.459514	-2.311746	-1.890142
6	2.271688	-1.586454	-1.934404
6	3.282993	-3.835710	1.543777
9	2.223102	-4.353779	2.176127
6	4.376663	-2.285046	-3.077042
9	4.063163	-3.234035	-3.973341
6	-0.965810	-0.966364	-0.455265
16	-1.599411	-2.512078	-0.152750
7	-1.668181	0.178883	-0.330294
6	-3.075418	0.286072	-0.013075
6	-3.219547	1.243204	1.187598
6	-4.659867	1.378901	1.726319

6	-4.707757	0.910203	3.189007
6	-3.795759	1.817418	4.030598
6	-2.379646	1.812154	3.419515
7	-2.333567	0.799355	2.320616
6	-2.702114	-0.545954	2.864542
6	-4.186617	-0.534922	3.309478
6	-4.991628	-1.580248	2.573963
6	-6.256009	-1.469286	2.174984
6	-3.879218	0.841528	-1.186050
6	-5.082725	0.225768	-1.656556
6	-5.769210	0.877017	-2.725176
7	-5.329129	2.026369	-3.312250
6	-4.211413	2.541674	-2.865718
6	-3.452315	1.990246	-1.805276
6	-6.970536	0.310229	-3.213829
6	-7.484645	-0.845065	-2.682770
6	-6.795873	-1.496016	-1.627811
6	-5.619661	-0.972888	-1.133021
9	4.146916	-4.834354	1.310021
9	3.885306	-3.005114	2.420353
9	5.656810	-2.489069	-2.729594
9	4.320763	-1.108817	-3.725630
1	-2.805740	2.211293	0.883740
1	-4.986790	2.420208	1.659673
1	-5.339351	0.784920	1.110607
1	-1.600298	1.522297	4.127135
1	-2.101998	2.769448	2.973373
1	-3.764677	1.459344	5.063430
1	-4.190602	2.836357	4.047764
1	-5.732047	0.969918	3.565663
1	-4.207164	-0.803249	4.374040
1	-2.010823	-0.728021	3.687429
1	-2.494417	-1.285728	2.087044
1	-4.463349	-2.515277	2.382666
1	-6.752065	-2.285350	1.658827
1	-6.840378	-0.565523	2.330384
1	-3.433816	-0.709773	0.253310
1	-2.530197	2.479508	-1.498232
1	-5.121575	-1.523350	-0.344252
1	-3.865147	3.454028	-3.348115
1	-7.471261	0.825245	-4.027050
1	-8.407030	-1.253328	-3.078236
1	-1.175082	1.084481	-0.464122
1	0.552661	0.238437	-1.150782
1	1.027935	-2.433098	1.108685
1	2.031540	-0.968347	-2.793784
1	4.734554	-3.612969	-0.736620
8	-7.232089	-2.644586	-1.048752
6	-8.369375	-3.280267	-1.600285
1	-8.502542	-4.201807	-1.032919
1	-9.269920	-2.663451	-1.496575
1	-8.216487	-3.529482	-2.656562
1	-1.333190	0.780121	1.993500
6	0.619376	2.721723	-0.753049
8	1.215479	1.792638	-1.359339
8	-0.591377	2.756438	-0.427077
1	3.987940	3.669643	3.549317
6	5.072707	3.527986	0.569438
1	5.561611	2.987448	1.379261
1	5.455305	3.133024	-0.374655
1	5.366608	4.582396	0.634434
1	2.558888	5.323204	-3.325689
1	1.959470	3.663887	-3.115081

si-si-PathA_TS-rev

Number of imaginary frequencies : 0

Electronic energy : =-3483.6719321
Zero-point correction= 0.924464
Thermal correction to Energy= 0.983729
Thermal correction to Enthalpy= 0.984673
Thermal correction to Gibbs Free Energy= 0.826101
Sum of electronic and zero-point Energies= -3482.747468
Sum of electronic and thermal Energies= -3482.688204
Sum of electronic and thermal Enthalpies= -3482.687259
Sum of electronic and thermal Free Energies= -3482.845831

Cartesian Coordinates

6 1.760723 4.085117 -2.995098
6 3.207443 3.614677 -3.165797
6 3.850959 4.057417 -1.855497
7 2.789370 3.803596 -0.889371
6 1.468600 3.841808 -1.499513
6 2.935382 3.924810 0.482962
6 1.878562 3.893631 1.326950
8 0.342563 0.713578 3.620089
8 0.299119 1.414361 1.578031
1 0.859252 4.648456 -1.071380
1 1.057204 3.559699 -3.645314
1 1.686578 5.155882 -3.210773
1 4.752349 3.485077 -1.613607
1 4.130538 5.123641 -1.898703
1 0.881980 3.780722 0.914445
6 1.980302 3.922676 2.829739
1 2.598170 3.108158 3.232577
1 0.987086 3.813206 3.274811
6 2.817779 0.668210 1.175429
1 2.243270 1.185451 0.407651
1 2.619569 -0.044773 3.239047
6 4.158081 0.256864 0.788627
6 4.613843 0.689732 -0.466863
6 4.970390 -0.573671 1.574281
6 5.874775 0.317720 -0.917694
1 3.944836 1.300980 -1.073122
6 6.223371 -0.953222 1.113078
1 4.610486 -0.945248 2.528513
6 6.676122 -0.507227 -0.129598
1 6.221635 0.644880 -1.892453
1 6.845927 -1.606191 1.716274
1 7.651953 -0.816923 -0.490492
7 0.877165 0.881980 2.530038
6 2.224217 0.442648 2.359338
7 0.408453 -0.841209 -0.539150
6 1.488368 -1.728089 -0.464554
6 1.750018 -2.552820 0.633201
6 2.937735 -3.274615 0.674992
6 3.874912 -3.211196 -0.351594
6 3.596301 -2.395152 -1.441128
6 2.423828 -1.652519 -1.501525
6 3.247559 -4.046210 1.923428
9 2.207586 -4.780115 2.339001
6 4.547500 -2.352562 -2.601330
9 4.231710 -3.266311 -3.534017
6 -0.878790 -1.000680 -0.155033
16 -1.543734 -2.436935 0.460044

7	-1.584713	0.142120	-0.314912
6	-3.011503	0.284113	-0.139211
6	-3.264039	1.536949	0.721516
6	-4.739714	1.745680	1.116361
6	-4.871000	1.725750	2.646937
6	-4.041204	2.881557	3.228608
6	-2.580185	2.743803	2.751719
7	-2.445298	1.465406	1.985324
6	-2.819453	0.308347	2.859604
6	-4.324274	0.402678	3.219793
6	-5.062566	-0.845846	2.798415
6	-6.295520	-0.909452	2.303175
6	-3.747030	0.445511	-1.466201
6	-4.908952	-0.322948	-1.792170
6	-5.551445	-0.034249	-3.032874
7	-5.100624	0.907884	-3.909160
6	-4.017533	1.568872	-3.583067
6	-3.307737	1.378408	-2.372237
6	-6.716639	-0.757897	-3.384392
6	-7.233905	-1.725061	-2.560968
6	-6.586004	-2.018168	-1.334205
6	-5.447269	-1.334788	-0.964471
9	4.290738	-4.872343	1.766980
9	3.557508	-3.217278	2.943943
9	5.811265	-2.606944	-2.227020
9	4.540209	-1.159165	-3.215722
1	-2.855235	2.399655	0.184133
1	-5.100239	2.700701	0.725225
1	-5.351750	0.958838	0.669850
1	-1.863308	2.684197	3.573167
1	-2.271094	3.546180	2.078280
1	-4.085538	2.862696	4.320992
1	-4.450619	3.839406	2.898613
1	-5.919006	1.848520	2.932169
1	-4.392428	0.466812	4.313701
1	-2.168377	0.373583	3.732385
1	-2.565590	-0.608355	2.319795
1	-4.509093	-1.774868	2.941687
1	-6.739093	-1.862732	2.032982
1	-6.904102	-0.025186	2.129902
1	-3.372831	-0.604764	0.379464
1	-2.416038	1.970786	-2.173973
1	-4.980605	-1.616478	-0.028381
1	-3.662947	2.310313	-4.296595
1	-7.186186	-0.519888	-4.333295
1	-8.126990	-2.261982	-2.857706
1	-1.091901	0.998206	-0.654382
1	0.664187	0.073613	-0.997983
1	1.043538	-2.603675	1.453445
1	2.233148	-0.986767	-2.337959
1	4.801138	-3.770910	-0.296058
8	-7.028639	-2.962843	-0.464131
6	-8.124013	-3.768412	-0.856061
1	-8.269852	-4.490173	-0.052173
1	-9.039417	-3.176929	-0.975833
1	-7.913033	-4.307282	-1.786870
1	-1.442341	1.368514	1.727261
6	0.697670	2.521555	-1.306498
8	1.340776	1.459519	-1.532006
8	-0.517532	2.598651	-0.989479
1	2.398929	4.859560	3.218086
6	4.354566	4.038508	0.971992
1	4.387758	4.135881	2.057160
1	4.938844	3.154410	0.692256
1	4.854024	4.911802	0.538557

1	3.698316	4.042274	-4.042984
1	3.233333	2.523276	-3.236422

si-si-PathA_TS-for

Number of imaginary frequencies : 0

Electronic energy : =-3483.6916382
 Zero-point correction= 0.927238
 Thermal correction to Energy= 0.984574
 Thermal correction to Enthalpy= 0.985518
 Thermal correction to Gibbs Free Energy= 0.833365
 Sum of electronic and zero-point Energies= -3482.764400
 Sum of electronic and thermal Energies= -3482.707064
 Sum of electronic and thermal Enthalpies= -3482.706120
 Sum of electronic and thermal Free Energies= -3482.858273

 Cartesian Coordinates

6	0.704010	5.305697	-0.871223
6	1.518603	5.331318	-2.166789
6	2.883492	4.779782	-1.744796
7	2.611950	4.001943	-0.506950
6	1.156118	3.990509	-0.240882
6	3.541795	3.447648	0.202028
6	3.213673	2.613917	1.402904
8	0.427667	-0.251971	3.044412
8	0.395979	1.337492	1.505464
1	0.954479	3.915798	0.826071
1	-0.373622	5.295420	-1.032283
1	0.965122	6.152028	-0.227723
1	3.327570	4.114790	-2.488654
1	3.594482	5.574033	-1.500329
1	2.224190	2.889730	1.770560
6	4.222243	2.769252	2.538797
1	5.215854	2.397357	2.277852
1	3.866010	2.193044	3.397008
6	3.019060	1.111695	0.938009
1	2.306348	1.163162	0.109561
1	2.845874	-0.419577	2.632767
6	4.290064	0.479733	0.415501
6	4.543539	0.525514	-0.960197
6	5.226668	-0.138295	1.249115
6	5.707922	-0.022341	-1.490549
1	3.799652	0.982554	-1.612797
6	6.387035	-0.699502	0.719184
1	5.045381	-0.196507	2.318468
6	6.631048	-0.641434	-0.650122
1	5.881328	0.004813	-2.561446
1	7.097093	-1.187992	1.379615
1	7.529628	-1.087635	-1.064525
7	1.072068	0.462151	2.210350
6	2.363981	0.335257	2.029159
7	0.369009	-0.725610	-0.960083
6	1.451368	-1.614143	-0.800465
6	1.722068	-2.202459	0.440169
6	2.869365	-2.968060	0.587445
6	3.759845	-3.162575	-0.468792
6	3.471470	-2.577277	-1.691945
6	2.322511	-1.807327	-1.866430
6	3.225584	-3.501169	1.943492
9	2.151144	-3.697172	2.713193

6	4.382905	-2.800659	-2.861857
9	4.014752	-3.865611	-3.593540
6	-0.914719	-0.958687	-0.581517
16	-1.508085	-2.500076	-0.190157
7	-1.660311	0.160908	-0.583743
6	-3.031628	0.266718	-0.137940
6	-3.080431	1.296207	1.011078
6	-4.485556	1.483068	1.626585
6	-4.450634	1.107435	3.115327
6	-3.477466	2.049561	3.841078
6	-2.103572	1.981568	3.145028
7	-2.127604	0.909241	2.105838
6	-2.480949	-0.389909	2.756197
6	-3.935741	-0.333870	3.287700
6	-4.796274	-1.408565	2.666662
6	-6.085115	-1.309734	2.351182
6	-3.963708	0.709279	-1.260639
6	-5.158935	-0.008834	-1.584164
6	-5.993425	0.538837	-2.603866
7	-5.690062	1.677362	-3.290175
6	-4.569613	2.284047	-2.985433
6	-3.677413	1.845205	-1.976459
6	-7.200839	-0.124127	-2.930534
6	-7.579846	-1.277150	-2.291592
6	-6.740375	-1.827941	-1.290957
6	-5.555358	-1.209870	-0.953310
9	3.891677	-4.664503	1.867478
9	4.031663	-2.648581	2.612812
9	5.652575	-3.013722	-2.482944
9	4.386770	-1.746781	-3.698092
1	-2.680226	2.237979	0.621212
1	-4.808786	2.521886	1.512360
1	-5.207880	0.858815	1.094970
1	-1.281478	1.716884	3.813184
1	-1.841773	2.908362	2.629392
1	-3.388301	1.756088	4.891257
1	-3.859457	3.073819	3.818209
1	-5.449756	1.205315	3.548753
1	-3.893874	-0.540944	4.365580
1	-1.743078	-0.528102	3.543296
1	-2.322873	-1.185053	2.024486
1	-4.285854	-2.355715	2.484640
1	-6.616431	-2.146239	1.907017
1	-6.653840	-0.395189	2.502122
1	-3.333389	-0.714735	0.228311
1	-2.767081	2.408517	-1.783123
1	-4.943353	-1.687383	-0.198707
1	-4.333519	3.185202	-3.548763
1	-7.817311	0.315263	-3.708061
1	-8.510770	-1.760875	-2.562721
1	-1.202640	1.067583	-0.776029
1	0.608811	0.219553	-1.292416
1	1.053346	-2.027052	1.279517
1	2.109024	-1.341001	-2.823134
1	4.661640	-3.749725	-0.332200
8	-7.036157	-2.967217	-0.611774
6	-8.205646	-3.675283	-0.974407
1	-8.226970	-4.563708	-0.343139
1	-9.110538	-3.083883	-0.790370
1	-8.179161	-3.984050	-2.025751
1	-1.104835	0.898216	1.743350
6	0.462555	2.788453	-0.940662
8	1.172809	1.991120	-1.588458
8	-0.779257	2.785801	-0.783154
1	4.314314	3.813650	2.851875

6	4.969478	3.641424	-0.204668
1	5.608167	2.887326	0.250947
1	5.099054	3.601589	-1.286954
1	5.300582	4.629235	0.142319
1	1.609801	6.326311	-2.604028
1	1.062555	4.668323	-2.906435

si-re-PathA_TS

Number of imaginary frequencies : 1
The smallest frequency is : -318.3379 cm(-1)

Electronic energy : =-3483.6585306
Zero-point correction= 0.925200
Thermal correction to Energy= 0.982821
Thermal correction to Enthalpy= 0.983766
Thermal correction to Gibbs Free Energy= 0.829968
Sum of electronic and zero-point Energies= -3482.733331
Sum of electronic and thermal Energies= -3482.675709
Sum of electronic and thermal Enthalpies= -3482.674765
Sum of electronic and thermal Free Energies= -3482.828562

Cartesian Coordinates

6	1.589469	-3.043845	3.248912
6	2.849589	-2.283540	3.667306
6	3.916541	-2.878757	2.754793
7	3.181059	-3.175754	1.516637
6	1.724080	-3.142163	1.719126
6	3.755220	-3.688418	0.415266
6	3.057410	-3.814427	-0.787230
8	0.302324	-0.520470	-2.110575
8	1.104481	-2.441400	-2.764064
1	1.286039	-4.058273	1.314184
1	0.667451	-2.539399	3.547115
1	1.588687	-4.049563	3.682107
1	2.724730	-1.221369	3.447495
1	3.097147	-2.410333	4.722947
1	4.744263	-2.193180	2.553974
1	4.328712	-3.804591	3.178610
1	1.987988	-3.617760	-0.769736
6	3.515698	-4.724741	-1.898288
1	3.454681	-5.784091	-1.623223
1	4.547278	-4.525734	-2.210158
6	3.526301	-1.866223	-1.699383
1	3.578804	-2.457109	-2.609817
1	2.377391	-0.144993	-0.949728
6	4.809961	-1.428914	-1.120319
6	6.009848	-1.755412	-1.760451
6	4.848983	-0.711948	0.085521
6	7.230399	-1.367908	-1.214478
1	5.981183	-2.308627	-2.695897
6	6.070510	-0.328261	0.628934
1	3.918508	-0.495693	0.609470
6	7.262785	-0.654877	-0.018932
1	8.154677	-1.619934	-1.724805
1	6.091127	0.236248	1.555020
1	8.213160	-0.348161	0.406538
7	1.250076	-1.356022	-2.172982
6	2.422723	-1.031287	-1.562149
7	0.077275	1.420744	0.301252
6	0.943724	2.507908	0.236202

6	0.692885	3.732528	-0.390078
6	1.684330	4.711612	-0.389985
6	2.923302	4.517345	0.203777
6	3.162057	3.288320	0.814516
6	2.197183	2.297700	0.839297
6	1.415953	5.997317	-1.120291
9	0.133278	6.371772	-1.028142
6	4.509006	3.025434	1.420444
9	4.956811	4.077305	2.122223
6	-1.241074	1.273790	0.002213
16	-2.332154	2.514068	-0.372956
7	-1.598033	-0.026531	0.050141
6	-2.940966	-0.540646	-0.069478
6	-2.901604	-1.822655	-0.923143
6	-4.307787	-2.314259	-1.333922
6	-4.450469	-2.247988	-2.862897
6	-3.438266	-3.219833	-3.488076
6	-2.032808	-2.893077	-2.946779
7	-2.096190	-1.613121	-2.175525
6	-2.651501	-0.521694	-3.033177
6	-4.130291	-0.831819	-3.382394
6	-5.055495	0.263760	-2.907482
6	-6.278616	0.105446	-2.407978
6	-3.539856	-0.889856	1.291624
6	-4.819884	-0.419323	1.720113
6	-5.287167	-0.874854	2.989384
7	-4.569275	-1.701958	3.801165
6	-3.389287	-2.086707	3.381294
6	-2.834684	-1.712661	2.134611
6	-6.560558	-0.450625	3.440125
6	-7.344185	0.384748	2.686000
6	-6.870859	0.846011	1.430700
6	-5.634119	0.454941	0.964299
9	2.164889	7.006486	-0.648265
9	1.695874	5.887678	-2.430420
9	5.436396	2.766547	0.483980
9	4.492030	1.967981	2.252137
1	-2.345129	-2.585540	-0.371158
1	-4.461585	-3.342991	-0.996021
1	-5.066808	-1.696204	-0.847828
1	-1.281023	-2.748748	-3.723401
1	-1.653129	-3.648852	-2.256579
1	-3.458315	-3.129811	-4.578061
1	-3.701470	-4.251137	-3.239508
1	-5.464992	-2.530668	-3.155932
1	-4.205275	-0.861777	-4.477413
1	-2.007925	-0.478507	-3.913758
1	-2.532624	0.418887	-2.487280
1	-4.662776	1.275105	-3.018303
1	-6.874129	0.962329	-2.109083
1	-6.732944	-0.872325	-2.268112
1	-3.551624	0.216412	-0.563993
1	-1.851795	-2.081827	1.848011
1	-5.305193	0.857581	0.013704
1	-2.822929	-2.739887	4.043172
1	-6.894618	-0.810619	4.407744
1	-8.313808	0.692778	3.058627
1	-0.861020	-0.747389	0.176121
1	0.543509	0.561016	0.644802
1	-0.262265	3.920578	-0.860173
1	2.390340	1.350525	1.335019
1	3.675941	5.298017	0.199355
8	-7.580572	1.677672	0.625667
6	-8.805605	2.191605	1.111992
1	-9.170955	2.875128	0.345318

1	-9.546206	1.397639	1.264385
1	-8.665562	2.744770	2.047823
1	-1.098552	-1.310460	-1.963854
6	1.025839	-1.944784	1.050124
8	1.457252	-0.799276	1.327052
8	0.029950	-2.222630	0.329353
1	2.873294	-4.570190	-2.769509
6	5.205938	-4.054408	0.537595
1	5.805565	-3.179793	0.812584
1	5.336601	-4.809748	1.320464
1	5.596745	-4.454728	-0.395398

re-si-PathA_TS

Number of imaginary frequencies : 1

The smallest frequency is : -246.3456 cm(-1)

Electronic energy : =-3483.6596173

Zero-point correction= 0.925037

Thermal correction to Energy= 0.983157

Thermal correction to Enthalpy= 0.984102

Thermal correction to Gibbs Free Energy= 0.828551

Sum of electronic and zero-point Energies= -3482.734580

Sum of electronic and thermal Energies= -3482.676460

Sum of electronic and thermal Enthalpies= -3482.675516

Sum of electronic and thermal Free Energies= -3482.831066

Cartesian Coordinates

6	1.821354	-3.022799	3.945597
6	3.029731	-2.083931	3.835050
6	3.694663	-2.469741	2.507283
7	2.684852	-3.248427	1.784766
6	1.401716	-3.266947	2.491349
6	2.872865	-3.701917	0.536283
6	4.044854	-3.444287	-0.169038
8	0.435144	-2.433991	-3.030192
6	0.507447	-2.133761	1.947718
8	-0.667467	-2.422026	1.616426
8	1.052766	-1.000708	1.890769
8	0.575782	-1.862375	-0.936672
1	0.899403	-4.227203	2.363553
1	1.007535	-2.601198	4.539835
1	2.115187	-3.976781	4.394470
1	2.694215	-1.048014	3.791059
1	3.717238	-2.193646	4.675896
1	3.979783	-1.585224	1.927115
1	4.591474	-3.086657	2.645508
6	4.435583	-4.238317	-1.383362
1	5.398247	-3.888447	-1.763967
1	3.703252	-4.144399	-2.195949
6	3.265042	-1.507631	-1.145115
1	2.755123	-1.203597	-0.230947
1	2.792509	-2.014829	-3.234008
6	4.616594	-0.957330	-1.371515
6	5.185413	-0.139534	-0.387881
6	5.343272	-1.201887	-2.544783
6	6.439391	0.430793	-0.570044
1	4.627006	0.058386	0.522173
6	6.603439	-0.641025	-2.722292
1	4.930620	-1.836665	-3.322736
6	7.154142	0.177836	-1.738828

1	6.851462	1.075857	0.198409
1	7.155005	-0.840865	-3.635553
1	8.134883	0.619578	-1.883930
7	1.111671	-2.059418	-2.054544
6	2.462467	-1.857627	-2.219590
7	0.300426	1.037651	0.273890
6	1.297637	2.008285	0.207810
6	1.339869	3.100457	-0.662197
6	2.428767	3.970938	-0.608273
6	3.480855	3.793025	0.276794
6	3.429201	2.692472	1.130837
6	2.364006	1.811184	1.103820
6	2.446157	5.119241	-1.577201
9	2.579245	4.695058	-2.844710
6	4.522609	2.496861	2.139282
9	4.361511	3.275477	3.218424
6	-1.000942	1.041569	-0.108134
16	-1.796139	2.259840	-0.973352
7	-1.620167	-0.095780	0.288197
6	-3.024021	-0.395976	0.122655
6	-3.143561	-1.874743	-0.290133
6	-4.560849	-2.276864	-0.750708
6	-4.528436	-2.676198	-2.234717
6	-3.640866	-3.920355	-2.389213
6	-2.266888	-3.635357	-1.752025
7	-2.182773	-2.179322	-1.411817
6	-2.447826	-1.345836	-2.630083
6	-3.914487	-1.549450	-3.088218
6	-4.684941	-0.250240	-3.099582
6	-5.970093	-0.092301	-2.793272
6	-3.818701	-0.173715	1.407199
6	-5.023580	0.596138	1.443689
6	-5.702418	0.678558	2.696324
7	-5.247718	0.087998	3.837421
6	-4.126195	-0.585005	3.764309
6	-3.379141	-0.749927	2.573185
6	-6.912886	1.408718	2.772380
6	-7.441215	2.034238	1.672160
6	-6.756309	1.963147	0.432301
6	-5.573037	1.264109	0.325805
9	1.308447	5.827492	-1.527252
9	3.456654	5.968315	-1.337520
9	5.730413	2.795049	1.629288
9	4.583564	1.226102	2.581509
1	-2.789687	-2.489693	0.542082
1	-4.925468	-3.116804	-0.152779
1	-5.248627	-1.442350	-0.590938
1	-1.425213	-3.840130	-2.415192
1	-2.117327	-4.175841	-0.814819
1	-3.524358	-4.165986	-3.448832
1	-4.104838	-4.780539	-1.900451
1	-5.540136	-2.898257	-2.583995
1	-3.878005	-1.909180	-4.124769
1	-1.719455	-1.671311	-3.371885
1	-2.225812	-0.306563	-2.371542
1	-4.111970	0.621734	-3.416982
1	-6.440932	0.884242	-2.847580
1	-6.600468	-0.916427	-2.468148
1	-3.412531	0.245446	-0.669560
1	-2.461351	-1.334460	2.590112
1	-5.075344	1.266995	-0.636101
1	-3.769329	-1.043126	4.684920
1	-7.408147	1.455284	3.736884
1	-8.371530	2.582670	1.760874
1	-1.100994	-0.790094	0.847843

1	0.568285	0.221134	0.866629
1	0.535996	3.270078	-1.365964
1	2.335476	0.954378	1.772218
1	4.317213	4.481678	0.299100
8	-7.202794	2.561643	-0.702477
6	-8.356602	3.375830	-0.618402
1	-8.498853	3.800291	-1.612463
1	-9.244864	2.792486	-0.348745
1	-8.222257	4.190913	0.101897
1	-1.199916	-1.991865	-1.105044
1	4.540337	-5.308278	-1.166344
6	1.769721	-4.499792	-0.102743
1	1.881562	-5.559285	0.157732
1	0.781933	-4.158181	0.207070
1	1.834514	-4.424015	-1.190692
1	4.854587	-2.960808	0.365411

re-re-PathA_TS

Number of imaginary frequencies : 1
The smallest frequency is : -306.7472 cm(-1)

Electronic energy : =-3483.6630997
Zero-point correction= 0.926735
Thermal correction to Energy= 0.984300
Thermal correction to Enthalpy= 0.985244
Thermal correction to Gibbs Free Energy= 0.832926
Sum of electronic and zero-point Energies= -3482.736365
Sum of electronic and thermal Energies= -3482.678800
Sum of electronic and thermal Enthalpies= -3482.677856
Sum of electronic and thermal Free Energies= -3482.830174

Cartesian Coordinates

6	2.499853	-1.722512	4.070291
6	3.497020	-0.732495	3.464859
6	4.079650	-1.512889	2.291613
7	2.993651	-2.416453	1.868228
6	1.880617	-2.403627	2.847999
6	3.212433	-3.404203	0.979731
6	4.385186	-3.425931	0.226964
8	0.869621	-0.401167	-0.511174
6	0.674692	-1.615226	2.274213
8	-0.197290	-2.275002	1.651011
8	0.658387	-0.382761	2.495200
8	1.399493	-2.431011	-1.073139
1	1.558677	-3.426069	3.054142
1	1.739236	-1.235893	4.681700
1	3.024220	-2.468827	4.676884
1	2.962872	0.150917	3.113217
1	4.276546	-0.422302	4.163651
1	4.395727	-0.878597	1.462214
1	4.938808	-2.121962	2.605897
1	5.218456	-2.835332	0.589973
6	3.968297	-1.850189	-1.304073
1	3.545728	-2.664716	-1.884083
1	3.279121	0.111525	-0.559144
6	5.357777	-1.472211	-1.633017
6	6.017015	-2.137394	-2.674117
6	6.034317	-0.452416	-0.950823
6	7.314602	-1.785399	-3.033456
1	5.498215	-2.925551	-3.213302

6	7.327589	-0.098058	-1.313271
1	5.545260	0.075733	-0.138647
6	7.973066	-0.763708	-2.354877
1	7.808755	-2.305661	-3.847853
1	7.832810	0.702500	-0.782108
1	8.983814	-0.485341	-2.635680
7	1.727704	-1.254220	-0.804346
6	3.060792	-0.904877	-0.852823
7	-0.365877	1.652505	0.965886
6	0.572635	2.624212	0.614786
6	0.268177	3.904161	0.145312
6	1.308630	4.787215	-0.129399
6	2.641401	4.440731	0.059185
6	2.923890	3.166580	0.542234
6	1.910385	2.263329	0.819151
6	1.000144	6.185836	-0.583114
9	-0.262276	6.321222	-1.004035
6	4.353880	2.742411	0.686547
9	5.114471	3.693214	1.244392
6	-1.505092	1.280210	0.330112
16	-2.332414	2.184496	-0.832819
7	-1.900652	0.046922	0.730007
6	-3.098177	-0.618542	0.277875
6	-2.805137	-2.109015	0.020348
6	-3.942878	-2.791930	-0.771522
6	-3.413413	-3.251189	-2.139016
6	-2.352092	-4.332205	-1.897989
6	-1.293646	-3.776249	-0.926315
7	-1.520560	-2.305188	-0.740879
6	-1.523798	-1.603735	-2.059008
6	-2.738862	-2.087884	-2.894487
6	-3.646466	-0.940550	-3.270838
6	-4.973886	-0.979127	-3.355071
6	-4.233054	-0.533702	1.296233
6	-5.552529	-0.107730	0.948082
6	-6.550218	-0.189140	1.965354
7	-6.291895	-0.599702	3.238844
6	-5.059292	-0.935035	3.528879
6	-4.000241	-0.927946	2.590023
6	-7.881081	0.176183	1.648417
6	-8.222907	0.610227	0.393390
6	-7.223669	0.712973	-0.608582
6	-5.918591	0.364971	-0.332852
9	1.183353	7.075631	0.408645
9	1.805588	6.567392	-1.588517
9	4.909754	2.455056	-0.505001
9	4.481722	1.631248	1.439828
1	-2.617815	-2.598685	0.979318
1	-4.323644	-3.655201	-0.218386
1	-4.774208	-2.093153	-0.893382
1	-0.273750	-3.882761	-1.290338
1	-1.352638	-4.216654	0.071136
1	-1.886900	-4.619328	-2.845555
1	-2.812486	-5.227969	-1.473325
1	-4.231998	-3.658195	-2.738333
1	-2.341531	-2.499153	-3.831934
1	-0.562916	-1.841103	-2.518228
1	-1.545214	-0.529523	-1.857656
1	-3.132776	-0.009464	-3.511827
1	-5.539757	-0.102219	-3.653162
1	-5.550655	-1.871614	-3.124773
1	-3.398543	-0.141719	-0.657076
1	-3.008493	-1.244886	2.904063
1	-5.185503	0.492574	-1.120396
1	-4.863703	-1.247605	4.552941

1	-8.621524	0.100436	2.438046
1	-9.249968	0.881352	0.179921
1	-1.277991	-0.479500	1.347859
1	0.040617	0.900179	1.549529
1	-0.761184	4.200389	-0.002196
1	2.126440	1.260966	1.179547
1	3.437939	5.143940	-0.162043
8	-7.475443	1.147100	-1.869813
6	-8.789286	1.567721	-2.181534
1	-8.761897	1.894808	-3.221134
1	-9.511510	0.748415	-2.084893
1	-9.103960	2.408057	-1.552149
1	-0.731799	-1.949020	-0.163097
6	4.751171	-4.609121	-0.629613
1	3.992680	-4.825281	-1.391784
1	5.693330	-4.417031	-1.149688
1	4.886786	-5.525601	-0.042259
6	2.151810	-4.458859	0.822444
1	2.326463	-5.263733	1.548560
1	1.156699	-4.040864	0.978579
1	2.199286	-4.893404	-0.175789

si-si-PathB_TS

Number of imaginary frequencies : 1

The smallest frequency is : -295.2974 cm(-1)

Electronic energy : =-3483.6563608

Zero-point correction= 0.922881

Thermal correction to Energy= 0.980980

Thermal correction to Enthalpy= 0.981924

Thermal correction to Gibbs Free Energy= 0.827041

Sum of electronic and zero-point Energies= -3482.733480

Sum of electronic and thermal Energies= -3482.675381

Sum of electronic and thermal Enthalpies= -3482.674437

Sum of electronic and thermal Free Energies= -3482.829320

Cartesian Coordinates

6	-3.077108	1.590896	2.377192
6	-3.941697	0.750486	3.318692
6	-4.831414	-0.035964	2.355906
7	-3.987669	-0.203542	1.161996
6	-2.768914	0.600447	1.240621
6	-4.401626	-0.794383	0.023879
6	-3.527112	-1.047740	-1.029394
8	-0.456525	-1.631799	-0.947816
6	-1.528101	-0.214517	1.608195
8	-0.425593	0.386691	1.234687
8	-1.587212	-1.255053	2.241765
8	0.047305	-3.025625	-2.547367
1	-2.596255	1.108295	0.290929
1	-2.168598	1.985526	2.836385
1	-3.647934	2.432591	1.971345
1	-3.312088	0.062154	3.888868
1	-4.526784	1.352083	4.016055
1	-5.132583	-1.009431	2.753692
1	-5.736277	0.530034	2.100890
1	-2.544179	-0.586872	-0.973745
6	-2.668580	-2.933612	-0.321186
1	-2.165224	-2.380823	0.463132
1	-2.085093	-4.146729	-2.081392

6	-3.822179	-3.726695	0.136443
6	-4.163331	-3.653920	1.495032
6	-4.591179	-4.524269	-0.719383
6	-5.250739	-4.367070	1.987375
1	-3.557394	-3.028736	2.148317
6	-5.686333	-5.226756	-0.225283
1	-4.334889	-4.593039	-1.773035
6	-6.018209	-5.150467	1.125804
1	-5.499582	-4.314491	3.043044
1	-6.280284	-5.840290	-0.895318
1	-6.869872	-5.705070	1.507191
7	-0.716614	-2.659551	-1.646932
6	-1.873380	-3.348489	-1.386656
7	0.154814	1.226676	-1.583036
6	-0.898255	2.124494	-1.389783
6	-2.027819	1.946269	-2.199393
6	-3.180551	2.682037	-1.960689
6	-3.236167	3.628995	-0.943355
6	-2.100564	3.811415	-0.161844
6	-0.939692	3.073553	-0.362513
6	-4.427559	2.399881	-2.746770
9	-5.293653	1.648440	-2.035895
6	-2.134433	4.814131	0.957668
9	-1.369942	4.430515	1.991713
6	1.399784	1.232400	-0.985373
16	2.289164	2.628118	-0.671189
7	1.818681	-0.013692	-0.734797
6	3.078555	-0.407667	-0.143002
6	2.781971	-1.325355	1.064222
6	4.076152	-1.723153	1.822541
6	3.946903	-1.293489	3.290731
6	2.743982	-2.024473	3.902880
6	1.487968	-1.699638	3.056153
7	1.804689	-0.712348	1.999368
6	2.349447	0.507278	2.632570
6	3.681776	0.220731	3.384886
6	4.794620	1.112182	2.892235
6	6.064223	0.769031	2.686763
6	3.938985	-1.148095	-1.161366
6	5.324146	-0.850593	-1.362310
6	6.029952	-1.647016	-2.312512
7	5.448475	-2.647033	-3.034359
6	4.172446	-2.868445	-2.839121
6	3.377058	-2.148708	-1.914597
6	7.405795	-1.394475	-2.530082
6	8.067673	-0.403583	-1.851367
6	7.360881	0.395413	-0.917297
6	6.019376	0.177727	-0.684764
9	-5.078856	3.524815	-3.070945
9	-4.176784	1.733456	-3.881610
9	-3.383718	4.981748	1.428052
9	-1.698707	6.021302	0.573970
1	2.282521	-2.219841	0.671084
1	4.231089	-2.804967	1.765927
1	4.947773	-1.250566	1.363251
1	0.679547	-1.280772	3.661015
1	1.083177	-2.586755	2.561772
1	2.603120	-1.707778	4.941501
1	2.930418	-3.102649	3.914673
1	4.858553	-1.550226	3.838594
1	3.525472	0.461567	4.445836
1	1.577581	0.874919	3.315770
1	2.477322	1.270210	1.858238
1	4.500434	2.146157	2.703122
1	6.789129	1.493131	2.328364

1	6.429952	-0.241919	2.848799
1	3.581296	0.501333	0.190602
1	2.320417	-2.398686	-1.837750
1	5.525850	0.825425	0.030153
1	3.714188	-3.660450	-3.428540
1	7.918556	-2.015263	-3.257530
1	9.120833	-0.233958	-2.040709
1	1.137945	-0.765243	-0.879576
1	-0.168608	0.297209	-1.843939
1	-2.006235	1.207465	-2.995781
1	-0.093273	3.191629	0.300471
1	-4.141100	4.197335	-0.758029
8	7.937896	1.402565	-0.211270
6	9.301082	1.690179	-0.454810
1	9.550032	2.535940	0.186508
1	9.945694	0.842052	-0.195328
1	9.472579	1.971717	-1.500280
1	0.437698	-0.165745	1.473878
6	-4.000286	-1.405292	-2.411711
1	-3.137661	-1.618089	-3.049988
1	-4.633442	-2.300078	-2.417555
1	-4.567101	-0.593643	-2.878203
6	-5.839488	-1.214829	-0.028125
1	-6.045102	-1.814295	-0.912742
1	-6.116890	-1.799247	0.853595
1	-6.478368	-0.324407	-0.060407

si-re-PathB_TS

Number of imaginary frequencies : 1

The smallest frequency is : -319.3037 cm(-1)

Electronic energy : =-3483.6553098

Zero-point correction= 0.925997

Thermal correction to Energy= 0.983670

Thermal correction to Enthalpy= 0.984614

Thermal correction to Gibbs Free Energy= 0.830836

Sum of electronic and zero-point Energies= -3482.729313

Sum of electronic and thermal Energies= -3482.671640

Sum of electronic and thermal Enthalpies= -3482.670696

Sum of electronic and thermal Free Energies= -3482.824474

 Cartesian Coordinates

6	-3.652169	0.919513	2.285408
6	-4.685258	-0.034663	2.890197
6	-5.571054	-0.383220	1.695319
7	-4.664052	-0.285009	0.540326
6	-3.366733	0.294236	0.909266
6	-5.065696	-0.435422	-0.733331
6	-4.168717	-0.427457	-1.802733
8	-0.141693	-2.328317	-1.484432
6	-2.237617	-0.751242	1.028406
8	-1.149946	-0.452835	0.440846
8	-2.443113	-1.761298	1.722454
8	-1.447279	-1.331808	-2.911939
1	-3.091677	1.040774	0.159306
1	-2.747678	1.012942	2.892306
1	-4.079832	1.917464	2.148605
1	-4.182521	-0.932998	3.251526
1	-5.258362	0.416180	3.702546
1	-6.001500	-1.386886	1.760752

1	-6.389903	0.338966	1.585793
1	-3.142213	-0.139025	-1.595625
6	-3.632567	-2.541236	-1.895262
1	-3.670998	-2.380596	-2.969880
1	-2.148474	-3.168355	-0.398144
6	-4.767103	-3.276620	-1.302536
6	-5.796721	-3.743541	-2.126495
6	-4.851203	-3.484489	0.082873
6	-6.888702	-4.416059	-1.584392
1	-5.733496	-3.583783	-3.200099
6	-5.944831	-4.156369	0.619336
1	-4.077705	-3.084669	0.737094
6	-6.965340	-4.624209	-0.209886
1	-7.677402	-4.778248	-2.236312
1	-6.002625	-4.315315	1.692266
1	-7.815567	-5.148167	0.215628
7	-1.294299	-2.093691	-1.946630
6	-2.365712	-2.692483	-1.341767
7	0.398830	1.637507	-0.545600
6	0.055500	2.977983	-0.317429
6	0.761410	4.043998	-0.887020
6	0.319601	5.340145	-0.670581
6	-0.823100	5.612723	0.084150
6	-1.511034	4.545579	0.636908
6	-1.071151	3.237197	0.455537
6	1.034012	6.494592	-1.314145
9	1.151802	7.531261	-0.468955
6	-2.749299	4.753792	1.456055
9	-3.813140	4.142157	0.898474
6	1.622569	1.071527	-0.307240
16	2.952149	1.892271	0.323319
7	1.618523	-0.249425	-0.581440
6	2.660674	-1.166236	-0.165452
6	2.027219	-2.474512	0.351400
6	3.010399	-3.324783	1.187644
6	2.486107	-3.455451	2.626379
6	1.152545	-4.217109	2.588185
6	0.204098	-3.515758	1.595844
7	0.807321	-2.204905	1.191798
6	1.108603	-1.383839	2.401954
6	2.220845	-2.066034	3.239350
6	3.431166	-1.173526	3.384976
6	4.705299	-1.557651	3.393307
6	3.621275	-1.502493	-1.300317
6	5.041553	-1.452130	-1.148575
6	5.827197	-1.833465	-2.276458
7	5.291109	-2.222050	-3.467788
6	3.984690	-2.240248	-3.567123
6	3.107173	-1.894322	-2.511370
6	7.238689	-1.813809	-2.164209
6	7.858646	-1.441225	-0.999170
6	7.074301	-1.056566	0.118597
6	5.698406	-1.056095	0.039046
9	2.262909	6.166333	-1.727235
9	0.363295	6.950767	-2.385806
9	-3.062185	6.046322	1.596011
9	-2.623547	4.231331	2.688075
1	1.647756	-3.037132	-0.501182
1	3.112747	-4.319756	0.745621
1	4.000529	-2.863519	1.175605
1	-0.778969	-3.278574	2.006232
1	0.068124	-4.076677	0.668293
1	0.708051	-4.243186	3.587672
1	1.318197	-5.251499	2.276035
1	3.208758	-4.000737	3.239297

1	1.816361	-2.224154	4.247690
1	0.160131	-1.297520	2.937384
1	1.396990	-0.386227	2.060000
1	3.206434	-0.114839	3.520764
1	5.503533	-0.834492	3.526347
1	5.007882	-2.593966	3.263924
1	3.200473	-0.676993	0.648003
1	2.031266	-1.946736	-2.667404
1	5.145659	-0.728476	0.911904
1	3.570508	-2.549434	-4.524937
1	7.813252	-2.105847	-3.037145
1	8.940685	-1.437103	-0.943736
1	0.818008	-0.656520	-1.073067
1	-0.378198	0.975239	-0.428802
1	1.641460	3.850823	-1.488297
1	-1.588822	2.410196	0.932388
1	-1.158891	6.632488	0.236577
8	7.606798	-0.673849	1.307914
6	9.014650	-0.583648	1.409593
1	9.220489	-0.223372	2.417912
1	9.493750	-1.560592	1.274970
1	9.426047	0.128024	0.684801
1	0.068937	-1.661243	0.661590
6	-4.614326	-0.203697	-3.225897
1	-3.749322	-0.309011	-3.885764
1	-5.367928	-0.930588	-3.550963
1	-5.035101	0.796226	-3.380776
6	-6.531815	-0.684751	-0.937070
1	-6.861968	-1.556315	-0.361482
1	-7.111509	0.181597	-0.598977
1	-6.760991	-0.861944	-1.985446

re-si-PathB_TS

Number of imaginary frequencies : 1
The smallest frequency is : -257.6648 cm(-1)

Electronic energy : =-3483.6524606
Zero-point correction= 0.923522
Thermal correction to Energy= 0.981561
Thermal correction to Enthalpy= 0.982505
Thermal correction to Gibbs Free Energy= 0.826015
Sum of electronic and zero-point Energies= -3482.728939
Sum of electronic and thermal Energies= -3482.670900
Sum of electronic and thermal Enthalpies= -3482.669956
Sum of electronic and thermal Free Energies= -3482.826445

Cartesian Coordinates

6	-2.547306	-1.207740	4.511896
6	-2.937420	-2.658286	4.216192
6	-3.771275	-2.549103	2.937851
7	-3.295179	-1.321132	2.296734
6	-2.307960	-0.619971	3.110578
6	-3.792056	-0.867063	1.131102
6	-4.734094	-1.589957	0.407398
8	-1.152029	-0.456644	-2.248182
6	-0.873296	-0.934550	2.673680
8	-0.097200	0.119685	2.721554
8	-0.513495	-2.066600	2.399067
8	-1.155711	-1.291186	-0.241337
1	-2.466531	0.459025	3.085885

1	-1.667268	-1.116515	5.152887
1	-3.375599	-0.671345	4.984352
1	-2.040773	-3.248987	4.021907
1	-3.497906	-3.120570	5.030606
1	-3.632658	-3.407251	2.272252
1	-4.845363	-2.455351	3.148146
6	-5.513183	-0.962331	-0.714437
1	-6.249155	-1.670504	-1.101944
1	-4.867093	-0.663441	-1.551247
6	-3.225389	-2.882227	-0.781414
1	-2.636140	-3.023499	0.121447
1	-2.991412	-1.960627	-2.775090
6	-4.186818	-3.945314	-1.119616
6	-4.308465	-5.039082	-0.252660
6	-4.976425	-3.909351	-2.276814
6	-5.189525	-6.075306	-0.534367
1	-3.692472	-5.076698	0.642507
6	-5.863408	-4.943717	-2.554203
1	-4.906031	-3.066514	-2.957902
6	-5.972457	-6.028260	-1.686054
1	-5.264821	-6.919778	0.143118
1	-6.471113	-4.904379	-3.452477
1	-6.664617	-6.834405	-1.907106
7	-1.618914	-1.246867	-1.403287
6	-2.665593	-2.071069	-1.752651
7	-0.013080	1.692419	-0.631530
6	-0.760611	2.864501	-0.678732
6	-0.462950	4.034639	0.033077
6	-1.351356	5.100022	-0.013768
6	-2.547479	5.043229	-0.725926
6	-2.828589	3.876375	-1.422095
6	-1.944812	2.805631	-1.421781
6	-1.065749	6.333636	0.795128
9	0.223509	6.433528	1.138057
6	-4.123448	3.703645	-2.159811
9	-4.861072	4.820600	-2.167182
6	1.273786	1.446021	-0.224979
16	2.492190	2.605128	-0.124832
7	1.435401	0.137076	0.053424
6	2.697877	-0.569607	0.156790
6	2.731072	-1.442299	1.427612
6	4.126426	-2.093025	1.621805
6	4.709470	-1.630752	2.966629
6	3.781241	-2.125782	4.084237
6	2.352470	-1.605127	3.792163
7	2.352102	-0.677737	2.637391
6	3.291129	0.427496	2.911836
6	4.755893	-0.092370	3.040241
6	5.673354	0.582286	2.050835
6	6.657231	0.013822	1.357108
6	2.895295	-1.457543	-1.069730
6	4.061077	-1.390931	-1.896314
6	4.132670	-2.298124	-2.995560
7	3.150944	-3.195831	-3.294388
6	2.091806	-3.210950	-2.524284
6	1.920741	-2.366021	-1.401927
6	5.277457	-2.273912	-3.828180
6	6.310649	-1.401596	-3.598548
6	6.233257	-0.496718	-2.509404
6	5.129899	-0.490979	-1.682692
9	-1.395362	7.450892	0.127445
9	-1.779349	6.346599	1.935428
9	-4.873527	2.734492	-1.597327
9	-3.930039	3.336461	-3.434910
1	1.951285	-2.206410	1.326179

1	4.042310	-3.184298	1.614089
1	4.792671	-1.817984	0.799792
1	1.939668	-1.056675	4.645291
1	1.656907	-2.412947	3.552098
1	4.137883	-1.763345	5.053953
1	3.789985	-3.219330	4.121856
1	5.713244	-2.044357	3.103061
1	5.118054	0.176956	4.042346
1	2.954966	0.900733	3.839291
1	3.195824	1.172751	2.117014
1	5.498622	1.651742	1.922252
1	7.268054	0.594827	0.672969
1	6.887382	-1.046039	1.431911
1	3.481639	0.186671	0.210126
1	1.006928	-2.447693	-0.816502
1	5.116104	0.229189	-0.873203
1	1.310867	-3.926211	-2.776624
1	5.306913	-2.972316	-4.658180
1	7.174108	-1.407375	-4.253029
1	0.591386	-0.438754	0.018143
1	-0.471465	0.889883	-1.067286
1	0.447212	4.104822	0.612358
1	-2.172974	1.906949	-1.991060
1	-3.233258	5.882337	-0.736501
8	7.209406	0.399496	-2.213051
6	8.335025	0.466755	-3.066640
1	8.968423	1.259257	-2.667261
1	8.898047	-0.474217	-3.067887
1	8.047775	0.721265	-4.093329
1	0.913012	-0.177300	2.584013
1	-6.054689	-0.063141	-0.397025
1	-5.182517	-2.455968	0.881304
6	-3.311746	0.459036	0.608320
1	-3.983481	1.260656	0.939441
1	-2.292862	0.696612	0.916791
1	-3.346729	0.453687	-0.484176

re-re-PathB_TS

Number of imaginary frequencies : 1

The smallest frequency is : -280.3740 cm(-1)

Electronic energy : =-3483.6537899

Zero-point correction= 0.923088

Thermal correction to Energy= 0.981208

Thermal correction to Enthalpy= 0.982152

Thermal correction to Gibbs Free Energy= 0.825462

Sum of electronic and zero-point Energies= -3482.730702

Sum of electronic and thermal Energies= -3482.672582

Sum of electronic and thermal Enthalpies= -3482.671638

Sum of electronic and thermal Free Energies= -3482.828328

Cartesian Coordinates

6	3.076209	-2.669539	-4.035506
6	3.721074	-3.753545	-3.166866
6	4.347989	-2.961937	-2.017860
7	3.574271	-1.708749	-1.945433
6	2.561904	-1.650597	-3.013226
6	4.029381	-0.632856	-1.269330
6	5.056267	-0.772779	-0.342189
8	0.613047	-2.201502	0.474987

6	1.192532	-2.078875	-2.463098
8	0.350892	-1.079887	-2.316060
8	0.944570	-3.244039	-2.222617
8	1.840558	-0.405235	0.580170
1	2.487548	-0.642725	-3.419894
1	2.275580	-3.051995	-4.671177
1	3.825844	-2.185457	-4.669275
1	2.951770	-4.427241	-2.791305
1	4.473922	-4.331706	-3.706001
1	4.312767	-3.491709	-1.063531
1	5.394331	-2.709052	-2.230642
1	5.657448	-1.673057	-0.395412
6	5.708254	0.414391	0.315538
1	6.199015	1.076564	-0.407572
1	6.474859	0.074727	1.016777
6	3.962359	-1.735179	1.396628
1	3.820619	-0.709384	1.721860
1	2.664166	-3.469704	0.941888
6	5.092346	-2.454631	2.013581
6	5.863252	-1.793344	2.977331
6	5.413289	-3.778582	1.684201
6	6.924214	-2.439803	3.603839
1	5.614558	-0.769726	3.244068
6	6.474425	-4.422420	2.308154
1	4.829532	-4.307600	0.935895
6	7.233009	-3.755139	3.269601
1	7.505791	-1.916166	4.355701
1	6.711698	-5.448414	2.045302
1	8.060620	-4.260987	3.756311
7	1.713198	-1.650346	0.667088
6	2.817491	-2.402325	0.990833
7	-0.131633	1.547208	-0.066841
6	0.455837	2.813049	-0.044920
6	-0.088840	3.975893	-0.596992
6	0.645607	5.159051	-0.549574
6	1.916561	5.224841	0.005453
6	2.448144	4.056697	0.542786
6	1.731067	2.871509	0.535372
6	0.038101	6.380407	-1.180833
9	-0.000989	6.272759	-2.519684
6	3.846767	4.034877	1.083665
9	4.719357	3.573156	0.163712
6	-1.437407	1.149872	-0.094737
16	-2.771731	2.175547	-0.215449
7	-1.539027	-0.192805	-0.013414
6	-2.786112	-0.924941	0.087305
6	-2.686449	-2.231741	-0.723982
6	-4.083235	-2.891996	-0.876155
6	-4.461750	-2.917275	-2.366359
6	-3.452457	-3.813823	-3.093719
6	-2.030094	-3.290544	-2.780789
7	-2.083257	-1.998298	-2.058783
6	-2.883840	-1.039406	-2.846607
6	-4.364122	-1.511121	-2.987401
6	-5.337092	-0.489832	-2.452855
6	-6.449637	-0.733630	-1.763574
6	-3.129017	-1.243289	1.541872
6	-4.392648	-0.920725	2.131842
6	-4.603672	-1.326686	3.483571
7	-3.665031	-1.973936	4.230520
6	-2.512881	-2.226242	3.661555
6	-2.200667	-1.886037	2.323432
6	-5.849441	-1.049563	4.096430
6	-6.849995	-0.399624	3.420859
6	-6.632567	0.016466	2.082882

6	-5.429427	-0.234753	1.458412
9	-1.223750	6.574821	-0.774863
9	0.730257	7.493222	-0.895637
9	3.961544	3.223152	2.147779
9	4.273205	5.248949	1.449408
1	-1.991503	-2.903963	-0.206437
1	-4.066595	-3.915733	-0.489555
1	-4.829347	-2.342165	-0.295624
1	-1.445747	-3.130304	-3.692145
1	-1.458636	-3.981827	-2.158934
1	-3.646328	-3.797002	-4.171390
1	-3.559460	-4.850259	-2.759435
1	-5.474358	-3.312773	-2.490216
1	-4.577177	-1.615540	-4.060573
1	-2.399370	-0.954161	-3.823977
1	-2.820771	-0.055385	-2.370726
1	-5.089650	0.546429	-2.688715
1	-7.093431	0.076203	-1.434559
1	-6.758007	-1.739296	-1.488958
1	-3.561867	-0.290262	-0.343334
1	-1.219446	-2.139431	1.928733
1	-5.304675	0.128326	0.445743
1	-1.767687	-2.736747	4.269189
1	-5.982509	-1.372422	5.123815
1	-7.793509	-0.203568	3.915968
1	-0.687550	-0.750717	0.088844
1	0.533834	0.794188	0.121902
1	-1.071039	3.956196	-1.050300
1	2.152751	1.974732	0.982370
1	2.471944	6.154593	0.022250
8	-7.566290	0.672283	1.345141
6	-8.787923	1.014307	1.969477
1	-9.366177	1.557642	1.221690
1	-9.348850	0.123799	2.277021
1	-8.627905	1.662955	2.838654
1	-0.602945	-1.455550	-2.078651
1	4.996140	1.030287	0.876972
6	3.399524	0.699647	-1.566021
1	3.793105	1.078845	-2.517961
1	2.312643	0.632552	-1.643284
1	3.655289	1.426849	-0.797708

Scheme 1(b) Details

Cartesian Coordinates of optimized geometries at the SMD_(toluene)/M06-2X/6-31G** Level of Theory

Stationary points relevant to Scheme 3 and 4, Figs. 1 and 5

Dicarbonyl compound (7-oxo-7-phenylhept-5-enal)

Number of imaginary frequencies : 0

Electronic energy=	-653.9768412
Zero-point correction=	0.240677
Thermal correction to Energy=	0.255128
Thermal correction to Enthalpy=	0.256072
Thermal correction to Gibbs Free Energy=	0.196558
Sum of electronic and zero-point Energies=	-653.736164
Sum of electronic and thermal Energies=	-653.721713
Sum of electronic and thermal Enthalpies=	-653.720769
Sum of electronic and thermal Free Energies=	-653.780283

 Cartesian Coordinates

6	4.938846	-0.221145	-0.520083
6	4.180486	-1.243038	0.285336
1	4.668225	-0.185629	-1.598849
1	4.474561	-1.150604	1.335017
6	2.668598	-1.073180	0.102630
6	2.163942	0.263227	0.664767
1	2.149806	-1.900513	0.597976
1	2.416377	-1.136625	-0.963555
1	2.429894	0.317285	1.728870
1	2.665029	1.102087	0.167107
6	0.679955	0.395916	0.517857
6	0.069155	1.376150	-0.154535
1	0.079637	-0.373867	1.003849
1	0.645178	2.184114	-0.601899
6	-1.403225	1.564997	-0.225794
8	-1.857559	2.688733	-0.358335
6	-2.329628	0.389194	-0.120817
6	-1.988964	-0.883222	-0.589305
6	-3.607751	0.612146	0.401003
6	-2.912974	-1.922496	-0.522012
1	-1.011888	-1.052873	-1.030351
6	-4.522009	-0.430100	0.484197
1	-3.864918	1.611644	0.736901
6	-4.174730	-1.699418	0.022485
1	-2.648475	-2.905392	-0.898793
1	-5.507820	-0.255240	0.903319
1	-4.891623	-2.512623	0.081430
8	5.775338	0.526088	-0.074199
1	4.483579	-2.234516	-0.075122

 trans- β -nitrostyrene

Number of imaginary frequencies : 0

Electronic energy=	-513.9497907
Zero-point correction=	0.138635
Thermal correction to Energy=	0.147647
Thermal correction to Enthalpy=	0.148591
Thermal correction to Gibbs Free Energy=	0.103123
Sum of electronic and zero-point Energies=	-513.811155
Sum of electronic and thermal Energies=	-513.802144
Sum of electronic and thermal Enthalpies=	-513.801200
Sum of electronic and thermal Free Energies=	-513.846668

 Cartesian Coordinates

8	-3.811807	-0.926976	0.000176
8	-3.243224	1.158472	0.000126
6	-0.617822	0.453308	-0.000084
1	-0.921660	1.497631	-0.000107
1	-1.500084	-1.535213	-0.000059
6	0.819347	0.178530	-0.000048
6	1.344155	-1.122553	-0.000110
6	1.701600	1.266034	0.000051
6	2.716571	-1.323994	-0.000072
1	0.676856	-1.978712	-0.000194
6	3.077177	1.062558	0.000093
1	1.300494	2.275751	0.000098
6	3.586510	-0.232511	0.000031
1	3.112328	-2.334348	-0.000125
1	3.749370	1.914237	0.000170
1	4.659531	-0.395387	0.000060
7	-2.978795	-0.033306	-0.000130
6	-1.591707	-0.458503	-0.000087

(S)-Proline

Number of imaginary frequencies : 0

Electronic energy= -401.0031889
Zero-point correction= 0.146558
Thermal correction to Energy= 0.154007
Thermal correction to Enthalpy= 0.154952
Thermal correction to Gibbs Free Energy= 0.113851
Sum of electronic and zero-point Energies= -400.856631
Sum of electronic and thermal Energies= -400.849182
Sum of electronic and thermal Enthalpies= -400.848237
Sum of electronic and thermal Free Energies= -400.889338

Cartesian Coordinates

6	-0.724841	-0.711330	1.075508
6	-1.741866	-0.903502	-0.053334
6	-2.011431	0.534529	-0.480638
7	-0.675193	1.137519	-0.450348
6	0.127360	0.485430	0.595634
6	1.452753	0.039031	0.003837
8	2.537184	0.452536	0.337418
8	1.299907	-0.892790	-0.952247
1	0.382883	1.158187	1.420091
1	-0.126462	-1.602183	1.279557
1	-1.240133	-0.431195	1.999198
1	-1.287438	-1.456353	-0.879761
1	-2.644137	-1.426402	0.271022
1	-2.441422	0.608677	-1.483883
1	-2.710513	1.009013	0.226516
1	2.187390	-1.107601	-1.280540
1	-0.702397	2.142306	-0.327174

(RR)-Cinchona-Thiourea

Number of imaginary frequencies : 0

Electronic energy= -2412.6833757
Zero-point correction= 0.544852
Thermal correction to Energy= 0.580303
Thermal correction to Enthalpy= 0.581247
Thermal correction to Gibbs Free Energy= 0.473713
Sum of electronic and zero-point Energies= -2412.138524
Sum of electronic and thermal Energies= -2412.103073
Sum of electronic and thermal Enthalpies= -2412.102129
Sum of electronic and thermal Free Energies= -2412.209663

Cartesian Coordinates

7	-1.813249	0.685511	0.688788
6	-3.096229	0.238353	0.335597
6	-3.434662	-1.108848	0.173600
6	-4.748728	-1.446443	-0.128262
6	-5.747827	-0.487398	-0.253895
6	-5.400394	0.844360	-0.067896
6	-4.092183	1.211841	0.218223
6	-5.094242	-2.891670	-0.360478
9	-4.277671	-3.717651	0.305725
6	-6.435058	1.920269	-0.237977
9	-7.671359	1.467673	0.006119

6	-0.576025	0.173767	0.388847
16	-0.287766	-1.216003	-0.502147
7	0.423196	0.937592	0.886174
6	1.832632	0.700411	0.614433
6	2.587657	1.980792	1.036913
6	4.063008	1.982708	0.559456
6	4.283287	3.222221	-0.322328
6	4.007898	4.472899	0.527028
6	2.563490	4.368169	1.091777
7	1.870490	3.182128	0.568132
6	1.855361	3.250363	-0.899258
6	3.295883	3.226295	-1.503038
6	3.461646	2.108382	-2.501127
6	4.501910	1.286893	-2.627878
6	2.373302	-0.492655	1.389989
6	3.276175	-1.443660	0.816560
6	3.781749	-2.461073	1.678951
7	3.437596	-2.574728	2.993532
6	2.590051	-1.698591	3.471930
6	2.037191	-0.641582	2.711409
6	4.690597	-3.412751	1.155594
6	5.084657	-3.380119	-0.157115
6	4.566374	-2.378539	-1.017113
6	3.680018	-1.437422	-0.538516
9	-6.349787	-3.166047	0.025301
9	-5.007406	-3.214773	-1.659928
9	-6.436186	2.414493	-1.486084
9	-6.212841	2.956183	0.586652
1	2.547805	2.025672	2.132584
1	4.740692	2.017754	1.418223
1	4.294765	1.069380	0.007568
1	1.968775	5.247426	0.826306
1	2.570830	4.294811	2.183883
1	4.121875	5.373062	-0.086279
1	4.737798	4.540099	1.339877
1	5.312668	3.241174	-0.693363
1	3.444947	4.166435	-2.052620
1	1.330887	4.170780	-1.173578
1	1.258039	2.417228	-1.285249
1	2.627678	1.994476	-3.196119
1	4.518575	0.519072	-3.395106
1	5.372107	1.338979	-1.978647
1	1.963091	0.529407	-0.459593
1	1.338218	0.046410	3.178025
1	3.306360	-0.702223	-1.241497
1	2.314982	-1.804499	4.519907
1	5.063886	-4.172293	1.834654
1	5.781682	-4.121883	-0.528324
1	0.231798	1.908645	1.129088
1	-1.811318	1.589806	1.145946
1	-2.685612	-1.879068	0.290695
1	-3.843680	2.260606	0.355746
1	-6.770750	-0.770778	-0.474391
8	4.896991	-2.279131	-2.330719
6	5.750594	-3.265025	-2.879171
1	5.850139	-3.022056	-3.937411
1	6.742865	-3.244709	-2.413040
1	5.321472	-4.268739	-2.781170

 (RR)-Cinchona-(S)-Proline-complex

Number of imaginary frequencies : 0

Electronic energy= -2813.7278194
 Zero-point correction= 0.692843
 Thermal correction to Energy= 0.736730
 Thermal correction to Enthalpy= 0.737674

Thermal correction to Gibbs Free Energy=	0.608583
Sum of electronic and zero-point Energies=	-2813.034976
Sum of electronic and thermal Energies=	-2812.991089
Sum of electronic and thermal Enthalpies=	-2812.990145
Sum of electronic and thermal Free Energies=	-2813.119236

Cartesian Coordinates

6	-3.610026	3.981576	-0.124502
6	-4.444450	3.998987	1.177521
6	-3.900476	2.806320	2.005121
7	-2.615692	2.420167	1.396269
6	-2.842336	2.644406	-0.039143
6	-1.551068	2.634693	-0.832871
8	-0.511840	3.069967	-0.134376
8	-1.493681	2.286557	-1.993694
1	-3.467853	1.829414	-0.421552
1	-2.890662	4.807150	-0.135389
1	-4.214455	4.049628	-1.030548
1	-5.511539	3.880002	0.977257
1	-4.314316	4.944198	1.709662
1	-4.582916	1.953445	1.929986
1	-3.761653	3.033966	3.063863
1	0.391702	2.833521	-0.665962
1	-1.909687	3.099976	1.682502
7	-1.338660	-0.095017	0.655214
6	-2.506640	-0.798139	0.322730
6	-2.694494	-1.445855	-0.902613
6	-3.921960	-2.033836	-1.178958
6	-4.986488	-1.970091	-0.283730
6	-4.791206	-1.303594	0.917943
6	-3.563222	-0.731933	1.233130
6	-4.094936	-2.785250	-2.469243
9	-3.334168	-2.280456	-3.449653
6	-5.921418	-1.137582	1.890861
9	-5.525783	-1.342487	3.155611
6	-0.043214	-0.388865	0.344728
16	0.477969	-1.844540	-0.324784
7	0.798741	0.625971	0.648635
6	2.225083	0.635228	0.374610
6	2.657928	2.004520	-0.200397
6	4.095761	1.928579	-0.779985
6	4.041026	2.235584	-2.285784
6	3.548238	3.677520	-2.461709
6	2.192154	3.811107	-1.730576
7	1.718917	2.495454	-1.240522
6	1.632896	1.553114	-2.376156
6	3.039772	1.308778	-3.002632
6	3.397832	-0.156704	-3.013045
6	4.590123	-0.689934	-2.755113
6	3.041750	0.326946	1.626235
6	4.052777	-0.685055	1.662929
6	4.786828	-0.826828	2.878961
7	4.551426	-0.075695	3.991768
6	3.598189	0.819520	3.926652
6	2.825077	1.059384	2.766383
6	5.816162	-1.796415	2.948590
6	6.115902	-2.597880	1.877308
6	5.374323	-2.465892	0.675233
6	4.361874	-1.534809	0.576407
9	-3.757766	-4.077454	-2.337721
9	-5.368556	-2.757163	-2.892060
9	-6.934745	-1.975228	1.640863
9	-6.424890	0.112154	1.848722
1	2.609411	2.743934	0.609829
1	4.747580	2.653767	-0.283140
1	4.524005	0.938766	-0.603399
1	1.411396	4.207939	-2.385889
1	2.263135	4.473642	-0.862401
1	3.437533	3.907812	-3.525851

1	4.278070	4.379965	-2.048734
1	5.036153	2.123795	-2.726057
1	2.994981	1.629854	-4.052577
1	0.928436	1.985799	-3.089419
1	1.185058	0.620134	-2.019786
1	2.577806	-0.823691	-3.283159
1	4.745528	-1.763187	-2.802904
1	5.452628	-0.088253	-2.479016
1	2.398559	-0.137824	-0.375443
1	2.058570	1.829514	2.795241
1	3.808810	-1.492917	-0.354419
1	3.412684	1.405890	4.824747
1	6.359003	-1.882297	3.884208
1	6.908803	-3.331455	1.960731
1	0.378387	1.497594	0.953217
1	-1.548263	0.752796	1.200905
1	-1.894557	-1.475947	-1.630739
1	-3.417849	-0.228353	2.184406
1	-5.942702	-2.421216	-0.521840
8	5.599375	-3.225409	-0.426331
6	6.616474	-4.206919	-0.365486
1	6.618306	-4.697715	-1.339064
1	7.600698	-3.757039	-0.189735
1	6.411524	-4.953441	0.410440

H₂O

Number of imaginary frequencies : 0

Electronic energy=	-76.3880966
Zero-point correction=	0.021600
Thermal correction to Energy=	0.024436
Thermal correction to Enthalpy=	0.025380
Thermal correction to Gibbs Free Energy=	0.003952
Sum of electronic and zero-point Energies=	-76.366496
Sum of electronic and thermal Energies=	-76.363661
Sum of electronic and thermal Enthalpies=	-76.362717
Sum of electronic and thermal Free Energies=	-76.384145

Cartesian Coordinates

8	0.000000	-0.000000	0.118449
1	-0.000000	0.759279	-0.473797
1	-0.000000	-0.759279	-0.473797

[2]

Number of imaginary frequencies : 0

Electronic energy	=-3467.7354408
Zero-point correction=	0.938863
Thermal correction to Energy=	0.998309
Thermal correction to Enthalpy=	0.999253
Thermal correction to Gibbs Free Energy=	0.837989
Sum of electronic and zero-point Energies=	-3466.796578
Sum of electronic and thermal Energies=	-3466.737132
Sum of electronic and thermal Enthalpies=	-3466.736188
Sum of electronic and thermal Free Energies=	-3466.897452

Cartesian Coordinates

6	2.941480	-2.695250	-4.283038
6	4.432830	-2.974495	-4.022087
6	4.918983	-1.671004	-3.378116

7	3.806080	-1.229538	-2.530611
6	2.590018	-1.525528	-3.307932
6	2.249621	0.856830	-0.900545
6	3.587629	1.103495	-0.261131
6	4.513458	1.960552	-1.122606
6	1.451140	-1.887725	-2.350616
8	1.729736	-2.730182	-1.459123
8	1.231862	0.620309	-0.278763
8	0.327392	-1.339511	-2.515107
1	2.233408	0.864082	-2.008390
1	4.035120	0.107570	-0.148493
1	2.294839	-0.637034	-3.876334
1	2.324292	-3.576136	-4.090423
1	2.770849	-2.387054	-5.318086
1	4.981377	-3.246065	-4.927781
1	4.542816	-3.790816	-3.300498
1	5.103108	-0.908881	-4.146381
1	5.829443	-1.781140	-2.784038
1	-0.418910	0.151773	-1.419748
1	3.772766	-1.860478	-1.727254
1	3.436988	1.513622	0.744000
1	4.491153	1.573537	-2.149188
1	5.541872	1.846336	-0.768974
6	4.157606	3.456299	-1.101600
1	4.889058	3.997957	-1.714223
1	4.239466	3.838111	-0.077767
6	2.789202	3.736341	-1.635839
6	1.789616	4.273741	-0.925475
1	2.591023	3.477911	-2.677449
1	1.946358	4.560158	0.110426
6	0.467229	4.533670	-1.548538
8	0.263339	4.324963	-2.737306
6	-0.642025	5.055651	-0.687412
6	-0.684196	4.831679	0.692974
6	-1.706828	5.715551	-1.312406
6	-1.786859	5.249051	1.434067
1	0.119862	4.299042	1.191820
6	-2.795089	6.152823	-0.566823
1	-1.660780	5.877883	-2.384814
6	-2.839203	5.912720	0.806795
1	-1.824533	5.053044	2.500662
1	-3.612423	6.673877	-1.054873
1	-3.695593	6.239741	1.387970
7	0.898622	-1.984139	1.021220
6	2.062695	-1.598753	1.681314
6	2.166320	-0.583258	2.639492
6	3.420739	-0.231397	3.124905
6	4.591034	-0.844867	2.690068
6	4.470241	-1.853137	1.741585
6	3.232952	-2.236287	1.244863
6	3.516894	0.953149	4.040883
9	2.463301	1.054686	4.859976
6	5.684103	-2.482758	1.127628
9	5.826594	-2.085145	-0.156112
6	-0.381049	-1.529465	1.133399
16	-1.097911	-0.921164	2.536331
7	-1.034748	-1.657355	-0.043932
6	-2.402221	-1.267094	-0.311348
6	-2.411052	-0.407296	-1.594195
6	-3.750467	0.308368	-1.868793
6	-3.535378	1.830683	-1.832145
6	-2.561450	2.225776	-2.953927
6	-1.280352	1.380225	-2.828289
7	-1.327444	0.635710	-1.530324
6	-1.509473	1.588596	-0.392956
6	-2.903582	2.254625	-0.492664
6	-3.732251	1.995469	0.742319
6	-5.046003	1.787387	0.787905
6	-3.307478	-2.473713	-0.532099
6	-4.584487	-2.607393	0.097232

6	-5.358827	-3.755433	-0.246933
7	-4.933916	-4.715592	-1.115911
6	-3.748194	-4.566290	-1.652026
6	-2.902071	-3.461299	-1.394275
6	-6.637662	-3.917844	0.339167
6	-7.140159	-2.999505	1.224707
6	-6.363334	-1.864678	1.573142
6	-5.111959	-1.679410	1.024529
9	4.620887	0.918867	4.800874
9	3.569109	2.104554	3.337334
9	5.605411	-3.819953	1.101387
9	6.813540	-2.155058	1.766644
1	-2.110094	-1.043585	-2.430619
1	-4.137359	0.012340	-2.847698
1	-4.488805	0.007097	-1.121943
1	-0.379822	1.997299	-2.808652
1	-1.170074	0.624397	-3.607181
1	-2.305560	3.287254	-2.874880
1	-3.020008	2.063791	-3.932602
1	-4.489449	2.345016	-1.973979
1	-2.737002	3.338849	-0.538064
1	-0.694013	2.307815	-0.479304
1	-1.361638	1.032568	0.536876
1	-3.173037	2.016525	1.678710
1	-5.554064	1.631237	1.734181
1	-5.664690	1.754873	-0.105549
1	-2.752477	-0.679674	0.539497
1	-1.933094	-3.408272	-1.885241
1	-4.551629	-0.806721	1.338982
1	-3.417053	-5.344101	-2.337298
1	-7.206529	-4.799118	0.061756
1	-8.122224	-3.150884	1.656732
1	-0.474572	-1.877165	-0.878889
1	1.115268	-2.421428	0.104073
1	1.280767	-0.065362	2.982297
1	3.161026	-3.006167	0.480948
1	5.559085	-0.541268	3.070211
8	-6.783995	-0.912586	2.444261
6	-8.037480	-1.093891	3.075676
1	-8.163892	-0.241084	3.742983
1	-8.857867	-1.104371	2.348367
1	-8.060553	-2.016848	3.666098

[2-3]TS

Number of imaginary frequencies : 1
The smallest frequency is : -76.5173

Electronic energy= -3467.7312633
Zero-point correction= 0.940266
Thermal correction to Energy= 0.998557
Thermal correction to Enthalpy= 0.999501
Thermal correction to Gibbs Free Energy= 0.841638
Sum of electronic and zero-point Energies= -3466.790997
Sum of electronic and thermal Energies= -3466.732706
Sum of electronic and thermal Enthalpies= -3466.731762
Sum of electronic and thermal Free Energies= -3466.889625

Cartesian Coordinates

6	-1.309236	-4.755788	-1.605714
6	-2.654723	-5.005138	-0.887058
6	-2.857342	-3.755277	0.012592
7	-1.770430	-2.825637	-0.328944
6	-0.648731	-3.670524	-0.748147
6	-0.921728	-1.542768	1.034161
6	0.405319	-2.801397	-1.441620
8	-0.036228	-1.866013	-2.164450

8	-0.030794	-2.184896	1.624884
8	1.611633	-3.050591	-1.210600
1	-0.204584	-4.092997	0.160192
1	-1.474545	-4.353366	-2.610648
1	-0.696146	-5.654947	-1.694389
1	-2.615624	-5.911098	-0.277463
1	-3.472435	-5.125213	-1.600816
1	-2.754232	-4.017577	1.071272
1	-3.822855	-3.264537	-0.125887
1	1.722127	-2.097657	0.899974
1	-2.023682	-2.249122	-1.132943
7	0.396007	0.778327	-1.352373
6	-0.835902	1.427865	-1.185099
6	-1.021597	2.706058	-0.647515
6	-2.316697	3.198357	-0.509439
6	-3.439117	2.474622	-0.898485
6	-3.231988	1.218482	-1.456387
6	-1.954734	0.699646	-1.611144
6	-2.517029	4.529171	0.157938
9	-3.579633	5.180405	-0.332154
6	-4.394317	0.343887	-1.824322
9	-5.535617	1.024329	-1.943140
6	1.526115	0.830531	-0.588975
16	1.962525	2.095297	0.439576
7	2.262653	-0.299168	-0.726052
6	3.623389	-0.483315	-0.258334
6	3.768917	-1.867087	0.403461
6	5.106523	-2.033032	1.157850
6	4.828812	-2.272984	2.649290
6	4.043269	-3.586256	2.793099
6	2.778712	-3.513870	1.914754
7	2.649154	-2.126214	1.369468
6	2.606659	-1.135207	2.489000
6	3.968341	-1.133912	3.230377
6	4.602233	0.237578	3.216715
6	5.896952	0.514194	3.082195
6	4.619008	-0.404213	-1.411096
6	5.760306	0.456044	-1.387318
6	6.635242	0.399558	-2.512995
7	6.422032	-0.408732	-3.589638
6	5.355692	-1.169738	-3.576475
6	4.428325	-1.207904	-2.507711
6	7.788669	1.221046	-2.522749
6	8.077794	2.059588	-1.476858
6	7.202730	2.117097	-0.361755
6	6.066992	1.336343	-0.324525
9	-2.728519	4.382141	1.480808
9	-1.452171	5.329727	0.023409
9	-4.597320	-0.608302	-0.883364
9	-4.182333	-0.313313	-2.974798
1	3.636838	-2.630252	-0.363549
1	5.663154	-2.879437	0.746220
1	5.721924	-1.141334	1.018289
1	1.855205	-3.708758	2.462083
1	2.811808	-4.173314	1.045300
1	3.771179	-3.746269	3.840365
1	4.663693	-4.430731	2.482705
1	5.771132	-2.344916	3.198610
1	3.764743	-1.380358	4.280757
1	1.771843	-1.441997	3.119421
1	2.360261	-0.160990	2.056636
1	3.903739	1.063388	3.356101
1	6.252994	1.539334	3.103920
1	6.650237	-0.256771	2.940328
1	3.820716	0.301033	0.473496
1	3.573360	-1.879967	-2.563687
1	5.421028	1.433800	0.540407
1	5.196038	-1.806633	-4.444398
1	8.437256	1.162922	-3.390778
1	8.969014	2.674670	-1.511628

1	1.909533	-1.047444	-1.328538
1	0.295238	-0.108153	-1.867208
1	-0.172888	3.301275	-0.342547
1	-1.803924	-0.277671	-2.064737
1	-4.440905	2.866569	-0.759989
8	7.415937	2.917807	0.713003
6	8.526884	3.794092	0.681577
1	8.486460	4.363936	1.610010
1	9.474307	3.244014	0.640885
1	8.469292	4.486013	-0.166436
6	-2.172354	-1.086961	1.746928
1	-2.954869	-0.868528	1.012695
1	-2.522978	-1.887450	2.409827
1	-0.643380	-0.901172	0.179972
6	-1.853711	0.172186	2.560372
6	-3.082935	0.716218	3.310369
1	-1.455994	0.949523	1.892457
1	-1.065165	-0.055720	3.285383
1	-3.491462	-0.071399	3.954142
1	-2.765510	1.543083	3.955329
6	-4.134449	1.205257	2.365474
6	-5.256057	0.540493	2.068303
1	-3.945543	2.150573	1.856093
1	-5.475062	-0.405320	2.555799
6	-6.213553	1.077480	1.068018
8	-6.136878	2.233190	0.677615
6	-7.289959	0.179003	0.537739
6	-7.261541	-1.209696	0.694290
6	-8.338030	0.767887	-0.176621
6	-8.276808	-1.995099	0.156596
1	-6.437985	-1.690285	1.212199
6	-9.355505	-0.015304	-0.704973
1	-8.332723	1.845186	-0.305304
6	-9.327006	-1.399368	-0.536772
1	-8.246218	-3.073353	0.276563
1	-10.170212	0.450314	-1.250359
1	-10.120566	-2.013639	-0.951120

[3]

Number of imaginary frequencies : 0

Electronic energy=	-3467.7440246
Zero-point correction=	0.941308
Thermal correction to Energy=	0.999009
Thermal correction to Enthalpy=	0.999953
Thermal correction to Gibbs Free Energy=	0.843892
Sum of electronic and zero-point Energies=	-3466.802717
Sum of electronic and thermal Energies=	-3466.745015
Sum of electronic and thermal Enthalpies=	-3466.744071
Sum of electronic and thermal Free Energies=	-3466.900133

Cartesian Coordinates

6	-3.122859	-2.167067	4.198636
6	-4.022066	-1.013492	4.644084
6	-4.241219	-0.195782	3.364395
7	-3.116747	-0.588396	2.437271
6	-2.195685	-1.516160	3.176166
6	-2.388462	0.581846	1.750123
6	-3.414222	1.293439	0.871254
6	-2.853437	2.417124	-0.000941
6	-1.608462	-2.520959	2.163866
8	-2.386866	-2.815541	1.218480
8	-1.387370	0.076385	0.978607
8	-0.459750	-2.936390	2.383265
1	-4.236289	1.680649	1.483927

1	-1.412376	-0.917248	3.648819
1	-3.706780	-2.944996	3.694783
1	-2.563398	-2.626762	5.014204
1	-3.507939	-0.403361	5.391892
1	-4.968131	-1.348183	5.072263
1	-4.185826	0.879671	3.539521
1	-5.182174	-0.421046	2.861432
1	-0.489443	-0.081512	1.441516
1	-3.460266	-1.192822	1.666247
1	-3.836413	0.528390	0.208805
1	-3.589473	2.602174	-0.788094
7	-1.490804	-1.800633	-1.278778
6	-2.645418	-1.168665	-1.735371
6	-2.708507	-0.089263	-2.630367
6	-3.942287	0.479510	-2.925802
6	-5.132878	0.026910	-2.363618
6	-5.057693	-1.062952	-1.506866
6	-3.846121	-1.669352	-1.207997
6	-4.004654	1.675560	-3.833672
9	-2.894753	1.829670	-4.561130
6	-6.263406	-1.541264	-0.756805
9	-6.410465	-2.869983	-0.814278
6	-0.191278	-1.355599	-1.241656
16	0.511336	-0.293612	-2.350287
7	0.477458	-1.892989	-0.206645
6	1.872084	-1.673998	0.128287
6	1.985744	-1.247190	1.606025
6	3.455301	-0.931041	1.994459
6	3.520605	0.478737	2.593904
6	2.604234	0.533583	3.823449
6	1.173751	0.131068	3.381714
7	1.101552	-0.096528	1.924008
6	1.538330	1.128411	1.222401
6	3.006384	1.510761	1.576429
6	3.844413	1.683099	0.335626
6	5.094811	1.267438	0.143189
6	2.681155	-2.947179	-0.090528
6	3.900443	-2.967067	-0.837975
6	4.581078	-4.217295	-0.936977
7	4.120537	-5.370514	-0.373844
6	2.996226	-5.308447	0.296036
6	2.245072	-4.121734	0.471254
6	5.802721	-4.276266	-1.649532
6	6.344099	-3.160166	-2.234365
6	5.665603	-1.918669	-2.133851
6	4.467627	-1.829272	-1.457703
9	-5.041029	1.596432	-4.682832
9	-4.178866	2.815741	-3.133592
9	-7.398303	-0.984265	-1.191775
9	-6.151152	-1.230223	0.558119
1	1.599006	-2.072856	2.208838
1	3.820266	-1.665524	2.719432
1	4.107527	-0.993241	1.119784
1	0.451794	0.918292	3.631142
1	0.847957	-0.796549	3.863434
1	2.605835	1.544116	4.244172
1	2.972824	-0.147881	4.596564
1	4.548071	0.719326	2.884234
1	2.977552	2.485512	2.082564
1	0.844877	1.921549	1.517355
1	1.402260	0.974142	0.146784
1	3.352291	2.228533	-0.471618
1	5.606314	1.456165	-0.795601
1	5.652529	0.719818	0.899071
1	2.235865	-0.878220	-0.522012
1	1.327233	-4.150951	1.055528
1	3.988885	-0.857425	-1.415160
1	2.639044	-6.235961	0.739914
1	6.298139	-5.239705	-1.713211
1	7.282848	-3.236735	-2.770044

1	-0.028764	-2.465399	0.470513
1	-1.718722	-2.432839	-0.504501
1	-1.805462	0.298356	-3.079652
1	-3.814725	-2.507808	-0.517917
1	-6.080536	0.500738	-2.593139
8	6.134404	-0.767122	-2.681590
6	7.370902	-0.810726	-3.364855
1	7.560843	0.206445	-3.708939
1	8.187708	-1.123323	-2.703298
1	7.330102	-1.478885	-4.233051
1	-1.942082	2.068363	-0.499632
1	-2.038971	1.203499	2.590515
6	-2.587567	3.757942	0.716993
1	-2.664695	4.564993	-0.018203
1	-3.372815	3.929700	1.464822
6	-1.239716	3.838641	1.363665
6	-0.220677	4.537074	0.854323
1	-1.057141	3.274162	2.279555
1	-0.353522	5.106356	-0.061414
6	1.119530	4.511738	1.495148
8	1.253911	4.205891	2.671622
6	2.314685	4.813726	0.647213
6	2.256342	4.794531	-0.749979
6	3.541229	5.036896	1.283353
6	3.412162	4.995618	-1.500190
1	1.321896	4.587498	-1.261259
6	4.691589	5.240180	0.534116
1	3.570105	5.035329	2.368537
6	4.627499	5.218743	-0.859630
1	3.363395	4.965632	-2.583758
1	5.641030	5.409356	1.031721
1	5.528874	5.371718	-1.445152

[3-4]TS

Number of imaginary frequencies : 1
The smallest frequency is : -1124.1990

Electronic energy=	-3467.7355607
Zero-point correction=	0.936101
Thermal correction to Energy=	0.993695
Thermal correction to Enthalpy=	0.994640
Thermal correction to Gibbs Free Energy=	0.839596
Sum of electronic and zero-point Energies=	-3466.799460
Sum of electronic and thermal Energies=	-3466.741865
Sum of electronic and thermal Enthalpies=	-3466.740921
Sum of electronic and thermal Free Energies=	-3466.895964

Cartesian Coordinates

6	-0.765531	5.623189	-1.169341
6	0.229798	6.262740	-0.200660
6	1.202456	5.121542	0.123217
7	0.424062	3.868720	-0.101693
6	-0.935330	4.216118	-0.589448
6	0.404588	2.884703	1.034026
6	1.814772	2.362980	1.272476
6	1.868036	1.329912	2.409276
6	-1.205352	3.151611	-1.661608
8	-0.087187	2.642186	-2.075077
8	-0.392426	1.820203	0.664164
8	-2.334165	2.860457	-2.033719
1	2.508925	3.188666	1.455465
1	-1.686781	4.173255	0.204208
1	-0.330298	5.553916	-2.172409
1	-1.716295	6.152553	-1.242967
1	-0.288784	6.578094	0.710248

1	0.738435	7.132762	-0.619669
1	1.550726	5.159143	1.158270
1	2.076320	5.116506	-0.532869
1	-1.370720	1.945729	0.869608
1	0.584669	3.169422	-1.170981
1	2.123100	1.893288	0.330003
1	0.858642	0.947164	2.588996
7	-0.174378	-0.327328	-1.440539
6	1.164657	-0.724225	-1.339338
6	1.614042	-1.984339	-0.923172
6	2.983587	-2.215854	-0.825033
6	3.930208	-1.251459	-1.148106
6	3.469299	-0.018949	-1.589504
6	2.111473	0.242873	-1.699764
6	3.471652	-3.507131	-0.236012
9	2.589719	-4.502445	-0.364498
6	4.434399	1.084018	-1.912567
9	4.546190	1.292779	-3.232636
6	-1.257255	-0.689079	-0.681364
16	-1.317018	-2.020886	0.354767
7	-2.285385	0.165786	-0.842411
6	-3.601881	0.044491	-0.243099
6	-4.014872	1.362356	0.447620
6	-5.375906	1.192632	1.179658
6	-5.181152	1.474522	2.676658
6	-4.729174	2.931769	2.834927
6	-3.469717	3.140249	1.954288
7	-2.984988	1.862835	1.391352
6	-2.755892	0.913250	2.499504
6	-4.074659	0.574194	3.257827
6	-4.363952	-0.906531	3.245082
6	-5.553749	-1.485973	3.102188
6	-4.637928	-0.310796	-1.306902
6	-5.484946	-1.459785	-1.209163
6	-6.456118	-1.643540	-2.238184
7	-6.586653	-0.804467	-3.305387
6	-5.771121	0.218173	-3.372704
6	-4.788065	0.511008	-2.396412
6	-7.336572	-2.748939	-2.157374
6	-7.273156	-3.639432	-1.115650
6	-6.298594	-3.460689	-0.101056
6	-5.420944	-2.398688	-0.154951
9	4.625424	-3.908705	-0.794771
9	3.721936	-3.369495	1.084085
9	5.659661	0.833828	-1.439386
9	4.027018	2.253490	-1.376445
1	-4.086035	2.130586	-0.330684
1	-6.117752	1.884940	0.768995
1	-5.765447	0.182317	1.030615
1	-2.651063	3.585133	2.531146
1	-3.687701	3.808358	1.114632
1	-4.508185	3.144119	3.886078
1	-5.529180	3.611036	2.525628
1	-6.119844	1.312756	3.215078
1	-3.936475	0.860254	4.310160
1	-2.027770	1.382226	3.169921
1	-2.280122	0.015181	2.091988
1	-3.489151	-1.544065	3.384940
1	-5.655894	-2.566873	3.112212
1	-6.467165	-0.914704	2.956136
1	-3.537077	-0.750028	0.500052
1	-4.160370	1.390238	-2.524719
1	-4.684086	-2.317489	0.634791
1	-5.879348	0.876124	-4.233165
1	-8.067180	-2.866391	-2.951024
1	-7.962110	-4.474926	-1.082297
1	-2.185381	0.938904	-1.499252
1	-0.255250	0.599689	-1.859847
1	0.909296	-2.758819	-0.657374
1	1.773466	1.216222	-2.044430

1	4.992080	-1.443795	-1.035678
8	-6.164848	-4.295715	0.961839
6	-7.029850	-5.411511	1.047332
1	-6.746254	-5.943018	1.956008
1	-8.079497	-5.104279	1.125028
1	-6.909072	-6.082219	0.188673
1	2.215694	1.799025	3.335869
1	0.012868	3.418155	1.919422
6	2.756131	0.132744	2.052259
1	2.747544	-0.613772	2.853445
1	2.306196	-0.353257	1.173968
6	4.168344	0.491489	1.703567
6	5.221789	-0.307814	1.895599
1	4.347321	1.440946	1.195082
1	5.098210	-1.284796	2.356156
6	6.561677	0.094893	1.394072
8	6.882339	1.268337	1.305021
6	7.504097	-0.985015	0.952616
6	7.082791	-2.302708	0.749769
6	8.831197	-0.636055	0.682971
6	7.978979	-3.259155	0.279380
1	6.052784	-2.587385	0.939456
6	9.728099	-1.594509	0.230775
1	9.135058	0.394911	0.832357
6	9.301935	-2.907296	0.026326
1	7.638581	-4.275650	0.109225
1	10.759224	-1.321601	0.029217
1	10.001852	-3.653908	-0.336205

[4]*_anti*

Number of imaginary frequencies : 0

Electronic energy=	-3467.7393067
Zero-point correction=	0.939167
Thermal correction to Energy=	0.997088
Thermal correction to Enthalpy=	0.998033
Thermal correction to Gibbs Free Energy=	0.841397
Sum of electronic and zero-point Energies=	-3466.800140
Sum of electronic and thermal Energies=	-3466.742218
Sum of electronic and thermal Enthalpies=	-3466.741274
Sum of electronic and thermal Free Energies=	-3466.897910

Cartesian Coordinates

6	0.406989	-3.909858	-1.116813
6	-0.102282	-5.141906	-1.875777
6	-0.887121	-5.877662	-0.778057
6	-0.130483	-5.554810	0.530098
7	0.821026	-4.504857	0.140979
6	1.501235	-3.740137	1.132101
6	2.221319	-4.639881	2.142038
6	3.132075	-5.721347	1.550868
6	-0.748005	-2.897430	-1.036686
8	-1.245972	-2.404820	-2.022812
8	-1.225580	-2.598220	0.176988
8	0.589002	-2.887444	1.876219
1	1.253139	-3.414180	-1.607708
1	-0.708216	-4.877297	-2.742910
1	0.760217	-5.728066	-2.203646
1	-1.906596	-5.482892	-0.727021
1	-0.959378	-6.951326	-0.959290
1	-0.823411	-5.220431	1.314608
1	0.410364	-6.425354	0.918377
1	1.442441	-5.110552	2.753098
1	-0.577178	-2.824575	0.938317
1	2.601485	-6.240124	0.745147

1	3.338285	-6.464425	2.327759
1	2.202046	-3.087370	0.598941
1	2.792911	-3.996429	2.821150
6	4.480163	-5.217728	1.004861
1	5.030773	-6.080519	0.608367
1	5.085089	-4.786029	1.810743
6	4.281622	-4.213904	-0.081333
6	4.818720	-2.989385	-0.118344
1	3.579512	-4.482187	-0.873488
1	5.522962	-2.674424	0.645786
6	4.359452	-2.018320	-1.144951
8	3.395975	-2.277967	-1.855634
6	5.023651	-0.681480	-1.249773
6	6.163917	-0.330408	-0.517931
6	4.438642	0.261587	-2.103330
6	6.693771	0.953246	-0.626811
1	6.656216	-1.049930	0.127836
6	4.964721	1.542152	-2.209295
1	3.564235	-0.030026	-2.673519
6	6.091756	1.890368	-1.463603
1	7.578626	1.220589	-0.058254
1	4.495555	2.264051	-2.871021
1	6.504463	2.891463	-1.540586
7	-2.636431	-0.058745	0.212668
6	-4.030256	0.082792	0.137137
6	-4.760384	0.969211	0.935621
6	-6.144145	0.998717	0.825998
6	-6.831899	0.154811	-0.040955
6	-6.094404	-0.733263	-0.811490
6	-4.706207	-0.771473	-0.735936
6	-6.920819	1.993764	1.640649
9	-7.133789	3.133138	0.964349
6	-6.783761	-1.700757	-1.730079
9	-6.243020	-1.692119	-2.957301
6	-1.678027	0.892864	0.393273
16	-1.965137	2.541226	0.570419
7	-0.424114	0.372292	0.413094
6	0.769898	1.194801	0.339418
6	2.023185	0.426789	0.820590
6	3.171337	1.435271	1.108805
6	3.493449	1.411697	2.611763
6	4.066406	0.029862	2.938282
6	3.048202	-1.022901	2.442315
7	1.766750	-0.407472	2.022817
6	1.256189	0.420962	3.133076
6	2.222951	1.600912	3.462761
6	1.549940	2.944989	3.333138
6	2.098783	4.067934	2.874840
6	1.015714	1.688402	-1.088350
6	1.352519	3.042993	-1.404337
6	1.688904	3.333360	-2.759701
7	1.669459	2.401745	-3.756383
6	1.287603	1.189444	-3.438722
6	0.958694	0.786888	-2.121508
6	2.063411	4.654778	-3.104533
6	2.090054	5.657700	-2.169429
6	1.725826	5.372164	-0.828696
6	1.361356	4.094740	-0.461212
9	-8.128360	1.517469	1.983945
9	-6.282805	2.323015	2.772542
9	-8.088751	-1.428513	-1.862087
9	-6.685846	-2.962805	-1.278055
1	2.323381	-0.274272	0.028407
1	4.068797	1.164495	0.544900
1	2.887692	2.440080	0.789272
1	2.817338	-1.754001	3.223943
1	3.440774	-1.572594	1.579374
1	4.236033	-0.068175	4.015574
1	5.031368	-0.104946	2.438359
1	4.225690	2.188967	2.849173

1	2.518999	1.500098	4.516458
1	1.133039	-0.242917	3.994190
1	0.262011	0.787060	2.861329
1	0.516183	2.978069	3.681240
1	1.534060	4.994406	2.843559
1	3.120455	4.111888	2.505169
1	0.606511	2.046397	1.003166
1	0.668250	-0.246614	-1.950051
1	1.059119	3.930777	0.566202
1	1.249193	0.457433	-4.243597
1	2.317768	4.847689	-4.141822
1	2.374090	6.660537	-2.465088
1	-0.320449	-0.630162	0.309404
1	-2.298007	-0.986827	-0.034712
1	-4.252627	1.620322	1.633624
1	-4.138270	-1.457170	-1.360205
1	-7.913078	0.185793	-0.107603
8	1.710109	6.308616	0.155418
6	1.983291	7.650334	-0.198752
1	1.874211	8.231211	0.717481
1	3.005565	7.769806	-0.576941
1	1.272519	8.022130	-0.945731
1	0.948364	-1.948082	1.913966

[4-5]TS-anti

Number of imaginary frequencies : 1
The smallest frequency is : -168.5960

Electronic energy= -3467.7214477
Zero-point correction= 0.936984
Thermal correction to Energy= 0.994965
Thermal correction to Enthalpy= 0.995909
Thermal correction to Gibbs Free Energy= 0.839320
Sum of electronic and zero-point Energies= -3466.784463
Sum of electronic and thermal Energies= -3466.726483
Sum of electronic and thermal Enthalpies= -3466.725539
Sum of electronic and thermal Free Energies= -3466.882128

Cartesian Coordinates

6	-0.023545	-3.814916	-1.130300
6	-0.702815	-4.982974	-1.845130
6	-1.467214	-5.652105	-0.696113
6	-0.501725	-5.560563	0.494528
7	0.397552	-4.443348	0.135807
6	1.320387	-3.945944	0.916967
6	1.920784	-4.762249	2.029267
6	2.794773	-5.928565	1.527068
6	-1.042885	-2.668479	-0.917991
8	-1.478600	-2.126319	-1.930891
8	-1.362778	-2.388279	0.291140
8	0.395612	-2.653092	2.180740
1	0.856591	-3.424100	-1.648507
1	-1.346969	-4.625377	-2.648208
1	0.049265	-5.661061	-2.260813
1	-2.377232	-5.086375	-0.478367
1	-1.749264	-6.684279	-0.908363
1	-1.007846	-5.335453	1.437272
1	0.085249	-6.475366	0.617806
1	1.106104	-5.143394	2.650327
1	-0.405300	-2.582047	1.594654
1	2.268985	-6.476202	0.736582
1	2.935133	-6.629933	2.354454
1	1.903651	-3.148658	0.463103
1	2.512098	-4.090683	2.657663
6	4.178474	-5.504985	1.001731

1	4.693307	-6.399202	0.630226
1	4.782554	-5.088827	1.815488
6	4.029330	-4.503528	-0.094701
6	4.559925	-3.276648	-0.115287
1	3.350379	-4.767780	-0.908484
1	5.253777	-2.957297	0.657212
6	4.103863	-2.305935	-1.148911
8	3.082609	-2.533728	-1.786667
6	4.841331	-1.024088	-1.346512
6	6.045865	-0.730867	-0.697553
6	4.268825	-0.074571	-2.201923
6	6.655615	0.506451	-0.889870
1	6.523618	-1.461123	-0.052572
6	4.874707	1.160561	-2.389515
1	3.342701	-0.323258	-2.707716
6	6.067622	1.452855	-1.726726
1	7.589935	0.731059	-0.385684
1	4.414471	1.891074	-3.047994
1	6.541461	2.419457	-1.866551
7	-2.583976	0.079432	0.424619
6	-3.964104	0.249372	0.268773
6	-4.720804	1.187236	0.979003
6	-6.096603	1.228869	0.792881
6	-6.749699	0.350086	-0.066472
6	-5.985270	-0.583027	-0.753970
6	-4.604055	-0.636739	-0.601514
6	-6.901740	2.271377	1.514176
9	-7.073313	3.374949	0.769658
6	-6.636477	-1.575311	-1.672955
9	-6.084172	-1.561281	-2.894951
6	-1.610722	1.013103	0.566415
16	-1.846068	2.677872	0.696470
7	-0.369286	0.455927	0.595459
6	0.843925	1.232228	0.432070
6	2.076975	0.409215	0.867295
6	3.320804	1.328342	1.023736
6	3.787677	1.290132	2.487135
6	4.244601	-0.140336	2.792626
6	3.063598	-1.087063	2.466445
7	1.837975	-0.340289	2.122691
6	1.508355	0.574898	3.229387
6	2.632266	1.635843	3.447272
6	2.102658	3.044942	3.345139
6	2.706116	4.086989	2.777547
6	1.037658	1.679041	-1.018347
6	1.465660	2.996151	-1.380400
6	1.751336	3.236079	-2.756808
7	1.601674	2.293148	-3.731976
6	1.132467	1.124791	-3.369161
6	0.841476	0.771177	-2.028712
6	2.213866	4.516010	-3.147444
6	2.370676	5.529350	-2.236330
6	2.053971	5.297442	-0.873386
6	1.607001	4.060268	-0.461545
9	-8.129744	1.822682	1.824190
9	-6.317303	2.657864	2.656923
9	-7.948190	-1.342156	-1.822760
9	-6.509227	-2.832265	-1.212102
1	2.261585	-0.352370	0.094475
1	4.133954	0.988372	0.375775
1	3.082977	2.350753	0.725120
1	2.822285	-1.737055	3.314651
1	3.299270	-1.734187	1.612305
1	4.539919	-0.231815	3.843021
1	5.118304	-0.388308	2.179860
1	4.618323	1.987359	2.632313
1	3.010780	1.514625	4.472090
1	1.366377	-0.042404	4.121917
1	0.546203	1.047855	3.009068
1	1.127885	3.201177	3.810167

1	2.241451	5.067856	2.769738
1	3.674969	4.008522	2.290545
1	0.757093	2.109254	1.077132
1	0.459042	-0.226461	-1.825813
1	1.345580	3.940560	0.583108
1	0.985130	0.386761	-4.155604
1	2.427930	4.670467	-4.200172
1	2.719544	6.500156	-2.567698
1	-0.314466	-0.549459	0.456193
1	-2.251919	-0.887352	0.260199
1	-4.237787	1.865718	1.668831
1	-4.003766	-1.348317	-1.165519
1	-7.825391	0.389719	-0.191014
8	2.164722	6.248660	0.090840
6	2.520143	7.558354	-0.306412
1	2.506191	8.162894	0.600809
1	3.526489	7.590973	-0.740937
1	1.800653	7.970611	-1.023059
1	0.822816	-1.746820	2.138487

[5]_{anti}

Number of imaginary frequencies : 0

Electronic energy=	-3467.7249544
Zero-point correction=	0.937904
Thermal correction to Energy=	0.997008
Thermal correction to Enthalpy=	0.997952
Thermal correction to Gibbs Free Energy=	0.838338
Sum of electronic and zero-point Energies=	-3466.787050
Sum of electronic and thermal Energies=	-3466.727946
Sum of electronic and thermal Enthalpies=	-3466.727002
Sum of electronic and thermal Free Energies=	-3466.886617

Cartesian Coordinates

6	-0.670792	-4.029797	-1.228635
6	-1.441368	-5.151078	-1.908826
6	-2.215591	-5.763927	-0.739393
6	-1.189988	-5.777562	0.395333
7	-0.294167	-4.636574	0.073901
6	0.657542	-4.200408	0.819417
6	1.096415	-4.890909	2.073378
6	1.918873	-6.172271	1.807145
6	-1.543354	-2.756318	-0.976255
8	-2.545549	-2.603136	-1.669551
8	-1.085113	-1.989665	-0.073538
8	-0.203166	-2.351726	2.498985
1	0.248392	-3.721410	-1.734289
1	-2.093918	-4.742369	-2.678926
1	-0.755334	-5.880198	-2.351623
1	-3.056390	-5.114010	-0.482800
1	-2.598492	-6.764638	-0.942972
1	-1.617168	-5.630350	1.389287
1	-0.595732	-6.694710	0.392815
1	0.210536	-5.132594	2.667009
1	-0.826806	-2.303373	1.756674
1	1.413326	-6.801175	1.065847
1	1.953990	-6.750037	2.734682
1	1.185264	-3.330373	0.438946
1	1.678915	-4.174819	2.656565
6	3.357769	-5.901605	1.332599
1	3.827580	-6.861611	1.088706
1	3.939514	-5.440632	2.138015
6	3.339286	-5.005093	0.138785
6	3.934890	-3.811736	0.055811
1	2.707728	-5.310494	-0.698504

1	4.597997	-3.464585	0.844099
6	3.601340	-2.899004	-1.073364
8	2.569529	-3.075596	-1.710219
6	4.484020	-1.733677	-1.367322
6	5.745395	-1.569549	-0.782897
6	4.004681	-0.767577	-2.259233
6	6.507881	-0.443607	-1.083079
1	6.145265	-2.320061	-0.107823
6	4.757813	0.362823	-2.546180
1	3.030578	-0.918349	-2.710914
6	6.012247	0.523735	-1.955564
1	7.487944	-0.320125	-0.633890
1	4.366078	1.114014	-3.225930
1	6.604219	1.406013	-2.177904
7	-2.469772	0.472866	0.253043
6	-3.844073	0.720813	0.173864
6	-4.492525	1.764465	0.845607
6	-5.871705	1.888845	0.736456
6	-6.636257	0.996614	-0.008519
6	-5.979080	-0.042871	-0.653454
6	-4.598864	-0.189210	-0.574488
6	-6.556772	3.041508	1.412573
9	-6.675138	4.101785	0.596989
6	-6.751455	-1.052445	-1.451981
9	-6.285449	-1.158523	-2.705473
6	-1.425315	1.336779	0.407861
16	-1.530037	3.016911	0.520261
7	-0.241139	0.685629	0.449225
6	1.048527	1.335671	0.364862
6	2.129910	0.339662	0.832611
6	3.520909	1.016844	0.963253
6	4.025584	0.834131	2.402390
6	4.161656	-0.671908	2.667005
6	2.773996	-1.321530	2.430602
7	1.751999	-0.318201	2.099533
6	1.661143	0.652085	3.197938
6	3.012463	1.407780	3.412363
6	2.820842	2.902510	3.366653
6	3.599847	3.796910	2.761869
6	1.356634	1.787726	-1.062125
6	1.970483	3.042845	-1.371928
6	2.300827	3.288885	-2.737678
7	2.036866	2.409017	-3.746795
6	1.425624	1.294416	-3.427730
6	1.073360	0.939721	-2.103307
6	2.935785	4.506812	-3.080911
6	3.226583	5.453765	-2.132621
6	2.876968	5.216399	-0.778598
6	2.257143	4.040765	-0.412713
9	-7.801005	2.717957	1.804373
9	-5.891418	3.458520	2.499029
9	-8.054028	-0.742809	-1.536873
9	-6.673790	-2.280139	-0.910110
1	2.174285	-0.464495	0.081942
1	4.231900	0.564115	0.265195
1	3.460168	2.077502	0.713648
1	2.427345	-1.863220	3.317556
1	2.803903	-2.038836	1.600924
1	4.508424	-0.849848	3.690350
1	4.910569	-1.094002	1.986794
1	4.996937	1.323448	2.524543
1	3.377007	1.164128	4.420560
1	1.372622	0.095569	4.095109
1	0.844111	1.346869	2.980612
1	1.944433	3.262647	3.908277
1	3.366756	4.856390	2.794370
1	4.487556	3.515291	2.201157
1	1.033249	2.205079	1.026471
1	0.580475	-0.012478	-1.921649
1	1.995037	3.915851	0.631390

1	1.200895	0.607836	-4.242615
1	3.177307	4.667514	-4.126629
1	3.709783	6.378043	-2.426412
1	-0.259352	-0.326164	0.331249
1	-2.193136	-0.495121	0.041091
1	-3.924092	2.461744	1.445059
1	-4.092890	-1.005074	-1.090870
1	-7.712129	1.105499	-0.076581
8	3.122876	6.103866	0.220396
6	3.690131	7.352315	-0.124470
1	3.770519	7.913607	0.806827
1	4.689988	7.236378	-0.559138
1	3.051309	7.906126	-0.822116
1	0.349902	-1.555739	2.346632

[4]_syn

Number of imaginary frequencies : 0

Electronic energy=	-3467.7400595
Zero-point correction=	0.939343
Thermal correction to Energy=	0.997331
Thermal correction to Enthalpy=	0.998275
Thermal correction to Gibbs Free Energy=	0.841102
Sum of electronic and zero-point Energies=	-3466.800716
Sum of electronic and thermal Energies=	-3466.742728
Sum of electronic and thermal Enthalpies=	-3466.741784
Sum of electronic and thermal Free Energies=	-3466.898958

Cartesian Coordinates

6	-2.617993	-4.467238	-0.483430
6	-3.798744	-5.427464	-0.271057
6	-4.011181	-5.342659	1.243368
6	-2.585080	-5.246633	1.802211
7	-1.780571	-4.762971	0.668298
6	-0.581434	-4.058393	0.970466
6	0.252286	-3.758458	-0.267639
6	0.771179	-5.014060	-0.965294
6	-3.159098	-3.035239	-0.636609
8	-3.843298	-2.728667	-1.585697
8	-2.869817	-2.144447	0.311723
8	-0.894682	-2.833874	1.672127
1	-2.098612	-4.682590	-1.424136
1	-4.670171	-5.139576	-0.860165
1	-3.487441	-6.434644	-0.562238
1	-4.571088	-4.433281	1.485772
1	-4.563249	-6.193255	1.646966
1	-2.529304	-4.558180	2.652924
1	-2.207896	-6.223193	2.131369
1	1.101379	-3.146178	0.056533
1	-2.143651	-2.440197	0.966025
1	-0.046551	-5.537198	-1.470247
1	1.161010	-5.706505	-0.208031
1	0.008083	-4.681616	1.659311
1	-0.329290	-3.135531	-0.963677
6	1.889870	-4.698933	-1.971955
1	1.526139	-4.013269	-2.746206
1	2.189368	-5.628790	-2.470152
6	3.068852	-4.106323	-1.267669
6	3.618236	-2.916101	-1.527984
1	3.482124	-4.680917	-0.436286
1	3.253158	-2.304130	-2.347386
6	4.714111	-2.397656	-0.662916
8	4.919528	-2.893802	0.437620
6	5.528250	-1.234986	-1.132104
6	5.396193	-0.682461	-2.409263

6	6.449395	-0.677957	-0.234895
6	6.156935	0.424974	-2.774769
1	4.704578	-1.100779	-3.131608
6	7.206314	0.425562	-0.599874
1	6.550522	-1.127592	0.747833
6	7.055430	0.982809	-1.870731
1	6.026772	0.858415	-3.761096
1	7.912076	0.855797	0.103406
1	7.637020	1.854908	-2.153537
7	-2.404242	0.658573	0.010594
6	-3.656973	1.277900	-0.130558
6	-3.982613	2.533470	0.391422
6	-5.276517	3.018067	0.237045
6	-6.267578	2.285726	-0.406742
6	-5.931959	1.031363	-0.899167
6	-4.645196	0.523413	-0.772472
6	-5.596439	4.392505	0.752607
9	-5.346778	5.339708	-0.165234
6	-6.950623	0.192623	-1.616762
9	-6.680926	0.101276	-2.928364
6	-1.159030	1.186233	0.160880
16	-0.780393	2.824532	0.151688
7	-0.197150	0.235529	0.314768
6	1.211776	0.569652	0.472283
6	2.008950	-0.599286	1.096809
6	3.356165	-0.091578	1.681357
6	3.355555	-0.302672	3.203523
6	3.326610	-1.814687	3.458465
6	2.130164	-2.401455	2.673459
7	1.251809	-1.328085	2.143054
6	0.866724	-0.425274	3.247952
6	2.100823	0.312087	3.848671
6	1.977480	1.811628	3.729197
6	2.956761	2.672780	3.460609
6	1.847599	0.926270	-0.871843
6	2.709021	2.050267	-1.065915
6	3.292572	2.208981	-2.358573
7	3.050292	1.368378	-3.403553
6	2.228229	0.369625	-3.194087
6	1.616051	0.104370	-1.947141
6	4.174443	3.294375	-2.581889
6	4.465399	4.195356	-1.590470
6	3.862242	4.049617	-0.313940
6	2.999136	3.004612	-0.065195
9	-6.890798	4.510280	1.088128
9	-4.870826	4.701069	1.837477
9	-8.188926	0.695065	-1.502208
9	-6.979868	-1.061502	-1.141885
1	2.201596	-1.334970	0.305739
1	4.186855	-0.656958	1.254054
1	3.517313	0.957945	1.428794
1	1.511667	-3.053568	3.299236
1	2.486168	-2.985257	1.816083
1	3.228228	-2.017068	4.530128
1	4.258192	-2.271653	3.112994
1	4.258082	0.134525	3.640762
1	2.134156	0.082367	4.922598
1	0.366443	-1.043397	3.999761
1	0.127886	0.287223	2.868341
1	0.976327	2.206579	3.910298
1	2.766196	3.740739	3.421610
1	3.978883	2.355612	3.268636
1	1.258053	1.432508	1.141571
1	0.952444	-0.751707	-1.851799
1	2.538362	2.953513	0.914844
1	2.026200	-0.286452	-4.040254
1	4.607378	3.392283	-3.572419
1	5.141972	5.017153	-1.792614
1	-0.468293	-0.739391	0.382191
1	-2.469976	-0.355876	-0.063872

1	-3.241086	3.118051	0.916872
1	-4.410681	-0.466666	-1.161545
1	-7.273321	2.675507	-0.509497
8	4.084176	4.903716	0.717366
6	4.905153	6.031376	0.483805
1	4.919939	6.591627	1.418936
1	5.930098	5.739461	0.226311
1	4.497356	6.669211	-0.308900
1	-0.074927	-2.238753	1.791182

[4-5]TS_{syn}

Number of imaginary frequencies : 1
The smallest frequency is : -168.2121

Electronic energy=	-3467.7222195
Zero-point correction=	0.937241
Thermal correction to Energy=	0.995205
Thermal correction to Enthalpy=	0.996149
Thermal correction to Gibbs Free Energy=	0.839282
Sum of electronic and zero-point Energies=	-3466.784978
Sum of electronic and thermal Energies=	-3466.727014
Sum of electronic and thermal Enthalpies=	-3466.726070
Sum of electronic and thermal Free Energies=	-3466.882938

Cartesian Coordinates

6	-2.543427	-4.139523	-0.692682
6	-3.932260	-4.773586	-0.721520
6	-4.554119	-4.248332	0.575324
6	-3.405642	-4.358402	1.579464
7	-2.193479	-4.218959	0.741449
6	-1.013026	-4.012651	1.273115
6	0.225747	-4.031052	0.432892
6	0.702252	-5.464780	0.170136
6	-2.566005	-2.680428	-1.235591
8	-3.317814	-2.440922	-2.174516
8	-1.760920	-1.860413	-0.669448
8	-1.024172	-2.112621	1.851082
1	-1.808539	-4.701032	-1.278857
1	-4.470108	-4.464905	-1.616762
1	-3.852754	-5.865146	-0.697003
1	-4.847797	-3.201848	0.442166
1	-5.431838	-4.811536	0.895162
1	-3.409779	-3.574918	2.340868
1	-3.385638	-5.337748	2.068965
1	1.003778	-3.481390	0.966542
1	-1.425284	-1.839348	0.992086
1	-0.090008	-6.047907	-0.312145
1	0.926633	-5.957809	1.123683
1	-0.921956	-4.294978	2.318742
1	0.038815	-3.500120	-0.504737
6	1.954484	-5.473778	-0.720985
1	1.706597	-5.087412	-1.715884
1	2.288680	-6.510889	-0.844494
6	3.059306	-4.664913	-0.117951
6	3.656564	-3.621885	-0.703838
1	3.384183	-4.935410	0.888617
1	3.378342	-3.333211	-1.712690
6	4.729728	-2.875156	0.011877
8	4.977958	-3.120337	1.184619
6	5.498551	-1.816433	-0.713155
6	5.101382	-1.303357	-1.951527
6	6.633356	-1.287692	-0.083794
6	5.823032	-0.273376	-2.549397
1	4.218627	-1.681439	-2.454024
6	7.357514	-0.267936	-0.684324

1	6.923948	-1.689020	0.881694
6	6.949472	0.243446	-1.917105
1	5.489277	0.134120	-3.498250
1	8.236832	0.135429	-0.192371
1	7.507756	1.049473	-2.383151
7	-2.258496	0.792395	-0.295214
6	-3.584092	1.234377	-0.270715
6	-4.066967	2.367038	0.395109
6	-5.431836	2.636627	0.371517
6	-6.342498	1.815427	-0.282420
6	-5.845656	0.696364	-0.939592
6	-4.489593	0.404963	-0.949285
6	-5.929536	3.887314	1.038931
9	-5.928506	4.934668	0.197790
6	-6.770134	-0.252924	-1.646296
9	-6.444746	-0.396924	-2.937857
6	-1.095512	1.321818	0.164442
16	-0.878892	2.887405	0.754566
7	-0.078383	0.414322	0.106576
6	1.323848	0.761028	0.256547
6	2.115937	-0.333836	1.009941
6	3.478585	0.225254	1.510553
6	3.488033	0.224357	3.049157
6	3.431135	-1.235753	3.515685
6	2.217735	-1.898370	2.821877
7	1.358710	-0.897552	2.150025
6	0.995671	0.158711	3.116989
6	2.249517	0.937888	3.619607
6	2.154717	2.415501	3.333213
6	3.144487	3.214163	2.938669
6	1.966879	1.007168	-1.108607
6	2.737339	2.173772	-1.409913
6	3.324719	2.254189	-2.708433
7	3.153194	1.303607	-3.670722
6	2.409034	0.268293	-3.369625
6	1.811174	0.071516	-2.102222
6	4.129192	3.374847	-3.027388
6	4.342524	4.381884	-2.121305
6	3.737123	4.310697	-0.840185
6	2.946682	3.233799	-0.500069
9	-7.190945	3.747944	1.478412
9	-5.174138	4.232859	2.090953
9	-8.047075	0.154238	-1.596932
9	-6.727454	-1.481930	-1.099955
1	2.281582	-1.173421	0.318669
1	4.302762	-0.400621	1.158350
1	3.650331	1.230000	1.116018
1	1.592037	-2.451377	3.531647
1	2.568144	-2.601697	2.057804
1	3.332873	-1.278978	4.605543
1	4.348063	-1.762177	3.236570
1	4.402062	0.700809	3.416002
1	2.287992	0.833753	4.713126
1	0.476686	-0.335740	3.943831
1	0.275634	0.831854	2.640998
1	1.168198	2.852091	3.493619
1	2.976989	4.274640	2.777654
1	4.151752	2.849501	2.752786
1	1.343604	1.677574	0.847202
1	1.224426	-0.829619	-1.938314
1	2.486499	3.236456	0.481198
1	2.265758	-0.477041	-4.150528
1	4.566791	3.411610	-4.019931
1	4.960959	5.228437	-2.394900
1	-0.290707	-0.477285	-0.335271
1	-2.169856	-0.169285	-0.662196
1	-3.390168	3.020036	0.927400
1	-4.124685	-0.471000	-1.487781
1	-7.402778	2.037890	-0.277578
8	3.889329	5.267030	0.110212

6	4.637763	6.421606	-0.218170
1	4.612592	7.057772	0.666688
1	5.680373	6.175313	-0.451009
1	4.192555	6.962490	-1.061124
1	-0.117134	-1.656998	1.886507

[5]_syn

Number of imaginary frequencies : 0

Electronic energy=	-3467.726875
Zero-point correction=	0.936753
Thermal correction to Energy=	0.996272
Thermal correction to Enthalpy=	0.997217
Thermal correction to Gibbs Free Energy=	0.834968
Sum of electronic and zero-point Energies=	-3466.790122
Sum of electronic and thermal Energies=	-3466.730603
Sum of electronic and thermal Enthalpies=	-3466.729658
Sum of electronic and thermal Free Energies=	-3466.891907

Cartesian Coordinates

6	-2.946127	-3.827092	-0.848902
6	-4.473889	-3.772989	-0.803353
6	-4.737826	-3.083960	0.537693
6	-3.733035	-3.758961	1.466734
7	-2.580440	-4.044698	0.568864
6	-1.406087	-4.277853	1.024740
6	-0.178321	-4.454955	0.213862
6	0.521844	-5.782375	0.527875
6	-2.357153	-2.479951	-1.386288
8	-2.828480	-2.090055	-2.452517
8	-1.468509	-1.926287	-0.668302
8	-1.155383	-1.886985	2.110942
1	-2.555079	-4.646261	-1.456618
1	-4.855551	-3.221075	-1.661525
1	-4.897743	-4.782260	-0.806620
1	-4.518917	-2.013187	0.462012
1	-5.762622	-3.198359	0.892207
1	-3.375145	-3.138566	2.290667
1	-4.110196	-4.713158	1.845711
1	0.462690	-3.609932	0.503158
1	-1.471127	-1.761414	1.201286
1	-0.113864	-6.617799	0.217672
1	0.672624	-5.877209	1.610186
1	-1.317955	-4.351644	2.105520
1	-0.377910	-4.349989	-0.854089
6	1.876607	-5.883337	-0.186691
1	1.744530	-5.752087	-1.266494
1	2.274481	-6.893055	-0.027653
6	2.867649	-4.895379	0.341886
6	3.517848	-3.979549	-0.383546
1	3.087970	-4.938309	1.410083
1	3.358705	-3.907889	-1.455161
6	4.535544	-3.105463	0.267750
8	4.754953	-3.193277	1.467495
6	5.310205	-2.136675	-0.566064
6	4.870037	-1.689065	-1.815434
6	6.500227	-1.626616	-0.031086
6	5.611174	-0.743262	-2.519937
1	3.935987	-2.047256	-2.236820
6	7.242841	-0.692503	-0.738784
1	6.820738	-1.975198	0.945309
6	6.795865	-0.247634	-1.983511
1	5.252801	-0.379799	-3.477279
1	8.166900	-0.305076	-0.321834
1	7.369176	0.491493	-2.534449

7	-2.184923	0.802275	-0.370335
6	-3.518596	1.209428	-0.321668
6	-4.014923	2.257295	0.464232
6	-5.382745	2.504811	0.482111
6	-6.288665	1.732630	-0.237182
6	-5.780539	0.694447	-1.006898
6	-4.417474	0.437475	-1.070714
6	-5.895379	3.669635	1.281106
9	-5.943299	4.792937	0.547623
6	-6.699589	-0.223422	-1.758206
9	-6.318114	-0.386924	-3.031225
6	-1.028838	1.396973	0.049046
16	-0.850132	3.023941	0.455349
7	-0.009327	0.508887	0.087246
6	1.389821	0.864348	0.224623
6	2.144553	-0.209751	1.043638
6	3.535114	0.305519	1.511407
6	3.555872	0.350350	3.049477
6	3.407285	-1.087357	3.566245
6	2.128448	-1.685582	2.929119
7	1.353756	-0.659884	2.206786
6	1.065214	0.461053	3.116262
6	2.370866	1.167693	3.596519
6	2.375748	2.637614	3.260245
6	3.412659	3.357465	2.835912
6	2.032199	1.032947	-1.151193
6	2.878813	2.135901	-1.486898
6	3.452800	2.146770	-2.793570
7	3.205442	1.188419	-3.731038
6	2.392709	0.215602	-3.398104
6	1.792969	0.091753	-2.122900
6	4.321002	3.206477	-3.151520
6	4.606897	4.222797	-2.276539
6	4.013221	4.223741	-0.988436
6	3.164649	3.205879	-0.609354
9	-7.141391	3.450705	1.732734
9	-5.123622	3.930681	2.344839
9	-7.964729	0.216088	-1.765754
9	-6.717146	-1.456248	-1.206699
1	2.268499	-1.095396	0.401581
1	4.327035	-0.366036	1.167061
1	3.745775	1.290589	1.088513
1	1.467514	-2.127358	3.682556
1	2.388767	-2.470860	2.209543
1	3.335529	-1.085798	4.659385
1	4.279134	-1.683239	3.284325
1	4.501716	0.777557	3.396728
1	2.403979	1.098379	4.693165
1	0.505527	0.046761	3.960861
1	0.398223	1.163589	2.605225
1	1.420948	3.143973	3.410897
1	3.312942	4.420086	2.637797
1	4.393626	2.922457	2.660137
1	1.419088	1.812570	0.764531
1	1.128141	-0.748505	-1.936523
1	2.720993	3.263622	0.377945
1	2.189316	-0.535308	-4.160126
1	4.746891	3.188344	-4.149641
1	5.272502	5.021915	-2.579978
1	-0.226839	-0.451029	-0.175242
1	-2.050216	-0.139636	-0.749216
1	-3.343677	2.861934	1.057673
1	-4.041257	-0.365239	-1.704932
1	-7.352799	1.931574	-0.195208
8	4.232375	5.196600	-0.067297
6	5.041281	6.296641	-0.436177
1	5.057493	6.960479	0.428390
1	6.067307	5.986288	-0.666902
1	4.621290	6.835330	-1.293580
1	-0.278985	-1.431263	2.102107

[6]*_anti*

Number of imaginary frequencies : 0

Electronic energy= -3467.733534
Zero-point correction= 0.937882
Thermal correction to Energy= 0.996572
Thermal correction to Enthalpy= 0.997517
Thermal correction to Gibbs Free Energy= 0.842424
Sum of electronic and zero-point Energies= -3466.795471
Sum of electronic and thermal Energies= -3466.736781
Sum of electronic and thermal Enthalpies= -3466.735837
Sum of electronic and thermal Free Energies= -3466.890929

Cartesian Coordinates

6	4.478504	-0.207263	-1.456330
6	3.974999	1.153325	-1.924378
7	2.965415	0.799037	-2.955084
6	3.044518	-0.634451	-3.321261
6	4.367328	-1.083035	-2.707333
6	2.055153	1.592576	-3.381187
6	1.913851	2.995797	-2.912546
6	1.127539	3.880420	-3.880841
6	1.802511	-1.407176	-2.747029
8	1.988641	-2.608383	-2.508524
8	0.743086	-0.737574	-2.608157
1	3.007279	-0.723180	-4.410276
1	4.333339	-2.148907	-2.486523
1	5.198278	-0.884502	-3.391414
1	3.808214	-0.571751	-0.672069
1	5.490760	-0.155344	-1.053523
1	3.485103	1.726501	-1.136623
1	4.754561	1.746304	-2.414428
1	1.408715	2.919957	-1.934355
1	1.144461	0.328038	-1.136008
8	1.364103	0.926343	-0.398359
1	1.638620	3.909516	-4.848974
1	0.495598	0.972270	0.042017
1	2.904682	3.424040	-2.718532
7	1.078688	-2.311259	0.158736
6	2.305136	-2.180162	0.804572
6	3.358569	-2.979253	0.346070
6	4.638248	-2.804357	0.860394
6	4.901261	-1.863659	1.848068
6	3.840726	-1.082288	2.299065
6	2.557297	-1.215343	1.788309
6	5.770197	-3.572876	0.247412
9	6.225072	-2.956745	-0.865294
6	4.113202	0.013475	3.287550
9	4.470063	1.156225	2.664385
6	-0.167023	-1.911505	0.570763
16	-0.618432	-1.748209	2.188573
7	-0.985342	-1.724000	-0.480546
6	-2.359493	-1.271677	-0.387971
6	-2.457915	0.144500	-0.988144
6	-3.891122	0.729524	-0.970426
6	-3.788408	2.238338	-0.682115
6	-2.720734	2.847900	-1.604472
6	-1.353612	2.227134	-1.213934
7	-1.525315	1.069967	-0.324211
6	-2.073660	1.522248	0.964016
6	-3.310720	2.450413	0.764389
6	-4.321565	2.194243	1.846750
6	-5.595220	1.838814	1.693050
6	-3.300590	-2.214092	-1.120048

6	-4.577946	-2.583302	-0.587966
6	-5.398643	-3.428563	-1.392662
7	-5.023228	-3.897145	-2.617492
6	-3.843610	-3.543829	-3.062593
6	-2.951745	-2.704523	-2.353507
6	-6.672815	-3.808899	-0.907780
6	-7.132189	-3.379235	0.310776
6	-6.315173	-2.539240	1.110790
6	-5.064772	-2.158835	0.670750
9	6.816240	-3.685850	1.076984
9	5.407359	-4.807636	-0.122110
9	5.114951	-0.295236	4.121743
9	3.038609	0.308630	4.033718
1	-2.106499	0.058878	-2.026797
1	-4.392883	0.544790	-1.925872
1	-4.491832	0.249356	-0.192717
1	-0.724467	2.947354	-0.685387
1	-0.790238	1.891289	-2.094305
1	-2.699756	3.935918	-1.476813
1	-2.964646	2.635129	-2.651974
1	-4.754208	2.726748	-0.843631
1	-2.970704	3.493893	0.858702
1	-1.280896	2.031392	1.521015
1	-2.340456	0.634682	1.545262
1	-3.925262	2.290363	2.859537
1	-6.232073	1.649837	2.551742
1	-6.052405	1.720372	0.714292
1	-2.606058	-1.243756	0.673158
1	-1.989318	-2.465394	-2.798009
1	-4.479251	-1.522113	1.325410
1	-3.552371	-3.927875	-4.038708
1	-7.275732	-4.453925	-1.538618
1	-8.112725	-3.687136	0.653618
1	-0.511521	-1.554138	-1.374267
1	1.158103	-2.648641	-0.805813
1	3.175143	-3.708348	-0.437144
1	1.759267	-0.567563	2.125033
1	5.898837	-1.741226	2.254303
8	-6.694198	-2.065715	2.324090
6	-7.964217	-2.441477	2.818826
1	-8.061512	-1.962228	3.793246
1	-8.771802	-2.090865	2.165329
1	-8.043570	-3.527483	2.945563
1	0.134108	3.447844	-4.053572
1	1.351151	1.178190	-4.099574
6	0.981871	5.317833	-3.347753
1	0.563473	5.946123	-4.140260
1	1.972970	5.714826	-3.099412
6	0.090205	5.356336	-2.145006
6	0.517063	5.391185	-0.880126
1	-0.982943	5.269729	-2.319957
1	1.578693	5.444637	-0.647717
6	-0.455640	5.249569	0.241863
8	-1.591417	5.687463	0.155383
6	-0.022029	4.460719	1.435985
6	1.052472	3.569270	1.355188
6	-0.787155	4.516679	2.606031
6	1.358037	2.737278	2.427866
1	1.626461	3.477427	0.437933
6	-0.471920	3.695841	3.682554
1	-1.631605	5.197951	2.646656
6	0.598044	2.802423	3.592930
1	2.184435	2.040432	2.345181
1	-1.065358	3.740461	4.590203
1	0.835948	2.148901	4.426438

Number of imaginary frequencies : 1
The smallest frequency is : -1247.9007

Electronic energy= -3467.7017948
Zero-point correction= 0.930635
Thermal correction to Energy= 0.989309
Thermal correction to Enthalpy= 0.990253
Thermal correction to Gibbs Free Energy= 0.827782
Sum of electronic and zero-point Energies= -3466.771160
Sum of electronic and thermal Energies= -3466.712486
Sum of electronic and thermal Enthalpies= -3466.711541
Sum of electronic and thermal Free Energies= -3466.874013

.....
Cartesian Coordinates

.....
6 -2.994654 1.920086 -1.441691
6 -3.384885 0.498721 -1.017694
7 -2.793142 -0.354247 -2.065299
6 -2.081118 0.450316 -3.070467
6 -2.760532 1.809355 -2.952180
6 -2.686790 -1.657885 -1.973707
6 -2.980942 -2.429914 -0.829903
6 -3.077167 -3.934010 -1.000046
6 -0.567725 0.508531 -2.695071
8 0.049941 1.552041 -2.943032
8 -0.091867 -0.537505 -2.151932
1 -2.178588 -0.014516 -4.056045
1 -2.124179 2.602918 -3.341420
1 -3.710440 1.804930 -3.495435
1 -2.059370 2.206737 -0.949650
1 -3.754127 2.655249 -1.173078
1 -2.977192 0.220728 -0.040917
1 -4.468695 0.338881 -1.005611
1 -1.819212 -2.018194 -0.217024
1 -0.568289 -0.871712 -0.585336
8 -0.848239 -1.318137 0.253931
1 -2.356929 -4.263529 -1.758175
1 0.016665 -1.802021 0.571325
1 -3.701748 -1.995435 -0.133876
7 1.238647 1.893129 -0.324147
6 0.705247 3.106839 0.118230
6 0.047814 3.875708 -0.853685
6 -0.604417 5.047126 -0.499123
6 -0.603727 5.513071 0.810111
6 0.060986 4.749082 1.761260
6 0.701154 3.554774 1.444440
6 -1.345854 5.779796 -1.578334
9 -2.289084 4.995543 -2.139783
6 0.122654 5.216646 3.188037
9 -0.122234 4.216572 4.049479
6 2.093722 1.009106 0.280694
16 3.068692 1.356426 1.614003
7 2.077272 -0.190460 -0.338647
6 3.061978 -1.239609 -0.155035
6 2.393345 -2.625702 -0.020539
6 3.449046 -3.702944 0.355032
6 3.067770 -4.328816 1.705895
6 1.717749 -5.036575 1.537824
6 0.703575 -3.999466 0.997329
7 1.286135 -2.639802 0.966818
6 1.761437 -2.285249 2.317390
6 2.899946 -3.242901 2.786348
6 4.152359 -2.483515 3.148777
6 5.407635 -2.841407 2.887344
6 4.028939 -1.265914 -1.338338
6 5.449248 -1.196733 -1.182070
6 6.239469 -1.277104 -2.367958
7 5.708899 -1.392523 -3.618447
6 4.403545 -1.423067 -3.720237

6	3.525023	-1.366443	-2.612010
6	7.649865	-1.234563	-2.254216
6	8.265598	-1.118016	-1.034586
6	7.477444	-1.026412	0.141320
6	6.101105	-1.057980	0.064528
9	-1.966034	6.873384	-1.117796
9	-0.535540	6.165901	-2.573994
9	-0.768576	6.187784	3.438817
9	1.333257	5.703457	3.499294
1	1.926211	-2.864612	-0.984576
1	3.490360	-4.483513	-0.411194
1	4.444611	-3.255419	0.409638
1	-0.196738	-3.954778	1.618926
1	0.388135	-4.239748	-0.023523
1	1.382399	-5.443600	2.496984
1	1.816369	-5.875487	0.842472
1	3.831859	-5.048651	2.013964
1	2.557920	-3.744159	3.702670
1	0.895143	-2.340359	2.983242
1	2.092745	-1.242246	2.304881
1	3.980092	-1.555629	3.696284
1	6.243260	-2.223760	3.201429
1	5.655904	-3.749686	2.343859
1	3.599757	-1.010866	0.765784
1	2.451661	-1.391526	-2.789068
1	5.545443	-0.961336	0.989733
1	3.991199	-1.504034	-4.724213
1	8.227091	-1.296397	-3.171028
1	9.347259	-1.088657	-0.980106
1	1.433260	-0.297997	-1.132296
1	0.990780	1.678948	-1.296958
1	0.024528	3.526301	-1.883227
1	1.186310	2.977432	2.219209
1	-1.112894	6.429850	1.080246
8	8.007273	-0.904455	1.385278
6	9.412769	-0.796550	1.503957
1	9.615683	-0.672597	2.567951
1	9.918930	-1.700958	1.146448
1	9.796522	0.075921	0.962718
1	-2.795997	-4.434506	-0.066260
1	-2.182680	-2.133619	-2.815039
6	-4.485745	-4.411235	-1.407938
1	-4.442072	-5.482980	-1.639252
1	-4.806381	-3.886788	-2.315379
6	-5.471029	-4.200137	-0.304726
6	-6.538450	-3.397159	-0.347645
1	-5.287753	-4.735347	0.628174
1	-6.779607	-2.844128	-1.250418
6	-7.429494	-3.291528	0.841571
8	-7.261088	-4.008351	1.814559
6	-8.553286	-2.298917	0.831943
6	-8.649064	-1.256306	-0.094376
6	-9.530530	-2.425443	1.825375
6	-9.709894	-0.356940	-0.027741
1	-7.891428	-1.122703	-0.859561
6	-10.593285	-1.534857	1.884769
1	-9.434178	-3.233582	2.542577
6	-10.684181	-0.497860	0.956758
1	-9.775280	0.454958	-0.744937
1	-11.350992	-1.645216	2.653868
1	-11.513248	0.201440	1.002969

[7] *anti*

Number of imaginary frequencies : 0

Electronic energy= -3467.7408058

Zero-point correction=	0.937123
Thermal correction to Energy=	0.996353
Thermal correction to Enthalpy=	0.997298
Thermal correction to Gibbs Free Energy=	0.837879
Sum of electronic and zero-point Energies=	-3466.803683
Sum of electronic and thermal Energies=	-3466.744452
Sum of electronic and thermal Enthalpies=	-3466.743508
Sum of electronic and thermal Free Energies=	-3466.902927

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

6	4.264513	0.571600	-2.884112
6	4.029978	2.004500	-2.404290
7	2.703464	2.319069	-2.906926
6	2.199710	1.302991	-3.835503
6	3.457256	0.507731	-4.184624
6	2.124821	3.535710	-2.689224
6	2.650357	4.534140	-1.946943
6	2.007975	5.880942	-1.772280
6	1.121174	0.453859	-3.128766
8	1.266177	-0.780147	-3.045135
8	0.144567	1.110820	-2.637763
1	1.736947	1.780726	-4.707244
1	3.216579	-0.511449	-4.486633
1	3.998347	1.009804	-4.993135
1	3.844497	-0.135299	-2.161957
1	5.322785	0.339070	-3.015635
1	4.062177	2.098049	-1.310741
1	4.770820	2.706734	-2.818416
1	1.036945	3.163595	-0.416604
1	0.587541	1.907400	-1.210097
8	0.582900	2.314388	-0.311089
1	2.489911	6.629041	-2.416244
1	-0.996129	2.076708	0.136882
1	3.631607	4.403731	-1.493993
7	0.796233	-1.494707	-0.404202
6	1.936328	-2.131958	0.083845
6	2.886013	-2.492503	-0.883581
6	4.088880	-3.069010	-0.504007
6	4.383286	-3.314259	0.832405
6	3.432921	-2.952051	1.780142
6	2.219901	-2.364857	1.434503
6	5.058662	-3.474390	-1.576186
9	5.066410	-2.599575	-2.595966
6	3.768927	-3.111111	3.234214
9	4.431465	-2.032845	3.705118
6	-0.407813	-1.223098	0.168595
16	-0.995714	-1.888365	1.605449
7	-1.107178	-0.338951	-0.583675
6	-2.536842	-0.135020	-0.512515
6	-2.843114	1.368217	-0.632275
6	-4.335339	1.696282	-0.397131
6	-4.478206	2.607015	0.831230
6	-3.769175	3.935610	0.535809
6	-2.316952	3.636746	0.117147
7	-2.028509	2.181426	0.338048
6	-2.293391	1.814801	1.764791
6	-3.807107	1.972518	2.064838
6	-4.419201	0.677283	2.542241
6	-5.643109	0.233713	2.266866
6	-3.256636	-0.866054	-1.646068
6	-4.386312	-1.714804	-1.421425
6	-5.010553	-2.281770	-2.572491
7	-4.567096	-2.077630	-3.845120
6	-3.507936	-1.323917	-4.002967
6	-2.822191	-0.691994	-2.937012
6	-6.150034	-3.103309	-2.398102
6	-6.659201	-3.365408	-1.152139
6	-6.026412	-2.814736	-0.008627
6	-4.911637	-2.014467	-0.143911

9	6.313779	-3.558462	-1.109908
9	4.754376	-4.672307	-2.098418
9	4.559075	-4.169843	3.456918
9	2.678456	-3.250066	4.000417
1	-2.505639	1.704447	-1.618918
1	-4.753828	2.194324	-1.276116
1	-4.894690	0.769106	-0.252625
1	-1.588249	4.186895	0.714242
1	-2.130681	3.830368	-0.941869
1	-3.780665	4.573461	1.424163
1	-4.286522	4.470872	-0.264305
1	-5.535932	2.790194	1.036851
1	-3.896593	2.692659	2.888956
1	-1.677470	2.490325	2.361599
1	-1.931518	0.793301	1.914559
1	-3.780153	0.078926	3.192644
1	-6.000442	-0.709697	2.667667
1	-6.331188	0.776516	1.623130
1	-2.877528	-0.507891	0.454610
1	-1.948903	-0.080665	-3.157891
1	-4.453087	-1.639079	0.762739
1	-3.154620	-1.180716	-5.022272
1	-6.605238	-3.520892	-3.290177
1	-7.533003	-3.998063	-1.051536
1	-0.641742	0.058817	-1.418577
1	0.868344	-1.252912	-1.408496
1	2.677078	-2.293054	-1.931997
1	1.507176	-2.085257	2.198609
1	5.322972	-3.767812	1.126317
8	-6.459309	-3.032125	1.259933
6	-7.577158	-3.879506	1.446433
1	-7.735172	-3.935721	2.523599
1	-8.477352	-3.469817	0.973193
1	-7.387205	-4.887119	1.059550
1	0.954047	5.843919	-2.077333
1	1.150280	3.654924	-3.161459
6	2.117180	6.405100	-0.320912
1	1.786768	7.448964	-0.290977
1	3.170498	6.383005	-0.019918
6	1.297235	5.600456	0.634219
6	1.770788	4.636452	1.433414
1	0.223204	5.790730	0.652857
1	2.831742	4.403162	1.449454
6	0.854226	3.866574	2.316331
8	-0.285152	4.265994	2.536328
6	1.339777	2.600178	2.936037
6	2.397510	1.867958	2.388132
6	0.677478	2.117251	4.070209
6	2.787503	0.667073	2.971037
1	2.889209	2.212008	1.484271
6	1.072895	0.921167	4.654229
1	-0.140927	2.698547	4.484184
6	2.128864	0.195087	4.104517
1	3.600361	0.091954	2.539968
1	0.561016	0.551480	5.536852
1	2.436093	-0.742880	4.555998

[6]_{syn}

Number of imaginary frequencies : 0

Electronic energy=	-3467.7236918
Zero-point correction=	0.936011
Thermal correction to Energy=	0.995683
Thermal correction to Enthalpy=	0.996627
Thermal correction to Gibbs Free Energy=	0.833500
Sum of electronic and zero-point Energies=	-3466.787681

Sum of electronic and thermal Energies=	-3466.728009
Sum of electronic and thermal Enthalpies=	-3466.727065
Sum of electronic and thermal Free Energies=	-3466.890192

Cartesian Coordinates

6	4.589021	-1.703516	3.378486
6	4.509055	-2.765154	2.274238
7	3.116611	-3.293641	2.358927
6	2.315905	-2.499850	3.311261
6	3.385701	-1.999450	4.287451
6	2.696188	-4.294328	1.682470
6	1.343584	-4.906267	1.797277
6	1.274128	-6.221668	1.013827
6	1.688791	-1.311495	2.531818
8	2.380552	-0.905939	1.553135
8	0.621514	-0.858305	2.958955
1	1.538427	-3.113793	3.764180
1	3.038659	-1.122808	4.836836
1	3.622980	-2.788743	5.007105
1	4.494709	-0.710750	2.938216
1	5.536070	-1.762235	3.916010
1	4.664004	-2.354555	1.276774
1	5.186047	-3.604760	2.443947
1	0.625637	-4.170952	1.402518
8	0.618108	-2.464888	-0.028807
1	0.464570	-6.836392	1.418349
1	1.119956	-5.057595	2.859856
7	1.793657	1.328755	0.042548
6	2.936634	1.726702	-0.644346
6	4.084033	0.963136	-0.351755
6	5.298292	1.258247	-0.938222
6	5.430705	2.316504	-1.837546
6	4.297009	3.061958	-2.117911
6	3.054526	2.791655	-1.540916
6	6.491878	0.399732	-0.641562
9	7.590906	1.131971	-0.410604
6	4.374819	4.224526	-3.067488
9	5.614215	4.401867	-3.549944
6	0.477006	1.681223	-0.046414
16	-0.182157	2.795471	-1.130879
7	-0.271531	0.994320	0.838988
6	-1.697504	1.168073	1.027434
6	-2.322671	-0.179430	1.446257
6	-3.875564	-0.113456	1.395003
6	-4.380665	-1.134407	0.361422
6	-3.981635	-2.538143	0.840058
6	-2.449805	-2.538275	1.081672
7	-1.829184	-1.288953	0.609095
6	-2.176234	-1.081274	-0.803166
6	-3.710762	-0.901423	-1.006878
6	-4.042063	0.401641	-1.688046
6	-5.060058	1.215066	-1.412926
6	-1.990943	2.218374	2.096139
6	-2.924595	3.285064	1.907413
6	-3.157899	4.152570	3.016308
7	-2.523073	4.025526	4.216246
6	-1.654592	3.051515	4.337831
6	-1.359493	2.123166	3.311872
6	-4.096047	5.203822	2.876327
6	-4.775630	5.404743	1.702190
6	-4.528958	4.550722	0.596908
6	-3.619940	3.520184	0.699211
9	6.301532	-0.384387	0.436879
9	6.785690	-0.419670	-1.665328
9	4.011804	5.371934	-2.474287
9	3.558436	4.061110	-4.119613
1	-1.976413	-0.401881	2.462380
1	-4.301757	-0.346010	2.376542
1	-4.210086	0.893714	1.132000

1	-1.963220	-3.370258	0.560487
1	-2.210174	-2.635590	2.146027
1	-4.253953	-3.285064	0.085076
1	-4.519443	-2.791700	1.759088
1	-5.468889	-1.066029	0.264574
1	-4.050549	-1.699914	-1.681230
1	-1.808624	-1.956473	-1.346309
1	-1.617608	-0.216701	-1.178544
1	-3.368763	0.672245	-2.503906
1	-5.216354	2.130282	-1.975591
1	-5.768411	1.013324	-0.613248
1	-2.116773	1.485657	0.071300
1	-0.632740	1.334276	3.494095
1	-3.451358	2.908767	-0.179063
1	-1.149346	2.964378	5.298323
1	-4.258169	5.847282	3.735037
1	-5.487969	6.217716	1.626204
1	0.176208	0.352908	1.501671
1	1.980028	0.550920	0.695110
1	3.998817	0.138201	0.348293
1	2.193858	3.400393	-1.783297
1	6.384942	2.550421	-2.295029
8	-5.152764	4.685474	-0.603146
6	-6.039586	5.772798	-0.773379
1	-6.398372	5.711147	-1.801191
1	-6.896399	5.707394	-0.092148
1	-5.532516	6.733954	-0.628572
1	2.197836	-6.789093	1.174184
1	-0.145230	-1.940262	0.315349
1	1.375949	-1.888190	0.145887
1	3.421422	-4.730279	0.992574
6	1.040864	-5.993068	-0.491193
1	1.451516	-6.844063	-1.048094
1	1.562298	-5.090507	-0.831796
6	-0.419225	-5.892284	-0.804757
6	-1.032049	-4.878235	-1.421554
1	-1.034337	-6.742041	-0.505397
1	-0.474228	-3.994048	-1.718064
6	-2.503450	-4.971186	-1.657481
8	-3.185554	-5.757211	-1.018021
6	-3.149677	-4.091870	-2.685400
6	-2.427522	-3.239575	-3.526554
6	-4.546142	-4.132803	-2.784926
6	-3.096028	-2.418826	-4.431135
1	-1.344091	-3.203711	-3.481003
6	-5.211552	-3.319756	-3.692668
1	-5.089324	-4.808520	-2.132190
6	-4.486125	-2.453634	-4.511169
1	-2.529438	-1.751369	-5.072313
1	-6.294295	-3.351990	-3.758853
1	-5.004410	-1.807055	-5.212467

[6-7]TS-syn

Number of imaginary frequencies : 1
The smallest frequency is : -1167.3438

Electronic energy=	-3467.7056651
Zero-point correction=	0.930753
Thermal correction to Energy=	0.989759
Thermal correction to Enthalpy=	0.990704
Thermal correction to Gibbs Free Energy=	0.826225
Sum of electronic and zero-point Energies=	-3466.774912
Sum of electronic and thermal Energies=	-3466.715906
Sum of electronic and thermal Enthalpies=	-3466.714962
Sum of electronic and thermal Free Energies=	-3466.879440

Cartesian Coordinates

6	1.234225	4.146674	3.082344
6	2.524054	3.934650	2.292133
7	2.590202	2.468521	2.127854
6	1.630130	1.766544	2.990553
6	1.130987	2.874013	3.930794
6	3.296454	1.860613	1.207962
6	3.248317	0.485969	0.884454
6	4.427191	-0.075687	0.105683
6	0.485888	1.199902	2.121212
8	0.067104	1.969879	1.203523
8	0.074456	0.056835	2.378786
1	2.122418	0.943463	3.513925
1	0.117610	2.675305	4.285091
1	1.791386	2.936634	4.801134
1	0.387072	4.210667	2.397462
1	1.273781	5.054476	3.686344
1	2.521409	4.417328	1.313133
1	3.401575	4.266803	2.856964
1	2.182252	0.462394	0.027738
8	1.151700	0.373470	-0.723060
1	4.705394	0.618958	-0.696349
1	2.863503	-0.166051	1.674451
7	-2.412111	1.484174	0.028357
6	-2.984959	2.682017	-0.404402
6	-2.178303	3.821583	-0.252581
6	-2.665466	5.073379	-0.584445
6	-3.955068	5.238238	-1.086079
6	-4.742042	4.105511	-1.229097
6	-4.285759	2.832656	-0.889687
6	-1.771345	6.271521	-0.455726
9	-2.442213	7.349617	-0.023367
6	-6.136314	4.222788	-1.777363
9	-6.549108	5.497752	-1.837681
6	-2.664496	0.185776	-0.307472
16	-3.818988	-0.328944	-1.428917
7	-1.827961	-0.659170	0.335243
6	-1.920522	-2.105125	0.286137
6	-0.508939	-2.721694	0.244124
6	-0.581552	-4.252464	-0.010058
6	0.144753	-4.576091	-1.324452
6	1.621494	-4.192387	-1.161882
6	1.682720	-2.701939	-0.747291
7	0.342661	-2.078067	-0.785010
6	-0.224811	-2.240782	-2.138112
6	-0.435084	-3.745917	-2.486945
6	-1.871438	-4.041922	-2.843233
6	-2.565975	-5.129159	-2.516080
6	-2.678681	-2.655119	1.493001
6	-3.792780	-3.544701	1.366521
6	-4.365157	-4.048318	2.573112
7	-3.925404	-3.700799	3.815742
6	-2.925974	-2.856953	3.886693
6	-2.267025	-2.313222	2.758050
6	-5.448283	-4.956270	2.490378
6	-5.957459	-5.354351	1.280922
6	-5.397897	-4.839116	0.083907
6	-4.344805	-3.950775	0.129968
9	-0.759685	6.058340	0.403331
9	-1.216319	6.609353	-1.631125
9	-7.021822	3.549904	-1.027267
9	-6.223993	3.721237	-3.019226
1	-0.020292	-2.506431	1.202145
1	-0.111242	-4.799561	0.813047
1	-1.623721	-4.579020	-0.058221
1	2.326478	-2.123925	-1.418565
1	2.068926	-2.580298	0.270758
1	2.157865	-4.355587	-2.102052
1	2.092847	-4.823065	-0.402309

1	0.059247	-5.643683	-1.547824
1	0.166568	-3.967890	-3.379356
1	0.473866	-1.763819	-2.831873
1	-1.162999	-1.678923	-2.191142
1	-2.361989	-3.272657	-3.442091
1	-3.599248	-5.249036	-2.826789
1	-2.144203	-5.932664	-1.917223
1	-2.452339	-2.362747	-0.629691
1	-1.439351	-1.623551	2.907617
1	-3.972389	-3.565046	-0.810980
1	-2.590748	-2.578742	4.884365
1	-5.862148	-5.325997	3.422870
1	-6.787398	-6.050264	1.250089
1	-1.212723	-0.291225	1.074140
1	-1.553368	1.631717	0.581164
1	-1.170924	3.706738	0.136793
1	-4.934666	1.973315	-0.992466
1	-4.335428	6.219914	-1.343688
8	-5.847337	-5.173206	-1.153999
6	-6.976832	-6.019074	-1.247778
1	-7.183786	-6.127581	-2.312733
1	-6.778345	-7.008968	-0.820032
1	-7.851603	-5.578127	-0.755853
1	4.129097	-1.006895	-0.388562
1	0.715637	-0.577435	-0.653208
1	0.553439	1.010108	-0.276693
1	3.912516	2.519196	0.592687
6	5.659562	-0.351088	0.985739
1	5.360492	-1.026556	1.798603
1	5.999536	0.582529	1.449745
6	6.768307	-0.980076	0.205627
6	7.982600	-0.453375	0.025566
1	6.560382	-1.937160	-0.274436
1	8.240108	0.503344	0.470146
6	8.987579	-1.161808	-0.814861
8	8.680718	-2.146934	-1.466126
6	10.389306	-0.633024	-0.869727
6	10.902690	0.255784	0.079385
6	11.212396	-1.078176	-1.909631
6	12.219239	0.697661	-0.016459
1	10.291133	0.588949	0.911419
6	12.521481	-0.627279	-2.011427
1	10.801798	-1.778129	-2.629870
6	13.026507	0.263087	-1.063964
1	12.614820	1.381444	0.727652
1	13.151149	-0.968424	-2.826927
1	14.050346	0.615665	-1.141247

[7]_syn

Number of imaginary frequencies : 0

Electronic energy= -3467.7393421
Zero-point correction= 0.938014
Thermal correction to Energy= 0.997719
Thermal correction to Enthalpy= 0.998663
Thermal correction to Gibbs Free Energy= 0.836612
Sum of electronic and zero-point Energies= -3466.801328
Sum of electronic and thermal Energies= -3466.741623
Sum of electronic and thermal Enthalpies= -3466.740679
Sum of electronic and thermal Free Energies= -3466.902730

Cartesian Coordinates

6	4.026788	-0.414496	4.396769
6	4.678399	-1.526294	3.560200
7	3.569858	-2.430128	3.244744

6	2.300005	-1.930197	3.714599
6	2.717813	-1.039314	4.896118
6	3.677835	-3.397887	2.291826
6	2.702682	-4.145901	1.730108
6	3.048811	-5.288919	0.812660
6	1.571839	-1.074996	2.664385
8	2.293983	-0.467352	1.819450
8	0.321432	-0.994517	2.741609
1	1.639452	-2.748573	4.019679
1	1.953199	-0.301445	5.150139
1	2.896864	-1.670456	5.771797
1	3.803288	0.440686	3.755808
1	4.671309	-0.078431	5.211405
1	5.135452	-1.124350	2.649194
1	5.450989	-2.064126	4.124565
1	1.363832	-2.816645	0.146533
8	1.054099	-1.956427	-0.173314
1	2.699616	-6.242056	1.235423
1	1.659776	-4.002972	2.016844
7	1.510874	1.571445	0.114813
6	2.592838	2.044182	-0.632797
6	3.809864	1.379377	-0.403506
6	4.959780	1.786177	-1.055820
6	4.944828	2.852568	-1.953390
6	3.740098	3.505667	-2.161789
6	2.564877	3.126602	-1.513757
6	6.244900	1.040816	-0.839895
9	7.288929	1.876498	-0.728794
6	3.665853	4.649748	-3.133243
9	4.881729	5.116117	-3.454834
6	0.166598	1.677766	-0.063091
16	-0.618426	2.505133	-1.306532
7	-0.504051	0.974701	0.882360
6	-1.944932	0.905692	1.006678
6	-2.337417	-0.521172	1.437945
6	-3.846902	-0.810663	1.287186
6	-4.057387	-1.917782	0.241270
6	-3.401925	-3.208151	0.756104
6	-1.932547	-2.912904	1.112393
7	-1.585376	-1.539679	0.627551
6	-1.860094	-1.417747	-0.837351
6	-3.382812	-1.543082	-1.093085
6	-3.932469	-0.321114	-1.789007
6	-5.117568	0.246298	-1.577584
6	-2.480451	1.886050	2.045565
6	-3.571637	2.771400	1.783010
6	-4.009931	3.595766	2.862214
7	-3.434065	3.585541	4.097357
6	-2.425885	2.771792	4.289878
6	-1.917733	1.899979	3.297407
6	-5.100650	4.473983	2.653137
6	-5.739986	4.544046	1.442150
6	-5.296645	3.729060	0.368782
6	-4.232862	2.868330	0.537200
9	6.215624	0.284743	0.268174
9	6.519505	0.219303	-1.866912
9	2.959099	5.676284	-2.638201
9	3.067960	4.289167	-4.280055
1	-1.990453	-0.683377	2.460480
1	-4.263342	-1.129643	2.246675
1	-4.369401	0.102837	0.993237
1	-1.231995	-3.601813	0.635130
1	-1.737531	-2.911890	2.186711
1	-3.451052	-3.991488	-0.006043
1	-3.929175	-3.574306	1.640589
1	-5.126000	-2.084321	0.083291
1	-3.523240	-2.387358	-1.781255
1	-1.279130	-2.210560	-1.309200
1	-1.449580	-0.461094	-1.172277
1	-3.280555	0.097417	-2.557109

1	-5.430647	1.114762	-2.148525
1	-5.817196	-0.120035	-0.830118
1	-2.372558	1.125973	0.027170
1	-1.084104	1.243527	3.538391
1	-3.919233	2.286300	-0.321400
1	-1.973061	2.777373	5.279578
1	-5.412094	5.090529	3.489959
1	-6.571713	5.226142	1.312805
1	0.017034	0.462642	1.606006
1	1.793315	0.895782	0.845621
1	3.837470	0.549667	0.297863
1	1.646092	3.669807	-1.687260
1	5.848642	3.169737	-2.461313
8	-5.869492	3.738918	-0.861800
6	-6.928253	4.647406	-1.098231
1	-7.210271	4.514234	-2.142942
1	-7.795462	4.430245	-0.463632
1	-6.611119	5.684894	-0.942650
1	4.139667	-5.366772	0.749392
1	-0.563189	-1.428893	0.757459
1	1.644614	-1.335842	0.294901
1	4.710429	-3.593466	2.000183
6	2.498089	-5.184191	-0.621028
1	2.963958	-5.979036	-1.221215
1	2.787308	-4.229429	-1.076190
6	1.018834	-5.382509	-0.712870
6	0.195230	-4.700055	-1.519572
1	0.585731	-6.182907	-0.110206
1	0.584834	-3.902106	-2.143563
6	-1.243571	-5.068144	-1.588657
8	-1.741973	-5.807209	-0.750619
6	-2.100226	-4.513209	-2.688791
6	-1.648624	-3.562013	-3.610823
6	-3.430842	-4.947617	-2.750588
6	-2.522883	-3.034491	-4.557905
1	-0.622399	-3.211837	-3.596632
6	-4.298328	-4.429802	-3.703582
1	-3.763826	-5.692521	-2.035128
6	-3.846783	-3.464160	-4.603512
1	-2.166686	-2.288598	-5.260830
1	-5.327035	-4.773067	-3.744282
1	-4.526433	-3.050088	-5.341594

[8]

Number of imaginary frequencies : 0

Electronic energy=	-3905.3030147
Zero-point correction=	1.052055
Thermal correction to Energy=	1.119025
Thermal correction to Enthalpy=	1.119969
Thermal correction to Gibbs Free Energy=	0.944655
Sum of electronic and zero-point Energies=	-3904.250960
Sum of electronic and thermal Energies=	-3904.183989
Sum of electronic and thermal Enthalpies=	-3904.183045
Sum of electronic and thermal Free Energies=	-3904.358360

Cartesian Coordinates

6	-1.571716	-1.009121	5.300472
6	-2.805668	-1.873438	5.028677
6	-3.845781	-0.834984	4.616043
7	-3.052430	0.166946	3.905308
6	-1.624980	0.016703	4.150428
6	-3.618683	1.358655	3.524367
6	-3.007063	2.445205	3.016802
8	-0.032241	1.981398	-1.174152

8	-0.417342	1.504836	0.890659
1	-1.176998	0.976325	4.432883
1	-0.633570	-1.568331	5.309765
1	-1.676461	-0.491328	6.259713
1	-4.627225	-1.251744	3.969773
1	-4.335334	-0.397087	5.499719
1	-1.932167	2.438823	2.837710
6	-3.763887	3.710118	2.718218
1	-4.840481	3.517128	2.787039
6	-2.933009	0.743468	0.244079
1	-2.493527	0.439413	1.190346
1	-2.378243	1.681017	-1.646949
6	-4.281605	0.261212	-0.014029
6	-4.798170	-0.674890	0.893993
6	-5.031401	0.623620	-1.142084
6	-6.048702	-1.239934	0.677010
1	-4.176536	-0.965666	1.739835
6	-6.281910	0.057982	-1.352670
1	-4.633709	1.337705	-1.856823
6	-6.788857	-0.874635	-0.446512
1	-6.438629	-1.979604	1.368473
1	-6.860118	0.334960	-2.228353
1	-7.760895	-1.325030	-0.621880
7	-0.793442	1.648241	-0.272117
6	-2.158978	1.411637	-0.622799
7	-0.550175	-1.485383	-0.383876
6	-1.605151	-1.805681	-1.245996
6	-1.807615	-1.172631	-2.475225
6	-2.984890	-1.406556	-3.175359
6	-3.962193	-2.278027	-2.702062
6	-3.736435	-2.916606	-1.489077
6	-2.579369	-2.678746	-0.755947
6	-3.236623	-0.586937	-4.405289
9	-2.189066	-0.583910	-5.238998
6	-4.730218	-3.919446	-0.979052
9	-4.429538	-5.164250	-1.385689
6	0.760149	-1.285101	-0.666917
16	1.477718	-1.502663	-2.185417
7	1.437439	-0.870767	0.429487
6	2.877241	-0.803701	0.543290
6	3.219420	0.474448	1.327663
6	4.727344	0.792797	1.391683
6	5.001120	2.129268	0.686276
6	4.260586	3.246343	1.436734
6	2.771618	2.870505	1.563957
7	2.511754	1.661543	0.717100
6	2.930353	1.920507	-0.701677
6	4.468237	2.095826	-0.759638
6	5.112808	1.075605	-1.667993
6	6.302343	0.505693	-1.493347
6	3.449978	-2.010807	1.283185
6	4.540157	-2.784079	0.770909
6	5.009274	-3.859914	1.582807
7	4.465901	-4.183796	2.790337
6	3.457726	-3.461954	3.210938
6	2.915890	-2.365481	2.497453
6	6.095643	-4.642258	1.123229
6	6.704927	-4.385150	-0.078165
6	6.232087	-3.320756	-0.886825
6	5.169069	-2.546021	-0.472700
9	-4.304609	-1.007495	-5.094624
9	-3.465335	0.707281	-4.083204
9	-5.975152	-3.664901	-1.411844
9	-4.767684	-3.952452	0.362384
1	2.776765	0.385458	2.324932
1	5.053629	0.850145	2.433617
1	5.290376	-0.014233	0.916675
1	2.106171	3.662691	1.218027
1	2.484945	2.600519	2.582439
1	4.362883	4.189422	0.890839

1	4.692024	3.389391	2.430339
1	6.074134	2.337067	0.683915
1	4.651608	3.085031	-1.200853
1	2.395464	2.819199	-1.013906
1	2.564156	1.087543	-1.308910
1	4.532818	0.816576	-2.554849
1	6.689303	-0.212902	-2.209102
1	6.928755	0.716396	-0.629847
1	3.291986	-0.749875	-0.464462
1	2.071920	-1.820302	2.915925
1	4.829450	-1.764819	-1.141464
1	3.027538	-3.735285	4.172852
1	6.428958	-5.455544	1.759416
1	7.535106	-5.000882	-0.402830
1	0.928054	-0.767153	1.333782
1	-0.829546	-1.460267	0.633243
1	-1.069420	-0.469955	-2.846798
1	-2.431814	-3.147270	0.212389
1	-4.879852	-2.440752	-3.255227
8	6.775175	-2.999807	-2.090030
6	7.817356	-3.816400	-2.588992
1	8.077544	-3.407850	-3.565839
1	8.701532	-3.785597	-1.941442
1	7.489956	-4.855231	-2.711285
1	1.492641	1.474035	0.724645
6	-0.838269	-0.545423	2.951657
8	-1.475540	-1.243731	2.117352
8	0.397984	-0.313824	2.937184
1	-3.541428	4.477910	3.475093
1	-3.121974	-2.462701	5.891815
1	-2.604923	-2.546069	4.190265
6	-3.452742	4.329753	1.345639
1	-4.081018	5.223439	1.221593
1	-3.708601	3.639253	0.534665
6	-2.025000	4.761379	1.239876
6	-1.247751	4.702540	0.151527
1	-1.575776	5.183303	2.140805
1	-1.629335	4.302714	-0.782981
6	0.153168	5.186195	0.238565
8	0.611079	5.593829	1.298064
6	1.046208	5.143881	-0.969232
6	0.649974	4.639711	-2.211096
6	2.361244	5.601353	-0.806678
6	1.561186	4.568614	-3.262268
1	-0.356568	4.271068	-2.366600
6	3.267833	5.537774	-1.856946
1	2.649148	6.005972	0.158811
6	2.869568	5.010882	-3.086926
1	1.247093	4.161732	-4.217777
1	4.282580	5.900206	-1.721804
1	3.577274	4.950784	-3.908022
1	-4.701965	1.377331	3.654965

[8-9]TS

Number of imaginary frequencies : 1

The smallest frequency is : -250.2911

Electronic energy=	-3905.2911079
Zero-point correction=	1.051978
Thermal correction to Energy=	1.117879
Thermal correction to Enthalpy=	1.118824
Thermal correction to Gibbs Free Energy=	0.945941
Sum of electronic and zero-point Energies=	-3904.239130
Sum of electronic and thermal Energies=	-3904.173229
Sum of electronic and thermal Enthalpies=	-3904.172284
Sum of electronic and thermal Free Energies=	-3904.345167

Cartesian Coordinates

6	-1.168883	-0.086649	5.342617
6	-2.182650	-1.233282	5.442984
6	-3.394889	-0.718043	4.654277
7	-2.834949	0.316173	3.772554
6	-1.384439	0.402943	3.902969
6	-3.605981	1.147331	3.069361
6	-3.219864	2.091125	2.141250
8	-0.281602	1.904683	-1.323639
8	-0.427903	1.170956	0.718293
1	-1.046799	1.429328	3.738459
1	-0.137421	-0.400744	5.508882
1	-1.416106	0.713706	6.047274
1	-3.873057	-1.508349	4.068383
1	-4.147171	-0.264135	5.309523
1	-2.162089	2.318342	2.024155
6	-4.229526	3.123215	1.694460
1	-5.178571	2.630083	1.443783
6	-3.014433	0.564758	0.419172
1	-2.432913	-0.014442	1.131763
1	-2.681440	1.554181	-1.524601
6	-4.388315	0.100656	0.190455
6	-4.835678	-0.998885	0.937602
6	-5.237323	0.666205	-0.769187
6	-6.099752	-1.530988	0.720627
1	-4.155969	-1.442970	1.663592
6	-6.503525	0.129807	-0.985879
1	-4.906870	1.517676	-1.356839
6	-6.933569	-0.969905	-0.246637
1	-6.426534	-2.398678	1.284114
1	-7.152640	0.567295	-1.737711
1	-7.916743	-1.394123	-0.425057
7	-0.961920	1.437515	-0.389918
6	-2.303098	1.224979	-0.568227
7	-0.521417	-1.815879	-0.285889
6	-1.623340	-2.085768	-1.109932
6	-1.889048	-1.360083	-2.275074
6	-3.096606	-1.550277	-2.934103
6	-4.049102	-2.458806	-2.476205
6	-3.759599	-3.187384	-1.330962
6	-2.562875	-3.005144	-0.644557
6	-3.421787	-0.645132	-4.085133
9	-2.375196	-0.464843	-4.899742
6	-4.733983	-4.207294	-0.819803
9	-4.431060	-5.445611	-1.241635
6	0.776387	-1.624348	-0.634447
16	1.393961	-1.839960	-2.198102
7	1.518817	-1.243716	0.425722
6	2.943178	-0.993209	0.432663
6	3.161072	0.391999	1.073205
6	4.621698	0.889355	1.071902
6	4.722453	2.192946	0.263701
6	3.848376	3.267650	0.931335
6	2.415015	2.723735	1.091323
7	2.314625	1.418390	0.368925
6	2.695073	1.603139	-1.068010
6	4.193763	1.975329	-1.166200
6	4.957710	0.976771	-2.002433
6	6.206334	0.563588	-1.801071
6	3.702264	-2.036180	1.245843
6	4.876529	-2.687072	0.751120
6	5.540970	-3.587129	1.636935
7	5.100005	-3.864012	2.896767
6	4.005698	-3.266864	3.298365
6	3.274679	-2.341427	2.514385
6	6.721361	-4.233788	1.198554
6	7.233837	-4.014856	-0.054382
6	6.563630	-3.131458	-0.938106

6	5.409103	-2.489229	-0.543682
9	-4.439188	-1.105393	-4.825336
9	-3.783452	0.584159	-3.652899
9	-5.989284	-3.956724	-1.220864
9	-4.743455	-4.253993	0.524449
1	2.746084	0.350888	2.085099
1	4.954798	1.062462	2.098986
1	5.273722	0.123949	0.644264
1	1.659451	3.375700	0.649306
1	2.140578	2.525922	2.129643
1	3.836599	4.174340	0.317994
1	4.256146	3.534299	1.909710
1	5.761062	2.532331	0.232172
1	4.245561	2.943458	-1.684697
1	2.043452	2.390841	-1.442475
1	2.440060	0.682188	-1.598607
1	4.410836	0.585319	-2.861779
1	6.669271	-0.158059	-2.467212
1	6.808118	0.907389	-0.963319
1	3.289187	-0.994678	-0.601712
1	2.378878	-1.879677	2.925469
1	4.927904	-1.840786	-1.265376
1	3.660038	-3.503548	4.302983
1	7.205403	-4.912237	1.893485
1	8.140001	-4.523374	-0.361259
1	1.051556	-1.073395	1.336616
1	-0.747079	-1.777475	0.729683
1	-1.173405	-0.622591	-2.623816
1	-2.360574	-3.556193	0.268921
1	-4.995355	-2.580446	-2.990476
8	6.999163	-2.863608	-2.196767
6	8.127598	-3.570620	-2.675317
1	8.272556	-3.243759	-3.705280
1	9.027997	-3.335307	-2.095727
1	7.957580	-4.653249	-2.663297
1	1.309041	1.136649	0.418415
6	-0.629479	-0.536014	2.936391
8	-1.301190	-1.399287	2.317382
8	0.616017	-0.378936	2.904254
1	-4.451428	3.808630	2.524982
1	-2.443705	-1.487187	6.471718
1	-1.779489	-2.125428	4.957472
6	-3.785713	3.981056	0.498946
1	-4.575732	4.719619	0.309913
1	-3.687128	3.377535	-0.406353
6	-2.513122	4.720768	0.765483
6	-1.426874	4.701406	-0.015279
1	-2.477796	5.338034	1.664744
1	-1.413151	4.097173	-0.916920
6	-0.246656	5.537272	0.335879
8	-0.211672	6.175535	1.376060
6	0.915969	5.609631	-0.616080
6	1.010768	4.821589	-1.767888
6	1.953323	6.498868	-0.307515
6	2.129243	4.922329	-2.593886
1	0.236504	4.105877	-2.021398
6	3.061363	6.606982	-1.138797
1	1.865567	7.100327	0.591334
6	3.152661	5.814879	-2.284183
1	2.195061	4.303169	-3.483621
1	3.855820	7.305622	-0.895819
1	4.018180	5.894969	-2.935013
1	-4.674817	0.987633	3.224639

Electronic energy= -3905.3193271
 Zero-point correction= 1.056443
 Thermal correction to Energy= 1.121263
 Thermal correction to Enthalpy= 1.122207
 Thermal correction to Gibbs Free Energy= 0.955517
 Sum of electronic and zero-point Energies= -3904.262884
 Sum of electronic and thermal Energies= -3904.198065
 Sum of electronic and thermal Enthalpies= -3904.197120
 Sum of electronic and thermal Free Energies= -3904.363810

 Cartesian Coordinates

6	-0.814686	0.523901	5.351873
6	-1.755150	-0.598041	5.806713
6	-3.071017	-0.271014	5.096285
7	-2.658093	0.539006	3.916029
6	-1.189442	0.676076	3.877748
6	-3.495079	0.995616	3.061159
6	-3.155703	1.731782	1.817264
8	-0.332889	1.751984	-1.421535
8	-0.412285	1.102964	0.697104
1	-0.906035	1.627246	3.426958
1	0.241548	0.273195	5.448665
1	-1.015926	1.450142	5.899418
1	-3.613658	-1.148846	4.743230
1	-3.729940	0.349295	5.708569
1	-2.143011	2.140272	1.887230
6	-4.181098	2.854335	1.600565
1	-5.167374	2.417017	1.406541
6	-3.067997	0.650078	0.660561
1	-2.442918	-0.145255	1.081397
1	-2.758398	1.381514	-1.484542
6	-4.414353	0.047826	0.320649
6	-4.832881	-1.086942	1.025355
6	-5.258690	0.572923	-0.661871
6	-6.064505	-1.679375	0.762732
1	-4.157345	-1.526569	1.759061
6	-6.486797	-0.026747	-0.936525
1	-4.953701	1.444690	-1.233738
6	-6.892767	-1.152538	-0.225426
1	-6.362030	-2.571393	1.304212
1	-7.123776	0.385562	-1.713118
1	-7.844168	-1.625879	-0.446884
7	-1.032107	1.352113	-0.427644
6	-2.326664	1.192677	-0.512665
7	-0.552655	-1.892024	-0.171604
6	-1.660655	-2.129078	-1.004053
6	-1.911404	-1.352230	-2.139739
6	-3.099483	-1.538164	-2.835406
6	-4.047234	-2.477672	-2.433005
6	-3.774838	-3.247165	-1.311184
6	-2.592367	-3.079549	-0.595496
6	-3.408886	-0.612817	-3.974877
9	-2.344192	-0.396748	-4.755279
6	-4.740121	-4.306299	-0.869495
9	-4.409706	-5.517313	-1.347671
6	0.746137	-1.743378	-0.543098
16	1.325080	-2.036758	-2.108363
7	1.520746	-1.363841	0.490669
6	2.927188	-1.027352	0.434498
6	3.072430	0.409280	0.977777
6	4.507429	0.982381	0.943067
6	4.543076	2.238409	0.057716
6	3.607339	3.307231	0.648019
6	2.216024	2.685504	0.864237
7	2.172865	1.340684	0.219491
6	2.549661	1.462606	-1.223528
6	4.028768	1.899093	-1.352840
6	4.846245	0.888344	-2.120878

6	6.121096	0.572696	-1.906451
6	3.769622	-1.976896	1.279239
6	4.960679	-2.594555	0.780783
6	5.697914	-3.412678	1.688461
7	5.312129	-3.642581	2.975830
6	4.202330	-3.078202	3.382214
6	3.399726	-2.234735	2.575909
6	6.893194	-4.025786	1.242667
6	7.353465	-3.849835	-0.037236
6	6.613636	-3.045306	-0.940286
6	5.441298	-2.440340	-0.539681
9	-4.396284	-1.078240	-4.754021
9	-3.810171	0.600051	-3.532182
9	-5.993442	-4.057763	-1.278351
9	-4.771049	-4.423454	0.470624
1	2.669100	0.407443	1.995173
1	4.830711	1.232715	1.957608
1	5.199569	0.229060	0.558291
1	1.406399	3.254657	0.406480
1	1.973697	2.531752	1.918527
1	3.534525	4.158311	-0.038309
1	4.002431	3.679754	1.596844
1	5.563022	2.628743	0.004825
1	4.034907	2.831617	-1.935306
1	1.858475	2.190896	-1.640175
1	2.336586	0.505607	-1.705581
1	4.317786	0.395397	-2.938663
1	6.624281	-0.169352	-2.519020
1	6.705985	1.021272	-1.106912
1	3.237969	-1.074948	-0.609773
1	2.493007	-1.800453	2.991280
1	4.905629	-1.854713	-1.276217
1	3.901156	-3.277209	4.409276
1	7.433060	-4.642801	1.953584
1	8.271978	-4.332405	-0.349284
1	1.068575	-1.138171	1.390254
1	-0.773280	-1.800396	0.830420
1	-1.198972	-0.585986	-2.435316
1	-2.393526	-3.673304	0.291585
1	-4.978590	-2.594376	-2.974894
8	6.997079	-2.819752	-2.224348
6	8.154503	-3.479996	-2.699546
1	8.259173	-3.188551	-3.744918
1	9.051517	-3.170476	-2.150246
1	8.048075	-4.569275	-2.640179
1	1.134640	1.055192	0.307090
6	-0.558633	-0.475831	3.041196
8	-1.324038	-1.338073	2.560796
8	0.688618	-0.410511	2.986611
1	-4.268616	3.432346	2.529975
1	-1.886044	-0.641173	6.888454
1	-1.377453	-1.563735	5.462051
6	-3.825738	3.825506	0.464204
1	-4.649558	4.545775	0.380723
1	-3.757997	3.298346	-0.489816
6	-2.561602	4.587961	0.718315
6	-1.472149	4.558344	-0.056632
1	-2.541810	5.237742	1.594890
1	-1.436518	3.916300	-0.932163
6	-0.317727	5.447985	0.259837
8	-0.288421	6.102060	1.290785
6	0.806127	5.564958	-0.730324
6	0.941201	4.702447	-1.823701
6	1.760911	6.568355	-0.522476
6	2.019533	4.847108	-2.694638
1	0.241761	3.886219	-1.980609
6	2.827064	6.718447	-1.400989
1	1.644268	7.223749	0.334587
6	2.958371	5.856057	-2.490126
1	2.120751	4.169722	-3.537565

1	3.557794	7.504492	-1.238646
1	3.791055	5.970189	-3.177659
1	-4.545019	0.773046	3.262150

[10]

Number of imaginary frequencies : 0

Electronic energy=	-3905.318206
Zero-point correction=	1.057013
Thermal correction to Energy=	1.121901
Thermal correction to Enthalpy=	1.122845
Thermal correction to Gibbs Free Energy=	0.950471
Sum of electronic and zero-point Energies=	-3904.261193
Sum of electronic and thermal Energies=	-3904.196305
Sum of electronic and thermal Enthalpies=	-3904.195361
Sum of electronic and thermal Free Energies=	-3904.367735

Cartesian Coordinates

7	-1.729358	0.010895	0.090762
6	-3.027648	-0.032563	0.023419
6	0.223196	2.871694	2.355852
6	-3.728939	-2.424469	-0.489505
6	-3.049078	1.000833	2.728563
6	-3.221496	-2.308635	-1.783765
6	-3.195643	-3.407568	-2.638514
8	-1.051085	-1.043357	0.441895
6	-4.173849	-4.773600	-0.919120
6	-0.726344	1.740594	2.588779
6	1.579646	2.570782	2.196311
8	-1.079521	1.099922	-0.148374
6	-4.197836	-3.671952	-0.068051
6	2.510421	3.583165	1.999863
6	-5.196306	-0.894774	0.953632
6	-3.763149	-1.247498	0.487674
6	-2.176622	1.959533	2.397794
6	-0.187156	4.208980	2.334357
6	-3.672434	-4.644132	-2.211403
6	-5.265693	-0.249524	2.349155
6	2.094355	4.914001	1.983390
8	-0.290972	0.655090	2.969616
6	0.747527	5.225424	2.158356
6	-4.540539	1.088416	2.587076
1	-3.496988	0.882538	-0.308198
1	-5.739373	-1.844312	1.040625
1	-4.889537	-0.975725	3.080518
1	3.555605	3.334339	1.843187
1	-2.810339	-3.292353	-3.647276
1	-4.798039	1.836146	1.827575
1	-4.544351	-5.733158	-0.570773
1	-2.507244	2.875345	1.917585
1	-2.643496	0.090102	3.173769
1	-4.579911	-3.787137	0.944917
1	-4.929230	1.485312	3.535501
1	-2.858549	-1.344858	-2.128292
1	-3.229672	-1.603077	1.381469
1	-1.231372	4.468215	2.473459
1	2.820773	5.704795	1.820895
1	0.420178	6.260004	2.139764
1	-6.327715	-0.104850	2.575361
1	1.890285	1.530612	2.205723
1	-3.655325	-5.499102	-2.879853
7	1.546972	1.423519	-0.819123
6	1.806361	2.773682	-1.060645
6	0.689952	3.620103	-0.959999
6	0.830137	4.981395	-1.163183

6	2.066449	5.545341	-1.466995
6	3.156522	4.694388	-1.579708
6	3.049539	3.318325	-1.391746
6	-0.367214	5.877761	-1.042098
9	-0.053467	7.040404	-0.443505
6	4.516494	5.288134	-1.804986
9	5.106989	5.607309	-0.637970
6	2.349864	0.399924	-0.428138
16	4.024229	0.461210	-0.197288
7	1.621184	-0.712673	-0.171677
6	2.159647	-2.017680	0.145340
6	1.239332	-2.710650	1.169468
6	1.888818	-3.952976	1.814516
6	2.061963	-3.713540	3.322397
6	0.669903	-3.555807	3.951368
6	-0.084744	-2.431348	3.216685
7	0.853711	-1.754219	2.266734
6	2.044358	-1.227430	3.000262
6	2.852470	-2.416323	3.586226
6	4.278776	-2.409401	3.088108
6	5.010717	-3.474044	2.770214
6	2.250805	-2.915169	-1.085931
6	3.440373	-3.625079	-1.437883
6	3.371645	-4.474773	-2.582167
7	2.249339	-4.621577	-3.341632
6	1.185446	-3.941792	-2.991409
6	1.136294	-3.079961	-1.869529
6	4.521302	-5.213018	-2.955042
6	5.688404	-5.128271	-2.240089
6	5.754991	-4.277583	-1.106898
6	4.656443	-3.539263	-0.721651
9	-0.884680	6.194331	-2.240052
9	-1.354273	5.317815	-0.325700
9	4.457711	6.418610	-2.526487
9	5.341920	4.446741	-2.440302
1	0.291264	-2.952396	0.681904
1	1.258869	-4.831893	1.652726
1	2.852477	-4.152175	1.339421
1	-0.455848	-1.649054	3.879721
1	-0.915617	-2.794335	2.607923
1	0.764154	-3.318961	5.014957
1	0.112981	-4.492590	3.870455
1	2.579429	-4.561472	3.778427
1	2.891412	-2.274457	4.674194
1	1.652830	-0.551549	3.760548
1	2.634348	-0.637229	2.292534
1	4.733595	-1.421167	3.012092
1	6.037351	-3.365691	2.435273
1	4.622721	-4.488164	2.822169
1	3.150787	-1.870713	0.577749
1	0.208539	-2.560991	-1.635521
1	4.768648	-2.885189	0.135079
1	0.296167	-4.068680	-3.605827
1	4.444808	-5.851066	-3.829405
1	6.551094	-5.706810	-2.548264
1	0.593618	-0.668501	-0.229966
1	0.535624	1.222841	-0.711825
1	-0.274858	3.199473	-0.687445
1	3.920025	2.684435	-1.484122
1	2.176752	6.615545	-1.603970
8	6.870007	-4.135385	-0.345608
6	8.044679	-4.812339	-0.750687
1	8.818104	-4.525360	-0.037804
1	7.914967	-5.900513	-0.718661
1	8.356190	-4.510931	-1.757300
1	0.311266	-0.980693	1.835987
6	-8.994988	0.638777	-1.451791
6	-9.135187	-0.885012	-1.408826
6	-7.807666	-1.308968	-0.778106
7	-7.427298	-0.236268	0.159586

6	-8.296031	0.932012	-0.121119
6	-6.002726	-0.053956	-0.045550
1	-7.707784	1.853718	-0.131390
1	-9.950573	1.157222	-1.551645
1	-8.357809	0.932336	-2.293809
1	-9.965837	-1.180573	-0.761335
1	-9.268990	-1.349221	-2.388047
1	-7.848050	-2.296931	-0.307434
1	-5.739326	1.005407	0.013499
6	-6.687814	-1.300360	-1.820807
8	-5.710297	-0.474637	-1.396680
8	-6.661655	-1.874278	-2.873488
1	-9.034535	1.017823	0.683696

[10-11]TS

Number of imaginary frequencies : 1

The smallest frequency is : -371.0329

Electronic energy=	-3905.3066568
Zero-point correction=	1.056381
Thermal correction to Energy=	1.120408
Thermal correction to Enthalpy=	1.121352
Thermal correction to Gibbs Free Energy=	0.951576
Sum of electronic and zero-point Energies=	-3904.250276
Sum of electronic and thermal Energies=	-3904.186249
Sum of electronic and thermal Enthalpies=	-3904.185305
Sum of electronic and thermal Free Energies=	-3904.355080

Cartesian Coordinates

7	-1.772673	-0.082089	-0.030375
6	-3.081658	0.079103	0.273566
6	0.432975	3.024815	2.204321
6	-3.927415	-2.232314	-0.452692
6	-2.816250	1.038541	2.108514
6	-3.456057	-2.050839	-1.753667
6	-3.500925	-3.091461	-2.676777
8	-1.166768	-1.149304	0.301979
6	-4.492583	-4.525501	-1.022161
6	-0.518878	1.860671	2.213686
6	1.800745	2.745385	2.125229
8	-1.149551	0.886304	-0.529329
6	-4.441967	-3.482746	-0.100538
6	2.733733	3.772264	2.034112
6	-5.288837	-0.695293	1.095800
6	-3.890894	-1.137869	0.614225
6	-1.908473	2.082881	1.976341
6	0.018097	4.361281	2.240235
6	-4.018444	-4.333202	-2.316302
6	-5.192604	0.080001	2.417980
6	2.309257	5.099331	2.048553
8	-0.039225	0.730687	2.468141
6	0.951024	5.391088	2.168547
6	-4.278970	1.312560	2.395197
1	-3.520680	0.906524	-0.271011
1	-5.871183	-1.605166	1.283889
1	-4.835406	-0.604233	3.197020
1	3.788634	3.536237	1.929080
1	-3.137755	-2.926483	-3.686722
1	-4.647284	2.075466	1.698456
1	-4.896930	-5.488758	-0.725598
1	-2.257757	3.068655	1.689346
1	-2.405761	0.131533	2.560818
1	-4.799588	-3.647144	0.914502
1	-4.324478	1.777436	3.388083
1	-3.065898	-1.083989	-2.058608

1	-3.412748	-1.604070	1.488243
1	-1.034243	4.606984	2.333575
1	3.035172	5.902418	1.960822
1	0.615586	6.423105	2.188921
1	-6.202618	0.388498	2.711177
1	2.117671	1.707145	2.098402
1	-4.056628	-5.141750	-3.039413
7	1.645974	1.354770	-0.790762
6	1.972296	2.689427	-1.048000
6	0.893807	3.585199	-0.977997
6	1.097179	4.936596	-1.187924
6	2.363721	5.440025	-1.476480
6	3.414909	4.540216	-1.562953
6	3.243038	3.171493	-1.363726
6	-0.062011	5.886446	-1.109356
9	0.270537	7.021239	-0.471012
6	4.804960	5.066906	-1.770116
9	5.398142	5.350504	-0.596035
6	2.392122	0.286763	-0.401488
16	4.061605	0.273165	-0.147787
7	1.607546	-0.795271	-0.177990
6	2.077602	-2.121314	0.163314
6	1.149022	-2.734736	1.229179
6	1.747059	-3.992193	1.896542
6	1.958798	-3.724546	3.394737
6	0.588958	-3.467327	4.042282
6	-0.112755	-2.321488	3.286319
7	0.845350	-1.730787	2.303158
6	2.077903	-1.255077	3.004788
6	2.829320	-2.470328	3.608049
6	4.241953	-2.560524	3.079979
6	4.903912	-3.673072	2.772204
6	2.093081	-3.055242	-1.042787
6	3.241285	-3.827564	-1.401015
6	3.104257	-4.712437	-2.512078
7	1.956470	-4.834407	-3.237404
6	0.933587	-4.095448	-2.885138
6	0.951775	-3.196119	-1.792128
6	4.209833	-5.513811	-2.887478
6	5.398727	-5.455761	-2.206565
6	5.533751	-4.569374	-1.107340
6	4.478977	-3.770700	-0.719676
9	-0.491414	6.249500	-2.330075
9	-1.113905	5.358795	-0.466307
9	4.809871	6.201593	-2.487304
9	5.593565	4.187378	-2.401443
1	0.180037	-2.946346	0.771902
1	1.070309	-4.841261	1.767414
1	2.690442	-4.251961	1.410320
1	-0.425927	-1.499570	3.932184
1	-0.975062	-2.654361	2.704596
1	0.717817	-3.204900	5.096153
1	-0.023707	-4.371239	4.000512
1	2.433077	-4.589309	3.865846
1	2.901400	-2.302096	4.690645
1	1.734642	-0.538109	3.751273
1	2.681971	-0.710795	2.273139
1	4.751404	-1.602402	2.971917
1	5.927795	-3.631965	2.414608
1	4.459742	-4.661811	2.857144
1	3.084390	-2.012152	0.569497
1	0.051425	-2.632975	-1.553059
1	4.643416	-3.094259	0.111093
1	0.022756	-4.201722	-3.471468
1	4.080683	-6.179152	-3.734973
1	6.226777	-6.082117	-2.516062
1	0.594981	-0.711613	-0.302586
1	0.636312	1.190334	-0.746359
1	-0.093052	3.213450	-0.712875
1	4.085390	2.498558	-1.435636

1	2.524359	6.502867	-1.620894
8	6.674856	-4.450337	-0.382009
6	7.808566	-5.187813	-0.798563
1	8.615089	-4.908547	-0.120287
1	7.636851	-6.268116	-0.724538
1	8.098788	-4.933477	-1.824261
1	0.373007	-0.891394	1.907938
6	-9.146062	0.866674	-1.204194
6	-9.294162	-0.656558	-1.166745
6	-7.946535	-1.091654	-0.589526
7	-7.528696	-0.030641	0.345234
6	-8.396467	1.146943	0.101512
6	-6.109090	0.139549	0.097934
1	-7.801225	2.063807	0.074217
1	-10.101073	1.392123	-1.265274
1	-8.538551	1.161840	-2.067356
1	-10.101744	-0.952607	-0.490966
1	-9.465955	-1.112544	-2.143913
1	-7.971331	-2.084801	-0.128116
1	-5.837306	1.197075	0.147729
6	-6.864950	-1.074679	-1.671649
8	-5.859524	-0.275771	-1.261010
8	-6.884533	-1.620483	-2.739164
1	-9.104163	1.234594	0.933294

[11]

Number of imaginary frequencies : 0

Electronic energy=	-3905.3421979
Zero-point correction=	1.058719
Thermal correction to Energy=	1.122645
Thermal correction to Enthalpy=	1.123589
Thermal correction to Gibbs Free Energy=	0.954781
Sum of electronic and zero-point Energies=	-3904.283479
Sum of electronic and thermal Energies=	-3904.219553
Sum of electronic and thermal Enthalpies=	-3904.218609
Sum of electronic and thermal Free Energies=	-3904.387417

Cartesian Coordinates

7	-1.607671	-1.328961	0.303005
6	-2.997672	-0.912522	0.694673
6	0.073021	2.346291	2.348724
6	-3.844624	-3.080430	-0.425051
6	-2.866857	-0.192735	2.064765
6	-3.364505	-2.702037	-1.680289
6	-3.340828	-3.610567	-2.734726
8	-1.130527	-2.306255	0.834147
6	-4.295502	-5.295976	-1.311259
6	-0.701095	1.084299	2.215308
6	1.439291	2.375588	2.054348
8	-1.014128	-0.631877	-0.511544
6	-4.307626	-4.388620	-0.256742
6	2.148988	3.573270	2.072941
6	-5.304536	-1.742350	1.228640
6	-3.883116	-2.156009	0.783727
6	-2.036547	1.062649	2.026218
6	-0.558132	3.544269	2.713979
6	-3.806035	-4.909703	-2.555893
6	-5.223844	-1.071021	2.606256
6	1.503913	4.761382	2.401263
8	-0.045142	-0.094773	2.253035
6	0.149351	4.739635	2.733729
6	-4.270407	0.125967	2.605756
1	-3.308928	-0.216420	-0.089011
1	-5.891252	-2.664513	1.317195

1	-4.880564	-1.810284	3.338843
1	3.202384	3.570828	1.809777
1	-2.964680	-3.294409	-3.702442
1	-4.689954	0.951173	2.016021
1	-4.659527	-6.307098	-1.157220
1	-2.560332	2.004302	1.896506
1	-2.381417	-0.921438	2.728606
1	-4.670772	-4.704056	0.719482
1	-4.157698	0.514155	3.622777
1	-3.015981	-1.688836	-1.857612
1	-3.485220	-2.741848	1.623048
1	-1.606314	3.539937	2.993985
1	2.052830	5.697575	2.406894
1	-0.359475	5.658124	3.007765
1	-6.225446	-0.753058	2.914688
1	1.953560	1.464350	1.770810
1	-3.789515	-5.614334	-3.381052
7	1.078637	1.462968	-0.921034
6	0.896883	2.831713	-1.176208
6	-0.300815	3.382826	-0.696176
6	-0.566088	4.728643	-0.861574
6	0.334065	5.565759	-1.520019
6	1.496406	5.001741	-2.019146
6	1.792750	3.646165	-1.865046
6	-1.826193	5.321718	-0.303891
9	-1.563991	6.322406	0.552461
6	2.487704	5.844956	-2.770003
9	3.705521	5.795914	-2.210077
6	2.219971	0.763155	-0.626662
16	3.789871	1.312153	-0.899155
7	1.942383	-0.410783	-0.024706
6	2.901711	-1.443615	0.320573
6	2.595706	-1.980290	1.735582
6	3.685508	-2.986115	2.196412
6	4.332794	-2.461203	3.486707
6	3.248030	-2.383377	4.568478
6	2.100764	-1.489419	4.033648
7	2.448423	-0.887355	2.728026
6	3.698330	-0.121809	2.872085
6	4.893211	-1.040928	3.274760
6	6.033415	-0.930175	2.293235
6	6.803693	-1.920941	1.849152
6	2.861277	-2.582336	-0.696099
6	4.036630	-3.079658	-1.344263
6	3.870928	-4.177543	-2.240936
7	2.663281	-4.746213	-2.519076
6	1.609765	-4.245677	-1.923540
6	1.659824	-3.170889	-1.003545
6	5.012110	-4.716204	-2.882272
6	6.265538	-4.206132	-2.660332
6	6.425786	-3.106692	-1.779423
6	5.333763	-2.554280	-1.144350
9	-2.600047	5.842098	-1.270073
9	-2.571064	4.419044	0.355149
9	2.122341	7.134175	-2.817711
9	2.630308	5.425030	-4.036985
1	1.612790	-2.469102	1.694651
1	3.242716	-3.969808	2.380905
1	4.441198	-3.116752	1.417397
1	1.876551	-0.667772	4.721099
1	1.176236	-2.057594	3.892013
1	3.666312	-1.968004	5.491096
1	2.878078	-3.386627	4.800914
1	5.132660	-3.135824	3.806832
1	5.271952	-0.689206	4.244559
1	3.517111	0.647779	3.629028
1	3.901862	0.398823	1.929389
1	6.232309	0.081976	1.935946
1	7.603378	-1.735491	1.138709
1	6.660107	-2.953510	2.157719

1	3.885972	-0.974641	0.312690
1	0.732745	-2.826164	-0.553487
1	5.511152	-1.705258	-0.495353
1	0.648411	-4.700300	-2.156832
1	4.857030	-5.550787	-3.558299
1	7.119827	-4.642553	-3.163690
1	0.964232	-0.647483	0.126301
1	0.215198	0.997609	-0.654642
1	-1.004884	2.751031	-0.162585
1	2.709356	3.236199	-2.266506
1	0.128047	6.623432	-1.641037
8	7.629436	-2.538051	-1.507968
6	8.768185	-3.035280	-2.183809
1	9.608413	-2.428652	-1.845057
1	8.961091	-4.085055	-1.933082
1	8.668085	-2.931694	-3.270434
1	0.940815	-0.092690	2.453891
6	-9.093280	0.048459	-1.014557
6	-9.271741	-1.470988	-1.064145
6	-7.937559	-1.964687	-0.503484
7	-7.508833	-0.968747	0.495706
6	-8.347287	0.241166	0.308958
6	-6.083068	-0.819824	0.275618
1	-7.730906	1.144139	0.332179
1	-10.037215	0.595573	-1.050981
1	-8.474758	0.379325	-1.856711
1	-10.089729	-1.788926	-0.411313
1	-9.444888	-1.867773	-2.066512
1	-7.985355	-2.982238	-0.101349
1	-5.782171	0.223662	0.397668
6	-6.845639	-1.902568	-1.574044
8	-5.826912	-1.152459	-1.103503
8	-6.864533	-2.376904	-2.674751
1	-9.057977	0.301610	1.140349

[12]

Number of imaginary frequencies : 0

Electronic energy=	-3905.3278818
Zero-point correction=	1.058947
Thermal correction to Energy=	1.122962
Thermal correction to Enthalpy=	1.123906
Thermal correction to Gibbs Free Energy=	0.954094
Sum of electronic and zero-point Energies=	-3904.268934
Sum of electronic and thermal Energies=	-3904.204920
Sum of electronic and thermal Enthalpies=	-3904.203976
Sum of electronic and thermal Free Energies=	-3904.373788

Cartesian Coordinates

7	1.252048	-1.895938	-1.206916
6	2.256336	-1.452947	-0.177837
6	-1.288190	-2.186816	3.267115
6	3.911415	-1.235031	-2.097603
6	1.465991	-0.719348	0.915395
6	4.250625	-2.590608	-2.133045
6	4.832270	-3.147132	-3.268766
8	0.766170	-1.042322	-1.924732
6	4.731688	-1.010526	-4.371034
6	-0.435462	-1.192620	2.509667
6	-1.086936	-3.574184	3.250807
8	0.943594	-3.078163	-1.240227
6	4.144470	-0.458212	-3.236106
6	-1.946306	-4.428382	3.935634
6	4.308797	-0.014921	0.172914
6	3.304061	-0.573538	-0.872046

6	0.451270	-1.635204	1.559503
6	-2.340665	-1.684649	4.041132
6	5.081644	-2.357899	-4.388611
6	3.511386	0.759532	1.239434
6	-3.019868	-3.915410	4.662818
8	-0.665859	0.051047	2.797976
6	-3.206977	-2.537567	4.721778
6	2.456391	-0.111163	1.924133
1	2.667955	-2.388851	0.206853
1	4.964217	0.689011	-0.352624
1	3.013641	1.599053	0.739493
1	-1.769793	-5.499653	3.910728
1	5.093212	-4.200934	-3.276123
1	2.926966	-0.917623	2.501310
1	4.908669	-0.388475	-5.242986
1	0.604571	-2.703179	1.429356
1	0.971005	0.115891	0.404605
1	3.865141	0.590953	-3.229156
1	1.873534	0.478912	2.637830
1	4.084318	-3.220567	-1.264506
1	2.761898	0.311069	-1.230518
1	-2.446927	-0.606651	4.108866
1	-3.688734	-4.583970	5.195701
1	-4.021422	-2.122751	5.309131
1	4.194765	1.183335	1.977908
1	-0.245891	-3.999782	2.711889
1	5.536992	-2.793202	-5.272660
7	-0.796743	1.746286	0.806191
6	0.229352	2.638890	0.456556
6	0.881126	2.594010	-0.782825
6	1.974874	3.418724	-1.001888
6	2.444340	4.294644	-0.023866
6	1.798009	4.316891	1.202109
6	0.701397	3.494205	1.451124
6	2.785422	3.270687	-2.253925
9	3.126874	4.450343	-2.786057
6	2.251067	5.258653	2.281371
9	1.427630	6.312653	2.394867
6	-1.836367	1.336135	0.046049
16	-2.254983	1.951309	-1.472255
7	-2.527488	0.334256	0.662679
6	-3.726290	-0.294582	0.157399
6	-3.588387	-1.821537	0.303105
6	-4.727217	-2.604539	-0.384680
6	-4.155358	-3.454143	-1.529448
6	-3.195376	-4.496183	-0.938290
6	-2.147934	-3.776747	-0.066890
7	-2.276193	-2.295051	-0.278758
6	-2.145389	-1.980880	-1.743195
6	-3.353057	-2.578459	-2.509833
6	-4.140789	-1.509815	-3.230028
6	-5.460342	-1.478963	-3.396394
6	-4.991211	0.160557	0.880178
6	-6.104619	0.735865	0.188656
6	-7.254661	1.061861	0.969623
7	-7.324602	0.877463	2.318607
6	-6.276292	0.369915	2.915815
6	-5.093612	-0.011307	2.237215
6	-8.391696	1.601441	0.322207
6	-8.410996	1.808701	-1.033342
6	-7.264757	1.490797	-1.805367
6	-6.135419	0.976666	-1.203118
9	3.943850	2.622414	-1.988758
9	2.156435	2.559535	-3.196782
9	3.478659	5.739776	2.043227
9	2.276065	4.658418	3.480063
1	-3.513805	-2.068673	1.368883
1	-5.226952	-3.251289	0.341498
1	-5.471567	-1.899881	-0.763048
1	-1.119423	-4.036145	-0.325159

1	-2.297425	-3.950214	1.000174
1	-2.704204	-5.049017	-1.743875
1	-3.745554	-5.217471	-0.329209
1	-4.967435	-3.958868	-2.058766
1	-2.939828	-3.244518	-3.278349
1	-1.195905	-2.414115	-2.056574
1	-2.069067	-0.895226	-1.846828
1	-3.538685	-0.711435	-3.665409
1	-5.934686	-0.669579	-3.943113
1	-6.119890	-2.241683	-2.989660
1	-3.797064	-0.035262	-0.899363
1	-4.278756	-0.448079	2.808268
1	-5.276950	0.784326	-1.834705
1	-6.342680	0.230717	3.993306
1	-9.250481	1.844327	0.939274
1	-9.296577	2.222092	-1.500738
1	-2.251170	0.148556	1.631747
1	-0.628715	1.165624	1.686758
1	0.548003	1.898559	-1.544767
1	0.208648	3.507500	2.418930
1	3.306706	4.925388	-0.210742
8	-7.198358	1.664082	-3.149475
6	-8.321386	2.219245	-3.808779
1	-8.049204	2.282986	-4.862379
1	-9.206298	1.580230	-3.705293
1	-8.549330	3.224380	-3.436358
6	8.545017	-2.225808	0.353248
6	8.265052	-1.664631	-1.053446
6	6.991898	-0.848366	-0.861649
7	6.199285	-1.718785	0.028941
6	7.167055	-2.190863	1.032416
6	5.185345	-1.077088	0.833048
1	9.242150	-1.596925	0.913606
1	8.957914	-3.234841	0.323659
1	9.089597	-1.066651	-1.445983
1	8.063188	-2.479916	-1.753913
1	7.230624	0.117795	-0.385229
1	6.452872	-0.658638	-1.792185
1	-1.500951	-1.836354	0.243256
1	4.567334	-1.866886	1.281124
1	6.858720	-3.154691	1.455578
6	7.052543	-1.136457	2.134809
8	7.825879	-0.896998	3.021482
8	5.898947	-0.462755	1.952832

[12-13]TS

Number of imaginary frequencies : 1
The smallest frequency is : -1263.0881

Electronic energy= -3905.3172595
Zero-point correction= 1.054845
Thermal correction to Energy= 1.118264
Thermal correction to Enthalpy= 1.119208
Thermal correction to Gibbs Free Energy= 0.952277
Sum of electronic and zero-point Energies= -3904.262414
Sum of electronic and thermal Energies= -3904.198995
Sum of electronic and thermal Enthalpies= -3904.198051
Sum of electronic and thermal Free Energies= -3904.364983

Cartesian Coordinates

7	1.239433	-1.721029	-1.724720
6	2.090762	-1.393508	-0.531985
6	-1.168586	-2.831321	2.946638
6	3.925495	-0.942667	-2.228432
6	1.170607	-0.817261	0.557100

6	4.302824	-2.279924	-2.381151
6	4.987533	-2.698914	-3.518285
8	0.828407	-0.791756	-2.392729
6	4.915269	-0.457819	-4.390705
6	-0.563153	-1.652654	2.218685
6	-0.826610	-4.164538	2.691996
8	0.983208	-2.895572	-1.940724
6	4.226240	-0.042737	-3.254329
6	-1.440570	-5.197736	3.394944
6	4.095564	-0.030706	0.207132
6	3.198800	-0.433817	-0.993256
6	0.110607	-1.850001	0.971252
6	-2.115317	-2.558807	3.941322
6	5.302339	-1.788306	-4.523588
6	3.189515	0.579778	1.290173
6	-2.400085	-4.914183	4.363947
8	-0.792733	-0.518743	2.710989
6	-2.733282	-3.589835	4.639959
6	2.070145	-0.367021	1.724394
1	2.482368	-2.362610	-0.213302
1	4.785343	0.742481	-0.149611
1	2.752209	1.496812	0.879253
1	-1.163050	-6.226889	3.189734
1	5.276432	-3.740739	-3.616814
1	2.489142	-1.259414	2.210083
1	5.139628	0.258147	-5.175237
1	0.455773	-2.874772	0.818879
1	0.704405	0.076182	0.121339
1	3.916432	0.993224	-3.159161
1	1.447089	0.120528	2.477576
1	4.085745	-3.003657	-1.601531
1	2.692678	0.494435	-1.289613
1	-2.341734	-1.520437	4.160448
1	-2.878539	-5.722125	4.908528
1	-3.468990	-3.361683	5.404974
1	3.788764	0.871292	2.155031
1	-0.069459	-4.408368	1.953651
1	5.836992	-2.116243	-5.409661
7	-0.853088	1.810011	0.950660
6	0.180577	2.726885	0.687419
6	0.849165	2.771476	-0.542022
6	1.955304	3.597341	-0.676355
6	2.415585	4.390349	0.373952
6	1.742893	4.331790	1.584480
6	0.633664	3.505793	1.749445
6	2.790385	3.530330	-1.920157
9	3.142438	4.741856	-2.366543
6	2.178511	5.192041	2.737029
9	1.389258	6.267809	2.875601
6	-1.855178	1.400488	0.117731
16	-2.280953	2.171238	-1.318836
7	-2.467652	0.298820	0.598242
6	-3.635525	-0.353230	0.049789
6	-3.402814	-1.877479	-0.000293
6	-4.566801	-2.599511	-0.726925
6	-4.044833	-3.217784	-2.032430
6	-3.036653	-4.316196	-1.671802
6	-1.998218	-3.717020	-0.701941
7	-2.111518	-2.230555	-0.665542
6	-2.055314	-1.703217	-2.056095
6	-3.299618	-2.164160	-2.871764
6	-4.133265	-1.002751	-3.355501
6	-5.459145	-0.972604	-3.468560
6	-4.873336	-0.053612	0.894117
6	-6.013652	0.635754	0.372239
6	-7.124953	0.813000	1.251240
7	-7.132200	0.393447	2.548408
6	-6.057853	-0.205477	2.996167
6	-4.911456	-0.458267	2.204971
6	-8.287206	1.457067	0.764346

6	-8.365310	1.908497	-0.528283
6	-7.255117	1.742754	-1.394844
6	-6.103095	1.130663	-0.947735
9	3.941490	2.863599	-1.672963
9	2.179545	2.883005	-2.918705
9	3.432386	5.637408	2.582294
9	2.126022	4.521840	3.897637
1	-3.298812	-2.246277	1.028185
1	-4.984354	-3.384039	-0.088725
1	-5.369681	-1.886919	-0.932469
1	-0.971660	-3.948357	-0.996493
1	-2.147516	-4.068258	0.323010
1	-2.547703	-4.687426	-2.577845
1	-3.543947	-5.162156	-1.199842
1	-4.874158	-3.641386	-2.605679
1	-2.919094	-2.671265	-3.768637
1	-1.137187	-2.089572	-2.497023
1	-1.969746	-0.613636	-2.010368
1	-3.562371	-0.124481	-3.661160
1	-5.968189	-0.092070	-3.849413
1	-6.088313	-1.811809	-3.181889
1	-3.773107	0.027450	-0.962433
1	-4.070901	-0.979716	2.656287
1	-5.271744	1.062022	-1.637629
1	-6.072146	-0.529840	4.035028
1	-9.116015	1.579010	1.453856
1	-9.269497	2.395364	-0.873904
1	-2.147557	-0.033464	1.508293
1	-0.709444	1.230972	1.782551
1	0.525191	2.141995	-1.363385
1	0.120099	3.457528	2.705045
1	3.289560	5.021489	0.252994
8	-7.247610	2.159714	-2.686120
6	-8.387462	2.840736	-3.175085
1	-8.159439	3.104030	-4.208068
1	-9.278296	2.202003	-3.156906
1	-8.583191	3.757149	-2.606625
6	8.347562	-2.187351	0.477938
6	8.180833	-1.445718	-0.861201
6	6.877649	-0.677018	-0.675831
7	6.029642	-1.674747	0.002939
6	6.909584	-2.282236	1.013947
6	4.925731	-1.175048	0.786565
1	8.962364	-1.621151	1.182948
1	8.801981	-3.171232	0.356111
1	9.023222	-0.792160	-1.094847
1	8.059033	-2.162064	-1.678682
1	7.051077	0.213225	-0.047388
1	6.420398	-0.361628	-1.616384
1	-1.087707	-1.899019	0.073726
1	4.283698	-2.029227	1.042001
1	6.594287	-3.306327	1.248598
6	6.654886	-1.417036	2.249265
8	7.326500	-1.312148	3.238855
8	5.507302	-0.735204	2.054782

[13]

Number of imaginary frequencies : 0

Electronic energy=	-3905.3483592
Zero-point correction=	1.057666
Thermal correction to Energy=	1.122477
Thermal correction to Enthalpy=	1.123421
Thermal correction to Gibbs Free Energy=	0.951135
Sum of electronic and zero-point Energies=	-3904.290694
Sum of electronic and thermal Energies=	-3904.225882

Sum of electronic and thermal Enthalpies= -3904.224938
Sum of electronic and thermal Free Energies= -3904.397225

Cartesian Coordinates

7	1.132814	1.736950	1.743972
6	2.197247	1.522894	0.697796
6	-1.054718	3.488065	-2.711352
6	3.569397	0.454947	2.557791
6	1.487357	1.299639	-0.649324
6	4.004050	1.664697	3.105068
6	4.500513	1.716507	4.404437
8	0.480498	0.769997	2.085096
6	4.115978	-0.646921	4.649256
6	-0.288387	2.322578	-2.184070
6	-0.760339	4.806892	-2.352960
8	0.966997	2.872894	2.156472
6	3.614566	-0.694669	3.351814
6	-1.545861	5.850515	-2.832000
6	4.149567	0.053773	0.054957
6	3.066065	0.334907	1.130252
6	0.689697	2.543208	-1.050862
6	-2.138699	3.226823	-3.557837
6	4.566183	0.560242	5.177580
6	3.423970	-0.240877	-1.268168
6	-2.630855	5.582520	-3.662999
8	-0.495241	1.205538	-2.641183
6	-2.926861	4.268727	-4.027972
6	2.523734	0.911357	-1.715227
1	2.749175	2.465472	0.691605
1	4.687478	-0.850654	0.362570
1	2.808518	-1.130988	-1.108144
1	-1.313560	6.873025	-2.553236
1	4.838980	2.664118	4.811697
1	3.131536	1.790957	-1.968392
1	4.144876	-1.551331	5.248663
1	1.376060	3.356084	-1.319548
1	0.796251	0.457965	-0.504645
1	3.256487	-1.636862	2.946916
1	1.992709	0.629546	-2.629439
1	3.979625	2.575393	2.514776
1	2.409887	-0.544747	1.100317
1	-2.351476	2.197713	-3.828988
1	-3.246368	6.398392	-4.028884
1	-3.771037	4.060028	-4.677083
1	4.143282	-0.482652	-2.053121
1	0.073916	5.030858	-1.696184
1	4.954857	0.602910	6.190158
7	-0.723038	-1.396632	-1.406020
6	0.346060	-2.298323	-1.342163
6	0.841491	-2.796275	-0.129446
6	1.982593	-3.585595	-0.141314
6	2.657081	-3.892403	-1.323050
6	2.158204	-3.383334	-2.511909
6	1.009187	-2.597183	-2.531999
6	2.596769	-4.043786	1.149287
9	2.864331	-5.355479	1.143313
6	2.911043	-3.585880	-3.794849
9	2.085375	-3.753033	-4.837155
6	-1.876729	-1.368082	-0.666327
16	-2.417760	-2.621182	0.308002
7	-2.552618	-0.213026	-0.840238
6	-3.813436	0.097969	-0.193715
6	-4.007994	1.630385	-0.253979
6	-5.178188	2.083111	0.660970
6	-4.620793	3.037068	1.728793
6	-4.050977	4.269644	1.015040
6	-2.999662	3.785078	-0.019095
7	-2.756510	2.337763	0.087693
6	-2.347418	2.030662	1.466771

6	-3.467016	2.373035	2.503506
6	-3.839259	1.175967	3.340852
6	-5.062417	0.810689	3.719868
6	-4.982329	-0.600391	-0.880246
6	-6.034449	-1.251532	-0.161402
6	-7.112412	-1.787426	-0.927163
7	-7.173675	-1.725328	-2.287864
6	-6.175727	-1.148398	-2.909316
6	-5.064993	-0.572047	-2.249568
6	-8.181328	-2.425594	-0.252222
6	-8.196650	-2.543106	1.113773
6	-7.115997	-2.023533	1.871147
6	-6.059158	-1.398954	1.244106
9	3.773255	-3.414493	1.361575
9	1.823331	-3.786521	2.209506
9	3.722272	-4.649024	-3.741585
9	3.677217	-2.516561	-4.075348
1	-4.218737	1.894493	-1.299069
1	-5.944231	2.600317	0.074210
1	-5.661651	1.221153	1.126738
1	-2.040363	4.293616	0.127088
1	-3.324693	3.998101	-1.043358
1	-3.596480	4.946990	1.745809
1	-4.855279	4.820560	0.517148
1	-5.415991	3.335775	2.418887
1	-3.060919	3.124543	3.195150
1	-1.440300	2.605395	1.679718
1	-2.067377	0.974518	1.525622
1	-2.990861	0.574406	3.672030
1	-5.220324	-0.068295	4.337127
1	-5.953151	1.361768	3.428328
1	-3.755583	-0.222487	0.851232
1	-4.274138	-0.111733	-2.835269
1	-5.251001	-1.035740	1.867669
1	-6.229364	-1.114513	-3.996118
1	-8.988766	-2.822321	-0.859024
1	-9.027147	-3.038671	1.602095
1	-2.049425	0.591019	-1.205564
1	-0.610726	-0.651348	-2.088654
1	0.347893	-2.547614	0.802293
1	0.628963	-2.209255	-3.472676
1	3.553908	-4.502455	-1.309400
8	-7.047479	-2.104379	3.225267
6	-8.080681	-2.790374	3.904793
1	-7.815994	-2.761889	4.962057
1	-9.051712	-2.300340	3.766422
1	-8.150564	-3.835396	3.581336
6	8.519605	1.750133	0.995198
6	8.046052	0.783477	2.096699
6	6.751166	0.209791	1.531490
7	6.123883	1.403811	0.932172
6	7.226365	2.086732	0.236205
6	5.165754	1.179778	-0.123300
1	9.229641	1.276390	0.311943
1	8.995196	2.643278	1.402041
1	8.779468	0.009274	2.329023
1	7.819451	1.335017	3.013473
1	6.976648	-0.559937	0.774074
1	6.100262	-0.223954	2.293326
1	0.082837	2.924601	-0.216167
1	4.656965	2.135225	-0.314319
1	7.032803	3.163166	0.151113
6	7.163544	1.486889	-1.169922
8	8.009620	1.484873	-2.021035
8	5.951384	0.913221	-1.326656

Stationary Points Relevant to Fig. S5
Different Possibilities for the Catalyst Dyad (Proline with Cinchona-Thiourea)

Conf-1 (0.0)

Number of imaginary frequencies : 1

Electronic energy = -2813.7276851
Zero-point correction= 0.692279
Thermal correction to Energy= 0.735416
Thermal correction to Enthalpy= 0.736360
Thermal correction to Gibbs Free Energy= 0.611922
Sum of electronic and zero-point Energies= -2813.035407
Sum of electronic and thermal Energies= -2812.992269
Sum of electronic and thermal Enthalpies= -2812.991325
Sum of electronic and thermal Free Energies= -2813.115763

Cartesian Coordinates

6	-3.576785	4.001958	-0.143787
6	-4.459584	4.000448	1.125990
6	-3.933370	2.807543	1.965710
7	-2.629943	2.428531	1.392719
6	-2.812471	2.664637	-0.047346
6	-1.494124	2.658821	-0.795388
8	-0.491149	3.138781	-0.072774
8	-1.385063	2.271314	-1.939653
1	-3.424318	1.852412	-0.456341
1	-2.857217	4.826901	-0.115233
1	-4.147106	4.083586	-1.070677
1	-5.516555	3.869294	0.883890
1	-4.362287	4.943525	1.668733
1	-4.610107	1.952220	1.870258
1	-3.825010	3.033540	3.028361
1	0.434758	2.918218	-0.567151
1	-1.934414	3.107194	1.705944
7	-1.354977	-0.084457	0.628690
6	-2.520251	-0.785769	0.284360
6	-2.700370	-1.429304	-0.944470
6	-3.924194	-2.021786	-1.227640
6	-4.992844	-1.965783	-0.336943
6	-4.805744	-1.301925	0.867539
6	-3.581539	-0.726462	1.189963
6	-4.087811	-2.771939	-2.519879
9	-3.325286	-2.262218	-3.496286
6	-5.940805	-1.144160	1.836117
9	-5.549943	-1.352982	3.101751
6	-0.057924	-0.370235	0.317735
16	0.470855	-1.810477	-0.377618
7	0.782976	0.638368	0.644846
6	2.215034	0.632285	0.404028
6	2.689178	2.025186	-0.067044
6	4.142459	1.955952	-0.609826
6	4.138404	2.361616	-2.092551
6	3.678152	3.821515	-2.187583
6	2.302379	3.935269	-1.490669
7	1.790421	2.600625	-1.100554
6	1.722822	1.734713	-2.296920
6	3.142505	1.501682	-2.895637
6	3.476657	0.032937	-2.985197
6	4.658110	-0.531376	-2.744501
6	2.995508	0.220872	1.650305
6	3.990059	-0.808009	1.639515
6	4.693402	-1.045037	2.859017
7	4.444963	-0.367620	4.015186
6	3.506390	0.544920	3.991390
6	2.762491	0.875205	2.834013
6	5.705604	-2.034614	2.885444
6	6.018156	-2.766599	1.769326

6	5.306780	-2.540571	0.563010
6	4.311663	-1.587892	0.504873
9	-3.745146	-4.062733	-2.388554
9	-5.359782	-2.749545	-2.948277
9	-6.949832	-1.984577	1.578057
9	-6.448798	0.103820	1.797096
1	2.631895	2.711339	0.787986
1	4.793650	2.631478	-0.046624
1	4.544308	0.947008	-0.487574
1	1.550602	4.387923	-2.143848
1	2.356513	4.541615	-0.581155
1	3.606243	4.124461	-3.236842
1	4.408010	4.479759	-1.707075
1	5.143958	2.258933	-2.510585
1	3.135271	1.887973	-3.924277
1	1.049032	2.225512	-3.002190
1	1.242148	0.792879	-2.014232
1	2.649447	-0.605722	-3.298693
1	4.799269	-1.602566	-2.849301
1	5.525574	0.041898	-2.426419
1	2.392069	-0.091378	-0.393268
1	2.005361	1.651904	2.900298
1	3.781681	-1.474157	-0.433288
1	3.310364	1.072394	4.923107
1	6.224117	-2.192887	3.825316
1	6.797555	-3.517531	1.820364
1	0.367979	1.502436	0.976856
1	-1.566824	0.752906	1.188640
1	-1.897185	-1.453907	-1.669100
1	-3.442294	-0.225899	2.143805
1	-5.945796	-2.420986	-0.580244
8	5.546529	-3.228625	-0.581836
6	6.542685	-4.232760	-0.559864
1	6.560110	-4.660834	-1.562386
1	7.530609	-3.815376	-0.331861
1	6.303645	-5.022232	0.161966

 Conf-2 (0.7)

Number of imaginary frequencies : 0

Electronic energy = -2813.728735
 Zero-point correction= 0.693489
 Thermal correction to Energy= 0.736967
 Thermal correction to Enthalpy= 0.737911
 Thermal correction to Gibbs Free Energy= 0.613805
 Sum of electronic and zero-point Energies= -2813.035246
 Sum of electronic and thermal Energies= -2812.991768
 Sum of electronic and thermal Enthalpies= -2812.990824
 Sum of electronic and thermal Free Energies= -2813.114930

 Cartesian Coordinates

6	2.771135	4.329973	-2.165818
6	3.713073	3.217699	-2.636074
6	4.569059	2.986260	-1.396984
7	3.581734	3.038694	-0.310919
6	2.494458	3.973132	-0.696637
6	1.182927	3.210554	-0.494182
8	0.739592	2.523639	-1.450776
8	0.668537	3.278245	0.660779
1	2.475245	4.856064	-0.049644
1	1.851589	4.386879	-2.750001
1	3.282018	5.296903	-2.219081
1	4.302335	3.488570	-3.514729
1	3.134754	2.315988	-2.860552
1	5.332763	3.774299	-1.311179

1	5.082677	2.019241	-1.404033
1	-0.590951	2.677244	0.966621
7	1.365003	-0.255310	-0.435505
6	2.534488	-0.970800	-0.125552
6	2.607104	-2.364820	-0.089059
6	3.826882	-2.969636	0.197876
6	4.980833	-2.228435	0.428662
6	4.891027	-0.842846	0.363459
6	3.684763	-0.210356	0.095645
6	3.913653	-4.469481	0.186312
9	2.759865	-5.043754	0.547957
6	6.119099	-0.002194	0.553541
9	6.749485	0.232512	-0.612487
6	0.080592	-0.474129	-0.021712
16	-0.430052	-1.813324	0.874649
7	-0.732704	0.538323	-0.379948
6	-2.158500	0.579032	-0.152308
6	-2.562702	1.989195	0.328315
6	-4.001122	2.024036	0.896826
6	-3.950073	2.363025	2.395899
6	-3.403550	3.788271	2.546397
6	-2.059311	3.871545	1.798604
7	-1.625067	2.503186	1.378361
6	-1.569349	1.602245	2.562686
6	-2.996526	1.414059	3.148977
6	-3.403597	-0.039635	3.169953
6	-4.622275	-0.522850	2.941271
6	-2.937329	0.258946	-1.426665
6	-4.014263	-0.680891	-1.463257
6	-4.700095	-0.834506	-2.705323
7	-4.362626	-0.156997	-3.838642
6	-3.349878	0.671090	-3.770310
6	-2.611584	0.914910	-2.587858
6	-5.789709	-1.736021	-2.777455
6	-6.192330	-2.460242	-1.685003
6	-5.497958	-2.317643	-0.456046
6	-4.429539	-1.452334	-0.353881
9	4.215436	-4.937740	-1.037014
9	4.868282	-4.918413	1.016604
9	7.011951	-0.589587	1.362039
9	5.827697	1.200211	1.077120
1	-2.446283	2.684687	-0.510620
1	-4.597638	2.777122	0.373921
1	-4.485282	1.058151	0.734081
1	-1.252450	4.278732	2.410579
1	-2.120059	4.470157	0.886951
1	-3.268593	4.028586	3.605029
1	-4.109251	4.512520	2.131685
1	-4.952887	2.301490	2.826677
1	-2.964628	1.749720	4.193998
1	-0.885921	2.071050	3.274012
1	-1.126044	0.653796	2.247270
1	-2.604415	-0.736138	3.425725
1	-4.820487	-1.588297	3.001295
1	-5.465167	0.110763	2.676142
1	-2.388746	-0.153913	0.623435
1	-1.784399	1.620818	-2.615752
1	-3.915440	-1.400564	0.598462
1	-3.083361	1.197867	-4.684522
1	-6.294595	-1.833891	-3.732976
1	-7.029630	-3.142214	-1.771543
1	-0.296100	1.340492	-0.883746
1	1.533803	0.655686	-0.863773
1	1.725529	-2.963935	-0.274637
1	3.612615	0.878286	0.072458
1	5.919824	-2.718946	0.659960
8	-5.825398	-3.001337	0.669590
6	-6.880978	-3.941003	0.597097
1	-6.956368	-4.385924	1.589444
1	-7.833623	-3.458600	0.348491

1	-6.668831	-4.729683	-0.133766
1	3.997615	3.294553	0.577409

 Conf-3 (0.7)

Number of imaginary frequencies : 0

Electronic energy = -2813.7265899
 Zero-point correction= 0.693912
 Thermal correction to Energy= 0.737765
 Thermal correction to Enthalpy= 0.738709
 Thermal correction to Gibbs Free Energy= 0.611974
 Sum of electronic and zero-point Energies= -2813.032678
 Sum of electronic and thermal Energies= -2812.988825
 Sum of electronic and thermal Enthalpies= -2812.987881
 Sum of electronic and thermal Free Energies= -2813.114615

 Cartesian Coordinates

6	2.459768	-3.319528	2.995657
6	3.584057	-2.438425	2.450419
6	4.231920	-3.377038	1.429471
7	3.133918	-4.189112	0.867041
6	1.952570	-4.022030	1.721014
6	0.850726	-3.177828	1.067455
8	1.063305	-2.721586	-0.112489
8	-0.194643	-2.958344	1.714072
1	1.488920	-4.985073	1.968726
1	1.658329	-2.779914	3.502699
1	2.870764	-4.061829	3.687540
1	4.278220	-2.089446	3.218597
1	3.164006	-1.554890	1.950755
1	4.950999	-4.032277	1.938248
1	4.775055	-2.851552	0.639302
1	-0.388335	-2.419756	-0.668638
1	2.888032	-3.843841	-0.056051
7	1.413639	0.136072	0.288673
6	2.592306	0.845124	0.029901
6	2.739823	2.205241	0.311571
6	3.963960	2.818254	0.074077
6	5.054350	2.112739	-0.422929
6	4.896017	0.756239	-0.681504
6	3.680523	0.120162	-0.464024
6	4.134014	4.265390	0.442882
9	2.993487	4.953635	0.310034
6	6.036533	-0.012703	-1.283411
9	5.957257	-1.325053	-1.010789
6	0.115593	0.542500	0.102103
16	-0.360527	1.948846	-0.689944
7	-0.750406	-0.376678	0.577180
6	-2.147699	-0.477467	0.208510
6	-2.430890	-1.929078	-0.229293
6	-3.795890	-2.092517	-0.932700
6	-3.573104	-2.567621	-2.376618
6	-2.907533	-3.951782	-2.336019
6	-1.624804	-3.862411	-1.485136
7	-1.353407	-2.429155	-1.153862
6	-1.256006	-1.625829	-2.407884
6	-2.630275	-1.607091	-3.128706
6	-3.138517	-0.195633	-3.307694
6	-4.401558	0.212150	-3.211315
6	-3.075580	-0.121310	1.362336
6	-4.146730	0.814740	1.223696
6	-4.971353	1.026728	2.368833
7	-4.774648	0.399269	3.562388
6	-3.772440	-0.439691	3.649966
6	-2.898615	-0.737067	2.576276

6	-6.054382	1.933728	2.274072
6	-6.323428	2.606544	1.110149
6	-5.496593	2.400526	-0.024097
6	-4.430979	1.527609	0.036225
9	4.527696	4.404360	1.719760
9	5.062190	4.866210	-0.316663
9	7.222279	0.421525	-0.834683
9	6.060389	0.103243	-2.620823
1	-2.341899	-2.570830	0.650306
1	-4.408899	-2.822123	-0.396473
1	-4.334909	-1.141991	-0.916693
1	-0.740277	-4.236307	-2.004291
1	-1.706861	-4.387035	-0.530370
1	-2.668433	-4.281476	-3.351185
1	-3.591421	-4.686605	-1.904474
1	-4.529891	-2.634548	-2.900682
1	-2.475458	-2.021224	-4.133465
1	-0.474133	-2.094545	-3.009203
1	-0.917265	-0.621667	-2.139295
1	-2.372527	0.536708	-3.566435
1	-4.664903	1.251727	-3.379037
1	-5.218846	-0.459008	-2.959264
1	-2.311797	0.202500	-0.629213
1	-2.093648	-1.453735	2.726314
1	-3.817738	1.428106	-0.851712
1	-3.624685	-0.929111	4.610524
1	-6.664650	2.076820	3.159870
1	-7.160062	3.293627	1.068148
1	-0.396420	-1.158856	1.138439
1	1.521139	-0.881884	0.286405
1	1.909414	2.774260	0.709814
1	3.564943	-0.939216	-0.680169
1	6.003037	2.606789	-0.600652
8	-5.690482	3.029104	-1.211103
6	-6.714865	4.002716	-1.289514
1	-6.660022	4.416370	-2.296645
1	-7.705883	3.559154	-1.138279
1	-6.559779	4.807630	-0.562284

 Conf-4 (1.0)

Number of imaginary frequencies : 1

Electronic energy = -2813.7278194
 Zero-point correction= 0.692842
 Thermal correction to Energy= 0.735787
 Thermal correction to Enthalpy= 0.736731
 Thermal correction to Gibbs Free Energy= 0.613584
 Sum of electronic and zero-point Energies= -2813.034978
 Sum of electronic and thermal Energies= -2812.992033
 Sum of electronic and thermal Enthalpies= -2812.991088
 Sum of electronic and thermal Free Energies= -2813.114235

 Cartesian Coordinates

6	-3.609918	3.981569	-0.124926
6	-4.444476	3.999156	1.177005
6	-3.900572	2.806607	2.004826
7	-2.615774	2.420317	1.396120
6	-2.842290	2.644386	-0.039329
6	-1.550955	2.634560	-0.832941
8	-0.511822	3.070092	-0.134445
8	-1.493411	2.286068	-1.993646
1	-3.467788	1.829361	-0.421700
1	-2.890521	4.807112	-0.135840
1	-4.214251	4.049537	-1.031046
1	-5.511542	3.880121	0.976646

1	-4.314412	4.944443	1.709026
1	-4.583030	1.953737	1.929780
1	-3.761818	3.034417	3.063541
1	0.391780	2.833600	-0.665936
1	-1.909738	3.100104	1.682323
7	-1.338666	-0.094995	0.655272
6	-2.506655	-0.798109	0.322816
6	-2.694544	-1.445828	-0.902521
6	-3.922011	-2.033838	-1.178818
6	-4.986518	-1.970089	-0.283566
6	-4.791200	-1.303580	0.918097
6	-3.563216	-0.731898	1.233241
6	-4.095015	-2.785239	-2.469112
9	-3.334254	-2.280443	-3.449527
6	-5.921401	-1.137552	1.891024
9	-5.525722	-1.342219	3.155796
6	-0.043209	-0.388868	0.344798
16	0.477980	-1.844581	-0.324546
7	0.798729	0.626013	0.648703
6	2.225043	0.635267	0.374650
6	2.657928	2.004573	-0.200314
6	4.095784	1.928648	-0.779836
6	4.041123	2.235650	-2.285632
6	3.548350	3.677590	-2.461561
6	2.192210	3.811152	-1.730528
7	1.718960	2.495501	-1.240480
6	1.632999	1.553145	-2.376099
6	3.039893	1.308852	-3.002530
6	3.397971	-0.156631	-3.012978
6	4.590269	-0.689868	-2.755091
6	3.041750	0.326921	1.626240
6	4.052763	-0.685101	1.662844
6	4.786863	-0.826968	2.878835
7	4.551551	-0.075864	3.991681
6	3.598327	0.819376	3.926649
6	2.825140	1.059299	2.766436
6	5.816147	-1.796619	2.948371
6	6.115789	-2.598059	1.877043
6	5.374165	-2.465958	0.675005
6	4.361767	-1.534818	0.576265
9	-3.757884	-4.077449	-2.337637
9	-5.368652	-2.757116	-2.891904
9	-6.934651	-1.975331	1.641180
9	-6.425007	0.112130	1.848703
1	2.609353	2.743977	0.609914
1	4.747567	2.653838	-0.282948
1	4.524028	0.938840	-0.603235
1	1.411499	4.207955	-2.385918
1	2.263105	4.473728	-0.862375
1	3.437745	3.907933	-3.525701
1	4.278155	4.380006	-2.048487
1	5.036266	2.123851	-2.725864
1	2.995120	1.629953	-4.052468
1	0.928559	1.985818	-3.089388
1	1.185163	0.620169	-2.019721
1	2.577944	-0.823620	-3.283090
1	4.745680	-1.763123	-2.802904
1	5.452793	-0.088202	-2.479021
1	2.398507	-0.137745	-0.375443
1	2.058630	1.829417	2.795390
1	3.808699	-1.492813	-0.354553
1	3.412891	1.405730	4.824766
1	6.359030	-1.882574	3.883961
1	6.908641	-3.331693	1.960393
1	0.378322	1.497683	0.953084
1	-1.548218	0.752850	1.200906
1	-1.894636	-1.475911	-1.630679
1	-3.417840	-0.228302	2.184508
1	-5.942723	-2.421259	-0.521634
8	5.599144	-3.225423	-0.426623

6	6.616124	-4.207031	-0.365851
1	6.617912	-4.697774	-1.339456
1	7.600410	-3.757287	-0.190077
1	6.411127	-4.953593	0.410028

 Conf-5 (1.4)

Number of imaginary frequencies : 0

Electronic energy = -2813.7289488
 Zero-point correction= 0.694868
 Thermal correction to Energy= 0.738130
 Thermal correction to Enthalpy= 0.739074
 Thermal correction to Gibbs Free Energy= 0.615476
 Sum of electronic and zero-point Energies= -2813.034081
 Sum of electronic and thermal Energies= -2812.990819
 Sum of electronic and thermal Enthalpies= -2812.989875
 Sum of electronic and thermal Free Energies= -2813.113473

 Cartesian Coordinates

6	-0.623225	-4.655770	-2.511661
6	0.519786	-4.034809	-3.318761
6	-0.003926	-2.626710	-3.583500
7	-0.655487	-2.251363	-2.312530
6	-1.086766	-3.504525	-1.615953
6	-0.365017	-3.447742	-0.263574
8	-0.896906	-2.652759	0.598793
8	0.713211	-4.037000	-0.118234
1	-2.167771	-3.502231	-1.444474
1	-0.308624	-5.517461	-1.921463
1	-1.434783	-4.959508	-3.180903
1	0.748774	-4.574392	-4.240309
1	1.419652	-4.001598	-2.696089
1	-0.723512	-2.647612	-4.413408
1	0.781294	-1.906420	-3.835406
1	0.268209	-2.136191	1.426071
7	-1.661166	-0.067827	-0.225331
6	-2.937107	0.493511	-0.129423
6	-3.239731	1.796917	-0.541085
6	-4.549875	2.246976	-0.457265
6	-5.580894	1.435085	0.008917
6	-5.268309	0.138473	0.391886
6	-3.963034	-0.336022	0.330348
6	-4.896073	3.625813	-0.944495
9	-3.824822	4.424203	-1.016108
6	-6.336147	-0.760585	0.945261
9	-6.155773	-2.035143	0.565460
6	-0.438998	0.523201	-0.018212
16	-0.195317	2.064787	0.618217
7	0.550664	-0.339172	-0.335709
6	1.916143	-0.270413	0.138756
6	2.264762	-1.517635	0.990732
6	3.591173	-1.334256	1.763012
6	3.313927	-1.370954	3.273715
6	2.788508	-2.768264	3.631846
6	1.578889	-3.086370	2.732693
7	1.179740	-1.856079	1.975949
6	0.913871	-0.743864	2.931343
6	2.228325	-0.346887	3.658515
6	2.580300	1.102074	3.415687
6	3.801357	1.602617	3.243289
6	2.896921	-0.214688	-1.024896
6	3.888873	0.803811	-1.160228
6	4.771682	0.704087	-2.276911
7	4.692341	-0.286621	-3.210307
6	3.757765	-1.192218	-3.057506

6	2.844830	-1.202789	-1.976072
6	5.788348	1.677779	-2.430639
6	5.937651	2.702879	-1.531580
6	5.051801	2.803106	-0.427720
6	4.045787	1.876305	-0.253844
9	-5.445035	3.589314	-2.170891
9	-5.792917	4.220946	-0.142791
9	-7.560291	-0.389463	0.545548
9	-6.343049	-0.756036	2.288197
1	2.294517	-2.390732	0.334370
1	4.292581	-2.131422	1.500860
1	4.055814	-0.387146	1.477505
1	0.699158	-3.394949	3.301816
1	1.774122	-3.848566	1.977936
1	2.503187	-2.800321	4.687591
1	3.570898	-3.516345	3.480407
1	4.233029	-1.163906	3.828472
1	2.046942	-0.453405	4.736242
1	0.152361	-1.109046	3.623763
1	0.490004	0.095787	2.376229
1	1.730301	1.785243	3.411341
1	3.952618	2.667684	3.097830
1	4.693463	0.981356	3.237149
1	1.994156	0.628792	0.751973
1	2.107366	-2.000832	-1.904551
1	3.383448	2.008298	0.594113
1	3.704074	-1.977485	-3.810139
1	6.448534	1.582460	-3.286588
1	6.726936	3.431063	-1.675255
1	0.285740	-1.112657	-0.967922
1	-1.617695	-1.088800	-0.091691
1	-2.461109	2.446967	-0.917493
1	-3.733066	-1.352301	0.640214
1	-6.598511	1.804859	0.066724
8	5.128414	3.785920	0.503763
6	6.127975	4.775931	0.350008
1	5.995434	5.468454	1.181395
1	7.134229	4.343734	0.400374
1	6.011081	5.322600	-0.592677
1	-1.448610	-1.641204	-2.485415

 Conf-6 (1.9)

Number of imaginary frequencies : 0

Electronic energy = -2813.7233927
 Zero-point correction= 0.693915
 Thermal correction to Energy= 0.737947
 Thermal correction to Enthalpy= 0.738891
 Thermal correction to Gibbs Free Energy= 0.610662
 Sum of electronic and zero-point Energies= -2813.029477
 Sum of electronic and thermal Energies= -2812.985445
 Sum of electronic and thermal Enthalpies= -2812.984501
 Sum of electronic and thermal Free Energies= -2813.112730

 Cartesian Coordinates

6	2.255919	4.943586	-1.174492
6	1.763859	5.600451	0.117098
6	0.442062	6.220803	-0.326406
7	-0.135869	5.200068	-1.212591
6	0.968755	4.396960	-1.804538
6	0.668247	2.945096	-1.429326
8	-0.055662	2.279979	-2.201345
8	1.110881	2.516979	-0.307375
1	0.968064	4.467513	-2.896062
1	2.992930	4.157664	-1.001201

1	2.697950	5.698140	-1.833541
1	2.458797	6.337497	0.525530
1	1.585222	4.824515	0.867322
1	0.632930	7.170278	-0.848668
1	-0.232699	6.430639	0.511829
1	-0.197512	2.043530	0.538466
7	1.610307	-0.352439	-0.532539
6	2.844956	-0.959631	-0.287131
6	3.053116	-2.341051	-0.391821
6	4.319946	-2.854808	-0.162018
6	5.403641	-2.035508	0.150153
6	5.186761	-0.668500	0.224137
6	3.922356	-0.125769	0.013989
6	4.564438	-4.330539	-0.303022
9	3.429122	-5.038111	-0.292581
6	6.316111	0.271438	0.531468
9	6.599275	1.062318	-0.516848
6	0.351232	-0.807466	-0.231388
16	0.002957	-2.162645	0.712861
7	-0.584450	0.018324	-0.736503
6	-1.955197	0.106571	-0.283261
6	-2.224349	1.557313	0.175741
6	-3.567935	1.715098	0.918865
6	-3.305380	2.198420	2.352841
6	-2.644063	3.582498	2.283236
6	-1.362091	3.483627	1.432568
7	-1.118453	2.047061	1.076977
6	-0.992524	1.232671	2.321868
6	-2.344368	1.240909	3.085645
6	-2.857654	-0.164014	3.297372
6	-4.125232	-0.564476	3.237558
6	-2.946424	-0.253241	-1.382352
6	-4.004917	-1.192655	-1.179272
6	-4.894094	-1.412972	-2.273395
7	-4.769634	-0.788741	-3.478789
6	-3.775461	0.051603	-3.626796
6	-2.840647	0.356176	-2.607745
6	-5.963595	-2.326428	-2.111987
6	-6.159996	-2.996544	-0.931777
6	-5.270900	-2.779808	0.152081
6	-4.215726	-1.901547	0.025536
9	5.200045	-4.617493	-1.452220
9	5.341323	-4.795042	0.688633
9	7.441954	-0.376717	0.856090
9	6.013412	1.089244	1.553146
1	-2.161729	2.209849	-0.700878
1	-4.201646	2.437600	0.397537
1	-4.099268	0.760094	0.923399
1	-0.471958	3.816612	1.971379
1	-1.402554	4.037285	0.489182
1	-2.406689	3.934970	3.291193
1	-3.333744	4.303832	1.837569
1	-4.248059	2.267699	2.901692
1	-2.153914	1.666705	4.079467
1	-0.184209	1.684987	2.899637
1	-0.683405	0.222932	2.040655
1	-2.089806	-0.898752	3.543282
1	-4.390740	-1.601007	3.420207
1	-4.944180	0.109400	2.998498
1	-2.067702	-0.576233	0.560592
1	-2.043763	1.069337	-2.809137
1	-3.553557	-1.792389	0.876319
1	-3.683457	0.536679	-4.596619
1	-6.624012	-2.478094	-2.959548
1	-6.986870	-3.690487	-0.839275
1	-0.286403	0.778347	-1.382931
1	1.645576	0.662954	-0.668999
1	2.232431	-2.999121	-0.643250
1	3.764293	0.947076	0.094526
1	6.386566	-2.455843	0.330219

8	-5.392787	-3.402625	1.352045
6	-6.409507	-4.376751	1.496349
1	-6.301022	-4.778305	2.503907
1	-7.408045	-3.936741	1.391230
1	-6.290958	-5.190027	0.771486
1	-0.711153	5.611745	-1.937923

Stationary Points relevant to Scheme S5, Figs. S4 and S6 and Table S5
Proline Enamine Formation in the Absence of Cinchona-Thiourea and
Conformational Analysis of the Transition States

[2]_conf-1

Number of imaginary frequencies : 0

Electronic energy=	-1055.0065587
Zero-point correction=	0.390600
Thermal correction to Energy=	0.413126
Thermal correction to Enthalpy=	0.414070
Thermal correction to Gibbs Free Energy=	0.337383
Sum of electronic and zero-point Energies=	-1054.615959
Sum of electronic and thermal Energies=	-1054.593433
Sum of electronic and thermal Enthalpies=	-1054.592489
Sum of electronic and thermal Free Energies=	-1054.669176

Cartesian Coordinates

6	-0.944305	-2.921418	-0.220088
6	-1.620892	-2.925937	-1.610883
6	-2.489974	-1.647131	-1.614406
7	-1.943174	-0.764201	-0.573715
6	-1.567305	-1.711826	0.492302
6	-3.760854	0.704402	0.734444
6	-2.829671	1.885935	0.676640
6	-0.635177	-1.031323	1.494759
8	-1.224340	-0.313034	2.453506
8	-3.832111	-0.053702	1.686610
8	0.568674	-1.107337	1.438604
1	-1.850241	1.547731	1.029295
1	-2.492224	-1.997777	1.011288
1	0.130686	-2.748238	-0.307340
1	-1.099604	-3.848291	0.336971
1	-2.223879	-3.821382	-1.779979
1	-0.867470	-2.878379	-2.400682
1	-3.526687	-1.886088	-1.347178
1	-2.499996	-1.127854	-2.576302
1	-2.200237	-0.283870	2.334139
1	-1.066515	-0.385949	-0.941824
1	-3.191378	2.608795	1.419924
1	-4.466090	0.584792	-0.110255
6	-2.730421	2.532089	-0.705464
6	-1.334194	3.136160	-0.952898
1	-3.493118	3.308016	-0.819659
1	-2.926727	1.776112	-1.476630
1	-1.378542	3.805212	-1.819429
1	-1.022177	3.731177	-0.087556
6	-0.356344	2.039254	-1.228685
6	0.648018	1.637680	-0.443185
1	-0.522396	1.480089	-2.152000
1	0.885846	2.150850	0.484996
6	1.453716	0.446781	-0.839477
8	0.982961	-0.395601	-1.593074
6	2.842123	0.306806	-0.313538

6	3.556964	1.400026	0.181080
6	3.442318	-0.954847	-0.352075
6	4.863617	1.232806	0.630495
1	3.104358	2.386833	0.198974
6	4.740982	-1.122526	0.108188
1	2.867603	-1.790984	-0.736113
6	5.453033	-0.027792	0.598901
1	5.419856	2.085769	1.005913
1	5.200999	-2.105388	0.088755
1	6.468875	-0.159209	0.958871

[2-3]TS_conf-1

Number of imaginary frequencies : 1
The smallest frequency is : -126.8538

Electronic energy=	-1055.0028652
Zero-point correction=	0.391720
Thermal correction to Energy=	0.412476
Thermal correction to Enthalpy=	0.413420
Thermal correction to Gibbs Free Energy=	0.341357
Sum of electronic and zero-point Energies=	-1054.611145
Sum of electronic and thermal Energies=	-1054.590389
Sum of electronic and thermal Enthalpies=	-1054.589445
Sum of electronic and thermal Free Energies=	-1054.661508

Cartesian Coordinates

6	-0.894822	-2.706876	-0.602972
6	-1.569108	-2.363224	-1.952186
6	-2.600321	-1.280295	-1.603524
7	-2.076836	-0.619232	-0.391599
6	-1.511496	-1.733947	0.407841
6	-3.423254	0.292753	0.705405
6	-2.791737	1.673657	0.804717
6	-0.547990	-1.188669	1.472038
8	-1.122556	-0.526395	2.458942
8	-3.541896	-0.411906	1.743436
8	0.650378	-1.349380	1.405709
1	-1.786911	1.555873	1.225531
1	-2.366594	-2.180466	0.928471
1	0.181933	-2.537411	-0.647694
1	-1.070327	-3.740053	-0.296246
1	-2.043643	-3.226858	-2.422460
1	-0.826966	-1.960011	-2.643743
1	-3.569018	-1.719301	-1.337639
1	-2.758596	-0.541340	-2.392719
1	-2.140056	-0.475855	2.319856
1	-1.306475	-0.003464	-0.667631
1	-3.376233	2.202390	1.565807
1	-4.203423	0.205232	-0.073801
6	-2.766364	2.475536	-0.501959
6	-1.415373	3.185185	-0.734031
1	-3.568939	3.218303	-0.505486
1	-2.964692	1.812348	-1.356481
1	-1.519017	3.911660	-1.546893
1	-1.119528	3.728314	0.169543
6	-0.398267	2.155262	-1.099891
6	0.584765	1.681937	-0.325911
1	-0.537124	1.675764	-2.071975
1	0.808093	2.113995	0.646529
6	1.371708	0.505424	-0.799860
8	0.860372	-0.291985	-1.575792
6	2.768655	0.324893	-0.318144
6	3.494387	1.381133	0.237550
6	3.363699	-0.933225	-0.452465
6	4.807297	1.181431	0.652911

1	3.043291	2.364223	0.332934
6	4.669307	-1.133438	-0.027353
1	2.780137	-1.741238	-0.880751
6	5.392287	-0.075547	0.524860
1	5.371563	2.004630	1.079057
1	5.126180	-2.113359	-0.121381
1	6.413586	-0.233361	0.857851

[2-3]TS_conf-2

Number of imaginary frequencies : 1

The smallest frequency is : -142.6404

Electronic energy=	-1054.9982838
Zero-point correction=	0.391841
Thermal correction to Energy=	0.412647
Thermal correction to Enthalpy=	0.413591
Thermal correction to Gibbs Free Energy=	0.340965
Sum of electronic and zero-point Energies=	-1054.606443
Sum of electronic and thermal Energies=	-1054.585637
Sum of electronic and thermal Enthalpies=	-1054.584693
Sum of electronic and thermal Free Energies=	-1054.657318

Cartesian Coordinates

6	-1.642296	-2.681436	-1.021030
6	-2.787933	-2.100793	-1.869106
6	-2.974320	-0.655962	-1.339069
7	-1.940946	-0.452323	-0.295445
6	-1.679647	-1.817606	0.229250
6	-2.315708	0.650296	1.258443
6	-3.258578	1.738368	0.785609
6	-0.415667	-1.858182	1.100721
8	-0.543712	-1.324279	2.297867
8	-2.737006	-0.151591	2.143720
8	0.612880	-2.362074	0.705234
1	-3.392163	2.353223	1.686285
1	-2.543493	-2.063931	0.858776
1	-0.670297	-2.545622	-1.503096
1	-1.767967	-3.742255	-0.795771
1	-3.708401	-2.672205	-1.728068
1	-2.551215	-2.111993	-2.934549
1	-3.955228	-0.525806	-0.871361
1	-2.857993	0.101987	-2.115448
1	-1.489514	-0.900237	2.399175
1	-1.075377	-0.137075	-0.748064
1	-4.236155	1.286097	0.587409
1	-1.259946	0.958590	1.306466
6	-2.840798	2.653086	-0.370407
6	-1.411482	3.230228	-0.297147
1	-3.551541	3.484876	-0.397149
1	-2.954465	2.134788	-1.329280
1	-1.373897	4.125805	-0.929672
1	-1.163167	3.541460	0.723992
6	-0.414694	2.240433	-0.808669
6	0.687260	1.800122	-0.193429
1	-0.655955	1.788355	-1.774128
1	1.019216	2.214443	0.755607
6	1.409726	0.625944	-0.756928
8	0.817462	-0.157548	-1.492411
6	2.824726	0.386974	-0.372053
6	3.651273	1.431395	0.051235
6	3.323809	-0.917104	-0.450758
6	4.978124	1.175395	0.380164
1	3.264522	2.445197	0.104093
6	4.644525	-1.170710	-0.104442
1	2.650758	-1.712586	-0.752995

6	5.471864	-0.125390	0.305996
1	5.624888	1.987279	0.696513
1	5.031003	-2.183714	-0.148987
1	6.504909	-0.326822	0.572806

[2-3]TS_conf-3

Number of imaginary frequencies : 1
 The smallest frequency is : -157.8137

Electronic energy=	-1054.9963941
Zero-point correction=	0.391569
Thermal correction to Energy=	0.412268
Thermal correction to Enthalpy=	0.413212
Thermal correction to Gibbs Free Energy=	0.339458
Sum of electronic and zero-point Energies=	-1054.604825
Sum of electronic and thermal Energies=	-1054.584126
Sum of electronic and thermal Enthalpies=	-1054.583182
Sum of electronic and thermal Free Energies=	-1054.656936

 Cartesian Coordinates

6	2.622702	-1.750004	1.297881
6	1.432029	-2.240087	0.461151
6	1.050416	-0.989774	-0.323224
7	2.362343	-0.405900	-0.709925
6	3.308696	-0.692896	0.420854
6	2.561013	1.345726	-1.291057
6	1.313426	2.061436	-0.812376
6	4.659725	-1.114703	-0.180079
8	5.168965	-0.237249	-1.016457
8	3.686219	1.737040	-0.833056
8	5.178340	-2.177134	0.080207
1	0.423147	1.472740	-1.060336
1	3.474396	0.256425	0.939592
1	3.327962	-2.544475	1.544775
1	2.269405	-1.293874	2.226742
1	0.601381	-2.611535	1.063710
1	1.749018	-3.032473	-0.225736
1	0.525240	-0.280427	0.320851
1	0.445593	-1.165683	-1.215499
1	4.628931	0.666858	-0.997101
1	2.688544	-0.919942	-1.529610
1	1.247999	2.981364	-1.408049
1	2.497876	1.064658	-2.358771
6	1.355650	2.421675	0.671793
6	-0.027856	2.836634	1.210381
1	2.082106	3.222265	0.828368
1	1.715405	1.565393	1.257575
1	0.093038	3.299295	2.195814
1	-0.486681	3.575995	0.544347
6	-0.886888	1.619500	1.325954
6	-1.928827	1.306258	0.549534
1	-0.575662	0.877576	2.064161
1	-2.299496	2.004621	-0.195876
6	-2.552808	-0.040564	0.662717
8	-1.949346	-0.963820	1.190375
6	-3.917531	-0.260043	0.089938
6	-4.765485	0.797022	-0.253085
6	-4.354550	-1.577953	-0.080167
6	-6.032824	0.536705	-0.766075
1	-4.452365	1.824939	-0.101053
6	-5.614938	-1.836311	-0.601271
1	-3.686955	-2.385125	0.202826
6	-6.455289	-0.777654	-0.946233
1	-6.690392	1.360552	-1.023782
1	-5.946647	-2.860527	-0.738481

1 -7.441623 -0.977806 -1.353362

[2-3]TS_conf-4

Number of imaginary frequencies : 1

The smallest frequency is : -125.0335

Electronic energy= -1054.9979403
Zero-point correction= 0.392185
Thermal correction to Energy= 0.412848
Thermal correction to Enthalpy= 0.413792
Thermal correction to Gibbs Free Energy= 0.341379
Sum of electronic and zero-point Energies= -1054.605755
Sum of electronic and thermal Energies= -1054.585093
Sum of electronic and thermal Enthalpies= -1054.584148
Sum of electronic and thermal Free Energies= -1054.656562

Cartesian Coordinates

6	0.853887	-2.540518	0.791689
6	0.208439	-1.712216	1.925739
6	1.071884	-0.444614	2.026725
7	1.744799	-0.303240	0.718839
6	2.035342	-1.699559	0.297058
6	3.393174	0.697210	0.783017
6	3.055798	1.879841	-0.117936
6	2.285862	-1.780553	-1.216667
8	3.295693	-1.051961	-1.659217
8	4.302164	-0.107377	0.434401
8	1.607847	-2.469503	-1.941860
1	2.740481	1.489320	-1.091880
1	2.971633	-1.968114	0.801554
1	0.158736	-2.685123	-0.036369
1	1.193583	-3.521693	1.128892
1	0.187755	-2.245228	2.878543
1	-0.821411	-1.454105	1.666573
1	1.855461	-0.560834	2.783468
1	0.507277	0.464276	2.250466
1	3.828797	-0.648117	-0.875100
1	1.068046	0.087162	0.056764
1	4.014144	2.378568	-0.296835
1	3.292661	0.924300	1.861613
6	2.044550	2.867768	0.486926
6	0.923764	3.305918	-0.477688
1	2.566321	3.759623	0.846180
1	1.568085	2.416504	1.367884
1	0.307562	4.069869	0.006401
1	1.364610	3.745203	-1.378996
6	0.094366	2.111697	-0.823099
6	-1.051972	1.769916	-0.223921
1	0.502441	1.410445	-1.553036
1	-1.540289	2.437275	0.482038
6	-1.625777	0.420062	-0.474434
8	-0.890859	-0.494602	-0.827959
6	-3.080286	0.180079	-0.249059
6	-3.990345	1.229867	-0.094514
6	-3.533824	-1.143157	-0.212581
6	-5.340629	0.956776	0.100674
1	-3.652775	2.260116	-0.146960
6	-4.880148	-1.413373	-0.008316
1	-2.813046	-1.942892	-0.350604
6	-5.783935	-0.362642	0.149641
1	-6.047406	1.772413	0.212813
1	-5.228803	-2.440424	0.024594
1	-6.837106	-0.573349	0.307681

[2-3]TS_conf-5

Number of imaginary frequencies : 1
The smallest frequency is : -144.5635

Electronic energy= -1054.9930013
Zero-point correction= 0.391062
Thermal correction to Energy= 0.412231
Thermal correction to Enthalpy= 0.413175
Thermal correction to Gibbs Free Energy= 0.336690
Sum of electronic and zero-point Energies= -1054.601940
Sum of electronic and thermal Energies= -1054.580770
Sum of electronic and thermal Enthalpies= -1054.579826
Sum of electronic and thermal Free Energies= -1054.656311

Cartesian Coordinates

6	5.568474	-1.289904	0.761244
6	4.599656	-2.483229	0.574061
6	3.226078	-1.836061	0.301693
7	3.524771	-0.446419	-0.117090
6	4.653947	-0.071481	0.777596
6	2.220938	0.855011	0.054402
6	0.928822	0.130140	-0.264125
6	5.292116	1.262914	0.358649
8	4.584907	2.328358	0.653782
8	2.375413	1.366320	1.211425
8	6.369052	1.294879	-0.195925
1	0.133218	0.855693	-0.057020
1	4.189725	0.065008	1.759813
1	6.267295	-1.197505	-0.073425
1	6.155620	-1.355621	1.678673
1	4.553605	-3.121782	1.457981
1	4.907472	-3.108083	-0.267135
1	2.633857	-1.761156	1.218797
1	2.632958	-2.345257	-0.459437
1	3.637188	2.042763	1.022008
1	3.849911	-0.442630	-1.087387
1	0.780811	-0.692442	0.445137
1	2.604630	1.429390	-0.812263
6	0.824806	-0.347736	-1.710001
6	-0.479595	-1.109832	-1.988755
1	1.667629	-1.001782	-1.964544
1	0.889762	0.516429	-2.383028
1	-0.456692	-1.479093	-3.021583
1	-0.548101	-1.983852	-1.330306
6	-1.683959	-0.239500	-1.816818
6	-2.680089	-0.458615	-0.953926
1	-1.742100	0.655068	-2.438719
1	-2.659705	-1.325013	-0.299969
6	-3.813023	0.503631	-0.858292
8	-3.790457	1.562934	-1.462762
6	-4.984842	0.160990	0.011893
6	-5.250941	-1.139148	0.450628
6	-5.854977	1.197127	0.367165
6	-6.370418	-1.396359	1.236977
1	-4.606013	-1.963221	0.164168
6	-6.963860	0.941935	1.162515
1	-5.639131	2.198166	0.008503
6	-7.223028	-0.357096	1.598691
1	-6.577160	-2.409737	1.565904
1	-7.628475	1.753073	1.442202
1	-8.091647	-0.560142	2.217513

[2-3]TS_conf-6

Number of imaginary frequencies : 1
The smallest frequency is : -135.9219

Electronic energy= -1054.9979709
Zero-point correction= 0.392361
Thermal correction to Energy= 0.412737
Thermal correction to Enthalpy= 0.413681
Thermal correction to Gibbs Free Energy= 0.343506
Sum of electronic and zero-point Energies= -1054.605610
Sum of electronic and thermal Energies= -1054.585234
Sum of electronic and thermal Enthalpies= -1054.584290
Sum of electronic and thermal Free Energies= -1054.654465

Cartesian Coordinates

6 -0.978896 -2.548618 1.188272
6 -1.150938 -1.349652 2.151048
6 0.176419 -0.585969 2.059618
7 0.647928 -0.848725 0.682278
6 0.349727 -2.288771 0.468647
6 2.426161 -0.542079 0.136183
6 2.915941 0.575032 1.040872
6 0.375402 -2.611063 -1.036835
8 1.572582 -2.668547 -1.570570
8 3.024149 -1.664150 0.159917
8 -0.647404 -2.778497 -1.668571
1 3.503115 0.115019 1.840966
1 1.180152 -2.820209 0.946327
1 -1.786415 -2.592099 0.455037
1 -0.945925 -3.504584 1.714426
1 -1.372792 -1.651781 3.176268
1 -1.966327 -0.704539 1.806937
1 0.931525 -0.985844 2.744688
1 0.077238 0.489020 2.225045
1 2.304159 -2.369326 -0.871144
1 0.067644 -0.292654 0.049431
1 2.076513 1.104141 1.498859
1 2.069175 -0.186194 -0.846135
6 3.765730 1.595465 0.267370
6 3.008184 2.284705 -0.893343
1 4.660966 1.112062 -0.136632
1 4.107378 2.357364 0.975766
1 3.578411 3.168593 -1.200517
1 2.951189 1.622849 -1.762714
6 1.629560 2.691241 -0.477327
6 0.499198 2.149203 -0.946886
1 1.540360 3.426783 0.323793
1 0.539321 1.404056 -1.737145
6 -0.805677 2.503834 -0.327181
8 -0.933907 3.529240 0.320563
6 -1.940377 1.520393 -0.412578
6 -1.898588 0.344240 -1.173057
6 -3.070634 1.784680 0.371586
6 -2.962125 -0.555990 -1.137798
1 -1.051595 0.108153 -1.811563
6 -4.132954 0.891751 0.400734
1 -3.088103 2.698595 0.955527
6 -4.077431 -0.283814 -0.350547
1 -2.898437 -1.471183 -1.716361
1 -5.003819 1.107044 1.011753
1 -4.904806 -0.986087 -0.321936

[3]_conf-1

Number of imaginary frequencies : 0

Electronic energy= -1055.0091523
 Zero-point correction= 0.394935
 Thermal correction to Energy= 0.415573
 Thermal correction to Enthalpy= 0.416517
 Thermal correction to Gibbs Free Energy= 0.344893
 Sum of electronic and zero-point Energies= -1054.614217
 Sum of electronic and thermal Energies= -1054.593579
 Sum of electronic and thermal Enthalpies= -1054.592635
 Sum of electronic and thermal Free Energies= -1054.664259

 Cartesian Coordinates

6	-0.544203	-2.552968	-0.315726
6	-1.208710	-2.493220	-1.713888
6	-2.405885	-1.549350	-1.554422
7	-2.071243	-0.711980	-0.361674
6	-1.404266	-1.685342	0.590958
6	-3.290950	0.058561	0.271314
6	-2.897419	1.509627	0.545518
6	-0.701613	-0.850335	1.705334
8	-1.497756	-0.387427	2.576140
8	-3.720589	-0.608631	1.375842
8	0.515022	-0.672616	1.599003
1	-1.972954	1.509366	1.133549
1	-2.227908	-2.254999	1.022241
1	0.468525	-2.149693	-0.341328
1	-0.500816	-3.568650	0.081476
1	-1.547607	-3.470565	-2.061512
1	-0.504692	-2.092781	-2.443776
1	-3.324187	-2.085282	-1.298284
1	-2.594072	-0.897865	-2.410384
1	-2.948542	-0.535561	2.048415
1	-1.344958	-0.036127	-0.645596
1	-3.677477	1.881539	1.214816
1	-4.063682	0.007627	-0.504646
6	-2.787408	2.417451	-0.692145
6	-1.433458	3.149870	-0.769407
1	-3.596421	3.152966	-0.683731
1	-2.922815	1.836999	-1.616594
1	-1.483559	3.931085	-1.535167
1	-1.216656	3.629872	0.190396
6	-0.381221	2.151821	-1.123365
6	0.529815	1.619841	-0.302040
1	-0.433373	1.747249	-2.136662
1	0.657357	1.956869	0.722311
6	1.366188	0.493653	-0.813043
8	0.907718	-0.241804	-1.679639
6	2.754496	0.307826	-0.307594
6	3.367229	1.243771	0.528073
6	3.462802	-0.827845	-0.712266
6	4.675605	1.044526	0.956708
1	2.831766	2.133905	0.841200
6	4.765750	-1.029125	-0.278304
1	2.972210	-1.540311	-1.367474
6	5.373500	-0.091823	0.557059
1	5.148373	1.774558	1.605616
1	5.310995	-1.915169	-0.587672
1	6.392515	-0.248987	0.897191

 [3-4]TS_conf-1

Number of imaginary frequencies : 1
 The smallest frequency is : -344.1426

Electronic energy= -1055.0044712
 Zero-point correction= 0.390285
 Thermal correction to Energy= 0.411225

Thermal correction to Enthalpy= 0.412169
 Thermal correction to Gibbs Free Energy= 0.336756
 Sum of electronic and zero-point Energies= -1054.614186
 Sum of electronic and thermal Energies= -1054.593246
 Sum of electronic and thermal Enthalpies= -1054.592302
 Sum of electronic and thermal Free Energies= -1054.667715

Cartesian Coordinates

6	3.748632	-1.552141	1.602023
6	2.374753	-1.312273	2.235526
6	1.451789	-1.274958	1.019257
7	2.266072	-0.591194	-0.028941
6	3.717415	-0.681459	0.340549
6	1.798253	0.759921	-0.478682
6	1.712806	1.774242	0.647830
6	1.251174	3.148218	0.151849
6	4.376408	-1.322516	-0.917838
8	3.499910	-1.558815	-1.833652
8	2.690061	1.231340	-1.435631
8	5.575770	-1.539189	-0.914880
1	2.697729	1.871316	1.116782
1	4.132293	0.314409	0.502661
1	3.861503	-2.605980	1.325821
1	4.582205	-1.285649	2.252433
1	2.354260	-0.345175	2.749553
1	2.082881	-2.086909	2.947433
1	0.509582	-0.743679	1.169529
1	1.230841	-2.284944	0.663852
1	2.874102	0.525786	-2.078716
1	2.432365	-1.187248	-0.993433
1	1.017475	1.400666	1.408301
1	2.016724	3.571173	-0.503977
1	1.161916	3.812454	1.018043
1	0.799439	0.573061	-0.899843
6	-0.087472	3.119206	-0.604989
1	-0.385061	4.155014	-0.810064
1	0.030520	2.626556	-1.576452
6	-1.165442	2.449276	0.186763
6	-1.910919	1.423139	-0.237216
1	-1.342706	2.815820	1.199497
1	-1.776783	1.021495	-1.238215
6	-2.921367	0.802684	0.664597
8	-2.931998	1.051580	1.859235
6	-3.911718	-0.161063	0.085534
6	-4.180586	-0.237089	-1.284307
6	-4.603034	-0.995848	0.969754
6	-5.124284	-1.142506	-1.761661
1	-3.679068	0.424050	-1.983688
6	-5.534610	-1.907390	0.491138
1	-4.392114	-0.913478	2.030952
6	-5.795050	-1.982257	-0.877045
1	-5.336073	-1.190583	-2.824908
1	-6.060817	-2.559153	1.181262
1	-6.524146	-2.693088	-1.253309

[3-4]TS_conf-2

Number of imaginary frequencies : 1
 The smallest frequency is : -200.6002

Electronic energy= -1055.004481
 Zero-point correction= 0.390971
 Thermal correction to Energy= 0.411784
 Thermal correction to Enthalpy= 0.412728
 Thermal correction to Gibbs Free Energy= 0.338180
 Sum of electronic and zero-point Energies= -1054.613510

Sum of electronic and thermal Energies= -1054.592697
 Sum of electronic and thermal Enthalpies= -1054.591753
 Sum of electronic and thermal Free Energies= -1054.666301

Cartesian Coordinates

6	3.287031	-1.599006	1.788853
6	1.854433	-1.288205	2.235644
6	1.105929	-1.190673	0.908134
7	2.091619	-0.549621	-0.013039
6	3.473955	-0.722411	0.545887
6	1.762502	0.828395	-0.505729
6	1.601539	1.844986	0.610437
6	1.251260	3.235990	0.073072
6	4.264043	-1.389778	-0.621347
8	3.515870	-1.567540	-1.654107
8	2.788350	1.246511	-1.343983
8	5.437891	-1.672026	-0.449276
1	2.536021	1.899925	1.178351
1	3.914497	0.248951	0.775689
1	3.380430	-2.655980	1.517632
1	4.037127	-1.382037	2.549868
1	1.817054	-0.325118	2.756226
1	1.428286	-2.050137	2.891162
1	0.184219	-0.605069	0.937513
1	0.876528	-2.183474	0.511858
1	3.019974	0.526199	-1.955146
1	2.337225	-1.142541	-0.944509
1	0.816174	1.502685	1.293939
1	2.087646	3.615745	-0.519751
1	1.123810	3.911060	0.925938
1	0.811913	0.698166	-1.044345
6	-0.024083	3.263586	-0.787788
1	-0.248882	4.308947	-1.031739
1	0.140539	2.744610	-1.738319
6	-1.190571	2.669765	-0.065204
6	-1.914354	1.625996	-0.484530
1	-1.454399	3.107340	0.899312
1	-1.705500	1.161676	-1.444268
6	-3.036133	1.111787	0.349682
8	-3.403752	1.715156	1.344412
6	-3.712612	-0.167082	-0.044674
6	-3.184205	-1.055072	-0.987193
6	-4.917680	-0.481079	0.592881
6	-3.857010	-2.235998	-1.289812
1	-2.240770	-0.846050	-1.481011
6	-5.592386	-1.654076	0.283871
1	-5.307856	0.214958	1.327784
6	-5.062184	-2.533535	-0.660025
1	-3.439736	-2.923619	-2.018336
1	-6.530953	-1.885809	0.777046
1	-5.588396	-3.451424	-0.902952

[3-4]TS_conf-3

Number of imaginary frequencies : 1
 The smallest frequency is : -780.0364

Electronic energy= -1055.0029901
 Zero-point correction= 0.389605
 Thermal correction to Energy= 0.410715
 Thermal correction to Enthalpy= 0.411659
 Thermal correction to Gibbs Free Energy= 0.336887
 Sum of electronic and zero-point Energies= -1054.613385
 Sum of electronic and thermal Energies= -1054.592276
 Sum of electronic and thermal Enthalpies= -1054.591331
 Sum of electronic and thermal Free Energies= -1054.666103

 Cartesian Coordinates

6	2.977853	-2.579693	0.827113
6	3.814932	-1.767149	1.814516
6	3.162855	-0.386195	1.750639
7	2.731199	-0.241805	0.326688
6	2.753984	-1.595594	-0.324278
6	3.404661	0.837647	-0.461404
6	3.111963	2.222383	0.134828
6	1.662295	2.503865	0.546546
6	1.352344	-1.714179	-0.980311
8	0.633874	-0.664855	-0.708562
8	3.031154	0.701987	-1.798164
8	1.047199	-2.702738	-1.617041
1	3.444295	2.946327	-0.617239
1	3.538262	-1.645530	-1.082027
1	2.018520	-2.855749	1.278308
1	3.463805	-3.492959	0.482605
1	4.852560	-1.705275	1.469781
1	3.813070	-2.173872	2.827640
1	3.835394	0.427570	2.024439
1	2.274127	-0.333872	2.385525
1	2.066987	0.614557	-1.853166
1	1.568561	-0.136155	0.099548
1	3.760711	2.366438	1.005090
1	1.651639	3.402130	1.173012
1	1.289586	1.696057	1.189253
1	4.485770	0.651434	-0.430257
6	0.679548	2.712881	-0.619991
1	0.898511	3.673875	-1.101010
1	0.800503	1.940251	-1.382871
6	-0.737932	2.663352	-0.138370
6	-1.542697	1.632274	-0.406740
1	-1.100021	3.465507	0.505072
1	-1.176171	0.816541	-1.021550
6	-2.912232	1.546531	0.162404
8	-3.461701	2.517017	0.658818
6	-3.601648	0.216064	0.120496
6	-2.919640	-0.971227	-0.169768
6	-4.969852	0.175098	0.409807
6	-3.607812	-2.181932	-0.174986
1	-1.852021	-0.969653	-0.375251
6	-5.653817	-1.032738	0.394570
1	-5.476869	1.106278	0.641439
6	-4.971961	-2.214044	0.100508
1	-3.073494	-3.099814	-0.398404
1	-6.717230	-1.057495	0.611155
1	-5.506162	-3.159316	0.088206

[3-4]TS_conf-4

Number of imaginary frequencies : 1
 The smallest frequency is : -544.8688

Electronic energy=	-1055.0049368
Zero-point correction=	0.390650
Thermal correction to Energy=	0.411348
Thermal correction to Enthalpy=	0.412292
Thermal correction to Gibbs Free Energy=	0.339211
Sum of electronic and zero-point Energies=	-1054.614286
Sum of electronic and thermal Energies=	-1054.593589
Sum of electronic and thermal Enthalpies=	-1054.592645
Sum of electronic and thermal Free Energies=	-1054.665726

 Cartesian Coordinates

6	1.633730	-2.728099	-0.078269
6	0.294597	-2.090049	-0.449618
6	0.722036	-0.827051	-1.197207
7	1.980254	-0.396965	-0.511823
6	2.470715	-1.523166	0.352901
6	1.917016	0.926985	0.187482
6	1.834232	2.051040	-0.847768
6	1.575338	3.420525	-0.203062
6	3.981658	-1.621551	0.001075
8	4.295010	-0.781052	-0.927808
8	3.039805	1.064392	0.998269
8	4.681348	-2.438210	0.574599
1	1.059445	1.834739	-1.592696
1	2.334207	-1.278238	1.407824
1	2.086451	-3.208142	-0.953238
1	1.563355	-3.470136	0.717574
1	-0.252532	-1.806535	0.456446
1	-0.347568	-2.729348	-1.059108
1	-0.016499	-0.024318	-1.151773
1	0.954041	-1.034130	-2.244957
1	3.830616	0.952723	0.443531
1	2.973167	-0.380225	-1.110945
1	2.793161	2.056670	-1.381737
1	2.067577	4.201965	-0.788426
1	2.036859	3.437353	0.790733
1	1.046357	0.899329	0.853323
6	0.076702	3.777565	-0.097099
1	-0.020696	4.725202	0.444213
1	-0.338095	3.920031	-1.101120
6	-0.663643	2.692145	0.609904
6	-1.550348	1.866608	0.043101
1	-0.382959	2.495388	1.645854
1	-1.884020	2.024425	-0.979478
6	-2.006409	0.656091	0.778161
8	-1.359437	0.232387	1.726792
6	-3.222157	-0.075441	0.306748
6	-4.123059	0.474383	-0.610544
6	-3.460688	-1.351622	0.828879
6	-5.244845	-0.249411	-1.004589
1	-3.968001	1.473987	-1.004024
6	-4.575230	-2.075526	0.428264
1	-2.759337	-1.753822	1.552674
6	-5.468061	-1.524405	-0.491083
1	-5.946369	0.182641	-1.710769
1	-4.752490	-3.066711	0.833056
1	-6.341761	-2.088365	-0.802668

[3-4]TS_conf-5

Number of imaginary frequencies : 1

The smallest frequency is : -125.5442

Electronic energy= -1055.002498
 Zero-point correction= 0.390994
 Thermal correction to Energy= 0.411894
 Thermal correction to Enthalpy= 0.412838
 Thermal correction to Gibbs Free Energy= 0.337775
 Sum of electronic and zero-point Energies= -1054.611504
 Sum of electronic and thermal Energies= -1054.590604
 Sum of electronic and thermal Enthalpies= -1054.589660
 Sum of electronic and thermal Free Energies= -1054.664723

 Cartesian Coordinates

6	-2.406461	-2.387607	0.531602
6	-1.854586	-1.746573	1.808871
6	-2.899391	-0.677006	2.119806

7	-3.306185	-0.169106	0.776048
6	-2.948463	-1.195061	-0.262639
6	-2.931957	1.244747	0.434193
6	-1.438364	1.502776	0.500868
6	-1.104871	2.950348	0.138004
6	-4.295108	-1.454781	-1.005382
8	-5.241219	-0.719803	-0.534783
8	-3.371739	1.502052	-0.857506
8	-4.322893	-2.287797	-1.895842
1	-0.924904	0.818492	-0.184049
1	-2.218000	-0.784891	-0.961439
1	-3.222140	-3.077223	0.773316
1	-1.657448	-2.939979	-0.036385
1	-0.885069	-1.276076	1.611530
1	-1.734034	-2.453238	2.632383
1	-2.545787	0.146900	2.742249
1	-3.782646	-1.115982	2.591000
1	-4.283257	1.177169	-0.958916
1	-4.408208	-0.241486	0.547720
1	-1.078261	1.285779	1.514156
1	-1.713579	3.632420	0.743329
1	-1.373132	3.128240	-0.907962
1	-3.457750	1.858848	1.181869
6	0.378936	3.276384	0.363634
1	0.550466	4.325587	0.093533
1	0.629198	3.166796	1.425417
6	1.272559	2.407840	-0.463412
6	2.205853	1.581763	0.019106
1	1.131068	2.431931	-1.544997
1	2.376604	1.508040	1.089227
6	2.991858	0.718889	-0.905403
8	2.737455	0.677976	-2.097752
6	4.086263	-0.138013	-0.343261
6	4.689011	0.109572	0.893527
6	4.524362	-1.217185	-1.117878
6	5.714239	-0.715270	1.348525
1	4.385495	0.959627	1.495878
6	5.535691	-2.048571	-0.655968
1	4.053758	-1.386291	-2.080789
6	6.132530	-1.797672	0.579253
1	6.187415	-0.511957	2.303876
1	5.861945	-2.891256	-1.257047
1	6.926121	-2.444596	0.940149

[3-4]TS_conf-6

Number of imaginary frequencies : 1
The smallest frequency is : -264.6583

Electronic energy= -1054.9990945
Zero-point correction= 0.390196
Thermal correction to Energy= 0.411230
Thermal correction to Enthalpy= 0.412174
Thermal correction to Gibbs Free Energy= 0.336574
Sum of electronic and zero-point Energies= -1054.608899
Sum of electronic and thermal Energies= -1054.587865
Sum of electronic and thermal Enthalpies= -1054.586921
Sum of electronic and thermal Free Energies= -1054.662520

Cartesian Coordinates

6	4.932506	0.005549	-1.832087
6	4.752651	-1.512341	-1.803954
6	3.445072	-1.685034	-1.029321
7	3.434754	-0.551371	-0.052847
6	4.516531	0.425509	-0.422477
6	3.410750	-0.932676	1.400476

6	2.077528	-1.580447	1.777816
6	0.840230	-0.687839	1.589213
6	3.806884	1.809597	-0.352836
8	2.552517	1.674974	-0.084233
8	3.685342	0.195409	2.161619
8	4.454578	2.819221	-0.568405
1	2.184613	-1.840049	2.835102
1	5.338306	0.372235	0.293805
1	4.259598	0.455670	-2.570535
1	5.949299	0.325689	-2.060996
1	5.575678	-1.980388	-1.253950
1	4.700188	-1.966767	-2.795279
1	3.373499	-2.633669	-0.494110
1	2.574763	-1.586893	-1.683218
1	3.069885	0.902868	1.904459
1	2.627650	0.241232	-0.154411
1	1.949450	-2.525934	1.237723
1	1.097442	0.369953	1.724877
1	0.117007	-0.918992	2.376792
1	4.236041	-1.635834	1.565566
6	0.127776	-0.858291	0.236930
1	0.814638	-0.636610	-0.589782
1	-0.195855	-1.899402	0.121127
6	-1.043415	0.066932	0.135394
6	-2.320702	-0.321081	0.085051
1	-0.830221	1.136214	0.132355
1	-2.574667	-1.376858	0.100163
6	-3.411417	0.691956	0.046731
8	-3.171555	1.879967	0.181235
6	-4.827220	0.230673	-0.137507
6	-5.159529	-1.044501	-0.603395
6	-5.847976	1.142194	0.153237
6	-6.494369	-1.402422	-0.771214
1	-4.384494	-1.758745	-0.860557
6	-7.179050	0.780666	-0.003133
1	-5.570899	2.131684	0.501492
6	-7.504040	-0.494208	-0.465723
1	-6.745479	-2.391208	-1.141608
1	-7.965513	1.490959	0.231362
1	-8.544533	-0.777546	-0.591373

[3-4]TS_conf-7

Number of imaginary frequencies : 1
The smallest frequency is : -162.1972

Electronic energy= -1055.0004048
Zero-point correction= 0.391070
Thermal correction to Energy= 0.411843
Thermal correction to Enthalpy= 0.412787
Thermal correction to Gibbs Free Energy= 0.338268
Sum of electronic and zero-point Energies= -1054.609335
Sum of electronic and thermal Energies= -1054.588562
Sum of electronic and thermal Enthalpies= -1054.587618
Sum of electronic and thermal Free Energies= -1054.662137

Cartesian Coordinates

6	4.822062	-1.139291	0.377895
6	4.859947	0.103278	1.271880
6	3.414633	0.215960	1.757755
7	2.600080	-0.279666	0.607012
6	3.486440	-1.008339	-0.360359
6	1.635996	0.693642	-0.011886
6	2.313825	1.923570	-0.601603
6	1.415710	3.165219	-0.641143
6	2.753921	-2.365556	-0.589431

8	1.718465	-2.474084	0.165038
8	0.968875	0.033752	-1.037057
8	3.223435	-3.154834	-1.393172
1	2.634023	1.661591	-1.615717
1	3.572647	-0.455102	-1.296877
1	4.819675	-2.047228	0.990769
1	5.659746	-1.204816	-0.316943
1	5.128719	0.985945	0.681623
1	5.563719	0.019861	2.102335
1	3.103048	1.227905	2.024733
1	3.228443	-0.442289	2.609635
1	0.627553	-0.815118	-0.706519
1	1.986913	-1.200966	0.818004
1	3.213923	2.166069	-0.026580
1	1.952157	3.942344	-1.193187
1	1.280687	3.549820	0.377852
1	0.960566	0.974159	0.810528
6	0.030566	2.953384	-1.282263
1	-0.323872	3.925906	-1.647299
1	0.103031	2.285006	-2.145934
6	-0.988597	2.444098	-0.309910
6	-1.776692	1.378293	-0.478707
1	-1.104993	3.008746	0.617007
1	-1.699261	0.773416	-1.376121
6	-2.745309	0.998859	0.586249
8	-2.670845	1.483870	1.704549
6	-3.814332	-0.003290	0.272389
6	-4.131622	-0.388425	-1.033455
6	-4.532762	-0.546510	1.342792
6	-5.151300	-1.308125	-1.262688
1	-3.603218	0.038737	-1.879292
6	-5.542558	-1.470985	1.113795
1	-4.278944	-0.228129	2.348450
6	-5.852624	-1.853577	-0.191212
1	-5.397076	-1.598172	-2.279138
1	-6.089429	-1.895990	1.949504
1	-6.641868	-2.576896	-0.371382

[3-4]TS_conf-8

Number of imaginary frequencies : 1

The smallest frequency is : -430.7477

Electronic energy=	-1054.9985124
Zero-point correction=	0.390286
Thermal correction to Energy=	0.411132
Thermal correction to Enthalpy=	0.412076
Thermal correction to Gibbs Free Energy=	0.336914
Sum of electronic and zero-point Energies=	-1054.608227
Sum of electronic and thermal Energies=	-1054.587381
Sum of electronic and thermal Enthalpies=	-1054.586437
Sum of electronic and thermal Free Energies=	-1054.661598

Cartesian Coordinates

6	4.566121	-1.099720	-0.302160
6	4.789555	0.291017	0.296526
6	3.547024	0.495624	1.165510
7	2.462569	-0.245024	0.454150
6	3.062597	-1.128795	-0.595924
6	1.275935	0.564894	0.007679
6	1.658361	1.713368	-0.941414
6	1.463795	3.134275	-0.390253
6	2.409808	-2.517251	-0.328466
8	1.693013	-2.491755	0.741960
8	0.408474	-0.297806	-0.654089
8	2.648386	-3.443281	-1.084788

1	1.054232	1.586297	-1.845860
1	2.813819	-0.769745	-1.596406
1	4.813104	-1.872364	0.434450
1	5.154875	-1.291835	-1.199661
1	4.825080	1.045369	-0.496476
1	5.710019	0.367987	0.878871
1	3.262356	1.541895	1.293738
1	3.673256	0.046784	2.153750
1	0.235935	-1.070087	-0.089038
1	2.020127	-1.151233	1.010656
1	2.702541	1.589296	-1.248897
1	2.079778	3.825620	-0.973696
1	1.825946	3.192979	0.644338
1	0.836751	0.942707	0.941106
6	0.003122	3.626356	-0.442817
1	-0.038723	4.651854	-0.059618
1	-0.334662	3.641621	-1.484937
6	-0.861939	2.719053	0.368206
6	-1.700635	1.810441	-0.133505
1	-0.702543	2.715757	1.447535
1	-1.895877	1.756720	-1.200736
6	-2.261897	0.757571	0.755804
8	-1.752903	0.532389	1.844119
6	-3.424924	-0.053027	0.281130
6	-4.222227	0.344455	-0.795794
6	-3.725849	-1.235737	0.964180
6	-5.307485	-0.434996	-1.185355
1	-4.012773	1.270724	-1.321519
6	-4.801743	-2.018222	0.567485
1	-3.099898	-1.524092	1.802198
6	-5.594054	-1.617496	-0.508290
1	-5.928208	-0.120107	-2.017940
1	-5.025502	-2.940346	1.094061
1	-6.436775	-2.227870	-0.817836

[3-4]TS_conf-9

Number of imaginary frequencies : 1
The smallest frequency is : -259.5661

Electronic energy= -1054.9992509
Zero-point correction= 0.390574
Thermal correction to Energy= 0.411301
Thermal correction to Enthalpy= 0.412245
Thermal correction to Gibbs Free Energy= 0.339009
Sum of electronic and zero-point Energies= -1054.608677
Sum of electronic and thermal Energies= -1054.587950
Sum of electronic and thermal Enthalpies= -1054.587006
Sum of electronic and thermal Free Energies= -1054.660242

Cartesian Coordinates

6	0.041385	-2.116245	1.224140
6	-1.023518	-1.923435	2.309978
6	-2.329208	-2.080275	1.532132
7	-2.047054	-1.439057	0.214799
6	-0.557736	-1.415522	0.000475
6	-2.755669	-0.153311	-0.102933
6	-2.553575	0.918251	0.960170
6	-3.047005	2.304047	0.494411
6	-0.375287	-2.172369	-1.351650
8	-1.511222	-2.502916	-1.858772
8	-2.257737	0.307303	-1.317010
8	0.750752	-2.388094	-1.771846
1	-1.484498	0.962700	1.195559
1	-0.213566	-0.384176	-0.105541
1	0.185862	-3.180860	1.013574

1	1.012643	-1.692740	1.486248
1	-0.959833	-0.915411	2.733430
1	-0.944881	-2.644512	3.126216
1	-3.201037	-1.618110	1.998173
1	-2.549214	-3.135232	1.347699
1	-2.266744	-0.417425	-1.964940
1	-2.213498	-2.102112	-0.698787
1	-3.073883	0.608798	1.870993
1	-3.834165	2.667993	1.160183
1	-3.483904	2.225052	-0.505434
1	-3.819297	-0.426151	-0.174865
6	-1.916976	3.354430	0.458543
1	-2.328700	4.298651	0.084959
1	-1.550129	3.531285	1.476171
6	-0.791590	2.899370	-0.414194
6	0.400340	2.505421	0.046811
1	-0.986233	2.790872	-1.480463
1	0.620453	2.545438	1.110962
6	1.368571	1.834247	-0.861479
8	1.241074	1.860999	-2.072396
6	2.435617	0.998162	-0.220988
6	3.051157	1.351042	0.984511
6	2.782562	-0.197745	-0.855969
6	4.021060	0.521067	1.538363
1	2.796966	2.285393	1.477135
6	3.727704	-1.040860	-0.281367
1	2.272855	-0.481662	-1.769979
6	4.353264	-0.678567	0.909821
1	4.515329	0.806908	2.461616
1	3.967601	-1.982746	-0.763915
1	5.097740	-1.333141	1.352960

[3-4]TS_conf-10

Number of imaginary frequencies : 1

The smallest frequency is : -369.3475

Electronic energy=	-1054.9994914
Zero-point correction=	0.390820
Thermal correction to Energy=	0.411482
Thermal correction to Enthalpy=	0.412426
Thermal correction to Gibbs Free Energy=	0.339675
Sum of electronic and zero-point Energies=	-1054.608671
Sum of electronic and thermal Energies=	-1054.588009
Sum of electronic and thermal Enthalpies=	-1054.587065
Sum of electronic and thermal Free Energies=	-1054.659817

Cartesian Coordinates

6	-0.619329	-2.123900	1.434718
6	-1.801876	-1.797464	2.353426
6	-2.980752	-1.756243	1.382022
7	-2.411536	-1.152584	0.142360
6	-0.918654	-1.328601	0.159604
6	-2.882306	0.220467	-0.232350
6	-2.647879	1.253924	0.866146
6	-2.794131	2.702833	0.357086
6	-0.625213	-2.085623	-1.169985
8	-1.703047	-2.256484	-1.855265
8	-2.197268	0.598663	-1.381400
8	0.513807	-2.449120	-1.413194
1	-1.641425	1.109227	1.275480
1	-0.429389	-0.352346	0.137025
1	-0.595115	-3.194990	1.209394
1	0.348752	-1.849641	1.856249
1	-1.666594	-0.815408	2.818484
1	-1.950634	-2.534643	3.145050

1	-3.838182	-1.174071	1.724181
1	-3.320229	-2.765994	1.135693
1	-2.176975	-0.141009	-2.012322
1	-2.515629	-1.780840	-0.812733
1	-3.356775	1.057558	1.676097
1	-3.472874	3.260970	1.007611
1	-3.237981	2.703209	-0.643115
1	-3.960942	0.107831	-0.421090
6	-1.448297	3.457455	0.311111
1	-1.620766	4.452660	-0.114640
1	-1.075222	3.594213	1.332787
6	-0.434115	2.718359	-0.501362
6	0.660911	2.139578	0.002686
1	-0.642072	2.569545	-1.558885
1	0.904653	2.235312	1.058146
6	1.497149	1.244939	-0.845758
8	1.182976	0.979262	-1.993107
6	2.699480	0.611196	-0.217088
6	3.422846	1.248200	0.795478
6	3.101952	-0.646395	-0.677909
6	4.551309	0.638846	1.334888
1	3.123220	2.232157	1.144818
6	4.217718	-1.260846	-0.120248
1	2.507214	-1.137244	-1.441839
6	4.945204	-0.617982	0.880617
1	5.121397	1.142660	2.109067
1	4.520642	-2.244095	-0.466000
1	5.819834	-1.097998	1.309244

[3-4]TS_conf-11

Number of imaginary frequencies : 1

The smallest frequency is : -69.8786

Electronic energy= -1054.997332
 Zero-point correction= 0.392870
 Thermal correction to Energy= 0.413487
 Thermal correction to Enthalpy= 0.414431
 Thermal correction to Gibbs Free Energy= 0.341224
 Sum of electronic and zero-point Energies= -1054.604462
 Sum of electronic and thermal Energies= -1054.583845
 Sum of electronic and thermal Enthalpies= -1054.582901
 Sum of electronic and thermal Free Energies= -1054.656108

Cartesian Coordinates

6	1.757531	-2.718595	-0.355036
6	0.420953	-2.150833	-0.835276
6	0.800872	-0.776565	-1.391560
7	2.049231	-0.385184	-0.641458
6	2.432007	-1.510825	0.283817
6	1.970051	0.936201	0.088305
6	1.840915	2.093383	-0.896034
6	1.545427	3.427092	-0.191577
6	3.997851	-1.542181	0.248004
8	4.440326	-1.244272	-0.891470
8	3.143626	1.146159	0.793137
8	4.566024	-1.832194	1.303539
1	1.062635	1.882438	-1.637706
1	2.023170	-1.309994	1.279618
1	2.366192	-3.053170	-1.202353
1	1.654714	-3.542401	0.352332
1	-0.259842	-2.023141	0.012567
1	-0.072613	-2.766785	-1.589543
1	0.033305	-0.019019	-1.225434
1	1.048020	-0.806520	-2.454117
1	3.279126	0.474417	1.478361

1	2.915802	-0.397371	-1.247502
1	2.798555	2.148890	-1.424791
1	2.004467	4.243601	-0.755200
1	2.024373	3.422983	0.793487
1	1.092895	0.824717	0.740832
6	0.038934	3.732610	-0.047213
1	-0.077577	4.647921	0.543850
1	-0.397000	3.913523	-1.035926
6	-0.656143	2.588229	0.611343
6	-1.553353	1.787590	0.026327
1	-0.331683	2.330280	1.620867
1	-1.940981	2.011895	-0.964880
6	-1.953791	0.516553	0.688909
8	-1.195085	-0.022451	1.485104
6	-3.254013	-0.121557	0.326269
6	-4.250804	0.570309	-0.368363
6	-3.475114	-1.445722	0.719474
6	-5.453385	-0.060396	-0.672589
1	-4.100494	1.606934	-0.653695
6	-4.671363	-2.076573	0.406060
1	-2.696575	-1.960389	1.273375
6	-5.660842	-1.383556	-0.291632
1	-6.229368	0.480746	-1.203996
1	-4.837836	-3.106087	0.706217
1	-6.597425	-1.876099	-0.534018

[4]-anti_conf-1

Number of imaginary frequencies : 0

Electronic energy= -1055.0155917
 Zero-point correction= 0.392784
 Thermal correction to Energy= 0.414164
 Thermal correction to Enthalpy= 0.415109
 Thermal correction to Gibbs Free Energy= 0.341660
 Sum of electronic and zero-point Energies= -1054.622808
 Sum of electronic and thermal Energies= -1054.601427
 Sum of electronic and thermal Enthalpies= -1054.600483
 Sum of electronic and thermal Free Energies= -1054.673931

 Cartesian Coordinates

6	1.905224	-1.301936	-0.848086
6	3.193485	-1.972007	-1.341742
6	4.186639	-1.570579	-0.242308
6	3.751506	-0.147403	0.162878
7	2.409185	-0.013228	-0.407363
6	1.565268	1.068989	-0.045106
6	2.256430	2.427296	-0.197825
6	1.335861	3.628226	-0.455396
6	1.258024	-2.223493	0.209549
8	1.010262	-3.377411	-0.047933
8	0.997231	-1.722487	1.416352
8	1.051143	0.944626	1.314799
1	1.161539	-1.173743	-1.642861
1	3.079331	-3.050149	-1.453027
1	3.476126	-1.534305	-2.302770
1	4.081431	-2.250769	0.609069
1	5.226816	-1.607650	-0.570158
1	3.758086	-0.031500	1.257352
1	4.417526	0.617673	-0.253303
1	2.962292	2.352714	-1.030491
1	1.115295	-0.743561	1.449431
1	0.975513	3.580339	-1.490081
1	1.685399	1.349765	1.922818
1	2.861903	2.610483	0.702696
1	1.954732	4.528530	-0.393729

6	0.117774	3.781636	0.482080
1	0.349624	3.424106	1.489892
1	-0.118921	4.849157	0.563376
1	0.664178	1.019204	-0.666046
6	-1.094534	3.082728	-0.056065
6	-1.710285	2.035881	0.497792
1	-1.481048	3.453036	-1.007086
1	-1.338030	1.604029	1.421334
6	-2.851317	1.385176	-0.203911
8	-3.593555	2.018632	-0.935794
6	-3.022624	-0.091851	-0.030548
6	-2.015234	-0.887105	0.523554
6	-4.195489	-0.690856	-0.499803
6	-2.173804	-2.267655	0.607185
1	-1.094165	-0.437200	0.881254
6	-4.362042	-2.066022	-0.401711
1	-4.960121	-0.058914	-0.940172
6	-3.350564	-2.854688	0.148256
1	-1.372577	-2.874875	1.017229
1	-5.276637	-2.527964	-0.760357
1	-3.479147	-3.930704	0.215010

[4-5]TS-anti_conf-1

Number of imaginary frequencies : 1
The smallest frequency is : -257.9318

Electronic energy= -1054.9838945
Zero-point correction= 0.388003
Thermal correction to Energy= 0.409837
Thermal correction to Enthalpy= 0.410781
Thermal correction to Gibbs Free Energy= 0.333134
Sum of electronic and zero-point Energies= -1054.595891
Sum of electronic and thermal Energies= -1054.574057
Sum of electronic and thermal Enthalpies= -1054.573113
Sum of electronic and thermal Free Energies= -1054.650760

.....
Cartesian Coordinates

6	-4.246910	-0.685708	-0.542384
6	-4.149688	-2.115993	-1.059151
6	-2.885296	-2.618208	-0.352962
6	-1.933441	-1.414475	-0.399037
7	-2.834313	-0.257877	-0.575848
6	-2.434417	0.979704	-0.634285
6	-1.001915	1.322054	-0.908944
6	-0.721638	2.822492	-0.884267
6	-4.856211	-0.637431	0.901519
8	-5.776904	-1.423628	1.108090
8	-4.374975	0.219779	1.704297
8	-2.507727	1.750772	1.264110
1	-4.831797	-0.020418	-1.184634
1	-5.042762	-2.674772	-0.784682
1	-4.020497	-2.128309	-2.146377
1	-3.127040	-2.863855	0.684857
1	-2.443732	-3.499600	-0.820273
1	-1.348723	-1.294358	0.517774
1	-1.246614	-1.459744	-1.250421
1	-0.766648	0.915005	-1.904399
1	-3.330011	1.119112	1.486732
1	-0.959330	3.214692	0.108578
1	-1.770967	1.411355	1.789319
1	-0.353499	0.793580	-0.201566
1	-1.384343	3.329135	-1.594567
6	0.736374	3.140453	-1.251409
1	0.957720	2.773062	-2.260272
1	0.860993	4.229375	-1.264994

1	-3.200173	1.712037	-0.879577
6	1.699634	2.549821	-0.269789
6	2.583602	1.588099	-0.551700
1	1.652170	2.912189	0.758157
1	2.665420	1.199209	-1.562691
6	3.477459	1.044070	0.508519
8	3.610814	1.617370	1.576602
6	4.210579	-0.236025	0.241996
6	3.847831	-1.107963	-0.788770
6	5.269944	-0.577582	1.089454
6	4.537622	-2.302753	-0.971270
1	3.012995	-0.874350	-1.441448
6	5.966276	-1.763680	0.898325
1	5.530679	0.103921	1.892617
6	5.599814	-2.628595	-0.132744
1	4.244887	-2.979211	-1.767755
1	6.793479	-2.018625	1.552988
1	6.140609	-3.558314	-0.279834

[4-5]TS-anti_conf-2

Number of imaginary frequencies : 1

The smallest frequency is : -258.0795

Electronic energy=	-1054.9841915
Zero-point correction=	0.388445
Thermal correction to Energy=	0.410237
Thermal correction to Enthalpy=	0.411181
Thermal correction to Gibbs Free Energy=	0.333642
Sum of electronic and zero-point Energies=	-1054.595747
Sum of electronic and thermal Energies=	-1054.573954
Sum of electronic and thermal Enthalpies=	-1054.573010
Sum of electronic and thermal Free Energies=	-1054.650549

Cartesian Coordinates

6	-4.528874	-0.581427	-0.498139
6	-4.586194	-2.003850	-1.042278
6	-3.334874	-2.629594	-0.415494
6	-2.283829	-1.514987	-0.502260
7	-3.086506	-0.279443	-0.594263
6	-2.582259	0.920229	-0.645328
6	-1.142576	1.147263	-0.993985
6	-0.755598	2.623804	-0.995660
6	-5.064756	-0.504949	0.972903
8	-6.049587	-1.199318	1.209879
8	-4.465266	0.283673	1.767082
8	-2.491655	1.648348	1.262132
1	-5.080865	0.146040	-1.101179
1	-5.509477	-2.487989	-0.728339
1	-4.517088	-2.004908	-2.135064
1	-3.539326	-2.870445	0.631466
1	-3.002005	-3.538527	-0.918726
1	-1.628754	-1.471755	0.372681
1	-1.664276	-1.599480	-1.400932
1	-0.987325	0.719053	-1.995577
1	-3.354936	1.084444	1.516705
1	-0.967095	3.048055	-0.009591
1	-1.760315	1.243397	1.747303
1	-0.501512	0.574583	-0.314115
1	-1.380035	3.162132	-1.717009
6	0.720838	2.832872	-1.358508
1	0.935083	2.404121	-2.344453
1	0.910241	3.911239	-1.424728
1	-3.293100	1.721533	-0.833837
6	1.638542	2.250177	-0.330813
6	2.576809	1.327241	-0.562900

1	1.525978	2.607297	0.694166
1	2.738280	0.949981	-1.567863
6	3.441640	0.847056	0.551131
8	3.330087	1.311329	1.673922
6	4.472836	-0.206206	0.275637
6	4.481263	-0.985790	-0.885129
6	5.455679	-0.416667	1.249486
6	5.459551	-1.959527	-1.067509
1	3.719490	-0.857712	-1.646587
6	6.437870	-1.379452	1.061217
1	5.430700	0.190756	2.147983
6	6.440641	-2.153346	-0.099122
1	5.455289	-2.566470	-1.967103
1	7.201417	-1.529944	1.817581
1	7.206275	-2.908639	-0.246547

[4-5]TS-anti_conf-3

Number of imaginary frequencies : 1
The smallest frequency is : -330.2062

Electronic energy= -1054.9880359
Zero-point correction= 0.388871
Thermal correction to Energy= 0.410028
Thermal correction to Enthalpy= 0.410972
Thermal correction to Gibbs Free Energy= 0.337870
Sum of electronic and zero-point Energies= -1054.599165
Sum of electronic and thermal Energies= -1054.578008
Sum of electronic and thermal Enthalpies= -1054.577064
Sum of electronic and thermal Free Energies= -1054.650166

Cartesian Coordinates

6	1.692750	-1.405215	-0.775597
6	2.852224	-2.167866	-1.410255
6	4.020023	-1.775421	-0.497193
6	3.775109	-0.287814	-0.207186
7	2.329939	-0.115893	-0.445988
6	1.672444	0.996089	-0.230807
6	2.400228	2.313925	-0.159169
6	1.539632	3.559184	-0.408816
6	1.144103	-2.171863	0.466814
8	0.917022	-3.364186	0.292361
8	0.953460	-1.513188	1.545704
8	1.003273	0.906155	1.639528
1	0.854192	-1.226100	-1.455871
1	2.646687	-3.237212	-1.415846
1	3.024908	-1.819640	-2.433539
1	3.966277	-2.350995	0.431550
1	4.999700	-1.943409	-0.946771
1	4.023130	-0.003389	0.820126
1	4.330655	0.360130	-0.892928
1	3.190813	2.286388	-0.919686
1	0.999998	-0.188709	1.635532
1	1.221018	3.567233	-1.458099
1	1.684592	1.183471	2.266683
1	2.914120	2.389217	0.805286
1	2.200745	4.422208	-0.287301
6	0.301278	3.734949	0.494984
1	0.494411	3.341968	1.497044
1	0.105151	4.809349	0.593127
1	0.635451	0.993947	-0.558455
6	-0.926622	3.093870	-0.081914
6	-1.602372	2.082634	0.468738
1	-1.271201	3.476182	-1.044448
1	-1.262959	1.648070	1.403585
6	-2.754474	1.471525	-0.251993

8	-3.454036	2.128819	-1.005153
6	-2.981486	0.003480	-0.073038
6	-2.028421	-0.815319	0.540593
6	-4.146455	-0.565621	-0.597565
6	-2.229218	-2.190890	0.624526
1	-1.111637	-0.400323	0.946233
6	-4.357182	-1.934380	-0.497250
1	-4.869626	0.083134	-1.081570
6	-3.397515	-2.747209	0.109302
1	-1.461726	-2.813527	1.075154
1	-5.265573	-2.373267	-0.898187
1	-3.560724	-3.818614	0.175735

[4-5]TS-anti_conf-4

Number of imaginary frequencies : 1

The smallest frequency is : -254.9969

Electronic energy=	-1054.9853764
Zero-point correction=	0.388674
Thermal correction to Energy=	0.410252
Thermal correction to Enthalpy=	0.411196
Thermal correction to Gibbs Free Energy=	0.335395
Sum of electronic and zero-point Energies=	-1054.596703
Sum of electronic and thermal Energies=	-1054.575124
Sum of electronic and thermal Enthalpies=	-1054.574180
Sum of electronic and thermal Free Energies=	-1054.649982

Cartesian Coordinates

6	-0.711129	-1.216323	0.390649
6	-0.602458	-1.274019	1.907342
6	-2.071826	-1.447828	2.312863
6	-2.842370	-0.549468	1.330781
7	-1.899601	-0.362335	0.209183
6	-2.123055	0.354720	-0.853181
6	-3.209093	1.387575	-0.924040
6	-2.891245	2.663957	-0.125076
6	-0.914270	-2.639701	-0.238328
8	-0.325702	-3.559249	0.323007
8	-1.636442	-2.706362	-1.281297
8	-2.907794	-0.869145	-2.300786
1	0.142331	-0.737642	-0.103015
1	0.021420	-2.113961	2.208236
1	-0.186158	-0.338960	2.297092
1	-2.359846	-2.492633	2.168169
1	-2.273929	-1.175450	3.349754
1	-3.765837	-1.008198	0.965009
1	-3.079614	0.425597	1.764912
1	-4.151637	0.959822	-0.567675
1	-2.357286	-1.683059	-1.903213
1	-2.986712	2.474008	0.949940
1	-3.833986	-1.067401	-2.111294
1	-3.340783	1.633738	-1.979720
1	-3.660478	3.399415	-0.377451
6	-1.503084	3.264585	-0.398306
1	-1.292886	3.288349	-1.474248
1	-1.512996	4.306288	-0.053073
1	-1.273443	0.462101	-1.521185
6	-0.409472	2.556087	0.340577
6	0.726489	2.089513	-0.186594
1	-0.553430	2.421515	1.414335
1	0.931442	2.199951	-1.247443
6	1.731324	1.424897	0.692198
8	1.626560	1.474939	1.908062
6	2.870313	0.684943	0.062849
6	2.897262	0.349372	-1.294744

6	3.926135	0.286995	0.890624
6	3.968081	-0.370564	-1.815908
1	2.078086	0.624521	-1.951076
6	4.998824	-0.420733	0.367132
1	3.882043	0.544425	1.943618
6	5.020649	-0.750366	-0.988131
1	3.977290	-0.638644	-2.867265
1	5.817585	-0.721656	1.012665
1	5.856611	-1.309071	-1.397484

[4-5]TS-anti_conf-5

Number of imaginary frequencies : 1

The smallest frequency is : -247.8602

Electronic energy=	-1054.9872301
Zero-point correction=	0.390050
Thermal correction to Energy=	0.411200
Thermal correction to Enthalpy=	0.412144
Thermal correction to Gibbs Free Energy=	0.337560
Sum of electronic and zero-point Energies=	-1054.597180
Sum of electronic and thermal Energies=	-1054.576030
Sum of electronic and thermal Enthalpies=	-1054.575086
Sum of electronic and thermal Free Energies=	-1054.649671

Cartesian Coordinates

6	4.006935	-0.585398	0.188813
6	4.335929	-1.426966	1.415996
6	2.940779	-1.810475	1.919658
6	2.125948	-0.525369	1.736511
7	2.833917	0.185112	0.654319
6	2.405045	1.287680	0.106697
6	1.428112	2.179606	0.812414
6	0.976113	3.383290	-0.031991
6	3.705939	-1.469365	-1.071719
8	4.374691	-2.497679	-1.163547
8	2.859130	-1.016029	-1.896916
8	1.225649	0.794119	-1.474133
1	4.799048	0.119804	-0.082382
1	4.938033	-2.286518	1.126519
1	4.868655	-0.832183	2.165654
1	2.535761	-2.603995	1.284898
1	2.926798	-2.155386	2.954699
1	1.087474	-0.708164	1.442508
1	2.132754	0.098710	2.636583
1	1.927174	2.514024	1.731738
1	1.885406	0.021003	-1.712754
1	1.280652	3.226375	-1.070716
1	0.369320	0.377264	-1.271507
1	0.570444	1.577861	1.129662
1	1.464075	4.296160	0.320162
6	-0.552379	3.586396	-0.002961
1	-0.897186	3.764885	1.021848
1	-0.800516	4.470085	-0.600746
1	3.075160	1.736911	-0.622800
6	-1.201839	2.367673	-0.570549
6	-1.973883	1.511623	0.106338
1	-0.927514	2.111390	-1.594090
1	-2.302886	1.726457	1.120685
6	-2.328915	0.204866	-0.507760
8	-1.552834	-0.329847	-1.290969
6	-3.612196	-0.458888	-0.140599
6	-4.627773	0.225916	0.533476
6	-3.800174	-1.795185	-0.508483
6	-5.819623	-0.423171	0.840319
1	-4.498360	1.270263	0.800701

6	-4.987099	-2.443013	-0.194274
1	-3.003045	-2.305743	-1.038812
6	-5.996911	-1.756814	0.480946
1	-6.610428	0.111235	1.356527
1	-5.129749	-3.481425	-0.475239
1	-6.925615	-2.263747	0.724151

[4-5]TS-anti_conf-6

Number of imaginary frequencies : 1

The smallest frequency is : -271.3403

Electronic energy=	-1054.98027
Zero-point correction=	0.387877
Thermal correction to Energy=	0.409718
Thermal correction to Enthalpy=	0.410662
Thermal correction to Gibbs Free Energy=	0.332861
Sum of electronic and zero-point Energies=	-1054.592393
Sum of electronic and thermal Energies=	-1054.570552
Sum of electronic and thermal Enthalpies=	-1054.569608
Sum of electronic and thermal Free Energies=	-1054.647409

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Cartesian Coordinates

6	4.229882	-0.164955	-0.321115
6	4.664476	0.777290	-1.437275
6	3.493561	1.766323	-1.484483
6	2.253422	0.890012	-1.251673
7	2.792153	-0.325798	-0.610700
6	2.070836	-1.346875	-0.246233
6	0.679710	-1.539862	-0.770241
6	-0.016631	-2.768896	-0.188547
6	4.482804	0.469268	1.090532
8	5.530673	1.098624	1.203905
8	3.606323	0.257971	1.985677
8	1.577080	-1.088079	1.719024
1	4.710178	-1.147338	-0.353870
1	5.611374	1.250606	-1.183093
1	4.758675	0.237417	-2.385036
1	3.600657	2.488744	-0.670728
1	3.426578	2.316547	-2.424114
1	1.514305	1.361295	-0.596176
1	1.761695	0.606758	-2.187483
1	0.766082	-1.641377	-1.862618
1	2.464883	-0.518790	1.876197
1	-0.115961	-2.646989	0.893513
1	0.849381	-0.460237	1.817976
1	0.098926	-0.627922	-0.590671
1	0.614651	-3.649238	-0.354939
6	-1.395567	-3.026859	-0.816324
1	-1.273406	-3.193287	-1.894669
1	-1.817788	-3.942021	-0.390926
1	2.623674	-2.220335	0.091086
6	-2.341710	-1.884924	-0.597020
6	-3.441134	-1.945168	0.160222
1	-2.103844	-0.946792	-1.098210
1	-3.748697	-2.879617	0.625802
6	-4.410715	-0.828023	0.312010
8	-5.587614	-1.071912	0.512291
6	-3.942910	0.593726	0.199130
6	-2.669527	1.000449	0.610216
6	-4.849920	1.546193	-0.273904
6	-2.303331	2.341050	0.530964
1	-1.980395	0.268593	1.020776
6	-4.477041	2.881042	-0.370623
1	-5.843389	1.219897	-0.564391
6	-3.202583	3.279794	0.030846

1	-1.321004	2.656523	0.869094
1	-5.180799	3.613604	-0.752564
1	-2.914270	4.324195	-0.036129

[4]-syn_conf-1

Number of imaginary frequencies : 0

Electronic energy= -1055.0152519
 Zero-point correction= 0.392138
 Thermal correction to Energy= 0.414111
 Thermal correction to Enthalpy= 0.415055
 Thermal correction to Gibbs Free Energy= 0.337106
 Sum of electronic and zero-point Energies= -1054.623114
 Sum of electronic and thermal Energies= -1054.601141
 Sum of electronic and thermal Enthalpies= -1054.600197
 Sum of electronic and thermal Free Energies= -1054.678146

 Cartesian Coordinates

6	2.678469	-1.221861	-0.558918
6	3.569513	-2.210198	-1.319659
6	4.968576	-1.824977	-0.821730
6	4.891082	-0.299618	-0.613332
7	3.458983	0.000725	-0.664654
6	3.022084	1.288681	-0.251612
6	1.545273	1.532309	-0.519071
6	1.141081	2.981117	-0.259977
6	2.403706	-1.779684	0.855223
8	2.004964	-2.911000	0.997514
8	2.608786	-0.988500	1.903251
8	3.213441	1.528393	1.169757
1	1.700573	-1.104039	-1.037307
1	3.301845	-3.244747	-1.106294
1	3.471715	-2.022208	-2.392122
1	5.165259	-2.322697	0.132993
1	5.762576	-2.109927	-1.514100
1	5.345094	-0.019673	0.349359
1	5.413064	0.259607	-1.399977
1	0.955180	0.863527	0.120966
1	2.885664	-0.075503	1.658402
1	1.776434	3.649948	-0.852895
1	4.134963	1.769511	1.327784
1	1.334667	1.259786	-1.560149
1	1.319390	3.220999	0.793336
1	3.629606	2.032648	-0.786615
6	-0.327300	3.255603	-0.616694
1	-0.500477	3.048940	-1.679209
1	-0.531204	4.321527	-0.454619
6	-1.272819	2.454217	0.220764
6	-2.170792	1.583115	-0.248561
1	-1.211605	2.580264	1.302781
1	-2.258629	1.405239	-1.316262
6	-3.033515	0.816753	0.692519
8	-2.882905	0.904823	1.899753
6	-4.083487	-0.096551	0.133514
6	-4.573200	0.015543	-1.170874
6	-4.600520	-1.083665	0.979012
6	-5.565315	-0.850782	-1.621900
1	-4.206003	0.791006	-1.834970
6	-5.578931	-1.956948	0.523297
1	-4.215235	-1.150374	1.991096
6	-6.062891	-1.841004	-0.779472
1	-5.950065	-0.751764	-2.631859
1	-5.966624	-2.727591	1.181844
1	-6.829444	-2.521591	-1.136986

[4-5]TS-syn_conf-1

Number of imaginary frequencies : 1

The smallest frequency is : -266.3023

Electronic energy= -1054.9849174
Zero-point correction= 0.388610
Thermal correction to Energy= 0.410318
Thermal correction to Enthalpy= 0.411263
Thermal correction to Gibbs Free Energy= 0.333334
Sum of electronic and zero-point Energies= -1054.596308
Sum of electronic and thermal Energies= -1054.574599
Sum of electronic and thermal Enthalpies= -1054.573655
Sum of electronic and thermal Free Energies= -1054.651584

Cartesian Coordinates

6	-3.945947	0.208443	-0.686022
6	-5.421113	-0.150853	-0.845774
6	-5.911408	-0.162614	0.604629
6	-4.766588	-0.848658	1.352373
7	-3.574085	-0.536118	0.535007
6	-2.360103	-0.725334	0.979150
6	-1.167059	-0.587968	0.085646
6	-1.050752	-1.791871	-0.859335
6	-3.738793	1.757774	-0.567996
8	-4.356211	2.419651	-1.397771
8	-2.933241	2.182975	0.317586
8	-1.869551	0.880949	2.111814
1	-3.335102	-0.136915	-1.524786
1	-5.916401	0.591402	-1.470090
1	-5.531706	-1.142833	-1.296421
1	-6.029038	0.865722	0.960013
1	-6.859083	-0.685001	0.743308
1	-4.626598	-0.475307	2.370260
1	-4.894867	-1.935128	1.386976
1	-0.281439	-0.514492	0.719648
1	-2.322861	1.492593	1.378637
1	-1.942064	-1.863904	-1.491835
1	-2.434689	0.932871	2.893206
1	-1.244292	0.348859	-0.475933
1	-1.002892	-2.718674	-0.274184
1	-2.274718	-1.376375	1.846160
6	0.194429	-1.687635	-1.753646
1	0.175407	-0.741618	-2.305958
1	0.159826	-2.499970	-2.489618
6	1.459264	-1.805142	-0.964122
6	2.393823	-0.857589	-0.848529
1	1.621518	-2.738933	-0.423695
1	2.276110	0.097172	-1.351533
6	3.592176	-1.098406	0.003700
8	3.679691	-2.104759	0.688646
6	4.689661	-0.077886	0.028517
6	4.805284	0.946247	-0.916053
6	5.646742	-0.186469	1.043452
6	5.862689	1.848980	-0.842136
1	4.088824	1.039131	-1.725248
6	6.694316	0.720359	1.122609
1	5.545748	-0.991999	1.762975
6	6.803230	1.741006	0.178352
1	5.951463	2.636973	-1.582993
1	7.428109	0.633800	1.917583
1	7.622731	2.450627	0.237384

[4-5]TS-syn_conf-2

Number of imaginary frequencies : 1
The smallest frequency is : -290.4352

Electronic energy= -1054.985198
Zero-point correction= 0.388858
Thermal correction to Energy= 0.410276
Thermal correction to Enthalpy= 0.411220
Thermal correction to Gibbs Free Energy= 0.334772
Sum of electronic and zero-point Energies= -1054.596340
Sum of electronic and thermal Energies= -1054.574922
Sum of electronic and thermal Enthalpies= -1054.573978
Sum of electronic and thermal Free Energies= -1054.650426

Cartesian Coordinates

6	-3.097170	-1.053359	-0.837152
6	-3.021795	-2.578271	-0.860941
6	-2.767078	-2.916034	0.610999
6	-1.760391	-1.848009	1.041718
7	-2.066025	-0.702777	0.159008
6	-1.602567	0.498217	0.386285
6	-1.749107	1.586959	-0.633567
6	-1.341664	2.982526	-0.155410
6	-4.529950	-0.552102	-0.449887
8	-5.449536	-1.110814	-1.039248
8	-4.619403	0.401831	0.389046
8	-2.816708	1.360475	1.737477
1	-2.838455	-0.605980	-1.801296
1	-3.952078	-2.988998	-1.250763
1	-2.184127	-2.913046	-1.481432
1	-3.696745	-2.806736	1.178193
1	-2.382678	-3.924786	0.768916
1	-1.862293	-1.550185	2.088977
1	-0.728142	-2.165720	0.861873
1	-2.786728	1.604164	-0.978146
1	-3.641908	0.951946	1.193861
1	-2.103348	3.362032	0.527735
1	-2.773242	0.874740	2.571086
1	-1.124047	1.279732	-1.484414
1	-1.324712	3.638378	-1.032138
1	-0.770252	0.547022	1.083148
6	0.023221	3.044058	0.547470
1	-0.029569	2.560993	1.529815
1	0.260453	4.099142	0.731125
6	1.114815	2.435032	-0.273845
6	1.927205	1.452656	0.129601
1	1.244889	2.811739	-1.289783
1	1.839025	1.043407	1.132553
6	2.953948	0.894251	-0.793312
8	2.947252	1.170215	-1.981503
6	3.988617	-0.040176	-0.242717
6	4.281686	-0.126986	1.121475
6	4.699583	-0.831984	-1.150529
6	5.269480	-0.999499	1.569854
1	3.765310	0.502690	1.838935
6	5.675183	-1.711646	-0.700872
1	4.468831	-0.741289	-2.206914
6	5.960408	-1.796836	0.661691
1	5.500978	-1.054266	2.628734
1	6.216894	-2.329956	-1.409492
1	6.724723	-2.482025	1.015022

[4-5]TS-syn_conf-3

Number of imaginary frequencies : 1

The smallest frequency is : -307.9748

Electronic energy= -1054.9843925
Zero-point correction= 0.388364
Thermal correction to Energy= 0.409832
Thermal correction to Enthalpy= 0.410776
Thermal correction to Gibbs Free Energy= 0.334485
Sum of electronic and zero-point Energies= -1054.596028
Sum of electronic and thermal Energies= -1054.574561
Sum of electronic and thermal Enthalpies= -1054.573617
Sum of electronic and thermal Free Energies= -1054.649908

Cartesian Coordinates

6 -3.978426 -0.430080 -0.240736
6 -4.546511 -1.626855 -1.001216
6 -3.340877 -2.569081 -1.072037
6 -2.174160 -1.623163 -1.365044
7 -2.611754 -0.334893 -0.787109
6 -1.782020 0.660706 -0.601851
6 -2.285442 2.011268 -0.176516
6 -1.308365 3.167256 -0.404204
6 -4.029321 -0.664222 1.305727
8 -5.114793 -1.046047 1.730569
8 -2.983044 -0.412212 1.987539
8 -0.820196 0.283979 1.112104
1 -4.522128 0.496486 -0.446846
1 -5.396847 -2.041884 -0.461846
1 -4.860755 -1.329544 -2.007069
1 -3.196486 -3.053058 -0.101159
1 -3.437122 -3.345350 -1.832576
1 -1.234244 -1.937727 -0.903437
1 -2.012626 -1.490798 -2.439538
1 -2.586270 1.944545 0.874379
1 -1.743711 -0.072813 1.533458
1 -1.810150 4.075636 -0.058699
1 -0.233684 -0.472868 0.985762
1 -3.196681 2.213929 -0.752229
1 -1.148163 3.299076 -1.481966
1 -0.847359 0.601048 -1.157152
6 0.055963 3.060800 0.297886
1 -0.060515 2.676880 1.314786
1 0.466680 4.077047 0.368804
6 1.054735 2.239582 -0.456875
6 1.846427 1.296706 0.064252
1 1.165232 2.453817 -1.522061
1 1.776289 1.049373 1.118936
6 2.813490 0.571284 -0.802498
8 2.700227 0.583896 -2.018613
6 3.931521 -0.191772 -0.158561
6 4.267696 -0.043486 1.190317
6 4.677797 -1.061559 -0.961322
6 5.332165 -0.761105 1.728302
1 3.718311 0.644671 1.824067
6 5.734300 -1.782514 -0.421956
1 4.410611 -1.153561 -2.008963
6 6.062006 -1.633408 0.925647
1 5.592232 -0.636547 2.774493
1 6.306983 -2.458381 -1.049060
1 6.889257 -2.194810 1.349009

[4-5]TS-syn_conf-4

Number of imaginary frequencies : 1
The smallest frequency is : -310.1021

Electronic energy= -1054.9822162

Zero-point correction= 0.388688
 Thermal correction to Energy= 0.410164
 Thermal correction to Enthalpy= 0.411108
 Thermal correction to Gibbs Free Energy= 0.334573
 Sum of electronic and zero-point Energies= -1054.593528
 Sum of electronic and thermal Energies= -1054.572052
 Sum of electronic and thermal Enthalpies= -1054.571108
 Sum of electronic and thermal Free Energies= -1054.647644

Cartesian Coordinates

6	3.929695	0.632752	0.981236
6	5.438714	0.841447	1.088628
6	5.928345	0.390539	-0.291162
6	5.077535	-0.849002	-0.577930
7	3.844262	-0.617721	0.203735
6	2.763298	-1.330050	0.026128
6	1.585950	-1.193963	0.948740
6	0.562961	-2.325976	0.824832
6	3.233215	1.853097	0.289354
8	3.551999	2.947404	0.741423
8	2.390525	1.616645	-0.635682
8	1.831222	-0.553990	-1.584837
1	3.450792	0.491705	1.954415
1	5.655544	1.885227	1.311189
1	5.860972	0.204480	1.872850
1	5.716418	1.170521	-1.028774
1	6.995733	0.167221	-0.324121
1	4.828850	-0.968853	-1.635994
1	5.555031	-1.766202	-0.218961
1	1.134253	-0.207670	0.797347
1	2.079561	0.428459	-1.220715
1	-0.133411	-2.234654	1.664935
1	2.332169	-0.692201	-2.398904
1	1.986395	-1.202819	1.970377
1	1.079382	-3.285228	0.952386
1	2.903291	-2.273198	-0.499084
6	-0.258276	-2.374162	-0.475307
1	-0.909972	-3.253287	-0.429876
1	0.411161	-2.491617	-1.333142
6	-1.086345	-1.142258	-0.673263
6	-2.407495	-1.092450	-0.474063
1	-0.570310	-0.233827	-0.981635
1	-2.952195	-1.984352	-0.176100
6	-3.159852	0.174895	-0.678299
8	-2.660403	1.120869	-1.263070
6	-4.562305	0.274014	-0.151347
6	-5.085628	-0.627144	0.780439
6	-5.353930	1.338456	-0.594675
6	-6.384247	-0.468122	1.256119
1	-4.479295	-1.443111	1.159270
6	-6.652611	1.490907	-0.127495
1	-4.926992	2.036702	-1.307052
6	-7.170055	0.586003	0.799486
1	-6.781086	-1.166949	1.985558
1	-7.262852	2.316323	-0.480195
1	-8.183832	0.706059	1.168903

[4-5]TS-syn_conf-5

Number of imaginary frequencies : 1
 The smallest frequency is : -282.4925

Electronic energy= -1054.9825989
 Zero-point correction= 0.388700
 Thermal correction to Energy= 0.410187
 Thermal correction to Enthalpy= 0.411131

Thermal correction to Gibbs Free Energy=	0.335289
Sum of electronic and zero-point Energies=	-1054.593899
Sum of electronic and thermal Energies=	-1054.572412
Sum of electronic and thermal Enthalpies=	-1054.571468
Sum of electronic and thermal Free Energies=	-1054.647310

Cartesian Coordinates

6	-3.413405	0.897034	0.500576
6	-4.383531	2.080459	0.536243
6	-5.301968	1.778692	-0.651696
6	-4.330751	1.277405	-1.722197
7	-3.207610	0.709152	-0.945486
6	-2.329170	-0.082368	-1.502959
6	-1.068689	-0.550609	-0.828095
6	-1.170220	-1.397631	0.447620
6	-4.068538	-0.345659	1.184483
8	-4.265144	-0.218822	2.389022
8	-4.367897	-1.340262	0.445951
8	-3.199838	-1.892711	-1.638694
1	-2.461134	1.120507	0.986802
1	-4.900281	2.118955	1.494963
1	-3.846527	3.021722	0.378841
1	-6.001250	0.982124	-0.382890
1	-5.873292	2.643435	-0.992464
1	-4.761082	0.505699	-2.366110
1	-3.951578	2.092726	-2.346632
1	-0.475793	0.354734	-0.634082
1	-3.758772	-1.687467	-0.752907
1	-1.874365	-2.215823	0.290921
1	-3.829038	-1.903943	-2.371128
1	-0.519473	-1.127026	-1.578459
1	-1.542088	-0.812434	1.293377
1	-2.291630	-0.018590	-2.587421
6	0.203173	-1.979969	0.816191
1	0.550658	-2.653168	0.024051
1	0.082340	-2.579972	1.726307
6	1.223620	-0.916044	1.067421
6	2.385231	-0.796581	0.417151
1	0.992827	-0.172225	1.832076
1	2.657190	-1.510234	-0.355287
6	3.312656	0.325129	0.728505
8	2.953825	1.270417	1.411672
6	4.703965	0.287385	0.170455
6	5.286421	-0.881105	-0.328784
6	5.445992	1.473377	0.184035
6	6.591524	-0.860727	-0.812678
1	4.738267	-1.817349	-0.321366
6	6.743184	1.495559	-0.310140
1	4.982740	2.367505	0.588238
6	7.317663	0.326993	-0.810117
1	7.041119	-1.773524	-1.190104
1	7.310695	2.420669	-0.304539
1	8.333223	0.342585	-1.193475

[4-5]TS-syn_conf-6

Number of imaginary frequencies : 1
The smallest frequency is : -282.5019

Electronic energy=	-1054.9825989
Zero-point correction=	0.388699
Thermal correction to Energy=	0.410186
Thermal correction to Enthalpy=	0.411130
Thermal correction to Gibbs Free Energy=	0.335290
Sum of electronic and zero-point Energies=	-1054.593900
Sum of electronic and thermal Energies=	-1054.572413

Sum of electronic and thermal Enthalpies= -1054.571468
 Sum of electronic and thermal Free Energies= -1054.647309

Cartesian Coordinates

6	-3.413150	0.897064	0.500418
6	-4.382835	2.080841	0.535931
6	-5.301431	1.779210	-0.651924
6	-4.330485	1.277253	-1.722369
7	-3.207403	0.708937	-0.945612
6	-2.329052	-0.082741	-1.502991
6	-1.068615	-0.551020	-0.828064
6	-1.170228	-1.397962	0.447698
6	-4.068698	-0.345349	1.184461
8	-4.265857	-0.218055	2.388862
8	-4.367697	-1.340237	0.446178
8	-3.199868	-1.893018	-1.638503
1	-2.460798	1.120248	0.986621
1	-4.899533	2.119658	1.494663
1	-3.845495	3.021883	0.378359
1	-6.001078	0.983030	-0.382915
1	-5.872384	2.644130	-0.992865
1	-4.761147	0.505433	-2.365926
1	-3.951149	2.092215	-2.347171
1	-0.475675	0.354301	-0.634078
1	-3.758668	-1.687602	-0.752671
1	-1.874314	-2.216202	0.290983
1	-3.829156	-1.904228	-2.370862
1	-0.519402	-1.127514	-1.578373
1	-1.542216	-0.812730	1.293378
1	-2.291516	-0.019110	-2.587460
6	0.203163	-1.980197	0.816442
1	0.550748	-2.653459	0.024400
1	0.082283	-2.580113	1.726608
6	1.223549	-0.916204	1.067641
6	2.385147	-0.796706	0.417354
1	0.992722	-0.172365	1.832265
1	2.657128	-1.510384	-0.355053
6	3.312523	0.325062	0.728645
8	2.953682	1.270324	1.411842
6	4.703795	0.287403	0.170497
6	5.286273	-0.881048	-0.328810
6	5.445769	1.473431	0.184045
6	6.591338	-0.860599	-0.812802
1	4.738167	-1.817320	-0.321375
6	6.742923	1.495683	-0.310226
1	4.982508	2.367532	0.588297
6	7.317420	0.327155	-0.810271
1	7.040948	-1.773368	-1.190278
1	7.310391	2.420819	-0.304640
1	8.332951	0.342804	-1.193704

[4-5]TS-syn_conf-7

Number of imaginary frequencies : 1
 The smallest frequency is : -255.4315

Electronic energy= -1054.9842338
 Zero-point correction= 0.389748
 Thermal correction to Energy= 0.410970
 Thermal correction to Enthalpy= 0.411914
 Thermal correction to Gibbs Free Energy= 0.337489
 Sum of electronic and zero-point Energies= -1054.594486
 Sum of electronic and thermal Energies= -1054.573264
 Sum of electronic and thermal Enthalpies= -1054.572320
 Sum of electronic and thermal Free Energies= -1054.646745

Cartesian Coordinates

```

-----
6   -3.724639 -0.457019 -0.743764
6   -4.144878 -1.847433 -1.225278
6   -3.119101 -2.748665 -0.528595
6   -1.812132 -1.957406 -0.645681
7   -2.256370 -0.554595 -0.790264
6   -1.422959  0.441339 -0.671295
6   -1.854513  1.858480 -0.924423
6   -0.710213  2.852410 -1.159615
6   -4.274728 -0.223302  0.703126
8   -5.498806 -0.138904  0.766902
8   -3.433205 -0.203087  1.653790
8   -1.136150  0.654158  1.343772
1   -4.072999  0.348014 -1.394363
1   -5.176018 -2.053513 -0.938978
1   -4.050404 -1.923099 -2.313889
1   -3.387205 -2.864144  0.524821
1   -3.034411 -3.739760 -0.976860
1   -1.173474 -2.044250  0.237587
1   -1.236699 -2.237299 -1.533394
1   -2.496978  2.179772 -0.096949
1   -2.068762  0.231076  1.553126
1   -1.152177  3.754464 -1.593845
1   -0.406639  0.083643  1.632782
1   -2.481677  1.841134 -1.824088
1   -0.032435  2.448520 -1.921744
1   -0.371039  0.189959 -0.780756
6    0.094300  3.275434  0.079734
1   -0.593580  3.643159  0.846181
1    0.735644  4.120076 -0.200823
6    0.940029  2.180238  0.666339
6    1.802962  1.408849 -0.005647
1    0.802151  1.966756  1.721874
1    2.038676  1.581002 -1.053643
6    2.377464  0.219843  0.671019
8    1.747246 -0.354516  1.553196
6    3.711533 -0.292525  0.238760
6    4.560476  0.471485 -0.567214
6    4.122590 -1.556781  0.674362
6    5.804509 -0.026675 -0.940302
1    4.260053  1.464329 -0.887096
6    5.361787 -2.055470  0.295630
1    3.456081 -2.131486  1.309316
6    6.202812 -1.291113 -0.513737
1    6.463255  0.572269 -1.560625
1    5.676977 -3.038342  0.630810
1    7.171771 -1.681441 -0.809381

```

[4-5]TS-syn_conf-8

Number of imaginary frequencies : 1

The smallest frequency is : -314.3175

```

Electronic energy=      -1054.9841633
Zero-point correction=      0.388997
Thermal correction to Energy=      0.410220
Thermal correction to Enthalpy=      0.411164
Thermal correction to Gibbs Free Energy=      0.337542
Sum of electronic and zero-point Energies=      -1054.595166
Sum of electronic and thermal Energies=      -1054.573943
Sum of electronic and thermal Enthalpies=      -1054.572999
Sum of electronic and thermal Free Energies=      -1054.646621

```

Cartesian Coordinates

```

-----
6   -1.024855 -1.360975 -0.723790

```

6	0.084881	-2.347098	-0.370873
6	-0.195388	-2.645773	1.105656
6	-0.621534	-1.288349	1.674537
7	-1.111134	-0.543442	0.497547
6	-1.755670	0.589318	0.612228
6	-2.111728	1.412691	-0.594553
6	-2.422839	2.868451	-0.243653
6	-2.369076	-2.084904	-1.066386
8	-2.267193	-3.032522	-1.838491
8	-3.441000	-1.617257	-0.558899
8	-3.649352	0.180919	1.081514
1	-0.763370	-0.724445	-1.574186
1	0.021761	-3.225997	-1.011285
1	1.066865	-1.875679	-0.486896
1	-1.018819	-3.361769	1.187445
1	0.668788	-3.052688	1.634236
1	-1.416314	-1.365823	2.422487
1	0.223934	-0.744055	2.107562
1	-2.958760	0.938954	-1.098392
1	-3.606428	-0.637505	0.387706
1	-3.329341	2.911896	0.367620
1	-3.713408	-0.204828	1.964758
1	-1.264571	1.368975	-1.286554
1	-2.634359	3.401420	-1.175403
1	-1.631094	1.092606	1.568078
6	-1.270189	3.583588	0.505215
1	-1.250318	3.274066	1.555793
1	-1.462158	4.661268	0.494046
6	0.046178	3.272516	-0.134795
6	0.931719	2.403616	0.364355
1	0.242546	3.685989	-1.124832
1	0.752575	1.937651	1.329528
6	2.073637	1.937225	-0.466645
8	2.408246	2.528938	-1.478221
6	2.724704	0.637003	-0.096988
6	2.690366	0.105380	1.196078
6	3.371636	-0.074096	-1.113340
6	3.283950	-1.125632	1.464751
1	2.231131	0.658650	2.009476
6	3.951430	-1.308544	-0.848049
1	3.401082	0.357435	-2.108591
6	3.904474	-1.838528	0.441292
1	3.265049	-1.525336	2.474043
1	4.439783	-1.859631	-1.645194
1	4.357580	-2.803029	0.648280

[5]-anti_conf-1

Number of imaginary frequencies : 0

Electronic energy= -1054.9981802
 Zero-point correction= 0.389206
 Thermal correction to Energy= 0.411907
 Thermal correction to Enthalpy= 0.412851
 Thermal correction to Gibbs Free Energy= 0.336429
 Sum of electronic and zero-point Energies= -1054.608974
 Sum of electronic and thermal Energies= -1054.586273
 Sum of electronic and thermal Enthalpies= -1054.585329
 Sum of electronic and thermal Free Energies= -1054.661751

 Cartesian Coordinates

6	1.698709	-1.477725	-1.009252
6	2.959465	-2.280166	-1.329034
6	3.825281	-1.998138	-0.092416
6	3.550951	-0.520975	0.223031
7	2.283161	-0.224707	-0.486881

6	1.807871	0.954050	-0.642679
6	2.528553	2.167207	-0.158830
6	1.835185	3.506990	-0.412544
6	0.891008	-2.243845	0.098476
8	0.402427	-3.300866	-0.297947
8	0.878156	-1.733341	1.251564
8	1.137001	0.734687	2.090856
1	1.055486	-1.254682	-1.861792
1	2.710738	-3.333760	-1.453083
1	3.440984	-1.909821	-2.240139
1	3.495634	-2.621549	0.741450
1	4.887472	-2.177942	-0.262563
1	3.393084	-0.304769	1.282458
1	4.324144	0.143133	-0.172447
1	3.511566	2.166262	-0.652814
1	1.049129	-0.206157	1.775410
1	1.587264	3.611660	-1.476051
1	0.840139	0.714033	3.007098
1	2.707360	2.026935	0.913850
1	2.568285	4.287356	-0.189734
6	0.582381	3.738541	0.452557
1	0.748691	3.320160	1.450650
1	0.433075	4.819053	0.561597
1	0.864916	1.032812	-1.183203
6	-0.662527	3.152573	-0.141009
6	-1.316478	2.101609	0.360208
1	-1.051509	3.616726	-1.048769
1	-0.926906	1.597773	1.240412
6	-2.549354	1.591061	-0.305693
8	-3.206302	2.302713	-1.048921
6	-2.938654	0.171011	-0.056758
6	-2.040841	-0.742230	0.502209
6	-4.211130	-0.258434	-0.449535
6	-2.401474	-2.078105	0.657431
1	-1.043523	-0.439266	0.804979
6	-4.580704	-1.584327	-0.270513
1	-4.891132	0.462591	-0.892089
6	-3.674328	-2.494899	0.277628
1	-1.667922	-2.777775	1.045222
1	-5.571137	-1.915729	-0.566983
1	-3.961714	-3.534829	0.400633

[6]-anti_conf-1

Number of imaginary frequencies : 0

Electronic energy= -1054.9994387
 Zero-point correction= 0.390497
 Thermal correction to Energy= 0.412760
 Thermal correction to Enthalpy= 0.413705
 Thermal correction to Gibbs Free Energy= 0.337625
 Sum of electronic and zero-point Energies= -1054.608942
 Sum of electronic and thermal Energies= -1054.586678
 Sum of electronic and thermal Enthalpies= -1054.585734
 Sum of electronic and thermal Free Energies= -1054.661814

 Cartesian Coordinates

6	4.346407	-1.421978	1.435464
6	3.683038	-0.078506	1.733907
7	3.517230	0.510659	0.386065
6	4.282249	-0.231654	-0.627824
6	5.196509	-1.130955	0.194800
6	2.654942	1.402120	0.065535
6	1.704958	2.012564	1.035392
6	0.804973	3.085690	0.416523
6	3.276625	-1.052330	-1.560627

8	3.825563	-1.960765	-2.181006
8	2.087890	-0.642366	-1.571020
1	4.810738	0.474774	-1.272892
1	5.444038	-2.019724	-0.384581
1	6.119412	-0.610646	0.472582
1	3.567104	-2.152957	1.198145
1	4.923688	-1.785774	2.286726
1	2.706113	-0.171448	2.207770
1	4.335264	0.587564	2.309354
1	1.109024	1.176902	1.431141
1	1.327690	-1.109361	0.007912
8	1.011089	-1.126197	0.933800
1	0.119893	3.432014	1.196129
1	1.405548	3.949704	0.112053
1	0.057044	-1.279806	0.863362
1	2.269007	2.425616	1.881101
1	2.639465	1.685976	-0.983463
6	-0.026037	2.601735	-0.789923
1	0.625141	2.463540	-1.661572
1	-0.750547	3.379884	-1.049194
6	-0.719710	1.307144	-0.501905
6	-2.023447	1.178545	-0.237487
1	-0.094297	0.416938	-0.477080
1	-2.680730	2.043140	-0.259334
6	-2.597465	-0.147609	0.106658
8	-1.887159	-1.086658	0.441889
6	-4.082265	-0.326738	0.057252
6	-4.924577	0.565037	-0.613507
6	-4.629063	-1.450603	0.685840
6	-6.297024	0.337015	-0.648342
1	-4.515112	1.425572	-1.132522
6	-5.999460	-1.670379	0.660092
1	-3.958795	-2.139483	1.189214
6	-6.835305	-0.775250	-0.007130
1	-6.945507	1.026454	-1.179261
1	-6.419200	-2.540185	1.155135
1	-7.906750	-0.948488	-0.030786

[6-7]TS-anti_conf-1

Number of imaginary frequencies : 1
The smallest frequency is : -1303.3118

Electronic energy= -1054.9752638
Zero-point correction= 0.384353
Thermal correction to Energy= 0.405621
Thermal correction to Enthalpy= 0.406566
Thermal correction to Gibbs Free Energy= 0.331920
Sum of electronic and zero-point Energies= -1054.590911
Sum of electronic and thermal Energies= -1054.569642
Sum of electronic and thermal Enthalpies= -1054.568698
Sum of electronic and thermal Free Energies= -1054.643344

Cartesian Coordinates

6	4.781261	-1.023287	1.385209
6	4.007488	0.293099	1.508605
7	3.564664	0.558774	0.129502
6	4.118373	-0.416360	-0.819961
6	5.302028	-1.003360	-0.055733
6	2.580519	1.361712	-0.188752
6	1.724832	2.011673	0.725417
6	0.746300	3.062804	0.215644
6	3.066034	-1.515508	-1.199792
8	3.515063	-2.451088	-1.851296
8	1.857716	-1.314796	-0.841380
1	4.412528	0.090154	-1.743557

1	5.551096	-1.989859	-0.446235
1	6.177640	-0.351168	-0.138550
1	4.093677	-1.864693	1.518938
1	5.570979	-1.104312	2.133721
1	3.140383	0.216468	2.169903
1	4.641135	1.121341	1.845185
1	1.128828	0.801517	1.020227
1	1.338773	-0.880177	0.401529
8	0.873690	-0.441915	1.243610
1	0.048962	3.290821	1.028583
1	1.260290	4.001338	-0.026806
1	-0.081923	-0.630403	1.140182
1	2.162802	2.238059	1.698518
1	2.337366	1.362894	-1.251206
6	-0.092631	2.629281	-1.006195
1	0.540262	2.539884	-1.895809
1	-0.829259	3.411680	-1.213867
6	-0.780375	1.326960	-0.727605
6	-2.021920	1.226045	-0.241986
1	-0.204472	0.412555	-0.876918
1	-2.645658	2.108540	-0.119098
6	-2.567121	-0.089402	0.175050
8	-1.824673	-0.974034	0.589761
6	-4.038319	-0.322313	0.108483
6	-4.888621	0.533932	-0.597342
6	-4.565455	-1.445678	0.754479
6	-6.253876	0.271840	-0.650355
1	-4.485791	1.393768	-1.123342
6	-5.929100	-1.700828	0.706907
1	-3.888477	-2.104127	1.288753
6	-6.774211	-0.841009	0.005262
1	-6.910315	0.933398	-1.206152
1	-6.336713	-2.569947	1.213011
1	-7.840354	-1.042091	-0.033087

[6-7]TS-anti_conf-2

Number of imaginary frequencies : 1
The smallest frequency is : -1399.6171

Electronic energy=	-1054.9716192
Zero-point correction=	0.382224
Thermal correction to Energy=	0.403845
Thermal correction to Enthalpy=	0.404789
Thermal correction to Gibbs Free Energy=	0.330305
Sum of electronic and zero-point Energies=	-1054.589395
Sum of electronic and thermal Energies=	-1054.567774
Sum of electronic and thermal Enthalpies=	-1054.566830
Sum of electronic and thermal Free Energies=	-1054.641314

Cartesian Coordinates

6	-0.151198	-2.355839	1.606016
6	-0.749747	-0.947047	1.686018
7	-0.913148	-0.558526	0.276072
6	-0.414267	-1.593817	-0.637312
6	0.553458	-2.378107	0.245156
6	-1.577092	0.495978	-0.122057
6	-2.395024	1.311869	0.692136
6	-2.803096	2.662222	0.140369
6	-1.559394	-2.504428	-1.180345
8	-1.190531	-3.470373	-1.833902
8	-2.770267	-2.161678	-0.940501
1	0.075951	-1.122713	-1.495122
1	0.704784	-3.380746	-0.154215
1	1.515821	-1.860918	0.302994
1	-0.955781	-3.097895	1.623259

1	0.520295	-2.558479	2.442242
1	-1.716937	-0.919701	2.195710
1	-0.069852	-0.231766	2.165297
1	-3.335681	0.305564	0.691620
1	-3.309403	-1.470919	0.006491
8	-3.855548	-0.860048	0.773890
1	-3.077534	2.564757	-0.917282
1	-3.691922	3.029835	0.661768
1	-4.796343	-0.872298	0.557093
1	-2.135899	1.316728	1.753840
1	-1.616854	0.627333	-1.204751
6	-1.683171	3.730800	0.279101
1	-1.437482	3.846806	1.340406
1	-2.055741	4.691488	-0.089946
6	-0.477223	3.297067	-0.487802
6	0.527600	2.595167	0.049457
1	-0.476473	3.440773	-1.568663
1	0.534064	2.401770	1.117996
6	1.539529	1.939044	-0.819191
8	1.595893	2.178221	-2.014150
6	2.439033	0.896809	-0.218359
6	2.606455	0.725561	1.160441
6	3.135995	0.062673	-1.100401
6	3.460075	-0.262602	1.645872
1	2.101399	1.374853	1.867711
6	3.980762	-0.927641	-0.615358
1	3.000048	0.211200	-2.166724
6	4.144969	-1.090729	0.760382
1	3.594192	-0.381120	2.716468
1	4.511829	-1.573639	-1.307011
1	4.807212	-1.862070	1.140884

[6-7]TS-anti_conf-3

Number of imaginary frequencies : 1
The smallest frequency is : -1369.3472

Electronic energy= -1054.9722685
Zero-point correction= 0.383262
Thermal correction to Energy= 0.404687
Thermal correction to Enthalpy= 0.405631
Thermal correction to Gibbs Free Energy= 0.331929
Sum of electronic and zero-point Energies= -1054.589007
Sum of electronic and thermal Energies= -1054.567582
Sum of electronic and thermal Enthalpies= -1054.566637
Sum of electronic and thermal Free Energies= -1054.640340

Cartesian Coordinates

6	3.617170	-2.399575	-0.544311
6	3.697316	-0.886295	-0.769882
7	2.286018	-0.476932	-0.855379
6	1.379078	-1.630915	-0.801456
6	2.286342	-2.794190	-1.193951
6	1.861896	0.761278	-0.745149
6	2.659606	1.861706	-0.378738
6	2.086008	3.272269	-0.364375
6	0.755380	-1.827862	0.614756
8	0.138646	-2.870813	0.781001
8	0.863141	-0.862579	1.457926
1	0.544193	-1.481760	-1.493121
1	1.880767	-3.736491	-0.826436
1	2.389332	-2.845925	-2.282300
1	3.579909	-2.608198	0.529942
1	4.478554	-2.920982	-0.964338
1	4.188681	-0.359490	0.052625
1	4.200510	-0.628518	-1.708560

1	2.714962	1.331087	0.904575
1	1.911194	-0.128039	1.709551
8	2.757944	0.562965	1.911026
1	2.881826	3.939454	-0.020969
1	1.818508	3.615256	-1.372231
1	2.606658	1.020526	2.748117
1	3.715030	1.793158	-0.646108
1	0.778594	0.866143	-0.770641
6	0.874704	3.461563	0.575147
1	0.785086	4.530920	0.803446
1	1.058906	2.942235	1.522959
6	-0.429406	3.015451	-0.010029
6	-1.189944	2.015313	0.447153
1	-0.782808	3.555927	-0.889443
1	-0.872061	1.422585	1.301267
6	-2.466959	1.681664	-0.249564
8	-2.996060	2.489602	-0.996363
6	-3.068362	0.326734	-0.048141
6	-2.380227	-0.713114	0.584569
6	-4.345298	0.092685	-0.572212
6	-2.961000	-1.975696	0.684837
1	-1.387593	-0.563896	0.998369
6	-4.929968	-1.160250	-0.454355
1	-4.857627	0.908925	-1.070792
6	-4.235592	-2.197150	0.172452
1	-2.395419	-2.774714	1.152107
1	-5.923334	-1.334822	-0.855999
1	-4.689833	-3.179944	0.256406

[6-7]TS-anti_conf-4

Number of imaginary frequencies : 1
The smallest frequency is : -1417.8706

Electronic energy= -1054.973267
Zero-point correction= 0.382970
Thermal correction to Energy= 0.404083
Thermal correction to Enthalpy= 0.405027
Thermal correction to Gibbs Free Energy= 0.333168
Sum of electronic and zero-point Energies= -1054.590297
Sum of electronic and thermal Energies= -1054.569184
Sum of electronic and thermal Enthalpies= -1054.568240
Sum of electronic and thermal Free Energies= -1054.640099

Cartesian Coordinates

6	3.206019	-2.599108	0.752230
6	3.544040	-1.112600	0.591307
7	2.518093	-0.627578	-0.346965
6	1.643369	-1.713530	-0.809075
6	2.497832	-2.955501	-0.560051
6	2.265794	0.633007	-0.601126
6	2.802442	1.728813	0.113666
6	2.518097	3.149948	-0.362142
6	0.308093	-1.787254	-0.011386
8	-0.435003	-2.705965	-0.329146
8	0.075240	-0.902372	0.890082
1	1.379788	-1.559975	-1.858322
1	1.873870	-3.846692	-0.495178
1	3.225677	-3.084927	-1.367517
1	2.515384	-2.728675	1.591608
1	4.095632	-3.200449	0.945585
1	3.482982	-0.557513	1.530913
1	4.531957	-0.954460	0.144371
1	2.051332	1.345428	1.200388
1	0.850137	-0.108386	1.516431
8	1.468515	0.643213	2.098817

1	3.223194	3.828712	0.125814
1	2.695085	3.251481	-1.440507
1	0.888665	1.154258	2.676710
1	3.795614	1.567444	0.535244
1	1.442126	0.775869	-1.301926
6	1.084120	3.641405	-0.051960
1	0.974842	4.664427	-0.430087
1	0.925773	3.664292	1.032269
6	0.097173	2.726713	-0.698939
6	-0.734666	1.897441	-0.065558
1	0.158388	2.638920	-1.785706
1	-0.863494	1.931679	1.013450
6	-1.425079	0.812301	-0.820457
8	-0.926276	0.365977	-1.844457
6	-2.711984	0.280444	-0.292311
6	-3.526401	1.055328	0.537239
6	-3.114873	-1.004340	-0.666784
6	-4.745679	0.553874	0.981720
1	-3.218159	2.058719	0.818044
6	-4.325397	-1.507998	-0.207659
1	-2.450393	-1.599842	-1.282902
6	-5.142790	-0.728752	0.611244
1	-5.383913	1.161283	1.615587
1	-4.631728	-2.512040	-0.483181
1	-6.089890	-1.124472	0.965569

[6-7]TS-*anti*_conf-5

Number of imaginary frequencies : 1
The smallest frequency is : -1364.3869

Electronic energy=	-1054.9681956
Zero-point correction=	0.382844
Thermal correction to Energy=	0.404676
Thermal correction to Enthalpy=	0.405620
Thermal correction to Gibbs Free Energy=	0.328626
Sum of electronic and zero-point Energies=	-1054.585352
Sum of electronic and thermal Energies=	-1054.563520
Sum of electronic and thermal Enthalpies=	-1054.562575
Sum of electronic and thermal Free Energies=	-1054.639569

Cartesian Coordinates

6	-1.999894	-2.328803	1.154994
6	-1.400341	-0.919276	1.077943
7	-1.979543	-0.361860	-0.157591
6	-2.862773	-1.325772	-0.823198
6	-2.344871	-2.663758	-0.300953
6	-1.876802	0.895038	-0.508105
6	-1.356476	1.920995	0.308151
6	-1.056672	3.261617	-0.332466
6	-4.364234	-1.111671	-0.447587
8	-5.126872	-1.976527	-0.856725
8	-4.675901	-0.056671	0.204443
1	-2.776085	-1.219565	-1.907919
1	-3.108026	-3.434451	-0.405260
1	-1.447681	-2.966570	-0.850586
1	-2.915042	-2.305678	1.754395
1	-1.309750	-3.039161	1.612272
1	-1.676128	-0.292509	1.930529
1	-0.308363	-0.925180	0.981895
1	-2.503562	1.856506	1.057463
1	-4.013688	0.702732	1.038156
8	-3.502608	1.405765	1.728851
1	-1.913658	3.593771	-0.929514
1	-0.913426	4.012003	0.451969
1	-4.129987	2.093223	1.985917

1	-0.629872	1.596316	1.054937
1	-2.397569	1.158369	-1.430994
6	0.190739	3.232359	-1.242320
1	0.362064	4.238010	-1.645085
1	0.002718	2.563071	-2.090205
6	1.403707	2.778532	-0.496932
6	2.041916	1.623536	-0.711232
1	1.768119	3.416838	0.309147
1	1.714494	0.959044	-1.505197
6	3.214636	1.244405	0.122017
8	3.716660	2.038555	0.900585
6	3.777532	-0.140562	-0.004289
6	3.105957	-1.180303	-0.655126
6	5.020872	-0.392037	0.585844
6	3.673289	-2.450063	-0.716721
1	2.132343	-1.016257	-1.104814
6	5.590639	-1.656021	0.515299
1	5.523626	0.423482	1.094969
6	4.916454	-2.688056	-0.137347
1	3.144769	-3.253749	-1.219293
1	6.559359	-1.839764	0.968943
1	5.359838	-3.677389	-0.193650

[6-7]TS-anti_conf-6

Number of imaginary frequencies : 1
The smallest frequency is : -1375.9780

Electronic energy=	-1054.9655193
Zero-point correction=	0.382527
Thermal correction to Energy=	0.404546
Thermal correction to Enthalpy=	0.405490
Thermal correction to Gibbs Free Energy=	0.326772
Sum of electronic and zero-point Energies=	-1054.582992
Sum of electronic and thermal Energies=	-1054.560973
Sum of electronic and thermal Enthalpies=	-1054.560029
Sum of electronic and thermal Free Energies=	-1054.638748

Cartesian Coordinates

6	-6.146078	-0.388834	-0.816984
6	-4.824571	-1.127352	-1.051706
7	-3.808161	-0.073472	-0.886136
6	-4.420955	1.243233	-0.663775
6	-5.831590	1.055308	-1.219298
6	-2.527892	-0.303635	-0.727491
6	-1.954791	-1.578485	-0.542013
6	-0.444607	-1.751357	-0.529997
6	-4.449587	1.639139	0.847913
8	-5.071553	2.660881	1.102607
8	-3.796175	0.909902	1.673225
1	-3.850574	2.012446	-1.191420
1	-6.511422	1.789921	-0.788637
1	-5.831013	1.160599	-2.308954
1	-6.402967	-0.428285	0.246349
1	-6.966429	-0.831614	-1.383774
1	-4.650682	-1.927091	-0.326973
1	-4.746571	-1.538734	-2.064287
1	-2.500374	-1.591376	0.714476
1	-3.565981	-0.371117	1.681978
8	-3.298365	-1.451549	1.718476
1	-0.225204	-2.740976	-0.113385
1	-0.034404	-1.755595	-1.547600
1	-2.883659	-1.642538	2.569295
1	-2.502111	-2.407755	-0.992266
1	-1.931796	0.591525	-0.549781
6	0.304110	-0.698938	0.303690

1	-0.174288	-0.626121	1.290771
1	0.239073	0.291430	-0.159633
6	1.740475	-1.076764	0.479461
6	2.787930	-0.346431	0.088339
1	1.945669	-2.039169	0.949823
1	2.641852	0.615246	-0.394532
6	4.171207	-0.862391	0.285754
8	4.369035	-2.011555	0.644723
6	5.330284	0.049064	0.016200
6	5.201388	1.439162	-0.049110
6	6.592294	-0.532880	-0.145413
6	6.320231	2.234929	-0.278977
1	4.236439	1.911238	0.103645
6	7.705258	0.260579	-0.387857
1	6.675553	-1.612623	-0.077767
6	7.569818	1.647034	-0.455591
1	6.215378	3.314330	-0.319362
1	8.679816	-0.197885	-0.522203
1	8.439749	2.268724	-0.643932

[6-7]TS-anti_conf-7

Number of imaginary frequencies : 1
The smallest frequency is : -1351.3651

Electronic energy= -1054.9654873
Zero-point correction= 0.382192
Thermal correction to Energy= 0.404252
Thermal correction to Enthalpy= 0.405196
Thermal correction to Gibbs Free Energy= 0.326846
Sum of electronic and zero-point Energies= -1054.583295
Sum of electronic and thermal Energies= -1054.561236
Sum of electronic and thermal Enthalpies= -1054.560291
Sum of electronic and thermal Free Energies= -1054.638642

Cartesian Coordinates

6	-6.107897	-0.228538	-1.019127
6	-4.771813	-0.923948	-1.301203
7	-3.770238	0.073991	-0.886812
6	-4.398642	1.330492	-0.458152
6	-5.771551	1.263051	-1.122915
6	-2.498326	-0.187140	-0.711514
6	-1.927535	-1.476215	-0.735894
6	-0.418395	-1.654357	-0.690217
6	-4.519917	1.437086	1.096535
8	-5.165298	2.395267	1.498694
8	-3.909533	0.565155	1.807644
1	-3.798066	2.179216	-0.796550
1	-6.477805	1.909847	-0.602910
1	-5.705360	1.570876	-2.171406
1	-6.435724	-0.463974	-0.001610
1	-6.887459	-0.548857	-1.711884
1	-4.639270	-1.843233	-0.724036
1	-4.629952	-1.146461	-2.364726
1	-2.530034	-1.711747	0.467135
1	-3.663811	-0.698737	1.586479
8	-3.383559	-1.763219	1.439494
1	-0.207891	-2.670610	-0.337651
1	0.018336	-1.586985	-1.694278
1	-3.002387	-2.095993	2.262010
1	-2.452325	-2.210504	-1.348757
1	-1.917647	0.657183	-0.340389
6	0.303586	-0.657457	0.229492
1	-0.213818	-0.632735	1.199409
1	0.262509	0.355389	-0.185833
6	1.730429	-1.050572	0.443790

6	2.790922	-0.320345	0.089135
1	1.916539	-2.017737	0.911801
1	2.656673	0.643779	-0.391284
6	4.167357	-0.834765	0.330320
8	4.350481	-1.970163	0.737854
6	5.338896	0.058707	0.049768
6	5.218122	1.437792	-0.144264
6	6.606810	-0.531299	0.005873
6	6.349505	2.212276	-0.385178
1	4.249781	1.923158	-0.086019
6	7.733415	0.240157	-0.243749
1	6.683149	-1.601028	0.170153
6	7.605436	1.614779	-0.441307
1	6.248962	3.283473	-0.527646
1	8.712552	-0.226347	-0.285106
1	8.485563	2.219555	-0.637083

[6-7]TS-anti_conf-8

Number of imaginary frequencies : 1
The smallest frequency is : -1395.5049

Electronic energy=	-1054.9659977
Zero-point correction=	0.382230
Thermal correction to Energy=	0.404067
Thermal correction to Enthalpy=	0.405011
Thermal correction to Gibbs Free Energy=	0.327804
Sum of electronic and zero-point Energies=	-1054.583768
Sum of electronic and thermal Energies=	-1054.561931
Sum of electronic and thermal Enthalpies=	-1054.560987
Sum of electronic and thermal Free Energies=	-1054.638194

Cartesian Coordinates

6	4.242758	-1.973691	-0.757828
6	4.057028	-0.456712	-0.868185
7	2.595856	-0.287158	-0.823949
6	1.894140	-1.577691	-0.805926
6	2.947128	-2.542054	-1.347307
6	1.987782	0.848708	-0.579773
6	2.624241	2.041196	-0.182511
6	1.823604	3.323871	-0.013699
6	1.421546	-1.979501	0.628770
8	1.001862	-3.121674	0.739368
8	1.450152	-1.079775	1.544901
1	1.000120	-1.522457	-1.433544
1	2.729128	-3.561320	-1.029404
1	2.973575	-2.503718	-2.440951
1	4.324817	-2.256668	0.296701
1	5.141911	-2.313361	-1.274068
1	4.518270	0.090232	-0.041210
1	4.434512	-0.056349	-1.815587
1	2.861545	1.447598	1.036566
1	2.369386	-0.200534	1.774387
8	3.107857	0.616510	1.980756
1	2.462559	4.037098	0.515814
1	1.592134	3.787704	-0.981499
1	2.940998	0.977845	2.860471
1	3.646743	2.177491	-0.537336
1	0.904688	0.768087	-0.509768
6	0.520257	3.157334	0.794653
1	0.259484	4.133979	1.222457
1	0.687331	2.472564	1.635422
6	-0.658282	2.703376	-0.011028
6	-1.421132	1.640173	0.264401
1	-0.924601	3.304774	-0.881302
1	-1.177897	0.997561	1.105577

6	-2.584713	1.307742	-0.605529
8	-2.781145	1.914371	-1.646362
6	-3.509512	0.203852	-0.191853
6	-3.481510	-0.375644	1.079902
6	-4.447560	-0.243932	-1.129503
6	-4.374626	-1.392197	1.405499
1	-2.777616	-0.034750	1.830855
6	-5.332389	-1.262994	-0.806228
1	-4.461306	0.222852	-2.108945
6	-5.295977	-1.839704	0.463294
1	-4.346316	-1.836428	2.395056
1	-6.051009	-1.611729	-1.541119
1	-5.985949	-2.638619	0.716878

[7]-anti_conf-1

Number of imaginary frequencies : 0

Electronic energy=	-1055.0107809
Zero-point correction=	0.389562
Thermal correction to Energy=	0.412203
Thermal correction to Enthalpy=	0.413147
Thermal correction to Gibbs Free Energy=	0.335508
Sum of electronic and zero-point Energies=	-1054.621219
Sum of electronic and thermal Energies=	-1054.598578
Sum of electronic and thermal Enthalpies=	-1054.597634
Sum of electronic and thermal Free Energies=	-1054.675273

Cartesian Coordinates

6	4.714622	-0.901174	1.536835
6	3.861642	0.366670	1.579269
7	3.361924	0.459869	0.215796
6	4.099419	-0.365261	-0.724628
6	5.284662	-0.878304	0.115490
6	2.424061	1.377243	-0.175109
6	1.824988	2.289991	0.614721
6	0.722985	3.214808	0.155545
6	3.300196	-1.541508	-1.306704
8	3.746969	-2.157341	-2.246239
8	2.145289	-1.864402	-0.747570
1	4.447682	0.209699	-1.589011
1	5.643630	-1.845717	-0.238976
1	6.106461	-0.158880	0.050346
1	4.071970	-1.777736	1.673189
1	5.485916	-0.916008	2.308901
1	3.027431	0.290959	2.286774
1	4.455037	1.255016	1.844264
1	0.941174	0.213415	1.286053
1	1.872241	-1.322156	0.037966
8	0.869363	-0.753149	1.308428
1	0.052592	3.405805	1.001692
1	1.128212	4.194300	-0.132885
1	-0.062694	-0.935764	1.086552
1	2.161905	2.403820	1.642618
1	2.133613	1.274618	-1.221176
6	-0.139927	2.686800	-1.008691
1	0.473195	2.576458	-1.910447
1	-0.910653	3.430462	-1.233891
6	-0.783186	1.376837	-0.665497
6	-2.054170	1.239538	-0.272497
1	-0.166586	0.479822	-0.704709
1	-2.718510	2.098624	-0.237814
6	-2.585625	-0.086778	0.129260
8	-1.841309	-0.987682	0.501847
6	-4.059794	-0.319346	0.085617
6	-4.927378	0.527860	-0.610574

6	-4.571487	-1.442910	0.744014
6	-6.291656	0.256412	-0.641230
1	-4.542657	1.387347	-1.150161
6	-5.934281	-1.705810	0.721069
1	-3.882480	-2.096089	1.269177
6	-6.795784	-0.855165	0.028599
1	-6.960083	0.910977	-1.191015
1	-6.327855	-2.574500	1.238991
1	-7.861231	-1.062391	0.008330

[6]-syn_conf-1

Number of imaginary frequencies : 0

Electronic energy=	-1054.9949702
Zero-point correction=	0.391175
Thermal correction to Energy=	0.413331
Thermal correction to Enthalpy=	0.414275
Thermal correction to Gibbs Free Energy=	0.339864
Sum of electronic and zero-point Energies=	-1054.603795
Sum of electronic and thermal Energies=	-1054.581640
Sum of electronic and thermal Enthalpies=	-1054.580696
Sum of electronic and thermal Free Energies=	-1054.655107

Cartesian Coordinates

6	3.608214	-2.697997	0.274087
6	4.077954	-1.267707	0.538716
7	3.137524	-0.423752	-0.240372
6	2.212655	-1.243827	-1.061348
6	2.909151	-2.606224	-1.088761
6	3.059943	0.849231	-0.124319
6	2.097707	1.671124	-0.905053
6	1.908427	3.085083	-0.346751
6	0.823835	-1.278355	-0.307186
8	-0.151981	-0.907827	-0.972163
8	0.902954	-1.664778	0.883868
1	2.096107	-0.782168	-2.042774
1	2.188563	-3.411520	-1.242467
1	3.641421	-2.638551	-1.902632
1	2.883865	-2.989940	1.032558
1	4.447389	-3.395793	0.271495
1	4.030177	-0.970416	1.587476
1	5.083744	-1.085952	0.149334
1	1.144927	1.129779	-0.913978
1	1.265385	-0.106184	1.733829
8	1.373739	0.850228	1.913940
1	2.048461	3.060536	0.739116
1	2.448178	1.704824	-1.947059
1	2.652992	3.769059	-0.765644
1	0.449567	1.125945	2.019489
1	3.754361	1.319747	0.570395
6	0.486409	3.603663	-0.647715
1	0.430256	4.668478	-0.400827
1	0.268284	3.493062	-1.716154
6	-0.479963	2.813473	0.177243
6	-1.205072	1.782040	-0.261074
1	-0.488500	3.026508	1.246834
1	-1.232747	1.507700	-1.311634
6	-1.892885	0.890567	0.712077
8	-1.550272	0.870573	1.887503
6	-3.014966	0.030166	0.239470
6	-3.734136	0.333139	-0.918134
6	-3.368134	-1.084148	1.005197
6	-4.805734	-0.467206	-1.302848
1	-3.471695	1.204178	-1.510978
6	-4.427846	-1.890369	0.611930

1	-2.786940	-1.308052	1.893490
6	-5.150175	-1.580226	-0.540570
1	-5.369983	-0.223172	-2.197307
1	-4.692807	-2.763145	1.200210
1	-5.981492	-2.208798	-0.845114

[6-7]TS-syn_conf-1

Number of imaginary frequencies : 1
The smallest frequency is : -1219.3418

Electronic energy=	-1054.975152
Zero-point correction=	0.383934
Thermal correction to Energy=	0.405340
Thermal correction to Enthalpy=	0.406284
Thermal correction to Gibbs Free Energy=	0.331375
Sum of electronic and zero-point Energies=	-1054.591218
Sum of electronic and thermal Energies=	-1054.569812
Sum of electronic and thermal Enthalpies=	-1054.568868
Sum of electronic and thermal Free Energies=	-1054.643777

Cartesian Coordinates

6	5.024139	-1.804748	0.170446
6	5.079925	-0.281477	0.245887
7	3.769300	0.125473	-0.290847
6	3.111802	-0.964262	-1.033931
6	4.198947	-2.047117	-1.098119
6	3.167619	1.246509	0.020687
6	1.828072	1.581746	-0.270715
6	1.423336	3.051301	-0.202105
6	1.850480	-1.439203	-0.249878
8	0.820226	-1.614811	-0.894923
8	2.038745	-1.563134	1.006325
1	2.797358	-0.604867	-2.017228
1	3.762809	-3.047195	-1.140138
1	4.818029	-1.905768	-1.990497
1	4.483061	-2.191535	1.035838
1	6.019991	-2.249678	0.126894
1	5.205922	0.109359	1.257121
1	5.870619	0.120953	-0.397861
1	1.259196	0.990536	0.828883
1	1.200355	-0.557481	1.637006
8	0.791882	0.379124	1.857392
1	1.562139	3.428568	0.819395
1	1.365428	1.010261	-1.079362
1	2.040123	3.678143	-0.856931
1	-0.184798	0.315469	1.837695
1	3.756489	1.923109	0.642770
6	-0.047963	3.237468	-0.613887
1	-0.329806	4.286224	-0.464035
1	-0.163023	3.010932	-1.679559
6	-0.939321	2.345701	0.189276
6	-1.706315	1.372449	-0.312058
1	-0.914435	2.475718	1.272867
1	-1.777462	1.210317	-1.384152
6	-2.447380	0.465898	0.598833
8	-2.024165	0.240053	1.729345
6	-3.713205	-0.170193	0.136258
6	-4.381284	0.256092	-1.015482
6	-4.250821	-1.206178	0.907379
6	-5.575079	-0.351315	-1.391718
1	-3.983060	1.072035	-1.610253
6	-5.438108	-1.815192	0.526242
1	-3.717386	-1.519462	1.798540
6	-6.100856	-1.387485	-0.624157
1	-6.095249	-0.016091	-2.283178

1	-5.849086	-2.623814	1.121959
1	-7.029750	-1.863850	-0.922702

[6-7]TS-syn_conf-2

Number of imaginary frequencies : 1
The smallest frequency is : -1204.2827

Electronic energy=	-1054.9758103
Zero-point correction=	0.384876
Thermal correction to Energy=	0.406064
Thermal correction to Enthalpy=	0.407008
Thermal correction to Gibbs Free Energy=	0.333720
Sum of electronic and zero-point Energies=	-1054.590935
Sum of electronic and thermal Energies=	-1054.569746
Sum of electronic and thermal Enthalpies=	-1054.568802
Sum of electronic and thermal Free Energies=	-1054.642090

Cartesian Coordinates

6	4.271836	-2.362570	0.101957
6	4.679605	-0.902950	-0.075413
7	3.416218	-0.250645	-0.459089
6	2.408000	-1.222786	-0.930016
6	3.190597	-2.543291	-0.969793
6	3.140587	1.012345	-0.232047
6	1.867525	1.596244	-0.379670
6	1.698819	3.111078	-0.427207
6	1.223185	-1.256622	0.083110
8	0.083652	-1.108158	-0.362371
8	1.588245	-1.380865	1.296695
1	2.027128	-0.913792	-1.907250
1	2.539868	-3.397798	-0.774176
1	3.647467	-2.677979	-1.955660
1	3.827659	-2.498258	1.089240
1	5.116474	-3.042818	-0.021824
1	5.078002	-0.440714	0.829793
1	5.405730	-0.786944	-0.888354
1	1.365782	1.248979	0.841986
1	1.106746	-0.122264	1.895454
8	0.906604	0.892483	1.997509
1	1.921542	3.550357	0.553339
1	1.187514	1.042943	-1.029571
1	2.372307	3.585796	-1.150185
1	-0.071538	0.972216	2.011733
1	3.960020	1.594090	0.193426
6	0.245647	3.458696	-0.822721
1	0.092978	4.539109	-0.732455
1	0.086921	3.181403	-1.870667
6	-0.714754	2.706109	0.044622
6	-1.396803	1.627257	-0.351987
1	-0.776086	3.002177	1.093189
1	-1.364657	1.290761	-1.384597
6	-2.140597	0.794600	0.624583
8	-1.852550	0.817761	1.818256
6	-3.247325	-0.076170	0.141890
6	-3.897482	0.167076	-1.070603
6	-3.653921	-1.144306	0.947068
6	-4.950604	-0.648910	-1.471757
1	-3.596831	1.004891	-1.692348
6	-4.694411	-1.966986	0.537315
1	-3.133830	-1.318277	1.883073
6	-5.345208	-1.717678	-0.670993
1	-5.461533	-0.452266	-2.408739
1	-4.999602	-2.804431	1.156368
1	-6.161355	-2.359248	-0.988889

[6-7]TS-syn_conf-3

Number of imaginary frequencies : 1
The smallest frequency is : -1387.3435

Electronic energy= -1054.9736927
Zero-point correction= 0.383652
Thermal correction to Energy= 0.404939
Thermal correction to Enthalpy= 0.405883
Thermal correction to Gibbs Free Energy= 0.333075
Sum of electronic and zero-point Energies= -1054.590041
Sum of electronic and thermal Energies= -1054.568754
Sum of electronic and thermal Enthalpies= -1054.567810
Sum of electronic and thermal Free Energies= -1054.640618

Cartesian Coordinates

6	-0.850779	-2.871416	-1.256900
6	-0.610698	-1.533398	-1.946042
7	-1.562235	-0.638455	-1.262332
6	-2.636847	-1.387104	-0.588938
6	-2.358622	-2.846452	-0.986358
6	-1.372139	0.655147	-1.125420
6	-2.126011	1.551304	-0.337978
6	-1.964526	3.051158	-0.597996
6	-2.546205	-1.147978	0.933852
8	-3.558653	-0.825421	1.542128
8	-1.353428	-1.231579	1.421000
1	-3.611681	-1.026427	-0.927678
1	-2.665066	-3.540167	-0.200890
1	-2.915059	-3.093466	-1.895745
1	-0.304983	-2.892265	-0.311257
1	-0.539987	-3.715599	-1.874675
1	0.406828	-1.153463	-1.830758
1	-0.861913	-1.580513	-3.011893
1	-1.616636	1.317295	0.957721
1	-1.234830	-0.053475	1.993812
8	-1.271620	1.054721	2.129116
1	-1.860120	3.262400	-1.669466
1	-3.145727	1.222784	-0.124385
1	-2.882888	3.552175	-0.279219
1	-2.049982	1.209864	2.685912
1	-0.490636	1.028797	-1.646759
6	-0.782052	3.707086	0.155707
1	-0.812046	4.787974	-0.019162
1	-0.898516	3.533624	1.230225
6	0.526205	3.149950	-0.307418
6	1.197891	2.189675	0.335900
1	0.907375	3.486131	-1.273160
1	0.831433	1.806609	1.284865
6	2.407476	1.571460	-0.268869
8	3.098824	2.164788	-1.080394
6	2.731789	0.164422	0.130184
6	1.763254	-0.683785	0.677456
6	4.026420	-0.313506	-0.093699
6	2.095783	-1.994518	1.012250
1	0.738112	-0.353357	0.824706
6	4.357654	-1.617901	0.250111
1	4.758259	0.357360	-0.532373
6	3.392371	-2.458701	0.806187
1	1.336600	-2.639624	1.443902
1	5.366928	-1.983060	0.088074
1	3.653398	-3.477145	1.077543

[6-7]TS-syn_conf-4

Number of imaginary frequencies : 1
The smallest frequency is : -1318.2567

Electronic energy= -1054.9725483
Zero-point correction= 0.384161
Thermal correction to Energy= 0.405512
Thermal correction to Enthalpy= 0.406456
Thermal correction to Gibbs Free Energy= 0.332796
Sum of electronic and zero-point Energies= -1054.588387
Sum of electronic and thermal Energies= -1054.567037
Sum of electronic and thermal Enthalpies= -1054.566093
Sum of electronic and thermal Free Energies= -1054.639752

Cartesian Coordinates

6	0.190814	-2.820390	-1.181370
6	-0.163255	-1.364065	-1.462993
7	0.668955	-0.626639	-0.495046
6	1.112018	-1.490365	0.614604
6	0.400583	-2.823905	0.336520
6	1.159536	0.572831	-0.719039
6	2.123618	1.261123	0.049197
6	2.239548	2.763483	-0.144561
6	2.654983	-1.610446	0.558099
8	3.300487	-1.384516	1.578965
8	3.120219	-1.851716	-0.612346
1	0.834938	-1.043493	1.574318
1	0.992895	-3.672571	0.684817
1	-0.565980	-2.840697	0.849142
1	1.124844	-3.077034	-1.684766
1	-0.599622	-3.501607	-1.502283
1	0.069567	-1.036915	-2.478029
1	-1.220749	-1.166174	-1.250758
1	3.333193	0.727974	-0.421187
1	4.007521	-0.830167	-0.749489
8	4.426117	0.176884	-0.678712
1	3.234933	3.098316	0.165355
1	2.213773	0.926085	1.086325
1	2.150641	3.007867	-1.210672
1	4.891689	0.150037	0.171779
1	0.817495	1.028807	-1.649864
6	1.188615	3.575019	0.656061
1	1.267318	3.304544	1.714686
1	1.412288	4.642678	0.561843
6	-0.183028	3.281443	0.145585
6	-0.976779	2.331132	0.651475
1	-0.512731	3.791874	-0.759776
1	-0.657630	1.777967	1.529418
6	-2.218113	1.936053	-0.061122
8	-2.717091	2.654461	-0.911557
6	-2.794180	0.575114	0.207074
6	-2.394445	-0.234125	1.276028
6	-3.743877	0.089832	-0.699943
6	-2.937446	-1.507532	1.431665
1	-1.676707	0.119691	2.007929
6	-4.271642	-1.186729	-0.553497
1	-4.046462	0.731703	-1.520659
6	-3.866293	-1.989697	0.512584
1	-2.634997	-2.122009	2.273977
1	-5.000036	-1.557997	-1.267264
1	-4.280665	-2.985972	0.631462

[6-7]TS-syn_conf-5

Number of imaginary frequencies : 1

The smallest frequency is : -1264.1884

Electronic energy= -1054.9711966
Zero-point correction= 0.383778
Thermal correction to Energy= 0.405319
Thermal correction to Enthalpy= 0.406263
Thermal correction to Gibbs Free Energy= 0.331965
Sum of electronic and zero-point Energies= -1054.587419
Sum of electronic and thermal Energies= -1054.565878
Sum of electronic and thermal Enthalpies= -1054.564934
Sum of electronic and thermal Free Energies= -1054.639232

Cartesian Coordinates

6	4.928460	-1.387800	0.486448
6	4.838739	0.066844	0.035863
7	3.450435	0.176752	-0.447612
6	2.857656	-1.142608	-0.729855
6	4.036377	-2.108747	-0.529505
6	2.767221	1.297178	-0.452413
6	1.382257	1.444632	-0.672896
6	0.859539	2.835435	-1.045878
6	1.695488	-1.411092	0.260530
8	0.641456	-1.844992	-0.202418
8	1.951655	-1.098126	1.473303
1	2.454129	-1.157935	-1.745686
1	3.696261	-3.086399	-0.182568
1	4.567903	-2.247120	-1.476319
1	4.501251	-1.488276	1.486060
1	5.956629	-1.753746	0.489006
1	5.013469	0.790814	0.833551
1	5.525591	0.270534	-0.793571
1	0.943480	1.175751	0.613325
1	1.049095	-0.112058	1.800573
8	0.514633	0.822790	1.752506
1	1.704828	3.511625	-1.216047
1	0.910134	0.603106	-1.184471
1	0.327940	2.776385	-2.002470
1	-0.433602	0.645676	1.667487
1	3.344707	2.179885	-0.172001
6	-0.052631	3.498354	-0.008575
1	0.466211	3.554295	0.959301
1	-0.234665	4.541511	-0.299624
6	-1.386626	2.859689	0.225431
6	-1.843065	1.724594	-0.314101
1	-2.050515	3.376631	0.918965
1	-1.244724	1.137236	-1.004296
6	-3.202951	1.224766	0.041516
8	-4.068174	1.981071	0.450403
6	-3.466277	-0.241042	-0.094200
6	-2.425432	-1.171227	-0.159803
6	-4.793693	-0.682778	-0.098168
6	-2.710754	-2.531977	-0.232222
1	-1.381499	-0.871720	-0.129267
6	-5.075856	-2.038889	-0.189330
1	-5.587259	0.054330	-0.028236
6	-4.033192	-2.965300	-0.256119
1	-1.888055	-3.238643	-0.266650
1	-6.106561	-2.379156	-0.203191
1	-4.255899	-4.026135	-0.321280

[6-7]TS-syn_conf-6

Number of imaginary frequencies : 1
The smallest frequency is : -1313.9650

Electronic energy= -1054.9677453

Zero-point correction= 0.383167
 Thermal correction to Energy= 0.405098
 Thermal correction to Enthalpy= 0.406042
 Thermal correction to Gibbs Free Energy= 0.328749
 Sum of electronic and zero-point Energies= -1054.584578
 Sum of electronic and thermal Energies= -1054.562648
 Sum of electronic and thermal Enthalpies= -1054.561703
 Sum of electronic and thermal Free Energies= -1054.638996

Cartesian Coordinates

6	-6.310730	-0.385357	1.486419
6	-5.096535	-1.284468	1.696591
7	-4.239659	-0.964572	0.540120
6	-4.995268	-0.297185	-0.536045
6	-6.447498	-0.358020	-0.039893
6	-2.928472	-1.037566	0.564737
6	-2.029858	-0.558274	-0.409336
6	-0.604086	-1.090664	-0.374594
6	-4.460676	1.149893	-0.676430
8	-4.147201	1.553061	-1.793335
8	-4.302385	1.763574	0.439087
1	-4.837268	-0.816253	-1.484871
1	-7.029470	0.492130	-0.401323
1	-6.923529	-1.276173	-0.398354
1	-6.090118	0.618470	1.854214
1	-7.199547	-0.772807	1.987603
1	-4.555910	-1.091817	2.625082
1	-5.373215	-2.344100	1.654351
1	-1.941157	0.790721	-0.057278
1	-2.992991	2.118691	0.347246
8	-1.927291	2.042497	0.114212
1	-0.301690	-1.274616	0.663808
1	-2.449776	-0.422508	-1.409546
1	-0.534721	-2.054996	-0.895013
1	-1.880561	2.409189	-0.782774
1	-2.518707	-1.455815	1.485523
6	0.393776	-0.112155	-1.014078
1	0.058129	0.106226	-2.037748
1	0.394694	0.833616	-0.461292
6	1.772459	-0.686489	-1.065357
6	2.847609	-0.157674	-0.474106
1	1.906140	-1.621509	-1.610891
1	2.764464	0.764904	0.092105
6	4.164583	-0.845200	-0.557758
8	4.268729	-1.955166	-1.054388
6	5.375271	-0.159860	0.002985
6	5.409593	1.208338	0.286934
6	6.518101	-0.935804	0.223628
6	6.570111	1.789517	0.790480
1	4.543795	1.833593	0.096177
6	7.671078	-0.357883	0.737417
1	6.476792	-1.993534	-0.014750
6	7.697875	1.007227	1.022155
1	6.592726	2.853860	1.001182
1	8.551091	-0.967632	0.916304
1	8.599623	1.460395	1.422299

[6-7]TS-syn_conf-7

Number of imaginary frequencies : 1
 The smallest frequency is : -1295.5559

Electronic energy= -1054.967479
 Zero-point correction= 0.383582
 Thermal correction to Energy= 0.405423
 Thermal correction to Enthalpy= 0.406367

Thermal correction to Gibbs Free Energy=	0.329136
Sum of electronic and zero-point Energies=	-1054.583897
Sum of electronic and thermal Energies=	-1054.562056
Sum of electronic and thermal Enthalpies=	-1054.561112
Sum of electronic and thermal Free Energies=	-1054.638343

Cartesian Coordinates

6	3.586200	-2.826301	-0.893816
6	3.196863	-1.697176	-1.843708
7	2.436384	-0.778422	-0.977457
6	1.999009	-1.431431	0.269405
6	2.380821	-2.902181	0.049621
6	2.365420	0.518212	-1.168552
6	1.851845	1.479366	-0.272665
6	1.488636	2.836719	-0.851372
6	2.756200	-0.776803	1.454467
8	2.109973	-0.430105	2.438688
8	4.004948	-0.579840	1.237113
1	0.926930	-1.275710	0.417811
1	2.606324	-3.402408	0.993479
1	1.552191	-3.433385	-0.429515
1	4.475602	-2.538350	-0.330851
1	3.774445	-3.761564	-1.424025
1	4.047725	-1.175431	-2.285655
1	2.541441	-2.059273	-2.644175
1	2.939302	1.698110	0.566004
1	4.099572	0.767400	1.461080
8	3.839925	1.823217	1.443532
1	1.466145	3.582436	-0.048446
1	1.156212	1.093032	0.476564
1	2.269275	3.160549	-1.549802
1	3.364138	1.946733	2.279404
1	2.828576	0.865561	-2.094603
6	0.132292	2.849117	-1.586166
1	-0.022327	3.842036	-2.026608
1	0.155124	2.121356	-2.406051
6	-0.999634	2.545333	-0.659078
6	-1.765317	1.450989	-0.706327
1	-1.196035	3.262758	0.138850
1	-1.599357	0.696642	-1.470146
6	-2.836871	1.242018	0.306092
8	-2.953342	1.988253	1.263881
6	-3.772132	0.081458	0.141633
6	-3.940768	-0.589209	-1.072987
6	-4.521208	-0.314887	1.254688
6	-4.843373	-1.644625	-1.170385
1	-3.391093	-0.278780	-1.955467
6	-5.411567	-1.376008	1.160061
1	-4.385199	0.223321	2.186956
6	-5.573639	-2.042998	-0.054091
1	-4.977741	-2.153575	-2.119503
1	-5.982340	-1.683775	2.030400
1	-6.272292	-2.870486	-0.130131

[6-7]TS-syn_conf-8

Number of imaginary frequencies : 1
The smallest frequency is : -1315.6727

Electronic energy=	-1054.9694002
Zero-point correction=	0.384541
Thermal correction to Energy=	0.405983
Thermal correction to Enthalpy=	0.406927
Thermal correction to Gibbs Free Energy=	0.331642
Sum of electronic and zero-point Energies=	-1054.584860
Sum of electronic and thermal Energies=	-1054.563418

Sum of electronic and thermal Enthalpies= -1054.562473
 Sum of electronic and thermal Free Energies= -1054.637758

Cartesian Coordinates

```

6 -5.117912 -1.764000 -0.106963
6 -5.133949 -0.246364 -0.261783
7 -3.803425 0.153954 0.230329
6 -3.175968 -0.906134 1.040325
6 -4.285376 -1.961211 1.164200
6 -3.161316 1.214630 -0.204020
6 -1.817587 1.564242 0.037259
6 -1.415377 3.013987 -0.208247
6 -1.927183 -1.416575 0.280292
8 -0.859382 -1.477382 0.888688
8 -2.113621 -1.624373 -0.969683
1 -2.850056 -0.501910 2.002139
1 -3.871189 -2.967284 1.253903
1 -4.890414 -1.759161 2.053786
1 -4.602332 -2.213133 -0.957866
1 -6.124202 -2.179024 -0.027041
1 -5.268376 0.094109 -1.290112
1 -5.902770 0.210213 0.372091
1 -1.128175 0.782525 -0.900512
1 -1.081746 -0.853645 -1.482031
8 -0.392736 -0.019586 -1.543543
1 -2.119329 3.478371 -0.908900
1 -1.364378 1.099481 0.917586
1 -1.483519 3.586996 0.725309
1 0.247887 -0.260891 -0.851622
1 -3.744814 1.841396 -0.880718
6 0.002262 3.171473 -0.782561
1 0.054437 2.724950 -1.781545
1 0.212719 4.243781 -0.889967
6 1.054375 2.567074 0.092919
6 1.964185 1.679693 -0.322703
1 1.078853 2.870795 1.140704
1 1.972392 1.360549 -1.360985
6 2.989346 1.141257 0.612425
8 3.174030 1.647718 1.706657
6 3.800215 -0.042620 0.178678
6 3.444300 -0.843013 -0.911191
6 4.940017 -0.364491 0.923324
6 4.220512 -1.946906 -1.252285
1 2.551375 -0.631022 -1.490655
6 5.720323 -1.458736 0.575008
1 5.194446 0.258969 1.774149
6 5.360914 -2.251696 -0.514915
1 3.931591 -2.569044 -2.092981
1 6.606955 -1.699102 1.152996
1 5.967606 -3.110287 -0.785542
  
```

[7]-syn_conf-1

Number of imaginary frequencies : 0

Electronic energy= -1055.0080115
 Zero-point correction= 0.389659
 Thermal correction to Energy= 0.412480
 Thermal correction to Enthalpy= 0.413424
 Thermal correction to Gibbs Free Energy= 0.335878
 Sum of electronic and zero-point Energies= -1054.618353
 Sum of electronic and thermal Energies= -1054.595531
 Sum of electronic and thermal Enthalpies= -1054.594587
 Sum of electronic and thermal Free Energies= -1054.672134

Cartesian Coordinates

6	4.356310	-2.352155	0.017531
6	4.703202	-0.872009	-0.185911
7	3.470529	-0.274241	-0.705992
6	2.414394	-1.250749	-0.904217
6	3.170872	-2.586615	-0.927298
6	3.164137	1.049084	-0.491740
6	1.970716	1.632336	-0.716130
6	1.684927	3.102813	-0.500406
6	1.385869	-1.158555	0.227699
8	0.192894	-1.055558	0.045500
8	1.960819	-1.159846	1.428453
1	1.865740	-1.066591	-1.834250
1	2.540645	-3.427503	-0.628693
1	3.521510	-2.769101	-1.947370
1	4.047826	-2.522164	1.050402
1	5.200936	-3.007442	-0.205111
1	5.003224	-0.393201	0.752339
1	5.518538	-0.745852	-0.909731
1	1.107663	1.252646	1.608480
1	1.359300	-0.665961	2.046608
8	0.730820	0.899343	2.429616
1	1.913618	3.407921	0.529865
1	1.155612	1.032993	-1.114093
1	2.305666	3.732302	-1.149792
1	-0.233735	0.896428	2.274491
1	4.000327	1.638469	-0.115430
6	0.206476	3.427643	-0.797411
1	0.034876	4.498147	-0.641444
1	-0.004923	3.202971	-1.848649
6	-0.704231	2.629731	0.082071
6	-1.450139	1.601665	-0.336541
1	-0.710445	2.875494	1.145511
1	-1.470532	1.327628	-1.387809
6	-2.228006	0.772680	0.615441
8	-1.985665	0.781680	1.818027
6	-3.324204	-0.092213	0.090888
6	-3.943044	0.151036	-1.138573
6	-3.751931	-1.162774	0.882370
6	-4.981547	-0.668872	-1.569461
1	-3.634673	0.992703	-1.750928
6	-4.776831	-1.989536	0.443022
1	-3.261066	-1.332968	1.834692
6	-5.393869	-1.741438	-0.782899
1	-5.468248	-0.471372	-2.519083
1	-5.096983	-2.827727	1.053458
1	-6.198137	-2.385534	-1.124906

Stationary Points Relevant to Fig. S7 and Table S6

Conformational Analysis of the Transition States Involved in Enamine Formation in Proline Cinchona-Thiourea Dual Catalytic Pathway

[2-3]TS_Cinchona-Thiourea_conf-1

Number of imaginary frequencies : 1

The smallest frequency is : -76.5173

Electronic energy= -3467.7312633

Zero-point correction= 0.940266

Thermal correction to Energy= 0.998557

Thermal correction to Enthalpy= 0.999501

Thermal correction to Gibbs Free Energy= 0.841638

Sum of electronic and zero-point Energies= -3466.790997

Sum of electronic and thermal Energies= -3466.732706

Sum of electronic and thermal Enthalpies= -3466.731762

Sum of electronic and thermal Free Energies= -3466.889625

..... Cartesian Coordinates			
6	-1.309236	-4.755788	-1.605714
6	-2.654723	-5.005138	-0.887058
6	-2.857342	-3.755277	0.012592
7	-1.770430	-2.825637	-0.328944
6	-0.648731	-3.670524	-0.748147
6	-0.921728	-1.542768	1.034161
6	0.405319	-2.801397	-1.441620
8	-0.036228	-1.866013	-2.164450
8	-0.030794	-2.184896	1.624884
8	1.611633	-3.050591	-1.210600
1	-0.204584	-4.092997	0.160192
1	-1.474545	-4.353366	-2.610648
1	-0.696146	-5.654947	-1.694389
1	-2.615624	-5.911098	-0.277463
1	-3.472435	-5.125213	-1.600816
1	-2.754232	-4.017577	1.071272
1	-3.822855	-3.264537	-0.125887
1	1.722127	-2.097657	0.899974
1	-2.023682	-2.249122	-1.132943
7	0.396007	0.778327	-1.352373
6	-0.835902	1.427865	-1.185099
6	-1.021597	2.706058	-0.647515
6	-2.316697	3.198357	-0.509439
6	-3.439117	2.474622	-0.898485
6	-3.231988	1.218482	-1.456387
6	-1.954734	0.699646	-1.611144
6	-2.517029	4.529171	0.157938
9	-3.579633	5.180405	-0.332154
6	-4.394317	0.343887	-1.824322
9	-5.535617	1.024329	-1.943140
6	1.526115	0.830531	-0.588975
16	1.962525	2.095297	0.439576
7	2.262653	-0.299168	-0.726052
6	3.623389	-0.483315	-0.258334
6	3.768917	-1.867087	0.403461
6	5.106523	-2.033032	1.157850
6	4.828812	-2.272984	2.649290
6	4.043269	-3.586256	2.793099
6	2.778712	-3.513870	1.914754
7	2.649154	-2.126214	1.369468
6	2.606659	-1.135207	2.489000
6	3.968341	-1.133912	3.230377
6	4.602233	0.237578	3.216715
6	5.896952	0.514194	3.082195
6	4.619008	-0.404213	-1.411096
6	5.760306	0.456044	-1.387318
6	6.635242	0.399558	-2.512995
7	6.422032	-0.408732	-3.589638
6	5.355692	-1.169738	-3.576475
6	4.428325	-1.207904	-2.507711
6	7.788669	1.221046	-2.522749
6	8.077794	2.059588	-1.476858
6	7.202730	2.117097	-0.361755
6	6.066992	1.336343	-0.324525
9	-2.728519	4.382141	1.480808
9	-1.452171	5.329727	0.023409
9	-4.597320	-0.608302	-0.883364
9	-4.182333	-0.313313	-2.974798
1	3.636838	-2.630252	-0.363549
1	5.663154	-2.879437	0.746220
1	5.721924	-1.141334	1.018289
1	1.855205	-3.708758	2.462083
1	2.811808	-4.173314	1.045300
1	3.771179	-3.746269	3.840365
1	4.663693	-4.430731	2.482705
1	5.771132	-2.344916	3.198610

1	3.764743	-1.380358	4.280757
1	1.771843	-1.441997	3.119421
1	2.360261	-0.160990	2.056636
1	3.903739	1.063388	3.356101
1	6.252994	1.539334	3.103920
1	6.650237	-0.256771	2.940328
1	3.820716	0.301033	0.473496
1	3.573360	-1.879967	-2.563687
1	5.421028	1.433800	0.540407
1	5.196038	-1.806633	-4.444398
1	8.437256	1.162922	-3.390778
1	8.969014	2.674670	-1.511628
1	1.909533	-1.047444	-1.328538
1	0.295238	-0.108153	-1.867208
1	-0.172888	3.301275	-0.342547
1	-1.803924	-0.277671	-2.064737
1	-4.440905	2.866569	-0.759989
8	7.415937	2.917807	0.713003
6	8.526884	3.794092	0.681577
1	8.486460	4.363936	1.610010
1	9.474307	3.244014	0.640885
1	8.469292	4.486013	-0.166436
6	-2.172354	-1.086961	1.746928
1	-2.954869	-0.868528	1.012695
1	-2.522978	-1.887450	2.409827
1	-0.643380	-0.901172	0.179972
6	-1.853711	0.172186	2.560372
6	-3.082935	0.716218	3.310369
1	-1.455994	0.949523	1.892457
1	-1.065165	-0.055720	3.285383
1	-3.491462	-0.071399	3.954142
1	-2.765510	1.543083	3.955329
6	-4.134449	1.205257	2.365474
6	-5.256057	0.540493	2.068303
1	-3.945543	2.150573	1.856093
1	-5.475062	-0.405320	2.555799
6	-6.213553	1.077480	1.068018
8	-6.136878	2.233190	0.677615
6	-7.289959	0.179003	0.537739
6	-7.261541	-1.209696	0.694290
6	-8.338030	0.767887	-0.176621
6	-8.276808	-1.995099	0.156596
1	-6.437985	-1.690285	1.212199
6	-9.355505	-0.015304	-0.704973
1	-8.332723	1.845186	-0.305304
6	-9.327006	-1.399368	-0.536772
1	-8.246218	-3.073353	0.276563
1	-10.170212	0.450314	-1.250359
1	-10.120566	-2.013639	-0.951120

[2-3]TS_Cinchona-Thiourea_conf-2

Number of imaginary frequencies : 1
The smallest frequency is : -39.6581

Electronic energy= -3467.7303115
Zero-point correction= 0.939908
Thermal correction to Energy= 0.997982
Thermal correction to Enthalpy= 0.998926
Thermal correction to Gibbs Free Energy= 0.841917
Sum of electronic and zero-point Energies= -3466.790403
Sum of electronic and thermal Energies= -3466.732330
Sum of electronic and thermal Enthalpies= -3466.731386
Sum of electronic and thermal Free Energies= -3466.888394

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

6	-0.340986	5.795004	-0.928782
6	0.817499	6.430073	-0.151624
6	1.573398	5.218450	0.437219
7	0.634371	4.076077	0.369337
6	-0.679820	4.578604	-0.062410
6	0.197255	2.977829	2.150940
6	0.830108	1.672265	1.718998
6	2.344333	1.701313	1.542906
6	-1.419724	3.449229	-0.789692
8	-0.732298	2.807849	-1.631543
8	-1.028648	3.066783	2.294017
8	-2.617641	3.221026	-0.495692
1	0.864398	3.670802	2.700643
1	0.326128	1.328956	0.804443
1	-1.257320	4.857114	0.825071
1	-0.003654	5.441517	-1.909477
1	-1.188355	6.469628	-1.070688
1	0.424353	7.055289	0.655823
1	1.460337	7.055349	-0.774764
1	1.871082	5.393273	1.477238
1	2.476140	4.976988	-0.130571
1	-2.544088	2.111859	1.238274
1	0.935929	3.416084	-0.348133
1	0.569786	0.948041	2.505698
1	2.805877	2.269444	2.361379
1	2.609616	2.220504	0.614084
6	2.919320	0.284610	1.503036
1	2.314599	-0.311511	0.803106
1	2.807540	-0.205335	2.477615
6	4.339412	0.201212	1.036226
6	5.179844	-0.804711	1.300458
1	4.693858	0.989793	0.371169
1	4.885285	-1.623068	1.950820
6	6.501350	-0.862215	0.626862
8	6.743926	-0.177030	-0.356724
6	7.538168	-1.801898	1.161832
6	7.469399	-2.326715	2.455228
6	8.619346	-2.134731	0.339564
6	8.468354	-3.177394	2.918894
1	6.648560	-2.057342	3.112062
6	9.609122	-2.993856	0.798487
1	8.661487	-1.709397	-0.657893
6	9.533992	-3.516594	2.089492
1	8.413830	-3.575817	3.926917
1	10.441250	-3.257708	0.153547
1	10.308115	-4.187438	2.449255
7	-0.362599	0.116190	-1.487455
6	1.001812	-0.166147	-1.629455
6	1.612894	-1.408501	-1.436209
6	3.000059	-1.506043	-1.549095
6	3.800043	-0.426211	-1.893276
6	3.168441	0.791947	-2.127366
6	1.796498	0.932484	-1.995668
6	3.630750	-2.817771	-1.178644
9	3.209774	-3.820623	-1.964431
6	3.977603	2.021748	-2.417998
9	4.079577	2.807177	-1.319751
6	-1.322850	-0.456243	-0.713278
16	-1.227465	-1.963030	0.040967
7	-2.388446	0.373579	-0.562727
6	-3.687972	-0.032537	-0.066707
6	-4.316086	1.099917	0.767288
6	-5.554986	0.622369	1.559116
6	-5.265520	0.706303	3.066381
6	-5.063268	2.182312	3.436755
6	-3.987360	2.782891	2.513540
7	-3.331415	1.672074	1.746721
6	-2.791859	0.641866	2.685704
6	-3.970206	-0.054171	3.416864
6	-3.996135	-1.541038	3.147884

6	-5.080287	-2.302993	3.025691
6	-4.645180	-0.371586	-1.206558
6	-5.325239	-1.626146	-1.291771
6	-6.250402	-1.790773	-2.365186
7	-6.478472	-0.836100	-3.311137
6	-5.807634	0.285358	-3.216773
6	-4.887417	0.567166	-2.178086
6	-6.972880	-3.004617	-2.464215
6	-6.796795	-4.017131	-1.555985
6	-5.862453	-3.856739	-0.500946
6	-5.139990	-2.689172	-0.378851
9	4.968204	-2.781640	-1.254368
9	3.313788	-3.160795	0.082934
9	3.410654	2.782236	-3.365913
9	5.220854	1.736577	-2.808565
1	-4.547343	1.937964	0.106831
1	-6.419900	1.245834	1.316292
1	-5.802545	-0.401849	1.269851
1	-3.185579	3.292648	3.045826
1	-4.392282	3.464198	1.763225
1	-4.758616	2.268026	4.483950
1	-6.000635	2.732166	3.321275
1	-6.104221	0.292253	3.631877
1	-3.798731	0.073183	4.493732
1	-2.127098	1.183153	3.359193
1	-2.190682	-0.057890	2.097144
1	-3.015363	-2.012291	3.072761
1	-4.995116	-3.370650	2.848572
1	-6.088947	-1.901435	3.085040
1	-3.534883	-0.905781	0.568247
1	-4.382950	1.531383	-2.160234
1	-4.416192	-2.628674	0.424813
1	-5.991388	1.034175	-3.984608
1	-7.672523	-3.104836	-3.287530
1	-7.364137	-4.934596	-1.657104
1	-2.357468	1.303568	-0.991316
1	-0.585853	1.088157	-1.759398
1	1.023216	-2.272675	-1.161287
1	1.320988	1.896825	-2.163389
1	4.880926	-0.512108	-1.929182
8	-5.621011	-4.811387	0.433311
6	-6.306103	-6.044496	0.320056
1	-5.953507	-6.661399	1.146858
1	-7.390866	-5.912770	0.409108
1	-6.075060	-6.547310	-0.626012

[2-3]TS_Cinchona-Thiourea_conf-3

Number of imaginary frequencies : 1

The smallest frequency is : -121.5673

Electronic energy=	-3467.7302479
Zero-point correction=	0.940280
Thermal correction to Energy=	0.998001
Thermal correction to Enthalpy=	0.998945
Thermal correction to Gibbs Free Energy=	0.843934
Sum of electronic and zero-point Energies=	-3466.789968
Sum of electronic and thermal Energies=	-3466.732247
Sum of electronic and thermal Enthalpies=	-3466.731303
Sum of electronic and thermal Free Energies=	-3466.886314

Cartesian Coordinates

6	2.992266	-2.165821	-4.217360
6	4.470353	-2.059875	-3.790481
6	4.499899	-0.779023	-2.953848
7	3.223784	-0.811755	-2.223070

6	2.217178	-1.289324	-3.191615
6	2.365110	0.706540	-1.186022
6	3.526519	1.016698	-0.251307
6	4.587072	1.934087	-0.862740
6	1.128169	-2.058689	-2.434738
8	1.543353	-2.885593	-1.581906
8	1.308468	0.227177	-0.729916
8	-0.069874	-1.807559	-2.709771
1	2.341440	1.306983	-2.119515
1	3.962717	0.067975	0.075629
1	1.766614	-0.416888	-3.677391
1	2.641341	-3.199737	-4.196484
1	2.843199	-1.780755	-5.228959
1	5.160670	-2.034563	-4.636691
1	4.743561	-2.905171	-3.151024
1	4.502956	0.107786	-3.599615
1	5.338437	-0.712978	-2.257362
1	-0.322654	0.154638	-1.372135
1	3.273637	-1.532920	-1.494800
1	3.095780	1.475121	0.647501
1	4.690723	1.720840	-1.934078
1	5.562983	1.736025	-0.409456
6	4.267675	3.428159	-0.670423
1	5.060851	4.023688	-1.138769
1	4.265111	3.660501	0.400384
6	2.952526	3.806448	-1.271155
6	1.893784	4.236460	-0.574600
1	2.840501	3.703767	-2.351605
1	1.969004	4.378292	0.498991
6	0.620461	4.569876	-1.259618
8	0.485404	4.434108	-2.468833
6	-0.525921	5.075407	-0.437897
6	-0.643029	4.812620	0.931407
6	-1.552019	5.761949	-1.098188
6	-1.781591	5.216181	1.624327
1	0.128875	4.261328	1.458869
6	-2.678327	6.181075	-0.400595
1	-1.446844	5.953639	-2.161479
6	-2.797323	5.900944	0.960905
1	-1.877349	4.990662	2.681481
1	-3.467488	6.718754	-0.916233
1	-3.683080	6.213693	1.504754
7	0.835393	-2.173501	0.976939
6	2.041284	-1.807929	1.568848
6	2.224010	-0.795743	2.520037
6	3.510240	-0.481409	2.943046
6	4.639542	-1.133840	2.458804
6	4.441451	-2.137998	1.518857
6	3.170533	-2.481921	1.081202
6	3.694702	0.702364	3.846811
9	2.644999	0.901934	4.652172
6	5.603220	-2.804480	0.846460
9	5.684619	-2.419974	-0.448702
6	-0.405915	-1.615397	1.091845
16	-1.044512	-0.924379	2.496266
7	-1.091121	-1.720222	-0.065089
6	-2.428939	-1.231964	-0.329171
6	-2.379203	-0.334813	-1.585767
6	-3.679957	0.453940	-1.843617
6	-3.389348	1.959950	-1.762095
6	-2.392253	2.336376	-2.870613
6	-1.155432	1.422724	-2.765415
7	-1.241370	0.643679	-1.491650
6	-1.378802	1.578924	-0.332746
6	-2.742052	2.310560	-0.410137
6	-3.582700	2.048270	0.816295
6	-4.904601	1.897761	0.857780
6	-3.394430	-2.379442	-0.600425
6	-4.662384	-2.494468	0.049461
6	-5.485605	-3.596159	-0.330926

7	-5.115691	-4.526887	-1.255471
6	-3.939761	-4.390140	-1.816287
6	-3.046242	-3.331072	-1.526645
6	-6.756359	-3.740818	0.276509
6	-7.207009	-2.846577	1.213321
6	-6.384487	-1.754523	1.592054
6	-5.137928	-1.589706	1.026256
9	4.783830	0.584147	4.619762
9	3.854034	1.836404	3.130761
9	5.490366	-4.138497	0.834837
9	6.773914	-2.499335	1.417808
1	-2.113430	-0.964445	-2.435659
1	-4.075340	0.206248	-2.832700
1	-4.437731	0.168288	-1.109794
1	-0.224293	1.993257	-2.724184
1	-1.083559	0.684384	-3.566617
1	-2.084631	3.381500	-2.761710
1	-2.855828	2.223422	-3.853832
1	-4.314436	2.528411	-1.890846
1	-2.532283	3.386775	-0.419822
1	-0.526030	2.258456	-0.401096
1	-1.261923	0.993049	0.582737
1	-3.023288	2.014519	1.752321
1	-5.419037	1.735997	1.799861
1	-5.524179	1.919146	-0.035328
1	-2.747527	-0.653677	0.539923
1	-2.089880	-3.278587	-2.044379
1	-4.542073	-0.748820	1.361901
1	-3.655166	-5.142651	-2.549289
1	-7.361819	-4.588578	-0.026816
1	-8.184627	-2.983472	1.659885
1	-0.605018	-2.075138	-0.897418
1	1.002314	-2.621398	0.060360
1	1.373275	-0.252141	2.907602
1	3.041711	-3.248907	0.321698
1	5.634030	-0.861053	2.791406
8	-6.755133	-0.824460	2.509199
6	-8.005461	-0.984109	3.151906
1	-8.090224	-0.155208	3.854994
1	-8.835832	-0.934191	2.437650
1	-8.056019	-1.928926	3.705148

[2-3]TS_Cinchona-Thiourea_conf-4

Number of imaginary frequencies : 1

The smallest frequency is : -127.1023

Electronic energy=	-3467.7302513
Zero-point correction=	0.940031
Thermal correction to Energy=	0.997552
Thermal correction to Enthalpy=	0.998496
Thermal correction to Gibbs Free Energy=	0.844252
Sum of electronic and zero-point Energies=	-3466.790221
Sum of electronic and thermal Energies=	-3466.732700
Sum of electronic and thermal Enthalpies=	-3466.731756
Sum of electronic and thermal Free Energies=	-3466.885999

Cartesian Coordinates

6	-3.333472	-4.027357	2.592085
6	-4.783883	-3.730223	2.157767
6	-4.798303	-2.207754	1.997997
7	-3.472950	-1.910304	1.436576
6	-2.514170	-2.787655	2.132358
6	-2.624710	-0.111182	1.304232
6	-1.364955	-3.121248	1.170532
8	-1.699413	-3.363362	-0.017621

8	-1.425808	-0.337620	1.033509
8	-0.196711	-3.116981	1.630869
1	-2.102877	-2.242734	2.989253
1	-2.956080	-4.944379	2.134034
1	-3.261376	-4.143343	3.676215
1	-5.527374	-4.093643	2.870721
1	-4.989304	-4.189722	1.185877
1	-4.885710	-1.712759	2.973159
1	-5.583526	-1.831121	1.340275
1	0.163064	-0.879134	1.679103
1	-3.450735	-2.208648	0.456332
7	-0.855506	-1.332972	-1.705295
6	-2.035520	-0.636314	-1.959591
6	-2.159035	0.753660	-2.090957
6	-3.422488	1.319472	-2.211886
6	-4.587133	0.555032	-2.213620
6	-4.447397	-0.822457	-2.106427
6	-3.198263	-1.418484	-1.993128
6	-3.544996	2.809111	-2.364102
9	-4.619188	3.284030	-1.711008
6	-5.649988	-1.719243	-2.086433
9	-6.796652	-1.033189	-2.007376
6	0.381520	-0.838708	-1.391146
16	1.088915	0.531393	-2.083737
7	0.998969	-1.607902	-0.473694
6	2.316843	-1.381217	0.084693
6	2.212376	-1.387803	1.624209
6	3.490210	-0.893837	2.336923
6	3.175209	0.390878	3.120493
6	2.150929	0.055345	4.216709
6	0.941975	-0.651568	3.571152
7	1.059313	-0.539512	2.085303
6	1.189911	0.901444	1.698382
6	2.554053	1.447544	2.183646
6	3.430905	1.873917	1.028858
6	4.760153	1.820142	0.989048
6	3.292595	-2.472420	-0.338986
6	4.565271	-2.185291	-0.922870
6	5.396957	-3.300362	-1.241480
7	5.030146	-4.595666	-1.028632
6	3.849279	-4.813858	-0.505097
6	2.947094	-3.786013	-0.139477
6	6.672859	-3.061844	-1.806994
6	7.121028	-1.788535	-2.048529
6	6.289642	-0.682652	-1.735205
6	5.038002	-0.880616	-1.191902
9	-2.471559	3.457643	-1.880197
9	-3.679375	3.176995	-3.645853
9	-5.612545	-2.554740	-1.024868
9	-5.720006	-2.497423	-3.173847
1	1.936456	-2.394913	1.940163
1	3.854474	-1.663331	3.023301
1	4.278543	-0.714026	1.602028
1	-0.012139	-0.193232	3.840563
1	0.888350	-1.719169	3.792866
1	1.831111	0.971889	4.721098
1	2.601097	-0.596694	4.969408
1	4.087271	0.784628	3.576056
1	2.340672	2.347784	2.777348
1	0.342050	1.402810	2.170420
1	1.059311	0.973307	0.614598
1	2.897496	2.288707	0.171928
1	5.304181	2.176079	0.119187
1	5.357184	1.418423	1.804512
1	2.654542	-0.403378	-0.262443
1	1.984742	-4.048771	0.296693
1	4.437293	-0.002911	-0.985469
1	3.567955	-5.852831	-0.344732
1	7.283903	-3.926585	-2.044100
1	8.102096	-1.638680	-2.483099

1	0.472066	-2.367983	-0.028647
1	-1.065457	-2.228971	-1.239003
1	-1.276069	1.377265	-2.077001
1	-3.114109	-2.496480	-1.878916
1	-5.564160	1.017195	-2.292354
8	6.655317	0.608145	-1.944414
6	7.928299	0.858528	-2.508319
1	8.011832	1.942202	-2.593342
1	8.734637	0.487112	-1.864891
1	8.022701	0.414275	-3.505759
6	-3.010719	0.484592	2.656323
1	-3.270184	-0.304498	3.369937
1	-2.108526	0.974423	3.040518
1	-3.314177	0.148774	0.478033
6	-4.148943	1.499798	2.543161
6	-3.802110	2.677590	1.610323
1	-4.391870	1.884564	3.539765
1	-5.053017	1.007087	2.164574
1	-3.747960	2.337407	0.570505
1	-4.609578	3.417614	1.661473
6	-2.504854	3.317196	1.992982
6	-1.414579	3.331182	1.219834
1	-2.434740	3.768389	2.983899
1	-1.447424	2.886972	0.229917
6	-0.154066	3.947502	1.714022
8	0.009034	4.166143	2.906487
6	0.929165	4.289639	0.736249
6	0.846736	3.998409	-0.629430
6	2.075895	4.920492	1.235695
6	1.904593	4.320659	-1.477546
1	-0.033634	3.526741	-1.050793
6	3.124433	5.248833	0.388330
1	2.120329	5.142203	2.297017
6	3.041540	4.943526	-0.970995
1	1.836645	4.080331	-2.533632
1	4.010644	5.734390	0.784300
1	3.864153	5.192003	-1.634506

[2-3]TS_Cinchona-Thiourea_conf-5

Number of imaginary frequencies : 1
 The smallest frequency is : -116.9322

Electronic energy= -3467.7316145
 Zero-point correction= 0.940417
 Thermal correction to Energy= 0.997920
 Thermal correction to Enthalpy= 0.998864
 Thermal correction to Gibbs Free Energy= 0.845737
 Sum of electronic and zero-point Energies= -3466.791198
 Sum of electronic and thermal Energies= -3466.733694
 Sum of electronic and thermal Enthalpies= -3466.732750
 Sum of electronic and thermal Free Energies= -3466.885877

 Cartesian Coordinates

6	-2.995606	-4.380682	2.493386
6	-4.495055	-4.035185	2.337942
6	-4.513155	-2.502529	2.303948
7	-3.263065	-2.148518	1.620572
6	-2.243227	-3.062045	2.161602
6	-2.470830	-0.273282	1.540272
6	-3.697967	0.429016	0.962339
6	-4.626813	0.985074	2.047610
6	-1.126828	-3.223588	1.121810
8	-1.508268	-3.444045	-0.054283
8	-1.420163	-0.390868	0.885625
8	0.062578	-3.109473	1.514274

1	-2.428816	-0.264346	2.652223
1	-4.231701	-0.266753	0.310520
1	-1.827272	-2.607249	3.068051
1	-2.700707	-5.173872	1.802850
1	-2.757615	-4.711552	3.506691
1	-5.114548	-4.447809	3.137403
1	-4.875113	-4.415982	1.385142
1	-4.473555	-2.087409	3.318856
1	-5.372025	-2.072576	1.783603
1	0.255743	-0.879617	1.497690
1	-3.339533	-2.363903	0.620477
1	-3.328312	1.233738	0.316179
1	-4.508287	0.400599	2.969875
1	-5.674330	0.879935	1.750155
6	-4.366987	2.475566	2.342056
1	-5.003823	2.794720	3.175349
1	-4.655036	3.059236	1.460569
6	-2.934585	2.765792	2.667219
6	-2.116031	3.422383	1.837145
1	-2.533669	2.405504	3.615963
1	-2.491276	3.787413	0.885192
6	-0.696329	3.695684	2.176595
8	-0.246440	3.503248	3.298271
6	0.181340	4.219812	1.083500
6	-0.064956	3.913291	-0.259205
6	1.287249	5.005862	1.424655
6	0.784278	4.396243	-1.251463
1	-0.906301	3.282091	-0.532747
6	2.120319	5.505201	0.431080
1	1.470875	5.221754	2.472969
6	1.868498	5.201111	-0.907423
1	0.593365	4.144491	-2.289828
1	2.970979	6.124221	0.697384
1	2.523449	5.586396	-1.682628
7	-0.675225	-1.439463	-1.774906
6	-1.854194	-0.773416	-2.099619
6	-1.978975	0.598996	-2.346398
6	-3.239437	1.148281	-2.543895
6	-4.402302	0.384886	-2.512765
6	-4.260746	-0.977165	-2.274809
6	-3.016039	-1.557329	-2.075113
6	-3.346622	2.642313	-2.623364
9	-2.267099	3.208279	-3.179279
6	-5.461023	-1.851994	-2.077204
9	-5.567313	-2.219260	-0.775966
6	0.566365	-0.922459	-1.528450
16	1.256514	0.393566	-2.334021
7	1.209774	-1.621551	-0.570696
6	2.492811	-1.275246	0.005376
6	2.343261	-1.210017	1.541104
6	3.548594	-0.552811	2.247385
6	3.082242	0.706117	2.995969
6	2.068486	0.288610	4.073074
6	0.924395	-0.499736	3.403274
7	1.103613	-0.448391	1.920452
6	1.127815	0.974948	1.462378
6	2.377936	1.683434	2.034747
6	3.230848	2.244821	0.923912
6	4.560681	2.278338	0.878932
6	3.566756	-2.301108	-0.331126
6	4.858096	-1.929508	-0.817967
6	5.789881	-2.984942	-1.049664
7	5.500600	-4.300699	-0.842614
6	4.300671	-4.597536	-0.407914
6	3.301621	-3.633075	-0.132284
6	7.086953	-2.661137	-1.515569
6	7.461379	-1.361659	-1.742010
6	6.531138	-0.314737	-1.514736
6	5.256964	-0.596507	-1.070038
9	-4.421630	3.044745	-3.311510

9	-3.460091	3.180684	-1.384851
9	-5.389379	-2.988398	-2.780487
9	-6.606287	-1.242314	-2.401984
1	2.155943	-2.220511	1.909414
1	3.995918	-1.258078	2.953180
1	4.315607	-0.299791	1.511826
1	-0.057869	-0.067652	3.608113
1	0.904153	-1.557991	3.670287
1	1.670937	1.176543	4.572396
1	2.554274	-0.331822	4.830527
1	3.937284	1.198107	3.467090
1	2.013027	2.532457	2.629416
1	0.190845	1.402934	1.818489
1	1.099230	0.976968	0.369672
1	2.665924	2.682269	0.098844
1	5.077268	2.727080	0.036215
1	5.185827	1.863000	1.665793
1	2.768880	-0.293540	-0.383511
1	2.331194	-3.956591	0.239416
1	4.579864	0.238433	-0.928890
1	4.082899	-5.652079	-0.250326
1	7.776586	-3.481344	-1.685978
1	8.461836	-1.145698	-2.097460
1	0.706074	-2.366735	-0.069703
1	-0.878886	-2.306411	-1.249988
1	-1.100684	1.229163	-2.363495
1	-2.934107	-2.618242	-1.852324
1	-5.377511	0.836793	-2.650545
8	6.822309	0.996205	-1.712770
6	8.102828	1.325195	-2.215804
1	8.117208	2.410750	-2.315185
1	8.898437	1.018703	-1.526556
1	8.277136	0.873718	-3.199162

[2-3]TS_Cinchona-Thiourea_conf-6

Number of imaginary frequencies : 1
 The smallest frequency is : -127.4959

Electronic energy= -3467.730246
 Zero-point correction= 0.940347
 Thermal correction to Energy= 0.997761
 Thermal correction to Enthalpy= 0.998705
 Thermal correction to Gibbs Free Energy= 0.845318
 Sum of electronic and zero-point Energies= -3466.789899
 Sum of electronic and thermal Energies= -3466.732485
 Sum of electronic and thermal Enthalpies= -3466.731541
 Sum of electronic and thermal Free Energies= -3466.884927

 Cartesian Coordinates

6	-3.338086	-4.005576	2.616206
6	-4.787685	-3.709510	2.178808
6	-4.800504	-2.187774	2.012161
7	-3.474826	-1.894747	1.449043
6	-2.516716	-2.770489	2.147604
6	-2.623936	-0.099566	1.304826
6	-1.370140	-3.112645	1.185402
8	-1.706302	-3.353138	-0.002846
8	-1.424473	-0.330272	1.039401
8	-0.202251	-3.117170	1.645746
1	-2.102051	-2.221935	3.000552
1	-2.961698	-4.926874	2.165955
1	-3.267083	-4.113057	3.701295
1	-5.532300	-4.069195	2.892494
1	-4.992224	-4.173154	1.208698
1	-4.887276	-1.688314	2.985064

1	-5.585350	-1.813160	1.352798
1	0.161878	-0.873257	1.685004
1	-3.453594	-2.198148	0.470354
7	-0.866253	-1.327467	-1.700211
6	-2.046457	-0.632644	-1.958785
6	-2.172604	0.754156	-2.106398
6	-3.438379	1.317155	-2.232174
6	-4.600894	0.552320	-2.222847
6	-4.458613	-0.824724	-2.098474
6	-3.209377	-1.417102	-1.980976
6	-3.542522	2.806269	-2.403169
9	-4.729474	3.273225	-1.986191
6	-5.660756	-1.721899	-2.067825
9	-6.806114	-1.035404	-1.973350
6	0.369737	-0.833094	-1.383524
16	1.075100	0.542981	-2.066481
7	0.988117	-1.607250	-0.470633
6	2.307892	-1.386280	0.085546
6	2.207387	-1.396249	1.625137
6	3.490267	-0.913804	2.336603
6	3.185667	0.369483	3.126354
6	2.161140	0.036281	4.223087
6	0.945621	-0.658975	3.577082
7	1.061052	-0.541585	2.091453
6	1.201217	0.900002	1.710352
6	2.570415	1.434134	2.194775
6	3.447733	1.857762	1.039288
6	4.776420	1.794048	0.995809
6	3.278259	-2.480269	-0.343304
6	4.548269	-2.196729	-0.934668
6	5.374564	-3.314190	-1.258948
7	5.005131	-4.608476	-1.044393
6	3.826923	-4.823313	-0.513548
6	2.930058	-3.792902	-0.142072
6	6.647662	-3.079310	-1.832245
6	7.098262	-1.807242	-2.075816
6	6.272276	-0.698991	-1.756650
6	5.023388	-0.893377	-1.205774
9	-2.595229	3.457278	-1.701816
9	-3.398680	3.179929	-3.681934
9	-5.611680	-2.560932	-1.009669
9	-5.743975	-2.496209	-3.157069
1	1.925071	-2.402174	1.938787
1	3.851017	-1.688761	3.018683
1	4.277998	-0.735923	1.600619
1	-0.004455	-0.194567	3.850342
1	0.884278	-1.727109	3.794163
1	1.849123	0.952695	4.732537
1	2.608234	-0.622510	4.971717
1	4.101248	0.755019	3.581899
1	2.365429	2.333919	2.792131
1	0.358030	1.405863	2.186187
1	1.069094	0.977382	0.627140
1	2.915277	2.279588	0.185184
1	5.320804	2.148622	0.125596
1	5.372536	1.385148	1.808364
1	2.647858	-0.408887	-0.260508
1	1.969568	-4.053029	0.299768
1	4.426795	-0.013884	-0.995126
1	3.543469	-5.861493	-0.351801
1	7.254572	-3.945810	-2.073496
1	8.077163	-1.660047	-2.516142
1	0.461791	-2.370497	-0.031166
1	-1.076566	-2.222436	-1.232537
1	-1.290803	1.380218	-2.101127
1	-3.123139	-2.493553	-1.854277
1	-5.578199	1.012092	-2.305322
8	6.640712	0.590814	-1.967132
6	7.911025	0.837704	-2.538581
1	7.997206	1.921167	-2.623682

1	8.720149	0.463667	-1.900171
1	7.998155	0.393595	-3.536763
6	-3.012781	0.511333	2.649389
1	-3.283538	-0.268878	3.368494
1	-2.109517	0.997932	3.034932
1	-3.310409	0.154476	0.474268
6	-4.143005	1.533331	2.518514
6	-3.781114	2.701371	1.578885
1	-4.392549	1.927838	3.509673
1	-5.046724	1.043066	2.135796
1	-3.707626	2.348760	0.544139
1	-4.589604	3.441267	1.608887
6	-2.490272	3.346328	1.975105
6	-1.382840	3.333100	1.226910
1	-2.442052	3.826546	2.953671
1	-1.394973	2.858760	0.250847
6	-0.130608	3.960774	1.727025
8	0.019693	4.196561	2.917692
6	0.959337	4.294261	0.753484
6	0.874407	4.011158	-0.613875
6	2.111735	4.911241	1.256942
6	1.936274	4.326527	-1.459548
1	-0.012795	3.554520	-1.037935
6	3.164534	5.232346	0.411995
1	2.157092	5.128330	2.319208
6	3.079585	4.934348	-0.948809
1	1.866370	4.093391	-2.517121
1	4.055539	5.706561	0.810929
1	3.905405	5.177232	-1.610423

[2-3]TS_Cinchona-Thiourea_conf-7

Number of imaginary frequencies : 1

The smallest frequency is : -122.7668

Electronic energy=	-3467.7187485
Zero-point correction=	0.939549
Thermal correction to Energy=	0.997894
Thermal correction to Enthalpy=	0.998838
Thermal correction to Gibbs Free Energy=	0.838636
Sum of electronic and zero-point Energies=	-3466.779200
Sum of electronic and thermal Energies=	-3466.720855
Sum of electronic and thermal Enthalpies=	-3466.719911
Sum of electronic and thermal Free Energies=	-3466.880113

Cartesian Coordinates

6	-1.701624	0.455252	-4.474910
6	-2.813411	1.487048	-4.198295
6	-3.187729	1.216096	-2.738982
7	-1.904761	0.891411	-2.100394
6	-1.163156	0.061609	-3.068873
6	-1.654605	-0.033354	-0.272767
6	-2.375151	0.974765	0.611375
6	-3.876356	0.722992	0.724524
6	0.340648	0.315879	-2.903023
8	0.677868	1.525454	-2.792309
8	-0.426862	-0.195109	-0.170537
8	1.111541	-0.672455	-2.886741
1	-2.291869	-0.858539	-0.658481
1	-2.176902	1.981368	0.231924
1	-1.368188	-0.992041	-2.848659
1	-0.909299	0.876294	-5.097746
1	-2.096705	-0.425829	-4.986512
1	-3.660635	1.398252	-4.882176
1	-2.415634	2.503447	-4.277849
1	-3.843432	0.339352	-2.659171

1	-3.664884	2.058384	-2.233613
1	0.887620	-1.322556	-0.728400
1	-1.356718	1.749881	-1.986012
1	-1.902444	0.921671	1.599660
1	-4.307711	0.579947	-0.274190
1	-4.365882	1.603196	1.155466
6	-4.193976	-0.503545	1.594089
1	-3.814984	-0.312257	2.606964
1	-3.666280	-1.386638	1.213654
6	-5.661484	-0.778365	1.662051
6	-6.256616	-1.879724	1.194534
1	-6.295016	-0.010952	2.108482
1	-5.668001	-2.673565	0.743428
6	-7.729201	-2.054048	1.314555
8	-8.404245	-1.301534	1.997244
6	-8.377441	-3.195366	0.589130
6	-7.769847	-3.840845	-0.491502
6	-9.651706	-3.597593	1.002091
6	-8.426947	-4.878764	-1.146409
1	-6.794934	-3.521299	-0.845190
6	-10.299981	-4.643513	0.358205
1	-10.115208	-3.077103	1.833851
6	-9.687419	-5.285557	-0.717806
1	-7.954616	-5.368906	-1.991671
1	-11.283728	-4.958938	0.690830
1	-10.195128	-6.100721	-1.224005
7	1.516467	2.187827	-0.272561
6	0.530300	3.001123	0.277791
6	0.182745	3.089572	1.631529
6	-0.904081	3.873427	2.004136
6	-1.661279	4.592705	1.085689
6	-1.291507	4.511466	-0.251615
6	-0.213795	3.738028	-0.657493
6	-1.360060	3.822171	3.433632
9	-0.344888	3.650047	4.288421
6	-2.081894	5.211944	-1.317214
9	-3.151443	5.847024	-0.825035
6	2.303326	1.224948	0.284033
16	2.815568	1.171199	1.891978
7	2.659111	0.305546	-0.641539
6	3.534759	-0.828090	-0.437717
6	2.834700	-2.098374	-0.958676
6	3.563179	-3.402950	-0.575237
6	2.633076	-4.274136	0.281395
6	1.396190	-4.639781	-0.554936
6	0.737929	-3.344910	-1.075051
7	1.420661	-2.172773	-0.448555
6	1.345640	-2.267718	1.041259
6	2.160364	-3.495095	1.525264
6	3.247207	-3.081309	2.490016
6	4.471441	-3.595754	2.574360
6	4.847986	-0.664898	-1.193298
6	6.122500	-0.833436	-0.569136
6	7.272685	-0.682565	-1.399901
7	7.205958	-0.384641	-2.728333
6	6.017600	-0.230368	-3.257715
6	4.809416	-0.365233	-2.532373
6	8.556599	-0.848822	-0.826445
6	8.712148	-1.153602	0.501435
6	7.566447	-1.301586	1.325034
6	6.301904	-1.139365	0.799671
9	-2.013087	4.935853	3.795783
9	-2.211455	2.794706	3.627741
9	-2.530982	4.331388	-2.238530
9	-1.347532	6.112117	-1.983797
1	2.716099	-2.000291	-2.038526
1	3.852193	-3.947942	-1.477947
1	4.480277	-3.168240	-0.029749
1	-0.318190	-3.266619	-0.807075
1	0.831165	-3.204760	-2.153303

1	0.688726	-5.208126	0.055625
1	1.685646	-5.272937	-1.397213
1	3.151880	-5.185980	0.588626
1	1.470939	-4.146554	2.078551
1	0.283896	-2.337232	1.282260
1	1.714157	-1.322948	1.448877
1	2.961785	-2.293758	3.188278
1	5.177192	-3.236432	3.316527
1	4.822613	-4.382630	1.911483
1	3.716720	-0.910247	0.634737
1	3.858753	-0.228309	-3.044966
1	5.462543	-1.245714	1.477548
1	5.980076	0.010998	-4.318096
1	9.414766	-0.726093	-1.479170
1	9.707599	-1.274527	0.911685
1	2.244238	0.368335	-1.575330
1	1.360431	2.051280	-1.284195
1	0.736935	2.534591	2.376030
1	0.040994	3.664359	-1.712600
1	-2.512270	5.185594	1.398894
8	7.632961	-1.605592	2.646069
6	8.911148	-1.680749	3.249109
1	8.733371	-1.884997	4.305071
1	9.511540	-2.493465	2.823752
1	9.455720	-0.734557	3.153413

[2-3]TS_Cinchona-Thiourea_conf-8

Number of imaginary frequencies : 1
The smallest frequency is : -120.0116

Electronic energy= -3467.7173655
Zero-point correction= 0.939584
Thermal correction to Energy= 0.997881
Thermal correction to Enthalpy= 0.998825
Thermal correction to Gibbs Free Energy= 0.838851
Sum of electronic and zero-point Energies= -3466.777781
Sum of electronic and thermal Energies= -3466.719485
Sum of electronic and thermal Enthalpies= -3466.718540
Sum of electronic and thermal Free Energies= -3466.878515

Cartesian Coordinates

6	-0.175506	4.726768	3.142380
6	1.208296	5.264722	2.721903
6	2.012395	3.991756	2.444850
7	1.030573	3.079657	1.840972
6	-0.218271	3.268242	2.603102
6	1.250518	1.057378	1.611663
6	2.510958	1.047681	0.757377
6	3.795313	1.080955	1.583999
6	-1.414360	2.996006	1.682135
8	-1.345831	3.517175	0.538150
8	0.165966	0.669170	1.141707
8	-2.351357	2.286822	2.121724
1	1.433300	0.993877	2.706921
1	2.472800	1.892557	0.063245
1	-0.231056	2.544273	3.425717
1	-0.982890	5.325811	2.715645
1	-0.292545	4.731775	4.228616
1	1.667847	5.905001	3.478379
1	1.127225	5.838289	1.793249
1	2.367936	3.541866	3.380745
1	2.864046	4.134439	1.776618
1	-1.477392	0.222722	1.770251
1	0.825891	3.385783	0.883876
1	2.465646	0.145525	0.136791

1	3.713208	1.862278	2.348871
1	4.642596	1.353356	0.946260
6	4.103233	-0.257067	2.280407
1	3.193818	-0.612378	2.787184
1	4.862217	-0.111792	3.055991
6	4.564553	-1.313380	1.325405
6	5.731435	-1.957525	1.419598
1	3.917534	-1.572335	0.487173
1	6.416397	-1.739699	2.233865
6	6.094205	-3.008760	0.430605
8	5.275674	-3.438927	-0.364767
6	7.490836	-3.556077	0.441921
6	8.553871	-2.902308	1.071767
6	7.726552	-4.760230	-0.229725
6	9.832937	-3.450156	1.034992
1	8.398019	-1.952552	1.572752
6	9.000023	-5.312601	-0.255012
1	6.892579	-5.247059	-0.724585
6	10.055911	-4.657421	0.378668
1	10.655611	-2.933246	1.518569
1	9.173763	-6.252409	-0.769426
1	11.052894	-5.086680	0.356604
7	-1.049419	1.652032	-1.450826
6	0.252259	1.812066	-1.917917
6	1.085841	0.803640	-2.417356
6	2.400221	1.110498	-2.752981
6	2.928774	2.390111	-2.620507
6	2.085406	3.382731	-2.135356
6	0.768745	3.111176	-1.793806
6	3.314025	-0.016724	-3.141101
9	2.680883	-0.969329	-3.834675
6	2.596662	4.764805	-1.860304
9	2.584289	5.019277	-0.530922
6	-1.797513	0.528204	-1.263173
16	-1.696123	-0.890289	-2.173721
7	-2.680740	0.701862	-0.254279
6	-3.642951	-0.270147	0.217105
6	-3.491180	-0.415247	1.744808
6	-4.286769	-1.599675	2.333451
6	-3.318404	-2.579057	3.012756
6	-2.609512	-1.847415	4.163942
6	-1.925348	-0.580057	3.610351
7	-2.043507	-0.579598	2.120902
6	-1.431630	-1.821188	1.555097
6	-2.246978	-3.057515	2.013148
6	-2.759991	-3.844392	0.830110
6	-3.943585	-4.444030	0.729170
6	-5.074963	0.158578	-0.079827
6	-6.036512	-0.723201	-0.664397
6	-7.358939	-0.215689	-0.834958
7	-7.727970	1.050494	-0.490953
6	-6.811242	1.830242	0.026431
6	-5.474212	1.427644	0.259306
6	-8.350224	-1.062449	-1.387640
6	-8.064682	-2.351925	-1.756065
6	-6.746964	-2.851327	-1.591715
6	-5.756180	-2.049827	-1.065523
9	4.347741	0.407510	-3.882958
9	3.837509	-0.608688	-2.049330
9	1.839451	5.710883	-2.429905
9	3.854309	4.942031	-2.280229
1	-3.773581	0.533462	2.204193
1	-5.015390	-1.233159	3.061685
1	-4.844692	-2.099787	1.538973
1	-0.857176	-0.542414	3.835616
1	-2.382611	0.351697	3.947763
1	-1.870666	-2.507841	4.626634
1	-3.333089	-1.571287	4.934976
1	-3.868766	-3.437800	3.405848
1	-1.559185	-3.715891	2.560291

1	-0.401199	-1.834371	1.912879
1	-1.400658	-1.707692	0.468307
1	-2.057329	-3.930982	0.000655
1	-4.212931	-5.002135	-0.161815
1	-4.691623	-4.399297	1.517054
1	-3.417898	-1.217663	-0.274974
1	-4.775306	2.129611	0.710352
1	-4.763144	-2.475360	-0.979221
1	-7.118170	2.839770	0.292528
1	-9.347231	-0.651377	-1.507869
1	-8.844471	-2.976937	-2.174527
1	-2.622138	1.556407	0.308376
1	-1.313838	2.430338	-0.825436
1	0.716796	-0.207606	-2.520594
1	0.133951	3.896431	-1.389963
1	3.960139	2.602171	-2.875735
8	-6.380872	-4.114434	-1.927790
6	-7.347352	-4.948840	-2.537920
1	-6.837172	-5.886119	-2.761098
1	-8.188869	-5.151101	-1.864841
1	-7.722281	-4.514388	-3.471550

[3-4]TS_Cinchona-Thiourea_conf-1

Number of imaginary frequencies : 1
The smallest frequency is : -1124.1990

Electronic energy=	-3467.7355607
Zero-point correction=	0.936101
Thermal correction to Energy=	0.993695
Thermal correction to Enthalpy=	0.994640
Thermal correction to Gibbs Free Energy=	0.839596
Sum of electronic and zero-point Energies=	-3466.799460
Sum of electronic and thermal Energies=	-3466.741865
Sum of electronic and thermal Enthalpies=	-3466.740921
Sum of electronic and thermal Free Energies=	-3466.895964

Cartesian Coordinates

6	-0.765531	5.623189	-1.169341
6	0.229798	6.262740	-0.200660
6	1.202456	5.121542	0.123217
7	0.424062	3.868720	-0.101693
6	-0.935330	4.216118	-0.589448
6	0.404588	2.884703	1.034026
6	1.814772	2.362980	1.272476
6	1.868036	1.329912	2.409276
6	-1.205352	3.151611	-1.661608
8	-0.087187	2.642186	-2.075077
8	-0.392426	1.820203	0.664164
8	-2.334165	2.860457	-2.033719
1	2.508925	3.188666	1.455465
1	-1.686781	4.173255	0.204208
1	-0.330298	5.553916	-2.172409
1	-1.716295	6.152553	-1.242967
1	-0.288784	6.578094	0.710248
1	0.738435	7.132762	-0.619669
1	1.550726	5.159143	1.158270
1	2.076320	5.116506	-0.532869
1	-1.370720	1.945729	0.869608
1	0.584669	3.169422	-1.170981
1	2.123100	1.893288	0.330003
1	0.858642	0.947164	2.588996
7	-0.174378	-0.327328	-1.440539
6	1.164657	-0.724225	-1.339338
6	1.614042	-1.984339	-0.923172
6	2.983587	-2.215854	-0.825033

6	3.930208	-1.251459	-1.148106
6	3.469299	-0.018949	-1.589504
6	2.111473	0.242873	-1.699764
6	3.471652	-3.507131	-0.236012
9	2.589719	-4.502445	-0.364498
6	4.434399	1.084018	-1.912567
9	4.546190	1.292779	-3.232636
6	-1.257255	-0.689079	-0.681364
16	-1.317018	-2.020886	0.354767
7	-2.285385	0.165786	-0.842411
6	-3.601881	0.044491	-0.243099
6	-4.014872	1.362356	0.447620
6	-5.375906	1.192632	1.179658
6	-5.181152	1.474522	2.676658
6	-4.729174	2.931769	2.834927
6	-3.469717	3.140249	1.954288
7	-2.984988	1.862835	1.391352
6	-2.755892	0.913250	2.499504
6	-4.074659	0.574194	3.257827
6	-4.363952	-0.906531	3.245082
6	-5.553749	-1.485973	3.102188
6	-4.637928	-0.310796	-1.306902
6	-5.484946	-1.459785	-1.209163
6	-6.456118	-1.643540	-2.238184
7	-6.586653	-0.804467	-3.305387
6	-5.771121	0.218173	-3.372704
6	-4.788065	0.511008	-2.396412
6	-7.336572	-2.748939	-2.157374
6	-7.273156	-3.639432	-1.115650
6	-6.298594	-3.460689	-0.101056
6	-5.420944	-2.398688	-0.154951
9	4.625424	-3.908705	-0.794771
9	3.721936	-3.369495	1.084085
9	5.659661	0.833828	-1.439386
9	4.027018	2.253490	-1.376445
1	-4.086035	2.130586	-0.330684
1	-6.117752	1.884940	0.768995
1	-5.765447	0.182317	1.030615
1	-2.651063	3.585133	2.531146
1	-3.687701	3.808358	1.114632
1	-4.508185	3.144119	3.886078
1	-5.529180	3.611036	2.525628
1	-6.119844	1.312756	3.215078
1	-3.936475	0.860254	4.310160
1	-2.027770	1.382226	3.169921
1	-2.280122	0.015181	2.091988
1	-3.489151	-1.544065	3.384940
1	-5.655894	-2.566873	3.112212
1	-6.467165	-0.914704	2.956136
1	-3.537077	-0.750028	0.500052
1	-4.160370	1.390238	-2.524719
1	-4.684086	-2.317489	0.634791
1	-5.879348	0.876124	-4.233165
1	-8.067180	-2.866391	-2.951024
1	-7.962110	-4.474926	-1.082297
1	-2.185381	0.938904	-1.499252
1	-0.255250	0.599689	-1.859847
1	0.909296	-2.758819	-0.657374
1	1.773466	1.216222	-2.044430
1	4.992080	-1.443795	-1.035678
8	-6.164848	-4.295715	0.961839
6	-7.029850	-5.411511	1.047332
1	-6.746254	-5.943018	1.956008
1	-8.079497	-5.104279	1.125028
1	-6.909072	-6.082219	0.188673
1	2.215694	1.799025	3.335869
1	0.012868	3.418155	1.919422
6	2.756131	0.132744	2.052259
1	2.747544	-0.613772	2.853445
1	2.306196	-0.353257	1.173968

6	4.168344	0.491489	1.703567
6	5.221789	-0.307814	1.895599
1	4.347321	1.440946	1.195082
1	5.098210	-1.284796	2.356156
6	6.561677	0.094893	1.394072
8	6.882339	1.268337	1.305021
6	7.504097	-0.985015	0.952616
6	7.082791	-2.302708	0.749769
6	8.831197	-0.636055	0.682971
6	7.978979	-3.259155	0.279380
1	6.052784	-2.587385	0.939456
6	9.728099	-1.594509	0.230775
1	9.135058	0.394911	0.832357
6	9.301935	-2.907296	0.026326
1	7.638581	-4.275650	0.109225
1	10.759224	-1.321601	0.029217
1	10.001852	-3.653908	-0.336205

[3-4]TS_Cinchona-Thiourea_conf-1

Number of imaginary frequencies : 1
The smallest frequency is : -1124.1990

Electronic energy=	-3467.7355607
Zero-point correction=	0.936101
Thermal correction to Energy=	0.993695
Thermal correction to Enthalpy=	0.994640
Thermal correction to Gibbs Free Energy=	0.839596
Sum of electronic and zero-point Energies=	-3466.799460
Sum of electronic and thermal Energies=	-3466.741865
Sum of electronic and thermal Enthalpies=	-3466.740921
Sum of electronic and thermal Free Energies=	-3466.895964

Cartesian Coordinates

6	-0.765531	5.623189	-1.169341
6	0.229798	6.262740	-0.200660
6	1.202456	5.121542	0.123217
7	0.424062	3.868720	-0.101693
6	-0.935330	4.216118	-0.589448
6	0.404588	2.884703	1.034026
6	1.814772	2.362980	1.272476
6	1.868036	1.329912	2.409276
6	-1.205352	3.151611	-1.661608
8	-0.087187	2.642186	-2.075077
8	-0.392426	1.820203	0.664164
8	-2.334165	2.860457	-2.033719
1	2.508925	3.188666	1.455465
1	-1.686781	4.173255	0.204208
1	-0.330298	5.553916	-2.172409
1	-1.716295	6.152553	-1.242967
1	-0.288784	6.578094	0.710248
1	0.738435	7.132762	-0.619669
1	1.550726	5.159143	1.158270
1	2.076320	5.116506	-0.532869
1	-1.370720	1.945729	0.869608
1	0.584669	3.169422	-1.170981
1	2.123100	1.893288	0.330003
1	0.858642	0.947164	2.588996
7	-0.174378	-0.327328	-1.440539
6	1.164657	-0.724225	-1.339338
6	1.614042	-1.984339	-0.923172
6	2.983587	-2.215854	-0.825033
6	3.930208	-1.251459	-1.148106
6	3.469299	-0.018949	-1.589504
6	2.111473	0.242873	-1.699764
6	3.471652	-3.507131	-0.236012

9	2.589719	-4.502445	-0.364498
6	4.434399	1.084018	-1.912567
9	4.546190	1.292779	-3.232636
6	-1.257255	-0.689079	-0.681364
16	-1.317018	-2.020886	0.354767
7	-2.285385	0.165786	-0.842411
6	-3.601881	0.044491	-0.243099
6	-4.014872	1.362356	0.447620
6	-5.375906	1.192632	1.179658
6	-5.181152	1.474522	2.676658
6	-4.729174	2.931769	2.834927
6	-3.469717	3.140249	1.954288
7	-2.984988	1.862835	1.391352
6	-2.755892	0.913250	2.499504
6	-4.074659	0.574194	3.257827
6	-4.363952	-0.906531	3.245082
6	-5.553749	-1.485973	3.102188
6	-4.637928	-0.310796	-1.306902
6	-5.484946	-1.459785	-1.209163
6	-6.456118	-1.643540	-2.238184
7	-6.586653	-0.804467	-3.305387
6	-5.771121	0.218173	-3.372704
6	-4.788065	0.511008	-2.396412
6	-7.336572	-2.748939	-2.157374
6	-7.273156	-3.639432	-1.115650
6	-6.298594	-3.460689	-0.101056
6	-5.420944	-2.398688	-0.154951
9	4.625424	-3.908705	-0.794771
9	3.721936	-3.369495	1.084085
9	5.659661	0.833828	-1.439386
9	4.027018	2.253490	-1.376445
1	-4.086035	2.130586	-0.330684
1	-6.117752	1.884940	0.768995
1	-5.765447	0.182317	1.030615
1	-2.651063	3.585133	2.531146
1	-3.687701	3.808358	1.114632
1	-4.508185	3.144119	3.886078
1	-5.529180	3.611036	2.525628
1	-6.119844	1.312756	3.215078
1	-3.936475	0.860254	4.310160
1	-2.027770	1.382226	3.169921
1	-2.280122	0.015181	2.091988
1	-3.489151	-1.544065	3.384940
1	-5.655894	-2.566873	3.112212
1	-6.467165	-0.914704	2.956136
1	-3.537077	-0.750028	0.500052
1	-4.160370	1.390238	-2.524719
1	-4.684086	-2.317489	0.634791
1	-5.879348	0.876124	-4.233165
1	-8.067180	-2.866391	-2.951024
1	-7.962110	-4.474926	-1.082297
1	-2.185381	0.938904	-1.499252
1	-0.255250	0.599689	-1.859847
1	0.909296	-2.758819	-0.657374
1	1.773466	1.216222	-2.044430
1	4.992080	-1.443795	-1.035678
8	-6.164848	-4.295715	0.961839
6	-7.029850	-5.411511	1.047332
1	-6.746254	-5.943018	1.956008
1	-8.079497	-5.104279	1.125028
1	-6.909072	-6.082219	0.188673
1	2.215694	1.799025	3.335869
1	0.012868	3.418155	1.919422
6	2.756131	0.132744	2.052259
1	2.747544	-0.613772	2.853445
1	2.306196	-0.353257	1.173968
6	4.168344	0.491489	1.703567
6	5.221789	-0.307814	1.895599
1	4.347321	1.440946	1.195082
1	5.098210	-1.284796	2.356156

6	6.561677	0.094893	1.394072
8	6.882339	1.268337	1.305021
6	7.504097	-0.985015	0.952616
6	7.082791	-2.302708	0.749769
6	8.831197	-0.636055	0.682971
6	7.978979	-3.259155	0.279380
1	6.052784	-2.587385	0.939456
6	9.728099	-1.594509	0.230775
1	9.135058	0.394911	0.832357
6	9.301935	-2.907296	0.026326
1	7.638581	-4.275650	0.109225
1	10.759224	-1.321601	0.029217
1	10.001852	-3.653908	-0.336205

[3-4]TS_Cinchona-Thiourea_conf-2

Number of imaginary frequencies : 1
The smallest frequency is : -1098.3675

Electronic energy=	-3467.7371898
Zero-point correction=	0.937312
Thermal correction to Energy=	0.994563
Thermal correction to Enthalpy=	0.995507
Thermal correction to Gibbs Free Energy=	0.842029
Sum of electronic and zero-point Energies=	-3466.799878
Sum of electronic and thermal Energies=	-3466.742627
Sum of electronic and thermal Enthalpies=	-3466.741683
Sum of electronic and thermal Free Energies=	-3466.895161

Cartesian Coordinates

6	-1.973782	2.236978	4.227064
6	-2.940955	3.260848	3.632335
6	-3.560728	2.515487	2.445349
7	-2.530752	1.519512	2.028073
6	-1.384091	1.583685	2.974036
6	-2.081205	1.596237	0.595866
6	-3.264480	1.299325	-0.331015
6	-2.876019	1.248137	-1.815358
6	-1.008978	0.109719	3.170059
8	-2.014860	-0.649429	2.856073
8	-1.121931	0.620736	0.400524
8	0.093974	-0.253399	3.554674
1	-4.072357	2.023567	-0.174437
1	-0.543035	2.152662	2.565534
1	-2.520381	1.487403	4.810358
1	-1.200956	2.672490	4.861623
1	-2.383459	4.129885	3.268212
1	-3.693001	3.609080	4.342703
1	-3.785191	3.187898	1.614352
1	-4.475330	1.981717	2.716299
1	-0.184944	0.916668	0.612177
1	-2.655248	0.263955	2.327859
1	-3.652089	0.321183	-0.023625
1	-3.553715	0.570321	-2.341493
7	-1.322612	-2.255206	0.480836
6	-2.566003	-2.309189	-0.151372
6	-2.795160	-2.393447	-1.530520
6	-4.102794	-2.372147	-2.006781
6	-5.204227	-2.259710	-1.167228
6	-4.962396	-2.199757	0.200134
6	-3.673534	-2.240390	0.708867
6	-4.323407	-2.390099	-3.493217
9	-3.375168	-3.078556	-4.138450
6	-6.088935	-1.976456	1.165139
9	-5.974300	-2.739098	2.260988
6	-0.067482	-2.021940	-0.018062

16	0.434233	-2.348646	-1.596443
7	0.749042	-1.509192	0.920983
6	2.151600	-1.180569	0.755151
6	2.424111	0.255859	1.252733
6	3.903613	0.653886	0.994048
6	3.936522	1.891648	0.088094
6	3.242749	3.047460	0.821109
6	1.826718	2.573229	1.238255
7	1.505108	1.254633	0.649878
6	1.678153	1.339329	-0.814380
6	3.156270	1.626889	-1.213434
6	3.717331	0.547290	-2.105854
6	4.954006	0.054821	-2.082176
6	3.025614	-2.162063	1.531284
6	4.082172	-2.906708	0.917456
6	4.869857	-3.740224	1.766740
7	4.641891	-3.879515	3.103780
6	3.645129	-3.204398	3.619716
6	2.815847	-2.328386	2.878024
6	5.949116	-4.464044	1.205313
6	6.247714	-4.381164	-0.130691
6	5.452656	-3.565271	-0.975294
6	4.390793	-2.852132	-0.461144
9	-5.507896	-2.931037	-3.814646
9	-4.318152	-1.144975	-4.008905
9	-7.284743	-2.227468	0.618850
9	-6.109371	-0.696885	1.590709
1	2.199474	0.277325	2.324875
1	4.409373	0.875108	1.939348
1	4.445091	-0.173025	0.527211
1	1.057372	3.285169	0.915930
1	1.747679	2.471593	2.325878
1	3.182490	3.922555	0.165438
1	3.823723	3.337585	1.702022
1	4.971136	2.162917	-0.143359
1	3.168001	2.560752	-1.793563
1	1.014944	2.143361	-1.157073
1	1.310586	0.409427	-1.261505
1	3.018263	0.156051	-2.847341
1	5.261982	-0.723546	-2.773870
1	5.701437	0.392617	-1.368499
1	2.368802	-1.245458	-0.311220
1	2.017402	-1.794836	3.389460
1	3.802893	-2.260414	-1.151952
1	3.468087	-3.330308	4.686314
1	6.534479	-5.087810	1.872951
1	7.081677	-4.945425	-0.530940
1	0.378905	-1.324642	1.851881
1	-1.434384	-1.965021	1.452096
1	-1.966107	-2.474811	-2.218591
1	-3.513940	-2.187515	1.782421
1	-6.212890	-2.232226	-1.561836
8	5.674418	-3.434400	-2.309521
6	6.730548	-4.178886	-2.884249
1	6.719388	-3.944420	-3.948940
1	7.702041	-3.891414	-2.464844
1	6.581321	-5.256985	-2.753797
1	-1.871964	0.817254	-1.896129
1	-1.674494	2.611084	0.454546
6	-2.915196	2.613558	-2.539303
1	-2.482761	2.501635	-3.538139
1	-3.959175	2.926455	-2.655932
6	-2.170995	3.637300	-1.749831
6	-0.901942	4.013751	-1.942578
1	-2.674148	4.052045	-0.876198
1	-0.347329	3.660583	-2.805558
6	-0.242881	4.862289	-0.918221
8	-0.808729	5.113253	0.139478
6	1.144515	5.377424	-1.154262
6	1.920060	5.014607	-2.260338

6	1.683597	6.243693	-0.194789
6	3.216664	5.506388	-2.398362
1	1.532418	4.345575	-3.021018
6	2.971299	6.741695	-0.339121
1	1.070825	6.512112	0.659112
6	3.742155	6.369962	-1.441380
1	3.813631	5.214662	-3.256417
1	3.378306	7.417621	0.406035
1	4.750699	6.755258	-1.553733

[3-4]TS_Cinchona-Thiourea_conf-3

Number of imaginary frequencies : 1
The smallest frequency is : -1021.4973

Electronic energy= -3467.7355109
Zero-point correction= 0.936362
Thermal correction to Energy= 0.993658
Thermal correction to Enthalpy= 0.994602
Thermal correction to Gibbs Free Energy= 0.840938
Sum of electronic and zero-point Energies= -3466.799149
Sum of electronic and thermal Energies= -3466.741853
Sum of electronic and thermal Enthalpies= -3466.740909
Sum of electronic and thermal Free Energies= -3466.894573

Cartesian Coordinates

6	-2.872431	-4.451473	2.187105
6	-4.240499	-3.851489	2.515665
6	-4.459752	-2.845539	1.383889
7	-3.092163	-2.382298	1.011026
6	-2.079380	-3.238409	1.678772
6	-2.851532	-0.907878	1.118930
6	-3.085930	-0.348317	2.533665
6	-4.137748	0.766995	2.520032
6	-1.109388	-3.605923	0.543475
8	-1.639866	-3.322039	-0.611797
8	-1.609020	-0.614121	0.582016
8	-0.013002	-4.100607	0.741935
1	-2.133485	0.042933	2.911214
1	-1.552875	-2.716142	2.483627
1	-2.967733	-5.191798	1.385000
1	-2.381698	-4.930648	3.034888
1	-4.201368	-3.332639	3.479468
1	-5.035151	-4.598431	2.565015
1	-5.075728	-1.992274	1.676215
1	-4.920154	-3.311683	0.508547
1	-0.838625	-0.867109	1.160642
1	-2.603974	-2.754903	-0.129440
1	-3.404295	-1.142469	3.219263
1	-4.333032	1.099845	3.545537
7	-0.824430	-0.927668	-2.191429
6	-2.005360	-0.182710	-2.278477
6	-2.084065	1.210267	-2.355846
6	-3.329216	1.831661	-2.305596
6	-4.514470	1.118921	-2.200814
6	-4.424122	-0.270893	-2.176516
6	-3.200638	-0.918559	-2.225711
6	-3.349825	3.332599	-2.248404
9	-2.475911	3.881381	-3.102014
6	-5.665415	-1.067624	-1.909601
9	-5.526982	-2.362076	-2.225545
6	0.374827	-0.517740	-1.637069
16	1.094271	0.979646	-1.911649
7	0.922318	-1.471841	-0.866710
6	2.181721	-1.373372	-0.146603
6	1.969924	-1.721105	1.342583

6	3.264845	-1.462189	2.163335
6	2.975416	-0.389885	3.223226
6	1.912310	-0.937112	4.185658
6	0.707857	-1.428781	3.343316
7	0.820515	-0.992405	1.936728
6	1.038759	0.470329	1.918012
6	2.403719	0.872465	2.548776
6	3.321965	1.535082	1.548129
6	4.651533	1.466159	1.527075
6	3.220898	-2.309738	-0.754983
6	4.477946	-1.843499	-1.255814
6	5.384729	-2.827199	-1.752969
7	5.098742	-4.159628	-1.797417
6	3.926705	-4.539850	-1.353749
6	2.958813	-3.656367	-0.817176
6	6.652108	-2.412621	-2.227540
6	7.022009	-1.092234	-2.218330
6	6.114320	-0.115705	-1.735453
6	4.868832	-0.484932	-1.273558
9	-4.560337	3.834249	-2.524910
9	-3.013076	3.769831	-1.019002
9	-6.728823	-0.595491	-2.568216
9	-5.977526	-1.024053	-0.593462
1	1.695854	-2.777667	1.396786
1	3.591955	-2.385364	2.652846
1	4.079726	-1.140651	1.508881
1	-0.236032	-1.040210	3.743749
1	0.642996	-2.522357	3.338269
1	1.602361	-0.151214	4.882607
1	2.325104	-1.758051	4.779954
1	3.888888	-0.145941	3.773803
1	2.197444	1.614963	3.333724
1	0.207817	0.911873	2.479177
1	0.952992	0.828661	0.885438
1	2.821707	2.139701	0.788713
1	5.224188	1.994896	0.770316
1	5.218688	0.879521	2.246175
1	2.507748	-0.337096	-0.235274
1	2.016122	-4.059821	-0.453785
1	4.207121	0.301944	-0.932812
1	3.707617	-5.605115	-1.399180
1	7.322779	-3.180685	-2.598811
1	8.000295	-0.806030	-2.585403
1	0.406109	-2.336512	-0.728916
1	-1.033508	-1.900540	-1.975546
1	-1.182806	1.802001	-2.435733
1	-3.164445	-2.004233	-2.196983
1	-5.472570	1.622709	-2.140793
8	6.400696	1.212079	-1.694947
6	7.657943	1.636764	-2.183327
1	7.675928	2.720598	-2.066401
1	8.483426	1.201866	-1.607472
1	7.783099	1.389443	-3.243974
1	-5.081478	0.363018	2.131791
1	-3.594181	-0.479918	0.435034
6	-3.731653	1.975823	1.661625
1	-3.503758	1.666289	0.634514
1	-4.584191	2.664259	1.606119
6	-2.557860	2.699174	2.239304
6	-1.387244	2.867623	1.619712
1	-2.666429	3.107249	3.245268
1	-1.233756	2.465730	0.621715
6	-0.276701	3.583856	2.307662
8	-0.299927	3.762541	3.516103
6	0.884377	4.067081	1.496098
6	0.891581	4.040214	0.098060
6	2.000364	4.561046	2.182173
6	2.011161	4.484679	-0.601841
1	0.027060	3.690142	-0.455919
6	3.115052	5.002599	1.483428

1	1.971635	4.580885	3.266780
6	3.123278	4.958709	0.088630
1	2.013049	4.455666	-1.686707
1	3.982622	5.371159	2.021544
1	3.998012	5.293874	-0.460341

[3-4]TS_Cinchona-Thiourea_conf-4

Number of imaginary frequencies : 1
The smallest frequency is : -1113.8294

Electronic energy=	-3467.7302065
Zero-point correction=	0.936070
Thermal correction to Energy=	0.993857
Thermal correction to Enthalpy=	0.994801
Thermal correction to Gibbs Free Energy=	0.836464
Sum of electronic and zero-point Energies=	-3466.794136
Sum of electronic and thermal Energies=	-3466.736349
Sum of electronic and thermal Enthalpies=	-3466.735405
Sum of electronic and thermal Free Energies=	-3466.893743

Cartesian Coordinates

6	0.784569	-4.423716	3.764817
6	-0.654938	-4.486705	4.275995
6	-1.487514	-4.041971	3.067217
7	-0.572887	-3.190720	2.250648
6	0.771157	-3.168230	2.887502
6	-1.054700	-1.808476	1.908882
6	-2.361669	-1.880572	1.123987
6	-2.805362	-0.508966	0.615371
6	1.725552	-3.266968	1.690236
8	1.109641	-3.797175	0.679545
8	-0.094522	-1.214246	1.115548
8	2.886028	-2.882101	1.730320
1	-3.152597	-2.324348	1.738751
1	0.942569	-2.250012	3.458747
1	1.007902	-5.298732	3.144776
1	1.533557	-4.361309	4.555221
1	-0.788239	-3.777570	5.099125
1	-0.941566	-5.477748	4.632256
1	-2.366426	-3.467002	3.365147
1	-1.819122	-4.883501	2.454278
1	0.622582	-0.707855	1.614024
1	-0.020017	-3.670830	1.190081
1	-2.195253	-2.551294	0.273317
1	-3.644291	-0.638388	-0.074713
7	0.883743	-1.888525	-1.546147
6	-0.407027	-2.203263	-1.977493
6	-1.332922	-1.318114	-2.541886
6	-2.617621	-1.767712	-2.835406
6	-3.029618	-3.070391	-2.585246
6	-2.089040	-3.946609	-2.054878
6	-0.795806	-3.536514	-1.772050
6	-3.597444	-0.765967	-3.380469
9	-3.049246	0.001745	-4.330236
6	-2.480670	-5.333597	-1.642124
9	-1.600649	-6.256028	-2.053640
6	1.462791	-0.669247	-1.294336
16	1.101637	0.765563	-2.104055
7	2.392116	-0.756074	-0.324396
6	3.227189	0.322512	0.168606
6	3.134867	0.399682	1.708699
6	3.916340	1.628958	2.250413
6	2.944992	2.543005	3.011727
6	2.387020	1.758228	4.206974
6	1.763018	0.444288	3.668793

7	1.731181	0.427645	2.192624
6	1.018942	1.630676	1.715808
6	1.759176	2.941955	2.114662
6	2.102621	3.776580	0.905798
6	3.226172	4.458814	0.695044
6	4.680660	0.107045	-0.242973
6	5.440124	1.096175	-0.944524
6	6.806766	0.790612	-1.221612
7	7.398949	-0.387532	-0.875691
6	6.660876	-1.275041	-0.256858
6	5.302562	-1.072440	0.086113
6	7.601674	1.753588	-1.888073
6	7.087149	2.966564	-2.268064
6	5.726062	3.263433	-2.001143
6	4.922018	2.343486	-1.361945
9	-4.678907	-1.356411	-3.910222
9	-4.038719	0.065496	-2.418870
9	-3.686006	-5.685578	-2.104202
9	-2.530808	-5.430171	-0.295591
1	3.553350	-0.530950	2.106672
1	4.717386	1.303614	2.921851
1	4.389482	2.173396	1.429309
1	0.734238	0.319754	4.026244
1	2.336475	-0.430928	3.991542
1	1.635693	2.357834	4.731248
1	3.186365	1.538872	4.921153
1	3.467634	3.437466	3.364106
1	1.070898	3.541309	2.726950
1	0.015126	1.596704	2.153208
1	0.893991	1.550725	0.631219
1	1.319309	3.821551	0.147194
1	3.366569	5.036609	-0.213467
1	4.050885	4.462941	1.403460
1	2.843929	1.244651	-0.268760
1	4.765914	-1.860786	0.609665
1	3.884851	2.611892	-1.200695
1	7.143155	-2.214258	0.008073
1	8.636933	1.496121	-2.086867
1	7.721604	3.683841	-2.774878
1	2.543940	-1.652541	0.134173
1	1.247100	-2.637394	-0.957457
1	-1.056264	-0.292033	-2.741833
1	-0.086020	-4.242481	-1.349582
1	-4.039904	-3.394348	-2.803253
8	5.137620	4.437372	-2.347135
6	5.920993	5.400504	-3.024640
1	5.259992	6.246683	-3.213569
1	6.766672	5.735850	-2.412691
1	6.292688	5.016849	-3.981647
1	-1.986165	-0.063259	0.040552
1	-1.192576	-1.280233	2.869491
6	-3.228643	0.448294	1.738788
1	-4.074339	0.028105	2.296509
1	-2.398687	0.564921	2.450179
6	-3.576408	1.802193	1.209083
6	-4.771679	2.389426	1.314960
1	-2.789930	2.343880	0.682156
1	-5.589596	1.887880	1.823900
6	-4.986713	3.753930	0.760911
8	-4.047037	4.441217	0.396372
6	-6.385336	4.288740	0.672611
6	-7.516627	3.474154	0.772142
6	-6.544022	5.660894	0.452329
6	-8.789145	4.027434	0.658201
1	-7.414228	2.403237	0.913601
6	-7.813373	6.213668	0.349842
1	-5.653583	6.274848	0.365980
6	-8.938617	5.396115	0.453114
1	-9.663755	3.388287	0.724756
1	-7.929565	7.280338	0.186041

1 -9.931786 5.826355 0.368272

[3-4]TS_Cinchona-Thiourea_conf-5

Number of imaginary frequencies : 1

The smallest frequency is : -1006.0054

Electronic energy= -3467.736391
Zero-point correction= 0.937798
Thermal correction to Energy= 0.994727
Thermal correction to Enthalpy= 0.995671
Thermal correction to Gibbs Free Energy= 0.843925
Sum of electronic and zero-point Energies= -3466.798593
Sum of electronic and thermal Energies= -3466.741664
Sum of electronic and thermal Enthalpies= -3466.740720
Sum of electronic and thermal Free Energies= -3466.892466

Cartesian Coordinates

6	-2.837169	-4.991976	1.086637
6	-4.178441	-4.500333	1.634955
6	-4.431363	-3.221789	0.833945
7	-3.073946	-2.678888	0.544663
6	-2.045954	-3.688748	0.905780
6	-2.802663	-1.290201	1.037603
6	-2.923285	-1.129778	2.561646
6	-3.830547	0.048611	2.934841
6	-1.120128	-3.717651	-0.324052
8	-1.694102	-3.129307	-1.333055
8	-1.585719	-0.870318	0.529738
8	-0.016074	-4.235454	-0.308688
1	-1.917304	-0.966290	2.967129
1	-1.486322	-3.410841	1.803588
1	-2.981409	-5.473176	0.112905
1	-2.319904	-5.694190	1.741390
1	-4.082848	-4.264133	2.700245
1	-4.982748	-5.229199	1.518525
1	-5.022631	-2.477902	1.373666
1	-4.933072	-3.429637	-0.115113
1	-0.807928	-1.266173	1.007908
1	-2.639918	-2.721321	-0.667161
1	-3.312420	-2.044453	3.024716
1	-3.846549	0.157538	4.025072
7	-0.819183	-0.367187	-2.172829
6	-1.998394	0.380772	-2.088760
6	-2.074644	1.764359	-1.894246
6	-3.319696	2.362748	-1.721055
6	-4.507245	1.643550	-1.760605
6	-4.417946	0.277141	-2.007497
6	-3.193242	-0.348615	-2.179369
6	-3.362716	3.821056	-1.365245
9	-2.342281	4.507975	-1.898156
6	-5.652783	-0.568777	-1.925440
9	-5.544398	-1.703701	-2.629114
6	0.362621	-0.128023	-1.496014
16	1.042512	1.394471	-1.266354
7	0.920292	-1.266059	-1.048008
6	2.180542	-1.374192	-0.331612
6	1.987525	-2.172778	0.974515
6	3.291275	-2.159510	1.820259
6	3.000142	-1.495372	3.172845
6	1.959104	-2.348663	3.911053
6	0.743363	-2.548754	2.969408
7	0.835884	-1.685432	1.774835
6	1.039644	-0.290719	2.218214
6	2.395514	-0.095370	2.956281
6	3.285169	0.887845	2.236585

6	4.614547	0.857621	2.164780
6	3.229889	-2.056709	-1.202816
6	4.476509	-1.437867	-1.536632
6	5.386459	-2.198580	-2.330978
7	5.115687	-3.452918	-2.792050
6	3.955660	-3.973569	-2.478793
6	2.984170	-3.319273	-1.683763
6	6.640516	-1.634525	-2.665611
6	6.995972	-0.379753	-2.241235
6	6.087401	0.376272	-1.458122
6	4.854152	-0.140166	-1.121452
9	-4.499514	4.407116	-1.760891
9	-3.282184	3.989650	-0.028863
9	-6.745141	0.074938	-2.349039
9	-5.892018	-0.935934	-0.645061
1	1.729345	-3.198119	0.697697
1	3.649437	-3.181844	1.980124
1	4.086060	-1.621100	1.296317
1	-0.194144	-2.314293	3.487300
1	0.678516	-3.583986	2.616420
1	1.655346	-1.845959	4.835462
1	2.389906	-3.315055	4.190891
1	3.917186	-1.428110	3.766193
1	2.172622	0.341897	3.938274
1	0.203385	-0.030885	2.874989
1	0.959831	0.366072	1.344114
1	2.756933	1.703875	1.740960
1	5.162401	1.624283	1.624458
1	5.205673	0.070286	2.626945
1	2.487542	-0.355682	-0.093093
1	2.049610	-3.830061	-1.460625
1	4.191967	0.486115	-0.535597
1	3.749990	-4.973788	-2.855984
1	7.311814	-2.234551	-3.271200
1	7.963751	0.025761	-2.511452
1	0.427885	-2.143137	-1.197805
1	-1.035091	-1.361144	-2.228206
1	-1.172935	2.359874	-1.862213
1	-3.156445	-1.417963	-2.368386
1	-5.466408	2.126693	-1.612010
8	6.360124	1.624980	-0.998216
6	7.596517	2.210729	-1.354616
1	7.600185	3.203325	-0.903290
1	8.444802	1.637214	-0.962407
1	7.696437	2.312301	-2.441588
1	-4.858532	-0.181330	2.627360
1	-3.577990	-0.691980	0.544631
6	-3.425951	1.386259	2.299310
1	-3.479051	1.337621	1.204405
1	-4.162306	2.139538	2.610018
6	-2.065840	1.863749	2.704325
6	-1.153555	2.330170	1.848341
1	-1.828867	1.872922	3.769892
1	-1.353724	2.338265	0.780877
6	0.139158	2.876253	2.339818
8	0.624699	2.494016	3.395840
6	0.824182	3.926404	1.522674
6	0.217382	4.518857	0.410713
6	2.106649	4.333541	1.906135
6	0.892360	5.493415	-0.317246
1	-0.790131	4.243403	0.119203
6	2.781448	5.302322	1.175249
1	2.557870	3.871622	2.778671
6	2.175478	5.881002	0.060224
1	0.413163	5.946702	-1.179113
1	3.779667	5.608004	1.471983
1	2.703716	6.637201	-0.512401

[3-4]TS_Cinchona-Thiourea_conf-6

Number of imaginary frequencies : 1
The smallest frequency is : -1027.1398

Electronic energy= -3467.7350007
Zero-point correction= 0.937292
Thermal correction to Energy= 0.994292
Thermal correction to Enthalpy= 0.995237
Thermal correction to Gibbs Free Energy= 0.843003
Sum of electronic and zero-point Energies= -3466.797709
Sum of electronic and thermal Energies= -3466.740708
Sum of electronic and thermal Enthalpies= -3466.739764
Sum of electronic and thermal Free Energies= -3466.891998

Cartesian Coordinates

6	-2.644490	-5.277874	0.166729
6	-4.008749	-4.965050	0.786222
6	-4.329148	-3.578438	0.224959
7	-3.002858	-2.916550	0.061267
6	-1.921628	-3.923868	0.225971
6	-2.806032	-1.644359	0.829185
6	-2.933147	-1.819040	2.353481
6	-4.043380	-0.929022	2.924482
6	-1.009294	-3.674937	-0.989893
8	-1.619800	-2.930148	-1.864889
8	-1.631881	-1.045826	0.404462
8	0.114110	-4.140272	-1.078916
1	-1.974044	-1.551787	2.812777
1	-1.368878	-3.787274	1.159910
1	-2.766189	-5.585378	-0.877929
1	-2.089041	-6.057966	0.688221
1	-3.926174	-4.923427	1.877300
1	-4.773830	-5.700718	0.530934
1	-4.969722	-2.976518	0.874393
1	-4.806070	-3.646511	-0.756668
1	-0.805961	-1.468976	0.770119
1	-2.581714	-2.711490	-1.127710
1	-3.133873	-2.865419	2.610262
1	-4.169270	-1.139461	3.992256
7	-0.918842	-0.041671	-2.298163
6	-2.043871	0.796668	-2.216921
6	-2.015709	2.171892	-2.452766
6	-3.188330	2.910573	-2.307337
6	-4.392530	2.321666	-1.941132
6	-4.410844	0.944295	-1.745320
6	-3.259443	0.187877	-1.897076
6	-3.121888	4.400182	-2.497349
9	-2.278088	4.740923	-3.480933
6	-5.654092	0.276578	-1.238010
9	-5.668036	-1.040622	-1.507934
6	0.256551	0.140050	-1.604578
16	0.854169	1.642749	-1.126530
7	0.871651	-1.025798	-1.340266
6	2.150165	-1.182680	-0.666421
6	2.026059	-2.185204	0.498462
6	3.350026	-2.259931	1.311529
6	3.072190	-1.825283	2.757113
6	2.077599	-2.816045	3.377516
6	0.849759	-2.918121	2.437210
7	0.880546	-1.875078	1.392067
6	1.047912	-0.561006	2.050309
6	2.423789	-0.427487	2.765988
6	3.274762	0.673243	2.178111
6	4.603412	0.688338	2.092541
6	3.211300	-1.662037	-1.652651
6	4.410575	-0.926558	-1.913160
6	5.337083	-1.496955	-2.836817

7	5.122272	-2.678071	-3.483622
6	4.003562	-3.310326	-3.229502
6	3.021960	-2.847469	-2.319780
6	6.546989	-0.812205	-3.102526
6	6.844492	0.378006	-2.488975
6	5.918785	0.945050	-1.576516
6	4.726337	0.308978	-1.303951
9	-4.321727	4.919346	-2.796621
9	-2.693977	5.019157	-1.385669
9	-6.767878	0.810850	-1.748451
9	-5.752091	0.382854	0.105080
1	1.794282	-3.162271	0.066740
1	3.742179	-3.282091	1.301803
1	4.113148	-1.618366	0.862469
1	-0.085390	-2.806854	2.998633
1	0.818898	-3.886828	1.926376
1	1.776866	-2.468068	4.371481
1	2.546762	-3.796735	3.502143
1	4.001103	-1.816276	3.335081
1	2.224416	-0.150352	3.811668
1	0.228615	-0.474812	2.772204
1	0.902391	0.229581	1.304736
1	2.723102	1.541673	1.814343
1	5.122921	1.540952	1.664250
1	5.221497	-0.140721	2.429288
1	2.414023	-0.200248	-0.275139
1	2.124813	-3.442276	-2.159635
1	4.046124	0.792813	-0.613720
1	3.841959	-4.250619	-3.753668
1	7.234110	-1.265481	-3.809612
1	7.780505	0.876532	-2.710756
1	0.436084	-1.886934	-1.661629
1	-1.182308	-1.023679	-2.373891
1	-1.092841	2.655667	-2.743515
1	-3.293893	-0.885093	-1.748565
1	-5.292652	2.914617	-1.822277
8	6.134613	2.119736	-0.928624
6	7.337404	2.814898	-1.192512
1	7.302893	3.718581	-0.583587
1	8.216575	2.225271	-0.907216
1	7.416042	3.098674	-2.248534
1	-4.993486	-1.178980	2.435816
1	-3.625505	-1.005194	0.480954
6	-3.776108	0.572602	2.728828
1	-3.618108	0.801574	1.668925
1	-4.669617	1.125009	3.044229
6	-2.601158	1.039654	3.526594
6	-1.479636	1.542007	3.003452
1	-2.662188	0.949449	4.611989
1	-1.370262	1.629363	1.925724
6	-0.360928	1.954430	3.898117
8	-0.333831	1.600736	5.067365
6	0.741189	2.801619	3.341577
6	0.701947	3.346884	2.054504
6	1.851441	3.045926	4.159703
6	1.765993	4.117231	1.590004
1	-0.146999	3.179688	1.401025
6	2.911265	3.811253	3.694478
1	1.861428	2.617840	5.156821
6	2.870395	4.345981	2.405795
1	1.730651	4.530376	0.587060
1	3.773790	3.987814	4.329298
1	3.702027	4.939224	2.037889

[3-4]TS_Cinchona-Thiourea_conf-7

Number of imaginary frequencies : 1

The smallest frequency is : -1015.1743

Electronic energy= -3467.7292646
Zero-point correction= 0.937425
Thermal correction to Energy= 0.995061
Thermal correction to Enthalpy= 0.996005
Thermal correction to Gibbs Free Energy= 0.838176
Sum of electronic and zero-point Energies= -3466.791839
Sum of electronic and thermal Energies= -3466.734203
Sum of electronic and thermal Enthalpies= -3466.733259
Sum of electronic and thermal Free Energies= -3466.891089

Cartesian Coordinates

6	2.899743	-0.120892	3.636839
6	4.012764	0.757298	3.058880
6	3.232619	1.862190	2.346688
7	1.998493	1.188097	1.853103
6	1.864795	-0.145939	2.502766
6	1.774210	1.197136	0.372045
6	2.817738	0.403239	-0.405529
6	2.695207	0.668085	-1.906400
6	0.406334	-0.159996	3.000884
8	-0.071730	1.051418	3.007860
8	0.477071	0.777876	0.127135
8	-0.176681	-1.179474	3.327455
1	2.671977	-0.667327	-0.209460
1	2.035395	-0.970288	1.806146
1	2.465644	0.355354	4.523110
1	3.223406	-1.125047	3.912764
1	4.601652	0.186995	2.331965
1	4.691493	1.148588	3.818884
1	3.769762	2.321635	1.514331
1	2.939091	2.656518	3.039981
1	0.365202	-0.206258	0.221030
1	0.889682	1.520543	2.410750
1	3.827441	0.653400	-0.058231
1	3.034234	1.688166	-2.124644
7	-2.004453	2.048895	0.989679
6	-1.574336	3.273322	0.456832
6	-2.266134	3.991223	-0.526300
6	-1.743776	5.195681	-0.980729
6	-0.554231	5.724800	-0.483402
6	0.101813	5.017523	0.512637
6	-0.402039	3.812607	0.986909
6	-2.451526	5.947192	-2.073242
9	-3.726792	5.567209	-2.208595
6	1.415308	5.480923	1.066732
9	1.423961	5.471378	2.409429
6	-2.392801	0.934823	0.285024
16	-3.063803	0.964184	-1.260604
7	-2.164939	-0.197408	0.978515
6	-2.544967	-1.536324	0.568636
6	-1.353714	-2.505483	0.694227
6	-1.730953	-3.901022	0.121897
6	-0.753148	-4.259495	-1.004133
6	0.657438	-4.326070	-0.403797
6	0.945719	-2.976328	0.305351
7	-0.120443	-1.988672	0.049124
6	-0.296427	-1.839742	-1.408217
6	-0.756230	-3.165478	-2.087783
6	-2.056145	-2.981397	-2.831374
6	-3.081865	-3.828660	-2.879704
6	-3.703432	-2.046022	1.420244
6	-4.941432	-2.486051	0.853844
6	-5.931761	-2.976121	1.757014
7	-5.759080	-3.021551	3.108761
6	-4.617385	-2.593089	3.586965
6	-3.558403	-2.104144	2.784587
6	-7.161585	-3.445048	1.235207

6	-7.414902	-3.439376	-0.112682
6	-6.431177	-2.945756	-1.007176
6	-5.226288	-2.474163	-0.530921
9	-2.445744	7.270477	-1.841579
9	-1.853323	5.765249	-3.262041
9	1.738684	6.712754	0.664317
9	2.420961	4.661491	0.685187
1	-1.103949	-2.584763	1.755923
1	-1.680420	-4.660471	0.908756
1	-2.757832	-3.896563	-0.252363
1	1.894622	-2.555730	-0.045977
1	1.017651	-3.097414	1.391542
1	1.392099	-4.512840	-1.194595
1	0.724983	-5.155450	0.306728
1	-1.019198	-5.225684	-1.444024
1	0.001788	-3.439254	-2.835683
1	0.668531	-1.508185	-1.809937
1	-1.009697	-1.028153	-1.588665
1	-2.130065	-2.047032	-3.390469
1	-3.973090	-3.594738	-3.453915
1	-3.083072	-4.776304	-2.346833
1	-2.848091	-1.464870	-0.475843
1	-2.634745	-1.782400	3.262905
1	-4.517578	-2.090403	-1.255156
1	-4.492988	-2.632178	4.667581
1	-7.897007	-3.813327	1.943073
1	-8.364488	-3.807490	-0.482417
1	-1.738408	-0.123796	1.898680
1	-1.510491	1.818468	1.850639
1	-3.196662	3.609955	-0.922194
1	0.123709	3.288039	1.779221
1	-0.161681	6.665192	-0.853600
8	-6.600126	-2.905899	-2.353904
6	-7.847369	-3.312172	-2.882622
1	-7.776033	-3.172242	-3.961509
1	-8.052056	-4.368503	-2.671901
1	-8.668137	-2.697292	-2.495381
1	1.640203	0.617918	-2.194820
1	1.831662	2.255263	0.089028
6	3.500996	-0.332679	-2.746232
1	3.108029	-1.346467	-2.597555
1	3.371219	-0.086082	-3.807117
6	4.958448	-0.298530	-2.412448
6	5.667460	-1.332992	-1.949866
1	5.477370	0.652792	-2.540767
1	5.198118	-2.303238	-1.818407
6	7.117667	-1.176241	-1.652725
8	7.703514	-0.136759	-1.907447
6	7.863378	-2.326069	-1.043427
6	7.226918	-3.412585	-0.435709
6	9.261405	-2.279877	-1.073583
6	7.979768	-4.438305	0.128968
1	6.144597	-3.459852	-0.377264
6	10.011316	-3.308981	-0.520914
1	9.738791	-1.425131	-1.541121
6	9.370189	-4.391094	0.081771
1	7.479739	-5.274546	0.606887
1	11.095309	-3.270074	-0.557208
1	9.954742	-5.195723	0.517080

[3-4]TS_Cinchona-Thiourea_conf-8

Number of imaginary frequencies : 1
The smallest frequency is : -990.0332

Electronic energy= -3467.7275126
Zero-point correction= 0.936008

Thermal correction to Energy=	0.993926
Thermal correction to Enthalpy=	0.994870
Thermal correction to Gibbs Free Energy=	0.837166
Sum of electronic and zero-point Energies=	-3466.791504
Sum of electronic and thermal Energies=	-3466.733586
Sum of electronic and thermal Enthalpies=	-3466.732642
Sum of electronic and thermal Free Energies=	-3466.890347

 Cartesian Coordinates

6	2.320398	-2.045925	4.687824
6	3.499756	-2.889614	4.197332
6	4.021396	-2.081002	3.009856
7	2.807433	-1.455642	2.410347
6	1.681740	-1.541207	3.382782
6	2.482221	-1.863132	1.004082
6	2.118535	-3.345756	0.898812
6	2.371652	-3.928601	-0.498514
6	1.181974	-0.088077	3.495916
8	2.042578	0.723026	2.942709
8	1.558611	-0.974269	0.477156
8	0.140666	0.215031	4.047392
1	1.071338	-3.495246	1.194116
1	0.879258	-2.195190	3.030058
1	2.684942	-1.194799	5.273330
1	1.605786	-2.596939	5.299950
1	3.148547	-3.872095	3.864784
1	4.263553	-3.040429	4.962522
1	4.546489	-2.673184	2.256385
1	4.692430	-1.282365	3.340421
1	0.655080	-1.021030	0.889206
1	2.730281	-0.175846	2.492634
1	2.730592	-3.898131	1.620351
1	2.526306	-5.009425	-0.403745
7	2.058272	2.061689	0.287650
6	3.167560	1.777745	-0.522325
6	3.376826	2.323318	-1.792835
6	4.515407	1.963957	-2.506298
6	5.464129	1.082071	-1.995985
6	5.258016	0.574942	-0.719880
6	4.132091	0.923074	0.013506
6	4.769213	2.599929	-3.844613
9	5.548417	3.688476	-3.731935
6	6.190806	-0.443296	-0.136201
9	6.344782	-0.279006	1.188848
6	0.730116	1.992991	-0.068370
16	0.151368	2.233428	-1.631891
7	-0.048291	1.710365	0.990932
6	-1.496243	1.614342	0.996131
6	-1.944903	0.292184	1.651931
6	-3.474163	0.090527	1.460444
6	-3.709718	-1.214657	0.688538
6	-3.157671	-2.370371	1.532831
6	-1.665145	-2.075900	1.838392
7	-1.188540	-0.871512	1.130454
6	-1.428276	-1.041780	-0.314373
6	-2.942287	-1.197258	-0.645210
6	-3.398543	-0.175872	-1.655696
6	-4.542319	0.505711	-1.647689
6	-2.105550	2.793430	1.746633
6	-3.062357	3.676767	1.153167
6	-3.557459	4.738580	1.967630
7	-3.160578	4.947411	3.255127
6	-2.282299	4.116333	3.758497
6	-1.730863	3.023420	3.047663
6	-4.514923	5.628723	1.424271
6	-4.980405	5.483056	0.142502
6	-4.490913	4.423433	-0.662807
6	-3.546217	3.548570	-0.169355
9	5.401543	1.759015	-4.678383

9	3.636809	2.987553	-4.441917
9	7.402695	-0.411448	-0.696395
9	5.716582	-1.699373	-0.299706
1	-1.700453	0.343183	2.716148
1	-3.974907	0.037959	2.432547
1	-3.908264	0.938848	0.923136
1	-1.038624	-2.919288	1.523050
1	-1.496586	-1.908249	2.907887
1	-3.262228	-3.317163	0.991108
1	-3.729487	-2.461987	2.461488
1	-4.778344	-1.363488	0.504960
1	-3.083358	-2.183852	-1.110147
1	-0.871847	-1.931591	-0.616904
1	-0.985243	-0.192251	-0.843574
1	-2.699239	-0.005068	-2.476286
1	-4.774756	1.218670	-2.432852
1	-5.284769	0.387813	-0.862568
1	-1.810640	1.628883	-0.047298
1	-1.015850	2.372341	3.547753
1	-3.194635	2.767215	-0.833079
1	-1.975516	4.292298	4.788002
1	-4.870337	6.430502	2.063234
1	-5.715025	6.179098	-0.244392
1	0.409990	1.546759	1.883222
1	2.219819	1.813801	1.260723
1	2.656533	3.011456	-2.213225
1	3.993226	0.515912	1.010246
1	6.338205	0.804813	-2.574347
8	-4.905878	4.201496	-1.936699
6	-5.830518	5.108361	-2.504411
1	-6.009985	4.757715	-3.521099
1	-6.780070	5.115225	-1.956272
1	-5.424608	6.126021	-2.543541
1	3.308227	-3.517596	-0.893412
1	3.415520	-1.697895	0.453532
6	1.241067	-3.696393	-1.502383
1	1.024425	-2.625453	-1.599590
1	1.572471	-4.037232	-2.491802
6	-0.002765	-4.455296	-1.132794
6	-1.227825	-4.237624	-1.623419
1	0.098587	-5.267115	-0.409719
1	-1.397974	-3.445955	-2.347686
6	-2.378455	-5.049131	-1.137877
8	-2.241594	-5.845382	-0.222033
6	-3.729218	-4.844889	-1.757403
6	-3.922265	-4.152694	-2.957399
6	-4.835976	-5.375481	-1.085396
6	-5.205033	-3.991686	-3.473084
1	-3.078574	-3.747758	-3.506479
6	-6.115627	-5.208591	-1.597668
1	-4.666606	-5.913337	-0.158313
6	-6.301320	-4.515129	-2.793237
1	-5.347157	-3.457322	-4.406678
1	-6.969894	-5.617646	-1.067629
1	-7.300994	-4.383371	-3.195389

[3-4]TS_Cinchona-Thiourea_conf-9

Number of imaginary frequencies : 1
The smallest frequency is : -979.7978

Electronic energy=	-3467.7273687
Zero-point correction=	0.936938
Thermal correction to Energy=	0.994719
Thermal correction to Enthalpy=	0.995663
Thermal correction to Gibbs Free Energy=	0.838328
Sum of electronic and zero-point Energies=	-3466.790431

Sum of electronic and thermal Energies=	-3466.732649
Sum of electronic and thermal Enthalpies=	-3466.731705
Sum of electronic and thermal Free Energies=	-3466.889041

 Cartesian Coordinates

6	-2.226168	-3.196167	-2.546863
6	-3.596468	-2.874061	-1.942304
6	-3.464171	-1.398243	-1.567449
7	-2.028971	-1.235350	-1.196505
6	-1.258254	-2.433070	-1.629341
6	-1.763762	-0.778573	0.200633
6	-2.120560	-1.811892	1.269722
6	-2.312432	-1.131555	2.638584
6	-0.046152	-1.833644	-2.369138
8	-0.273182	-0.582621	-2.652036
8	-0.447371	-0.351293	0.287963
8	0.958560	-2.472744	-2.630093
1	-1.313556	-2.548759	1.315318
1	-0.922079	-3.040712	-0.785473
1	-2.161901	-2.796795	-3.565211
1	-1.994682	-4.261302	-2.583433
1	-3.764933	-3.477901	-1.043283
1	-4.421738	-3.054279	-2.633847
1	-4.105291	-1.080227	-0.741021
1	-3.675801	-0.748561	-2.422065
1	0.190104	-1.109212	0.327165
1	-1.299087	-0.531977	-1.986176
1	-3.031050	-2.352031	0.982766
1	-1.944351	-0.100740	2.581990
7	0.998369	1.715712	-1.280137
6	0.082215	2.698050	-0.868421
6	0.459477	3.935702	-0.339152
6	-0.526156	4.845876	0.025432
6	-1.882272	4.569079	-0.130060
6	-2.238336	3.346295	-0.681120
6	-1.271392	2.421099	-1.052176
6	-0.121158	6.154018	0.644073
9	1.102712	6.535853	0.256811
6	-3.676439	2.940654	-0.809615
9	-3.918457	2.323488	-1.976667
6	1.981994	1.156237	-0.501902
16	2.683074	1.911632	0.831066
7	2.309568	-0.079740	-0.924694
6	3.373597	-0.905559	-0.387092
6	2.866852	-2.330347	-0.096290
6	3.975628	-3.151870	0.619978
6	3.438031	-3.640834	1.970760
6	2.237227	-4.553805	1.694180
6	1.213544	-3.759650	0.839634
7	1.606172	-2.344768	0.687787
6	1.799479	-1.754823	2.026575
6	2.948087	-2.451006	2.818146
6	4.011835	-1.464626	3.233443
6	5.329473	-1.654458	3.219508
6	4.542871	-0.974518	-1.364840
6	5.873726	-0.593161	-1.003781
6	6.885893	-0.744935	-1.998327
7	6.638807	-1.204419	-3.258050
6	5.403412	-1.524705	-3.552667
6	4.324749	-1.435570	-2.639915
6	8.221738	-0.408451	-1.672029
6	8.558160	0.055050	-0.425843
6	7.548358	0.213824	0.557522
6	6.236363	-0.096744	0.269444
9	-0.973765	7.139075	0.318523
9	-0.105973	6.085894	1.984929
9	-4.512668	3.978653	-0.712891
9	-4.017529	2.065005	0.158093
1	2.608703	-2.792700	-1.053165

1	4.269346	-4.010503	0.007654
1	4.871140	-2.541454	0.763489
1	0.224271	-3.794232	1.307364
1	1.119250	-4.177356	-0.168433
1	1.786064	-4.877625	2.638213
1	2.564089	-5.453397	1.163696
1	4.214068	-4.192361	2.510538
1	2.517303	-2.860769	3.742874
1	0.843970	-1.850800	2.555240
1	1.987448	-0.682023	1.908669
1	3.630208	-0.506670	3.590381
1	6.011307	-0.875299	3.546377
1	5.781212	-2.581537	2.875366
1	3.689549	-0.435757	0.544272
1	3.330961	-1.741873	-2.961653
1	5.500795	0.063071	1.048941
1	5.219037	-1.887875	-4.562149
1	8.972144	-0.534518	-2.445535
1	9.590328	0.299821	-0.204561
1	1.832486	-0.452437	-1.741747
1	0.585149	1.053901	-1.935561
1	1.507113	4.178944	-0.222510
1	-1.572472	1.471456	-1.483721
1	-2.636308	5.292752	0.158269
8	7.795697	0.668991	1.812987
6	9.114341	1.070519	2.128341
1	9.080549	1.432979	3.156044
1	9.818658	0.232223	2.068405
1	9.455865	1.881333	1.474404
1	-1.707105	-1.626208	3.403354
1	-2.397705	0.108630	0.325941
6	-3.777117	-1.138692	3.113806
1	-4.063955	-2.154328	3.409940
1	-3.857554	-0.504959	4.005511
6	-4.726668	-0.646101	2.066078
6	-5.782303	-1.339496	1.624618
1	-4.536634	0.334534	1.626058
1	-6.019158	-2.309928	2.053742
6	-6.648976	-0.805759	0.538636
8	-6.224077	0.027427	-0.247171
6	-8.045339	-1.328599	0.407128
6	-8.677719	-2.040801	1.430511
6	-8.736492	-1.067026	-0.780617
6	-9.983814	-2.491361	1.263424
1	-8.164802	-2.226992	2.368688
6	-10.035537	-1.526587	-0.950190
1	-8.233904	-0.501964	-1.558822
6	-10.660040	-2.240916	0.072373
1	-10.474494	-3.035385	2.063953
1	-10.564815	-1.327591	-1.876532
1	-11.676386	-2.599310	-0.058450

[4-5]TS-anti_Cinchona-Thiourea_conf-1

Number of imaginary frequencies : 1
The smallest frequency is : -168.5960

Electronic energy=	-3467.7214477
Zero-point correction=	0.936984
Thermal correction to Energy=	0.994965
Thermal correction to Enthalpy=	0.995909
Thermal correction to Gibbs Free Energy=	0.839320
Sum of electronic and zero-point Energies=	-3466.784463
Sum of electronic and thermal Energies=	-3466.726483
Sum of electronic and thermal Enthalpies=	-3466.725539
Sum of electronic and thermal Free Energies=	-3466.882128

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Cartesian Coordinates

6	-0.023545	-3.814916	-1.130300
6	-0.702815	-4.982974	-1.845130
6	-1.467214	-5.652105	-0.696113
6	-0.501725	-5.560563	0.494528
7	0.397552	-4.443348	0.135807
6	1.320387	-3.945944	0.916967
6	1.920784	-4.762249	2.029267
6	2.794773	-5.928565	1.527068
6	-1.042885	-2.668479	-0.917991
8	-1.478600	-2.126319	-1.930891
8	-1.362778	-2.388279	0.291140
8	0.395612	-2.653092	2.180740
1	0.856591	-3.424100	-1.648507
1	-1.346969	-4.625377	-2.648208
1	0.049265	-5.661061	-2.260813
1	-2.377232	-5.086375	-0.478367
1	-1.749264	-6.684279	-0.908363
1	-1.007846	-5.335453	1.437272
1	0.085249	-6.475366	0.617806
1	1.106104	-5.143394	2.650327
1	-0.405300	-2.582047	1.594654
1	2.268985	-6.476202	0.736582
1	2.935133	-6.629933	2.354454
1	1.903651	-3.148658	0.463103
1	2.512098	-4.090683	2.657663
6	4.178474	-5.504985	1.001731
1	4.693307	-6.399202	0.630226
1	4.782554	-5.088827	1.815488
6	4.029330	-4.503528	-0.094701
6	4.559925	-3.276648	-0.115287
1	3.350379	-4.767780	-0.908484
1	5.253777	-2.957297	0.657212
6	4.103863	-2.305935	-1.148911
8	3.082609	-2.533728	-1.786667
6	4.841331	-1.024088	-1.346512
6	6.045865	-0.730867	-0.697553
6	4.268825	-0.074571	-2.201923
6	6.655615	0.506451	-0.889870
1	6.523618	-1.461123	-0.052572
6	4.874707	1.160561	-2.389515
1	3.342701	-0.323258	-2.707716
6	6.067622	1.452855	-1.726726
1	7.589935	0.731059	-0.385684
1	4.414471	1.891074	-3.047994
1	6.541461	2.419457	-1.866551
7	-2.583976	0.079432	0.424619
6	-3.964104	0.249372	0.268773
6	-4.720804	1.187236	0.979003
6	-6.096603	1.228869	0.792881
6	-6.749699	0.350086	-0.066472
6	-5.985270	-0.583027	-0.753970
6	-4.604055	-0.636739	-0.601514
6	-6.901740	2.271377	1.514176
9	-7.073313	3.374949	0.769658
6	-6.636477	-1.575311	-1.672955
9	-6.084172	-1.561281	-2.894951
6	-1.610722	1.013103	0.566415
16	-1.846068	2.677872	0.696470
7	-0.369286	0.455927	0.595459
6	0.843925	1.232228	0.432070
6	2.076975	0.409215	0.867295
6	3.320804	1.328342	1.023736
6	3.787677	1.290132	2.487135
6	4.244601	-0.140336	2.792626
6	3.063598	-1.087063	2.466445
7	1.837975	-0.340289	2.122691
6	1.508355	0.574898	3.229387
6	2.632266	1.635843	3.447272

6	2.102658	3.044942	3.345139
6	2.706116	4.086989	2.777547
6	1.037658	1.679041	-1.018347
6	1.465660	2.996151	-1.380400
6	1.751336	3.236079	-2.756808
7	1.601674	2.293148	-3.731976
6	1.132467	1.124791	-3.369161
6	0.841476	0.771177	-2.028712
6	2.213866	4.516010	-3.147444
6	2.370676	5.529350	-2.236330
6	2.053971	5.297442	-0.873386
6	1.607001	4.060268	-0.461545
9	-8.129744	1.822682	1.824190
9	-6.317303	2.657864	2.656923
9	-7.948190	-1.342156	-1.822760
9	-6.509227	-2.832265	-1.212102
1	2.261585	-0.352370	0.094475
1	4.133954	0.988372	0.375775
1	3.082977	2.350753	0.725120
1	2.822285	-1.737055	3.314651
1	3.299270	-1.734187	1.612305
1	4.539919	-0.231815	3.843021
1	5.118304	-0.388308	2.179860
1	4.618323	1.987359	2.632313
1	3.010780	1.514625	4.472090
1	1.366377	-0.042404	4.121917
1	0.546203	1.047855	3.009068
1	1.127885	3.201177	3.810167
1	2.241451	5.067856	2.769738
1	3.674969	4.008522	2.290545
1	0.757093	2.109254	1.077132
1	0.459042	-0.226461	-1.825813
1	1.345580	3.940560	0.583108
1	0.985130	0.386761	-4.155604
1	2.427930	4.670467	-4.200172
1	2.719544	6.500156	-2.567698
1	-0.314466	-0.549459	0.456193
1	-2.251919	-0.887352	0.260199
1	-4.237787	1.865718	1.668831
1	-4.003766	-1.348317	-1.165519
1	-7.825391	0.389719	-0.191014
8	2.164722	6.248660	0.090840
6	2.520143	7.558354	-0.306412
1	2.506191	8.162894	0.600809
1	3.526489	7.590973	-0.740937
1	1.800653	7.970611	-1.023059
1	0.822816	-1.746820	2.138487

[4-5]TS-anti_Cinchona-Thiourea_conf-2

Number of imaginary frequencies : 1
The smallest frequency is : -165.6932

Electronic energy=	-3467.7170949
Zero-point correction=	0.936798
Thermal correction to Energy=	0.994882
Thermal correction to Enthalpy=	0.995826
Thermal correction to Gibbs Free Energy=	0.838549
Sum of electronic and zero-point Energies=	-3466.780297
Sum of electronic and thermal Energies=	-3466.722213
Sum of electronic and thermal Enthalpies=	-3466.721268
Sum of electronic and thermal Free Energies=	-3466.878545

Cartesian Coordinates

6	-0.531129	-3.698131	0.678537
6	-0.104342	-4.954355	1.437078

6	0.673028	-5.720838	0.360967
6	-0.154132	-5.502249	-0.912394
7	-0.888003	-4.246050	-0.643834
6	-1.632777	-3.617928	-1.510174
6	-2.232225	-4.319170	-2.691871
6	-3.388538	-5.252604	-2.293999
6	0.642203	-2.687334	0.612229
8	1.043209	-2.242753	1.684709
8	1.099657	-2.402404	-0.549346
8	-0.407519	-2.430467	-2.669995
1	-1.408047	-3.211675	1.117121
1	0.493845	-4.693170	2.309638
1	-0.986522	-5.515758	1.760506
1	1.666315	-5.280088	0.237434
1	0.794598	-6.781227	0.585769
1	0.458616	-5.383234	-1.809812
1	-0.872911	-6.310446	-1.076625
1	-1.450673	-4.880461	-3.210757
1	0.315595	-2.463184	-1.991094
1	-3.024880	-6.043792	-1.627759
1	-3.737856	-5.746459	-3.205230
1	-2.127553	-2.732738	-1.120747
1	-2.591401	-3.556566	-3.385979
6	-4.575267	-4.546238	-1.621864
1	-5.409554	-5.258612	-1.579841
1	-4.911979	-3.696697	-2.228542
6	-4.277545	-4.107313	-0.221902
6	-4.524462	-2.898197	0.293209
1	-3.816551	-4.844789	0.438470
1	-5.006452	-2.130823	-0.306082
6	-4.168918	-2.615007	1.715494
8	-3.693969	-3.492878	2.420385
6	-4.388191	-1.242937	2.263664
6	-4.615487	-0.129379	1.449111
6	-4.321073	-1.075685	3.652243
6	-4.762694	1.135318	2.012367
1	-4.658371	-0.235144	0.369777
6	-4.493927	0.180611	4.215012
1	-4.128879	-1.947178	4.269478
6	-4.709516	1.288567	3.394732
1	-4.913528	2.000282	1.373407
1	-4.440821	0.306068	5.291507
1	-4.815284	2.275258	3.834357
7	2.512054	-0.028831	-0.467134
6	3.883815	0.031731	-0.197270
6	4.754406	0.968677	-0.763243
6	6.110482	0.898288	-0.468190
6	6.633246	-0.091600	0.358197
6	5.756969	-1.023619	0.899108
6	4.393020	-0.966596	0.637941
6	7.030516	1.943166	-1.031858
9	7.108144	3.022245	-0.237384
6	6.262286	-2.125578	1.784438
9	5.678272	-2.102936	2.991606
6	1.614984	0.977010	-0.620980
16	1.966742	2.625249	-0.618402
7	0.347086	0.508353	-0.785329
6	-0.821713	1.357943	-0.662200
6	-2.060767	0.669526	-1.278202
6	-3.202047	1.698536	-1.513840
6	-3.481850	1.799593	-3.022307
6	-4.014582	0.439997	-3.490639
6	-2.979183	-0.635585	-3.078458
7	-1.743460	-0.029717	-2.544659
6	-1.204889	0.911274	-3.543666
6	-2.188661	2.093893	-3.806648
6	-1.551998	3.433228	-3.527940
6	-2.138174	4.494462	-2.977975
6	-1.101825	1.705740	0.802361
6	-1.451860	3.021192	1.243580

6	-1.752721	3.187211	2.628257
7	-1.690344	2.175440	3.539388
6	-1.323697	0.996058	3.103536
6	-1.028304	0.713717	1.748320
6	-2.131375	4.468835	3.097531
6	-2.196737	5.550376	2.256640
6	-1.862648	5.389411	0.887802
6	-1.493335	4.154686	0.399900
9	8.282648	1.479005	-1.176302
9	6.623303	2.374834	-2.234906
9	7.586760	-2.053044	1.979496
9	6.003722	-3.335722	1.259334
1	-2.393401	-0.110562	-0.576085
1	-4.119555	1.385232	-1.004214
1	-2.933087	2.673551	-1.102690
1	-2.693819	-1.262980	-3.929676
1	-3.384710	-1.300089	-2.303451
1	-4.160023	0.443325	-4.575582
1	-4.987796	0.238157	-3.031520
1	-4.225075	2.579000	-3.213544
1	-2.446031	2.082517	-4.874979
1	-1.021991	0.336802	-4.456899
1	-0.234262	1.270048	-3.188975
1	-0.509331	3.519232	-3.837854
1	-1.595571	5.423522	-2.835165
1	-3.171503	4.483499	-2.639692
1	-0.607994	2.273470	-1.219162
1	-0.709067	-0.292327	1.487196
1	-1.213066	4.091472	-0.645098
1	-1.259082	0.195958	3.838496
1	-2.359268	4.565194	4.154400
1	-2.487500	6.518592	2.646625
1	0.218941	-0.497638	-0.717217
1	2.105660	-0.976171	-0.384006
1	4.372662	1.732879	-1.426764
1	3.704290	-1.678601	1.088915
1	7.694811	-0.137596	0.569226
8	-1.882494	6.408919	-0.011018
6	-2.156412	7.710812	0.468086
1	-2.078581	8.372558	-0.395069
1	-3.168379	7.785564	0.883861
1	-1.427933	8.022733	1.225570
1	-0.774681	-1.505112	-2.599020

[4-5]TS-anti_Cinchona-Thiourea_conf-3

Number of imaginary frequencies : 1
The smallest frequency is : -180.8831

Electronic energy= -3467.7082535
Zero-point correction= 0.936612
Thermal correction to Energy= 0.995125
Thermal correction to Enthalpy= 0.996069
Thermal correction to Gibbs Free Energy= 0.833002
Sum of electronic and zero-point Energies= -3466.771642
Sum of electronic and thermal Energies= -3466.713129
Sum of electronic and thermal Enthalpies= -3466.712185
Sum of electronic and thermal Free Energies= -3466.875252

Cartesian Coordinates

6	2.540669	-0.302548	1.403747
6	3.687914	0.580060	1.900090
6	4.297914	1.075153	0.583424
6	4.234072	-0.150938	-0.337267
7	3.162526	-0.984503	0.254249
6	2.685694	-2.066619	-0.300939

6	3.504617	-2.943943	-1.198951
6	4.105090	-4.112780	-0.397622
6	1.332597	0.581582	1.007180
8	0.742253	1.140313	1.929771
8	1.068363	0.677291	-0.240169
8	1.415534	-1.412433	-1.756281
1	2.213003	-1.043825	2.137033
1	3.315555	1.379909	2.540349
1	4.408322	-0.022475	2.464053
1	3.684005	1.881144	0.172666
1	5.319365	1.443595	0.691940
1	3.967570	0.100206	-1.366852
1	5.168096	-0.716676	-0.338397
1	4.285362	-2.365762	-1.701336
1	1.310188	-0.513423	-1.351722
1	4.524659	-4.826118	-1.114913
1	3.298832	-4.640019	0.125859
1	1.885532	-2.552765	0.257625
1	2.843520	-3.340562	-1.970058
6	5.192338	-3.727055	0.613403
1	5.443009	-4.625598	1.192585
1	4.821230	-2.983646	1.329758
6	6.447021	-3.235452	-0.038976
6	7.146805	-2.163067	0.343432
1	6.827731	-3.809757	-0.885154
1	6.804121	-1.560623	1.179333
6	8.378619	-1.766500	-0.397096
8	8.783584	-2.438870	-1.330643
6	9.091730	-0.506194	-0.009132
6	8.794123	0.221745	1.147780
6	10.104298	-0.050932	-0.861434
6	9.494953	1.388000	1.441773
1	8.031944	-0.116574	1.841291
6	10.799064	1.114877	-0.570071
1	10.328235	-0.629135	-1.751545
6	10.493830	1.837555	0.583055
1	9.261236	1.944062	2.343799
1	11.578674	1.463052	-1.239904
1	11.036354	2.749235	0.812827
7	-1.444331	1.788280	-0.594100
6	-1.663004	3.171991	-0.560802
6	-2.606043	3.833906	-1.352377
6	-2.698248	5.218489	-1.278995
6	-1.864864	5.968053	-0.453375
6	-0.925805	5.294811	0.316413
6	-0.822176	3.908932	0.277200
6	-3.748643	5.926837	-2.085447
9	-4.884296	6.095812	-1.390244
6	0.023664	6.053603	1.197091
9	0.056468	5.553447	2.441213
6	-2.348386	0.777820	-0.608672
16	-4.015137	0.946802	-0.777567
7	-1.753893	-0.441685	-0.466149
6	-2.501636	-1.628514	-0.094153
6	-1.638781	-2.896183	-0.287781
6	-2.518279	-4.177468	-0.236534
6	-2.445972	-4.888359	-1.598330
6	-1.002067	-5.358950	-1.806597
6	-0.082280	-4.124510	-1.645859
7	-0.858906	-2.871246	-1.545934
6	-1.747659	-2.762393	-2.715290
6	-2.792161	-3.921262	-2.748209
6	-4.209662	-3.405601	-2.759065
6	-5.254740	-3.932213	-2.124399
6	-2.967452	-1.562287	1.363445
6	-4.279983	-1.945643	1.786405
6	-4.545002	-1.935360	3.187967
7	-3.631923	-1.548267	4.123651
6	-2.460428	-1.153259	3.691956
6	-2.082371	-1.148360	2.327853

6	-5.824042	-2.334806	3.646233
6	-6.810567	-2.715850	2.773340
6	-6.553057	-2.697948	1.378862
6	-5.318769	-2.313274	0.901764
9	-3.342264	7.151104	-2.461718
9	-4.068833	5.251770	-3.198622
9	-0.299981	7.350552	1.294348
9	1.283476	5.995656	0.729401
1	-0.894757	-2.916000	0.520650
1	-2.161378	-4.856866	0.544330
1	-3.551153	-3.926237	0.010718
1	0.600689	-4.019537	-2.495539
1	0.529237	-4.203620	-0.738347
1	-0.887481	-5.800703	-2.801567
1	-0.745433	-6.130294	-1.074111
1	-3.125617	-5.745475	-1.609593
1	-2.649925	-4.470332	-3.689578
1	-1.109682	-2.776763	-3.603999
1	-2.235582	-1.783986	-2.684454
1	-4.371228	-2.521664	-3.378343
1	-6.243084	-3.492641	-2.213987
1	-5.173130	-4.808403	-1.485656
1	-3.371149	-1.680545	-0.753365
1	-1.092879	-0.782240	2.064342
1	-5.182435	-2.284585	-0.172575
1	-1.746430	-0.818438	4.442247
1	-5.997256	-2.320845	4.717353
1	-7.780004	-3.014308	3.154093
1	-0.753922	-0.437363	-0.284309
1	-0.472058	1.510870	-0.380397
1	-3.248597	3.272046	-2.016795
1	-0.110056	3.378919	0.907680
1	-1.944722	7.048280	-0.415822
8	-7.475776	-3.046887	0.444277
6	-8.778851	-3.373542	0.886341
1	-9.357828	-3.583942	-0.013275
1	-8.777987	-4.264248	1.525864
1	-9.243000	-2.538866	1.424227
1	0.510874	-1.843371	-1.683276

[4-5]TS-anti_Cinchona-Thiourea_conf-4

Number of imaginary frequencies : 1

The smallest frequency is : -210.2683

Electronic energy=	-3467.7072823
Zero-point correction=	0.937285
Thermal correction to Energy=	0.995168
Thermal correction to Enthalpy=	0.996112
Thermal correction to Gibbs Free Energy=	0.838378
Sum of electronic and zero-point Energies=	-3466.769998
Sum of electronic and thermal Energies=	-3466.712114
Sum of electronic and thermal Enthalpies=	-3466.711170
Sum of electronic and thermal Free Energies=	-3466.868904

Cartesian Coordinates

6	-1.382519	-2.875095	-0.338984
6	-1.459682	-4.298019	0.211764
6	-1.115230	-5.121698	-1.033666
6	-1.881727	-4.407201	-2.152236
7	-2.004931	-3.019430	-1.660138
6	-2.529591	-2.021355	-2.347100
6	-3.453909	-2.349943	-3.495599
6	-4.590696	-1.346161	-3.739388
6	0.093066	-2.404044	-0.407604
8	0.743794	-2.472830	0.632653

8	0.524782	-1.950351	-1.528298
8	-1.106961	-1.158974	-3.280667
1	-1.954097	-2.149290	0.255108
1	-0.762709	-4.432902	1.038053
1	-2.478070	-4.515832	0.550202
1	-0.038243	-5.075031	-1.223105
1	-1.404059	-6.170520	-0.954125
1	-1.367507	-4.430745	-3.116885
1	-2.883432	-4.833582	-2.271394
1	-3.904397	-3.320458	-3.265787
1	-0.375806	-1.559603	-2.694797
1	-5.321305	-1.847424	-4.381592
1	-4.233169	-0.480682	-4.303499
1	-2.736589	-1.132308	-1.755253
1	-2.859206	-2.483353	-4.402582
6	-5.299272	-0.856505	-2.456522
1	-6.280755	-0.456707	-2.736192
1	-4.745774	-0.027093	-1.998137
6	-5.457518	-1.947726	-1.442380
6	-4.938359	-1.899551	-0.211520
1	-5.979847	-2.856815	-1.743001
1	-4.416563	-1.005757	0.122667
6	-5.009590	-3.077571	0.698572
8	-5.373863	-4.164115	0.276807
6	-4.583613	-2.917740	2.124757
6	-4.352376	-1.670661	2.715060
6	-4.418272	-4.079706	2.889240
6	-3.957406	-1.586546	4.048346
1	-4.490602	-0.751710	2.154849
6	-4.017670	-3.995586	4.215090
1	-4.609131	-5.039492	2.420025
6	-3.784269	-2.748003	4.795561
1	-3.762922	-0.613160	4.489579
1	-3.882883	-4.900679	4.798639
1	-3.464446	-2.682488	5.830786
7	2.610986	-0.184884	-0.678641
6	3.919672	-0.556581	-0.335826
6	5.031258	0.265377	-0.536835
6	6.296055	-0.216418	-0.221412
6	6.488970	-1.503888	0.270394
6	5.373601	-2.311506	0.449531
6	4.094291	-1.850119	0.160786
6	7.479063	0.692725	-0.392674
9	7.678148	1.464307	0.687096
6	5.518387	-3.703239	0.993712
9	4.996711	-3.812902	2.225546
6	1.973600	0.992461	-0.445780
16	2.667444	2.372005	0.228265
7	0.669369	0.948202	-0.825396
6	-0.305694	1.945251	-0.434250
6	-1.555420	1.850479	-1.348529
6	-2.426114	3.134365	-1.262100
6	-2.387288	3.856019	-2.621067
6	-3.099655	2.965897	-3.643961
6	-2.451313	1.566680	-3.557292
7	-1.205300	1.575432	-2.762034
6	-0.312433	2.624582	-3.288174
6	-0.936930	4.045439	-3.108705
6	-0.080860	4.947000	-2.252854
6	-0.512814	5.868644	-1.394638
6	-0.736332	1.754437	1.024462
6	-1.050429	2.835296	1.908749
6	-1.607376	2.502320	3.180527
7	-1.792210	1.220379	3.609879
6	-1.390425	0.260978	2.812806
6	-0.870427	0.479923	1.515993
6	-1.966912	3.549248	4.063446
6	-1.759377	4.865114	3.736966
6	-1.159218	5.190196	2.493753
6	-0.813047	4.194638	1.605785

9	8.613352	0.002075	-0.591170
9	7.326316	1.520653	-1.437295
9	6.801255	-4.085405	1.072437
9	4.879681	-4.601769	0.226653
1	-2.134972	0.976827	-1.012886
1	-3.464221	2.877833	-1.023321
1	-2.073885	3.791311	-0.466732
1	-2.211488	1.165821	-4.547854
1	-3.125355	0.854592	-3.071307
1	-2.993341	3.384762	-4.649833
1	-4.170657	2.906762	-3.424806
1	-2.889321	4.824730	-2.545013
1	-0.986893	4.512140	-4.102245
1	-0.143255	2.398668	-4.344946
1	0.652614	2.547578	-2.779781
1	0.995172	4.828994	-2.390562
1	0.184816	6.489003	-0.840674
1	-1.569245	6.040379	-1.202414
1	0.164207	2.924779	-0.555765
1	-0.546314	-0.380153	0.940985
1	-0.327757	4.486990	0.681368
1	-1.488213	-0.759750	3.177667
1	-2.398173	3.269856	5.019376
1	-2.036747	5.643666	4.437652
1	0.328094	0.063768	-1.192621
1	2.003274	-0.971320	-0.938560
1	4.905965	1.260712	-0.942131
1	3.216571	-2.471023	0.331766
1	7.483492	-1.869372	0.497435
8	-0.891325	6.462610	2.103171
6	-1.150203	7.509007	3.019403
1	-0.825909	8.426435	2.527575
1	-2.218704	7.587485	3.252527
1	-0.582696	7.379916	3.948206
1	-1.034646	-0.176374	-3.106973

[4-5]TS-syn_Cinchona-Thiourea_conf-1

Number of imaginary frequencies : 1

The smallest frequency is : -168.2121

Electronic energy=	-3467.7222195
Zero-point correction=	0.937241
Thermal correction to Energy=	0.995205
Thermal correction to Enthalpy=	0.996149
Thermal correction to Gibbs Free Energy=	0.839282
Sum of electronic and zero-point Energies=	-3466.784978
Sum of electronic and thermal Energies=	-3466.727014
Sum of electronic and thermal Enthalpies=	-3466.726070
Sum of electronic and thermal Free Energies=	-3466.882938

Cartesian Coordinates

6	-2.543427	-4.139523	-0.692682
6	-3.932260	-4.773586	-0.721520
6	-4.554119	-4.248332	0.575324
6	-3.405642	-4.358402	1.579464
7	-2.193479	-4.218959	0.741449
6	-1.013026	-4.012651	1.273115
6	0.225747	-4.031052	0.432892
6	0.702252	-5.464780	0.170136
6	-2.566005	-2.680428	-1.235591
8	-3.317814	-2.440922	-2.174516
8	-1.760920	-1.860413	-0.669448
8	-1.024172	-2.112621	1.851082
1	-1.808539	-4.701032	-1.278857
1	-4.470108	-4.464905	-1.616762

1	-3.852754	-5.865146	-0.697003
1	-4.847797	-3.201848	0.442166
1	-5.431838	-4.811536	0.895162
1	-3.409779	-3.574918	2.340868
1	-3.385638	-5.337748	2.068965
1	1.003778	-3.481390	0.966542
1	-1.425284	-1.839348	0.992086
1	-0.090008	-6.047907	-0.312145
1	0.926633	-5.957809	1.123683
1	-0.921956	-4.294978	2.318742
1	0.038815	-3.500120	-0.504737
6	1.954484	-5.473778	-0.720985
1	1.706597	-5.087412	-1.715884
1	2.288680	-6.510889	-0.844494
6	3.059306	-4.664913	-0.117951
6	3.656564	-3.621885	-0.703838
1	3.384183	-4.935410	0.888617
1	3.378342	-3.333211	-1.712690
6	4.729728	-2.875156	0.011877
8	4.977958	-3.120337	1.184619
6	5.498551	-1.816433	-0.713155
6	5.101382	-1.303357	-1.951527
6	6.633356	-1.287692	-0.083794
6	5.823032	-0.273376	-2.549397
1	4.218627	-1.681439	-2.454024
6	7.357514	-0.267936	-0.684324
1	6.923948	-1.689020	0.881694
6	6.949472	0.243446	-1.917105
1	5.489277	0.134120	-3.498250
1	8.236832	0.135429	-0.192371
1	7.507756	1.049473	-2.383151
7	-2.258496	0.792395	-0.295214
6	-3.584092	1.234377	-0.270715
6	-4.066967	2.367038	0.395109
6	-5.431836	2.636627	0.371517
6	-6.342498	1.815427	-0.282420
6	-5.845656	0.696364	-0.939592
6	-4.489593	0.404963	-0.949285
6	-5.929536	3.887314	1.038931
9	-5.928506	4.934668	0.197790
6	-6.770134	-0.252924	-1.646296
9	-6.444746	-0.396924	-2.937857
6	-1.095512	1.321818	0.164442
16	-0.878892	2.887405	0.754566
7	-0.078383	0.414322	0.106576
6	1.323848	0.761028	0.256547
6	2.115937	-0.333836	1.009941
6	3.478585	0.225254	1.510553
6	3.488033	0.224357	3.049157
6	3.431135	-1.235753	3.515685
6	2.217735	-1.898370	2.821877
7	1.358710	-0.897552	2.150025
6	0.995671	0.158711	3.116989
6	2.249517	0.937888	3.619607
6	2.154717	2.415501	3.333213
6	3.144487	3.214163	2.938669
6	1.966879	1.007168	-1.108607
6	2.737339	2.173772	-1.409913
6	3.324719	2.254189	-2.708433
7	3.153194	1.303607	-3.670722
6	2.409034	0.268293	-3.369625
6	1.811174	0.071516	-2.102222
6	4.129192	3.374847	-3.027388
6	4.342524	4.381884	-2.121305
6	3.737123	4.310697	-0.840185
6	2.946682	3.233799	-0.500069
9	-7.190945	3.747944	1.478412
9	-5.174138	4.232859	2.090953
9	-8.047075	0.154238	-1.596932
9	-6.727454	-1.481930	-1.099955

1	2.281582	-1.173421	0.318669
1	4.302762	-0.400621	1.158350
1	3.650331	1.230000	1.116018
1	1.592037	-2.451377	3.531647
1	2.568144	-2.601697	2.057804
1	3.332873	-1.278978	4.605543
1	4.348063	-1.762177	3.236570
1	4.402062	0.700809	3.416002
1	2.287992	0.833753	4.713126
1	0.476686	-0.335740	3.943831
1	0.275634	0.831854	2.640998
1	1.168198	2.852091	3.493619
1	2.976989	4.274640	2.777654
1	4.151752	2.849501	2.752786
1	1.343604	1.677574	0.847202
1	1.224426	-0.829619	-1.938314
1	2.486499	3.236456	0.481198
1	2.265758	-0.477041	-4.150528
1	4.566791	3.411610	-4.019931
1	4.960959	5.228437	-2.394900
1	-0.290707	-0.477285	-0.335271
1	-2.169856	-0.169285	-0.662196
1	-3.390168	3.020036	0.927400
1	-4.124685	-0.471000	-1.487781
1	-7.402778	2.037890	-0.277578
8	3.889329	5.267030	0.110212
6	4.637763	6.421606	-0.218170
1	4.612592	7.057772	0.666688
1	5.680373	6.175313	-0.451009
1	4.192555	6.962490	-1.061124
1	-0.117134	-1.656998	1.886507

[4-5]TS-syn_Cinchona-Thiourea_conf-2

Number of imaginary frequencies : 1

The smallest frequency is : -167.0845

Electronic energy=	-3467.7229268
Zero-point correction=	0.937987
Thermal correction to Energy=	0.995830
Thermal correction to Enthalpy=	0.996774
Thermal correction to Gibbs Free Energy=	0.840538
Sum of electronic and zero-point Energies=	-3466.784940
Sum of electronic and thermal Energies=	-3466.727097
Sum of electronic and thermal Enthalpies=	-3466.726152
Sum of electronic and thermal Free Energies=	-3466.882389

Cartesian Coordinates

6	2.532112	4.069895	-0.681599
6	3.962750	4.604924	-0.658830
6	4.511359	4.004185	0.638175
6	3.347731	4.169231	1.616384
7	2.151328	4.135698	0.745104
6	0.944764	3.995124	1.243020
6	-0.268968	4.147803	0.379738
6	-0.595464	5.629071	0.146792
6	2.471900	2.629793	-1.268194
8	3.214131	2.376394	-2.211323
8	1.620494	1.836086	-0.731592
8	0.813303	2.093407	1.737801
1	1.855181	4.696773	-1.271109
1	4.502432	4.281674	-1.547942
1	3.959575	5.698416	-0.606989
1	4.732652	2.943327	0.484169
1	5.418663	4.493776	0.994595
1	3.279013	3.369824	2.357763

1	3.383045	5.135633	2.130349
1	-1.105874	3.668385	0.890919
1	1.234872	1.836061	0.878901
1	0.251074	6.136516	-0.328371
1	-0.760566	6.120668	1.113127
1	0.849508	4.252362	2.294701
1	-0.118345	3.617546	-0.565703
6	-1.844693	5.797673	-0.733322
1	-1.645421	5.415825	-1.740780
1	-2.064321	6.868053	-0.824628
6	-3.025509	5.093024	-0.144084
6	-3.699998	4.104759	-0.739688
1	-3.329666	5.379431	0.864375
1	-3.432071	3.791406	-1.743611
6	-4.812005	3.418398	-0.024356
8	-5.233502	3.851727	1.037753
6	-5.372533	2.153855	-0.596136
6	-4.761375	1.461513	-1.647621
6	-6.511628	1.609877	0.012043
6	-5.269212	0.235600	-2.070275
1	-3.870873	1.849990	-2.130802
6	-7.023212	0.392193	-0.416928
1	-6.973571	2.156021	0.828265
6	-6.396447	-0.300400	-1.454227
1	-4.783672	-0.300759	-2.878959
1	-7.905156	-0.023627	0.059695
1	-6.783526	-1.259992	-1.782980
7	2.256954	-0.799552	-0.262967
6	3.596066	-1.192405	-0.190235
6	4.100252	-2.274754	0.540162
6	5.473093	-2.501039	0.556182
6	6.371542	-1.681752	-0.116639
6	5.853863	-0.611378	-0.836011
6	4.489466	-0.367170	-0.889146
6	5.992772	-3.704945	1.289761
9	6.019705	-4.792378	0.502110
6	6.763288	0.339745	-1.559538
9	6.420233	0.476188	-2.846863
6	1.099440	-1.367562	0.166280
16	0.925430	-2.924275	0.789455
7	0.049144	-0.507779	0.040603
6	-1.339996	-0.916847	0.124242
6	-2.228393	0.186942	0.743637
6	-3.600375	-0.411777	1.164787
6	-3.775589	-0.241669	2.681678
6	-3.806754	1.260111	2.988321
6	-2.513869	1.884808	2.410871
7	-1.585600	0.854033	1.898639
6	-1.296706	-0.114778	2.974375
6	-2.586802	-0.856209	3.444103
6	-2.442351	-2.353566	3.333960
6	-3.360762	-3.216641	2.903985
6	-1.885391	-1.288148	-1.255316
6	-2.638230	-2.478706	-1.504423
6	-3.159844	-2.658313	-2.821323
7	-2.936243	-1.786194	-3.845192
6	-2.199025	-0.732736	-3.589697
6	-1.668237	-0.437083	-2.312484
6	-3.955269	-3.798067	-3.093488
6	-4.218300	-4.732901	-2.125687
6	-3.671253	-4.568955	-0.826324
6	-2.893571	-3.470074	-0.529673
9	7.247239	-3.516621	1.730272
9	5.236414	-4.013134	2.352617
9	8.043166	-0.058199	-1.522963
9	6.719588	1.571902	-1.018258
1	-2.375926	0.977131	-0.007249
1	-4.417136	0.096009	0.647961
1	-3.657488	-1.465674	0.886909
1	-1.973803	2.469786	3.164077

1	-2.753332	2.555373	1.578252
1	-3.871225	1.424869	4.068852
1	-4.684321	1.727527	2.529451
1	-4.711478	-0.708873	3.003301
1	-2.729724	-0.632497	4.510729
1	-0.840555	0.448090	3.794525
1	-0.542230	-0.819319	2.608832
1	-1.479296	-2.743993	3.666219
1	-3.158426	-4.282796	2.879938
1	-4.341080	-2.901314	2.555141
1	-1.360239	-1.790273	0.777327
1	-1.083310	0.471441	-2.191098
1	-2.480862	-3.400557	0.470617
1	-2.011299	-0.052044	-4.418273
1	-4.344910	-3.907930	-4.100288
1	-4.828389	-5.595678	-2.365217
1	0.243278	0.382326	-0.412210
1	2.138638	0.139963	-0.669239
1	3.434028	-2.923760	1.090425
1	4.108506	0.467235	-1.479609
1	7.437839	-1.869876	-0.080821
8	-3.869990	-5.453988	0.182572
6	-4.637955	-6.611362	-0.085152
1	-4.654325	-7.182260	0.843388
1	-5.666452	-6.357098	-0.367065
1	-4.183549	-7.222904	-0.873060
1	-0.098513	1.650199	1.726087

[4-5]TS-syn_Cinchona-Thiourea_conf-3

Number of imaginary frequencies : 1
The smallest frequency is : -164.5216

Electronic energy=	-3467.7216592
Zero-point correction=	0.937266
Thermal correction to Energy=	0.995255
Thermal correction to Enthalpy=	0.996199
Thermal correction to Gibbs Free Energy=	0.839417
Sum of electronic and zero-point Energies=	-3466.784393
Sum of electronic and thermal Energies=	-3466.726404
Sum of electronic and thermal Enthalpies=	-3466.725460
Sum of electronic and thermal Free Energies=	-3466.882242

Cartesian Coordinates

6	-2.609162	-4.108610	-0.331318
6	-4.024040	-4.682842	-0.374121
6	-4.687685	-4.005403	0.828195
6	-3.598648	-4.058834	1.900345
7	-2.340665	-4.044410	1.121114
6	-1.184191	-3.816118	1.691754
6	0.092446	-3.946328	0.920856
6	0.551447	-5.408576	0.842615
6	-2.527116	-2.720384	-1.033189
8	-3.214161	-2.560504	-2.037138
8	-1.712291	-1.878432	-0.516684
8	-1.180635	-1.852549	2.072439
1	-1.872450	-4.764183	-0.807749
1	-4.500036	-4.443210	-1.323991
1	-3.998217	-5.768795	-0.238181
1	-4.927122	-2.967011	0.577594
1	-5.604680	-4.499157	1.152759
1	-3.608273	-3.205598	2.582313
1	-3.644108	-4.986439	2.480430
1	0.856741	-3.349733	1.423985
1	-1.502095	-1.664973	1.159550
1	-0.269585	-6.051394	0.506120

1	0.840409	-5.755862	1.841459
1	-1.155070	-3.982400	2.765271
1	-0.041001	-3.520095	-0.077735
6	1.733980	-5.560228	-0.127402
1	1.391566	-5.385791	-1.153534
1	2.103621	-6.591037	-0.073833
6	2.843116	-4.610567	0.200649
6	3.326172	-3.688655	-0.637514
1	3.270590	-4.664724	1.203724
1	2.942580	-3.608404	-1.651791
6	4.395600	-2.746196	-0.203215
8	4.607514	-2.544711	0.984816
6	5.177908	-2.036155	-1.257878
6	5.277319	-2.536843	-2.560205
6	5.829619	-0.843831	-0.925009
6	6.013780	-1.847814	-3.518553
1	4.796833	-3.473817	-2.825446
6	6.547468	-0.147789	-1.888197
1	5.755316	-0.469570	0.090565
6	6.636587	-0.647796	-3.186885
1	6.094202	-2.242890	-4.526013
1	7.030165	0.789888	-1.631874
1	7.189493	-0.098938	-3.942621
7	-2.122103	0.810610	-0.413162
6	-3.443578	1.257521	-0.504274
6	-3.966488	2.421211	0.071969
6	-5.326696	2.686005	-0.051661
6	-6.195102	1.830632	-0.720384
6	-5.658102	0.681514	-1.287580
6	-4.304500	0.393575	-1.196197
6	-5.869156	3.962844	0.525430
9	-5.868024	4.958657	-0.375956
6	-6.530329	-0.304613	-2.009729
9	-6.163361	-0.449873	-3.290447
6	-0.990740	1.364093	0.093580
16	-0.801122	2.971979	0.570498
7	0.014724	0.448005	0.188536
6	1.400666	0.789655	0.458631
6	2.089299	-0.256331	1.361186
6	3.420168	0.313852	1.929095
6	3.311510	0.407666	3.460932
6	3.172624	-1.018479	4.008911
6	1.995704	-1.693583	3.264911
7	1.223973	-0.713820	2.469804
6	0.820958	0.414155	3.332408
6	2.055502	1.190585	3.883998
6	2.028649	2.647306	3.493954
6	3.067262	3.392303	3.121099
6	2.201497	0.928969	-0.834568
6	2.987609	2.084640	-1.141258
6	3.747011	2.057046	-2.348524
7	3.723721	1.015005	-3.228550
6	2.964847	-0.008789	-2.929766
6	2.200244	-0.101719	-1.740925
6	4.571486	3.164314	-2.662527
6	4.645839	4.257636	-1.837126
6	3.869760	4.292239	-0.650533
6	3.055178	3.231185	-0.317367
9	-7.139587	3.819876	0.938100
9	-5.152357	4.387576	1.575152
9	-7.820873	0.060986	-2.002574
9	-6.462299	-1.525945	-1.450338
1	2.293638	-1.153187	0.760255
1	4.247266	-0.354590	1.677694
1	3.634921	1.293208	1.492890
1	1.302526	-2.185653	3.956621
1	2.382619	-2.445071	2.567257
1	2.991611	-0.990775	5.088719
1	4.095368	-1.580574	3.838425
1	4.208161	0.881856	3.871307

1	2.004076	1.159117	4.981464
1	0.221626	-0.008408	4.144879
1	0.163638	1.072146	2.754189
1	1.046303	3.118321	3.552081
1	2.943208	4.442590	2.876358
1	4.074210	2.991297	3.035957
1	1.377499	1.742797	0.987146
1	1.611589	-1.000037	-1.564728
1	2.462065	3.316177	0.585812
1	2.946657	-0.830537	-3.643809
1	5.143327	3.116917	-3.583849
1	5.285447	5.090355	-2.104638
1	-0.170981	-0.477047	-0.192896
1	-2.024380	-0.178658	-0.695345
1	-3.324836	3.099570	0.615766
1	-3.909191	-0.511761	-1.658516
1	-7.253987	2.049154	-0.791285
8	3.875099	5.339692	0.213590
6	4.650707	6.474243	-0.119786
1	4.488510	7.196071	0.680935
1	5.718910	6.232629	-0.172016
1	4.329489	6.916383	-1.070031
1	-0.262054	-1.427241	2.135627

[4-5]TS-syn_Cinchona-Thiourea_conf-4

Number of imaginary frequencies : 1
The smallest frequency is : -157.0006

Electronic energy=	-3467.7175441
Zero-point correction=	0.937760
Thermal correction to Energy=	0.995566
Thermal correction to Enthalpy=	0.996511
Thermal correction to Gibbs Free Energy=	0.840203
Sum of electronic and zero-point Energies=	-3466.779784
Sum of electronic and thermal Energies=	-3466.721978
Sum of electronic and thermal Enthalpies=	-3466.721034
Sum of electronic and thermal Free Energies=	-3466.877341

Cartesian Coordinates

6	-2.118752	-3.397249	-1.682956
6	-3.564579	-3.808714	-1.930594
6	-4.291795	-3.239400	-0.707959
6	-3.313886	-3.481621	0.444706
7	-1.992042	-3.571947	-0.215409
6	-0.874309	-3.580947	0.488710
6	0.432428	-3.964374	-0.140060
6	0.477010	-5.469774	-0.432496
6	-1.828580	-1.915137	-2.055055
8	-2.709804	-1.241014	-2.598216
8	-0.672622	-1.506216	-1.705373
8	-0.556727	-1.755923	0.942558
1	-1.386244	-4.032047	-2.190379
1	-3.934908	-3.391140	-2.866486
1	-3.642617	-4.900466	-1.959379
1	-4.447021	-2.168362	-0.855791
1	-5.261662	-3.705177	-0.526439
1	-3.305925	-2.670777	1.178354
1	-3.510732	-4.426840	0.961107
1	1.232273	-3.699602	0.556559
1	-0.740228	-1.458149	0.022943
1	-0.368458	-5.757897	-1.066622
1	0.377594	-6.033613	0.503001
1	-1.013775	-3.849758	1.533552
1	0.579382	-3.379260	-1.052450
6	1.787269	-5.861774	-1.135493

1	1.867348	-5.325787	-2.087819
1	1.758949	-6.934470	-1.358529
6	2.971202	-5.564307	-0.273318
6	3.893327	-4.630562	-0.526902
1	3.063030	-6.122193	0.659585
1	3.842941	-4.045780	-1.440087
6	4.983673	-4.384716	0.456376
8	5.139742	-5.127896	1.411534
6	5.876104	-3.191303	0.283961
6	5.696893	-2.230141	-0.717045
6	6.908551	-3.025436	1.214635
6	6.540138	-1.122861	-0.783070
1	4.901386	-2.324485	-1.448494
6	7.747208	-1.921081	1.149125
1	7.029881	-3.777067	1.987218
6	7.562368	-0.965331	0.149855
1	6.396855	-0.382240	-1.563567
1	8.543460	-1.800939	1.876602
1	8.215457	-0.099877	0.097318
7	-2.352727	0.812400	-0.507553
6	-3.676284	0.811988	-0.054219
6	-4.040244	0.987741	1.287052
6	-5.375314	0.876288	1.652018
6	-6.370392	0.566899	0.728956
6	-5.991527	0.378155	-0.592690
6	-4.667013	0.509026	-0.994018
6	-5.768305	1.124855	3.080457
9	-6.175311	2.388865	3.272712
6	-6.998430	-0.054348	-1.617782
9	-6.858695	0.614819	-2.770542
6	-1.247356	1.431353	0.020124
16	-1.303600	2.700699	1.133211
7	-0.106003	0.910327	-0.470881
6	1.224411	1.450434	-0.275814
6	2.233567	0.367885	0.178129
6	3.579892	1.039048	0.573788
6	3.858781	0.768504	2.060910
6	4.046574	-0.742616	2.238110
6	2.805253	-1.447513	1.638084
7	1.742074	-0.473529	1.297174
6	1.437689	0.343357	2.490272
6	2.664445	1.197485	2.932712
6	2.354548	2.673930	2.940199
6	3.166037	3.659978	2.563746
6	1.724015	2.073217	-1.579307
6	2.163275	3.430917	-1.676805
6	2.655587	3.867209	-2.943817
7	2.695487	3.071651	-4.050051
6	2.249323	1.846440	-3.928330
6	1.761651	1.302901	-2.715907
6	3.126982	5.195562	-3.073641
6	3.113973	6.065415	-2.013691
6	2.608648	5.633925	-0.760304
6	2.139571	4.346986	-0.601078
9	-6.784982	0.330884	3.457266
9	-4.754705	0.906477	3.930213
9	-8.258668	0.122313	-1.197830
9	-6.863518	-1.361086	-1.913425
1	2.383266	-0.325551	-0.659241
1	4.401914	0.631775	-0.023667
1	3.539533	2.113777	0.377572
1	2.378527	-2.173250	2.339186
1	3.064852	-1.990255	0.720735
1	4.156574	-0.987268	3.299799
1	4.957711	-1.070791	1.729581
1	4.764319	1.297360	2.373169
1	2.902872	0.922649	3.969668
1	1.135524	-0.352683	3.279085
1	0.570836	0.972637	2.265386
1	1.363990	2.931798	3.317609

1	2.852165	4.697573	2.623883
1	4.164569	3.478946	2.173554
1	1.145386	2.209183	0.504026
1	1.410909	0.273327	-2.707330
1	1.742963	4.072560	0.369136
1	2.271170	1.224878	-4.821444
1	3.497212	5.502130	-4.046493
1	3.482378	7.075849	-2.144164
1	-0.209509	0.140106	-1.143936
1	-2.227855	0.301489	-1.385652
1	-3.286695	1.197273	2.033531
1	-4.387558	0.336122	-2.028971
1	-7.405362	0.467982	1.035023
8	2.553257	6.433171	0.335233
6	2.961495	7.780765	0.198457
1	2.808421	8.241968	1.174300
1	4.021813	7.856382	-0.070081
1	2.357448	8.310698	-0.547063
1	0.377138	-1.348017	1.088662

[4-5]TS-syn_Cinchona-Thiourea_conf-5

Number of imaginary frequencies : 1
The smallest frequency is : -167.7198

Electronic energy= -3467.7137781
Zero-point correction= 0.937713
Thermal correction to Energy= 0.995759
Thermal correction to Enthalpy= 0.996703
Thermal correction to Gibbs Free Energy= 0.837318
Sum of electronic and zero-point Energies= -3466.776066
Sum of electronic and thermal Energies= -3466.718020
Sum of electronic and thermal Enthalpies= -3466.717075
Sum of electronic and thermal Free Energies= -3466.876460

Cartesian Coordinates

6	-2.731813	0.178619	-2.607337
6	-3.860372	1.178112	-2.839845
6	-4.082690	1.748990	-1.435677
6	-3.950621	0.523296	-0.527389
7	-3.108364	-0.411922	-1.308607
6	-2.663517	-1.530917	-0.782175
6	-2.048244	-2.597370	-1.643244
6	-3.071046	-3.282213	-2.562496
6	-1.337619	0.864985	-2.556192
8	-1.174875	1.897693	-3.196920
8	-0.451312	0.254828	-1.855041
8	-1.132032	-1.032849	0.298446
1	-2.684210	-0.601700	-3.372460
1	-3.561626	1.931271	-3.567613
1	-4.758805	0.658576	-3.189097
1	-3.302103	2.482855	-1.213772
1	-5.053142	2.233208	-1.318450
1	-3.466271	0.739667	0.428210
1	-4.918570	0.043718	-0.352871
1	-1.607781	-3.342636	-0.976502
1	-0.814187	-0.408911	-0.408715
1	-2.544840	-4.078012	-3.097486
1	-3.428933	-2.580921	-3.324874
1	-3.196213	-1.845027	0.110758
1	-1.238246	-2.150582	-2.227627
6	-4.286124	-3.883614	-1.841161
1	-3.972647	-4.469550	-0.968704
1	-4.768521	-4.585693	-2.534053
6	-5.321061	-2.872300	-1.448906
6	-5.975652	-2.835614	-0.283323

1	-5.589794	-2.127030	-2.200241
1	-5.759375	-3.558539	0.498508
6	-7.031241	-1.809521	-0.053979
8	-7.097649	-0.812712	-0.758376
6	-8.008494	-2.011415	1.060406
6	-8.175574	-3.241819	1.703115
6	-8.796783	-0.920814	1.444312
6	-9.115286	-3.376056	2.720972
1	-7.593938	-4.106363	1.400601
6	-9.726274	-1.053569	2.466736
1	-8.661179	0.023719	0.928010
6	-9.885968	-2.282548	3.106948
1	-9.247409	-4.335554	3.210335
1	-10.328715	-0.201771	2.765350
1	-10.614897	-2.388350	3.904356
7	1.222948	1.796240	-0.268777
6	0.898597	3.109091	0.087214
6	1.268834	3.754234	1.273344
6	0.815562	5.047467	1.510779
6	-0.006233	5.724357	0.617435
6	-0.366424	5.068063	-0.553133
6	0.079854	3.783890	-0.829538
6	1.259467	5.757175	2.758427
9	2.343695	6.518759	2.540218
6	-1.300556	5.717290	-1.533286
9	-0.876215	5.579426	-2.795634
6	2.085574	0.883339	0.251968
16	3.224312	1.172901	1.462418
7	1.920944	-0.337689	-0.327459
6	2.840463	-1.448092	-0.173100
6	2.093280	-2.796120	-0.060758
6	3.064505	-3.908197	0.430077
6	2.589789	-4.415504	1.802236
6	1.221979	-5.082769	1.615693
6	0.301093	-4.067809	0.895269
7	0.913145	-2.724656	0.830840
6	1.305108	-2.306508	2.190926
6	2.398044	-3.245997	2.787762
6	3.653594	-2.496533	3.159575
6	4.906095	-2.925142	3.017301
6	3.819417	-1.515243	-1.345547
6	5.239004	-1.550819	-1.173623
6	6.035543	-1.674971	-2.351668
7	5.514228	-1.729080	-3.609934
6	4.211903	-1.659632	-3.727484
6	3.328053	-1.559809	-2.627111
6	7.443297	-1.746792	-2.220946
6	8.050190	-1.698655	-0.992317
6	7.256694	-1.559387	0.175460
6	5.883646	-1.478363	0.082122
9	0.302593	6.575924	3.226985
9	1.573437	4.903615	3.742449
9	-1.446063	7.029226	-1.296136
9	-2.530260	5.171719	-1.479324
1	1.697406	-3.048813	-1.052827
1	3.084164	-4.742902	-0.278183
1	4.085114	-3.521772	0.496204
1	-0.665902	-3.970123	1.401345
1	0.107512	-4.385992	-0.134302
1	0.806437	-5.364446	2.588725
1	1.319470	-5.998402	1.024626
1	3.308080	-5.134910	2.205803
1	1.998403	-3.668884	3.720083
1	0.396609	-2.316719	2.800821
1	1.651604	-1.269159	2.148964
1	3.487531	-1.515844	3.607263
1	5.746690	-2.314711	3.332320
1	5.148374	-3.888296	2.574214
1	3.384586	-1.265997	0.754386
1	2.258461	-1.515887	-2.819198

1	5.323984	-1.340656	0.999773
1	3.807107	-1.691786	-4.737265
1	8.025317	-1.840502	-3.132010
1	9.129923	-1.757527	-0.925079
1	1.271933	-0.380658	-1.110718
1	0.651314	1.435749	-1.045470
1	1.891913	3.253085	1.999708
1	-0.208955	3.294468	-1.760289
1	-0.356463	6.727958	0.828874
8	7.778546	-1.496441	1.427239
6	9.185557	-1.537414	1.566310
1	9.384092	-1.455619	2.635209
1	9.600425	-2.482481	1.196719
1	9.666769	-0.699790	1.048546
1	-0.367229	-1.684891	0.432229

[4-5]TS-syn_Cinchona-Thiourea_conf-6

Number of imaginary frequencies : 1
The smallest frequency is : -168.8022

Electronic energy=	-3467.7153245
Zero-point correction=	0.937967
Thermal correction to Energy=	0.995995
Thermal correction to Enthalpy=	0.996939
Thermal correction to Gibbs Free Energy=	0.839517
Sum of electronic and zero-point Energies=	-3466.777358
Sum of electronic and thermal Energies=	-3466.719330
Sum of electronic and thermal Enthalpies=	-3466.718386
Sum of electronic and thermal Free Energies=	-3466.875807

Cartesian Coordinates

6	3.498139	-2.540284	-1.088580
6	4.862393	-1.828418	-1.039102
6	4.686070	-0.668370	-2.019919
6	3.927205	-1.325184	-3.167577
7	3.043395	-2.287148	-2.472691
6	1.881665	-2.623010	-2.987541
6	0.979366	-3.627609	-2.333286
6	1.472477	-5.089431	-2.474852
6	2.576235	-2.008291	0.037614
8	2.931140	-2.288309	1.182638
8	1.553042	-1.318083	-0.292603
8	0.817607	-0.970828	-2.770705
1	3.611432	-3.613935	-0.931937
1	5.102254	-1.522725	-0.020194
1	5.649434	-2.502349	-1.391680
1	4.069247	0.118652	-1.572029
1	5.629990	-0.226325	-2.341200
1	3.315848	-0.632892	-3.749201
1	4.603717	-1.870608	-3.835045
1	-0.002848	-3.514668	-2.796449
1	1.127834	-0.889764	-1.833208
1	2.379524	-5.136023	-3.087714
1	0.712476	-5.669428	-3.006307
1	1.805045	-2.495391	-4.063368
1	0.858973	-3.358718	-1.281039
6	1.764100	-5.775302	-1.124037
1	2.639808	-5.323621	-0.649478
1	2.012739	-6.823926	-1.324547
6	0.612042	-5.710811	-0.171091
6	0.607058	-4.967081	0.940304
1	-0.280027	-6.292877	-0.404829
1	1.474969	-4.367218	1.209127
6	-0.573750	-4.980853	1.851148
8	-1.493691	-5.764237	1.678107

6	-0.596012	-4.025191	3.002797
6	0.193199	-2.869597	3.031144
6	-1.458480	-4.304793	4.069873
6	0.105133	-2.000134	4.116578
1	0.875833	-2.626700	2.219522
6	-1.519744	-3.449819	5.162656
1	-2.066296	-5.202796	4.023983
6	-0.740926	-2.291373	5.183021
1	0.708655	-1.098239	4.127832
1	-2.178752	-3.677360	5.994541
1	-0.796925	-1.615700	6.030817
7	1.063493	1.286226	0.314929
6	2.201324	2.080129	0.466470
6	2.286481	3.461297	0.266722
6	3.516555	4.096794	0.424514
6	4.672044	3.409302	0.766174
6	4.569119	2.036366	0.973125
6	3.359589	1.375643	0.842220
6	3.563439	5.591493	0.270383
9	2.765811	6.017680	-0.719003
6	5.807021	1.237141	1.257277
9	5.544275	0.125373	1.957809
6	-0.189819	1.532688	-0.157673
16	-0.860776	3.050251	-0.444763
7	-0.863957	0.373910	-0.394407
6	-2.302511	0.297201	-0.583830
6	-2.681702	-0.831183	-1.563132
6	-4.186610	-0.725897	-1.942338
6	-4.302848	-0.476159	-3.455219
6	-3.729626	-1.698068	-4.184719
6	-2.289793	-1.928423	-3.660376
7	-1.849698	-0.822662	-2.786943
6	-1.984289	0.452583	-3.516071
6	-3.472040	0.751636	-3.877141
6	-3.932079	2.076236	-3.321429
6	-5.120802	2.348873	-2.787696
6	-3.018986	0.079885	0.748117
6	-4.046531	0.952944	1.226704
6	-4.664748	0.614871	2.467308
7	-4.310282	-0.470703	3.212527
6	-3.349116	-1.233197	2.752238
6	-2.680883	-0.998205	1.526296
6	-5.702419	1.441987	2.961268
6	-6.122719	2.551341	2.272856
6	-5.500050	2.888316	1.044439
6	-4.480386	2.109588	0.540708
9	3.161587	6.214684	1.389133
9	4.804147	6.027672	0.003778
9	6.717905	1.944732	1.937883
9	6.401960	0.838372	0.114290
1	-2.478853	-1.792872	-1.075017
1	-4.713319	-1.649737	-1.683472
1	-4.664690	0.081747	-1.381616
1	-1.569011	-2.006443	-4.482075
1	-2.228382	-2.852156	-3.075401
1	-3.727890	-1.524132	-5.265566
1	-4.351997	-2.577735	-3.995478
1	-5.351558	-0.332638	-3.732055
1	-3.539336	0.829885	-4.971433
1	-1.366487	0.369771	-4.415564
1	-1.548458	1.248676	-2.902831
1	-3.199417	2.881474	-3.395735
1	-5.356377	3.344521	-2.424624
1	-5.898929	1.597747	-2.677182
1	-2.608674	1.250758	-1.014224
1	-1.898268	-1.689774	1.222859
1	-4.018138	2.427187	-0.385764
1	-3.066486	-2.095021	3.353512
1	-6.155133	1.163914	3.907544
1	-6.919802	3.164183	2.676780

1	-0.388382	-0.491218	-0.144980
1	1.281960	0.286299	0.402128
1	1.409509	4.029155	-0.010208
1	3.303702	0.307342	1.045894
1	5.620772	3.921847	0.874798
8	-5.852454	3.969213	0.301057
6	-6.868019	4.818303	0.798841
1	-6.980733	5.615427	0.063763
1	-7.823122	4.289601	0.901485
1	-6.588607	5.257782	1.763464
1	-0.195988	-0.980636	-2.708377

[4-5]TS-syn_Cinchona-Thiourea_conf-7

Number of imaginary frequencies : 1
The smallest frequency is : -161.6834

Electronic energy=	-3467.7118663
Zero-point correction=	0.937740
Thermal correction to Energy=	0.995984
Thermal correction to Enthalpy=	0.996928
Thermal correction to Gibbs Free Energy=	0.836572
Sum of electronic and zero-point Energies=	-3466.774127
Sum of electronic and thermal Energies=	-3466.715882
Sum of electronic and thermal Enthalpies=	-3466.714938
Sum of electronic and thermal Free Energies=	-3466.875294

Cartesian Coordinates

6	0.593749	-3.959847	1.367056
6	-0.013361	-5.359152	1.399837
6	-1.330057	-5.118125	2.143946
6	-0.933061	-4.144764	3.256695
7	0.250326	-3.443659	2.709292
6	0.762661	-2.393657	3.306337
6	2.068354	-1.815671	2.854213
6	3.248975	-2.693044	3.293637
6	-0.011173	-3.093038	0.225527
8	-0.371655	-3.666726	-0.796302
8	-0.048896	-1.831843	0.452174
8	-0.450126	-0.899648	2.868070
1	1.680211	-3.963119	1.237574
1	-0.154462	-5.736466	0.388176
1	0.632410	-6.040096	1.963814
1	-2.048486	-4.651144	1.463062
1	-1.777945	-6.029839	2.541571
1	-1.709150	-3.413816	3.496038
1	-0.638487	-4.669418	4.171356
1	2.169120	-0.821927	3.297554
1	-0.493493	-1.192529	1.922648
1	3.196681	-3.667914	2.796741
1	3.190893	-2.881013	4.371613
1	0.491848	-2.284388	4.353375
1	2.040286	-1.694654	1.767713
6	4.604711	-2.037652	2.974256
1	5.408346	-2.735451	3.228108
1	4.725234	-1.150350	3.608507
6	4.704918	-1.629117	1.537198
6	5.409947	-2.263439	0.597029
1	4.140050	-0.752658	1.220193
1	6.014960	-3.128068	0.850999
6	5.395645	-1.750917	-0.803529
8	4.771316	-0.739540	-1.085663
6	6.169200	-2.475684	-1.859980
6	6.670529	-3.769275	-1.684898
6	6.371527	-1.820824	-3.080331
6	7.366216	-4.395098	-2.715207

1	6.505130	-4.309168	-0.759004
6	7.074578	-2.441971	-4.103167
1	5.969497	-0.821045	-3.205605
6	7.573268	-3.731560	-3.921175
1	7.745273	-5.402364	-2.576480
1	7.232317	-1.925294	-5.044292
1	8.119315	-4.220584	-4.721877
7	-2.090306	-0.256743	-0.505824
6	-3.328595	-0.823574	-0.823511
6	-4.562361	-0.166713	-0.839278
6	-5.715879	-0.892114	-1.131074
6	-5.690379	-2.252620	-1.399742
6	-4.453007	-2.891020	-1.383878
6	-3.285008	-2.198803	-1.111850
6	-7.037130	-0.179647	-1.071232
9	-7.533649	-0.162220	0.178535
6	-4.378490	-4.354814	-1.710713
9	-4.299884	-4.572449	-3.032936
6	-1.704717	1.005986	-0.182225
16	-2.660905	2.392317	-0.296576
7	-0.420448	1.033741	0.272881
6	0.353364	2.247338	0.465304
6	1.200376	2.200621	1.758054
6	1.733437	3.623715	2.093009
6	1.119521	4.084779	3.425930
6	1.634317	3.158649	4.534053
6	1.341069	1.702661	4.098329
7	0.457111	1.653751	2.915297
6	-0.755787	2.448955	3.189513
6	-0.416222	3.957056	3.403782
6	-1.130807	4.849069	2.419624
6	-0.635864	5.931386	1.822717
6	1.277493	2.509654	-0.723881
6	1.241191	3.727943	-1.475775
6	2.204878	3.880355	-2.517192
7	3.121112	2.923812	-2.841125
6	3.101343	1.809311	-2.153015
6	2.203507	1.562945	-1.085248
6	2.221891	5.084011	-3.261951
6	1.335529	6.098515	-3.004013
6	0.370877	5.938703	-1.977107
6	0.322950	4.775938	-1.237928
9	-6.939366	1.096827	-1.465362
9	-7.960964	-0.771551	-1.844145
9	-5.468412	-5.010958	-1.277104
9	-3.309548	-4.941087	-1.152692
1	2.037881	1.510217	1.593989
1	2.824854	3.616359	2.179067
1	1.481763	4.322671	1.290872
1	0.861263	1.128031	4.898264
1	2.271859	1.190883	3.831795
1	1.133623	3.391325	5.479654
1	2.707860	3.303919	4.687708
1	1.407812	5.119337	3.634389
1	-0.778738	4.239270	4.402276
1	-1.221760	2.017134	4.080586
1	-1.457036	2.314082	2.360366
1	-2.162519	4.565079	2.208519
1	-1.239822	6.519338	1.138412
1	0.385207	6.270726	1.979593
1	-0.371096	3.056615	0.555758
1	2.276638	0.609558	-0.566522
1	-0.454376	4.689210	-0.488257
1	3.830377	1.044681	-2.410083
1	2.964600	5.174699	-4.047852
1	1.372718	7.007441	-3.592651
1	0.098826	0.159773	0.214562
1	-1.346716	-0.962137	-0.393736
1	-4.623288	0.891617	-0.631715
1	-2.327874	-2.720397	-1.125677

1	-6.601134	-2.799604	-1.615681
8	-0.546702	6.889114	-1.660077
6	-0.557032	8.083035	-2.417726
1	-1.366569	8.690233	-2.011717
1	0.386776	8.632532	-2.318949
1	-0.754858	7.885790	-3.477629
1	-0.073533	0.040714	2.839650

[6-7]TS-anti_Cinchona-Thiourea_conf-1

Number of imaginary frequencies : 1
The smallest frequency is : -1247.9007

Electronic energy=	-3467.7017948
Zero-point correction=	0.930635
Thermal correction to Energy=	0.989309
Thermal correction to Enthalpy=	0.990253
Thermal correction to Gibbs Free Energy=	0.827782
Sum of electronic and zero-point Energies=	-3466.771160
Sum of electronic and thermal Energies=	-3466.712486
Sum of electronic and thermal Enthalpies=	-3466.711541
Sum of electronic and thermal Free Energies=	-3466.874013

Cartesian Coordinates

6	-2.994654	1.920086	-1.441691
6	-3.384885	0.498721	-1.017694
7	-2.793142	-0.354247	-2.065299
6	-2.081118	0.450316	-3.070467
6	-2.760532	1.809355	-2.952180
6	-2.686790	-1.657885	-1.973707
6	-2.980942	-2.429914	-0.829903
6	-3.077167	-3.934010	-1.000046
6	-0.567725	0.508531	-2.695071
8	0.049941	1.552041	-2.943032
8	-0.091867	-0.537505	-2.151932
1	-2.178588	-0.014516	-4.056045
1	-2.124179	2.602918	-3.341420
1	-3.710440	1.804930	-3.495435
1	-2.059370	2.206737	-0.949650
1	-3.754127	2.655249	-1.173078
1	-2.977192	0.220728	-0.040917
1	-4.468695	0.338881	-1.005611
1	-1.819212	-2.018194	-0.217024
1	-0.568289	-0.871712	-0.585336
8	-0.848239	-1.318137	0.253931
1	-2.356929	-4.263529	-1.758175
1	0.016665	-1.802021	0.571325
1	-3.701748	-1.995435	-0.133876
7	1.238647	1.893129	-0.324147
6	0.705247	3.106839	0.118230
6	0.047814	3.875708	-0.853685
6	-0.604417	5.047126	-0.499123
6	-0.603727	5.513071	0.810111
6	0.060986	4.749082	1.761260
6	0.701154	3.554774	1.444440
6	-1.345854	5.779796	-1.578334
9	-2.289084	4.995543	-2.139783
6	0.122654	5.216646	3.188037
9	-0.122234	4.216572	4.049479
6	2.093722	1.009106	0.280694
16	3.068692	1.356426	1.614003
7	2.077272	-0.190460	-0.338647
6	3.061978	-1.239609	-0.155035
6	2.393345	-2.625702	-0.020539
6	3.449046	-3.702944	0.355032
6	3.067770	-4.328816	1.705895

6	1.717749	-5.036575	1.537824
6	0.703575	-3.999466	0.997329
7	1.286135	-2.639802	0.966818
6	1.761437	-2.285249	2.317390
6	2.899946	-3.242901	2.786348
6	4.152359	-2.483515	3.148777
6	5.407635	-2.841407	2.887344
6	4.028939	-1.265914	-1.338338
6	5.449248	-1.196733	-1.182070
6	6.239469	-1.277104	-2.367958
7	5.708899	-1.392523	-3.618447
6	4.403545	-1.423067	-3.720237
6	3.525023	-1.366443	-2.612010
6	7.649865	-1.234563	-2.254216
6	8.265598	-1.118016	-1.034586
6	7.477444	-1.026412	0.141320
6	6.101105	-1.057980	0.064528
9	-1.966034	6.873384	-1.117796
9	-0.535540	6.165901	-2.573994
9	-0.768576	6.187784	3.438817
9	1.333257	5.703457	3.499294
1	1.926211	-2.864612	-0.984576
1	3.490360	-4.483513	-0.411194
1	4.444611	-3.255419	0.409638
1	-0.196738	-3.954778	1.618926
1	0.388135	-4.239748	-0.023523
1	1.382399	-5.443600	2.496984
1	1.816369	-5.875487	0.842472
1	3.831859	-5.048651	2.013964
1	2.557920	-3.744159	3.702670
1	0.895143	-2.340359	2.983242
1	2.092745	-1.242246	2.304881
1	3.980092	-1.555629	3.696284
1	6.243260	-2.223760	3.201429
1	5.655904	-3.749686	2.343859
1	3.599757	-1.010866	0.765784
1	2.451661	-1.391526	-2.789068
1	5.545443	-0.961336	0.989733
1	3.991199	-1.504034	-4.724213
1	8.227091	-1.296397	-3.171028
1	9.347259	-1.088657	-0.980106
1	1.433260	-0.297997	-1.132296
1	0.990780	1.678948	-1.296958
1	0.024528	3.526301	-1.883227
1	1.186310	2.977432	2.219209
1	-1.112894	6.429850	1.080246
8	8.007273	-0.904455	1.385278
6	9.412769	-0.796550	1.503957
1	9.615683	-0.672597	2.567951
1	9.918930	-1.700958	1.146448
1	9.796522	0.075921	0.962718
1	-2.795997	-4.434506	-0.066260
1	-2.182680	-2.133619	-2.815039
6	-4.485745	-4.411235	-1.407938
1	-4.442072	-5.482980	-1.639252
1	-4.806381	-3.886788	-2.315379
6	-5.471029	-4.200137	-0.304726
6	-6.538450	-3.397159	-0.347645
1	-5.287753	-4.735347	0.628174
1	-6.779607	-2.844128	-1.250418
6	-7.429494	-3.291528	0.841571
8	-7.261088	-4.008351	1.814559
6	-8.553286	-2.298917	0.831943
6	-8.649064	-1.256306	-0.094376
6	-9.530530	-2.425443	1.825375
6	-9.709894	-0.356940	-0.027741
1	-7.891428	-1.122703	-0.859561
6	-10.593285	-1.534857	1.884769
1	-9.434178	-3.233582	2.542577
6	-10.684181	-0.497860	0.956758

1	-9.775280	0.454958	-0.744937
1	-11.350992	-1.645216	2.653868
1	-11.513248	0.201440	1.002969

[6-7]TS-anti_Cinchona-Thiourea_conf-2

Number of imaginary frequencies : 1
The smallest frequency is : -1291.4075

Electronic energy=	-3467.7094547
Zero-point correction=	0.931949
Thermal correction to Energy=	0.990018
Thermal correction to Enthalpy=	0.990962
Thermal correction to Gibbs Free Energy=	0.835723
Sum of electronic and zero-point Energies=	-3466.777505
Sum of electronic and thermal Energies=	-3466.719437
Sum of electronic and thermal Enthalpies=	-3466.718493
Sum of electronic and thermal Free Energies=	-3466.873732

Cartesian Coordinates

6	4.303601	0.387778	-2.645749
6	3.774599	1.785213	-2.294740
7	2.660601	1.998505	-3.235116
6	2.413646	0.789939	-4.036519
6	3.782541	0.123725	-4.064146
6	1.856516	3.034803	-3.186535
6	1.850266	3.999004	-2.160164
6	1.202636	5.355502	-2.406708
6	1.338132	-0.057538	-3.292150
8	1.534234	-1.272126	-3.150584
8	0.339454	0.604435	-2.868198
1	2.023549	1.072570	-5.018612
1	3.698543	-0.940000	-4.284777
1	4.418707	0.604496	-4.813306
1	3.878916	-0.351736	-1.962709
1	5.390055	0.330492	-2.569435
1	3.403151	1.846188	-1.265964
1	4.516026	2.576625	-2.444891
1	1.064194	3.172527	-1.352096
1	0.564074	1.498775	-1.453312
8	0.562971	2.176211	-0.731029
1	1.655002	5.855550	-3.271112
1	-0.415170	2.140309	-0.373290
1	2.771983	4.049372	-1.575777
7	0.909153	-1.603964	-0.369061
6	2.079689	-2.066181	0.228231
6	3.068601	-2.544654	-0.643313
6	4.304757	-2.941829	-0.152798
6	4.592551	-2.903181	1.206078
6	3.600060	-2.434148	2.060422
6	2.358434	-2.009657	1.599810
6	5.322465	-3.439112	-1.138168
9	5.010027	-4.652216	-1.615778
6	3.899810	-2.293292	3.525260
9	4.351550	-1.055247	3.819932
6	-0.319784	-1.310076	0.165920
16	-0.873877	-1.823432	1.674649
7	-1.050564	-0.570402	-0.689825
6	-2.473153	-0.315216	-0.589954
6	-2.783470	1.172890	-0.856681
6	-4.296105	1.458155	-0.642289
6	-4.457113	2.499773	0.474250
6	-3.793543	3.802475	0.012786
6	-2.330644	3.481269	-0.374926
7	-1.968159	2.090128	-0.021655
6	-2.224486	1.880363	1.419350

6	-3.739650	2.035355	1.756068
6	-4.302545	0.796284	2.406181
6	-5.503862	0.260685	2.200360
6	-3.227035	-1.180155	-1.599433
6	-4.284031	-2.067748	-1.222331
6	-4.938461	-2.783618	-2.269676
7	-4.589668	-2.679416	-3.583542
6	-3.595341	-1.881085	-3.882192
6	-2.888202	-1.110601	-2.928372
6	-6.005399	-3.653662	-1.940873
6	-6.416152	-3.822807	-0.643385
6	-5.755247	-3.120431	0.396519
6	-4.709866	-2.268063	0.110421
9	5.412515	-2.620203	-2.203493
9	6.546705	-3.526765	-0.600200
9	4.845553	-3.150366	3.932085
9	2.815965	-2.489082	4.287459
1	-2.495294	1.390843	-1.893250
1	-4.749442	1.833237	-1.565443
1	-4.820936	0.536108	-0.378810
1	-1.632355	4.135904	0.152315
1	-2.161999	3.597088	-1.451462
1	-3.820307	4.543385	0.818459
1	-4.336612	4.222199	-0.839724
1	-5.518532	2.671150	0.677687
1	-3.827655	2.847173	2.491857
1	-1.636063	2.626975	1.956412
1	-1.842009	0.894538	1.701286
1	-3.638289	0.320355	3.129645
1	-5.816255	-0.634498	2.729526
1	-6.215347	0.678669	1.492315
1	-2.776246	-0.570389	0.425734
1	-2.070010	-0.476958	-3.264455
1	-4.225365	-1.772054	0.942494
1	-3.317560	-1.815954	-4.932618
1	-6.487210	-4.183979	-2.755779
1	-7.236041	-4.496041	-0.423145
1	-0.605710	-0.288554	-1.572859
1	0.974209	-1.543502	-1.392920
1	2.865641	-2.573832	-1.711524
1	1.616135	-1.636791	2.292625
1	5.555140	-3.224031	1.585857
8	-6.095728	-3.234662	1.706307
6	-7.122356	-4.144190	2.051451
1	-7.212569	-4.097896	3.136946
1	-8.081259	-3.861315	1.601152
1	-6.868640	-5.168984	1.756689
1	0.135194	5.238316	-2.632388
1	1.065242	3.038099	-3.936287
6	1.376665	6.281447	-1.187003
1	0.991638	7.275487	-1.433979
1	2.447389	6.383816	-0.976368
6	0.666948	5.741908	0.014414
6	1.231785	4.965420	0.944851
1	-0.399349	5.949241	0.104253
1	2.292033	4.731712	0.902404
6	0.411004	4.377332	2.035919
8	-0.701661	4.819054	2.292696
6	0.952428	3.206710	2.789728
6	1.977387	2.403714	2.281228
6	0.359324	2.876719	4.013723
6	2.409192	1.289792	2.994367
1	2.411344	2.620711	1.311120
6	0.795654	1.768274	4.726406
1	-0.445447	3.503150	4.385676
6	1.823150	0.973066	4.217176
1	3.199689	0.662309	2.597290
1	0.335167	1.518562	5.676867
1	2.163764	0.101022	4.767219

[6-7]TS-anti_Cinchona-Thiourea_conf-3

Number of imaginary frequencies : 1
The smallest frequency is : -1244.0887

Electronic energy= -3467.7024173
Zero-point correction= 0.931808
Thermal correction to Energy= 0.990277
Thermal correction to Enthalpy= 0.991221
Thermal correction to Gibbs Free Energy= 0.829884
Sum of electronic and zero-point Energies= -3466.770609
Sum of electronic and thermal Energies= -3466.712141
Sum of electronic and thermal Enthalpies= -3466.711196
Sum of electronic and thermal Free Energies= -3466.872533

Cartesian Coordinates

6	-3.448881	1.193681	-0.999682
6	-3.532503	-0.175858	-0.312719
7	-2.944692	-1.102805	-1.298619
6	-2.478646	-0.383240	-2.492776
6	-3.354628	0.863590	-2.494065
6	-2.639225	-2.350595	-1.033956
6	-2.694157	-2.949035	0.241737
6	-2.654190	-4.463539	0.317490
6	-0.964345	-0.053058	-2.320693
8	-0.551709	1.031221	-2.750827
8	-0.273385	-0.945191	-1.734822
1	-2.596672	-1.016432	-3.377573
1	-2.899211	1.665150	-3.074508
1	-4.341512	0.630057	-2.906119
1	-2.536364	1.709250	-0.684222
1	-4.297759	1.831284	-0.750372
1	-2.959712	-0.215597	0.619131
1	-4.561330	-0.489789	-0.104371
1	-1.515419	-2.328617	0.619423
1	-0.494289	-1.113168	-0.078591
8	-0.591110	-1.474488	0.838577
1	-1.823313	-4.849657	-0.284707
1	0.364963	-1.821490	1.064694
1	-3.378561	-2.474585	0.946852
7	0.940060	1.821845	-0.397489
6	0.297106	2.992576	0.013089
6	-0.587584	3.564986	-0.913599
6	-1.352731	4.667852	-0.564159
6	-1.250057	5.257953	0.690332
6	-0.361591	4.689522	1.593920
6	0.401168	3.567156	1.284743
6	-2.317233	5.192602	-1.586858
9	-3.152429	4.222382	-2.010522
6	-0.207962	5.266932	2.972593
9	-0.466191	4.350933	3.920723
6	1.987710	1.130696	0.153906
16	3.086000	1.761417	1.269028
7	2.049784	-0.129511	-0.325127
6	3.179320	-1.026796	-0.174465
6	2.724638	-2.449672	0.219025
6	3.954769	-3.337492	0.559623
6	3.841833	-3.814194	2.016240
6	2.586041	-4.686464	2.138163
6	1.381775	-3.859089	1.627842
7	1.768806	-2.457669	1.353479
6	2.364575	-1.872198	2.568845
6	3.674915	-2.615938	2.972597
6	4.850405	-1.673344	3.049778
6	6.096319	-1.913309	2.646548
6	3.969811	-1.098956	-1.479353

6	5.375572	-0.843188	-1.548064
6	6.003057	-0.992208	-2.821256
7	5.329290	-1.335586	-3.955414
6	4.037944	-1.530191	-3.855564
6	3.316974	-1.428318	-2.641871
6	7.397495	-0.771594	-2.926072
6	8.148962	-0.416640	-1.835355
6	7.519785	-0.254235	-0.574277
6	6.162979	-0.458196	-0.438988
9	-3.076806	6.186915	-1.109048
9	-1.692418	5.655158	-2.679091
9	-1.034226	6.301761	3.184223
9	1.041116	5.701823	3.192978
1	2.170808	-2.869585	-0.630278
1	3.998661	-4.204381	-0.107418
1	4.880850	-2.775270	0.413870
1	0.567749	-3.836216	2.360029
1	0.976967	-4.270983	0.697471
1	2.436650	-4.985097	3.180679
1	2.701474	-5.601564	1.549638
1	4.728011	-4.393641	2.291241
1	3.529133	-3.022943	3.982907
1	1.608706	-1.942209	3.356736
1	2.547034	-0.808472	2.388502
1	4.630108	-0.706209	3.504184
1	6.873980	-1.164024	2.757539
1	6.391618	-2.851714	2.183621
1	3.803655	-0.618529	0.620668
1	2.242900	-1.602423	-2.650677
1	5.726472	-0.299639	0.540032
1	3.508910	-1.791281	-4.770214
1	7.850486	-0.893014	-3.904573
1	9.214495	-0.254947	-1.947230
1	1.320075	-0.412442	-0.992225
1	0.588092	1.463801	-1.292779
1	-0.695762	3.112277	-1.896417
1	1.066692	3.143848	2.024923
1	-1.846503	6.121620	0.956110
8	8.188590	0.103294	0.551578
6	9.567927	0.397828	0.441490
1	9.891443	0.700497	1.437610
1	10.144796	-0.480854	0.129707
1	9.748778	1.220931	-0.259309
1	-2.459663	-4.767686	1.351538
1	-2.174188	-2.892414	-1.858018
6	-3.958453	-5.130468	-0.175139
1	-3.872031	-6.216773	-0.053413
1	-4.083827	-4.924750	-1.244790
6	-5.149873	-4.631162	0.576406
6	-6.087730	-3.830367	0.060198
1	-5.230790	-4.894776	1.631649
1	-6.040028	-3.541957	-0.985553
6	-7.199025	-3.323487	0.909837
8	-7.400280	-3.786595	2.020441
6	-8.064144	-2.213046	0.389956
6	-7.773591	-1.499498	-0.777601
6	-9.195035	-1.867336	1.138271
6	-8.600655	-0.457276	-1.187309
1	-6.898591	-1.738393	-1.372838
6	-10.024037	-0.833543	0.724537
1	-9.403487	-2.425179	2.045114
6	-9.726977	-0.125381	-0.439719
1	-8.364816	0.095299	-2.091108
1	-10.901328	-0.575068	1.308741
1	-10.372294	0.685725	-0.762265

Number of imaginary frequencies : 1
The smallest frequency is : -1269.3976

Electronic energy= -3467.704938
Zero-point correction= 0.931412
Thermal correction to Energy= 0.989443
Thermal correction to Enthalpy= 0.990387
Thermal correction to Gibbs Free Energy= 0.834129
Sum of electronic and zero-point Energies= -3466.773526
Sum of electronic and thermal Energies= -3466.715495
Sum of electronic and thermal Enthalpies= -3466.714551
Sum of electronic and thermal Free Energies= -3466.870809

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Cartesian Coordinates

.....
6 4.196998 1.553760 1.140011
6 3.492651 2.213351 2.330289
7 2.471437 3.064245 1.695607
6 2.590488 3.057571 0.230056
6 4.019718 2.569153 0.005808
6 1.394966 3.514697 2.301423
6 0.981228 3.201038 3.608472
6 -0.235342 3.907886 4.193584
6 1.540370 2.095968 -0.395995
8 1.751469 1.693256 -1.546686
8 0.521633 1.807839 0.315269
1 2.403750 4.059077 -0.170913
1 4.137758 2.141432 -0.989724
1 4.724700 3.398144 0.119253
1 3.683243 0.619505 0.886204
1 5.240812 1.318445 1.350987
1 3.010876 1.488998 2.993716
1 4.166509 2.843001 2.921338
1 0.612628 1.900294 3.225638
1 0.636439 1.026017 1.760970
8 0.514513 0.755083 2.709094
1 -0.449078 3.440630 5.159658
1 -0.380413 0.214170 2.724695
1 1.772007 2.957368 4.319408
7 1.443921 -1.095547 -0.698464
6 2.759385 -1.563960 -0.767553
6 3.659827 -0.757021 -1.480349
6 5.012985 -1.055910 -1.484807
6 5.513316 -2.175220 -0.828203
6 4.608037 -2.980485 -0.149595
6 3.247913 -2.689823 -0.095677
6 5.968814 -0.080825 -2.106363
9 6.441598 0.783503 -1.183725
6 5.105886 -4.227444 0.525790
9 4.361274 -4.553034 1.592210
6 0.301156 -1.696731 -0.234702
16 0.068950 -3.363458 -0.129483
7 -0.630828 -0.781989 0.112939
6 -2.040667 -1.066743 0.310400
6 -2.609848 -0.395659 1.583381
6 -4.028489 -0.956809 1.885704
6 -4.005736 -1.677783 3.243792
6 -3.703474 -0.640503 4.330618
6 -2.401962 0.091928 3.929812
7 -1.741372 -0.561255 2.775663
6 -1.527784 -1.989161 3.088025
6 -2.883918 -2.732880 3.293840
6 -3.037532 -3.899163 2.349789
6 -4.149075 -4.274740 1.720372
6 -2.840360 -0.588935 -0.901748
6 -3.706675 -1.448467 -1.648420
6 -4.426511 -0.862948 -2.733230
7 -4.308353 0.445246 -3.097001
6 -3.481502 1.192545 -2.409001

6	-2.732178	0.719795	-1.304733
6	-5.313900	-1.673488	-3.481811
6	-5.491607	-3.000830	-3.187173
6	-4.765042	-3.582810	-2.116844
6	-3.888018	-2.822733	-1.372189
9	7.035880	-0.687113	-2.643419
9	5.392717	0.658781	-3.062881
9	6.373080	-4.089773	0.947855
9	5.086563	-5.283409	-0.302232
1	-2.656366	0.687023	1.405697
1	-4.764269	-0.146907	1.915429
1	-4.340082	-1.642904	1.093608
1	-1.678337	0.117177	4.751305
1	-2.611314	1.125670	3.642384
1	-3.589869	-1.135231	5.300427
1	-4.529450	0.071150	4.420642
1	-4.974159	-2.150094	3.432691
1	-2.879655	-3.151830	4.309865
1	-0.912398	-2.025992	3.991719
1	-0.946631	-2.438634	2.277652
1	-2.132556	-4.490180	2.203566
1	-4.157368	-5.145866	1.072666
1	-5.087563	-3.733711	1.814303
1	-2.125068	-2.149021	0.417250
1	-2.063881	1.410989	-0.793996
1	-3.340594	-3.321438	-0.581076
1	-3.381893	2.232940	-2.714754
1	-5.848274	-1.202761	-4.300524
1	-6.177571	-3.595184	-3.778801
1	-0.359755	0.203865	0.019766
1	1.329917	-0.151445	-1.078633
1	3.292631	0.126204	-1.994190
1	2.582328	-3.325629	0.470842
1	6.572717	-2.405613	-0.838963
8	-4.875576	-4.888373	-1.762682
6	-5.746237	-5.713203	-2.513174
1	-5.672748	-6.707186	-2.071491
1	-6.784747	-5.367767	-2.448777
1	-5.443539	-5.766361	-3.565289
1	-0.035081	4.965888	4.406709
1	0.713911	4.053327	1.646481
6	-1.504099	3.786342	3.321746
1	-2.380354	3.921055	3.969510
1	-1.554702	2.771015	2.910580
6	-1.625404	4.770375	2.198257
6	-1.709431	4.428295	0.908461
1	-1.669351	5.829681	2.454781
1	-1.636145	3.382328	0.618748
6	-1.881671	5.459283	-0.153783
8	-2.204618	6.602690	0.123121
6	-1.648268	5.050699	-1.574161
6	-0.935373	3.892767	-1.901343
6	-2.127684	5.877829	-2.595120
6	-0.705577	3.562338	-3.234672
1	-0.542122	3.246415	-1.123596
6	-1.914582	5.537793	-3.924655
1	-2.668283	6.779083	-2.324433
6	-1.202913	4.380192	-4.245757
1	-0.136656	2.668305	-3.468537
1	-2.299306	6.174785	-4.714804
1	-1.034151	4.119658	-5.286074

[6-7]TS-*anti*_Cinchona-Thiourea_conf-5

Number of imaginary frequencies : 1
The smallest frequency is : -1272.6086

Electronic energy= -3467.6993975
 Zero-point correction= 0.931488
 Thermal correction to Energy= 0.989968
 Thermal correction to Enthalpy= 0.990912
 Thermal correction to Gibbs Free Energy= 0.829256
 Sum of electronic and zero-point Energies= -3466.767909
 Sum of electronic and thermal Energies= -3466.709429
 Sum of electronic and thermal Enthalpies= -3466.708485
 Sum of electronic and thermal Free Energies= -3466.870141

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 Cartesian Coordinates

6	-1.471887	3.696232	-1.673924
6	-2.519442	2.588181	-1.507332
7	-2.214079	1.648607	-2.602743
6	-1.064562	2.109843	-3.394821
6	-1.075267	3.614438	-3.152168
6	-2.736608	0.450413	-2.706431
6	-3.556577	-0.171169	-1.743606
6	-4.326505	-1.410530	-2.168966
6	0.230133	1.431086	-2.855538
8	1.280628	2.084317	-2.881636
8	0.094296	0.241977	-2.423914
1	-1.196378	1.824472	-4.442963
1	-0.099643	4.053856	-3.356377
1	-1.828877	4.092558	-3.785300
1	-0.598543	3.475855	-1.050907
1	-1.855012	4.673991	-1.380271
1	-2.441381	2.071746	-0.545567
1	-3.545110	2.951428	-1.631767
1	-2.437833	-0.441681	-0.942426
1	-0.763042	0.004872	-1.041058
8	-1.343709	-0.326863	-0.304704
1	-5.200495	-1.135387	-2.773016
1	-0.829270	-1.153574	0.060337
1	-4.095590	0.511214	-1.083593
7	2.094495	1.666649	-0.134852
6	2.112664	2.952484	0.413451
6	1.992207	4.004216	-0.506040
6	1.897944	5.316488	-0.065592
6	1.948484	5.633898	1.285349
6	2.082324	4.583593	2.186825
6	2.154718	3.255752	1.780718
6	1.687527	6.379345	-1.103567
9	0.523870	6.192919	-1.760516
6	2.188683	4.892250	3.653862
9	1.671249	3.916078	4.412926
6	2.348008	0.439299	0.418127
16	3.161048	0.176595	1.874171
7	1.877076	-0.556357	-0.363546
6	2.259367	-1.951141	-0.256868
6	1.036709	-2.886958	-0.389636
6	1.446236	-4.354990	-0.083853
6	0.642754	-4.859854	1.123929
6	-0.840031	-4.865431	0.735384
6	-1.212349	-3.435392	0.276081
7	-0.095091	-2.487561	0.483745
6	0.291054	-2.507866	1.907401
6	0.812025	-3.916740	2.331137
6	2.201913	-3.849015	2.913259
6	3.192789	-4.715323	2.713385
6	3.275142	-2.302831	-1.343769
6	4.530842	-2.927202	-1.059739
6	5.359006	-3.261069	-2.173433
7	5.026080	-2.987399	-3.466653
6	3.885329	-2.380611	-3.680524
6	2.976960	-2.024689	-2.655217
6	6.596485	-3.906825	-1.937256
6	7.014081	-4.209673	-0.666816
6	6.197109	-3.861349	0.439189

6	4.986991	-3.230145	0.243551
9	1.648790	7.608938	-0.575679
9	2.651045	6.369909	-2.035077
9	1.546787	6.029206	3.968221
9	3.465133	5.049503	4.038359
1	0.657688	-2.796639	-1.415787
1	1.247845	-4.996223	-0.948561
1	2.518087	-4.415432	0.119735
1	-2.068077	-3.047650	0.838600
1	-1.473191	-3.406111	-0.787915
1	-1.453152	-5.168966	1.589722
1	-1.015959	-5.587162	-0.067757
1	0.962913	-5.871346	1.390767
1	0.153244	-4.287982	3.128736
1	-0.596179	-2.224781	2.481074
1	1.044840	-1.732933	2.074508
1	2.378438	-3.002353	3.578367
1	4.158830	-4.581552	3.189960
1	3.091243	-5.579254	2.061165
1	2.704675	-2.082249	0.729993
1	2.051315	-1.520625	-2.925361
1	4.410943	-2.968184	1.122964
1	3.637147	-2.153768	-4.715663
1	7.204377	-4.152450	-2.801854
1	7.966925	-4.703372	-0.518035
1	1.376223	-0.283543	-1.218753
1	1.917723	1.668494	-1.146029
1	1.939570	3.778901	-1.568828
1	2.237785	2.468236	2.515838
1	1.876177	6.659399	1.626968
8	6.539282	-4.117644	1.727800
6	7.811310	-4.682264	1.981250
1	7.893652	-4.763825	3.065262
1	7.906621	-5.681397	1.540119
1	8.617449	-4.039922	1.608340
1	-3.686683	-2.033891	-2.805461
1	-2.371232	-0.133764	-3.551052
6	-4.815696	-2.264623	-0.987057
1	-3.946016	-2.579816	-0.397227
1	-5.300326	-3.168222	-1.370757
6	-5.762858	-1.522932	-0.096692
6	-7.065032	-1.796225	0.024457
1	-5.369846	-0.690645	0.487551
1	-7.507070	-2.623612	-0.522816
6	-7.920508	-0.991264	0.939900
8	-7.431114	-0.183261	1.712077
6	-9.404866	-1.199820	0.911703
6	-10.060071	-1.834272	-0.147955
6	-10.153220	-0.708002	1.986351
6	-11.444420	-1.978824	-0.128304
1	-9.502254	-2.196573	-1.005249
6	-11.532595	-0.864087	2.011068
1	-9.629667	-0.207600	2.794262
6	-12.180136	-1.500811	0.952314
1	-11.948124	-2.464748	-0.957663
1	-12.105968	-0.489739	2.853192
1	-13.258828	-1.621887	0.969541

[6-7]TS-anti_Cinchona-Thiourea_conf-6

Number of imaginary frequencies : 1
The smallest frequency is : -1272.9665

Electronic energy= -3467.6992726
Zero-point correction= 0.931541
Thermal correction to Energy= 0.990028
Thermal correction to Enthalpy= 0.990972

Thermal correction to Gibbs Free Energy=	0.829310
Sum of electronic and zero-point Energies=	-3466.767732
Sum of electronic and thermal Energies=	-3466.709245
Sum of electronic and thermal Enthalpies=	-3466.708300
Sum of electronic and thermal Free Energies=	-3466.869963

Cartesian Coordinates

6	-1.491625	3.690929	-1.667887
6	-2.535486	2.580038	-1.497549
7	-2.229389	1.639593	-2.592057
6	-1.083379	2.103449	-3.387705
6	-1.098129	3.608303	-3.146927
6	-2.748253	0.439531	-2.692620
6	-3.563554	-0.183210	-1.726555
6	-4.330559	-1.425728	-2.148029
6	0.214751	1.429115	-2.851034
8	1.263196	2.085606	-2.879669
8	0.083681	0.239768	-2.418781
1	-1.216997	1.816363	-4.435152
1	-0.124391	4.050436	-3.354296
1	-1.854707	4.083281	-3.778883
1	-0.616311	3.474231	-1.046288
1	-1.877082	4.667930	-1.374796
1	-2.454052	2.065554	-0.535041
1	-3.562460	2.940032	-1.620705
1	-2.441705	-0.447596	-0.927896
1	-0.768840	0.004879	-1.032510
8	-1.345998	-0.327031	-0.293550
1	-5.204376	-1.154449	-2.754096
1	-0.827276	-1.151853	0.070114
1	-4.103401	0.498499	-1.066534
7	2.101606	1.673100	-0.137572
6	2.122885	2.959187	0.410414
6	1.974793	4.009685	-0.508980
6	1.885466	5.321521	-0.070595
6	1.967919	5.644492	1.279269
6	2.129837	4.598344	2.177596
6	2.199135	3.267789	1.773144
6	1.653405	6.381250	-1.107315
9	0.482635	6.185430	-1.748838
6	2.231696	4.874821	3.651229
9	1.307509	4.191920	4.346317
6	2.355789	0.445216	0.413627
16	3.176034	0.180453	1.865298
7	1.878965	-0.550124	-0.365088
6	2.262151	-1.944934	-0.260217
6	1.039715	-2.881709	-0.387918
6	1.451812	-4.349321	-0.083314
6	0.654048	-4.854482	1.128232
6	-0.830392	-4.861736	0.746133
6	-1.205912	-3.432371	0.287520
7	-0.088781	-2.483342	0.490182
6	0.303366	-2.502541	1.912194
6	0.827487	-3.910715	2.334349
6	2.219712	-3.841484	2.910661
6	3.210430	-4.707124	2.707183
6	3.274074	-2.295933	-1.350918
6	4.531595	-2.918784	-1.071472
6	5.355808	-3.252167	-2.188227
7	5.017621	-2.979289	-3.480250
6	3.875443	-2.373734	-3.689942
6	2.970591	-2.018460	-2.661288
6	6.594970	-3.896384	-1.956614
6	7.017867	-4.198219	-0.687681
6	6.204813	-3.850332	0.421334
6	4.993205	-3.220625	0.230157
9	1.612624	7.611425	-0.580759
9	2.604374	6.377817	-2.051777
9	2.064672	6.174450	3.936617

9	3.425324	4.510571	4.142837
1	0.656365	-2.791945	-1.412497
1	1.250177	-4.991090	-0.946869
1	2.524600	-4.408787	0.115592
1	-2.059791	-3.045038	0.853137
1	-1.470949	-3.403964	-0.775445
1	-1.439531	-5.165246	1.603319
1	-1.009174	-5.584142	-0.055774
1	0.976419	-5.865536	1.394066
1	0.172399	-4.282225	3.134867
1	-0.581776	-2.220094	2.489396
1	1.057032	-1.726749	2.075809
1	2.398306	-2.994303	3.574554
1	4.178289	-4.572340	3.179761
1	3.106902	-5.571485	2.055845
1	2.711341	-2.076058	0.724853
1	2.043302	-1.515488	-2.927829
1	4.420404	-2.958658	1.111688
1	3.623131	-2.147448	-4.724209
1	7.199796	-4.141644	-2.823458
1	7.971869	-4.690699	-0.542307
1	1.373389	-0.277854	-1.217648
1	1.913379	1.674608	-1.146671
1	1.900710	3.781389	-1.569943
1	2.311610	2.483496	2.508913
1	1.903536	6.670687	1.618633
8	6.552331	-4.105603	1.708736
6	7.826354	-4.667746	1.957611
1	7.912990	-4.748518	3.041350
1	7.921815	-5.666978	1.516733
1	8.629878	-4.024150	1.581227
1	-3.688922	-2.050376	-2.781425
1	-2.383100	-0.144783	-3.537250
6	-4.820117	-2.275993	-0.963455
1	-3.951068	-2.588521	-0.371294
1	-5.303596	-3.181289	-1.344596
6	-5.769179	-1.531562	-0.077349
6	-7.072239	-1.802477	0.039583
1	-5.376985	-0.698892	0.506874
1	-7.513660	-2.630130	-0.507781
6	-7.929573	-0.994086	0.950289
8	-7.441424	-0.185154	1.722278
6	-9.414230	-1.199928	0.917454
6	-10.066984	-1.836616	-0.142384
6	-10.165427	-0.702994	1.987765
6	-11.451688	-1.978299	-0.127164
1	-9.506963	-2.203045	-0.996469
6	-11.545201	-0.856128	2.008067
1	-9.643717	-0.200996	2.795876
6	-12.190277	-1.495117	0.949170
1	-11.953458	-2.465956	-0.956677
1	-12.120800	-0.477591	2.846793
1	-13.269274	-1.613877	0.962919

[6-7]TS-anti_Cinchona-Thiourea_conf-7

Number of imaginary frequencies : 1
The smallest frequency is : -1271.8337

Electronic energy=	-3467.7002391
Zero-point correction=	0.931778
Thermal correction to Energy=	0.989941
Thermal correction to Enthalpy=	0.990885
Thermal correction to Gibbs Free Energy=	0.833247
Sum of electronic and zero-point Energies=	-3466.768461
Sum of electronic and thermal Energies=	-3466.710298
Sum of electronic and thermal Enthalpies=	-3466.709354

Sum of electronic and thermal Free Energies= -3466.866992

Cartesian Coordinates			
6	-2.135267	-4.112595	-1.357233
6	-0.611878	-4.156447	-1.539371
7	-0.388093	-3.448813	-2.814852
6	-1.647796	-2.923694	-3.356892
6	-2.681269	-3.878965	-2.770863
6	0.795124	-3.155505	-3.292309
6	2.016582	-3.304647	-2.601683
6	3.313898	-3.263298	-3.401704
6	-1.852051	-1.459332	-2.859098
8	-3.014013	-1.080364	-2.661440
8	-0.798282	-0.769538	-2.694144
1	-1.608489	-2.919323	-4.450337
1	-3.675836	-3.434569	-2.773027
1	-2.698830	-4.811698	-3.342648
1	-2.402791	-3.264621	-0.719784
1	-2.521730	-5.018701	-0.889390
1	-0.074242	-3.645557	-0.735095
1	-0.221812	-5.175030	-1.636298
1	1.747644	-2.188897	-1.843771
1	0.335587	-1.169342	-1.603302
8	1.138372	-1.369260	-1.049209
1	3.803908	-4.241450	-3.349138
1	1.474445	-0.445178	-0.712290
1	2.000227	-4.025208	-1.781897
7	-2.591585	-0.168940	0.031483
6	-3.414627	-1.011051	0.784140
6	-4.376271	-1.737764	0.068034
6	-5.151393	-2.693387	0.709411
6	-5.031780	-2.933032	2.072480
6	-4.087846	-2.191982	2.774619
6	-3.270996	-1.252451	2.156099
6	-6.054399	-3.538522	-0.138922
9	-5.342149	-4.432242	-0.857720
6	-3.956987	-2.385781	4.258826
9	-2.692565	-2.223021	4.675033
6	-1.750677	0.838444	0.425466
16	-1.818749	1.619050	1.921165
7	-0.863486	1.154239	-0.543441
6	-0.077616	2.375058	-0.563244
6	1.390641	2.129474	-0.978860
6	2.227816	3.415916	-0.724137
6	3.322547	3.104676	0.308822
6	4.266773	2.068227	-0.308162
6	3.415431	0.847813	-0.729281
7	2.010561	0.978642	-0.280366
6	1.998523	1.164982	1.183262
6	2.720698	2.488571	1.587375
6	1.820488	3.397218	2.387121
6	1.739748	4.723011	2.295212
6	-0.704498	3.388821	-1.519318
6	-1.051097	4.718183	-1.119447
6	-1.573119	5.586404	-2.124423
7	-1.781865	5.201399	-3.415053
6	-1.488321	3.964610	-3.731337
6	-0.943814	3.025966	-2.822082
6	-1.900052	6.919154	-1.774269
6	-1.730843	7.384517	-0.495567
6	-1.228084	6.513690	0.504678
6	-0.902755	5.209737	0.197409
9	-6.934862	-4.237197	0.588882
9	-6.746391	-2.808827	-1.024441
9	-4.348990	-3.612924	4.637689
9	-4.707972	-1.509463	4.943576
1	1.403060	1.866197	-2.044061
1	2.691888	3.762613	-1.653104
1	1.584134	4.224663	-0.368741

1	3.808322	-0.069643	-0.283585
1	3.400366	0.721232	-1.817605
1	5.028869	1.767843	0.418625
1	4.785189	2.497099	-1.171175
1	3.874024	4.016679	0.556226
1	3.560500	2.219210	2.243020
1	2.498324	0.293150	1.615409
1	0.960181	1.155535	1.528108
1	1.195358	2.888193	3.122004
1	1.065359	5.289084	2.930207
1	2.328302	5.297046	1.583600
1	-0.090222	2.764371	0.455201
1	-0.731430	2.017227	-3.170663
1	-0.544916	4.579145	1.002691
1	-1.673935	3.664790	-4.761106
1	-2.293166	7.559723	-2.556971
1	-1.990571	8.409244	-0.257780
1	-0.910311	0.608747	-1.412102
1	-2.707335	-0.290116	-0.981607
1	-4.479005	-1.575874	-1.001958
1	-2.525733	-0.721083	2.730870
1	-5.642456	-3.677981	2.568573
8	-1.038624	6.891199	1.794881
6	-1.392281	8.210434	2.162427
1	-1.177049	8.293891	3.227956
1	-0.798689	8.954632	1.618074
1	-2.458658	8.402617	1.996642
1	3.095628	-3.086046	-4.460757
1	0.786886	-2.627026	-4.246367
6	4.299391	-2.180577	-2.936157
1	3.845379	-1.201891	-3.152821
1	5.230267	-2.234548	-3.510065
6	4.587985	-2.213322	-1.470744
6	5.796925	-2.134604	-0.906119
1	3.729967	-2.256109	-0.797433
1	6.699152	-2.102082	-1.510441
6	5.907903	-2.019102	0.573009
8	4.941490	-1.693993	1.248169
6	7.229997	-2.273629	1.225364
6	8.266577	-2.952290	0.577919
6	7.410071	-1.831015	2.539826
6	9.470901	-3.179206	1.237782
1	8.132303	-3.326988	-0.431863
6	8.616042	-2.047508	3.192705
1	6.590084	-1.317035	3.030381
6	9.648671	-2.721683	2.540712
1	10.270386	-3.713367	0.734703
1	8.753756	-1.693370	4.209270
1	10.591689	-2.893049	3.050499

[6-7]TS-syn_Cinchona-Thiourea_conf-1

Number of imaginary frequencies : 1
The smallest frequency is : -1167.3438

Electronic energy= -3467.7056651
Zero-point correction= 0.930753
Thermal correction to Energy= 0.989759
Thermal correction to Enthalpy= 0.990704
Thermal correction to Gibbs Free Energy= 0.826225
Sum of electronic and zero-point Energies= -3466.774912
Sum of electronic and thermal Energies= -3466.715906
Sum of electronic and thermal Enthalpies= -3466.714962
Sum of electronic and thermal Free Energies= -3466.879440

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Cartesian Coordinates
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6	1.234225	4.146674	3.082344
6	2.524054	3.934650	2.292133
7	2.590202	2.468521	2.127854
6	1.630130	1.766544	2.990553
6	1.130987	2.874013	3.930794
6	3.296454	1.860613	1.207962
6	3.248317	0.485969	0.884454
6	4.427191	-0.075687	0.105683
6	0.485888	1.199902	2.121212
8	0.067104	1.969879	1.203523
8	0.074456	0.056835	2.378786
1	2.122418	0.943463	3.513925
1	0.117610	2.675305	4.285091
1	1.791386	2.936634	4.801134
1	0.387072	4.210667	2.397462
1	1.273781	5.054476	3.686344
1	2.521409	4.417328	1.313133
1	3.401575	4.266803	2.856964
1	2.182252	0.462394	0.027738
8	1.151700	0.373470	-0.723060
1	4.705394	0.618958	-0.696349
1	2.863503	-0.166051	1.674451
7	-2.412111	1.484174	0.028357
6	-2.984959	2.682017	-0.404402
6	-2.178303	3.821583	-0.252581
6	-2.665466	5.073379	-0.584445
6	-3.955068	5.238238	-1.086079
6	-4.742042	4.105511	-1.229097
6	-4.285759	2.832656	-0.889687
6	-1.771345	6.271521	-0.455726
9	-2.442213	7.349617	-0.023367
6	-6.136314	4.222788	-1.777363
9	-6.549108	5.497752	-1.837681
6	-2.664496	0.185776	-0.307472
16	-3.818988	-0.328944	-1.428917
7	-1.827961	-0.659170	0.335243
6	-1.920522	-2.105125	0.286137
6	-0.508939	-2.721694	0.244124
6	-0.581552	-4.252464	-0.010058
6	0.144753	-4.576091	-1.324452
6	1.621494	-4.192387	-1.161882
6	1.682720	-2.701939	-0.747291
7	0.342661	-2.078067	-0.785010
6	-0.224811	-2.240782	-2.138112
6	-0.435084	-3.745917	-2.486945
6	-1.871438	-4.041922	-2.843233
6	-2.565975	-5.129159	-2.516080
6	-2.678681	-2.655119	1.493001
6	-3.792780	-3.544701	1.366521
6	-4.365157	-4.048318	2.573112
7	-3.925404	-3.700799	3.815742
6	-2.925974	-2.856953	3.886693
6	-2.267025	-2.313222	2.758050
6	-5.448283	-4.956270	2.490378
6	-5.957459	-5.354351	1.280922
6	-5.397897	-4.839116	0.083907
6	-4.344805	-3.950775	0.129968
9	-0.759685	6.058340	0.403331
9	-1.216319	6.609353	-1.631125
9	-7.021822	3.549904	-1.027267
9	-6.223993	3.721237	-3.019226
1	-0.020292	-2.506431	1.202145
1	-0.111242	-4.799561	0.813047
1	-1.623721	-4.579020	-0.058221
1	2.326478	-2.123925	-1.418565
1	2.068926	-2.580298	0.270758
1	2.157865	-4.355587	-2.102052
1	2.092847	-4.823065	-0.402309
1	0.059247	-5.643683	-1.547824
1	0.166568	-3.967890	-3.379356

1	0.473866	-1.763819	-2.831873
1	-1.162999	-1.678923	-2.191142
1	-2.361989	-3.272657	-3.442091
1	-3.599248	-5.249036	-2.826789
1	-2.144203	-5.932664	-1.917223
1	-2.452339	-2.362747	-0.629691
1	-1.439351	-1.623551	2.907617
1	-3.972389	-3.565046	-0.810980
1	-2.590748	-2.578742	4.884365
1	-5.862148	-5.325997	3.422870
1	-6.787398	-6.050264	1.250089
1	-1.212723	-0.291225	1.074140
1	-1.553368	1.631717	0.581164
1	-1.170924	3.706738	0.136793
1	-4.934666	1.973315	-0.992466
1	-4.335428	6.219914	-1.343688
8	-5.847337	-5.173206	-1.153999
6	-6.976832	-6.019074	-1.247778
1	-7.183786	-6.127581	-2.312733
1	-6.778345	-7.008968	-0.820032
1	-7.851603	-5.578127	-0.755853
1	4.129097	-1.006895	-0.388562
1	0.715637	-0.577435	-0.653208
1	0.553439	1.010108	-0.276693
1	3.912516	2.519196	0.592687
6	5.659562	-0.351088	0.985739
1	5.360492	-1.026556	1.798603
1	5.999536	0.582529	1.449745
6	6.768307	-0.980076	0.205627
6	7.982600	-0.453375	0.025566
1	6.560382	-1.937160	-0.274436
1	8.240108	0.503344	0.470146
6	8.987579	-1.161808	-0.814861
8	8.680718	-2.146934	-1.466126
6	10.389306	-0.633024	-0.869727
6	10.902690	0.255784	0.079385
6	11.212396	-1.078176	-1.909631
6	12.219239	0.697661	-0.016459
1	10.291133	0.588949	0.911419
6	12.521481	-0.627279	-2.011427
1	10.801798	-1.778129	-2.629870
6	13.026507	0.263087	-1.063964
1	12.614820	1.381444	0.727652
1	13.151149	-0.968424	-2.826927
1	14.050346	0.615665	-1.141247

[6-7]TS-syn_Cinchona-Thiourea_conf-2

Number of imaginary frequencies : 1
The smallest frequency is : -1171.3801

Electronic energy= -3467.7050533
Zero-point correction= 0.931061
Thermal correction to Energy= 0.989968
Thermal correction to Enthalpy= 0.990912
Thermal correction to Gibbs Free Energy= 0.826370
Sum of electronic and zero-point Energies= -3466.773992
Sum of electronic and thermal Energies= -3466.715085
Sum of electronic and thermal Enthalpies= -3466.714141
Sum of electronic and thermal Free Energies= -3466.878683

Cartesian Coordinates

6	1.294679	-4.821588	3.443596
6	-0.171172	-5.123829	3.139205
7	-0.813950	-3.795875	3.193741
6	0.053354	-2.781025	3.805386

6	1.212796	-3.609835	4.379409
6	-1.962260	-3.505134	2.631591
6	-2.525786	-2.218037	2.513816
6	-4.013559	-2.108377	2.188754
6	0.541158	-1.798555	2.718442
8	0.884038	-2.326943	1.616644
8	0.555364	-0.588490	2.998894
1	-0.495593	-2.222733	4.567929
1	2.139669	-3.034269	4.418063
1	0.964668	-3.926557	5.397065
1	1.817222	-4.552089	2.523937
1	1.797141	-5.674752	3.902108
1	-0.330136	-5.573707	2.157640
1	-0.616755	-5.765249	3.907182
1	-1.882785	-1.758663	1.381993
8	-1.297836	-1.276985	0.370573
1	-4.287196	-1.048744	2.206420
1	-2.155753	-1.485940	3.235537
7	2.442468	-0.843517	-0.159626
6	3.267477	-1.689311	-0.904154
6	3.070655	-3.063500	-0.692055
6	3.877644	-3.991422	-1.327272
6	4.891594	-3.594763	-2.196446
6	5.078438	-2.234773	-2.393177
6	4.292672	-1.275277	-1.756927
6	3.619514	-5.455454	-1.122635
9	4.756911	-6.166437	-1.124915
6	6.156435	-1.746010	-3.318946
9	6.961509	-2.738501	-3.726673
6	2.038173	0.441994	-0.373678
16	2.445292	1.387060	-1.713416
7	1.205781	0.863786	0.604608
6	0.713458	2.221652	0.738465
6	-0.751578	2.204663	1.217015
6	-1.367849	3.629348	1.171358
6	-2.542227	3.635293	0.180060
6	-3.621369	2.681837	0.709800
6	-2.963223	1.300821	0.941127
7	-1.580803	1.271801	0.415005
6	-1.597383	1.652752	-1.012232
6	-2.096071	3.117212	-1.201794
6	-1.077633	3.969307	-1.918633
6	-0.782244	5.241087	-1.659776
6	1.561227	3.020046	1.727878
6	2.161660	4.277151	1.398749
6	2.875119	4.949785	2.435890
7	3.030247	4.443637	3.692453
6	2.490561	3.276923	3.942337
6	1.744493	2.531356	2.998404
6	3.458328	6.209697	2.160129
6	3.352075	6.791858	0.922925
6	2.653991	6.115367	-0.109955
6	2.080866	4.883393	0.124099
9	2.994496	-5.701567	0.041503
9	2.844017	-5.966270	-2.093352
9	6.928915	-0.819560	-2.731359
9	5.642240	-1.175924	-4.419586
1	-0.767770	1.802783	2.237138
1	-1.724916	3.924873	2.162862
1	-0.610898	4.359559	0.872195
1	-3.520571	0.498363	0.444116
1	-2.907586	1.053882	2.006879
1	-4.441751	2.604723	-0.010937
1	-4.041380	3.066993	1.643457
1	-2.950834	4.645714	0.086893
1	-2.989143	3.083918	-1.841190
1	-2.252028	0.937967	-1.520295
1	-0.590828	1.511254	-1.419225
1	-0.556845	3.470150	-2.737314
1	-0.033182	5.772562	-2.238516

1	-1.259059	5.797865	-0.856870
1	0.764111	2.683289	-0.247789
1	1.328289	1.570602	3.292571
1	1.584707	4.394790	-0.705336
1	2.628461	2.878209	4.945874
1	3.993606	6.699563	2.966940
1	3.808322	7.758200	0.744192
1	1.077018	0.275477	1.440654
1	1.943052	-1.338397	0.595429
1	2.283397	-3.386334	-0.016564
1	4.481140	-0.221992	-1.915474
1	5.522594	-4.324090	-2.690643
8	2.505133	6.618386	-1.363196
6	3.136245	7.846996	-1.667395
1	2.919751	8.044769	-2.717461
1	2.737891	8.668142	-1.059617
1	4.222165	7.785892	-1.531112
1	-4.631095	-2.591253	2.957170
1	-1.266563	-0.223531	0.439876
1	-0.390228	-1.624447	0.508817
1	-2.462014	-4.352380	2.159617
6	-4.385527	-2.675292	0.807444
1	-4.167364	-3.751707	0.780259
1	-3.768330	-2.203680	0.034395
6	-5.838618	-2.469875	0.524148
6	-6.332750	-1.741397	-0.481067
1	-6.552840	-2.920878	1.214027
1	-5.666750	-1.259498	-1.190646
6	-7.804554	-1.553841	-0.609456
8	-8.569335	-1.995310	0.232816
6	-8.342532	-0.781760	-1.776491
6	-7.596747	-0.522178	-2.929904
6	-9.662204	-0.323941	-1.694444
6	-8.163876	0.189694	-3.983465
1	-6.581497	-0.891581	-3.027879
6	-10.222308	0.397113	-2.739858
1	-10.229563	-0.546208	-0.796786
6	-9.472330	0.655215	-3.886961
1	-7.583759	0.380646	-4.880555
1	-11.243321	0.757466	-2.664947
1	-9.910321	1.215980	-4.706934

[6-7]TS-syn_Cinchona-Thiourea_conf-3

Number of imaginary frequencies : 1
The smallest frequency is : -1243.5953

Electronic energy= -3467.7135721
Zero-point correction= 0.931843
Thermal correction to Energy= 0.989943
Thermal correction to Enthalpy= 0.990888
Thermal correction to Gibbs Free Energy= 0.835298
Sum of electronic and zero-point Energies= -3466.781730
Sum of electronic and thermal Energies= -3466.723629
Sum of electronic and thermal Enthalpies= -3466.722684
Sum of electronic and thermal Free Energies= -3466.878274

Cartesian Coordinates

6	3.460107	-2.484406	3.933986
6	3.933311	-3.222909	2.680874
7	2.684076	-3.722430	2.067040
6	1.510478	-3.488572	2.919572
6	2.136894	-3.174862	4.285480
6	2.611920	-4.200353	0.849573
6	1.430061	-4.488825	0.130106
6	1.513552	-5.498602	-1.016825

6	0.715064	-2.289324	2.361593
8	1.428423	-1.312641	1.973273
8	-0.521822	-2.368384	2.318715
1	0.871655	-4.374318	2.931389
1	1.480795	-2.554067	4.898613
1	2.320973	-4.111513	4.820561
1	3.281963	-1.434334	3.699412
1	4.193180	-2.549183	4.739607
1	4.456563	-2.572756	1.976380
1	4.570184	-4.078360	2.927686
1	1.147548	-3.218407	-0.324856
8	0.796584	-2.012361	-0.605621
1	0.527023	-5.553665	-1.490981
1	0.543794	-4.618135	0.758035
7	0.552105	1.149836	1.069884
6	1.659485	1.979885	0.876416
6	2.906767	1.373760	1.083730
6	4.074506	2.110045	0.964032
6	4.045687	3.459446	0.632703
6	2.804000	4.044446	0.415566
6	1.612220	3.336953	0.540056
6	5.381652	1.411319	1.193382
9	6.402443	2.039824	0.591096
6	2.751315	5.454241	-0.093821
9	3.770414	6.196223	0.364534
6	-0.687350	1.149565	0.498779
16	-1.313380	2.375144	-0.484828
7	-1.361426	0.017004	0.792973
6	-2.719519	-0.285262	0.383376
6	-2.791105	-1.730210	-0.154502
6	-4.173221	-2.022374	-0.798233
6	-3.969649	-2.378717	-2.279253
6	-3.124093	-3.657496	-2.352891
6	-1.809851	-3.406777	-1.572474
7	-1.711575	-1.999754	-1.132838
6	-1.810136	-1.120441	-2.316431
6	-3.199549	-1.260897	-3.008779
6	-3.912538	0.065104	-3.104883
6	-5.212545	0.288073	-2.924051
6	-3.696409	-0.125427	1.545378
6	-4.885899	0.665661	1.453250
6	-5.746766	0.682192	2.591173
7	-5.478578	0.010626	3.746930
6	-4.366604	-0.679782	3.797880
6	-3.449045	-0.783628	2.725111
6	-6.946640	1.431260	2.530924
6	-7.294120	2.136410	1.407196
6	-6.431137	2.127842	0.281988
6	-5.251647	1.414393	0.310810
9	5.690328	1.324626	2.498059
9	5.359134	0.149569	0.724717
9	1.614815	6.078119	0.236569
9	2.832843	5.479538	-1.440510
1	-2.597240	-2.406966	0.685880
1	-4.665672	-2.854496	-0.285170
1	-4.829445	-1.153474	-0.701204
1	-0.926039	-3.610771	-2.188344
1	-1.745461	-4.033467	-0.676030
1	-2.912517	-3.907289	-3.397353
1	-3.674255	-4.497816	-1.918699
1	-4.937984	-2.544342	-2.761219
1	-3.024012	-1.601119	-4.039055
1	-0.992773	-1.400701	-2.987270
1	-1.624779	-0.090261	-1.994936
1	-3.272753	0.909046	-3.367561
1	-5.629696	1.285227	-3.024624
1	-5.909084	-0.503804	-2.659867
1	-2.974372	0.412481	-0.414395
1	-2.552415	-1.387176	2.847930
1	-4.619437	1.456437	-0.567827

1	-4.159934	-1.205742	4.728435
1	-7.582834	1.426916	3.409994
1	-8.219113	2.700250	1.391461
1	-0.933695	-0.686258	1.406221
1	0.802377	0.271378	1.548227
1	2.946626	0.314734	1.323215
1	0.663390	3.826732	0.371173
1	4.961458	4.028752	0.518765
8	-6.696535	2.802233	-0.866735
6	-7.874080	3.583192	-0.926127
1	-7.878706	4.045509	-1.913617
1	-8.774537	2.967195	-0.815643
1	-7.874624	4.370185	-0.162885
1	1.715249	-6.502414	-0.623674
1	-0.251212	-1.928641	-0.693122
1	1.081153	-1.508744	0.184700
1	3.576653	-4.290095	0.348267
6	2.553362	-5.180095	-2.110370
1	2.577562	-6.023145	-2.809802
1	3.558772	-5.091508	-1.683890
6	2.175815	-3.924544	-2.825787
6	2.784119	-2.745159	-2.694598
1	1.264708	-3.949867	-3.425247
1	3.674648	-2.642433	-2.080226
6	2.140018	-1.521565	-3.247561
8	1.125384	-1.595875	-3.923732
6	2.725999	-0.187841	-2.912105
6	4.078146	-0.018254	-2.597525
6	1.880651	0.926090	-2.949732
6	4.584100	1.256345	-2.359660
1	4.750023	-0.870666	-2.571891
6	2.380690	2.194875	-2.684879
1	0.832244	0.777080	-3.187610
6	3.737862	2.361787	-2.410919
1	5.637094	1.387192	-2.129123
1	1.719397	3.055902	-2.690915
1	4.128101	3.357387	-2.226147

[6-7]TS-syn_Cinchona-Thiourea_conf-4

Number of imaginary frequencies : 1
The smallest frequency is : -1167.4477

Electronic energy= -3467.7056355
Zero-point correction= 0.931028
Thermal correction to Energy= 0.989873
Thermal correction to Enthalpy= 0.990817
Thermal correction to Gibbs Free Energy= 0.828114
Sum of electronic and zero-point Energies= -3466.774607
Sum of electronic and thermal Energies= -3466.715763
Sum of electronic and thermal Enthalpies= -3466.714819
Sum of electronic and thermal Free Energies= -3466.877522

Cartesian Coordinates

6	1.377974	3.795000	3.399911
6	2.640580	3.574646	2.567940
7	2.655917	2.115398	2.339089
6	1.673548	1.409379	3.172058
6	1.233680	2.482657	4.178688
6	3.327964	1.527763	1.381203
6	3.227072	0.172982	0.992031
6	4.372928	-0.386931	0.163950
6	0.498118	0.947786	2.282820
8	0.127759	1.781356	1.399653
8	0.016632	-0.177186	2.490255
1	2.131685	0.537000	3.643966

1	0.217931	2.306115	4.537989
1	1.907667	2.470363	5.040735
1	0.519631	3.937744	2.741505
1	1.471410	4.663902	4.053330
1	2.626813	4.099910	1.610973
1	3.542515	3.855057	3.121904
1	2.151500	0.221963	0.148546
8	1.117066	0.207157	-0.599970
1	4.647339	0.330493	-0.619084
1	2.834820	-0.504340	1.756380
7	-2.308792	1.580201	0.089720
6	-2.706306	2.836031	-0.374369
6	-1.807836	3.880656	-0.099665
6	-2.113809	5.181517	-0.458126
6	-3.306719	5.491110	-1.107181
6	-4.185666	4.451051	-1.372754
6	-3.913422	3.132240	-1.012328
6	-1.114852	6.270788	-0.198006
9	-1.710657	7.424101	0.137801
6	-5.466904	4.729222	-2.107570
9	-5.812892	6.023994	-2.041944
6	-2.662370	0.315127	-0.278228
16	-3.816497	-0.081380	-1.447319
7	-1.930569	-0.610541	0.382473
6	-2.141520	-2.042689	0.298892
6	-0.785048	-2.775392	0.267712
6	-0.981425	-4.287321	-0.029629
6	-0.269799	-4.635712	-1.346065
6	1.232635	-4.388326	-1.156139
6	1.418318	-2.925476	-0.685118
7	0.140724	-2.181036	-0.727285
6	-0.412298	-2.255259	-2.094668
6	-0.757363	-3.723267	-2.488849
6	-2.209475	-3.876272	-2.869302
6	-3.006661	-4.901382	-2.576608
6	-2.968659	-2.553902	1.477081
6	-4.158404	-3.331263	1.305024
6	-4.798325	-3.813778	2.485921
7	-4.353963	-3.542233	3.745928
6	-3.282099	-2.798152	3.859026
6	-2.552126	-2.287963	2.758435
6	-5.956066	-4.618184	2.358055
6	-6.472225	-4.938874	1.128600
6	-5.844542	-4.443772	-0.042639
6	-4.719561	-3.651930	0.047821
9	-0.266868	5.952890	0.795612
9	-0.361340	6.526910	-1.280506
9	-6.489392	4.015240	-1.616100
9	-5.365902	4.415954	-3.409163
1	-0.300868	-2.625801	1.239974
1	-0.567445	-4.894197	0.781875
1	-2.046406	-4.524829	-0.095600
1	2.128407	-2.385990	-1.320930
1	1.788180	-2.876614	0.344737
1	1.764211	-4.563186	-2.097015
1	1.638863	-5.084670	-0.416717
1	-0.445961	-5.684531	-1.602589
1	-0.168346	-3.974443	-3.381941
1	0.342084	-1.829386	-2.762782
1	-1.291893	-1.605644	-2.148794
1	-2.617066	-3.053322	-3.458884
1	-4.041940	-4.917110	-2.903300
1	-2.672454	-5.753229	-1.989556
1	-2.674168	-2.233653	-0.632628
1	-1.665229	-1.686184	2.943245
1	-4.296279	-3.276210	-0.875518
1	-2.942404	-2.580512	4.870242
1	-6.420349	-4.973501	3.272268
1	-7.358877	-5.558285	1.063813
1	-1.301616	-0.313753	1.140342

1	-1.481770	1.632308	0.703693
1	-0.871574	3.653523	0.402233
1	-4.631904	2.350522	-1.216551
1	-3.545653	6.511767	-1.383257
8	-6.294847	-4.705902	-1.297664
6	-7.465880	-5.486584	-1.435473
1	-7.653112	-5.561652	-2.506905
1	-7.330856	-6.494022	-1.024435
1	-8.327304	-5.009076	-0.954400
1	4.040503	-1.292188	-0.356305
1	0.624675	-0.718576	-0.554122
1	0.558367	0.863003	-0.131578
1	3.959098	2.193792	0.789547
6	5.619953	-0.720680	1.002411
1	5.328603	-1.427960	1.790548
1	5.982187	0.186738	1.500258
6	6.703777	-1.326983	0.171056
6	7.915948	-0.798872	-0.019229
1	6.478013	-2.264281	-0.338919
1	8.187484	0.139926	0.454167
6	8.898529	-1.479392	-0.907608
8	8.575355	-2.444349	-1.580783
6	10.298233	-0.947261	-0.982350
6	10.835156	-0.086109	-0.020905
6	11.094891	-1.359700	-2.055872
6	12.147937	0.361767	-0.137979
1	10.245690	0.220781	0.836704
6	12.400180	-0.902836	-2.178349
1	10.667116	-2.039298	-2.785587
6	12.928310	-0.039455	-1.218680
1	12.561361	1.024445	0.615487
1	13.008583	-1.218015	-3.020003
1	13.948986	0.318247	-1.312339

[6-7]TS-syn_Cinchona-Thiourea_conf-5

Number of imaginary frequencies : 1
 The smallest frequency is : -1194.3734

Electronic energy= -3467.706966
 Zero-point correction= 0.930544
 Thermal correction to Energy= 0.989081
 Thermal correction to Enthalpy= 0.990025
 Thermal correction to Gibbs Free Energy= 0.830226
 Sum of electronic and zero-point Energies= -3466.776422
 Sum of electronic and thermal Energies= -3466.717885
 Sum of electronic and thermal Enthalpies= -3466.716941
 Sum of electronic and thermal Free Energies= -3466.876740

 Cartesian Coordinates

6	4.902924	-2.035864	3.229704
6	4.499229	-3.405487	2.684805
7	3.031011	-3.423940	2.841330
6	2.543056	-2.305811	3.659484
6	3.829376	-1.745941	4.285079
6	2.229036	-4.218541	2.174365
6	0.821352	-4.145530	2.153149
6	0.041914	-5.330548	1.589122
6	1.862894	-1.265196	2.739101
8	2.448002	-1.065266	1.629119
8	0.823798	-0.717645	3.139607
1	1.821641	-2.658893	4.399872
1	3.733796	-0.684104	4.520458
1	4.046311	-2.284227	5.212869
1	4.855961	-1.291668	2.433131
1	5.911315	-2.048367	3.646448

1	4.761761	-3.549091	1.634572
1	4.929547	-4.218572	3.278862
1	0.635473	-3.178577	1.198825
8	0.414589	-2.303059	0.306314
1	-1.021231	-5.089593	1.688992
1	0.367395	-3.657716	3.018511
7	1.891913	1.167309	0.104848
6	3.006383	1.505442	-0.666610
6	4.090219	0.616784	-0.579470
6	5.271755	0.884811	-1.248443
6	5.415900	2.026934	-2.033363
6	4.338710	2.897549	-2.109582
6	3.141834	2.664404	-1.433794
6	6.400006	-0.101722	-1.170055
9	7.593871	0.507625	-1.135333
6	4.427782	4.134741	-2.958042
9	5.682615	4.380312	-3.362741
6	0.571672	1.478840	-0.032647
16	-0.084005	2.430303	-1.266662
7	-0.180281	0.881180	0.919947
6	-1.598806	1.120299	1.107568
6	-2.314877	-0.188404	1.495521
6	-3.858452	-0.016091	1.442054
6	-4.439074	-0.979077	0.391866
6	-4.142650	-2.416624	0.841401
6	-2.617599	-2.536051	1.075193
7	-1.911289	-1.315936	0.625030
6	-2.245581	-1.057611	-0.789979
6	-3.763509	-0.774246	-0.977583
6	-4.007135	0.558672	-1.638713
6	-4.955912	1.442202	-1.335063
6	-1.846829	2.168444	2.190232
6	-2.693881	3.303511	1.987840
6	-2.905809	4.165295	3.105646
7	-2.321431	3.975194	4.322594
6	-1.525468	2.943090	4.454717
6	-1.262608	2.010125	3.423088
6	-3.765485	5.280171	2.957601
6	-4.390462	5.548398	1.766886
6	-4.163320	4.701050	0.652346
6	-3.329328	3.608930	0.762244
9	6.314737	-0.881264	-0.077973
9	6.419888	-0.925801	-2.231224
9	3.999420	5.221587	-2.298708
9	3.670364	4.030879	-4.061085
1	-1.985520	-0.466549	2.503702
1	-4.301111	-0.231384	2.419695
1	-4.115792	1.017084	1.195279
1	-2.189618	-3.379898	0.523459
1	-2.379833	-2.673596	2.135511
1	-4.472050	-3.124245	0.072302
1	-4.691107	-2.649551	1.758867
1	-5.519389	-0.830184	0.303727
1	-4.157973	-1.540781	-1.660959
1	-1.940301	-1.948175	-1.345371
1	-1.628798	-0.225060	-1.145354
1	-3.327256	0.788198	-2.461119
1	-5.049461	2.374402	-1.883418
1	-5.666394	1.283904	-0.527535
1	-1.988960	1.475464	0.153503
1	-0.596674	1.172492	3.620630
1	-3.169086	3.008874	-0.125695
1	-1.057800	2.807351	5.428253
1	-3.911893	5.916654	3.824275
1	-5.044104	6.408688	1.685972
1	0.285297	0.378591	1.687566
1	2.095757	0.421614	0.790566
1	3.991266	-0.279034	0.026541
1	2.329673	3.375994	-1.499300
1	6.342138	2.235122	-2.556344

8	-4.733068	4.902093	-0.564389
6	-5.549539	6.043496	-0.736859
1	-5.869323	6.030211	-1.779094
1	-6.435209	6.009213	-0.091355
1	-4.994581	6.969176	-0.545158
1	0.198240	-6.237774	2.183397
1	-0.482493	-1.776773	0.531573
1	1.167986	-1.698471	0.479213
1	2.735041	-4.936312	1.525436
6	0.357169	-5.617244	0.092055
1	0.958893	-6.528255	0.002004
1	0.938969	-4.792207	-0.332000
6	-0.912272	-5.768009	-0.684824
6	-1.362236	-4.876602	-1.575286
1	-1.548904	-6.622611	-0.453783
1	-0.770535	-3.994116	-1.803835
6	-2.718860	-5.035319	-2.169326
8	-3.415547	-6.001432	-1.903037
6	-3.255712	-3.941984	-3.045467
6	-2.439928	-2.987898	-3.662311
6	-4.642537	-3.880189	-3.228152
6	-3.006030	-1.973402	-4.429958
1	-1.360303	-3.032353	-3.558855
6	-5.206874	-2.865966	-3.991977
1	-5.259487	-4.637427	-2.754829
6	-4.388517	-1.906561	-4.588142
1	-2.366380	-1.235078	-4.902907
1	-6.283513	-2.817525	-4.119780
1	-4.828529	-1.107579	-5.176798

[6-7]TS-syn_Cinchona-Thiourea_conf-6

Number of imaginary frequencies : 1
The smallest frequency is : -1220.3201

Electronic energy= -3467.7035402
Zero-point correction= 0.930658
Thermal correction to Energy= 0.989611
Thermal correction to Enthalpy= 0.990556
Thermal correction to Gibbs Free Energy= 0.827277
Sum of electronic and zero-point Energies= -3466.772882
Sum of electronic and thermal Energies= -3466.713929
Sum of electronic and thermal Enthalpies= -3466.712984
Sum of electronic and thermal Free Energies= -3466.876263

Cartesian Coordinates

6	0.857544	-4.233955	3.800181
6	-0.357239	-4.734816	3.017002
7	-1.185584	-3.524241	2.836436
6	-0.658841	-2.379309	3.582853
6	0.309002	-3.033251	4.579550
6	-2.132701	-3.417236	1.936542
6	-2.848033	-2.255018	1.579832
6	-4.154584	-2.490297	0.828723
6	0.097483	-1.452170	2.606587
8	0.666348	-2.041416	1.634232
8	0.102559	-0.234225	2.840099
1	-1.466201	-1.823127	4.064144
1	1.083720	-2.336471	4.905266
1	-0.247744	-3.365912	5.460999
1	1.635295	-3.907435	3.106960
1	1.266496	-5.008525	4.450741
1	-0.095901	-5.156282	2.044030
1	-0.930294	-5.472702	3.587788
1	-1.969379	-1.598137	0.696383
8	-1.187835	-0.978509	-0.047045

1	-4.960227	-2.768477	1.520068
1	-2.887114	-1.475250	2.347457
7	2.583616	-1.020715	-0.045448
6	3.309059	-2.038579	-0.665094
6	2.943745	-3.338292	-0.273566
6	3.621204	-4.437327	-0.767486
6	4.671731	-4.291788	-1.672031
6	5.021072	-3.004659	-2.052603
6	4.366276	-1.874661	-1.562513
6	3.184770	-5.814277	-0.360422
9	4.229247	-6.634155	-0.175337
6	6.126805	-2.792680	-3.048520
9	6.880117	-3.891126	-3.206496
6	2.373726	0.288709	-0.358644
16	3.069293	1.118872	-1.653245
7	1.478926	0.853342	0.486503
6	1.165843	2.267062	0.526112
6	-0.325175	2.466566	0.861966
6	-0.722354	3.957427	0.684648
6	-1.792884	4.064943	-0.411311
6	-3.037096	3.310244	0.071210
6	-2.610797	1.863138	0.416896
7	-1.205901	1.604768	0.031356
6	-1.041701	1.897341	-1.408065
6	-1.311973	3.400844	-1.716676
6	-0.127691	4.058714	-2.381533
6	0.323652	5.292420	-2.167153
6	2.018178	2.996984	1.564058
6	2.795536	4.157080	1.250996
6	3.486554	4.788795	2.328311
7	3.465068	4.324641	3.609806
6	2.768690	3.240581	3.846358
6	2.024722	2.547010	2.861803
6	4.236731	5.960905	2.066922
6	4.313451	6.494935	0.806261
6	3.640614	5.854646	-0.265684
6	2.905940	4.709302	-0.045755
9	2.476864	-5.802182	0.783658
9	2.405005	-6.388625	-1.291111
9	6.943847	-1.795751	-2.678204
9	5.646562	-2.467982	-4.259173
1	-0.486570	2.133439	1.893059
1	-1.116026	4.363781	1.621557
1	0.155412	4.552590	0.420470
1	-3.228832	1.131910	-0.111077
1	-2.693779	1.657799	1.489435
1	-3.805285	3.311124	-0.708957
1	-3.461443	3.805880	0.949442
1	-2.039285	5.114816	-0.595373
1	-2.143942	3.448087	-2.433148
1	-1.740321	1.247070	-1.943572
1	-0.032290	1.598307	-1.708643
1	0.382204	3.441008	-3.122698
1	1.183952	5.675317	-2.707521
1	-0.128964	5.963456	-1.441169
1	1.368518	2.669850	-0.466418
1	1.459757	1.661953	3.146049
1	2.435560	4.242323	-0.902084
1	2.766101	2.875293	4.871827
1	4.749218	6.423496	2.904129
1	4.893295	7.394623	0.637914
1	1.139052	0.324020	1.297089
1	1.971962	-1.374910	0.705426
1	2.124137	-3.465637	0.427975
1	4.678337	-0.884978	-1.867316
1	5.205405	-5.154086	-2.055002
8	3.673275	6.310256	-1.545210
6	4.459834	7.451469	-1.826264
1	4.362840	7.627043	-2.897968
1	4.099761	8.334962	-1.285672

1	5.515721	7.281646	-1.585850
1	-4.027573	-3.337511	0.142624
1	-1.115768	0.068421	0.101536
1	-0.334098	-1.361279	0.249578
1	-2.325149	-4.334578	1.377132
6	-4.609536	-1.267860	0.020916
1	-3.813554	-1.007069	-0.690613
1	-4.750325	-0.412130	0.691840
6	-5.870938	-1.541462	-0.733586
6	-7.025084	-0.890380	-0.564996
1	-5.847837	-2.347224	-1.468316
1	-7.101798	-0.088577	0.163238
6	-8.226859	-1.275582	-1.355662
8	-8.232317	-2.285711	-2.039864
6	-9.446664	-0.406190	-1.290171
6	-9.419667	0.899775	-0.792981
6	-10.649239	-0.930847	-1.776222
6	-10.581030	1.667319	-0.776765
1	-8.492271	1.335866	-0.437216
6	-11.809495	-0.168583	-1.749492
1	-10.649656	-1.942154	-2.169386
6	-11.776542	1.132589	-1.248452
1	-10.550862	2.683706	-0.397641
1	-12.740552	-0.584465	-2.121126
1	-12.682525	1.730370	-1.230249

[6-7]TS-syn_Cinchona-Thiourea_conf-7

Number of imaginary frequencies : 1
The smallest frequency is : -1177.7740

Electronic energy= -3467.7057193
Zero-point correction= 0.931459
Thermal correction to Energy= 0.989923
Thermal correction to Enthalpy= 0.990867
Thermal correction to Gibbs Free Energy= 0.830026
Sum of electronic and zero-point Energies= -3466.774260
Sum of electronic and thermal Energies= -3466.715796
Sum of electronic and thermal Enthalpies= -3466.714852
Sum of electronic and thermal Free Energies= -3466.875694

Cartesian Coordinates

6	3.147747	0.464271	4.123120
6	3.973857	-0.596000	3.400006
7	2.958974	-1.572018	2.954954
6	1.664114	-1.375956	3.617531
6	1.986389	-0.344953	4.712565
6	3.154427	-2.417952	1.972253
6	2.186644	-3.258729	1.380137
6	2.680936	-4.399226	0.483974
6	0.636464	-0.819970	2.608294
8	1.060851	0.097411	1.840624
8	-0.508478	-1.304730	2.620991
1	1.291894	-2.324699	4.012089
1	1.116442	0.266599	4.959757
1	2.305066	-0.867283	5.619991
1	2.771450	1.195070	3.405286
1	3.730197	0.981943	4.887065
1	4.525225	-0.221553	2.535264
1	4.669344	-1.094928	4.083807
1	1.545911	-2.372224	0.518548
8	0.922401	-1.622083	-0.258161
1	1.895229	-5.158846	0.424820
1	1.333875	-3.497501	2.020180
7	-0.655288	1.719857	0.345950
6	-0.058463	2.944625	0.038025

6	1.267760	3.090472	0.475190
6	1.940035	4.285471	0.283741
6	1.330155	5.364041	-0.352470
6	0.018472	5.207734	-0.776813
6	-0.690178	4.023490	-0.585909
6	3.369801	4.405454	0.724648
9	3.651729	5.642669	1.161117
6	-0.671431	6.335518	-1.491432
9	-0.065204	7.512837	-1.272323
6	-1.722624	1.065890	-0.196051
16	-2.664715	1.616871	-1.486049
7	-1.916137	-0.132909	0.397659
6	-3.046028	-1.004993	0.145940
6	-2.586474	-2.473688	0.211611
6	-3.716183	-3.437483	-0.242870
6	-3.242994	-4.215570	-1.480799
6	-2.029403	-5.064526	-1.077055
6	-0.970707	-4.120316	-0.457405
7	-1.369018	-2.704567	-0.605105
6	-1.606296	-2.412399	-2.033218
6	-2.793548	-3.249045	-2.594765
6	-3.876611	-2.368973	-3.169108
6	-5.190483	-2.561108	-3.076935
6	-4.159695	-0.774659	1.166681
6	-5.518484	-0.530361	0.790103
6	-6.473456	-0.398943	1.842499
7	-6.148245	-0.465971	3.164841
6	-4.888262	-0.660213	3.466210
6	-3.861115	-0.826375	2.506225
6	-7.833389	-0.186780	1.510848
6	-8.247255	-0.104816	0.205999
6	-7.293922	-0.222008	-0.837375
6	-5.961107	-0.421979	-0.548169
9	3.664039	3.552512	1.719124
9	4.226777	4.146430	-0.276199
9	-1.948728	6.463573	-1.104245
9	-0.688097	6.145864	-2.820688
1	-2.283789	-2.681265	1.244320
1	-3.962943	-4.140901	0.558550
1	-4.626565	-2.875973	-0.468550
1	0.007434	-4.238180	-0.937635
1	-0.837886	-4.307586	0.613447
1	-1.624048	-5.580845	-1.953245
1	-2.329261	-5.830145	-0.355447
1	-4.045063	-4.863192	-1.847212
1	-2.407923	-3.860574	-3.422527
1	-0.673283	-2.636321	-2.559653
1	-1.781588	-1.336718	-2.139316
1	-3.515986	-1.500328	-3.722659
1	-5.891478	-1.867658	-3.531158
1	-5.621487	-3.400125	-2.536187
1	-3.412943	-0.781653	-0.856172
1	-2.840181	-0.993831	2.842807
1	-5.270366	-0.477721	-1.380346
1	-4.639713	-0.702914	4.525195
1	-8.538367	-0.090550	2.330152
1	-9.295110	0.058319	-0.016153
1	-1.357707	-0.387684	1.223508
1	-0.100229	1.162007	1.012134
1	1.755770	2.256331	0.971833
1	-1.719284	3.944046	-0.908216
1	1.856903	6.300102	-0.497166
8	-7.617906	-0.145689	-2.154676
6	-8.966726	0.107391	-2.495633
1	-8.998298	0.155745	-3.584374
1	-9.628475	-0.697547	-2.154012
1	-9.313824	1.062757	-2.085463
1	3.555170	-4.894656	0.923309
1	-0.083280	-1.959246	-0.300548
1	0.940251	-0.780362	0.248743

1	4.159527	-2.374678	1.547897
6	3.048056	-3.973280	-0.959563
1	2.143713	-3.640344	-1.481845
1	3.455667	-4.837655	-1.493410
6	4.037338	-2.853485	-0.931669
6	5.358204	-2.964314	-1.101551
1	3.650602	-1.867631	-0.671781
1	5.816132	-3.904693	-1.397942
6	6.225465	-1.788741	-0.814362
8	5.851222	-0.925465	-0.033062
6	7.565704	-1.688526	-1.468266
6	7.926996	-2.491970	-2.553562
6	8.466077	-0.732734	-0.985875
6	9.177617	-2.342732	-3.146039
1	7.228251	-3.219378	-2.954736
6	9.716318	-0.591009	-1.572157
1	8.162899	-0.111000	-0.150037
6	10.073156	-1.397001	-2.653344
1	9.451298	-2.961071	-3.994713
1	10.414013	0.147781	-1.191196
1	11.049482	-1.283691	-3.114366

[6-7]TS-*syn*_Cinchona-Thiourea_conf-8

Number of imaginary frequencies : 1
The smallest frequency is : -1171.8704

Electronic energy= -3467.706737
Zero-point correction= 0.930969
Thermal correction to Energy= 0.989342
Thermal correction to Enthalpy= 0.990286
Thermal correction to Gibbs Free Energy= 0.831537
Sum of electronic and zero-point Energies= -3466.775768
Sum of electronic and thermal Energies= -3466.717395
Sum of electronic and thermal Enthalpies= -3466.716451
Sum of electronic and thermal Free Energies= -3466.875200

Cartesian Coordinates

6	2.570323	-1.961515	4.212329
6	3.372143	-2.539358	3.046437
7	2.342943	-3.176713	2.197948
6	1.027231	-3.197314	2.839890
6	1.359189	-2.897449	4.309603
6	2.545555	-3.487567	0.940738
6	1.582716	-3.933680	0.008185
6	2.106835	-4.505010	-1.315087
6	0.138607	-2.082963	2.241849
8	0.746908	-1.022814	1.897784
8	-1.081593	-2.297483	2.156956
1	0.539180	-4.163999	2.694359
1	0.509095	-2.454605	4.832475
1	1.630000	-3.827770	4.818684
1	2.241576	-0.949960	3.967954
1	3.155949	-1.933067	5.132618
1	3.909620	-1.787210	2.464444
1	4.075494	-3.307681	3.384681
1	0.937381	-2.741815	-0.351074
8	0.367451	-1.706694	-0.709894
1	1.342611	-5.160049	-1.744391
1	0.723747	-4.449722	0.443531
7	-0.250043	1.335732	0.838748
6	0.771471	2.271764	0.634637
6	2.069084	1.833987	0.940143
6	3.143524	2.701036	0.816793
6	2.965497	4.012052	0.384176
6	1.674905	4.434160	0.094833

6	0.573888	3.591577	0.221994
6	4.534741	2.207010	1.095755
9	5.302698	3.174008	1.627589
6	1.454818	5.834355	-0.403683
9	1.459893	5.891580	-1.745403
6	-1.432992	1.146746	0.184182
16	-2.090554	2.190666	-0.970397
7	-2.011977	-0.020896	0.540992
6	-3.305761	-0.494251	0.087228
6	-3.201381	-1.980853	-0.306313
6	-4.520161	-2.495833	-0.940782
6	-4.232073	-2.992042	-2.365527
6	-3.239977	-4.161488	-2.278507
6	-1.991722	-3.677755	-1.500217
7	-2.066832	-2.225398	-1.233072
6	-2.234053	-1.502511	-2.511735
6	-3.577384	-1.877651	-3.204066
6	-4.431866	-0.658276	-3.451317
6	-5.754095	-0.571353	-3.325298
6	-4.363409	-0.334472	1.176367
6	-5.604824	0.343207	0.956085
6	-6.529479	0.374972	2.042608
7	-6.278372	-0.183374	3.260901
6	-5.121978	-0.775752	3.425714
6	-4.136101	-0.881974	2.415098
6	-7.779314	1.014662	1.860676
6	-8.116605	1.599776	0.667195
6	-7.192270	1.575403	-0.407920
6	-5.963952	0.966294	-0.261342
9	4.546300	1.174963	1.950604
9	5.151629	1.803363	-0.025698
9	2.414528	6.670959	0.022616
9	0.278007	6.331725	0.001413
1	-2.953959	-2.543504	0.599698
1	-4.935999	-3.313294	-0.343505
1	-5.268708	-1.699397	-0.958637
1	-1.067161	-3.860492	-2.060281
1	-1.897497	-4.177282	-0.531014
1	-2.964864	-4.494332	-3.284396
1	-3.703600	-5.010776	-1.768253
1	-5.158514	-3.325746	-2.842425
1	-3.338007	-2.303957	-4.188333
1	-1.374288	-1.764970	-3.135675
1	-2.166453	-0.428625	-2.310400
1	-3.881517	0.225782	-3.777470
1	-6.276469	0.357427	-3.532859
1	-6.365316	-1.409856	-3.000798
1	-3.576526	0.099487	-0.785949
1	-3.203819	-1.399784	2.630803
1	-5.288587	0.995731	-1.107567
1	-4.932295	-1.213822	4.404106
1	-8.462482	1.023099	2.703654
1	-9.082145	2.078897	0.557247
1	-1.563678	-0.621589	1.241388
1	0.049962	0.536401	1.413582
1	2.222515	0.811813	1.277626
1	-0.422547	3.955397	0.012894
1	3.806858	4.689594	0.292398
8	-7.445021	2.132336	-1.620941
6	-8.657825	2.840306	-1.788664
1	-8.636539	3.237465	-2.803808
1	-9.528479	2.182528	-1.680535
1	-8.739072	3.672567	-1.079923
1	2.989863	-5.133264	-1.145825
1	-0.690836	-1.871206	-0.808070
1	0.508241	-1.151103	0.086399
1	3.563643	-3.288596	0.601187
6	2.479971	-3.432784	-2.373744
1	1.567068	-2.945510	-2.734090
1	2.968489	-3.921786	-3.222295

6	3.373967	-2.407334	-1.755826
6	4.704539	-2.330989	-1.851482
1	2.894241	-1.701302	-1.078692
1	5.271620	-2.965226	-2.528213
6	5.424690	-1.404508	-0.932973
8	4.930561	-1.117416	0.149240
6	6.760473	-0.861349	-1.319723
6	7.272798	-0.990770	-2.613500
6	7.497813	-0.177130	-0.347298
6	8.515656	-0.448987	-2.927742
1	6.697574	-1.494440	-3.383990
6	8.739789	0.356671	-0.660653
1	7.068115	-0.068880	0.643058
6	9.250508	0.219108	-1.951789
1	8.909059	-0.545278	-3.934487
1	9.310263	0.884691	0.096662
1	10.221008	0.639106	-2.197992

[6-7]TS-syn_Cinchona-Thiourea_conf-9

Number of imaginary frequencies : 1
The smallest frequency is : -1172.2596

Electronic energy= -3467.701345
Zero-point correction= 0.930929
Thermal correction to Energy= 0.989708
Thermal correction to Enthalpy= 0.990652
Thermal correction to Gibbs Free Energy= 0.828121
Sum of electronic and zero-point Energies= -3466.770416
Sum of electronic and thermal Energies= -3466.711637
Sum of electronic and thermal Enthalpies= -3466.710693
Sum of electronic and thermal Free Energies= -3466.873224

Cartesian Coordinates

6	2.412415	2.624898	3.423237
6	3.545888	2.050503	2.574427
7	3.129640	0.654650	2.331699
6	1.979146	0.264523	3.155366
6	1.882046	1.402779	4.181562
6	3.599030	-0.091034	1.360159
6	3.094606	-1.347697	0.964573
6	3.941234	-2.292714	0.112145
6	0.724208	0.197812	2.257729
8	0.629817	1.121948	1.391038
8	-0.077016	-0.732766	2.437878
1	2.147752	-0.713791	3.611460
1	0.860593	1.531990	4.544850
1	2.523006	1.172650	5.038075
1	1.634295	3.033767	2.776758
1	2.767710	3.411783	4.090531
1	3.678650	2.569070	1.622813
1	4.496049	2.046372	3.118542
1	2.093280	-0.944192	0.121220
8	1.113516	-0.632590	-0.636378
1	3.259128	-2.921257	-0.469218
1	2.492886	-1.857497	1.721131
7	-1.765495	1.718570	0.145352
6	-1.785420	3.059991	-0.242301
6	-0.607562	3.774899	0.034371
6	-0.525739	5.126959	-0.245599
6	-1.594980	5.813040	-0.818558
6	-2.751451	5.096722	-1.086684
6	-2.871143	3.736528	-0.802279
6	0.753561	5.862571	0.027299
9	0.524445	7.101767	0.486328
6	-3.929353	5.780704	-1.721405

9	-3.794867	7.115504	-1.728681
6	-2.490592	0.638604	-0.263150
16	-3.720378	0.664584	-1.422621
7	-2.067463	-0.494540	0.342171
6	-2.706800	-1.788931	0.205813
6	-1.644428	-2.902507	0.112226
6	-2.305380	-4.257771	-0.261610
6	-1.744284	-4.732099	-1.610981
6	-0.240481	-4.981236	-1.438879
6	0.397826	-3.679081	-0.896796
7	-0.581271	-2.570882	-0.867881
6	-1.134728	-2.386323	-2.224506
6	-1.921501	-3.648433	-2.692524
6	-3.347105	-3.316296	-3.058112
6	-4.429528	-4.046219	-2.798013
6	-3.638639	-2.073380	1.382731
6	-5.016727	-2.420017	1.211255
6	-5.763068	-2.726732	2.388282
7	-5.238499	-2.675897	3.645480
6	-3.982036	-2.323652	3.759985
6	-3.141466	-2.019802	2.662007
6	-7.121503	-3.103849	2.258852
6	-7.729715	-3.176801	1.031997
6	-6.989802	-2.856672	-0.134801
6	-5.666610	-2.480870	-0.042690
9	1.516761	5.232288	0.936676
9	1.501793	5.995199	-1.080311
9	-5.072785	5.497135	-1.079623
9	-4.096937	5.394629	-2.995756
1	-1.135934	-2.967769	1.081415
1	-2.098323	-5.010228	0.505798
1	-3.391474	-4.146329	-0.316229
1	1.234881	-3.353052	-1.523211
1	0.775255	-3.806763	0.123505
1	0.206833	-5.262252	-2.397736
1	-0.072642	-5.809385	-0.744022
1	-2.242776	-5.655395	-1.920971
1	-1.439271	-4.019708	-3.607693
1	-0.287183	-2.175988	-2.883758
1	-1.768601	-1.493935	-2.222765
1	-3.471590	-2.380405	-3.605130
1	-5.414838	-3.717353	-3.113522
1	-4.384465	-4.986181	-2.253721
1	-3.281662	-1.766107	-0.719925
1	-2.106656	-1.741038	2.847462
1	-5.154610	-2.216489	-0.959656
1	-3.576868	-2.277209	4.769384
1	-7.665275	-3.332957	3.169564
1	-8.770931	-3.468960	0.965784
1	-1.374620	-0.434887	1.100620
1	-0.947099	1.489991	0.731189
1	0.234602	3.251886	0.478382
1	-3.796132	3.214561	-1.006583
1	-1.529334	6.873188	-1.034308
8	-7.518695	-2.893828	-1.385792
6	-8.883771	-3.237400	-1.520664
1	-9.102047	-3.190726	-2.587790
1	-9.082358	-4.253235	-1.158725
1	-9.531785	-2.529011	-0.991457
1	4.506315	-2.978486	0.755793
1	0.351157	-1.353673	-0.623148
1	0.778651	0.154340	-0.154927
1	4.385556	0.387431	0.776704
6	4.916297	-1.607600	-0.859649
1	4.449639	-0.692262	-1.253061
1	5.095869	-2.252421	-1.725093
6	6.231721	-1.275604	-0.221776
6	7.429047	-1.519524	-0.760958
1	6.226289	-0.820743	0.769875
1	7.509858	-1.995670	-1.733215

6	8.667546	-1.160982	-0.014680
8	8.611222	-0.754698	1.134805
6	9.995772	-1.319865	-0.690578
6	10.131107	-1.502947	-2.069850
6	11.142263	-1.256496	0.109292
6	11.395975	-1.625184	-2.638262
1	9.258825	-1.528845	-2.713994
6	12.402616	-1.388946	-0.457074
1	11.018572	-1.103864	1.176326
6	12.530621	-1.574518	-1.833417
1	11.494853	-1.759312	-3.710650
1	13.286996	-1.348154	0.170678
1	13.515512	-1.677463	-2.278330

Stationary Points relevant to Fig. S9 and Table S8
Conformational Study of First-Michael-addition_path-A [8-9]TS

si-si_1-path-A

Number of imaginary frequencies : 1
The smallest frequency is : -250.2911

Electronic energy= -3905.2911079
Zero-point correction= 1.051978
Thermal correction to Energy= 1.117879
Thermal correction to Enthalpy= 1.118824
Thermal correction to Gibbs Free Energy= 0.945941
Sum of electronic and zero-point Energies= -3904.239130
Sum of electronic and thermal Energies= -3904.173229
Sum of electronic and thermal Enthalpies= -3904.172284
Sum of electronic and thermal Free Energies= -3904.345167

Cartesian Coordinates

6	-1.168883	-0.086649	5.342617
6	-2.182650	-1.233282	5.442984
6	-3.394889	-0.718043	4.654277
7	-2.834949	0.316173	3.772554
6	-1.384439	0.402943	3.902969
6	-3.605981	1.147331	3.069361
6	-3.219864	2.091125	2.141250
8	-0.281602	1.904683	-1.323639
8	-0.427903	1.170956	0.718293
1	-1.046799	1.429328	3.738459
1	-0.137421	-0.400744	5.508882
1	-1.416106	0.713706	6.047274
1	-3.873057	-1.508349	4.068383
1	-4.147171	-0.264135	5.309523
1	-2.162089	2.318342	2.024155
6	-4.229526	3.123215	1.694460
1	-5.178571	2.630083	1.443783
6	-3.014433	0.564758	0.419172
1	-2.432913	-0.014442	1.131763
1	-2.681440	1.554181	-1.524601
6	-4.388315	0.100656	0.190455
6	-4.835678	-0.998885	0.937602
6	-5.237323	0.666205	-0.769187
6	-6.099752	-1.530988	0.720627
1	-4.155969	-1.442970	1.663592
6	-6.503525	0.129807	-0.985879
1	-4.906870	1.517676	-1.356839
6	-6.933569	-0.969905	-0.246637
1	-6.426534	-2.398678	1.284114
1	-7.152640	0.567295	-1.737711
1	-7.916743	-1.394123	-0.425057

7	-0.961920	1.437515	-0.389918
6	-2.303098	1.224979	-0.568227
7	-0.521417	-1.815879	-0.285889
6	-1.623340	-2.085768	-1.109932
6	-1.889048	-1.360083	-2.275074
6	-3.096606	-1.550277	-2.934103
6	-4.049102	-2.458806	-2.476205
6	-3.759599	-3.187384	-1.330962
6	-2.562875	-3.005144	-0.644557
6	-3.421787	-0.645132	-4.085133
9	-2.375196	-0.464843	-4.899742
6	-4.733983	-4.207294	-0.819803
9	-4.431060	-5.445611	-1.241635
6	0.776387	-1.624348	-0.634447
16	1.393961	-1.839960	-2.198102
7	1.518817	-1.243716	0.425722
6	2.943178	-0.993209	0.432663
6	3.161072	0.391999	1.073205
6	4.621698	0.889355	1.071902
6	4.722453	2.192946	0.263701
6	3.848376	3.267650	0.931335
6	2.415015	2.723735	1.091323
7	2.314625	1.418390	0.368925
6	2.695073	1.603139	-1.068010
6	4.193763	1.975329	-1.166200
6	4.957710	0.976771	-2.002433
6	6.206334	0.563588	-1.801071
6	3.702264	-2.036180	1.245843
6	4.876529	-2.687072	0.751120
6	5.540970	-3.587129	1.636935
7	5.100005	-3.864012	2.896767
6	4.005698	-3.266864	3.298365
6	3.274679	-2.341427	2.514385
6	6.721361	-4.233788	1.198554
6	7.233837	-4.014856	-0.054382
6	6.563630	-3.131458	-0.938106
6	5.409103	-2.489229	-0.543682
9	-4.439188	-1.105393	-4.825336
9	-3.783452	0.584159	-3.652899
9	-5.989284	-3.956724	-1.220864
9	-4.743455	-4.253993	0.524449
1	2.746084	0.350888	2.085099
1	4.954798	1.062462	2.098986
1	5.273722	0.123949	0.644264
1	1.659451	3.375700	0.649306
1	2.140578	2.525922	2.129643
1	3.836599	4.174340	0.317994
1	4.256146	3.534299	1.909710
1	5.761062	2.532331	0.232172
1	4.245561	2.943458	-1.684697
1	2.043452	2.390841	-1.442475
1	2.440060	0.682188	-1.598607
1	4.410836	0.585319	-2.861779
1	6.669271	-0.158059	-2.467212
1	6.808118	0.907389	-0.963319
1	3.289187	-0.994678	-0.601712
1	2.378878	-1.879677	2.925469
1	4.927904	-1.840786	-1.265376
1	3.660038	-3.503548	4.302983
1	7.205403	-4.912237	1.893485
1	8.140001	-4.523374	-0.361259
1	1.051556	-1.073395	1.336616
1	-0.747079	-1.777475	0.729683
1	-1.173405	-0.622591	-2.623816
1	-2.360574	-3.556193	0.268921
1	-4.995355	-2.580446	-2.990476
8	6.999163	-2.863608	-2.196767
6	8.127598	-3.570620	-2.675317
1	8.272556	-3.243759	-3.705280
1	9.027997	-3.335307	-2.095727

1	7.957580	-4.653249	-2.663297
1	1.309041	1.136649	0.418415
6	-0.629479	-0.536014	2.936391
8	-1.301190	-1.399287	2.317382
8	0.616017	-0.378936	2.904254
1	-4.451428	3.808630	2.524982
1	-2.443705	-1.487187	6.471718
1	-1.779489	-2.125428	4.957472
6	-3.785713	3.981056	0.498946
1	-4.575732	4.719619	0.309913
1	-3.687128	3.377535	-0.406353
6	-2.513122	4.720768	0.765483
6	-1.426874	4.701406	-0.015279
1	-2.477796	5.338034	1.664744
1	-1.413151	4.097173	-0.916920
6	-0.246656	5.537272	0.335879
8	-0.211672	6.175535	1.376060
6	0.915969	5.609631	-0.616080
6	1.010768	4.821589	-1.767888
6	1.953323	6.498868	-0.307515
6	2.129243	4.922329	-2.593886
1	0.236504	4.105877	-2.021398
6	3.061363	6.606982	-1.138797
1	1.865567	7.100327	0.591334
6	3.152661	5.814879	-2.284183
1	2.195061	4.303169	-3.483621
1	3.855820	7.305622	-0.895819
1	4.018180	5.894969	-2.935013
1	-4.674817	0.987633	3.224639

si-si_2-path-A

Number of imaginary frequencies : 1
The smallest frequency is : -276.7684

Electronic energy= -3905.2924524
Zero-point correction= 1.052006
Thermal correction to Energy= 1.117714
Thermal correction to Enthalpy= 1.118658
Thermal correction to Gibbs Free Energy= 0.948321
Sum of electronic and zero-point Energies= -3904.240447
Sum of electronic and thermal Energies= -3904.174739
Sum of electronic and thermal Enthalpies= -3904.173795
Sum of electronic and thermal Free Energies= -3904.344131

Cartesian Coordinates

6	-1.291577	-0.610884	5.391264
6	-2.301328	-1.764328	5.353142
6	-3.486585	-1.188436	4.563997
7	-2.907565	-0.064459	3.813089
6	-1.459148	0.001759	3.993251
6	-3.664919	0.833426	3.183281
6	-3.257415	1.864616	2.358879
8	-0.087572	2.060255	-0.853792
8	-0.392238	1.156843	1.096692
1	-1.112389	1.035586	3.924991
1	-0.264747	-0.935919	5.564301
1	-1.568193	0.123105	6.154913
1	-1.873657	-2.610837	4.810166
1	-2.601284	-2.106824	6.344944
1	-3.922922	-1.923936	3.881876
1	-4.275089	-0.810682	5.224475
1	-4.736567	0.657657	3.296907
1	-2.196947	2.103695	2.314661
6	-4.246033	2.955339	2.014620
6	-3.814371	3.887930	0.870308

1	-4.414409	3.583712	2.900950
1	-5.218097	2.510324	1.764432
1	-3.882593	3.385085	-0.098077
1	-4.520413	4.728409	0.842339
6	-2.430575	4.423250	1.067030
6	-1.500080	4.520958	0.111788
1	-2.154354	4.741403	2.073668
1	-1.722448	4.212830	-0.904304
6	-0.134722	4.992737	0.450317
8	0.172293	5.249339	1.606987
6	0.898968	5.136160	-0.630219
6	0.704021	4.715232	-1.949050
6	2.136788	5.678435	-0.261877
6	1.736391	4.823147	-2.877662
1	-0.229104	4.257818	-2.253464
6	3.163742	5.793575	-1.190657
1	2.269410	6.005825	0.764701
6	2.965120	5.359937	-2.502296
1	1.581334	4.478055	-3.894644
1	4.117724	6.220806	-0.895676
1	3.767025	5.441575	-3.229736
6	-2.961788	0.575777	0.519371
1	-2.454169	-0.114993	1.189817
1	-2.457203	1.760224	-1.270650
6	-4.324158	0.187900	0.114134
6	-4.920322	-0.906955	0.755906
6	-5.024644	0.830252	-0.915089
6	-6.181538	-1.349931	0.378608
1	-4.357097	-1.424522	1.530976
6	-6.285235	0.381661	-1.298383
1	-4.581085	1.669333	-1.441727
6	-6.866016	-0.707364	-0.653655
1	-6.620764	-2.213282	0.867517
1	-6.808202	0.879356	-2.108922
1	-7.845175	-1.062505	-0.959287
7	-0.839414	1.512271	-0.025338
6	-2.159436	1.323154	-0.329915
7	-0.513103	-1.658686	-0.389390
6	-1.613931	-1.855931	-1.232343
6	-1.897825	-1.028687	-2.323373
6	-3.116522	-1.161111	-2.976988
6	-4.056904	-2.115758	-2.597119
6	-3.749935	-2.942915	-1.526327
6	-2.547659	-2.814835	-0.838366
6	-3.436561	-0.179150	-4.065143
9	-2.631719	-0.312650	-5.127619
6	-4.719323	-3.997126	-1.079091
9	-4.370510	-5.218126	-1.515951
6	0.774893	-1.367917	-0.705511
16	1.408889	-1.354986	-2.276364
7	1.498551	-1.094310	0.400028
6	2.929338	-0.901607	0.455875
6	3.192417	0.328026	1.344008
6	4.676792	0.735680	1.449501
6	4.860519	2.156059	0.896408
6	4.032542	3.133346	1.745384
6	2.567487	2.654544	1.786697
7	2.409933	1.512778	0.831686
6	2.828580	1.939855	-0.543169
6	4.348819	2.233422	-0.554721
6	5.078298	1.362628	-1.549550
6	6.310995	0.878802	-1.420681
6	3.641992	-2.112891	1.051483
6	4.785512	-2.709584	0.433371
6	5.402418	-3.798463	1.118232
7	4.941112	-4.297796	2.300344
6	3.873574	-3.740102	2.816465
6	3.191135	-2.643767	2.234409
6	6.551411	-4.399866	0.550478
6	7.076883	-3.959431	-0.637603

6	6.452370	-2.886553	-1.322937
6	5.329003	-2.283161	-0.799518
9	-4.698933	-0.294802	-4.500947
9	-3.286181	1.093241	-3.636446
9	-5.964782	-3.766156	-1.520915
9	-4.779547	-4.076713	0.262663
1	2.754126	0.123450	2.326580
1	5.000328	0.697278	2.493308
1	5.293978	0.028103	0.890501
1	1.858592	3.427280	1.481997
1	2.266893	2.281495	2.767999
1	4.086043	4.136632	1.311343
1	4.434743	3.188636	2.760087
1	5.915830	2.438120	0.937138
1	4.464194	3.273075	-0.889277
1	2.231846	2.821979	-0.775167
1	2.528224	1.150516	-1.237457
1	4.521866	1.141465	-2.461868
1	6.754089	0.262659	-2.197155
1	6.917785	1.058031	-0.536146
1	3.281479	-0.721437	-0.560929
1	2.310639	-2.235186	2.727555
1	4.879026	-1.482668	-1.372910
1	3.510134	-4.154838	3.754875
1	7.003195	-5.225661	1.090500
1	7.957523	-4.440733	-1.045828
1	1.028382	-1.086959	1.323634
1	-0.734424	-1.771476	0.621764
1	-1.191850	-0.255512	-2.608102
1	-2.337151	-3.436499	0.026973
1	-5.012523	-2.189501	-3.101700
8	6.902845	-2.392886	-2.505972
6	8.012882	-3.025581	-3.113713
1	8.181573	-2.499708	-4.053742
1	8.913382	-2.947142	-2.493242
1	7.806920	-4.080864	-3.326170
1	1.394618	1.267377	0.812907
6	-0.678177	-0.855792	2.970321
8	-1.340093	-1.626037	2.229928
8	0.569914	-0.731021	3.013382

si-si_3-path-A

Number of imaginary frequencies : 1
The smallest frequency is : -290.4720

Electronic energy= -3905.291533
Zero-point correction= 1.053424
Thermal correction to Energy= 1.119185
Thermal correction to Enthalpy= 1.120129
Thermal correction to Gibbs Free Energy= 0.948303
Sum of electronic and zero-point Energies= -3904.238109
Sum of electronic and thermal Energies= -3904.172348
Sum of electronic and thermal Enthalpies= -3904.171404
Sum of electronic and thermal Free Energies= -3904.343230

Cartesian Coordinates

6	-1.199861	1.573119	4.853012
6	-2.252038	0.554857	5.304847
6	-3.456520	0.868869	4.412046
7	-2.858283	1.485477	3.216691
6	-1.404960	1.600402	3.329808
6	-3.589420	1.981863	2.223797
6	-3.120077	2.450367	1.006824
8	-0.552062	1.503297	-2.393030
8	-0.466884	1.432106	-0.212770

1	-1.060888	2.530288	2.868076
1	-0.178378	1.293410	5.115597
1	-1.412497	2.561816	5.271663
1	-1.896976	-0.457988	5.100629
1	-2.498464	0.632417	6.365045
1	-4.023489	-0.024112	4.135981
1	-4.138066	1.586072	4.884061
1	-4.666768	1.922400	2.387412
1	-2.046215	2.587327	0.899592
6	-3.990861	3.310231	0.136685
6	-3.714604	4.819964	0.332788
1	-5.049501	3.113807	0.342961
1	-3.814887	3.056577	-0.919407
1	-4.427457	5.390393	-0.274169
1	-3.880064	5.085861	1.382149
6	-2.319947	5.189947	-0.074747
6	-1.348327	5.503522	0.791335
1	-2.110797	5.184372	-1.144122
1	-1.565683	5.550442	1.857480
6	0.027165	5.952503	0.456583
8	0.663866	6.575452	1.291747
6	0.644970	5.669838	-0.882076
6	0.373970	4.508458	-1.612120
6	1.600220	6.575389	-1.358913
6	1.035371	4.267139	-2.815254
1	-0.313876	3.762672	-1.224279
6	2.249747	6.340452	-2.564553
1	1.820927	7.458550	-0.767946
6	1.966092	5.185637	-3.295614
1	0.814087	3.355472	-3.361916
1	2.979242	7.053358	-2.935592
1	2.473723	5.000962	-4.237586
6	-2.969167	0.553351	-0.029809
1	-2.280537	0.231619	0.744864
1	-2.895115	0.864938	-2.220651
6	-4.304804	-0.067896	0.033814
6	-4.588341	-0.896271	1.129248
6	-5.270512	0.102423	-0.964208
6	-5.810033	-1.551780	1.217569
1	-3.817431	-1.030372	1.887554
6	-6.493003	-0.557571	-0.874076
1	-5.066278	0.743737	-1.816329
6	-6.762476	-1.387746	0.211143
1	-6.013251	-2.211523	2.055025
1	-7.233889	-0.428342	-1.656647
1	-7.710632	-1.912735	0.271802
7	-1.095240	1.280468	-1.297225
6	-2.409262	0.895267	-1.257716
7	-0.440521	-1.972485	0.156838
6	-1.533475	-2.487252	-0.562678
6	-1.801666	-2.127475	-1.886465
6	-2.989070	-2.544555	-2.474124
6	-3.917945	-3.319957	-1.783361
6	-3.626831	-3.685182	-0.476670
6	-2.447596	-3.273071	0.136948
6	-3.333332	-2.036198	-3.842883
9	-2.252102	-1.887475	-4.615750
6	-4.572885	-4.572640	0.277470
9	-4.295936	-5.873167	0.086595
6	0.857643	-1.873904	-0.226882
16	1.486979	-2.481769	-1.672592
7	1.601295	-1.228871	0.701099
6	3.017039	-0.938964	0.607985
6	3.227649	0.531484	1.028263
6	4.631916	1.099583	0.729974
6	4.515583	2.263262	-0.272340
6	3.679196	3.390600	0.357654
6	2.342624	2.803260	0.850159
7	2.221572	1.404548	0.338988
6	2.355941	1.371704	-1.150761

6	3.788206	1.800535	-1.549208
6	4.486628	0.726364	-2.348270
6	5.775234	0.400436	-2.282749
6	3.847587	-1.826663	1.527802
6	5.050030	-2.470255	1.098662
6	5.765773	-3.224027	2.076671
7	5.350778	-3.366298	3.367156
6	4.234766	-2.774728	3.713745
6	3.453167	-1.990613	2.832062
6	6.971460	-3.863252	1.699986
6	7.461219	-3.769257	0.422686
6	6.744915	-3.024039	-0.548874
6	5.562857	-2.396406	-0.216868
9	-4.185040	-2.849423	-4.483960
9	-3.933052	-0.827468	-3.781662
9	-5.847577	-4.390697	-0.099554
9	-4.511412	-4.358126	1.602656
1	2.975111	0.617351	2.088556
1	5.092608	1.455751	1.655532
1	5.273754	0.310917	0.330313
1	1.472658	3.342247	0.472438
1	2.267217	2.737381	1.937051
1	3.492419	4.174661	-0.384240
1	4.214958	3.846870	1.193558
1	5.511593	2.637930	-0.522972
1	3.685822	2.677044	-2.204918
1	1.582687	2.034260	-1.533820
1	2.104927	0.360125	-1.481702
1	3.849458	0.196725	-3.057811
1	6.185665	-0.379983	-2.915576
1	6.468084	0.882860	-1.597619
1	3.318039	-1.086304	-0.431100
1	2.542174	-1.523548	3.199271
1	5.044880	-1.858290	-1.002102
1	3.912329	-2.900642	4.745578
1	7.495276	-4.430821	2.462172
1	8.386288	-4.270085	0.163907
1	1.119237	-0.802709	1.507611
1	-0.683673	-1.610797	1.095891
1	-1.104564	-1.498760	-2.429702
1	-2.237847	-3.543932	1.167168
1	-4.847316	-3.622502	-2.253063
8	7.160413	-2.880333	-1.832983
6	8.331802	-3.564288	-2.235617
1	8.464694	-3.337782	-3.293684
1	9.213466	-3.217949	-1.683423
1	8.226727	-4.648295	-2.112771
1	1.271075	1.081063	0.575714
6	-0.643203	0.415373	2.697592
8	-1.282717	-0.637174	2.463788
8	0.592543	0.600176	2.538033

si-si_4-path-A

Number of imaginary frequencies : 1
The smallest frequency is : -278.0952

Electronic energy= -3905.291171
Zero-point correction= 1.052937
Thermal correction to Energy= 1.118449
Thermal correction to Enthalpy= 1.119393
Thermal correction to Gibbs Free Energy= 0.949517
Sum of electronic and zero-point Energies= -3904.238234
Sum of electronic and thermal Energies= -3904.172723
Sum of electronic and thermal Enthalpies= -3904.171778
Sum of electronic and thermal Free Energies= -3904.341654

Cartesian Coordinates

6	-1.190053	0.372659	5.362811
6	-2.187123	-0.775596	5.553910
6	-3.411047	-0.322947	4.750232
7	-2.855792	0.604005	3.751646
6	-1.404885	0.740660	3.886995
6	-3.626736	1.316559	2.931598
6	-3.202618	2.101404	1.875655
8	-0.253715	1.527787	-1.542466
8	-0.418576	1.290767	0.613979
1	-1.098366	1.762967	3.649951
1	-0.154229	0.090217	5.556187
1	-1.451810	1.223141	6.000600
1	-1.780586	-1.692077	5.119252
1	-2.432698	-0.965186	6.600157
1	-3.921339	-1.155539	4.258236
1	-4.135164	0.211682	5.376238
1	-4.697368	1.171256	3.085528
1	-2.135772	2.288026	1.780054
6	-4.122481	3.067784	1.188213
6	-3.856298	4.545443	1.562636
1	-5.169882	2.820791	1.396838
1	-3.977203	2.979865	0.100893
1	-4.474101	5.185247	0.923230
1	-4.153091	4.721577	2.600660
6	-2.404779	4.884609	1.384028
6	-1.812468	5.104705	0.205244
1	-1.764856	4.884046	2.265508
1	-2.382196	5.103379	-0.720432
6	-0.344264	5.323878	0.151781
8	0.291525	5.627298	1.151389
6	0.371639	5.125327	-1.148872
6	-0.173810	4.375281	-2.192184
6	1.667402	5.644973	-1.275217
6	0.568486	4.141277	-3.348049
1	-1.156535	3.926627	-2.093208
6	2.398377	5.429864	-2.435764
1	2.077047	6.220008	-0.450075
6	1.849027	4.671179	-3.473216
1	0.149330	3.530342	-4.140512
1	3.394808	5.849613	-2.537071
1	2.423337	4.490688	-4.376807
6	-2.964268	0.486148	0.399999
1	-2.356163	-0.028947	1.139099
1	-2.674133	1.228806	-1.657778
6	-4.315260	-0.064209	0.198043
6	-4.724954	-1.121047	1.023900
6	-5.171507	0.379551	-0.816336
6	-5.959680	-1.727494	0.832663
1	-4.037997	-1.477580	1.790354
6	-6.408629	-0.230175	-1.006637
1	-4.869461	1.193411	-1.468366
6	-6.802273	-1.285020	-0.187432
1	-6.256269	-2.562987	1.458227
1	-7.061439	0.113930	-1.802626
1	-7.760744	-1.769030	-0.346714
7	-0.941937	1.309668	-0.534155
6	-2.289506	1.077631	-0.660644
7	-0.407234	-1.779609	-0.149271
6	-1.478028	-2.163100	-0.969506
6	-1.742980	-1.534697	-2.189917
6	-2.919061	-1.831218	-2.865249
6	-3.840002	-2.752194	-2.368957
6	-3.551825	-3.381636	-1.166275
6	-2.385300	-3.092787	-0.463107
6	-3.252307	-1.026208	-4.085381
9	-2.189291	-0.839425	-4.876526
6	-4.492208	-4.414719	-0.619081
9	-4.158708	-5.654639	-1.013837

6	0.879013	-1.520233	-0.506183
16	1.535007	-1.825695	-2.036650
7	1.578972	-0.996564	0.519821
6	2.996866	-0.719449	0.522059
6	3.201352	0.680739	1.126707
6	4.659122	1.182939	1.065674
6	4.724633	2.473036	0.235767
6	3.873079	3.546535	0.930357
6	2.445374	3.003399	1.140939
7	2.320935	1.689583	0.434909
6	2.648940	1.860421	-1.017280
6	4.141663	2.238794	-1.171128
6	4.878734	1.236604	-2.026925
6	6.131115	0.818911	-1.860117
6	3.770533	-1.729524	1.364385
6	4.951583	-2.383490	0.891605
6	5.620581	-3.252760	1.804333
7	5.179241	-3.495959	3.071086
6	4.079160	-2.896288	3.453052
6	3.341954	-2.001684	2.640118
6	6.805984	-3.903533	1.386108
6	7.318847	-3.716316	0.128160
6	6.645544	-2.861188	-0.780962
6	5.485815	-2.216107	-0.406882
9	-4.215618	-1.592460	-4.824837
9	-3.698232	0.206204	-3.750537
9	-5.757583	-4.210817	-1.016914
9	-4.491167	-4.427421	0.725325
1	2.820529	0.655786	2.152098
1	5.030388	1.373261	2.076491
1	5.296513	0.412283	0.625860
1	1.683729	3.664958	0.728401
1	2.206828	2.816203	2.189973
1	3.841075	4.450479	0.314408
1	4.315210	3.816997	1.892584
1	5.759856	2.816300	0.159849
1	4.169857	3.200259	-1.702539
1	1.974020	2.636475	-1.384872
1	2.380609	0.929457	-1.525044
1	4.306347	0.848294	-2.870645
1	6.574450	0.099201	-2.541114
1	6.757254	1.160154	-1.039289
1	3.343744	-0.741720	-0.512161
1	2.439679	-1.536487	3.033543
1	4.999699	-1.591458	-1.146553
1	3.733465	-3.105834	4.463708
1	7.293546	-4.559172	2.100212
1	8.228121	-4.228176	-0.163517
1	1.097284	-0.788491	1.413260
1	-0.641172	-1.685450	0.857004
1	-1.054215	-0.784909	-2.566840
1	-2.185090	-3.569748	0.491568
1	-4.762080	-2.958889	-2.900138
8	7.082843	-2.625115	-2.045052
6	8.220522	-3.332885	-2.499185
1	8.368528	-3.030832	-3.536306
1	9.115333	-3.074646	-1.920662
1	8.061016	-4.416576	-2.461045
1	1.316828	1.390532	0.498063
6	-0.595418	-0.236966	3.001662
8	-1.212316	-1.187839	2.460750
8	0.638749	-0.008307	2.956586

si-si_5-path-A

Number of imaginary frequencies : 1
The smallest frequency is : -192.9981

Electronic energy= -3905.2881908
 Zero-point correction= 1.053141
 Thermal correction to Energy= 1.118997
 Thermal correction to Enthalpy= 1.119941
 Thermal correction to Gibbs Free Energy= 0.947736
 Sum of electronic and zero-point Energies= -3904.235050
 Sum of electronic and thermal Energies= -3904.169194
 Sum of electronic and thermal Enthalpies= -3904.168250
 Sum of electronic and thermal Free Energies= -3904.340455

 Cartesian Coordinates

8	-0.576426	-1.032831	-3.716564
8	-0.744953	-0.897413	-1.554165
6	-3.461608	-1.320912	-1.702638
1	-2.996189	-1.505483	-0.738766
1	-2.946244	-1.354028	-3.835769
6	-4.865724	-1.756274	-1.849416
6	-5.497708	-2.404336	-0.781844
6	-5.589080	-1.547323	-3.031846
6	-6.810494	-2.851692	-0.898293
1	-4.954918	-2.561061	0.144357
6	-6.899192	-1.993030	-3.147287
1	-5.126671	-1.023294	-3.863749
6	-7.514039	-2.650831	-2.081748
1	-7.279491	-3.360727	-0.062269
1	-7.445067	-1.823793	-4.070135
1	-8.537329	-3.000240	-2.174574
7	-1.272801	-1.063979	-2.676903
6	-2.627824	-1.269078	-2.808304
7	0.054753	-0.120258	1.275010
6	-1.028080	-0.770139	1.892636
6	-1.503107	-1.992469	1.412104
6	-2.591690	-2.595137	2.032321
6	-3.242575	-1.988581	3.102474
6	-2.776216	-0.755609	3.544704
6	-1.669303	-0.144968	2.961456
6	-3.040926	-3.943018	1.547422
9	-2.336166	-4.940816	2.094630
6	-3.542314	-0.039931	4.617097
9	-3.984383	-0.876179	5.566446
6	1.211366	-0.715336	0.881709
16	1.691446	-2.260733	1.385093
7	1.943434	0.063437	0.057299
6	3.286596	-0.244871	-0.386381
6	3.425823	-0.070289	-1.910028
6	4.718171	-0.712731	-2.457841
6	4.357365	-1.821424	-3.456653
6	3.619588	-1.177992	-4.639457
6	2.411072	-0.379887	-4.108612
7	2.251172	-0.665043	-2.645070
6	2.099150	-2.134931	-2.415092
6	3.416044	-2.854769	-2.806530
6	3.992806	-3.616096	-1.635900
6	5.281469	-3.747998	-1.330734
6	4.314565	0.657495	0.285574
6	5.446694	0.140891	0.988002
6	6.354563	1.093435	1.540180
7	6.179793	2.441660	1.440813
6	5.120289	2.870970	0.800663
6	4.162219	2.019586	0.199365
6	7.501431	0.625874	2.226018
6	7.754041	-0.714842	2.364521
6	6.845870	-1.659348	1.819806
6	5.715375	-1.237502	1.152909
9	-4.334567	-4.170644	1.840967
9	-2.910439	-4.056909	0.215098
9	-4.634086	0.566675	4.103957
9	-2.816790	0.911723	5.214072

1	3.367462	0.991369	-2.145562
1	5.329702	0.045426	-2.955080
1	5.308954	-1.114414	-1.631196
1	1.471159	-0.663565	-4.579116
1	2.531539	0.701820	-4.189031
1	3.284332	-1.951288	-5.336666
1	4.293196	-0.512814	-5.185833
1	5.265441	-2.316585	-3.810862
1	3.162291	-3.595354	-3.576511
1	1.245730	-2.436710	-3.023553
1	1.838428	-2.277364	-1.363157
1	3.253829	-4.111782	-1.006065
1	5.592745	-4.334382	-0.471974
1	6.073050	-3.279832	-1.910500
1	3.467000	-1.288139	-0.123601
1	3.313942	2.452286	-0.330276
1	5.040445	-1.998689	0.777353
1	4.994423	3.949829	0.730879
1	8.176331	1.369247	2.637446
1	8.641234	-1.041502	2.893799
1	1.583193	0.993179	-0.167663
1	-0.082541	0.858274	1.004146
1	-1.026813	-2.450287	0.552871
1	-1.305506	0.817230	3.310195
1	-4.097044	-2.461933	3.574046
8	7.020556	-3.001843	1.914333
6	8.125759	-3.480668	2.656365
1	8.052571	-4.568185	2.635863
1	9.077964	-3.177725	2.204857
1	8.089993	-3.138901	3.697099
1	1.391923	-0.189114	-2.323281
6	-1.015557	3.298501	-3.484019
6	-2.295660	3.040417	-4.283453
6	-3.182073	2.248190	-3.310977
7	-2.243417	1.698380	-2.320700
6	-0.859953	1.989245	-2.707427
6	-2.657843	1.187467	-1.162001
6	-3.960167	0.785963	-0.930031
6	0.207708	2.060408	-1.610311
8	-0.109031	2.231603	-0.410275
8	1.375759	1.933285	-2.057673
1	-0.525294	1.204466	-3.402527
1	-0.144191	3.509626	-4.105014
1	-1.151395	4.121507	-2.772134
1	-2.061989	2.430005	-5.160846
1	-2.786936	3.952907	-4.626105
1	-3.742513	1.448833	-3.807153
1	-3.902115	2.890310	-2.788870
1	-1.884648	1.010974	-0.425970
1	-4.716932	1.031337	-1.672630
6	-4.471256	0.563539	0.464379
6	-4.753890	1.909385	1.196686
1	-5.399295	-0.015825	0.424688
1	-3.749999	-0.018604	1.053819
1	-5.445367	1.729620	2.024251
1	-5.236595	2.598554	0.495606
6	-3.475536	2.481713	1.720706
6	-2.657493	3.312303	1.067023
1	-3.140374	2.120577	2.691240
1	-2.923615	3.724230	0.096588
6	-1.316118	3.636304	1.625627
8	-0.812239	2.953269	2.505330
6	-0.584593	4.824095	1.087147
6	0.804750	4.865808	1.234803
6	-1.248840	5.890613	0.478822
6	1.521789	5.959346	0.769780
1	1.298930	4.023833	1.708199
6	-0.529097	6.992688	0.022341
1	-2.330343	5.875373	0.380445
6	0.855056	7.025113	0.163498

1	2.601324	5.988186	0.879940
1	-1.049136	7.825597	-0.440304
1	1.416684	7.882130	-0.195872

si-si_6-path-A

Number of imaginary frequencies : 1

The smallest frequency is : -166.6022

Electronic energy= -3905.2876673
 Zero-point correction= 1.053822
 Thermal correction to Energy= 1.119455
 Thermal correction to Enthalpy= 1.120399
 Thermal correction to Gibbs Free Energy= 0.950201
 Sum of electronic and zero-point Energies= -3904.233845
 Sum of electronic and thermal Energies= -3904.168212
 Sum of electronic and thermal Enthalpies= -3904.167268
 Sum of electronic and thermal Free Energies= -3904.337466

 Cartesian Coordinates

8	0.095070	1.060668	3.930675
8	0.200878	0.072398	1.997392
6	2.627249	-0.987602	2.609902
1	2.073733	-1.386051	1.763986
1	2.257739	0.136592	4.458308
6	3.798271	-1.767470	3.042043
6	4.014050	-3.018654	2.454551
6	4.696851	-1.310044	4.014721
6	5.095763	-3.806159	2.834721
1	3.314355	-3.376081	1.706204
6	5.776813	-2.096676	4.394725
1	4.559405	-0.328061	4.459999
6	5.979442	-3.346439	3.807005
1	5.243148	-4.774093	2.366328
1	6.469746	-1.732421	5.146589
1	6.827841	-3.954590	4.104009
7	0.700115	0.335302	3.114050
6	1.930324	-0.174766	3.477928
7	-0.083565	-0.642226	-1.083954
6	0.899572	-1.560050	-1.479226
6	1.158439	-2.743377	-0.777647
6	2.174148	-3.586550	-1.214110
6	2.948501	-3.279434	-2.328047
6	2.693391	-2.090294	-3.000830
6	1.687434	-1.224069	-2.585656
6	2.455291	-4.873246	-0.492497
9	2.147686	-5.943845	-1.236489
6	3.534698	-1.771471	-4.204221
9	3.481097	-2.752690	-5.116132
6	-1.339111	-0.895742	-0.625911
16	-2.023371	-2.433636	-0.463699
7	-2.002438	0.238658	-0.312611
6	-3.397500	0.296926	0.066150
6	-3.589389	1.333068	1.186734
6	-4.997997	1.267822	1.816135
6	-4.880679	0.910093	3.304237
6	-4.103723	2.031102	4.009169
6	-2.752103	2.233677	3.295725
7	-2.571882	1.143750	2.282280
6	-2.664525	-0.199432	2.933522
6	-4.098246	-0.406204	3.486685
6	-4.746250	-1.636338	2.895386
6	-6.027458	-1.776093	2.564242
6	-4.294314	0.689599	-1.104232
6	-5.454350	-0.063061	-1.466153
6	-6.256136	0.451407	-2.527900

7	-5.950026	1.587724	-3.215526
6	-4.861194	2.230932	-2.871805
6	-4.006999	1.826594	-1.817317
6	-7.433412	-0.245557	-2.894220
6	-7.811294	-1.397046	-2.252623
6	-7.003027	-1.913607	-1.207688
6	-5.847895	-1.262925	-0.830640
9	3.762435	-4.985249	-0.183809
9	1.772540	-4.972735	0.656767
9	4.833911	-1.635380	-3.870050
9	3.160893	-0.636473	-4.803157
1	-3.362875	2.323287	0.787793
1	-5.500695	2.232785	1.707517
1	-5.600997	0.525491	1.288255
1	-1.896895	2.167905	3.966538
1	-2.688673	3.169401	2.737648
1	-3.941521	1.771700	5.059360
1	-4.679919	2.959527	3.985360
1	-5.875951	0.813622	3.745651
1	-4.003554	-0.581653	4.566450
1	-1.904984	-0.195410	3.716397
1	-2.380730	-0.945533	2.186051
1	-4.075095	-2.484752	2.755982
1	-6.400031	-2.710026	2.155416
1	-6.752271	-0.973191	2.674606
1	-3.674192	-0.692714	0.431358
1	-3.130335	2.426171	-1.579570
1	-5.250631	-1.716380	-0.048845
1	-4.624297	3.131021	-3.435583
1	-8.026875	0.166606	-3.703866
1	-8.718258	-1.906985	-2.554935
1	-1.540422	1.143561	-0.439316
1	0.157643	0.350707	-1.211288
1	0.566879	-2.996154	0.092288
1	1.513439	-0.287837	-3.111637
1	3.731789	-3.951696	-2.665571
8	-7.301338	-3.049489	-0.526338
6	-8.429735	-3.797456	-0.937673
1	-8.456642	-4.678250	-0.296035
1	-9.359832	-3.231635	-0.807264
1	-8.340687	-4.118005	-1.981993
1	-1.626291	1.248525	1.873824
6	1.479413	4.356896	1.495590
6	2.615745	4.325681	2.521792
6	3.323316	2.987255	2.254921
7	2.332597	2.184695	1.523966
6	1.047275	2.890396	1.457136
6	2.673715	1.079537	0.853939
6	3.823118	0.352294	1.081734
6	0.107140	2.551025	0.294887
8	0.566143	2.094216	-0.777037
8	-1.108111	2.775213	0.543997
1	0.486687	2.666089	2.376742
1	0.656166	5.015935	1.776531
1	1.847924	4.650602	0.507271
1	2.200519	4.332659	3.534124
1	3.302000	5.169960	2.429364
1	3.636338	2.488107	3.178293
1	4.210956	3.105855	1.619983
1	1.942571	0.723392	0.139175
1	4.560359	0.738924	1.783788
6	4.325376	-0.631930	0.067427
6	5.182208	0.048869	-1.041539
1	4.945761	-1.392944	0.553030
1	3.482106	-1.152215	-0.405167
1	5.672254	-0.728859	-1.634211
1	5.961348	0.650511	-0.560314
6	4.322605	0.898189	-1.920586
6	3.964181	2.158479	-1.659519
1	3.872033	0.438940	-2.796466

1	4.366037	2.687764	-0.799206
6	2.910616	2.823798	-2.471201
8	2.320665	2.243719	-3.366960
6	2.562298	4.236696	-2.116799
6	1.247238	4.663350	-2.319943
6	3.506711	5.122807	-1.591709
6	0.876144	5.958814	-1.981346
1	0.530798	3.948713	-2.709783
6	3.138563	6.428972	-1.275124
1	4.535191	4.802709	-1.449709
6	1.822136	6.843246	-1.461005
1	-0.150553	6.282570	-2.120054
1	3.877096	7.120551	-0.881769
1	1.531996	7.856768	-1.200923

si-si_7-path-A

Number of imaginary frequencies : 1

The smallest frequency is : -192.4777

Electronic energy=	-3905.2813968
Zero-point correction=	1.053655 <i>si-re</i>
Thermal correction to Energy=	1.119512
Thermal correction to Enthalpy=	1.120456
Thermal correction to Gibbs Free Energy=	0.947344
Sum of electronic and zero-point Energies=	-3904.227741
Sum of electronic and thermal Energies=	-3904.161885
Sum of electronic and thermal Enthalpies=	-3904.160941
Sum of electronic and thermal Free Energies=	-3904.334053

Cartesian Coordinates

8	-0.298439	-2.707299	-3.004914
8	-0.517806	-1.714060	-1.084762
6	-3.192122	-2.401130	-1.002117
1	-2.743372	-2.172198	-0.038720
1	-2.633076	-3.239485	-2.947448
6	-4.558925	-2.964964	-0.981651
6	-5.151556	-3.306703	0.238973
6	-5.284534	-3.173805	-2.163450
6	-6.430967	-3.855182	0.277170
1	-4.601555	-3.157299	1.162013
6	-6.559316	-3.721845	-2.124223
1	-4.850044	-2.889585	-3.118601
6	-7.137762	-4.065749	-0.902155
1	-6.871895	-4.120064	1.233003
1	-7.107502	-3.876072	-3.048377
1	-8.135832	-4.491030	-0.871932
7	-1.008089	-2.370515	-2.030909
6	-2.339619	-2.722901	-2.046401
7	0.239068	0.470919	1.205548
6	-0.753546	0.071055	2.118751
6	-1.157037	-1.265469	2.192477
6	-2.183663	-1.620449	3.057229
6	-2.852247	-0.667118	3.822742
6	-2.455222	0.659178	3.716237
6	-1.398983	1.035905	2.889277
6	-2.568588	-3.065912	3.170027
9	-2.381050	-3.720364	2.009899
6	-3.213808	1.729784	4.445001
9	-3.882272	1.242959	5.500018
6	1.434156	-0.153991	1.022472
16	2.065262	-1.293415	2.104012
7	2.064324	0.241188	-0.102971
6	3.436680	-0.092740	-0.429504
6	3.565158	-0.570792	-1.887049
6	4.923605	-1.249609	-2.164147

6	4.693460	-2.710896	-2.573654
6	3.895856	-2.720793	-3.885412
6	2.607274	-1.894319	-3.699480
7	2.468101	-1.540056	-2.248727
6	2.476166	-2.775886	-1.406774
6	3.868770	-3.452437	-1.502951
6	4.520110	-3.565248	-0.143694
6	5.816211	-3.430887	0.126692
6	4.359559	1.106532	-0.247368
6	5.542647	1.053306	0.552970
6	6.345972	2.231538	0.596474
7	6.027126	3.382452	-0.060870
6	4.922229	3.393454	-0.765215
6	4.059742	2.278720	-0.896158
6	7.538989	2.215802	1.359054
6	7.932130	1.097312	2.048235
6	7.126608	-0.069948	2.008862
6	5.955174	-0.085908	1.282218
9	-1.858783	-3.714784	4.101184
9	-3.865924	-3.209589	3.498426
9	-4.124228	2.317768	3.644949
9	-2.407628	2.702507	4.887462
1	3.389985	0.276263	-2.548614
1	5.447146	-0.722235	-2.966353
1	5.552717	-1.192237	-1.272910
1	1.705660	-2.441586	-3.967643
1	2.615019	-0.944156	-4.236515
1	3.648159	-3.749001	-4.164560
1	4.496359	-2.295582	-4.693620
1	5.652823	-3.214406	-2.719330
1	3.706229	-4.475748	-1.866538
1	1.667469	-3.396124	-1.795112
1	2.222134	-2.480090	-0.385701
1	3.836970	-3.798533	0.673260
1	6.190592	-3.548583	1.138659
1	6.552555	-3.195563	-0.637866
1	3.725837	-0.902260	0.241700
1	3.167108	2.357965	-1.514949
1	5.361718	-0.992955	1.306173
1	4.676792	4.320876	-1.278871
1	8.132777	3.123848	1.377774
1	8.850354	1.115725	2.623009
1	1.601850	0.932786	-0.697996
1	0.032153	1.273035	0.603339
1	-0.677920	-2.004248	1.559492
1	-1.092061	2.075234	2.807178
1	-3.668936	-0.952353	4.476195
8	7.443846	-1.216935	2.661885
6	8.584726	-1.214497	3.498654
1	8.626024	-2.204261	3.954036
1	9.505486	-1.045654	2.927767
1	8.501505	-0.459660	4.288937
1	1.564178	-1.054501	-2.128122
6	-1.192216	1.210356	-4.624068
6	-2.435708	0.498559	-5.164109
6	-3.254533	0.195069	-3.902442
7	-2.262013	0.195376	-2.820299
6	-0.911217	0.430019	-3.337593
6	-2.605379	0.157981	-1.536715
6	-3.856332	-0.198895	-1.072797
6	0.101798	1.116968	-2.407423
8	-0.273885	1.765786	-1.407984
8	1.293310	0.934211	-2.775188
1	-0.466492	-0.540600	-3.604829
1	-0.341457	1.187495	-5.306133
1	-1.416415	2.253498	-4.372373
1	-2.140683	-0.435643	-5.651794
1	-3.002391	1.093936	-5.882319
1	-3.774513	-0.767605	-3.952355
1	-4.001359	0.972029	-3.695840

1	-1.788126	0.305260	-0.844440
1	-4.671265	-0.300158	-1.787526
6	-4.260645	0.080040	0.348604
6	-4.918653	1.462143	0.518193
1	-4.981689	-0.676482	0.681483
1	-3.391105	-0.005160	1.012691
1	-5.347428	1.538416	1.526447
1	-5.766890	1.543782	-0.173162
6	-4.012932	2.646676	0.313842
6	-2.680256	2.591793	0.378433
1	-4.499790	3.606442	0.141216
1	-2.187937	1.654708	0.596492
6	-1.741696	3.736494	0.334045
8	-0.731435	3.702215	1.021936
6	-2.033629	4.920890	-0.529160
6	-1.513923	6.162607	-0.153437
6	-2.751562	4.799487	-1.721993
6	-1.737547	7.280519	-0.946504
1	-0.938864	6.229829	0.764614
6	-2.957344	5.917588	-2.525029
1	-3.118098	3.824197	-2.028031
6	-2.459696	7.158037	-2.133588
1	-1.345510	8.246751	-0.645260
1	-3.502725	5.821216	-3.458602
1	-2.629360	8.030637	-2.757089

si-si_8-path-A

Number of imaginary frequencies : 1

The smallest frequency is : -357.6759

Electronic energy=	-3905.2789741
Zero-point correction=	1.053836
Thermal correction to Energy=	1.119367
Thermal correction to Enthalpy=	1.120311
Thermal correction to Gibbs Free Energy=	0.950645
Sum of electronic and zero-point Energies=	-3904.225138
Sum of electronic and thermal Energies=	-3904.159607
Sum of electronic and thermal Enthalpies=	-3904.158663
Sum of electronic and thermal Free Energies=	-3904.328329

Cartesian Coordinates

6	-0.567083	1.217646	5.378614
6	-1.259385	-0.054869	5.879368
6	-2.616132	-0.035494	5.163488
7	-2.390727	0.824728	3.988551
6	-0.995205	1.254381	3.904504
6	-3.386466	1.260558	3.226722
6	-3.289421	1.985429	2.043769
8	-0.807972	1.969204	-1.680525
8	-0.531751	1.806999	0.482069
1	-0.928104	2.248958	3.457668
1	0.518850	1.192482	5.477028
1	-0.952704	2.099979	5.899287
1	-0.689387	-0.933631	5.567534
1	-1.373475	-0.084275	6.964113
1	-2.939793	-1.031925	4.849983
1	-3.401519	0.409619	5.783847
1	-4.371570	0.920644	3.549918
1	-2.322707	2.432876	1.822439
6	-4.521245	2.729641	1.572624
6	-4.592444	3.050458	0.075778
1	-4.578913	3.680573	2.121833
1	-5.416920	2.161240	1.851191
1	-4.783599	2.134656	-0.492863
1	-5.459224	3.697950	-0.100715

6	-3.356920	3.713312	-0.479380
6	-3.253600	4.153653	-1.737310
1	-2.485606	3.787461	0.171878
1	-4.084680	4.045706	-2.432814
6	-2.012434	4.656691	-2.373435
8	-1.912827	4.638945	-3.587952
6	-0.879136	5.210283	-1.553607
6	-1.074913	5.916763	-0.365351
6	0.409630	5.109490	-2.088985
6	0.007507	6.504127	0.288759
1	-2.076735	6.038684	0.033230
6	1.487779	5.694261	-1.436588
1	0.538688	4.580093	-3.027862
6	1.288328	6.393026	-0.243584
1	-0.155556	7.063258	1.204801
1	2.482679	5.628797	-1.868353
1	2.128570	6.862873	0.259767
6	-2.765081	0.362387	0.755807
1	-1.942129	0.165425	1.432959
1	-2.955665	0.877177	-1.392690
6	-3.848739	-0.640078	0.844647
6	-3.779783	-1.561314	1.901953
6	-4.881197	-0.755865	-0.091065
6	-4.733508	-2.561219	2.032133
1	-2.936559	-1.493634	2.588173
6	-5.835804	-1.762706	0.041369
1	-4.927348	-0.086400	-0.945566
6	-5.769870	-2.660276	1.103189
1	-4.658121	-3.281161	2.841382
1	-6.624251	-1.856670	-0.699112
1	-6.506369	-3.452455	1.192066
7	-1.201714	1.576329	-0.569165
6	-2.395695	0.917467	-0.470667
7	-0.285060	-1.854797	0.035394
6	-1.335883	-2.309748	-0.789935
6	-1.656990	-1.638472	-1.971018
6	-2.771954	-2.033179	-2.697869
6	-3.571241	-3.093739	-2.282660
6	-3.233242	-3.759472	-1.111721
6	-2.125419	-3.374281	-0.360185
6	-3.194629	-1.203904	-3.873312
9	-2.154889	-0.679011	-4.526314
6	-4.036473	-4.957729	-0.698807
9	-3.602422	-6.076323	-1.303865
6	0.978642	-1.550429	-0.367298
16	1.596740	-1.905700	-1.900052
7	1.692249	-0.928280	0.598373
6	3.092671	-0.572295	0.487213
6	3.314289	0.847206	1.043891
6	4.686281	1.439515	0.660782
6	4.474505	2.721725	-0.158128
6	3.721461	3.733770	0.719599
6	2.384531	3.114212	1.176353
7	2.240645	1.769332	0.541618
6	2.238160	1.907252	-0.947036
6	3.621558	2.430519	-1.409068
6	4.244862	1.494426	-2.417708
6	5.528005	1.150451	-2.498760
6	3.994968	-1.534684	1.248553
6	5.159706	-2.121571	0.663421
6	5.951954	-2.960289	1.503172
7	5.639525	-3.233180	2.801698
6	4.554256	-2.686970	3.292544
6	3.704944	-1.825211	2.558220
6	7.128375	-3.542383	0.971801
6	7.516951	-3.314180	-0.323111
6	6.722139	-2.486750	-1.158135
6	5.566419	-1.911295	-0.674465
9	-3.922328	-1.905568	-4.754117
9	-3.969134	-0.167440	-3.477682

9	-5.332934	-4.826495	-1.025337
9	-3.972799	-5.186024	0.621760
1	3.163882	0.826193	2.123539
1	5.258106	1.669924	1.563761
1	5.260622	0.705952	0.090984
1	1.514100	3.693683	0.858259
1	2.322033	2.946731	2.253136
1	3.533068	4.651862	0.156610
1	4.329435	3.997906	1.588969
1	5.440124	3.139389	-0.455711
1	3.448464	3.387557	-1.920003
1	1.409412	2.576524	-1.182733
1	1.995185	0.929568	-1.372497
1	3.547677	1.087746	-3.150818
1	5.876173	0.474540	-3.273179
1	6.278396	1.517205	-1.802764
1	3.337377	-0.590698	-0.575726
1	2.829664	-1.392721	3.039348
1	4.983116	-1.306951	-1.360287
1	4.315988	-2.916943	4.329296
1	7.714747	-4.176060	1.629177
1	8.423905	-3.771772	-0.699765
1	1.247559	-0.749443	1.502769
1	-0.503852	-1.685442	1.023303
1	-1.059653	-0.792484	-2.294564
1	-1.878208	-3.892069	0.561198
1	-4.444277	-3.387916	-2.855323
8	7.035034	-2.211208	-2.449424
6	8.179091	-2.830012	-3.006491
1	8.223668	-2.499670	-4.044441
1	9.096634	-2.520158	-2.492562
1	8.097473	-3.922729	-2.981464
1	1.317420	1.402594	0.827845
6	-0.097663	0.289369	3.096020
8	-0.567176	-0.824342	2.754432
8	1.070372	0.701873	2.897447

si-re_1-path-A

Number of imaginary frequencies : 1
The smallest frequency is : -300.2290

Electronic energy =-3905.2842098
Zero-point correction= 1.052392
Thermal correction to Energy= 1.118523
Thermal correction to Enthalpy= 1.119467
Thermal correction to Gibbs Free Energy= 0.943886
Sum of electronic and zero-point Energies= -3904.231818
Sum of electronic and thermal Energies= -3904.165687
Sum of electronic and thermal Enthalpies= -3904.164743
Sum of electronic and thermal Free Energies= -3904.340324

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Cartesian Coordinates

6	1.671285	-2.720916	3.354829
6	2.933488	-1.950276	3.760570
6	3.911064	-2.199467	2.603161
7	3.050281	-2.605285	1.478543
6	1.629361	-2.538755	1.828433
6	3.514171	-3.247578	0.413253
6	2.803199	-3.496026	-0.751595
8	0.432915	0.187608	-1.346458
8	0.699452	-1.758450	-2.285170
1	1.096825	-3.342614	1.313597
1	0.764005	-2.347029	3.835069
1	1.776077	-3.785897	3.588014
1	2.708782	-0.885071	3.826750

1	3.342307	-2.285624	4.715250
1	4.478031	-1.302368	2.342026
1	4.616538	-3.009922	2.817814
1	4.575077	-3.501373	0.454026
1	1.746257	-3.238554	-0.772458
6	3.213360	-4.621445	-1.660712
6	2.492178	-5.940313	-1.299658
1	4.297240	-4.778992	-1.607864
1	2.971736	-4.371785	-2.702714
1	2.844901	-6.730773	-1.973501
1	2.750732	-6.230239	-0.275629
6	1.009368	-5.806554	-1.439797
6	0.133399	-5.837985	-0.428963
1	0.614460	-5.641367	-2.443268
1	0.466651	-5.998660	0.593536
6	-1.324767	-5.706239	-0.687528
8	-1.779939	-5.692020	-1.821283
6	-2.247479	-5.601346	0.487328
6	-1.853775	-4.992026	1.681653
6	-3.559935	-6.061553	0.344224
6	-2.770496	-4.828592	2.716840
1	-0.842706	-4.609488	1.793136
6	-4.464647	-5.927927	1.389831
1	-3.852521	-6.518013	-0.596322
6	-4.072220	-5.303782	2.574471
1	-2.468067	-4.331844	3.633187
1	-5.478159	-6.300668	1.281752
1	-4.783348	-5.187127	3.386290
6	3.357945	-1.710025	-1.800392
1	3.052652	-2.265894	-2.683285
1	2.763515	0.146375	-0.761082
6	4.814370	-1.552610	-1.599748
6	5.708862	-2.200130	-2.456702
6	5.321036	-0.778455	-0.546750
6	7.083252	-2.073332	-2.270655
1	5.322357	-2.796378	-3.279454
6	6.691878	-0.650224	-0.363257
1	4.636942	-0.284097	0.138132
6	7.577139	-1.298869	-1.225024
1	7.767619	-2.574185	-2.948212
1	7.066721	-0.035865	0.448544
1	8.648173	-1.195342	-1.082537
7	1.173757	-0.765792	-1.690656
6	2.502991	-0.695370	-1.382192
7	0.717774	2.287024	0.702043
6	1.837683	3.089475	0.501641
6	1.871287	4.335970	-0.130402
6	3.092420	4.994376	-0.279611
6	4.287646	4.463390	0.177946
6	4.238920	3.223720	0.815094
6	3.046607	2.545100	0.983052
6	3.096389	6.296743	-1.029231
9	4.222967	6.995665	-0.818696
6	5.513846	2.646191	1.355184
9	5.985002	3.354698	2.392654
6	-0.593502	2.435756	0.370609
16	-1.331244	3.822660	-0.249225
7	-1.296612	1.305318	0.617999
6	-2.686491	1.134050	0.258339
6	-2.960106	-0.364114	0.026059
6	-4.410284	-0.651595	-0.411724
6	-4.404481	-1.725754	-1.508598
6	-3.544326	-2.900131	-1.021289
6	-2.077555	-2.441190	-0.953667
7	-2.044029	-0.940421	-1.025041
6	-2.418335	-0.499735	-2.401242
6	-3.773636	-1.146851	-2.788912
6	-4.611577	-0.143777	-3.541201
6	-5.865615	0.212309	-3.276240
6	-3.638525	1.643018	1.336821

6	-4.827173	2.380801	1.034906
6	-5.657684	2.746174	2.135744
7	-5.369458	2.435743	3.432009
6	-4.263224	1.774161	3.664177
6	-3.368909	1.356256	2.650158
6	-6.848365	3.470301	1.885209
6	-7.216700	3.823618	0.612969
6	-6.387098	3.464642	-0.480596
6	-5.217989	2.765285	-0.269302
9	2.999056	6.103516	-2.355114
9	2.067496	7.080706	-0.677775
9	6.487146	2.629894	0.430240
9	5.363285	1.377545	1.785873
1	-2.701067	-0.910318	0.939129
1	-4.990490	-0.980815	0.454221
1	-4.876561	0.261337	-0.787945
1	-1.480326	-2.794156	-1.796043
1	-1.571790	-2.711603	-0.025791
1	-3.619479	-3.763388	-1.688045
1	-3.888238	-3.220395	-0.031844
1	-5.423662	-2.063592	-1.713008
1	-3.565094	-1.984199	-3.468534
1	-1.590208	-0.798067	-3.046471
1	-2.466869	0.591828	-2.395889
1	-4.100807	0.332709	-4.378786
1	-6.370643	0.958734	-3.880807
1	-6.438126	-0.215913	-2.457930
1	-2.868941	1.691172	-0.664035
1	-2.462922	0.819647	2.917837
1	-4.614076	2.532888	-1.139751
1	-4.040923	1.540681	4.703801
1	-7.459535	3.736720	2.741287
1	-8.134282	4.377078	0.452486
1	-0.795438	0.455962	0.924184
1	0.977377	1.342350	1.040906
1	0.960329	4.783911	-0.502561
1	3.028301	1.580837	1.481801
1	5.225415	4.991601	0.047233
8	-6.679242	3.772940	-1.769097
6	-7.825552	4.562738	-2.019723
1	-7.848181	4.726420	-3.097393
1	-8.745337	4.048167	-1.717321
1	-7.765245	5.532072	-1.511598
1	-1.063175	-0.614937	-0.872932
6	0.969279	-1.194487	1.482005
8	1.674114	-0.166494	1.598460
8	-0.251215	-1.248674	1.183912

si-re_2-path-A

Number of imaginary frequencies : 1

The smallest frequency is : -291.3378

Electronic energy= -3905.2853601
 Zero-point correction= 1.053110
 Thermal correction to Energy= 1.119031
 Thermal correction to Enthalpy= 1.119975
 Thermal correction to Gibbs Free Energy= 0.946312
 Sum of electronic and zero-point Energies= -3904.232250
 Sum of electronic and thermal Energies= -3904.166329
 Sum of electronic and thermal Enthalpies= -3904.165385
 Sum of electronic and thermal Free Energies= -3904.339048

 Cartesian Coordinates

6	1.962845	-2.341877	3.416676
6	2.771828	-1.207335	4.066415
6	3.812098	-0.809832	2.998686

7	3.386715	-1.514824	1.777908
6	2.004745	-1.983708	1.920004
6	4.258611	-2.087795	0.951721
6	3.943288	-2.678978	-0.259634
8	0.791846	0.464678	-1.023302
8	1.409133	-1.480143	-1.765830
1	1.839692	-2.836011	1.261025
1	0.940483	-2.409062	3.796307
1	2.456660	-3.308196	3.568213
1	2.120714	-0.358138	4.275980
1	3.246595	-1.521036	4.997729
1	3.808588	0.267472	2.820728
1	4.828385	-1.127237	3.250534
1	5.307844	-1.954891	1.221075
1	2.892647	-2.816835	-0.504273
6	4.896892	-3.656165	-0.888543
6	4.639974	-5.100951	-0.391358
1	5.932901	-3.380225	-0.660458
1	4.793481	-3.633935	-1.981767
1	5.389068	-5.767281	-0.834458
1	4.764878	-5.129825	0.696515
6	3.271079	-5.573498	-0.768469
6	2.226294	-5.664288	0.062167
1	3.097420	-5.808538	-1.819113
1	2.335858	-5.423056	1.116641
6	0.894612	-6.064739	-0.470473
8	0.799135	-6.662940	-1.529210
6	-0.348755	-5.662496	0.271783
6	-0.333512	-4.806323	1.375988
6	-1.578846	-6.088725	-0.245669
6	-1.527479	-4.360110	1.938315
1	0.602757	-4.456757	1.794543
6	-2.769751	-5.656435	0.323560
1	-1.574528	-6.746587	-1.108646
6	-2.746078	-4.779963	1.411592
1	-1.501671	-3.671982	2.776526
1	-3.718971	-5.993795	-0.081968
1	-3.676117	-4.426583	1.848076
6	4.010702	-0.900850	-1.435806
1	3.758333	-1.570577	-2.254668
1	3.140240	0.918208	-0.537576
6	5.421099	-0.461457	-1.370398
6	6.336397	-0.920444	-2.323629
6	5.867304	0.409445	-0.367784
6	7.666502	-0.511445	-2.282501
1	5.996769	-1.590248	-3.109207
6	7.192752	0.823574	-0.331654
1	5.170692	0.764212	0.386747
6	8.097173	0.362638	-1.288547
1	8.364480	-0.871714	-3.031593
1	7.519397	1.509831	0.443613
1	9.132564	0.686871	-1.259410
7	1.690687	-0.357706	-1.282231
6	3.000209	-0.034498	-1.023594
7	-0.282996	2.368164	0.798258
6	0.586552	3.431316	0.557366
6	0.221711	4.718766	0.152250
6	1.212847	5.683357	-0.019030
6	2.556589	5.418616	0.209685
6	2.900075	4.136934	0.630633
6	1.940506	3.154300	0.805629
6	0.810254	7.043239	-0.514468
9	1.671890	7.994487	-0.119322
6	4.343542	3.781540	0.824128
9	5.072531	4.825005	1.241972
6	-1.485640	2.055260	0.246761
16	-2.462699	3.082934	-0.674579
7	-1.820355	0.772008	0.510165
6	-3.046090	0.133384	0.092345
6	-2.748479	-1.308967	-0.363749

6	-3.932635	-1.947665	-1.122761
6	-3.530606	-2.207834	-2.583562
6	-2.419232	-3.264159	-2.590728
6	-1.310190	-2.815954	-1.623758
7	-1.537327	-1.377704	-1.254461
6	-1.674762	-0.529492	-2.479228
6	-2.965390	-0.931525	-3.239203
6	-3.931093	0.224269	-3.356523
6	-5.259146	0.149045	-3.316901
6	-4.063845	0.055898	1.228385
6	-5.422485	0.473947	1.086045
6	-6.286929	0.263504	2.202007
7	-5.872009	-0.280227	3.380953
6	-4.609956	-0.618172	3.481142
6	-3.671579	-0.475815	2.431860
6	-7.648633	0.634962	2.089922
6	-8.144894	1.192199	0.939423
6	-7.278207	1.415658	-0.161773
6	-5.946292	1.068987	-0.084049
9	0.772333	7.091154	-1.856447
9	-0.406437	7.398606	-0.079134
9	4.907295	3.345344	-0.316249
9	4.506914	2.792526	1.726265
1	-2.462692	-1.901492	0.509700
1	-4.209460	-2.895586	-0.650306
1	-4.801861	-1.287616	-1.068969
1	-0.310810	-2.874349	-2.050214
1	-1.326258	-3.368134	-0.682545
1	-2.020867	-3.384468	-3.602492
1	-2.807713	-4.234538	-2.270846
1	-4.394003	-2.565148	-3.150782
1	-2.665301	-1.198977	-4.260891
1	-0.760809	-0.700045	-3.050504
1	-1.678275	0.514728	-2.155352
1	-3.466346	1.198222	-3.512948
1	-5.872777	1.036907	-3.433442
1	-5.788550	-0.787634	-3.160384
1	-3.451166	0.707405	-0.743161
1	-2.640885	-0.789093	2.585283
1	-5.316362	1.289893	-0.937813
1	-4.289288	-1.039437	4.432310
1	-8.286389	0.462678	2.950937
1	-9.191717	1.466011	0.884262
1	-1.135914	0.154117	0.973392
1	0.208106	1.565130	1.227683
1	-0.816777	4.964178	-0.020388
1	2.216730	2.159745	1.146409
1	3.310344	6.186544	0.078684
8	-7.686553	1.969640	-1.331694
6	-9.025018	2.418706	-1.425821
1	-9.124684	2.862658	-2.416514
1	-9.737313	1.590521	-1.332183
1	-9.247381	3.179358	-0.668706
1	-0.706109	-1.051497	-0.727787
6	0.943427	-0.913388	1.632149
8	1.234869	0.272240	1.896109
8	-0.169866	-1.354870	1.233884

si-re_3-path-A

Number of imaginary frequencies : 1
The smallest frequency is : -340.1789

Electronic energy= -3905.2829508
Zero-point correction= 1.053049
Thermal correction to Energy= 1.119013
Thermal correction to Enthalpy= 1.119957

Thermal correction to Gibbs Free Energy=	0.946284
Sum of electronic and zero-point Energies=	-3904.229901
Sum of electronic and thermal Energies=	-3904.163938
Sum of electronic and thermal Enthalpies=	-3904.162994
Sum of electronic and thermal Free Energies=	-3904.336666

Cartesian Coordinates

6	-1.807443	0.888007	4.744958
6	-2.477730	-0.484232	4.920005
6	-3.534068	-0.547154	3.797192
7	-3.237373	0.614529	2.937382
6	-1.883894	1.104092	3.223096
6	-4.211778	1.348663	2.410853
6	-4.086009	2.436556	1.559693
8	-0.384871	0.479917	-0.355437
8	-1.312810	2.440990	-0.176822
1	-1.783957	2.146322	2.919005
1	-0.777798	0.915005	5.106742
1	-2.380300	1.671541	5.250728
1	-1.744053	-1.278456	4.775479
1	-2.928475	-0.603453	5.906698
1	-3.445715	-1.466670	3.215020
1	-4.557801	-0.454603	4.170012
1	-5.213877	0.961427	2.602105
1	-3.103375	2.884791	1.420052
6	-5.287496	3.343556	1.360593
6	-4.882215	4.771114	0.940852
1	-5.873895	3.406996	2.283594
1	-5.966042	2.931444	0.599640
1	-5.780776	5.396111	0.902005
1	-4.203874	5.198145	1.687534
6	-4.221566	4.715750	-0.396748
6	-2.913630	4.853541	-0.622315
1	-4.846658	4.421858	-1.241470
1	-2.230877	5.132423	0.175890
6	-2.353291	4.489741	-1.952385
8	-3.008134	3.844142	-2.754136
6	-0.958238	4.914567	-2.292159
6	-0.326691	5.977836	-1.642045
6	-0.298927	4.248335	-3.330284
6	0.947384	6.380991	-2.036700
1	-0.839275	6.515305	-0.850056
6	0.980864	4.636177	-3.708459
1	-0.809274	3.429953	-3.827686
6	1.603062	5.708412	-3.065774
1	1.425758	7.222275	-1.544726
1	1.492339	4.112494	-4.510323
1	2.597332	6.020963	-3.371437
6	-3.801107	1.318788	-0.244814
1	-3.720529	2.283612	-0.741705
1	-2.562314	-0.500471	-0.076991
6	-5.067541	0.583346	-0.450740
6	-6.056064	1.115512	-1.284279
6	-5.288424	-0.663079	0.152575
6	-7.241648	0.419335	-1.509827
1	-5.877009	2.065934	-1.780475
6	-6.469050	-1.357573	-0.073220
1	-4.525886	-1.088599	0.799958
6	-7.451114	-0.815576	-0.904164
1	-7.995887	0.839383	-2.167707
1	-6.617298	-2.327257	0.390456
1	-8.372638	-1.360146	-1.083966
7	-1.409033	1.191719	-0.236240
6	-2.623865	0.573649	-0.155467
7	0.327568	-2.272172	0.258114
6	-0.529169	-3.177771	-0.359159
6	-0.252476	-3.951033	-1.489996
6	-1.230319	-4.815741	-1.981526
6	-2.476218	-4.945805	-1.389394

6	-2.736808	-4.173187	-0.257890
6	-1.791269	-3.304997	0.255641
6	-0.913725	-5.588216	-3.230903
9	-1.756444	-6.616879	-3.414444
6	-4.056426	-4.344887	0.434070
9	-4.138722	-5.526177	1.066246
6	1.567719	-1.812010	-0.050498
16	2.577837	-2.360947	-1.291115
7	1.932571	-0.809612	0.782753
6	3.202707	-0.123918	0.744762
6	2.984953	1.354530	1.120186
6	4.239084	2.222026	0.874555
6	3.912890	3.313135	-0.154675
6	2.821856	4.218669	0.433581
6	1.602645	3.355556	0.814750
7	1.838867	1.953326	0.347435
6	2.060890	1.936915	-1.129067
6	3.371714	2.692326	-1.459255
6	4.340263	1.812314	-2.212807
6	5.664703	1.797795	-2.084452
6	4.207802	-0.723648	1.726620
6	5.554012	-1.039380	1.362848
6	6.406742	-1.533223	2.394747
7	5.994727	-1.730954	3.678636
6	4.746622	-1.452390	3.963924
6	3.818769	-0.943044	3.024185
6	7.754288	-1.836912	2.081278
6	8.249655	-1.665445	0.814383
6	7.396287	-1.183829	-0.211309
6	6.077833	-0.886116	0.058747
9	-0.995985	-4.815268	-4.325941
9	0.329604	-6.088923	-3.205984
9	-5.083267	-4.301939	-0.430018
9	-4.281245	-3.393598	1.361344
1	2.651574	1.400539	2.159740
1	4.563741	2.684913	1.810745
1	5.060364	1.592961	0.524113
1	0.677452	3.678348	0.333939
1	1.430677	3.288218	1.890593
1	2.528267	4.974943	-0.299901
1	3.203868	4.739097	1.315975
1	4.808000	3.903244	-0.368769
1	3.100902	3.522064	-2.126127
1	1.173230	2.404010	-1.562706
1	2.074387	0.890428	-1.444511
1	3.880348	1.144953	-2.942936
1	6.276893	1.133086	-2.685574
1	6.191962	2.430731	-1.374779
1	3.592293	-0.195794	-0.272664
1	2.799522	-0.729163	3.338207
1	5.461325	-0.547482	-0.765177
1	4.428821	-1.623081	4.990879
1	8.381788	-2.211436	2.883415
1	9.285051	-1.906255	0.604626
1	1.259658	-0.459230	1.477744
1	-0.136839	-1.752130	1.024364
1	0.710228	-3.880282	-1.976939
1	-2.009378	-2.707868	1.137228
1	-3.219757	-5.626661	-1.788021
8	7.806068	-0.987732	-1.490901
6	9.135228	-1.338293	-1.825918
1	9.242355	-1.130615	-2.890845
1	9.864082	-0.737482	-1.268952
1	9.327638	-2.402468	-1.647698
1	0.971366	1.405203	0.519788
6	-0.775516	0.265494	2.562928
8	-1.052159	-0.914522	2.249093
8	0.346238	0.829407	2.477146

si-re_4-path-A

Number of imaginary frequencies : 1

The smallest frequency is : -295.7617

Electronic energy= -3905.2857186
 Zero-point correction= 1.053330
 Thermal correction to Energy= 1.118912
 Thermal correction to Enthalpy= 1.119856
 Thermal correction to Gibbs Free Energy= 0.949184
 Sum of electronic and zero-point Energies= -3904.232389
 Sum of electronic and thermal Energies= -3904.166807
 Sum of electronic and thermal Enthalpies= -3904.165863
 Sum of electronic and thermal Free Energies= -3904.336534

Cartesian Coordinates

6	-2.176317	1.756933	4.135355
6	-3.420776	0.862244	4.205735
6	-4.253138	1.272798	2.978035
7	-3.311315	2.016000	2.122762
6	-1.939820	1.883785	2.620475
6	-3.717398	2.936546	1.254147
6	-2.936834	3.570527	0.301021
8	-0.266997	0.165102	-0.772446
8	-0.485766	2.296199	-1.144132
1	-1.360098	2.767940	2.347766
1	-1.309085	1.334259	4.646485
1	-2.382574	2.747191	4.553420
1	-3.128670	-0.185087	4.113822
1	-3.977611	0.990235	5.135564
1	-4.639862	0.402281	2.442661
1	-5.090479	1.929831	3.234477
1	-4.795086	3.109975	1.250622
1	-1.861023	3.410387	0.317928
6	-3.401465	4.852497	-0.335823
6	-2.684794	6.091354	0.251027
1	-4.483779	4.968870	-0.209997
1	-3.210989	4.836899	-1.419396
1	-3.144286	6.995463	-0.164761
1	-2.820322	6.112661	1.337084
6	-1.224811	6.079871	-0.088798
6	-0.252196	5.822935	0.793334
1	-0.971361	6.277128	-1.130139
1	-0.493908	5.673060	1.844527
6	1.207564	5.840751	0.526891
8	1.973709	6.003172	1.465570
6	1.766800	5.651921	-0.854104
6	1.145786	4.857164	-1.823913
6	3.018055	6.219185	-1.124051
6	1.771842	4.641232	-3.051086
1	0.201497	4.367619	-1.609532
6	3.627941	6.021291	-2.356775
1	3.498021	6.812556	-0.352309
6	3.005212	5.228832	-3.321998
1	1.293618	4.006888	-3.791194
1	4.591428	6.476043	-2.563612
1	3.486433	5.064701	-4.281304
6	-3.177692	2.075183	-1.259462
1	-2.751824	2.855143	-1.885279
1	-2.666784	0.011882	-0.660505
6	-4.634375	1.860005	-1.372875
6	-5.401655	2.695172	-2.191489
6	-5.272416	0.838236	-0.655168
6	-6.777945	2.511882	-2.294662
1	-4.912273	3.484465	-2.756265
6	-6.644801	0.654455	-0.760768
1	-4.690058	0.190504	-0.005383

6	-7.401659	1.492729	-1.580304
1	-7.362425	3.161739	-2.938248
1	-7.120916	-0.148791	-0.208286
1	-8.473879	1.346663	-1.664462
7	-0.995715	1.163444	-0.967471
6	-2.352144	0.997826	-0.961327
7	-0.664009	-2.495771	0.494304
6	-1.702137	-3.299316	0.026261
6	-1.570631	-4.524826	-0.633062
6	-2.716430	-5.225858	-1.010964
6	-3.995232	-4.757502	-0.757182
6	-4.112193	-3.538553	-0.089754
6	-2.998798	-2.818207	0.299514
6	-2.525067	-6.523114	-1.744829
9	-2.112659	-6.324271	-3.006909
6	-5.486911	-3.001302	0.178873
9	-6.278882	-3.920902	0.750865
6	0.674719	-2.496670	0.240629
16	1.507633	-3.551048	-0.781281
7	1.311062	-1.507249	0.911461
6	2.705104	-1.180232	0.697994
6	2.936807	0.290651	1.090848
6	4.395855	0.757962	0.925511
6	4.412170	2.206988	0.414270
6	3.439551	3.042239	1.256979
6	2.006403	2.558450	0.973166
7	2.077838	1.227448	0.278190
6	2.609579	1.412487	-1.108602
6	3.913073	2.245442	-1.040237
6	4.873115	1.757286	-2.093270
6	6.111876	1.311895	-1.901551
6	3.642112	-2.061604	1.518637
6	4.883420	-2.554423	1.003716
6	5.694802	-3.320055	1.892025
7	5.342953	-3.601019	3.179432
6	4.191763	-3.143860	3.604612
6	3.309727	-2.369765	2.812214
6	6.935081	-3.821541	1.426902
6	7.369405	-3.584307	0.148420
6	6.558603	-2.826864	-0.735363
6	5.341400	-2.333912	-0.315925
9	-1.600556	-7.295458	-1.155047
9	-3.659409	-7.237837	-1.811252
9	-6.103381	-2.616280	-0.951314
9	-5.473359	-1.928553	0.994335
1	2.591726	0.426882	2.121555
1	4.911869	0.672543	1.885396
1	4.917958	0.111381	0.216964
1	1.461655	3.209772	0.286379
1	1.406191	2.402801	1.868346
1	3.518350	4.105210	1.011731
1	3.674867	2.932749	2.320248
1	5.422136	2.619582	0.479034
1	3.657227	3.288283	-1.278645
1	1.813921	1.897703	-1.676481
1	2.778375	0.418206	-1.528974
1	4.470731	1.767419	-3.107307
1	6.714544	0.968980	-2.736462
1	6.575494	1.270523	-0.919495
1	2.926903	-1.325747	-0.362437
1	2.363185	-2.036859	3.228220
1	4.755723	-1.780507	-1.041638
1	3.918607	-3.382298	4.630873
1	7.531239	-4.402735	2.122913
1	8.322894	-3.981425	-0.178632
1	0.751202	-0.835573	1.463033
1	-1.016241	-1.671557	1.012931
1	-0.590804	-4.930846	-0.842589
1	-3.110363	-1.882493	0.838122
1	-4.871018	-5.323246	-1.054031

8	6.912614	-2.541638	-2.013784
6	8.119579	-3.087385	-2.509151
1	8.191571	-2.764202	-3.547943
1	8.990113	-2.712920	-1.957668
1	8.110495	-4.182941	-2.475865
1	1.115983	0.840393	0.183601
6	-1.222657	0.614897	2.125002
8	-1.933848	-0.360326	1.801499
8	0.034768	0.652592	2.171313

si-re_5-path-A

Number of imaginary frequencies : 1

The smallest frequency is : -321.4132

Electronic energy=	-3905.2782751
Zero-point correction=	1.053050
Thermal correction to Energy=	1.119372
Thermal correction to Enthalpy=	1.120316
Thermal correction to Gibbs Free Energy=	0.942176
Sum of electronic and zero-point Energies=	-3904.225225
Sum of electronic and thermal Energies=	-3904.158903
Sum of electronic and thermal Enthalpies=	-3904.157959
Sum of electronic and thermal Free Energies=	-3904.336099

Cartesian Coordinates

6	-2.126225	-2.950227	-1.687185
6	-2.672488	-1.812322	-2.562835
6	-3.353130	-0.852770	-1.566786
7	-2.909862	-1.313904	-0.236990
6	-1.771215	-2.224895	-0.377505
6	-3.720066	-1.250711	0.813565
6	-3.430571	-1.592657	2.125822
8	0.835900	0.053691	1.645440
8	-0.286959	-1.288967	2.938031
1	-1.705199	-2.890049	0.483617
1	-1.258818	-3.451343	-2.121554
1	-2.902032	-3.695687	-1.487463
1	-1.850956	-1.298331	-3.063824
1	-3.372208	-2.171182	-3.319476
1	-3.038473	0.181340	-1.724725
1	-4.445320	-0.907487	-1.607739
1	-4.668917	-0.764849	0.598508
1	-2.505898	-2.129847	2.324933
6	-4.533961	-1.784867	3.144724
6	-5.945689	-1.363519	2.707026
1	-4.280464	-1.241154	4.065069
1	-4.567202	-2.843792	3.432377
1	-6.584817	-1.382955	3.599568
1	-5.957785	-0.330040	2.340247
6	-6.541400	-2.293066	1.695028
6	-7.161142	-1.925278	0.568738
1	-6.471263	-3.361949	1.902572
1	-7.249387	-0.873740	0.308594
6	-7.701651	-2.957020	-0.357816
8	-7.487123	-4.143968	-0.171912
6	-8.496018	-2.517200	-1.551029
6	-9.053021	-1.240005	-1.666124
6	-8.697939	-3.449453	-2.574672
6	-9.797755	-0.901435	-2.792796
1	-8.933717	-0.509642	-0.872821
6	-9.430240	-3.106781	-3.703247
1	-8.268557	-4.439509	-2.462317
6	-9.981406	-1.830192	-3.813375
1	-10.235520	0.088337	-2.873126
1	-9.575286	-3.833037	-4.496545

1	-10.556996	-1.561046	-4.693561
6	-2.511835	0.251769	2.696567
1	-2.382482	-0.233206	3.661299
1	-1.215829	1.232500	1.204107
6	-3.606625	1.241815	2.602793
6	-4.367043	1.566460	3.730631
6	-3.899033	1.868791	1.383784
6	-5.406660	2.489964	3.638886
1	-4.133280	1.102893	4.685396
6	-4.932862	2.790895	1.292782
1	-3.313742	1.620045	0.502132
6	-5.694186	3.100142	2.421580
1	-5.987008	2.737359	4.522176
1	-5.134921	3.276010	0.343304
1	-6.501645	3.822071	2.351282
7	-0.235175	-0.282524	2.195947
6	-1.352254	0.475083	1.960108
7	1.608192	1.476838	-0.768345
6	1.092311	2.768715	-0.748370
6	1.803786	3.949305	-0.521132
6	1.126315	5.168941	-0.540062
6	-0.233907	5.262458	-0.783582
6	-0.930422	4.076735	-1.020768
6	-0.291765	2.851269	-1.006659
6	1.921082	6.408492	-0.240809
9	1.255511	7.527555	-0.566536
6	-2.395357	4.164830	-1.332036
9	-2.620696	4.805077	-2.490070
6	2.827417	0.962615	-0.461716
16	4.229333	1.828364	-0.082400
7	2.800018	-0.391071	-0.483406
6	3.936449	-1.248526	-0.238182
6	3.469056	-2.499617	0.530285
6	4.642890	-3.336114	1.086145
6	4.569783	-3.365053	2.620990
6	3.272381	-4.077664	3.030112
6	2.081180	-3.380641	2.343820
7	2.571643	-2.130946	1.680593
6	3.241531	-1.243897	2.678743
6	4.530967	-1.932944	3.193024
6	5.755629	-1.090782	2.920923
6	6.966143	-1.536661	2.594489
6	4.599230	-1.707310	-1.535244
6	6.009298	-1.629606	-1.755808
6	6.502571	-2.149926	-2.989694
7	5.700725	-2.687590	-3.951929
6	4.411838	-2.718721	-3.718882
6	3.816258	-2.245496	-2.525594
6	7.896081	-2.113147	-3.238268
6	8.771851	-1.589981	-2.321930
6	8.276725	-1.062068	-1.101688
6	6.925145	-1.077379	-0.831124
9	2.225062	6.500092	1.064307
9	3.084089	6.425485	-0.907887
9	-3.067985	4.840985	-0.386351
9	-2.977701	2.954835	-1.436110
1	2.823165	-3.088176	-0.125625
1	4.594633	-4.356734	0.696665
1	5.590451	-2.905755	0.753774
1	1.300256	-3.064364	3.035302
1	1.622205	-3.979040	1.554833
1	3.154948	-4.047408	4.117220
1	3.310696	-5.128841	2.733080
1	5.431192	-3.903443	3.024941
1	4.438125	-2.019889	4.283585
1	2.497893	-1.071848	3.458433
1	3.431595	-0.285522	2.188411
1	5.607271	-0.016062	3.033463
1	7.790146	-0.848360	2.435400
1	7.184634	-2.593561	2.461979

1	4.652621	-0.688387	0.366050
1	2.737595	-2.312135	-2.401851
1	6.594183	-0.638069	0.102412
1	3.782466	-3.144079	-4.498360
1	8.246761	-2.514564	-4.183448
1	9.833040	-1.577150	-2.539775
1	1.905915	-0.875042	-0.642114
1	0.867717	0.761494	-0.889963
1	2.868433	3.919062	-0.335113
1	-0.844814	1.934917	-1.195036
1	-0.738287	6.222127	-0.796399
8	9.074276	-0.521315	-0.145293
6	10.459568	-0.415584	-0.413130
1	10.897854	0.072248	0.457794
1	10.922890	-1.400928	-0.541516
1	10.652317	0.197049	-1.301349
1	1.744392	-1.618559	1.319848
6	-0.432894	-1.492218	-0.574277
8	-0.475682	-0.330521	-1.039262
8	0.598891	-2.169130	-0.323623

si-re_6-path-A

Number of imaginary frequencies : 1

The smallest frequency is : -301.2556

Electronic energy= -3905.2762633
 Zero-point correction= 1.052448
 Thermal correction to Energy= 1.119005
 Thermal correction to Enthalpy= 1.119949
 Thermal correction to Gibbs Free Energy= 0.941517
 Sum of electronic and zero-point Energies= -3904.223816
 Sum of electronic and thermal Energies= -3904.157258
 Sum of electronic and thermal Enthalpies= -3904.156314
 Sum of electronic and thermal Free Energies= -3904.334746

 Cartesian Coordinates

6	0.547273	-0.022031	4.887578
6	0.588759	1.509381	5.007253
6	1.646434	1.953320	3.975843
7	1.945032	0.739467	3.194927
6	0.896755	-0.265041	3.408081
6	3.176668	0.466049	2.774235
6	3.562072	-0.577248	1.949468
8	-0.306009	-0.202364	-0.414123
8	1.382726	-1.565327	-0.253241
1	1.290306	-1.263405	3.216420
1	-0.422545	-0.449010	5.151991
1	1.315848	-0.482916	5.515750
1	-0.380557	1.932432	4.741516
1	0.845589	1.836381	6.016352
1	1.253868	2.728831	3.314520
1	2.572374	2.310750	4.435867
1	3.918687	1.225639	3.026021
1	2.837694	-1.353414	1.708638
6	5.023532	-0.953772	1.870912
6	5.313721	-2.042719	0.827049
1	5.366650	-1.328671	2.844596
1	5.631540	-0.063881	1.659084
1	4.702230	-2.922901	1.068496
1	5.024704	-1.723077	-0.179676
6	6.756937	-2.432627	0.834455
6	7.566935	-2.405658	-0.227413
1	7.183377	-2.753367	1.785816
1	7.194592	-2.087189	-1.196769
6	8.998605	-2.790561	-0.088314

8	9.501481	-2.959850	1.010431
6	9.827097	-2.953178	-1.326882
6	9.265506	-3.110998	-2.597347
6	11.218414	-2.973815	-1.183270
6	10.086175	-3.282179	-3.708480
1	8.188431	-3.125756	-2.727166
6	12.036411	-3.131712	-2.293752
1	11.636544	-2.861807	-0.188287
6	11.470134	-3.285855	-3.559241
1	9.643887	-3.413253	-4.690799
1	13.115303	-3.137287	-2.176060
1	12.108919	-3.411556	-4.428092
6	3.096544	0.497960	0.116925
1	3.485536	-0.384597	-0.380348
1	1.180396	1.597546	0.165402
6	3.982476	1.679190	0.139819
6	5.281749	1.583903	-0.370369
6	3.550842	2.906015	0.663246
6	6.130764	2.687817	-0.360754
1	5.624289	0.638546	-0.784794
6	4.395952	4.007709	0.669915
1	2.547953	2.998542	1.070039
6	5.689818	3.901471	0.158697
1	7.134538	2.598492	-0.763676
1	4.036870	4.952289	1.065566
1	6.348666	4.763854	0.163028
7	0.912334	-0.404808	-0.217246
6	1.717542	0.670646	0.045469
7	-2.361291	1.754169	0.139797
6	-1.981550	2.974854	-0.410423
6	-2.575484	3.617203	-1.499261
6	-2.072747	4.847508	-1.924330
6	-1.004279	5.470080	-1.301113
6	-0.430569	4.824975	-0.204793
6	-0.901473	3.604620	0.241231
6	-2.718863	5.481796	-3.123425
9	-2.300683	6.741846	-3.317210
6	0.729107	5.487012	0.478185
9	0.438633	6.742716	0.849658
6	-3.182540	0.764703	-0.299328
16	-4.202467	0.814419	-1.647361
7	-3.087428	-0.331300	0.489806
6	-3.840364	-1.549690	0.300950
6	-2.951511	-2.753366	0.670598
6	-3.566568	-4.106459	0.246805
6	-2.648906	-4.792373	-0.776606
6	-1.307115	-5.095329	-0.094154
6	-0.741966	-3.789870	0.499739
7	-1.589492	-2.643754	0.039316
6	-1.643172	-2.603202	-1.453244
6	-2.375539	-3.864238	-1.977244
6	-3.584398	-3.493768	-2.804501
6	-4.749778	-4.135224	-2.838761
6	-5.090049	-1.596013	1.177398
6	-6.378142	-1.958408	0.674717
6	-7.443444	-2.041887	1.620283
7	-7.292488	-1.772135	2.947715
6	-6.102293	-1.413063	3.361205
6	-4.971619	-1.316160	2.515761
6	-8.729557	-2.425510	1.168808
6	-8.967951	-2.711959	-0.150850
6	-7.910316	-2.611960	-1.090957
6	-6.647151	-2.237927	-0.684757
9	-2.450552	4.799906	-4.248708
9	-4.054570	5.518110	-3.006269
9	1.802488	5.565045	-0.326177
9	1.122734	4.829622	1.586269
1	-2.746999	-2.715048	1.743484
1	-3.688663	-4.752766	1.120423
1	-4.559406	-3.942722	-0.177635

1	0.272044	-3.563854	0.171291
1	-0.767027	-3.763351	1.590759
1	-0.604998	-5.516605	-0.819301
1	-1.446764	-5.835908	0.697370
1	-3.106381	-5.722991	-1.122618
1	-1.679685	-4.390201	-2.644282
1	-0.603321	-2.533162	-1.776990
1	-2.140601	-1.671086	-1.733997
1	-3.451265	-2.619501	-3.443120
1	-5.555311	-3.794638	-3.481521
1	-4.957336	-5.010504	-2.228053
1	-4.122165	-1.608980	-0.752134
1	-4.012493	-1.020488	2.934960
1	-5.880971	-2.147719	-1.445293
1	-5.997788	-1.190992	4.421580
1	-9.521906	-2.485130	1.907882
1	-9.962652	-3.003553	-0.465964
1	-2.394566	-0.347826	1.252501
1	-1.758382	1.482006	0.937295
1	-3.416531	3.165222	-2.006454
1	-0.451072	3.116470	1.101700
1	-0.632635	6.428088	-1.646598
8	-8.062621	-2.868600	-2.415387
6	-9.357375	-3.184360	-2.890265
1	-9.259117	-3.310704	-3.968750
1	-9.731741	-4.118044	-2.454117
1	-10.068734	-2.375529	-2.687932
1	-1.134144	-1.762300	0.344385
6	-0.362318	-0.030712	2.556840
8	-0.629164	1.150772	2.241312
8	-1.060144	-1.053484	2.324433

si-re_7-path-A

Number of imaginary frequencies : 1
 The smallest frequency is : -320.0780

Electronic energy= -3905.2766295
 Zero-point correction= 1.052419
 Thermal correction to Energy= 1.118706
 Thermal correction to Enthalpy= 1.119650
 Thermal correction to Gibbs Free Energy= 0.942508
 Sum of electronic and zero-point Energies= -3904.224210
 Sum of electronic and thermal Energies= -3904.157923
 Sum of electronic and thermal Enthalpies= -3904.156979
 Sum of electronic and thermal Free Energies= -3904.334122

 Cartesian Coordinates

6	1.007931	-1.217517	4.330217
6	1.227215	0.253056	4.720791
6	2.187673	0.802039	3.644983
7	2.249197	-0.257091	2.619551
6	1.127577	-1.186349	2.796198
6	3.385450	-0.557829	2.001148
6	3.569099	-1.477050	0.979756
8	-0.499624	-0.207215	-0.694494
8	0.945248	-1.821129	-0.895845
1	1.366656	-2.155285	2.358128
1	0.042639	-1.610615	4.655838
1	1.800796	-1.852242	4.738102
1	0.282817	0.796620	4.678059
1	1.643401	0.356211	5.724378
1	1.804122	1.722294	3.200471
1	3.197679	0.979008	4.025408
1	4.226617	0.084275	2.268692
1	2.754150	-2.153253	0.727832

6	4.977536	-1.926808	0.662565
6	5.054383	-2.874380	-0.532310
1	5.422403	-2.436561	1.527502
1	5.601063	-1.042555	0.478993
1	4.554811	-3.821288	-0.286569
1	4.489521	-2.479822	-1.388263
6	6.437901	-3.177402	-1.016359
6	7.573056	-2.633251	-0.566216
1	6.524091	-3.901114	-1.826429
1	7.573169	-1.911781	0.243607
6	8.875443	-3.030318	-1.167284
8	8.962024	-3.987826	-1.918217
6	10.097174	-2.229079	-0.827486
6	10.033111	-0.950392	-0.265565
6	11.345078	-2.788254	-1.121614
6	11.203356	-0.245323	0.002374
1	9.075040	-0.484832	-0.057183
6	12.511754	-2.089308	-0.842493
1	11.375760	-3.776249	-1.569273
6	12.441770	-0.815492	-0.278948
1	11.146310	0.750664	0.429746
1	13.476894	-2.533770	-1.063945
1	13.352986	-0.266781	-0.061617
6	3.014418	-0.119407	-0.604560
1	3.157699	-0.974905	-1.257001
1	1.350516	1.268168	-0.167247
6	4.094814	0.887347	-0.617370
6	5.247053	0.653293	-1.377066
6	3.999995	2.076518	0.117255
6	6.280038	1.586187	-1.406856
1	5.329904	-0.266541	-1.951480
6	5.025949	3.012343	0.079376
1	3.117812	2.270175	0.721384
6	6.170251	2.768984	-0.680420
1	7.165387	1.389464	-2.003676
1	4.926707	3.936771	0.639573
1	6.970388	3.501918	-0.709323
7	0.682677	-0.611673	-0.688193
6	1.689248	0.281578	-0.439728
7	-2.263352	1.739362	0.493847
6	-1.808267	2.997374	0.107639
6	-2.524145	3.947742	-0.625005
6	-1.932772	5.179623	-0.904539
6	-0.657109	5.507963	-0.472800
6	0.037917	4.556531	0.271985
6	-0.517408	3.323793	0.563538
6	-2.719751	6.159835	-1.727638
9	-2.188633	7.391737	-1.690295
6	1.438103	4.865200	0.711948
9	1.568978	6.135205	1.120233
6	-3.236080	0.933601	-0.005715
16	-4.369697	1.335991	-1.194493
7	-3.187551	-0.294764	0.561025
6	-4.095323	-1.377950	0.261315
6	-3.319253	-2.708663	0.291723
6	-4.135506	-3.887276	-0.284163
6	-3.426641	-4.443686	-1.528383
6	-2.066423	-5.005970	-1.093177
6	-1.284090	-3.903542	-0.353006
7	-2.030078	-2.609764	-0.480950
6	-2.241963	-2.271502	-1.920421
6	-3.175362	-3.327975	-2.563532
6	-4.415225	-2.690072	-3.144995
6	-5.641609	-3.206489	-3.151085
6	-5.236763	-1.467276	1.271977
6	-6.608221	-1.577856	0.884946
6	-7.569223	-1.717217	1.930361
7	-7.242387	-1.729028	3.253568
6	-5.976342	-1.601226	3.565937
6	-4.938991	-1.472392	2.611601

6	-8.936507	-1.852876	1.587939
6	-9.349353	-1.853760	0.280402
6	-8.392080	-1.704749	-0.756204
6	-7.054138	-1.562476	-0.456193
9	-2.772791	5.794589	-3.018301
9	-3.988754	6.258757	-1.304430
9	2.326663	4.688471	-0.281819
9	1.842336	4.075557	1.726609
1	-2.995868	-2.896393	1.318614
1	-4.234768	-4.677145	0.465498
1	-5.143961	-3.548980	-0.532997
1	-0.294697	-3.721228	-0.768782
1	-1.181189	-4.087235	0.718142
1	-1.504381	-5.346853	-1.967420
1	-2.209232	-5.867934	-0.436361
1	-4.029557	-5.237172	-1.977245
1	-2.625776	-3.779647	-3.399929
1	-1.243026	-2.243984	-2.359201
1	-2.649524	-1.257952	-1.960029
1	-4.253949	-1.721412	-3.619595
1	-6.468347	-2.675896	-3.612470
1	-5.876476	-4.165110	-2.694582
1	-4.497878	-1.207043	-0.738850
1	-3.909774	-1.376471	2.950107
1	-6.366171	-1.422206	-1.281109
1	-5.730270	-1.604421	4.626070
1	-9.647953	-1.956717	2.400611
1	-10.402851	-1.959862	0.050558
1	-2.424554	-0.519039	1.214946
1	-1.594113	1.259199	1.123068
1	-3.527408	3.732648	-0.966471
1	0.026095	2.594041	1.158457
1	-0.221191	6.475432	-0.693506
8	-8.717185	-1.692035	-2.074194
6	-10.085847	-1.773094	-2.423036
1	-10.123474	-1.713024	-3.510901
1	-10.529084	-2.722946	-2.101202
1	-10.658646	-0.940567	-1.998517
1	-1.440889	-1.859722	-0.072163
6	-0.197615	-0.666448	2.213473
8	-0.350064	0.573523	2.150476
8	-1.049489	-1.551375	1.933505

si-re_8-path-A

Number of imaginary frequencies : 1
 The smallest frequency is : -305.3023

Electronic energy= -3905.2714729
 Zero-point correction= 1.050344
 Thermal correction to Energy= 1.116398
 Thermal correction to Enthalpy= 1.117342
 Thermal correction to Gibbs Free Energy= 0.944360
 Sum of electronic and zero-point Energies= -3904.221129
 Sum of electronic and thermal Energies= -3904.155075
 Sum of electronic and thermal Enthalpies= -3904.154131
 Sum of electronic and thermal Free Energies= -3904.327113

 Cartesian Coordinates

6	4.067161	0.115809	-3.110411
6	2.557600	0.319493	-3.257475
6	2.032366	-0.200697	-1.919227
7	2.889405	-1.360362	-1.662612
6	4.201187	-1.182933	-2.301747
6	2.623440	-2.354507	-0.816235
6	3.577382	-3.216852	-0.287037

8	0.717562	-1.599495	2.743438
8	1.634979	-0.593296	1.043101
1	4.408962	-2.057791	-2.928085
1	4.497675	0.945388	-2.543321
1	4.585990	0.053338	-4.068137
1	2.270718	1.358011	-3.422308
1	2.152584	-0.292094	-4.070649
1	2.234070	0.552593	-1.143947
1	1.589954	-2.412923	-0.499837
1	4.581646	-3.184370	-0.703070
6	3.209870	-4.520480	0.377710
6	1.742235	-4.703979	0.787585
1	3.845810	-4.654866	1.262400
1	3.480360	-5.344958	-0.295764
1	1.699566	-5.593918	1.429892
1	1.377120	-3.869731	1.397799
6	0.817772	-4.938489	-0.367855
6	-0.393126	-4.391560	-0.499703
1	1.146828	-5.641284	-1.134573
1	-0.756523	-3.682792	0.238593
6	-1.259070	-4.773547	-1.645724
8	-0.785492	-5.264847	-2.656914
6	-2.749242	-4.617067	-1.519240
6	-3.374496	-4.146354	-0.359824
6	-3.537628	-5.033898	-2.598702
6	-4.765519	-4.103631	-0.280788
1	-2.791705	-3.831110	0.499004
6	-4.923590	-4.989121	-2.519894
1	-3.036928	-5.403697	-3.487356
6	-5.540979	-4.524932	-1.358007
1	-5.240179	-3.748875	0.629046
1	-5.525157	-5.317272	-3.361668
1	-6.624148	-4.494565	-1.291485
6	3.979792	-1.859437	1.430929
1	3.984958	-0.996507	0.768384
1	2.877186	-2.617912	3.185092
6	5.315135	-2.371272	1.802968
6	6.442825	-1.825095	1.174942
6	5.501076	-3.370875	2.767989
6	7.720091	-2.262615	1.500474
1	6.310833	-1.034729	0.441406
6	6.780640	-3.813182	3.087878
1	4.648445	-3.807314	3.278491
6	7.892436	-3.262841	2.455931
1	8.582241	-1.820288	1.011819
1	6.908565	-4.587135	3.837725
1	8.889612	-3.607567	2.710167
7	1.716549	-1.366228	2.046766
6	2.910177	-1.969040	2.323970
7	0.794020	2.012528	0.578723
6	1.899258	2.796820	0.253912
6	1.885341	4.041550	-0.386913
6	3.094261	4.654582	-0.704828
6	4.326578	4.074644	-0.426365
6	4.322856	2.841713	0.215467
6	3.138359	2.215598	0.566298
6	3.057369	6.019357	-1.335596
9	4.150692	6.250131	-2.079657
6	5.597630	2.091937	0.459506
9	5.737898	1.082906	-0.438215
6	-0.545478	2.140992	0.338511
16	-1.324602	3.576541	-0.069402
7	-1.177685	0.953699	0.484609
6	-2.616522	0.769770	0.462346
6	-3.045918	-0.185799	-0.669808
6	-4.578452	-0.408470	-0.676560
6	-5.078725	-0.383539	-2.126771
6	-4.215700	-1.351748	-2.944330
6	-2.776149	-0.795384	-2.985553
7	-2.608026	0.304994	-2.001890

6	-3.423662	1.456582	-2.442150
6	-4.900156	1.029340	-2.706960
6	-5.841750	2.084196	-2.187798
6	-6.867015	1.912735	-1.356455
6	-3.127377	0.268007	1.806665
6	-4.268742	0.854939	2.443552
6	-4.690332	0.282055	3.680008
7	-4.057102	-0.767853	4.276786
6	-3.004978	-1.261163	3.672489
6	-2.505791	-0.780784	2.436523
6	-5.822832	0.822718	4.336053
6	-6.519767	1.878677	3.808414
6	-6.097197	2.450641	2.581190
6	-4.994387	1.951406	1.920935
9	1.990056	6.176318	-2.128709
9	3.004054	6.990433	-0.410786
9	5.622825	1.513283	1.666760
9	6.682118	2.862259	0.346712
1	-2.517864	-1.138126	-0.526341
1	-4.818438	-1.365657	-0.204700
1	-5.080805	0.373684	-0.102933
1	-2.531118	-0.376116	-3.966809
1	-2.033121	-1.562088	-2.751454
1	-4.612989	-1.468007	-3.957496
1	-4.228760	-2.337368	-2.470278
1	-6.130255	-0.683766	-2.170126
1	-5.047157	0.965279	-3.794673
1	-2.956234	1.866948	-3.342413
1	-3.363928	2.233094	-1.675321
1	-5.622718	3.094425	-2.537532
1	-7.470806	2.755837	-1.036472
1	-7.144922	0.938741	-0.962517
1	-3.032811	1.756981	0.268087
1	-1.608955	-1.241881	2.031118
1	-4.715742	2.434630	0.990569
1	-2.497099	-2.088295	4.164869
1	-6.119580	0.367512	5.275486
1	-7.383172	2.269455	4.333503
1	-0.598881	0.131295	0.652752
1	1.059182	1.111433	0.982949
1	0.947908	4.516750	-0.639658
1	3.160030	1.249481	1.066196
1	5.252959	4.564643	-0.701585
8	-6.728686	3.495247	1.989723
6	-7.850477	4.055413	2.644551
1	-8.191598	4.873278	2.009392
1	-8.660447	3.324697	2.754083
1	-7.583935	4.455240	3.629834
1	-1.141633	0.562474	-2.119304
1	4.992946	-1.110936	-1.547110
6	0.527071	-0.407166	-1.871733
8	-0.029082	-1.400827	-1.428266
8	-0.089646	0.656161	-2.313778

re-si_1-path-A

Number of imaginary frequencies : 1
The smallest frequency is : -269.7898

Electronic energy=	-3905.286145
Zero-point correction=	1.052017
Thermal correction to Energy=	1.117901
Thermal correction to Enthalpy=	1.118845
Thermal correction to Gibbs Free Energy=	0.945789
Sum of electronic and zero-point Energies=	-3904.234128
Sum of electronic and thermal Energies=	-3904.168244
Sum of electronic and thermal Enthalpies=	-3904.167300

Sum of electronic and thermal Free Energies= -3904.340356

Cartesian Coordinates			
6	-1.334620	2.238637	4.582104
6	-2.822845	1.895878	4.424705
6	-3.218719	2.569034	3.105063
7	-1.955241	2.695667	2.376640
6	-0.808395	2.198055	3.142232
6	-1.856702	3.052128	1.105055
6	-2.907948	3.229058	0.211685
8	-0.128255	0.382942	-2.172178
6	-0.457093	0.756642	2.703180
8	0.768151	0.494262	2.596656
8	-1.418723	-0.027223	2.513798
8	-0.345224	1.008849	-0.098797
1	0.056807	2.847188	2.982966
1	-0.802418	1.540884	5.232068
1	-1.211602	3.248859	4.985023
1	-2.940166	0.815375	4.330682
1	-3.428345	2.250332	5.260824
1	-3.933748	1.978495	2.525890
1	-3.645150	3.569011	3.254914
1	-0.837969	3.110640	0.730575
1	-3.915376	3.316122	0.609889
6	-2.634980	3.846134	-1.133912
6	-2.284212	5.354293	-1.113158
1	-3.507862	3.697066	-1.779721
1	-1.797260	3.317462	-1.608992
1	-2.149436	5.694558	-2.145391
1	-3.114748	5.918873	-0.676490
6	-1.030830	5.590465	-0.327671
6	0.201904	5.618717	-0.848093
1	-1.113049	5.671886	0.755645
1	0.348927	5.561494	-1.922592
6	1.382552	5.724648	0.049693
8	1.252533	5.847604	1.257647
6	2.760834	5.668372	-0.544811
6	3.020757	5.160242	-1.822100
6	3.826596	6.109587	0.247507
6	4.329219	5.098669	-2.297684
1	2.213705	4.794018	-2.449019
6	5.129078	6.063156	-0.234310
1	3.608963	6.489015	1.240466
6	5.382752	5.554361	-1.507866
1	4.524067	4.699491	-3.288311
1	5.948356	6.418725	0.382349
1	6.399746	5.513505	-1.885143
6	-3.026333	1.047848	-0.280261
1	-2.619189	0.789775	0.698178
1	-2.546110	0.628158	-2.390734
6	-4.486536	0.881378	-0.443319
6	-5.239342	0.401340	0.635341
6	-5.133949	1.127120	-1.661736
6	-6.604432	0.170450	0.503308
1	-4.735661	0.164799	1.569635
6	-6.498422	0.894426	-1.794159
1	-4.568507	1.495469	-2.512442
6	-7.237327	0.417236	-0.713027
1	-7.167239	-0.223353	1.343219
1	-6.985435	1.081629	-2.745950
1	-8.301568	0.232598	-0.820334
7	-0.853661	0.726046	-1.222300
6	-2.206867	0.815741	-1.383495
7	-1.109654	-1.909388	0.473402
6	-2.335541	-2.285318	-0.091203
6	-2.569869	-2.253787	-1.469966
6	-3.855241	-2.471416	-1.947814
6	-4.922970	-2.735487	-1.093147
6	-4.671116	-2.776965	0.270876

6	-3.394432	-2.549503	0.777214
6	-4.095617	-2.285485	-3.416947
9	-3.207625	-2.953237	-4.164342
6	-5.779457	-3.057599	1.241667
9	-5.687969	-4.287803	1.770768
6	0.145154	-2.218723	0.050083
16	0.513241	-3.312546	-1.185654
7	1.084495	-1.555817	0.757821
6	2.507993	-1.643062	0.528388
6	3.088827	-0.231509	0.706045
6	4.596837	-0.106013	0.434387
6	4.860977	1.245450	-0.249259
6	4.106331	2.352329	0.505973
6	2.591491	2.127873	0.334433
7	2.376873	0.743865	-0.196508
6	2.860565	0.650517	-1.608228
6	4.308875	1.194664	-1.683641
6	5.103088	0.378813	-2.671444
6	6.279847	-0.203120	-2.458944
6	3.209989	-2.579208	1.502612
6	4.251511	-3.469810	1.093259
6	4.872217	-4.249296	2.114154
7	4.516698	-4.185807	3.428996
6	3.551699	-3.362732	3.757373
6	2.871095	-2.536514	2.831168
6	5.915383	-5.137577	1.757682
6	6.339350	-5.258998	0.459437
6	5.719282	-4.484981	-0.554977
6	4.696080	-3.615542	-0.241564
9	-5.319980	-2.683332	-3.789807
9	-3.985231	-0.985956	-3.767989
9	-6.990331	-2.962913	0.674394
9	-5.757795	-2.198386	2.280322
1	2.841735	0.104945	1.717171
1	5.139402	-0.183739	1.380074
1	4.938448	-0.923501	-0.207104
1	2.144897	2.812519	-0.392003
1	2.032414	2.181241	1.271597
1	4.377740	3.336357	0.112958
1	4.375899	2.332385	1.566114
1	5.930660	1.468150	-0.263213
1	4.264248	2.226466	-2.060287
1	2.150698	1.205827	-2.222026
1	2.795562	-0.399527	-1.904367
1	4.631315	0.263446	-3.647970
1	6.765297	-0.777516	-3.241349
1	6.804624	-0.135965	-1.509695
1	2.652339	-1.996482	-0.494043
1	2.084254	-1.870682	3.178301
1	4.243655	-3.065266	-1.059324
1	3.276555	-3.325383	4.809679
1	6.369623	-5.719698	2.552921
1	7.140935	-5.947006	0.218516
1	0.797550	-0.898544	1.506650
1	-1.187988	-1.291152	1.305065
1	-1.756564	-2.009332	-2.145509
1	-3.215024	-2.556285	1.848750
1	-5.923557	-2.880390	-1.481792
8	6.080462	-4.541302	-1.861398
6	7.076977	-5.471774	-2.237298
1	7.186386	-5.375267	-3.317802
1	8.038601	-5.249454	-1.759705
1	6.780028	-6.499331	-1.997996
1	1.340169	0.580415	-0.180179

re-si_2-path-A

Number of imaginary frequencies : 1
The smallest frequency is : -280.8817

Electronic energy= -3905.2890794
Zero-point correction= 1.053698
Thermal correction to Energy= 1.119252
Thermal correction to Enthalpy= 1.120196
Thermal correction to Gibbs Free Energy= 0.949174
Sum of electronic and zero-point Energies= -3904.235381
Sum of electronic and thermal Energies= -3904.169828
Sum of electronic and thermal Enthalpies= -3904.168883
Sum of electronic and thermal Free Energies= -3904.339905

.....
Cartesian Coordinates

.....
6 -0.356716 -4.384978 4.096695
6 -1.635093 -4.848484 3.384310
6 -2.567435 -3.631879 3.457543
7 -1.667804 -2.500030 3.683495
6 -0.260678 -2.903442 3.712649
6 -2.045641 -1.225294 3.647956
6 -3.291804 -0.760801 3.257656
8 -0.416422 1.717949 0.387409
6 0.389390 -2.728221 2.320549
8 1.577065 -2.321512 2.317005
8 -0.310101 -3.039953 1.324117
8 -0.233792 -0.047034 1.642474
1 0.291330 -2.302871 4.439771
1 0.529482 -4.945442 3.791836
1 -0.465492 -4.472758 5.182428
1 -1.410605 -5.071243 2.340384
1 -2.079549 -5.730543 3.848921
1 -3.137383 -3.488379 2.535725
1 -3.278921 -3.692447 4.290867
1 -1.246682 -0.522162 3.867055
1 -4.095877 -1.485848 3.162750
6 -3.721214 0.672299 3.434706
6 -2.574620 1.668561 3.697778
1 -4.456131 0.746828 4.246011
1 -4.255140 0.983015 2.526472
1 -2.309190 1.644165 4.762273
1 -1.681768 1.375808 3.136721
6 -2.972997 3.050740 3.281311
6 -2.458598 3.664903 2.211671
1 -3.772219 3.546836 3.832468
1 -1.673797 3.183945 1.632146
6 -2.976866 4.984990 1.763789
8 -3.586117 5.719283 2.524821
6 -2.765450 5.376284 0.332147
6 -2.296905 4.475626 -0.630697
6 -3.105771 6.678641 -0.050855
6 -2.178637 4.873482 -1.959980
1 -2.019065 3.460869 -0.361780
6 -2.969402 7.078617 -1.372925
1 -3.479458 7.359731 0.706922
6 -2.509246 6.173768 -2.330602
1 -1.836692 4.160827 -2.703391
1 -3.228492 8.092242 -1.662407
1 -2.412644 6.483161 -3.366849
6 -2.767170 -0.824366 1.047039
1 -2.056340 -1.633399 1.218836
1 -2.764124 1.167204 0.108878
6 -4.083049 -1.202697 0.493275
6 -4.346167 -2.554260 0.231593
6 -5.046428 -0.246592 0.138741
6 -5.539405 -2.942758 -0.366261
1 -3.582835 -3.295989 0.455792
6 -6.239902 -0.636996 -0.458805
1 -4.863930 0.808894 0.315579
6 -6.489760 -1.984165 -0.712150

1	-5.716672	-3.990470	-0.584632
1	-6.972952	0.114664	-0.733828
1	-7.418484	-2.286158	-1.186065
7	-0.931765	0.696013	0.907444
6	-2.244315	0.414282	0.681633
7	0.110352	-1.577193	-1.008146
6	-1.034845	-1.481896	-1.815353
6	-1.562880	-0.251165	-2.216351
6	-2.785120	-0.213628	-2.873263
6	-3.502328	-1.373679	-3.157087
6	-2.958108	-2.588366	-2.764343
6	-1.738539	-2.652058	-2.093907
6	-3.361150	1.136549	-3.181438
9	-2.500017	1.903469	-3.868402
6	-3.670865	-3.873054	-3.066629
9	-3.107746	-4.528177	-4.094306
6	1.282223	-0.905886	-1.147395
16	1.665350	0.090200	-2.465193
7	2.118139	-1.131357	-0.111130
6	3.421240	-0.528018	0.051231
6	3.429960	0.230774	1.390771
6	4.741977	0.975219	1.700358
6	4.416715	2.383722	2.218200
6	3.404538	2.263486	3.368243
6	2.078595	1.708411	2.811538
7	2.309814	1.241213	1.408452
6	2.581374	2.412756	0.518321
6	3.776482	3.217345	1.094141
6	4.695637	3.630332	-0.028431
6	6.013898	3.463083	-0.086668
6	4.551949	-1.547317	0.042201
6	5.780478	-1.303174	-0.652719
6	6.788447	-2.308105	-0.553555
7	6.629942	-3.466403	0.147383
6	5.486908	-3.651229	0.759075
6	4.419336	-2.720813	0.741512
6	8.025800	-2.106608	-1.211653
6	8.275052	-0.969289	-1.935080
6	7.271765	0.028486	-2.036103
6	6.052757	-0.141086	-1.413394
9	-4.493304	1.063641	-3.890798
9	-3.648608	1.817450	-2.050401
9	-4.958873	-3.679751	-3.384397
9	-3.638512	-4.716049	-2.017250
1	3.166165	-0.485238	2.177882
1	5.313276	0.411336	2.442303
1	5.355857	1.042369	0.799429
1	1.287273	2.459624	2.753752
1	1.702028	0.846973	3.366204
1	3.232873	3.237803	3.832594
1	3.800614	1.594830	4.137627
1	5.325807	2.874720	2.575017
1	3.376228	4.135186	1.545850
1	1.654639	2.985415	0.475381
1	2.773375	2.023567	-0.484145
1	4.191766	4.108600	-0.868859
1	6.577625	3.793915	-0.952670
1	6.582314	2.992974	0.711306
1	3.555115	0.167932	-0.777104
1	3.503411	-2.943712	1.283957
1	5.319773	0.648740	-1.538548
1	5.372989	-4.582001	1.311742
1	8.772812	-2.888028	-1.118397
1	9.232776	-0.842814	-2.425493
1	1.798055	-1.701485	0.697037
1	0.021472	-2.211734	-0.187674
1	-1.038743	0.664997	-1.961403
1	-1.335294	-3.606936	-1.769061
1	-4.464336	-1.326818	-3.653315
8	7.437713	1.184125	-2.726956

6	8.639431	1.360849	-3.452460
1	8.546122	2.322684	-3.957259
1	9.512140	1.388615	-2.789430
1	8.776109	0.574062	-4.203051
1	1.430755	0.779507	1.111894

re-si_3-path-A

Number of imaginary frequencies : 1

The smallest frequency is : -288.5862

Electronic energy= -3905.2803283
 Zero-point correction= 1.052210
 Thermal correction to Energy= 1.118291
 Thermal correction to Enthalpy= 1.119235
 Thermal correction to Gibbs Free Energy= 0.944289
 Sum of electronic and zero-point Energies= -3904.228118
 Sum of electronic and thermal Energies= -3904.162037
 Sum of electronic and thermal Enthalpies= -3904.161093
 Sum of electronic and thermal Free Energies= -3904.336039

Cartesian Coordinates

6	0.396558	-3.065352	4.195686
6	1.375843	-1.931723	4.538604
6	2.265259	-1.789197	3.289748
7	1.556048	-2.534267	2.250046
6	0.214495	-2.918510	2.681050
6	1.973866	-2.683000	1.002036
6	3.076162	-2.083086	0.403085
8	-0.334934	-1.878345	-2.563986
6	-0.791997	-1.797083	2.348729
8	-1.962134	-2.160702	2.083404
8	-0.355384	-0.618984	2.409974
8	-0.437692	-1.716361	-0.395987
1	-0.095663	-3.840116	2.183669
1	-0.551647	-2.987170	4.731519
1	0.840253	-4.041668	4.413743
1	0.825971	-1.003141	4.695814
1	1.963181	-2.146616	5.432948
1	2.364095	-0.739828	2.997390
1	3.265777	-2.218007	3.416319
1	1.324264	-3.304327	0.387098
1	3.774741	-1.542045	1.037085
6	3.616467	-2.727412	-0.852140
6	4.563866	-1.871220	-1.711499
1	2.769284	-3.037385	-1.479906
1	4.153207	-3.647052	-0.582189
1	4.940492	-2.493019	-2.530296
1	3.999163	-1.049577	-2.162500
6	5.712659	-1.296174	-0.944799
6	6.990747	-1.649324	-1.117679
1	5.496581	-0.533618	-0.194927
1	7.258408	-2.384204	-1.871023
6	8.065908	-1.006442	-0.315841
8	7.820181	-0.105273	0.469339
6	9.482139	-1.468972	-0.500860
6	9.815184	-2.678344	-1.117544
6	10.502053	-0.647465	-0.009141
6	11.149195	-3.055810	-1.244361
1	9.041478	-3.344865	-1.483382
6	11.832738	-1.018463	-0.146900
1	10.224786	0.282021	0.477174
6	12.158329	-2.224871	-0.766315
1	11.399488	-3.999820	-1.717823
1	12.618026	-0.370146	0.228701
1	13.198308	-2.517585	-0.873250

6	1.884258	-0.298231	-0.319033
1	1.272863	-0.336600	0.582378
1	1.688476	-0.581996	-2.497561
6	2.956226	0.729392	-0.335315
6	3.547517	1.132945	0.868129
6	3.376500	1.351912	-1.519117
6	4.549332	2.095986	0.891189
1	3.209067	0.689526	1.799804
6	4.379176	2.315359	-1.500708
1	2.900392	1.110620	-2.463140
6	4.978142	2.682012	-0.297813
1	4.988797	2.392557	1.837760
1	4.682094	2.788724	-2.429163
1	5.765895	3.428552	-0.283942
7	0.135089	-1.450868	-1.490383
6	1.277295	-0.701533	-1.507465
7	-1.239126	1.155743	0.552390
6	-0.305852	2.173989	0.332147
6	0.009180	2.681245	-0.932081
6	1.027696	3.619361	-1.054120
6	1.754811	4.065151	0.044476
6	1.443468	3.536431	1.289811
6	0.429964	2.598275	1.442500
6	1.366956	4.117057	-2.429563
9	0.421108	4.931515	-2.920207
6	2.209502	3.956532	2.510123
9	1.450618	4.669417	3.357693
6	-2.453340	0.954171	-0.013855
16	-3.177266	1.959029	-1.173788
7	-3.035086	-0.166911	0.465653
6	-4.335875	-0.681522	0.102370
6	-4.163094	-2.172235	-0.250785
6	-5.435614	-2.843870	-0.807178
6	-5.172118	-3.342598	-2.235662
6	-4.054148	-4.396472	-2.196128
6	-2.812695	-3.791547	-1.510037
7	-3.058688	-2.336112	-1.265366
6	-3.360903	-1.650718	-2.564788
6	-4.704143	-2.177222	-3.128996
6	-5.703994	-1.060581	-3.317341
6	-7.021091	-1.141560	-3.147394
6	-5.343799	-0.555949	1.241615
6	-6.650577	-0.003425	1.052756
6	-7.518926	0.010345	2.185118
7	-7.158554	-0.455335	3.414525
6	-5.946866	-0.934373	3.547045
6	-5.005220	-1.010865	2.492156
6	-8.826513	0.533174	2.039671
6	-9.271960	1.022295	0.838566
6	-8.404423	1.015245	-0.283021
6	-7.122773	0.518779	-0.173478
9	2.525048	4.794464	-2.452252
9	1.486529	3.102541	-3.306758
9	3.278824	4.705953	2.208150
9	2.653416	2.893778	3.208527
1	-3.785369	-2.681679	0.640970
1	-5.723880	-3.683233	-0.168561
1	-6.262132	-2.129305	-0.799344
1	-1.906978	-3.841040	-2.116623
1	-2.605130	-4.237314	-0.534784
1	-3.807189	-4.716030	-3.212557
1	-4.389651	-5.279256	-1.646057
1	-6.080897	-3.787555	-2.648995
1	-4.493305	-2.591439	-4.123792
1	-2.514790	-1.868212	-3.213894
1	-3.368611	-0.573658	-2.376575
1	-5.277173	-0.112390	-3.647458
1	-7.659678	-0.280426	-3.318919
1	-7.513716	-2.053390	-2.818178
1	-4.683047	-0.120505	-0.766453

1	-4.018000	-1.426301	2.683985
1	-6.497592	0.555478	-1.056842
1	-5.668911	-1.296215	4.535285
1	-9.464429	0.532866	2.917433
1	-10.277949	1.416460	0.757578
1	-2.536955	-0.736373	1.172119
1	-0.973170	0.495032	1.316947
1	-0.521751	2.323046	-1.805509
1	0.209988	2.174815	2.418972
1	2.558096	4.781798	-0.072179
8	-8.764445	1.484129	-1.506171
6	-10.042514	2.076152	-1.641170
1	-10.106183	2.422557	-2.672901
1	-10.844437	1.351685	-1.456608
1	-10.161227	2.932667	-0.967779
1	-2.168206	-1.954174	-0.874882

re-si_4-path-A

Number of imaginary frequencies : 1
 The smallest frequency is : -387.2431

Electronic energy= -3905.2739058
 Zero-point correction= 1.052675
 Thermal correction to Energy= 1.118245
 Thermal correction to Enthalpy= 1.119190
 Thermal correction to Gibbs Free Energy= 0.946808
 Sum of electronic and zero-point Energies= -3904.221231
 Sum of electronic and thermal Energies= -3904.155660
 Sum of electronic and thermal Enthalpies= -3904.154716
 Sum of electronic and thermal Free Energies= -3904.327097

 Cartesian Coordinates

6	1.355704	0.407970	5.017370
6	1.981160	1.619828	4.324875
6	3.273395	1.053703	3.737197
7	2.936115	-0.347438	3.459645
6	1.622945	-0.710869	4.017526
6	3.675605	-1.162605	2.734039
6	4.902406	-0.855852	2.134516
8	0.896712	-0.304099	-0.517213
6	0.567183	-0.818524	2.877359
8	0.820447	-1.673046	2.001474
8	-0.442924	-0.079148	2.962778
8	1.805657	0.987471	0.980255
1	1.698099	-1.700050	4.480137
1	0.286894	0.524472	5.191254
1	1.862971	0.198700	5.965284
1	1.324767	1.943418	3.512184
1	2.167064	2.461868	4.993524
1	3.565682	1.555437	2.813203
1	4.107832	1.089431	4.449507
1	3.215609	-2.134238	2.569018
1	5.385338	0.051627	2.492114
6	5.879698	-1.977014	1.835202
6	5.282687	-3.346990	1.480992
1	6.530902	-2.112196	2.708764
1	6.545906	-1.672688	1.017757
1	6.124101	-4.047983	1.397451
1	4.637813	-3.735137	2.276671
6	4.570298	-3.348760	0.167767
6	3.418469	-3.964706	-0.121511
1	5.074624	-2.826146	-0.644544
1	2.871431	-4.523466	0.633627
6	2.885327	-3.892906	-1.505742
8	3.249237	-3.021109	-2.283459

6	1.892553	-4.919782	-1.963863
6	1.152092	-4.645041	-3.119760
6	1.729308	-6.148027	-1.315833
6	0.261204	-5.586962	-3.622192
1	1.304424	-3.692909	-3.618753
6	0.847676	-7.096819	-1.829927
1	2.312950	-6.385145	-0.431696
6	0.113699	-6.817529	-2.980377
1	-0.308665	-5.368188	-4.519844
1	0.737602	-8.056113	-1.334612
1	-0.573600	-7.557510	-3.378337
6	4.289536	0.182758	0.281169
1	4.114139	1.072645	0.874797
1	3.106318	-1.097154	-1.086037
6	5.597717	0.159728	-0.406076
6	6.648924	0.927260	0.114124
6	5.820190	-0.571514	-1.580840
6	7.892588	0.949140	-0.503617
1	6.480903	1.515025	1.013625
6	7.067776	-0.551948	-2.197469
1	5.013624	-1.146671	-2.027526
6	8.107970	0.202262	-1.660783
1	8.692152	1.553494	-0.087027
1	7.222428	-1.120161	-3.109333
1	9.078130	0.217879	-2.147254
7	1.917880	0.120122	0.065345
6	3.140034	-0.329119	-0.327623
7	-0.685397	2.208336	0.165634
6	-0.292144	3.432492	-0.384838
6	-1.190248	4.453237	-0.716121
6	-0.703384	5.658416	-1.207527
6	0.658342	5.894846	-1.364787
6	1.538688	4.881300	-1.007621
6	1.080971	3.661221	-0.528162
6	-1.668403	6.772242	-1.496693
9	-1.831656	7.574472	-0.429650
6	3.013767	5.077745	-1.202571
9	3.414165	4.701231	-2.427816
6	-1.801043	1.467284	-0.108065
16	-2.918181	1.806527	-1.333104
7	-1.886994	0.384724	0.688071
6	-2.934190	-0.607223	0.589316
6	-2.342283	-2.008088	0.843225
6	-3.312749	-3.137095	0.428867
6	-2.717946	-3.922645	-0.752308
6	-1.441442	-4.624148	-0.273455
6	-0.522504	-3.573807	0.370045
7	-1.057876	-2.203656	0.085062
6	-1.226695	-2.011501	-1.385980
6	-2.318204	-2.982217	-1.907476
6	-3.456606	-2.247373	-2.573691
6	-4.743241	-2.584424	-2.531062
6	-4.058528	-0.365995	1.595938
6	-5.439821	-0.349275	1.224337
6	-6.394074	-0.194539	2.273907
7	-6.050941	-0.036542	3.583576
6	-4.773667	-0.024018	3.875116
6	-3.741229	-0.190985	2.920496
6	-7.773019	-0.203491	1.951943
6	-8.204999	-0.355584	0.659281
6	-7.253397	-0.493153	-0.383455
6	-5.903495	-0.481315	-0.104339
9	-1.238313	7.554427	-2.500309
9	-2.882695	6.318552	-1.831012
9	3.735442	4.362827	-0.323806
9	3.369036	6.364357	-1.059062
1	-2.043029	-2.075350	1.894051
1	-3.485186	-3.817677	1.267573
1	-4.279622	-2.706063	0.157372
1	0.493849	-3.587687	-0.026562

1	-0.455096	-3.650641	1.454859
1	-0.939406	-5.102625	-1.118629
1	-1.681219	-5.403735	0.454847
1	-3.439146	-4.662422	-1.109019
1	-1.844602	-3.607541	-2.677317
1	-0.244780	-2.197885	-1.824679
1	-1.468101	-0.959753	-1.559104
1	-3.163213	-1.376410	-3.160584
1	-5.491681	-2.003380	-3.060294
1	-5.106386	-3.437661	-1.963100
1	-3.331225	-0.560529	-0.426227
1	-2.702437	-0.175966	3.244222
1	-5.217014	-0.552404	-0.938748
1	-4.512951	0.114778	4.922863
1	-8.477857	-0.084350	2.768331
1	-9.267100	-0.359113	0.444945
1	-1.251138	0.292950	1.507858
1	0.075688	1.690120	0.621415
1	-2.254522	4.304658	-0.591983
1	1.782792	2.883657	-0.243291
1	1.020188	6.842929	-1.746332
8	-7.595430	-0.640980	-1.690063
6	-8.967800	-0.590891	-2.027716
1	-9.015770	-0.696285	-3.111792
1	-9.527970	-1.411323	-1.563646
1	-9.418467	0.366292	-1.740827
1	-0.336886	-1.545768	0.454135

re-si_5-path-A

Number of imaginary frequencies : 1

The smallest frequency is : -363.6339

Electronic energy=	-3905.2673339
Zero-point correction=	1.053524
Thermal correction to Energy=	1.118912
Thermal correction to Enthalpy=	1.119856
Thermal correction to Gibbs Free Energy=	0.948001
Sum of electronic and zero-point Energies=	-3904.213810
Sum of electronic and thermal Energies=	-3904.148422
Sum of electronic and thermal Enthalpies=	-3904.147478
Sum of electronic and thermal Free Energies=	-3904.319333

Cartesian Coordinates

6	1.235105	1.057740	4.798365
6	1.672016	2.324837	4.061694
6	3.045923	1.947565	3.510251
7	2.933933	0.501446	3.277471
6	1.692459	-0.044962	3.851180
6	3.800034	-0.215970	2.593021
6	4.961980	0.258241	1.969580
8	0.795361	0.258984	-0.636789
6	0.680632	-0.377404	2.714743
8	1.093060	-1.182017	1.853388
8	-0.454622	0.153246	2.794569
8	1.586082	1.664354	0.820151
1	1.921348	-0.987842	4.358463
1	0.158752	1.007728	4.955264
1	1.751354	0.970431	5.760299
1	0.986645	2.510660	3.230042
1	1.712843	3.210653	4.697344
1	3.276037	2.460691	2.575841
1	3.850323	2.131035	4.234108
1	3.512362	-1.258821	2.480835
1	5.270442	1.262142	2.253978
6	6.133846	-0.684803	1.751427

6	5.892804	-2.184960	1.984179
1	6.926579	-0.379398	2.444973
1	6.565045	-0.553610	0.750902
1	6.882150	-2.660341	2.018283
1	5.429387	-2.363331	2.960557
6	5.121743	-2.891582	0.910139
6	4.064900	-3.680605	1.143614
1	5.520886	-2.796692	-0.100199
1	3.691677	-3.804868	2.159194
6	3.400413	-4.583074	0.171577
8	2.718061	-5.505594	0.591651
6	3.551193	-4.397952	-1.309272
6	3.639580	-3.131262	-1.891351
6	3.489277	-5.529239	-2.127998
6	3.676160	-2.991979	-3.275975
1	3.644877	-2.259168	-1.246595
6	3.549573	-5.392925	-3.510221
1	3.391113	-6.505821	-1.664653
6	3.640862	-4.125405	-4.085604
1	3.727138	-2.002625	-3.721531
1	3.516990	-6.274247	-4.142584
1	3.676654	-4.021151	-5.165358
6	4.154703	1.070610	0.077849
1	3.933003	1.989510	0.609462
1	3.034246	-0.313370	-1.230349
6	5.435439	1.071598	-0.656152
6	6.385846	2.059397	-0.369240
6	5.750272	0.102210	-1.617271
6	7.610983	2.082281	-1.025380
1	6.155934	2.816339	0.376742
6	6.976764	0.121732	-2.272437
1	5.036540	-0.678676	-1.858239
6	7.911798	1.111254	-1.978791
1	8.331590	2.860642	-0.795463
1	7.199665	-0.638550	-3.014587
1	8.868442	1.127098	-2.490927
7	1.773084	0.794306	-0.068100
6	3.028971	0.438369	-0.458897
7	-1.399964	2.082406	0.178839
6	-1.394560	3.397366	-0.295942
6	-2.559592	4.117024	-0.584075
6	-2.461230	5.438471	-1.002873
6	-1.235961	6.083388	-1.130133
6	-0.089805	5.362647	-0.818044
6	-0.155358	4.036366	-0.410327
6	-3.731887	6.199439	-1.252494
9	-4.281098	6.638730	-0.106546
6	1.262734	5.992049	-0.979749
9	1.853668	5.623078	-2.128692
6	-2.252848	1.059510	-0.141843
16	-3.420351	1.115945	-1.366486
7	-2.012885	-0.036017	0.600201
6	-2.713291	-1.291751	0.446916
6	-1.708820	-2.451166	0.607066
6	-2.276076	-3.812360	0.143536
6	-1.487039	-4.314035	-1.080138
6	-0.038177	-4.580598	-0.648032
6	0.508350	-3.309439	0.022499
7	-0.459122	-2.184456	-0.181554
6	-0.730900	-1.993455	-1.637989
6	-1.452488	-3.249464	-2.194870
6	-2.785795	-2.903490	-2.812654
6	-3.895105	-3.635940	-2.754258
6	-3.827173	-1.457465	1.478389
6	-5.146399	-1.883298	1.126558
6	-6.078486	-2.062044	2.191875
7	-5.777317	-1.825660	3.500271
6	-4.565979	-1.408811	3.775250
6	-3.555249	-1.215759	2.802178
6	-7.388604	-2.504455	1.887816

6	-7.777179	-2.756451	0.597075
6	-6.853972	-2.559040	-0.461437
6	-5.572294	-2.124845	-0.199359
9	-3.528262	7.278719	-2.023778
9	-4.657893	5.442235	-1.856148
9	2.098697	5.636085	0.010079
9	1.199409	7.331852	-0.987460
1	-1.365896	-2.476245	1.646836
1	-2.200150	-4.547438	0.949653
1	-3.336355	-3.703968	-0.097864
1	1.449367	-2.961424	-0.405430
1	0.647587	-3.404914	1.098796
1	0.576777	-4.848033	-1.513943
1	0.011872	-5.415572	0.053431
1	-1.937073	-5.235114	-1.459881
1	-0.822595	-3.648144	-3.001220
1	0.241268	-1.822221	-2.102301
1	-1.316784	-1.077169	-1.750141
1	-2.803202	-1.972133	-3.379551
1	-4.804870	-3.312425	-3.249715
1	-3.949919	-4.572520	-2.204577
1	-3.135519	-1.313158	-0.559557
1	-2.572340	-0.866556	3.112690
1	-4.916464	-1.955577	-1.044591
1	-4.341447	-1.212095	4.821963
1	-8.077234	-2.634386	2.716284
1	-8.787156	-3.093131	0.395585
1	-1.375997	0.050702	1.429513
1	-0.519795	1.784839	0.607857
1	-3.529835	3.648664	-0.483304
1	0.749587	3.486759	-0.166536
1	-1.178843	7.115005	-1.455838
8	-7.160613	-2.773853	-1.767312
6	-8.484535	-3.155490	-2.086585
1	-8.521869	-3.233184	-3.173352
1	-8.741018	-4.128037	-1.649956
1	-9.211284	-2.404347	-1.756728
1	0.006014	-1.336847	0.203274

re-re_1-path-A

Number of imaginary frequencies : 1

The smallest frequency is : -254.3622

Electronic energy=	-3905.283585
Zero-point correction=	1.052811
Thermal correction to Energy=	1.119155
Thermal correction to Enthalpy=	1.120099
Thermal correction to Gibbs Free Energy=	0.941594
Sum of electronic and zero-point Energies=	-3904.230547
Sum of electronic and thermal Energies=	-3904.164203
Sum of electronic and thermal Enthalpies=	-3904.163259
Sum of electronic and thermal Free Energies=	-3904.341764

Cartesian Coordinates

6	-2.756293	-0.407575	-3.219622
6	-2.763158	1.121438	-3.372829
6	-3.126004	1.649265	-1.972271
7	-2.953451	0.494191	-1.075480
6	-2.298259	-0.621145	-1.770446
6	-3.683435	0.310252	0.022149
6	-4.381882	1.297208	0.695680
8	0.336172	0.753469	0.776474
6	-0.764511	-0.520501	-1.658210
8	-0.153743	-1.557510	-1.280340
8	-0.249862	0.569601	-1.992879

8	-1.418765	-0.208109	1.622108
1	-2.631113	-1.567076	-1.340563
1	-2.098869	-0.901471	-3.938666
1	-3.766263	-0.814701	-3.332965
1	-1.770766	1.471945	-3.652593
1	-3.484296	1.455526	-4.121394
1	-2.483879	2.476945	-1.662878
1	-4.170972	1.973598	-1.914794
1	-3.634641	-0.690091	0.445273
1	-4.548869	2.246490	0.192314
6	-5.388271	0.901655	1.742051
6	-6.811256	0.689784	1.175607
1	-5.447351	1.674953	2.517636
1	-5.060120	-0.025150	2.229890
1	-7.492742	0.424203	1.990552
1	-7.158906	1.640155	0.750576
6	-6.838597	-0.360250	0.111788
6	-7.448495	-1.545739	0.206218
1	-6.292298	-0.154435	-0.808568
1	-8.019124	-1.800265	1.093274
6	-7.364478	-2.513653	-0.921744
8	-6.759774	-2.234385	-1.945124
6	-8.042169	-3.846620	-0.796515
6	-8.557833	-4.335713	0.407706
6	-8.138517	-4.632257	-1.950705
6	-9.162161	-5.588908	0.453060
1	-8.482380	-3.757479	1.321876
6	-8.748895	-5.878043	-1.906558
1	-7.727244	-4.240880	-2.875110
6	-9.262592	-6.358691	-0.702198
1	-9.554851	-5.963929	1.392690
1	-8.823674	-6.477084	-2.808521
1	-9.739180	-7.333425	-0.664265
6	-2.698377	2.124748	1.888216
1	-2.905989	1.346457	2.617043
1	-0.958919	2.840442	0.743316
6	-3.278548	3.456437	2.158704
6	-3.908009	3.703532	3.383613
6	-3.192233	4.492255	1.219845
6	-4.425043	4.963974	3.671336
1	-3.972545	2.907414	4.120649
6	-3.701751	5.750710	1.510274
1	-2.724379	4.308326	0.257215
6	-4.321537	5.990290	2.736878
1	-4.903746	5.143847	4.628748
1	-3.614037	6.546239	0.776947
1	-4.721664	6.974015	2.961053
7	-0.832323	0.815501	1.198765
6	-1.488687	2.027417	1.218021
7	2.308812	1.313434	-1.169267
6	2.353417	2.703309	-1.056001
6	3.516918	3.461985	-0.914865
6	3.420789	4.851324	-0.856043
6	2.204254	5.511290	-0.948144
6	1.055391	4.739657	-1.111251
6	1.116047	3.357241	-1.165762
6	4.683482	5.640430	-0.658191
9	5.698763	5.144972	-1.380936
6	-0.272071	5.432656	-1.164593
9	-0.240542	6.528096	-1.935767
6	3.041730	0.369018	-0.522758
16	4.437389	0.643980	0.393051
7	2.492979	-0.858043	-0.668610
6	3.032663	-2.074520	-0.109250
6	1.881030	-2.948951	0.424381
6	2.386329	-4.111399	1.307737
6	1.835851	-3.952719	2.732289
6	0.306975	-4.066773	2.669856
6	-0.228733	-3.034852	1.658832
7	0.896188	-2.140864	1.230598

6	1.524218	-1.484505	2.415460
6	2.189644	-2.565639	3.307343
6	3.664433	-2.296066	3.493837
6	4.635982	-3.203536	3.554268
6	3.800752	-2.890522	-1.146697
6	5.099940	-3.434342	-0.902609
6	5.671832	-4.235499	-1.935644
7	5.055818	-4.477246	-3.127118
6	3.877436	-3.937990	-3.320263
6	3.208426	-3.144300	-2.358627
6	6.946242	-4.815737	-1.723821
6	7.633888	-4.622645	-0.553264
6	7.067402	-3.815626	0.466877
6	5.832527	-3.228957	0.288851
9	4.531776	6.926732	-1.010644
9	5.081631	5.631212	0.623813
9	-0.674117	5.833545	0.056110
9	-1.247671	4.635598	-1.642335
1	1.293013	-3.303916	-0.425328
1	2.059050	-5.069085	0.893460
1	3.478474	-4.117072	1.316000
1	-0.992347	-2.379572	2.073517
1	-0.617532	-3.484286	0.743191
1	-0.123936	-3.888047	3.659276
1	0.017296	-5.074920	2.362707
1	2.240529	-4.735416	3.379061
1	1.725285	-2.495705	4.299822
1	0.714268	-0.951187	2.916057
1	2.233526	-0.741854	2.040856
1	3.925476	-1.243951	3.612677
1	5.667901	-2.905697	3.710677
1	4.453006	-4.269501	3.442039
1	3.695561	-1.793147	0.711207
1	2.224870	-2.740560	-2.588606
1	5.458136	-2.596560	1.085447
1	3.400345	-4.131407	-4.279179
1	7.359906	-5.420277	-2.524419
1	8.606986	-5.080144	-0.420770
1	1.577657	-0.949983	-1.133270
1	1.389312	0.978268	-1.514197
1	4.482206	2.976944	-0.859199
1	0.220442	2.755355	-1.301260
1	2.151075	6.593586	-0.909541
8	7.682155	-3.573281	1.652854
6	8.979266	-4.101853	1.851575
1	9.290840	-3.769399	2.841966
1	8.977337	-5.197952	1.826313
1	9.687482	-3.720662	1.107108
1	0.489865	-1.402695	0.626291

re-re_2-path-A

Number of imaginary frequencies : 1
The smallest frequency is : -330.2854

Electronic energy= -3905.288664
Zero-point correction= 1.054342
Thermal correction to Energy= 1.119830
Thermal correction to Enthalpy= 1.120774
Thermal correction to Gibbs Free Energy= 0.949151
Sum of electronic and zero-point Energies= -3904.234322
Sum of electronic and thermal Energies= -3904.168834
Sum of electronic and thermal Enthalpies= -3904.167890
Sum of electronic and thermal Free Energies= -3904.339513

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

6	2.398678	-0.246109	4.784374
6	3.401547	0.772650	4.221281
6	3.943481	0.114409	2.941212
7	3.008605	-0.987652	2.652322
6	1.831770	-0.930206	3.534170
6	3.362143	-2.095334	2.007387
6	4.509874	-2.218070	1.231816
8	0.677097	0.118420	-0.048657
6	0.702431	-0.088118	2.902806
8	-0.415181	-0.652160	2.765819
8	0.984409	1.095695	2.614613
8	1.434590	-1.919872	0.041945
1	1.464511	-1.942410	3.711958
1	1.617149	0.221665	5.386798
1	2.910906	-0.993475	5.398870
1	2.889189	1.700216	3.970951
1	4.206582	0.988181	4.926580
1	3.984541	0.811871	2.102782
1	4.940562	-0.313617	3.092202
1	2.635460	-2.901889	2.049721
1	5.279997	-1.470666	1.393984
6	5.023450	-3.572019	0.773117
6	4.352993	-4.799664	1.399957
1	6.088870	-3.619981	1.018933
1	4.985928	-3.658276	-0.322780
1	5.001686	-5.673366	1.245919
1	4.302450	-4.673371	2.488916
6	2.991995	-5.183229	0.900027
6	2.400513	-4.770975	-0.225847
1	2.441859	-5.904932	1.504375
1	2.881616	-4.073377	-0.901067
6	1.067263	-5.310603	-0.602779
8	0.456893	-6.079700	0.125441
6	0.478554	-4.921799	-1.926551
6	0.817259	-3.740215	-2.593733
6	-0.465785	-5.787613	-2.492410
6	0.210544	-3.428996	-3.809288
1	1.511354	-3.037727	-2.140652
6	-1.051426	-5.487149	-3.715315
1	-0.719789	-6.696764	-1.956352
6	-0.714785	-4.304000	-4.374489
1	0.460161	-2.501054	-4.314055
1	-1.771830	-6.169874	-4.154328
1	-1.177884	-4.062369	-5.326194
6	3.904363	-1.174721	-0.568399
1	3.569361	-2.139810	-0.934840
1	3.017047	0.837506	-0.354521
6	5.228353	-0.720028	-1.046329
6	5.936746	-1.484012	-1.979773
6	5.792327	0.474781	-0.581844
6	7.177078	-1.056925	-2.447266
1	5.502938	-2.406900	-2.355938
6	7.025263	0.904478	-1.054814
1	5.262113	1.073969	0.152316
6	7.723300	0.137801	-1.987279
1	7.712940	-1.655431	-3.177160
1	7.440187	1.840642	-0.694760
1	8.687803	0.473337	-2.354689
7	1.626885	-0.685117	-0.104996
6	2.902021	-0.236652	-0.335514
7	-0.492434	2.538012	0.724734
6	0.386561	3.417013	0.091600
6	0.014817	4.458760	-0.760908
6	1.001137	5.289372	-1.290596
6	2.345178	5.129320	-0.985992
6	2.696153	4.098094	-0.117014
6	1.742260	3.247998	0.416406
6	0.586168	6.370609	-2.247470
9	-0.607930	6.889367	-1.929568
6	4.145257	3.893849	0.206393

9	4.753270	5.038764	0.545969
6	-1.638583	1.970566	0.261276
16	-2.499403	2.441123	-1.114361
7	-2.014998	0.929624	1.038353
6	-3.188360	0.117529	0.813855
6	-2.857574	-1.350714	1.140581
6	-3.962147	-2.321776	0.667302
6	-3.368737	-3.332134	-0.325429
6	-2.287478	-4.138311	0.405776
6	-1.223077	-3.166944	0.947324
7	-1.556207	-1.771907	0.506574
6	-1.594324	-1.684207	-0.981429
6	-2.713926	-2.609365	-1.519732
6	-3.655945	-1.839168	-2.412842
6	-4.982498	-1.938745	-2.451287
6	-4.363097	0.554992	1.684788
6	-5.683521	0.743177	1.168950
6	-6.696942	1.110124	2.104541
7	-6.461528	1.296589	3.434228
6	-5.234303	1.130853	3.861142
6	-4.154971	0.757905	3.025891
6	-8.021953	1.293948	1.641236
6	-8.346861	1.126413	0.319698
6	-7.335936	0.769850	-0.609663
6	-6.034572	0.588856	-0.192288
9	1.469391	7.381977	-2.273516
9	0.486875	5.911273	-3.505857
9	4.827355	3.394711	-0.840487
9	4.324968	3.028932	1.224877
1	-2.668518	-1.436609	2.213740
1	-4.385670	-2.852289	1.524390
1	-4.772698	-1.757659	0.201722
1	-0.223413	-3.367769	0.564738
1	-1.174063	-3.129431	2.036968
1	-1.821262	-4.862359	-0.267897
1	-2.735885	-4.699626	1.229913
1	-4.152211	-4.004213	-0.685856
1	-2.227223	-3.376635	-2.138959
1	-0.600126	-1.977498	-1.318150
1	-1.741473	-0.632459	-1.241670
1	-3.166220	-1.143128	-3.095394
1	-5.567082	-1.338411	-3.140963
1	-5.540010	-2.608026	-1.800829
1	-3.457726	0.207743	-0.240339
1	-3.162889	0.639497	3.454880
1	-5.296535	0.342390	-0.947530
1	-5.058589	1.289649	4.923423
1	-8.772858	1.573620	2.373124
1	-9.369994	1.273690	-0.004948
1	-1.388167	0.613953	1.792216
1	-0.022607	1.996628	1.473236
1	-1.026270	4.625752	-0.999988
1	2.016401	2.445933	1.097238
1	3.095130	5.796490	-1.396779
8	-7.572511	0.587549	-1.934083
6	-8.871435	0.863268	-2.421968
1	-8.827023	0.706692	-3.500002
1	-9.617441	0.183959	-1.993075
1	-9.163762	1.900541	-2.222244
1	-0.794501	-1.154907	0.842018

re-re_3-path-A

Number of imaginary frequencies : 1
The smallest frequency is : -329.8119

Electronic energy= -3905.2888597

Zero-point correction=	1.054953
Thermal correction to Energy=	1.120361
Thermal correction to Enthalpy=	1.121305
Thermal correction to Gibbs Free Energy=	0.949775
Sum of electronic and zero-point Energies=	-3904.233906
Sum of electronic and thermal Energies=	-3904.168498
Sum of electronic and thermal Enthalpies=	-3904.167554
Sum of electronic and thermal Free Energies=	-3904.339085

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

6	2.111580	-0.417794	4.920855
6	3.070831	0.708029	4.502448
6	3.757826	0.185186	3.226452
7	2.966309	-0.990185	2.825183
6	1.714336	-1.067363	3.588096
6	3.468644	-2.035098	2.177720
6	4.658376	-2.020823	1.457924
8	0.636114	0.004880	-0.054415
6	0.594159	-0.256703	2.904293
8	-0.510211	-0.841780	2.745933
8	0.866255	0.927674	2.609067
8	1.498086	-1.977014	0.190769
1	1.402450	-2.109330	3.676815
1	1.244918	-0.050071	5.474540
1	2.629124	-1.158633	5.538575
1	2.507893	1.610936	4.271409
1	3.801275	0.932898	5.282112
1	3.764946	0.931536	2.429221
1	4.785730	-0.142254	3.415862
1	2.822186	-2.907713	2.153313
1	5.334330	-1.194374	1.657945
6	5.330314	-3.300908	0.999088
6	4.616642	-4.606576	1.372532
1	6.332643	-3.336400	1.439519
1	5.501644	-3.273625	-0.086529
1	5.288436	-5.444898	1.145417
1	4.465631	-4.636252	2.457078
6	3.302962	-4.875598	0.692460
6	2.968232	-4.574218	-0.565915
1	2.540616	-5.390131	1.278161
1	3.655302	-4.079193	-1.246131
6	1.606570	-4.911299	-1.059680
8	0.874055	-5.670813	-0.441193
6	1.125538	-4.300212	-2.339782
6	1.613850	-3.080887	-2.820769
6	0.107662	-4.959678	-3.037921
6	1.077560	-2.522602	-3.978010
1	2.379276	-2.541971	-2.271676
6	-0.408147	-4.414139	-4.207865
1	-0.259147	-5.905579	-2.651182
6	0.070433	-3.189155	-4.673162
1	1.442396	-1.564552	-4.333392
1	-1.189062	-4.935932	-4.752120
1	-0.341260	-2.754499	-5.578609
6	3.961149	-1.094549	-0.350728
1	3.699585	-2.096206	-0.671100
1	2.935454	0.855924	-0.242796
6	5.244872	-0.557731	-0.856947
6	5.955105	-1.257167	-1.838343
6	5.756604	0.658638	-0.388428
6	7.147386	-0.748240	-2.347361
1	5.557487	-2.193280	-2.223033
6	6.941765	1.169500	-0.901347
1	5.220985	1.208859	0.380137
6	7.642796	0.465546	-1.880350
1	7.683736	-1.297414	-3.114659
1	7.317789	2.120341	-0.537110
1	8.570181	0.864612	-2.278513
7	1.630410	-0.742858	-0.005210

6	2.889547	-0.221414	-0.178141
7	-0.654142	2.368811	0.741931
6	0.179829	3.315662	0.149108
6	-0.240229	4.363908	-0.672741
6	0.704617	5.262004	-1.167175
6	2.053176	5.162614	-0.856949
6	2.451294	4.125165	-0.016228
6	1.539775	3.210079	0.482848
6	0.236279	6.348756	-2.092669
9	-0.965753	6.824565	-1.737864
6	3.907477	3.975015	0.304357
9	4.482068	5.146379	0.610279
6	-1.774087	1.766528	0.257684
16	-2.655340	2.243337	-1.103417
7	-2.101448	0.685264	0.998643
6	-3.241874	-0.167714	0.759234
6	-2.847366	-1.630627	1.040274
6	-3.904045	-2.639484	0.539051
6	-3.288798	-3.530966	-0.550234
6	-2.152356	-4.349947	0.078644
6	-1.172421	-3.388893	0.773975
7	-1.526998	-1.980533	0.403275
6	-1.542446	-1.816209	-1.081776
6	-2.685050	-2.675538	-1.681849
6	-3.664730	-1.828342	-2.457789
6	-4.983281	-1.997973	-2.521151
6	-4.416563	0.189555	1.666993
6	-5.747905	0.374183	1.181424
6	-6.759927	0.642107	2.151362
7	-6.511480	0.749366	3.487302
6	-5.272869	0.598464	3.886570
6	-4.194910	0.312751	3.015904
6	-8.096716	0.807448	1.715944
6	-8.432852	0.715476	0.389727
6	-7.422168	0.461869	-0.573404
6	-6.109588	0.302554	-0.183446
9	1.087398	7.387166	-2.118274
9	0.120835	5.910562	-3.357034
9	4.598942	3.468340	-0.732776
9	4.118534	3.143298	1.343723
1	-2.656908	-1.738214	2.110663
1	-4.251809	-3.261291	1.368850
1	-4.771779	-2.099643	0.152395
1	-0.139886	-3.538501	0.464523
1	-1.220012	-3.430266	1.863962
1	-1.619511	-4.923609	-0.685518
1	-2.553528	-5.061985	0.804537
1	-4.050376	-4.201715	-0.956818
1	-2.218949	-3.365047	-2.397246
1	-0.551260	-2.124958	-1.421338
1	-1.654584	-0.748151	-1.287520
1	-3.213117	-1.018817	-3.032754
1	-5.603785	-1.343589	-3.125299
1	-5.498541	-2.783117	-1.973079
1	-3.528338	-0.055960	-0.288548
1	-3.194077	0.193529	3.424685
1	-5.370029	0.140935	-0.958730
1	-5.086638	0.694977	4.954581
1	-8.847883	1.008486	2.472788
1	-9.465200	0.845571	0.087904
1	-1.471477	0.382349	1.756119
1	-0.160645	1.822798	1.471192
1	-1.286962	4.482914	-0.916295
1	1.851951	2.404702	1.143301
1	2.770950	5.878216	-1.242152
8	-7.669689	0.360936	-1.904855
6	-8.985246	0.614092	-2.359198
1	-8.950605	0.523283	-3.445099
1	-9.698630	-0.117637	-1.962321
1	-9.314267	1.625633	-2.094550

1 -0.788533 -1.363687 0.786746

re-re_4-path-A

Number of imaginary frequencies : 1

The smallest frequency is : -305.6500

Electronic energy= -3905.288499
Zero-point correction= 1.054791
Thermal correction to Energy= 1.120206
Thermal correction to Enthalpy= 1.121150
Thermal correction to Gibbs Free Energy= 0.950632
Sum of electronic and zero-point Energies= -3904.233708
Sum of electronic and thermal Energies= -3904.168293
Sum of electronic and thermal Enthalpies= -3904.167349
Sum of electronic and thermal Free Energies= -3904.337867

Cartesian Coordinates

6 2.054678 -0.188374 4.904968
6 2.960869 0.982368 4.492576
6 3.707306 0.475391 3.244952
7 2.968723 -0.726443 2.824325
6 1.712419 -0.866967 3.570752
6 3.534209 -1.752696 2.190643
6 4.733951 -1.688181 1.501435
8 0.656587 0.234945 -0.087686
6 0.556935 -0.125607 2.868249
8 -0.505488 -0.775780 2.674797
8 0.758708 1.078103 2.593450
8 1.523731 -1.720650 0.283413
1 1.456052 -1.923844 3.664214
1 1.162193 0.137129 5.443902
1 2.601255 -0.897305 5.535102
1 2.353896 1.847373 4.229868
1 3.656783 1.261817 5.286167
1 3.722900 1.218641 2.444493
1 4.738057 0.181304 3.472326
1 2.933601 -2.656622 2.161786
1 5.348114 -0.806656 1.662779
6 5.493375 -2.926826 1.083721
6 4.764106 -4.270161 1.221943
1 6.408002 -2.985817 1.685202
1 5.843597 -2.817630 0.047136
1 5.509179 -5.057065 1.045399
1 4.403341 -4.410584 2.246975
6 3.644077 -4.509882 0.251341
6 2.445386 -4.986465 0.608119
1 3.874611 -4.359434 -0.804405
1 2.230636 -5.185511 1.657458
6 1.375048 -5.466809 -0.300837
8 0.541528 -6.246373 0.137223
6 1.301090 -5.036752 -1.735108
6 1.659206 -3.750588 -2.150995
6 0.761198 -5.938679 -2.659240
6 1.485068 -3.375168 -3.481980
1 2.015952 -3.031952 -1.419608
6 0.609247 -5.568115 -3.989570
1 0.464529 -6.924897 -2.316131
6 0.970384 -4.284865 -4.402424
1 1.747410 -2.369154 -3.795217
1 0.202738 -6.274990 -4.705721
1 0.842468 -3.993264 -5.440275
6 3.976787 -0.865972 -0.397667
1 3.736963 -1.891245 -0.666702
1 2.953036 1.078522 -0.346123
6 5.250189 -0.330888 -0.925627

6	5.956334	-1.041678	-1.902095
6	5.753254	0.899803	-0.484925
6	7.135327	-0.527001	-2.436166
1	5.565136	-1.990646	-2.261144
6	6.925562	1.414579	-1.021813
1	5.222056	1.455288	0.282816
6	7.621387	0.701164	-1.997907
1	7.669625	-1.083740	-3.199400
1	7.296649	2.374562	-0.677066
1	8.539261	1.103539	-2.414394
7	1.650833	-0.503102	0.000310
6	2.908687	0.005209	-0.229843
7	-0.794356	2.471347	0.735288
6	0.016960	3.432766	0.130568
6	-0.437418	4.470845	-0.685229
6	0.481866	5.383610	-1.200997
6	1.837647	5.307368	-0.916375
6	2.270059	4.279375	-0.081063
6	1.384050	3.350628	0.439284
6	-0.019435	6.455600	-2.126497
9	-1.225948	6.910695	-1.759814
6	3.735652	4.146755	0.201652
9	4.308885	5.325078	0.481086
6	-1.872996	1.813771	0.229788
16	-2.748587	2.253589	-1.147900
7	-2.159856	0.712302	0.958580
6	-3.252482	-0.193756	0.690193
6	-2.793044	-1.647192	0.922118
6	-3.795467	-2.672636	0.347991
6	-3.116395	-3.492570	-0.760830
6	-1.969468	-4.293045	-0.130375
6	-1.033378	-3.318854	0.607096
7	-1.446654	-1.909780	0.301084
6	-1.438518	-1.675700	-1.174555
6	-2.515831	-2.571776	-1.841791
6	-3.510292	-1.744871	-2.621506
6	-4.821215	-1.956491	-2.710242
6	-4.448912	0.073683	1.598643
6	-5.780996	0.229070	1.104386
6	-6.811445	0.419749	2.073295
7	-6.581154	0.475755	3.415462
6	-5.342660	0.349969	3.823843
6	-4.245944	0.144249	2.954333
6	-8.148747	0.559391	1.630182
6	-8.468212	0.513230	0.297654
6	-7.440429	0.332213	-0.663995
6	-6.126976	0.199211	-0.266631
9	0.811405	7.509789	-2.169679
9	-0.141436	6.007170	-3.386684
9	4.402565	3.634719	-0.849468
9	3.982816	3.326181	1.241965
1	-2.620465	-1.795532	1.990796
1	-4.141699	-3.343902	1.138832
1	-4.672723	-2.148038	-0.038064
1	0.005846	-3.392129	0.290297
1	-1.069907	-3.415309	1.693965
1	-1.415335	-4.840047	-0.898853
1	-2.361462	-5.033282	0.571139
1	-3.839776	-4.175066	-1.214408
1	-1.994143	-3.215846	-2.562946
1	-0.424517	-1.914137	-1.502532
1	-1.608079	-0.608017	-1.337306
1	-3.077304	-0.909854	-3.173416
1	-5.450277	-1.311982	-3.316016
1	-5.321025	-2.768297	-2.187667
1	-3.539954	-0.065164	-0.355048
1	-3.245399	0.042859	3.368836
1	-5.375279	0.092581	-1.040362
1	-5.171739	0.403724	4.897288
1	-8.913439	0.703806	2.386314

1	-9.501293	0.622745	-0.009880
1	-1.522208	0.428250	1.716829
1	-0.288209	1.948191	1.473209
1	-1.490698	4.569386	-0.909492
1	1.723235	2.551364	1.093630
1	2.535720	6.032749	-1.319157
8	-7.671574	0.277674	-2.000759
6	-8.990061	0.502654	-2.460718
1	-8.940259	0.459461	-3.549007
1	-9.681882	-0.269740	-2.104324
1	-9.358993	1.489747	-2.158978
1	-0.746602	-1.284899	0.741451

re-re_5-path-A

Number of imaginary frequencies : 1
The smallest frequency is : -305.6500

Electronic energy=	-3905.288499
Zero-point correction=	1.054791
Thermal correction to Energy=	1.120206
Thermal correction to Enthalpy=	1.121150
Thermal correction to Gibbs Free Energy=	0.950632
Sum of electronic and zero-point Energies=	-3904.233708
Sum of electronic and thermal Energies=	-3904.168293
Sum of electronic and thermal Enthalpies=	-3904.167349
Sum of electronic and thermal Free Energies=	-3904.337867

Cartesian Coordinates

6	2.054678	-0.188374	4.904968
6	2.960869	0.982368	4.492576
6	3.707306	0.475391	3.244952
7	2.968723	-0.726443	2.824325
6	1.712419	-0.866967	3.570752
6	3.534209	-1.752696	2.190643
6	4.733951	-1.688181	1.501435
8	0.656587	0.234945	-0.087686
6	0.556935	-0.125607	2.868249
8	-0.505488	-0.775780	2.674797
8	0.758708	1.078103	2.593450
8	1.523731	-1.720650	0.283413
1	1.456052	-1.923844	3.664214
1	1.162193	0.137129	5.443902
1	2.601255	-0.897305	5.535102
1	2.353896	1.847373	4.229868
1	3.656783	1.261817	5.286167
1	3.722900	1.218641	2.444493
1	4.738057	0.181304	3.472326
1	2.933601	-2.656622	2.161786
1	5.348114	-0.806656	1.662779
6	5.493375	-2.926826	1.083721
6	4.764106	-4.270161	1.221943
1	6.408002	-2.985817	1.685202
1	5.843597	-2.817630	0.047136
1	5.509179	-5.057065	1.045399
1	4.403341	-4.410584	2.246975
6	3.644077	-4.509882	0.251341
6	2.445386	-4.986465	0.608119
1	3.874611	-4.359434	-0.804405
1	2.230636	-5.185511	1.657458
6	1.375048	-5.466809	-0.300837
8	0.541528	-6.246373	0.137223
6	1.301090	-5.036752	-1.735108
6	1.659206	-3.750588	-2.150995
6	0.761198	-5.938679	-2.659240
6	1.485068	-3.375168	-3.481980

1	2.015952	-3.031952	-1.419608
6	0.609247	-5.568115	-3.989570
1	0.464529	-6.924897	-2.316131
6	0.970384	-4.284865	-4.402424
1	1.747410	-2.369154	-3.795217
1	0.202738	-6.274990	-4.705721
1	0.842468	-3.993264	-5.440275
6	3.976787	-0.865972	-0.397667
1	3.736963	-1.891245	-0.666702
1	2.953036	1.078522	-0.346123
6	5.250189	-0.330888	-0.925627
6	5.956334	-1.041678	-1.902095
6	5.753254	0.899803	-0.484925
6	7.135327	-0.527001	-2.436166
1	5.565136	-1.990646	-2.261144
6	6.925562	1.414579	-1.021813
1	5.222056	1.455288	0.282816
6	7.621387	0.701164	-1.997907
1	7.669625	-1.083740	-3.199400
1	7.296649	2.374562	-0.677066
1	8.539261	1.103539	-2.414394
7	1.650833	-0.503102	0.000310
6	2.908687	0.005209	-0.229843
7	-0.794356	2.471347	0.735288
6	0.016960	3.432766	0.130568
6	-0.437418	4.470845	-0.685229
6	0.481866	5.383610	-1.200997
6	1.837647	5.307368	-0.916375
6	2.270059	4.279375	-0.081063
6	1.384050	3.350628	0.439284
6	-0.019435	6.455600	-2.126497
9	-1.225948	6.910695	-1.759814
6	3.735652	4.146755	0.201652
9	4.308885	5.325078	0.481086
6	-1.872996	1.813771	0.229788
16	-2.748587	2.253589	-1.147900
7	-2.159856	0.712302	0.958580
6	-3.252482	-0.193756	0.690193
6	-2.793044	-1.647192	0.922118
6	-3.795467	-2.672636	0.347991
6	-3.116395	-3.492570	-0.760830
6	-1.969468	-4.293045	-0.130375
6	-1.033378	-3.318854	0.607096
7	-1.446654	-1.909780	0.301084
6	-1.438518	-1.675700	-1.174555
6	-2.515831	-2.571776	-1.841791
6	-3.510292	-1.744871	-2.621506
6	-4.821215	-1.956491	-2.710242
6	-4.448912	0.073683	1.598643
6	-5.780996	0.229070	1.104386
6	-6.811445	0.419749	2.073295
7	-6.581154	0.475755	3.415462
6	-5.342660	0.349969	3.823843
6	-4.245944	0.144249	2.954333
6	-8.148747	0.559391	1.630182
6	-8.468212	0.513230	0.297654
6	-7.440429	0.332213	-0.663995
6	-6.126976	0.199211	-0.266631
9	0.811405	7.509789	-2.169679
9	-0.141436	6.007170	-3.386684
9	4.402565	3.634719	-0.849468
9	3.982816	3.326181	1.241965
1	-2.620465	-1.795532	1.990796
1	-4.141699	-3.343902	1.138832
1	-4.672723	-2.148038	-0.038064
1	0.005846	-3.392129	0.290297
1	-1.069907	-3.415309	1.693965
1	-1.415335	-4.840047	-0.898853
1	-2.361462	-5.033282	0.571139
1	-3.839776	-4.175066	-1.214408

1	-1.994143	-3.215846	-2.562946
1	-0.424517	-1.914137	-1.502532
1	-1.608079	-0.608017	-1.337306
1	-3.077304	-0.909854	-3.173416
1	-5.450277	-1.311982	-3.316016
1	-5.321025	-2.768297	-2.187667
1	-3.539954	-0.065164	-0.355048
1	-3.245399	0.042859	3.368836
1	-5.375279	0.092581	-1.040362
1	-5.171739	0.403724	4.897288
1	-8.913439	0.703806	2.386314
1	-9.501293	0.622745	-0.009880
1	-1.522208	0.428250	1.716829
1	-0.288209	1.948191	1.473209
1	-1.490698	4.569386	-0.909492
1	1.723235	2.551364	1.093630
1	2.535720	6.032749	-1.319157
8	-7.671574	0.277674	-2.000759
6	-8.990061	0.502654	-2.460718
1	-8.940259	0.459461	-3.549007
1	-9.681882	-0.269740	-2.104324
1	-9.358993	1.489747	-2.158978
1	-0.746602	-1.284899	0.741451

re-re_6-path-A

Number of imaginary frequencies : 1

The smallest frequency is : -306.9803

Electronic energy=	-3905.2881269
Zero-point correction=	1.054727
Thermal correction to Energy=	1.120136
Thermal correction to Enthalpy=	1.121080
Thermal correction to Gibbs Free Energy=	0.950289
Sum of electronic and zero-point Energies=	-3904.233399
Sum of electronic and thermal Energies=	-3904.167991
Sum of electronic and thermal Enthalpies=	-3904.167047
Sum of electronic and thermal Free Energies=	-3904.337838

Cartesian Coordinates

6	2.073033	-0.187833	4.898330
6	2.984949	0.975857	4.478673
6	3.723577	0.460457	3.229840
7	2.976453	-0.738607	2.816315
6	1.721815	-0.868577	3.567537
6	3.532079	-1.771349	2.184451
6	4.728387	-1.718929	1.488033
8	0.659336	0.223691	-0.084204
6	0.568267	-0.121375	2.867490
8	-0.499807	-0.764218	2.681258
8	0.778001	1.079895	2.587816
8	1.517577	-1.736367	0.283985
1	1.459436	-1.923562	3.664553
1	1.184616	0.145442	5.439199
1	2.617542	-0.897768	5.529169
1	2.382331	1.843826	4.215717
1	3.685777	1.253076	5.268675
1	3.740004	1.200829	2.426783
1	4.753557	0.161530	3.454467
1	2.925241	-2.671323	2.163762
1	5.351174	-0.842277	1.643156
6	5.474896	-2.965599	1.070643
6	4.736628	-4.303008	1.218005
1	6.392496	-3.029485	1.667090
1	5.819536	-2.863323	0.031511
1	5.475431	-5.095604	1.040075

1	4.380894	-4.437309	2.245613
6	3.608995	-4.539497	0.255274
6	2.410836	-5.009973	0.621931
1	3.832883	-4.393136	-0.802509
1	2.203381	-5.205921	1.673355
6	1.330604	-5.487272	-0.276929
8	0.498449	-6.263425	0.169815
6	1.243194	-5.058600	-1.710889
6	1.608040	-3.776944	-2.134534
6	0.681213	-5.956855	-2.625372
6	1.417833	-3.402430	-3.463648
1	1.982478	-3.060197	-1.410299
6	0.513472	-5.587703	-3.954122
1	0.379901	-6.939054	-2.275059
6	0.880535	-4.308587	-4.374541
1	1.685101	-2.399663	-3.783045
1	0.090119	-6.292038	-4.663015
1	0.739876	-4.017370	-5.410835
6	3.971910	-0.896039	-0.410037
1	3.725951	-1.920617	-0.676226
1	2.958221	1.053732	-0.359284
6	5.245717	-0.367377	-0.943687
6	5.949420	-1.085119	-1.916744
6	5.751719	0.864876	-0.510952
6	7.128846	-0.575941	-2.455071
1	5.556136	-2.035437	-2.269689
6	6.923871	1.374736	-1.052773
1	5.222596	1.425518	0.254413
6	7.617387	0.654195	-2.025271
1	7.661269	-1.138505	-3.215335
1	7.296644	2.336473	-0.714846
1	8.535325	1.052425	-2.445557
7	1.649908	-0.519991	-0.001526
6	2.908898	-0.019008	-0.239851
7	-0.766767	2.480082	0.730572
6	0.049138	3.437293	0.125241
6	-0.403270	4.482752	-0.682217
6	0.518132	5.392348	-1.198982
6	1.875237	5.305289	-0.923336
6	2.305869	4.270752	-0.095483
6	1.417109	3.344852	0.425835
6	0.016988	6.474968	-2.111839
9	-1.186252	6.930735	-1.735095
6	3.772226	4.127620	0.177647
9	4.357238	5.303026	0.444743
6	-1.849388	1.829076	0.224758
16	-2.717765	2.271012	-1.156566
7	-2.146861	0.733164	0.957944
6	-3.248632	-0.162487	0.692538
6	-2.804145	-1.618704	0.935779
6	-3.814106	-2.639674	0.366762
6	-3.139308	-3.476271	-0.731767
6	-2.001901	-4.281104	-0.090531
6	-1.057519	-3.308186	0.638084
7	-1.458496	-1.898497	0.318879
6	-1.446634	-1.676414	-1.158385
6	-2.527441	-2.571662	-1.820378
6	-3.512432	-1.744413	-2.611608
6	-4.823442	-1.951450	-2.709154
6	-4.444901	0.126738	1.595289
6	-5.777368	0.270803	1.098318
6	-6.806550	0.491569	2.062203
7	-6.575017	0.584314	3.402200
6	-5.336594	0.465431	3.812535
6	-4.241047	0.232438	2.948408
6	-8.143664	0.623505	1.616339
6	-8.464565	0.542206	0.285839
6	-7.438152	0.331263	-0.670978
6	-6.124928	0.205273	-0.271006
9	0.851581	7.526483	-2.147420

9	-0.112482	6.040004	-3.375855
9	4.426937	3.603006	-0.875064
9	4.020281	3.312010	1.221607
1	-2.635138	-1.760756	2.006102
1	-4.169330	-3.300613	1.162266
1	-4.685160	-2.111339	-0.027839
1	-0.018905	-3.393748	0.322090
1	-1.095049	-3.393429	1.725893
1	-1.452061	-4.841332	-0.852515
1	-2.402758	-5.010120	0.617844
1	-3.867182	-4.156723	-1.181067
1	-2.007953	-3.227100	-2.533266
1	-0.433418	-1.922634	-1.482911
1	-1.610029	-0.608882	-1.329553
1	-3.072111	-0.913256	-3.163560
1	-5.446529	-1.306596	-3.320679
1	-5.329542	-2.758892	-2.185747
1	-3.531742	-0.036546	-0.354362
1	-3.240600	0.140535	3.365112
1	-5.374964	0.073399	-1.042456
1	-5.164636	0.548447	4.884032
1	-8.907282	0.790749	2.368845
1	-9.497358	0.646393	-0.024383
1	-1.511744	0.446467	1.717144
1	-0.263177	1.954127	1.468533
1	-1.457473	4.590328	-0.897741
1	1.754675	2.540851	1.075348
1	2.575831	6.028385	-1.325849
8	-7.670885	0.239873	-2.005538
6	-8.987725	0.467704	-2.469598
1	-8.940169	0.393580	-3.556273
1	-9.687090	-0.286749	-2.090605
1	-9.343989	1.466928	-2.193614
1	-0.753062	-1.275885	0.753827

re-re_7-path-A

Number of imaginary frequencies : 1
 The smallest frequency is : -324.8144

Electronic energy= -3905.2825951
 Zero-point correction= 1.053948
 Thermal correction to Energy= 1.119881
 Thermal correction to Enthalpy= 1.120825
 Thermal correction to Gibbs Free Energy= 0.945010
 Sum of electronic and zero-point Energies= -3904.228647
 Sum of electronic and thermal Energies= -3904.162715
 Sum of electronic and thermal Enthalpies= -3904.161770
 Sum of electronic and thermal Free Energies= -3904.337585

 Cartesian Coordinates

6	0.695982	0.724993	4.967948
6	1.148085	2.112967	4.491377
6	2.182301	1.820646	3.393772
7	1.942685	0.419139	3.009500
6	0.772735	-0.141205	3.704891
6	2.867542	-0.349046	2.441838
6	4.022815	0.129475	1.839244
8	-0.245055	0.341711	-0.109244
6	-0.497366	0.002214	2.840378
8	-1.093183	-1.060827	2.520880
8	-0.842175	1.170371	2.555393
8	1.369303	-1.088288	0.171978
1	0.946613	-1.198946	3.909606
1	-0.307419	0.734821	5.398346
1	1.391358	0.329404	5.715172

1	0.301713	2.653009	4.069885
1	1.584905	2.704525	5.298375
1	2.073080	2.480335	2.530065
1	3.209747	1.902496	3.767380
1	2.609945	-1.402500	2.391518
1	4.330612	1.139376	2.095372
6	5.131937	-0.802709	1.413963
6	4.662844	-2.211022	1.056105
1	5.900835	-0.861693	2.195366
1	5.632291	-0.357268	0.544471
1	4.349903	-2.748394	1.962657
1	3.756068	-2.162511	0.434284
6	5.675020	-3.063056	0.357174
6	6.929853	-2.722150	0.047693
1	5.354758	-4.066073	0.075985
1	7.332504	-1.748783	0.305940
6	7.814890	-3.702846	-0.638130
8	7.480994	-4.867682	-0.780499
6	9.147013	-3.237410	-1.146301
6	9.456128	-1.887799	-1.339888
6	10.099138	-4.212137	-1.462220
6	10.703374	-1.520934	-1.837562
1	8.722399	-1.115985	-1.130097
6	11.347457	-3.844562	-1.946012
1	9.837522	-5.255162	-1.317055
6	11.651083	-2.496477	-2.134205
1	10.934091	-0.472255	-1.995273
1	12.085067	-4.606196	-2.178101
1	12.625663	-2.206636	-2.514753
6	3.243016	0.783399	-0.080595
1	3.474290	-0.211353	-0.452109
1	1.476190	2.106268	-0.091996
6	4.235405	1.834414	-0.394920
6	5.316105	1.541093	-1.235158
6	4.113593	3.129880	0.122580
6	6.247030	2.524379	-1.559397
1	5.412698	0.541537	-1.652045
6	5.037646	4.112063	-0.207618
1	3.285543	3.369961	0.782899
6	6.109890	3.811382	-1.047533
1	7.075939	2.284799	-2.218086
1	4.921216	5.114386	0.192382
1	6.833558	4.579313	-1.301756
7	0.969846	0.093133	0.013173
6	1.890475	1.109940	-0.033683
7	-2.582997	1.816119	0.493314
6	-2.200400	3.040437	-0.055274
6	-2.971645	3.814534	-0.923981
6	-2.474587	5.040206	-1.365454
6	-1.240028	5.525972	-0.960337
6	-0.493515	4.749873	-0.075535
6	-0.956284	3.525898	0.376684
6	-3.310149	5.831032	-2.331315
9	-4.600429	5.858423	-1.965689
6	0.873108	5.214440	0.325435
9	0.925518	6.539280	0.517649
6	-3.253738	0.781208	-0.076313
16	-4.133799	0.836773	-1.518692
7	-3.108884	-0.349225	0.652109
6	-3.715300	-1.620613	0.336051
6	-2.713861	-2.753911	0.632142
6	-3.156767	-4.100874	0.018967
6	-2.130123	-4.551246	-1.031125
6	-0.798706	-4.809532	-0.313694
6	-0.408254	-3.548057	0.480161
7	-1.336561	-2.430223	0.110153
6	-1.320025	-2.202658	-1.366543
6	-1.898885	-3.449437	-2.084642
6	-3.099671	-3.092994	-2.929534
6	-4.190184	-3.833902	-3.111168

6	-4.973393	-1.874064	1.163959
6	-6.209397	-2.302162	0.588190
6	-7.289715	-2.555305	1.485461
7	-7.198558	-2.391512	2.835540
6	-6.053913	-1.977016	3.319823
6	-4.913673	-1.710188	2.525246
6	-8.525775	-3.001680	0.957933
6	-8.700364	-3.194718	-0.388386
6	-7.626711	-2.933460	-1.278421
6	-6.413173	-2.489701	-0.798081
9	-2.896204	7.103737	-2.432128
9	-3.271508	5.307822	-3.567128
9	1.791213	4.924831	-0.615247
9	1.299941	4.628477	1.461968
1	-2.573466	-2.820492	1.713526
1	-3.240280	-4.861795	0.799938
1	-4.145799	-3.987934	-0.430858
1	0.596308	-3.193106	0.258169
1	-0.503225	-3.669755	1.560877
1	-0.020874	-5.054933	-1.042692
1	-0.894270	-5.661312	0.364551
1	-2.472219	-5.467163	-1.519918
1	-1.124276	-3.814810	-2.771788
1	-0.276918	-2.003628	-1.618329
1	-1.892370	-1.292339	-1.563525
1	-3.025265	-2.137164	-3.449039
1	-4.993181	-3.494149	-3.757526
1	-4.335595	-4.795857	-2.625718
1	-3.960416	-1.613702	-0.727879
1	-3.995175	-1.374623	3.001900
1	-5.634322	-2.276090	-1.520828
1	-5.997080	-1.843535	4.398458
1	-9.331617	-3.185354	1.661083
1	-9.657883	-3.537958	-0.761426
1	-2.466260	-0.349894	1.455261
1	-1.975853	1.539724	1.287859
1	-3.945434	3.469454	-1.244987
1	-0.376721	2.922058	1.070795
1	-0.873871	6.483753	-1.311528
8	-7.715788	-3.097115	-2.623002
6	-8.962045	-3.486494	-3.167598
1	-8.817131	-3.531426	-4.247204
1	-9.270191	-4.475090	-2.807012
1	-9.746247	-2.754737	-2.941913
1	-0.989856	-1.569982	0.576645

re-re_8-path-A

Number of imaginary frequencies : 1
 The smallest frequency is : -337.7303

Electronic energy= -3905.2868776
 Zero-point correction= 1.054077
 Thermal correction to Energy= 1.119661
 Thermal correction to Enthalpy= 1.120606
 Thermal correction to Gibbs Free Energy= 0.949345
 Sum of electronic and zero-point Energies= -3904.232801
 Sum of electronic and thermal Energies= -3904.167216
 Sum of electronic and thermal Enthalpies= -3904.166272
 Sum of electronic and thermal Free Energies= -3904.337533

 Cartesian Coordinates

6	2.024548	-0.394522	4.866830
6	2.971590	0.767104	4.522275
6	3.683151	0.327266	3.226607
7	2.949889	-0.871630	2.781080

6	1.673580	-0.985609	3.493703
6	3.528330	-1.904067	2.175759
6	4.730729	-1.821365	1.483231
8	0.638413	0.062130	-0.109608
6	0.573698	-0.137336	2.823531
8	-0.554714	-0.681828	2.692591
8	0.879552	1.037686	2.523397
8	1.456734	-1.922875	0.234707
1	1.358428	-2.029722	3.523079
1	1.137920	-0.070438	5.416316
1	2.542529	-1.154720	5.460199
1	2.398576	1.673891	4.335060
1	3.688562	0.959064	5.322976
1	3.649919	1.102242	2.458521
1	4.725317	0.045577	3.405000
1	2.939193	-2.816190	2.151466
1	5.305062	-0.910773	1.632463
6	5.590211	-3.036312	1.205412
6	4.870081	-4.391347	1.104551
1	6.347735	-3.109038	1.995556
1	6.151143	-2.868034	0.275972
1	5.640901	-5.168451	1.035553
1	4.284038	-4.600616	2.006131
6	4.013164	-4.441585	-0.116807
6	2.700081	-4.670865	-0.176163
1	4.518519	-4.215658	-1.057504
1	2.122605	-4.923787	0.710150
6	2.006054	-4.527241	-1.484364
8	2.463339	-3.805811	-2.355266
6	0.752539	-5.309315	-1.740704
6	0.385366	-6.404814	-0.953071
6	-0.016730	-4.976886	-2.861757
6	-0.731045	-7.166999	-1.291492
1	0.986797	-6.687021	-0.094290
6	-1.137257	-5.731210	-3.191530
1	0.293700	-4.134524	-3.472418
6	-1.491859	-6.831565	-2.409111
1	-1.002267	-8.026291	-0.686729
1	-1.728250	-5.470431	-4.064031
1	-2.360199	-7.427102	-2.672996
6	3.940242	-1.110978	-0.394995
1	3.645914	-2.114426	-0.689640
1	2.943136	0.858556	-0.341913
6	5.206761	-0.598999	-0.966365
6	5.880435	-1.339815	-1.942952
6	5.735057	0.633677	-0.564761
6	7.055510	-0.852875	-2.511510
1	5.459678	-2.284854	-2.277628
6	6.902233	1.121839	-1.136817
1	5.226328	1.212275	0.201563
6	7.568382	0.377140	-2.110137
1	7.565018	-1.432105	-3.275165
1	7.289505	2.086400	-0.823969
1	8.482450	0.757770	-2.554768
7	1.620859	-0.703516	-0.024932
6	2.883909	-0.213778	-0.225573
7	-0.528518	2.526743	0.602801
6	0.336946	3.434869	-0.004727
6	-0.042509	4.465398	-0.867818
6	0.932545	5.323272	-1.373997
6	2.272013	5.202745	-1.035221
6	2.630389	4.184716	-0.153689
6	1.688200	3.307967	0.357338
6	0.508163	6.388990	-2.344162
9	-0.696523	6.891512	-2.039161
6	4.076880	4.029413	0.207273
9	4.637484	5.197384	0.552128
6	-1.675941	1.962795	0.139321
16	-2.551985	2.448745	-1.222185
7	-2.040432	0.909624	0.903763

6	-3.218061	0.102859	0.691634
6	-2.884994	-1.373242	0.982524
6	-3.993478	-2.332197	0.496359
6	-3.426244	-3.264011	-0.582281
6	-2.328852	-4.125922	0.056158
6	-1.285047	-3.204451	0.713209
7	-1.584982	-1.785740	0.338145
6	-1.603801	-1.638163	-1.147664
6	-2.786789	-2.454782	-1.729542
6	-3.731985	-1.574452	-2.512433
6	-5.057110	-1.685666	-2.564999
6	-4.364279	0.517722	1.611770
6	-5.694534	0.749198	1.143689
6	-6.680388	1.068332	2.124752
7	-6.407174	1.183391	3.455114
6	-5.169358	0.988826	3.837974
6	-4.117019	0.648094	2.955667
6	-8.016725	1.278642	1.706895
6	-8.376758	1.181593	0.387306
6	-7.391185	0.878051	-0.587292
6	-6.079693	0.674647	-0.214499
9	1.374974	7.414420	-2.372951
9	0.424692	5.916372	-3.598464
9	4.801277	3.546871	-0.817980
9	4.259351	3.180590	1.237617
1	-2.690649	-1.481007	2.051622
1	-4.369261	-2.927131	1.333634
1	-4.834161	-1.753968	0.105769
1	-0.269513	-3.397253	0.367360
1	-1.295755	-3.233463	1.804583
1	-1.851345	-4.743992	-0.707510
1	-2.761369	-4.796754	0.803542
1	-4.217688	-3.906020	-0.978290
1	-2.359767	-3.180250	-2.434994
1	-0.626880	-1.990260	-1.487854
1	-1.669937	-0.569372	-1.367581
1	-3.249574	-0.791960	-3.099172
1	-5.651280	-1.011567	-3.173760
1	-5.603750	-2.439877	-2.004077
1	-3.514426	0.215714	-0.353296
1	-3.115641	0.491704	3.350840
1	-5.357984	0.477818	-0.998706
1	-4.963207	1.092323	4.901671
1	-8.747802	1.518781	2.472071
1	-9.408111	1.346954	0.099521
1	-1.422895	0.599025	1.667187
1	-0.060172	1.976434	1.344644
1	-1.081031	4.601446	-1.135281
1	1.969387	2.516355	1.047830
1	3.013119	5.888787	-1.430265
8	-7.662188	0.770438	-1.913388
6	-8.975773	1.060270	-2.351400
1	-8.960741	0.954364	-3.436364
1	-9.705909	0.356995	-1.934091
1	-9.267851	2.085302	-2.095756
1	-0.814404	-1.195371	0.705152

re-re_9-path-A

Number of imaginary frequencies : 2
The smallest frequency is : -305.1552

Electronic energy= -3905.2835932
Zero-point correction= 1.053532
Thermal correction to Energy= 1.118610
Thermal correction to Enthalpy= 1.119555
Thermal correction to Gibbs Free Energy= 0.947311

Sum of electronic and zero-point Energies=	-3904.230061
Sum of electronic and thermal Energies=	-3904.164983
Sum of electronic and thermal Enthalpies=	-3904.164039
Sum of electronic and thermal Free Energies=	-3904.336282

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Cartesian Coordinates
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6	-2.783838	-1.438622	-2.851233
6	-3.203744	0.033352	-2.978195
6	-3.680785	0.415704	-1.569083
7	-3.119522	-0.619922	-0.683853
6	-2.242777	-1.545074	-1.418264
6	-3.642703	-0.913853	0.502704
6	-4.517525	-0.095270	1.204787
8	0.130099	0.703533	0.875423
6	-0.770534	-1.086139	-1.349601
8	0.064716	-1.903796	-0.880756
8	-0.532272	0.052298	-1.809201
8	-1.244043	-0.620560	1.916638
1	-2.328859	-2.545585	-0.986209
1	-2.036664	-1.728230	-3.593517
1	-3.652955	-2.095728	-2.959642
1	-2.344583	0.640987	-3.256578
1	-3.996904	0.172034	-3.715164
1	-3.338101	1.407389	-1.264593
1	-4.773356	0.377676	-1.482526
1	-3.269012	-1.828654	0.958209
1	-4.998706	0.705900	0.649177
6	-5.292345	-0.631373	2.385821
6	-6.807168	-0.628607	2.158018
1	-5.107351	-0.012815	3.273610
1	-4.943686	-1.640141	2.640070
1	-7.321886	-0.850924	3.103064
1	-7.125225	0.390125	1.895826
6	-7.335407	-1.574868	1.124953
6	-6.644167	-2.535439	0.504695
1	-8.391009	-1.480202	0.870120
1	-5.592081	-2.691172	0.713223
6	-7.308698	-3.430527	-0.478509
8	-8.522015	-3.466450	-0.596865
6	-6.440245	-4.307465	-1.330666
6	-5.077555	-4.056012	-1.514412
6	-7.032512	-5.392081	-1.984314
6	-4.316362	-4.881331	-2.337407
1	-4.610972	-3.196461	-1.040263
6	-6.269848	-6.224778	-2.793427
1	-8.094523	-5.564435	-1.842260
6	-4.909914	-5.970601	-2.970427
1	-3.261015	-4.671901	-2.487561
1	-6.733963	-7.070604	-3.290412
1	-4.313813	-6.618007	-3.605931
6	-3.106178	1.269014	2.117905
1	-3.018978	0.552474	2.929540
1	-1.696940	2.356729	0.814456
6	-4.027320	2.405353	2.342166
6	-4.606044	2.594591	3.601913
6	-4.332944	3.306913	1.314531
6	-5.465719	3.665759	3.832238
1	-4.361572	1.911058	4.410519
6	-5.183178	4.379671	1.547282
1	-3.899308	3.167796	0.328007
6	-5.755975	4.560024	2.806632
1	-5.903190	3.803253	4.816018
1	-5.401122	5.076067	0.743685
1	-6.424529	5.395980	2.985970
7	-0.987272	0.485723	1.379068
6	-1.952676	1.463214	1.364603
7	1.774730	1.485248	-1.275827
6	1.465513	2.846462	-1.277827
6	2.404421	3.879688	-1.327828

6	1.960683	5.198815	-1.368291
6	0.609816	5.523142	-1.371330
6	-0.311440	4.480134	-1.342462
6	0.098655	3.156901	-1.299125
6	2.976535	6.305405	-1.375797
9	4.110430	5.943201	-1.991412
6	-1.774746	4.796363	-1.276510
9	-2.090161	5.892829	-1.978197
6	2.752473	0.827124	-0.600183
16	4.081832	1.535684	0.167663
7	2.518390	-0.505189	-0.580208
6	3.380198	-1.484303	0.038438
6	2.525200	-2.555633	0.740999
6	3.366448	-3.451427	1.677140
6	2.893980	-3.267520	3.127512
6	1.447017	-3.768096	3.220062
6	0.596557	-3.028046	2.170494
7	1.418485	-1.935049	1.554837
6	1.930086	-1.010101	2.610998
6	2.913955	-1.779418	3.531980
6	4.277359	-1.130028	3.550119
6	5.452090	-1.753157	3.600211
6	4.276903	-2.184133	-0.980156
6	5.690028	-2.315207	-0.807515
6	6.398691	-3.053347	-1.802194
7	5.802113	-3.603735	-2.896924
6	4.509962	-3.434887	-3.031848
6	3.705837	-2.739220	-2.098121
6	7.795832	-3.231156	-1.655308
6	8.473867	-2.709933	-0.583602
6	7.768666	-1.963227	0.395272
6	6.409377	-1.765786	0.278483
9	2.512695	7.400615	-1.999726
9	3.313186	6.684400	-0.131908
9	-2.178781	5.017973	-0.011078
9	-2.537154	3.787319	-1.742344
1	1.996453	-3.136606	-0.018571
1	3.260724	-4.501189	1.389438
1	4.423358	-3.193765	1.577272
1	-0.280912	-2.542437	2.593364
1	0.277286	-3.664391	1.343071
1	1.050114	-3.589833	4.223552
1	1.409974	-4.845241	3.038077
1	3.530799	-3.844737	3.802817
1	2.516697	-1.715089	4.553612
1	1.043473	-0.648872	3.134887
1	2.392448	-0.157852	2.105608
1	4.264636	-0.039700	3.544561
1	6.380211	-1.191189	3.627141
1	5.542890	-2.836605	3.607251
1	3.992073	-0.964436	0.778092
1	2.636364	-2.649403	-2.275614
1	5.923416	-1.159147	1.033348
1	4.048004	-3.871519	-3.915280
1	8.311405	-3.795377	-2.425533
1	9.542811	-2.864683	-0.498074
1	1.630018	-0.863279	-0.954209
1	0.949527	0.898852	-1.504491
1	3.461963	3.654909	-1.345201
1	-0.619104	2.340301	-1.285844
1	0.283033	6.556176	-1.411580
8	8.364741	-1.407601	1.481106
6	9.770679	-1.515004	1.597943
1	10.039066	-0.974697	2.505969
1	10.089828	-2.559348	1.695717
1	10.281157	-1.055191	0.743949
1	0.792176	-1.400905	0.923208

Number of imaginary frequencies : 2
The smallest frequency is : -305.6570

Electronic energy= -3905.2835932
Zero-point correction= 1.053540
Thermal correction to Energy= 1.118616
Thermal correction to Enthalpy= 1.119560
Thermal correction to Gibbs Free Energy= 0.947335
Sum of electronic and zero-point Energies= -3904.230053
Sum of electronic and thermal Energies= -3904.164977
Sum of electronic and thermal Enthalpies= -3904.164033
Sum of electronic and thermal Free Energies= -3904.336258

Cartesian Coordinates

6	-2.783496	-1.439138	-2.850774
6	-3.203465	0.032818	-2.977782
6	-3.680674	0.415167	-1.568727
7	-3.119567	-0.620504	-0.683438
6	-2.242665	-1.545603	-1.417716
6	-3.642665	-0.914266	0.503137
6	-4.517423	-0.095465	1.205167
8	0.130241	0.703731	0.876013
6	-0.770493	-1.086500	-1.348832
8	0.064880	-1.904203	-0.880311
8	-0.532449	0.052156	-1.807999
8	-1.243835	-0.620965	1.916594
1	-2.328752	-2.546129	-0.985699
1	-2.036179	-1.728695	-3.592934
1	-3.652555	-2.096289	-2.959346
1	-2.344324	0.640515	-3.256092
1	-3.996564	0.171434	-3.714829
1	-3.337968	1.406818	-1.264161
1	-4.773255	0.377176	-1.482301
1	-3.269046	-1.829049	0.958732
1	-4.998516	0.705633	0.649377
6	-5.292623	-0.631545	2.385989
6	-6.807393	-0.628307	2.157830
1	-5.107665	-0.013171	3.273906
1	-4.944323	-1.640458	2.640154
1	-7.322399	-0.850786	3.102680
1	-7.125106	0.390595	1.895882
6	-7.335630	-1.574103	1.124338
6	-6.644521	-2.534745	0.504041
1	-8.391121	-1.479009	0.869201
1	-5.592561	-2.690903	0.712881
6	-7.309038	-3.429359	-0.479606
8	-8.522311	-3.464599	-0.598597
6	-6.440628	-4.306695	-1.331397
6	-5.077718	-4.055951	-1.514462
6	-7.033163	-5.390916	-1.985461
6	-4.316576	-4.881567	-2.337206
1	-4.610893	-3.196718	-1.039975
6	-6.270561	-6.223917	-2.794318
1	-8.095335	-5.562716	-1.843937
6	-4.910411	-5.970434	-2.970654
1	-3.261047	-4.672674	-2.486832
1	-6.734891	-7.069433	-3.291629
1	-4.314356	-6.618063	-3.605975
6	-3.106358	1.268273	2.118218
1	-3.018917	0.551735	2.929834
1	-1.697229	2.356464	0.814988
6	-4.027422	2.404654	2.342773
6	-4.605886	2.593856	3.602640
6	-4.333179	3.306309	1.315261
6	-5.465440	3.665077	3.833201
1	-4.361311	1.910255	4.411156

6	-5.183292	4.379114	1.548242
1	-3.899754	3.167222	0.328639
6	-5.755828	4.559433	2.807716
1	-5.902712	3.802535	4.817075
1	-5.401346	5.075572	0.744729
1	-6.424279	5.395431	2.987241
7	-0.987220	0.485557	1.379338
6	-1.952815	1.462770	1.364912
7	1.774559	1.485128	-1.275507
6	1.465357	2.846338	-1.277785
6	2.404222	3.879590	-1.328109
6	1.960426	5.198690	-1.368904
6	0.609546	5.522978	-1.371946
6	-0.311664	4.479941	-1.342682
6	0.098489	3.156741	-1.299011
6	2.976274	6.305281	-1.376782
9	2.512229	7.400496	-2.000544
6	-1.774998	4.796026	-1.276639
9	-2.090485	5.892763	-1.977868
6	2.752471	0.827120	-0.600007
16	4.081980	1.535790	0.167477
7	2.518414	-0.505196	-0.579820
6	3.380348	-1.484251	0.038735
6	2.525479	-2.555585	0.741462
6	3.366896	-3.451236	1.677585
6	2.894659	-3.267131	3.128007
6	1.447758	-3.767832	3.220844
6	0.597061	-3.027953	2.171347
7	1.418814	-1.935002	1.555372
6	1.930476	-1.009851	2.611323
6	2.914560	-1.778967	3.532254
6	4.277911	-1.129457	3.550094
6	5.452712	-1.752470	3.599998
6	4.276898	-2.184119	-0.979970
6	5.690068	-2.315068	-0.807618
6	6.398555	-3.053359	-1.802313
7	5.801776	-3.603960	-2.896826
6	4.509592	-3.435180	-3.031516
6	3.705627	-2.739410	-2.097730
6	7.795732	-3.231093	-1.655678
6	8.473965	-2.709647	-0.584207
6	7.768942	-1.962765	0.394661
6	6.409621	-1.765395	0.278117
9	3.313390	6.684262	-0.133014
9	4.109948	5.943060	-1.992805
9	-2.179098	5.017058	-0.011121
9	-2.537302	3.787111	-1.742909
1	1.996691	-3.136648	-0.018009
1	3.261126	-4.501043	1.390061
1	4.423786	-3.193578	1.577494
1	-0.280323	-2.542297	2.594343
1	0.277614	-3.664416	1.344082
1	1.050994	-3.589529	4.224382
1	1.410801	-4.844996	3.038951
1	3.531634	-3.844187	3.803304
1	2.517452	-1.714534	4.553938
1	1.043907	-0.648630	3.135290
1	2.392682	-0.157621	2.105763
1	4.265083	-0.039130	3.544472
1	6.380781	-1.190408	3.626715
1	5.543619	-2.835909	3.607100
1	3.992317	-0.964355	0.778290
1	2.636109	-2.649690	-2.275005
1	5.923794	-1.158575	1.032925
1	4.047469	-3.871978	-3.914781
1	8.311169	-3.795441	-2.425902
1	9.542932	-2.864344	-0.498861
1	1.630093	-0.863400	-0.953807
1	0.949265	0.898690	-1.503781
1	3.461774	3.654853	-1.345487

1	-0.619248	2.340128	-1.285386
1	0.282720	6.555985	-1.412463
8	8.365227	-1.406892	1.480253
6	9.771197	-1.514201	1.596800
1	10.039764	-0.973649	2.504626
1	10.090414	-2.558506	1.694769
1	10.281462	-1.054585	0.742572
1	0.792327	-1.401045	0.923766

re-re_11-path-A

Number of imaginary frequencies : 1
The smallest frequency is : -326.4231

Electronic energy=	-3905.2830341
Zero-point correction=	1.053638
Thermal correction to Energy=	1.119430
Thermal correction to Enthalpy=	1.120374
Thermal correction to Gibbs Free Energy=	0.946984
Sum of electronic and zero-point Energies=	-3904.229396
Sum of electronic and thermal Energies=	-3904.163604
Sum of electronic and thermal Enthalpies=	-3904.162660
Sum of electronic and thermal Free Energies=	-3904.336050

Cartesian Coordinates

6	-2.471434	1.226175	3.937358
6	-3.620451	0.361529	3.407475
6	-4.080715	1.126360	2.169615
7	-2.852337	1.767271	1.676902
6	-1.755362	1.696744	2.669928
6	-2.838354	2.600974	0.646355
6	-3.922060	2.812780	-0.201885
8	-0.904758	-0.608979	-0.578509
6	-0.677772	0.707015	2.171389
8	0.277155	1.207581	1.523687
8	-0.845485	-0.500063	2.456408
8	-1.287068	1.406792	-1.302241
1	-1.300573	2.685591	2.765277
1	-1.796741	0.671668	4.590401
1	-2.864054	2.092041	4.480623
1	-3.234547	-0.619255	3.124242
1	-4.430519	0.234180	4.127844
1	-4.512447	0.495108	1.390987
1	-4.807615	1.910767	2.423788
1	-1.872462	3.056972	0.442137
1	-4.910278	2.583491	0.190151
6	-3.831976	3.910897	-1.231933
6	-3.947051	5.348323	-0.673033
1	-4.624147	3.770238	-1.975901
1	-2.872358	3.822199	-1.759003
1	-3.930752	6.050865	-1.513229
1	-4.907872	5.461495	-0.159657
6	-2.819659	5.650887	0.265882
6	-1.658996	6.202743	-0.103549
1	-2.915771	5.336456	1.304681
1	-1.509564	6.537844	-1.126004
6	-0.552473	6.344871	0.879920
8	-0.738924	6.170417	2.073282
6	0.817744	6.694475	0.378428
6	1.188464	6.560709	-0.963235
6	1.763083	7.133039	1.311699
6	2.486149	6.869179	-1.364979
1	0.478565	6.196999	-1.699381
6	3.053426	7.450022	0.908464
1	1.461517	7.218204	2.350475
6	3.417093	7.317612	-0.431593

1	2.768638	6.759064	-2.407456
1	3.778407	7.800461	1.636100
1	4.425940	7.565303	-0.746928
6	-3.879163	1.038751	-1.468632
1	-3.402482	1.695620	-2.189939
1	-3.368022	-0.907090	-0.540940
6	-5.318925	0.787546	-1.695892
6	-5.965826	1.437206	-2.754841
6	-6.058703	-0.093959	-0.897188
6	-7.316172	1.215721	-3.007697
1	-5.395312	2.101614	-3.398367
6	-7.404823	-0.321394	-1.154661
1	-5.577987	-0.619440	-0.078737
6	-8.039913	0.336429	-2.207325
1	-7.800211	1.723078	-3.836164
1	-7.959321	-1.017083	-0.532661
1	-9.092040	0.158263	-2.405332
7	-1.703264	0.278198	-0.938716
6	-3.055731	0.046176	-0.941819
7	0.159669	-2.638036	1.035586
6	-0.857772	-3.538980	0.718329
6	-0.672259	-4.850072	0.280042
6	-1.790755	-5.648912	0.040978
6	-3.084128	-5.186977	0.235584
6	-3.248699	-3.878402	0.688271
6	-2.160117	-3.059834	0.928299
6	-1.572676	-7.041982	-0.476676
9	-0.512077	-7.627997	0.098262
6	-4.636510	-3.338273	0.852818
9	-5.441912	-4.191521	1.499238
6	1.322207	-2.381705	0.383387
16	2.092169	-3.406349	-0.717467
7	1.798538	-1.157309	0.711322
6	3.045009	-0.601495	0.242510
6	2.857214	0.896751	-0.062025
6	4.052635	1.483531	-0.845037
6	3.579072	1.956928	-2.227510
6	2.589603	3.109017	-2.014966
6	1.462961	2.628330	-1.079957
7	1.603172	1.150707	-0.859498
6	1.597471	0.418444	-2.160185
6	2.848404	0.827068	-2.982741
6	3.694730	-0.373861	-3.333985
6	5.023865	-0.420099	-3.377195
6	4.161707	-0.740955	1.275174
6	5.452840	-1.264445	0.954567
6	6.430190	-1.263141	1.994462
7	6.179995	-0.823093	3.259871
6	4.973525	-0.384126	3.520766
6	3.935672	-0.317774	2.560848
6	7.731753	-1.742067	1.709714
6	8.065990	-2.206487	0.463511
6	7.086945	-2.222777	-0.562999
6	5.808800	-1.768474	-0.317214
9	-2.635998	-7.830875	-0.256357
9	-1.348710	-7.052421	-1.800972
9	-5.217546	-3.087798	-0.335311
9	-4.654601	-2.173769	1.533803
1	2.681135	1.425226	0.878438
1	4.483862	2.327291	-0.299077
1	4.834867	0.727251	-0.942643
1	0.467360	2.778857	-1.492932
1	1.499196	3.085266	-0.088881
1	2.175585	3.433830	-2.974715
1	3.099347	3.966950	-1.568732
1	4.433304	2.303059	-2.815470
1	2.488162	1.250361	-3.929872
1	0.655942	0.687025	-2.641207
1	1.565246	-0.650416	-1.931594
1	3.131509	-1.270517	-3.594255

1	5.542770	-1.331409	-3.656908
1	5.648191	0.434245	-3.127534
1	3.315424	-1.128937	-0.674494
1	2.963067	0.070320	2.854117
1	5.088264	-1.833265	-1.123825
1	4.783724	-0.045874	4.537674
1	8.456532	-1.728561	2.517229
1	9.070481	-2.567030	0.276753
1	1.195651	-0.530723	1.253936
1	-0.192093	-1.832480	1.585293
1	0.325698	-5.242691	0.136451
1	-2.284568	-2.036167	1.271512
1	-3.939191	-5.827700	0.050467
8	7.332334	-2.674367	-1.819665
6	8.614174	-3.202722	-2.100197
1	8.585253	-3.525238	-3.141196
1	9.398184	-2.445472	-1.981951
1	8.841942	-4.066109	-1.464596
1	0.780110	0.850150	-0.300405

re-re_12-path-A

Number of imaginary frequencies : 1

The smallest frequency is : -245.7452

Electronic energy= -3905.2806258
 Zero-point correction= 1.053725
 Thermal correction to Energy= 1.119642
 Thermal correction to Enthalpy= 1.120586
 Thermal correction to Gibbs Free Energy= 0.944979
 Sum of electronic and zero-point Energies= -3904.226901
 Sum of electronic and thermal Energies= -3904.160984
 Sum of electronic and thermal Enthalpies= -3904.160040
 Sum of electronic and thermal Free Energies= -3904.335647

Cartesian Coordinates

6	-2.228543	-2.207878	-2.774721
6	-2.822897	-0.806221	-2.982204
6	-3.230615	-0.342544	-1.570071
7	-2.581201	-1.299889	-0.655039
6	-1.607299	-2.126693	-1.372621
6	-3.153699	-1.712419	0.477465
6	-4.099136	-0.995160	1.182265
8	0.512399	0.241857	0.915710
6	-0.227908	-1.442893	-1.427387
8	0.773484	-2.165765	-1.167571
8	-0.211542	-0.240253	-1.769397
8	-0.647190	-1.371077	1.786968
1	-1.506842	-3.093439	-0.876349
1	-1.497135	-2.478136	-3.539947
1	-3.023812	-2.960453	-2.767178
1	-2.068044	-0.134235	-3.388047
1	-3.684127	-0.826612	-3.652738
1	-2.904067	0.678502	-1.362202
1	-4.313083	-0.411224	-1.417717
1	-2.769920	-2.646764	0.880997
1	-4.519552	-0.117569	0.698702
6	-4.965666	-1.643418	2.238323
6	-6.411672	-1.150453	2.153074
1	-4.602095	-1.411529	3.249058
1	-4.934287	-2.735752	2.145545
1	-6.993520	-1.543530	2.997471
1	-6.420228	-0.057812	2.281230
6	-7.147470	-1.476215	0.885177
6	-6.689727	-2.241777	-0.112356
1	-8.129152	-1.014309	0.784207

1	-5.690866	-2.668352	-0.078219
6	-7.360435	-2.416122	-1.426141
8	-6.675015	-2.602563	-2.419085
6	-8.852703	-2.337673	-1.546079
6	-9.710942	-2.717345	-0.509937
6	-9.389292	-1.927524	-2.770561
6	-11.090208	-2.671761	-0.693785
1	-9.299787	-3.072051	0.429618
6	-10.765592	-1.866705	-2.946652
1	-8.709639	-1.657782	-3.572460
6	-11.617828	-2.238397	-1.907117
1	-11.752135	-2.978399	0.109778
1	-11.176485	-1.533475	-3.894353
1	-12.693603	-2.196037	-2.046692
6	-2.684091	0.269296	2.357449
1	-2.514545	-0.593173	2.996106
1	-1.469241	1.671496	1.174693
6	-3.706084	1.233707	2.813138
6	-4.244751	1.114220	4.099128
6	-4.163418	2.262662	1.979390
6	-5.216310	2.006802	4.545338
1	-3.887364	0.326475	4.756833
6	-5.127654	3.155926	2.427394
1	-3.769124	2.352723	0.971628
6	-5.659763	3.028769	3.711246
1	-5.622997	1.904564	5.546464
1	-5.468295	3.951336	1.772025
1	-6.416143	3.725359	4.058523
7	-0.542893	-0.178353	1.418184
6	-1.606600	0.686486	1.596731
7	1.942161	1.445124	-1.206487
6	1.468178	2.748618	-1.042229
6	2.267663	3.892780	-1.030403
6	1.666895	5.142053	-0.885353
6	0.293022	5.288964	-0.763735
6	-0.491414	4.137772	-0.800688
6	0.075524	2.881480	-0.940933
6	2.551002	6.355829	-0.919499
9	2.995697	6.608833	-2.161990
6	-1.969147	4.262824	-0.589850
9	-2.480969	5.345213	-1.191103
6	3.037349	0.860653	-0.651609
16	4.301724	1.664114	0.132113
7	2.987417	-0.485009	-0.770384
6	3.998621	-1.391855	-0.280866
6	3.321042	-2.637184	0.321211
6	4.307344	-3.509046	1.129044
6	3.867157	-3.558346	2.599434
6	2.499593	-4.250995	2.663980
6	1.522931	-3.514366	1.727377
7	2.176670	-2.260737	1.228397
6	2.607199	-1.402768	2.372328
6	3.711342	-2.137094	3.177949
6	4.980898	-1.320833	3.245891
6	6.225623	-1.789824	3.207157
6	4.938358	-1.854578	-1.392102
6	6.361593	-1.838031	-1.261559
6	7.119368	-2.357689	-2.352928
7	6.556038	-2.838911	-3.496871
6	5.249026	-2.814230	-3.585041
6	4.399528	-2.337285	-2.558442
6	8.531734	-2.382025	-2.254087
6	9.178302	-1.920757	-1.136251
6	8.421922	-1.395995	-0.056936
6	7.046037	-1.348307	-0.125852
9	1.910977	7.458571	-0.500806
9	3.635930	6.204512	-0.147478
9	-2.275939	4.369243	0.717259
9	-2.644089	3.191766	-1.049583
1	2.841529	-3.196825	-0.484954

1	4.333645	-4.523447	0.721364
1	5.315439	-3.097844	1.041344
1	0.606178	-3.200420	2.222821
1	1.257125	-4.086585	0.836746
1	2.121408	-4.239526	3.690360
1	2.591859	-5.296547	2.359089
1	4.596431	-4.120470	3.188266
1	3.343050	-2.244101	4.206823
1	1.702094	-1.214898	2.952860
1	2.943486	-0.448987	1.957062
1	4.830220	-0.246754	3.359286
1	7.076799	-1.120141	3.277881
1	6.450828	-2.847412	3.093291
1	4.563174	-0.870608	0.495010
1	3.321829	-2.357189	-2.703959
1	6.516212	-0.906385	0.709657
1	4.812768	-3.194783	-4.506581
1	9.084499	-2.781422	-3.098279
1	10.260228	-1.954114	-1.090040
1	2.141571	-0.928691	-1.158501
1	1.186717	0.781484	-1.463514
1	3.341892	3.808667	-1.128773
1	-0.534447	1.981969	-0.972361
1	-0.156421	6.268420	-0.646631
8	8.982056	-0.921006	1.085092
6	10.393407	-0.855281	1.159684
1	10.622278	-0.406773	2.126715
1	10.848646	-1.851518	1.111324
1	10.808832	-0.224862	0.365083
1	1.466509	-1.741157	0.679737

re-re_13-path-A

Number of imaginary frequencies : 1
 The smallest frequency is : -267.2379

Electronic energy= -3905.2821952
 Zero-point correction= 1.054302
 Thermal correction to Energy= 1.120172
 Thermal correction to Enthalpy= 1.121116
 Thermal correction to Gibbs Free Energy= 0.946620
 Sum of electronic and zero-point Energies= -3904.227893
 Sum of electronic and thermal Energies= -3904.162023
 Sum of electronic and thermal Enthalpies= -3904.161079
 Sum of electronic and thermal Free Energies= -3904.335576

 Cartesian Coordinates

6	-2.748409	-1.209839	-3.344207
6	-3.295645	0.225077	-3.357029
6	-3.831406	0.436663	-1.932256
7	-3.192120	-0.617105	-1.125990
6	-2.213332	-1.379112	-1.915554
6	-3.733769	-1.095076	-0.009922
6	-4.725029	-0.465315	0.726417
8	-0.168422	0.586452	0.773186
6	-0.799273	-0.779829	-1.776677
8	0.118763	-1.569779	-1.428257
8	-0.675010	0.432974	-2.055816
8	-1.527195	-0.834586	1.703804
1	-2.198548	-2.416512	-1.574676
1	-1.973875	-1.374091	-4.096271
1	-3.553002	-1.933475	-3.510735
1	-2.489052	0.929128	-3.557586
1	-4.082976	0.360107	-4.100978
1	-3.590498	1.424817	-1.534064
1	-4.917391	0.294787	-1.880691

1	-3.267316	-1.995563	0.377851
1	-5.287799	0.328981	0.242390
6	-5.445524	-1.226844	1.804060
6	-6.560345	-2.153938	1.249674
1	-5.905914	-0.519447	2.503060
1	-4.728609	-1.827185	2.381051
1	-7.192541	-2.485798	2.079785
1	-7.187893	-1.579298	0.560679
6	-5.973400	-3.344289	0.555858
6	-5.779981	-3.423521	-0.765992
1	-5.647948	-4.164479	1.194770
1	-6.143883	-2.633537	-1.421579
6	-5.197225	-4.578757	-1.495613
8	-5.465438	-4.732838	-2.675778
6	-4.286410	-5.556747	-0.809141
6	-3.440046	-5.202519	0.246167
6	-4.240088	-6.859641	-1.315845
6	-2.573724	-6.143626	0.796597
1	-3.444059	-4.186875	0.627303
6	-3.386316	-7.801625	-0.756535
1	-4.882112	-7.114117	-2.152839
6	-2.551542	-7.444388	0.301852
1	-1.918174	-5.860833	1.614578
1	-3.365118	-8.813699	-1.147660
1	-1.880350	-8.179092	0.735610
6	-3.483341	0.967106	1.868369
1	-3.434718	0.198761	2.634230
1	-2.037229	2.164397	0.702771
6	-4.484265	2.034497	2.070680
6	-5.264716	2.042952	3.232488
6	-4.663354	3.055806	1.128553
6	-6.197485	3.053268	3.451343
1	-5.122046	1.263696	3.976446
6	-5.588580	4.066994	1.350504
1	-4.076869	3.057491	0.215063
6	-6.361216	4.067266	2.511950
1	-6.791538	3.050788	4.359684
1	-5.705068	4.856032	0.614620
1	-7.086921	4.855995	2.682473
7	-1.293254	0.303294	1.229055
6	-2.290176	1.248814	1.216653
7	1.430183	1.983200	-1.061556
6	0.955148	3.282166	-0.887472
6	1.716789	4.390299	-0.511431
6	1.102777	5.640130	-0.421168
6	-0.239772	5.829030	-0.708928
6	-0.981328	4.716021	-1.104478
6	-0.406792	3.460584	-1.191158
6	1.939163	6.802734	0.032803
9	3.147742	6.802901	-0.547820
6	-2.427152	4.909181	-1.450357
9	-2.590990	5.772066	-2.462988
6	2.431395	1.311918	-0.433289
16	3.612383	1.984649	0.571901
7	2.360605	-0.014444	-0.690280
6	3.283832	-1.008178	-0.194169
6	2.498041	-2.267198	0.217810
6	3.358864	-3.274089	1.011349
6	2.773526	-3.452290	2.420216
6	1.368831	-4.057032	2.283222
6	0.526683	-3.161840	1.352542
7	1.296784	-1.911727	1.055194
6	1.660901	-1.209090	2.323125
6	2.644703	-2.091109	3.134495
6	3.946608	-1.370322	3.395544
6	5.161845	-1.912229	3.412677
6	4.310938	-1.412365	-1.248823
6	5.715246	-1.456333	-0.985427
6	6.559084	-1.907784	-2.043938
7	6.093934	-2.273718	-3.271623

6	4.802421	-2.197125	-3.477909
6	3.872573	-1.776697	-2.497329
6	7.955083	-1.985207	-1.819990
6	8.505650	-1.638437	-0.613014
6	7.664908	-1.181500	0.434269
6	6.302540	-1.086832	0.246448
9	1.359021	7.979882	-0.248527
9	2.148362	6.776271	1.358996
9	-3.130932	5.400198	-0.414290
9	-3.025157	3.757061	-1.811879
1	2.066847	-2.715794	-0.679841
1	3.378927	-4.238449	0.496203
1	4.388595	-2.913383	1.064147
1	-0.411473	-2.834660	1.799344
1	0.311833	-3.620696	0.385303
1	0.896376	-4.134461	3.266957
1	1.434921	-5.066757	1.869194
1	3.409011	-4.120078	3.007542
1	2.180642	-2.277899	4.111914
1	0.714328	-1.033391	2.836822
1	2.079256	-0.236239	2.049710
1	3.845814	-0.305788	3.609943
1	6.038595	-1.310008	3.628667
1	5.337610	-2.965077	3.206013
1	3.789705	-0.587290	0.676575
1	2.813415	-1.746615	-2.743189
1	5.708568	-0.703472	1.067770
1	4.445268	-2.486134	-4.464503
1	8.574684	-2.329146	-2.641711
1	9.577493	-1.708557	-0.471389
1	1.546151	-0.383773	-1.200430
1	0.715177	1.367768	-1.490211
1	2.771638	4.282461	-0.298574
1	-0.989970	2.596635	-1.499733
1	-0.694095	6.811412	-0.641787
8	8.129013	-0.816954	1.656962
6	9.528379	-0.813638	1.866169
1	9.678990	-0.452119	2.883600
1	9.953983	-1.820049	1.777353
1	10.037250	-0.139409	1.167835
1	0.677025	-1.285315	0.507854

re-re_14-path-A

Number of imaginary frequencies : 1
The smallest frequency is : -339.9548

Electronic energy= -3905.2854612
Zero-point correction= 1.054558
Thermal correction to Energy= 1.119952
Thermal correction to Enthalpy= 1.120896
Thermal correction to Gibbs Free Energy= 0.950687
Sum of electronic and zero-point Energies= -3904.230903
Sum of electronic and thermal Energies= -3904.165509
Sum of electronic and thermal Enthalpies= -3904.164565
Sum of electronic and thermal Free Energies= -3904.334774

Cartesian Coordinates

6	-2.019624	1.585724	4.308960
6	-3.197901	0.616282	4.112495
6	-3.758625	0.949969	2.715274
7	-2.764692	1.855310	2.114426
6	-1.513166	1.837882	2.882126
6	-3.070059	2.839791	1.276075
6	-4.244879	2.906295	0.533983
8	-0.724714	-0.047834	-0.393335

6	-0.591532	0.688105	2.422133
8	0.603224	0.984828	2.162205
8	-1.106516	-0.452828	2.392947
8	-1.191722	2.067257	-0.629412
1	-0.993843	2.789415	2.754521
1	-1.241894	1.177539	4.958023
1	-2.366110	2.532320	4.735743
1	-2.843155	-0.412916	4.128965
1	-3.959043	0.741125	4.885142
1	-3.881096	0.056737	2.100321
1	-4.716317	1.477209	2.769576
1	-2.277489	3.563630	1.114875
1	-5.060004	2.266281	0.859303
6	-4.673024	4.179552	-0.163725
6	-3.705316	5.367192	-0.095115
1	-5.625309	4.506726	0.267941
1	-4.895189	3.970763	-1.220064
1	-4.217678	6.221541	-0.558434
1	-3.514005	5.648891	0.946856
6	-2.404836	5.199572	-0.822586
6	-1.233614	5.666093	-0.374690
1	-2.421279	4.722758	-1.803781
1	-1.171882	6.160699	0.591706
6	-0.006269	5.598351	-1.206761
8	-0.017422	5.178718	-2.353285
6	1.275128	6.095434	-0.607203
6	2.247954	6.619637	-1.463843
6	1.543349	5.988263	0.760077
6	3.469667	7.045441	-0.958093
1	2.027748	6.681328	-2.525128
6	2.779927	6.386804	1.262145
1	0.801547	5.564936	1.431740
6	3.739207	6.922876	0.405450
1	4.215942	7.465531	-1.624794
1	2.992008	6.284366	2.321603
1	4.696947	7.247566	0.800211
6	-3.773496	1.557293	-1.067213
1	-3.332153	2.396365	-1.599216
1	-3.123826	-0.481947	-0.511666
6	-5.142761	1.167588	-1.474942
6	-5.751468	1.788087	-2.570708
6	-5.839303	0.159020	-0.795870
6	-7.024718	1.403734	-2.984281
1	-5.212950	2.558451	-3.116286
6	-7.105177	-0.229298	-1.213276
1	-5.386215	-0.323696	0.065754
6	-7.703509	0.394542	-2.308113
1	-7.482046	1.888947	-3.840720
1	-7.622102	-1.024008	-0.685194
1	-8.693565	0.091120	-2.633082
7	-1.556793	0.868704	-0.560410
6	-2.884578	0.557654	-0.680011
7	-0.126441	-2.524102	0.805695
6	-1.188933	-3.334924	0.412315
6	-1.086455	-4.541256	-0.283327
6	-2.245510	-5.260565	-0.577663
6	-3.503485	-4.830233	-0.189511
6	-3.587986	-3.634562	0.524520
6	-2.460347	-2.891463	0.823948
6	-2.090324	-6.539227	-1.351235
9	-1.173144	-7.344993	-0.794106
6	-4.944020	-3.169181	0.962125
9	-5.570849	-4.085593	1.713635
6	1.093663	-2.321013	0.240979
16	1.794107	-3.244338	-0.990295
7	1.703266	-1.238515	0.776063
6	3.015448	-0.760119	0.405165
6	3.001990	0.780270	0.358619
6	4.260240	1.368595	-0.316756
6	3.854884	2.132452	-1.586991

6	2.970764	3.318978	-1.179235
6	1.803793	2.797811	-0.319895
7	1.793785	1.299973	-0.373856
6	1.727703	0.829320	-1.790494
6	3.029334	1.234044	-2.529813
6	3.748807	0.026828	-3.083025
6	5.066224	-0.151648	-3.143387
6	4.083279	-1.195311	1.406223
6	5.323007	-1.787906	1.012451
6	6.258303	-2.084871	2.048356
7	6.014680	-1.853473	3.369296
6	4.855457	-1.333116	3.689015
6	3.862207	-0.982625	2.744091
6	7.508852	-2.649123	1.698131
6	7.834159	-2.912141	0.392295
6	6.896838	-2.627301	-0.634048
6	5.667613	-2.084848	-0.326125
9	-3.238301	-7.230508	-1.422496
9	-1.687057	-6.311994	-2.610815
9	-5.751076	-2.919831	-0.085089
9	-4.890891	-2.034668	1.686798
1	2.870865	1.155189	1.376324
1	4.772459	2.047836	0.370564
1	4.958154	0.562953	-0.557051
1	0.826085	3.117883	-0.679307
1	1.893566	3.058902	0.736627
1	2.577553	3.824415	-2.066827
1	3.547822	4.055656	-0.611928
1	4.747362	2.493450	-2.104989
1	2.733247	1.850294	-3.388759
1	0.833466	1.294915	-2.209456
1	1.567448	-0.251779	-1.767114
1	3.097480	-0.748146	-3.488837
1	5.488276	-1.051595	-3.579303
1	5.775068	0.576865	-2.757347
1	3.244518	-1.157982	-0.585485
1	2.927484	-0.544464	3.087058
1	4.974555	-1.913183	-1.141281
1	4.670412	-1.161059	4.747666
1	8.202583	-2.865773	2.503912
1	8.799505	-3.344046	0.156489
1	1.188607	-0.649588	1.445223
1	-0.432449	-1.756634	1.432071
1	-0.119293	-4.915046	-0.590790
1	-2.531309	-1.962106	1.384064
1	-4.391022	-5.407283	-0.423405
8	7.136581	-2.862551	-1.949291
6	8.362336	-3.471744	-2.305803
1	8.334356	-3.591652	-3.389078
1	9.219563	-2.843220	-2.037297
1	8.472835	-4.457725	-1.840077
1	0.932499	0.970902	0.101401

re-re_15-path-A

Number of imaginary frequencies : 1

The smallest frequency is : -289.7023

Electronic energy= -3905.2818704

Zero-point correction= 1.054383

Thermal correction to Energy= 1.120007

Thermal correction to Enthalpy= 1.120951

Thermal correction to Gibbs Free Energy= 0.947297

Sum of electronic and zero-point Energies= -3904.227487

Sum of electronic and thermal Energies= -3904.161863

Sum of electronic and thermal Enthalpies= -3904.160919

Sum of electronic and thermal Free Energies= -3904.334574

Cartesian Coordinates

6	-2.392878	-2.412768	-2.522773
6	-3.038705	-1.037312	-2.759048
6	-3.417309	-0.528954	-1.353256
7	-2.755364	-1.461908	-0.423602
6	-1.769245	-2.288400	-1.124943
6	-3.274574	-1.821103	0.749608
6	-4.212670	-1.082998	1.449284
8	0.296188	0.350120	0.984290
6	-0.406770	-1.572326	-1.199910
8	0.608751	-2.235692	-0.854615
8	-0.424736	-0.403335	-1.643142
8	-0.781286	-1.250781	1.979704
1	-1.648509	-3.240133	-0.604760
1	-1.654651	-2.669979	-3.285766
1	-3.158269	-3.195735	-2.503444
1	-2.317123	-0.358480	-3.210867
1	-3.917268	-1.107632	-3.403787
1	-3.074660	0.493854	-1.184095
1	-4.497746	-0.575150	-1.174007
1	-2.851671	-2.721451	1.189289
1	-4.689677	-0.268134	0.913387
6	-5.021831	-1.691918	2.571329
6	-6.504446	-1.280904	2.466708
1	-4.656365	-1.368862	3.555827
1	-4.939422	-2.785028	2.553232
1	-7.066385	-1.753241	3.280099
1	-6.581981	-0.194087	2.592188
6	-7.068317	-1.684150	1.139751
6	-7.426354	-0.818558	0.185418
1	-7.134108	-2.755171	0.945573
1	-7.412533	0.252590	0.382939
6	-7.968581	-1.190881	-1.146152
8	-8.739969	-0.436861	-1.714605
6	-7.567122	-2.482595	-1.800167
6	-6.339642	-3.112863	-1.565653
6	-8.451165	-3.027889	-2.736856
6	-6.016558	-4.284162	-2.247099
1	-5.629681	-2.681429	-0.864191
6	-8.131005	-4.200903	-3.407525
1	-9.388101	-2.513536	-2.924387
6	-6.912252	-4.832136	-3.161763
1	-5.064009	-4.771292	-2.062228
1	-8.827937	-4.622729	-4.124579
1	-6.658916	-5.747414	-3.687587
6	-2.886393	0.327780	2.464000
1	-2.657803	-0.454506	3.182693
1	-1.750860	1.702190	1.173554
6	-3.949107	1.281910	2.849779
6	-4.459918	1.260364	4.151524
6	-4.481565	2.192274	1.926605
6	-5.480180	2.131576	4.526331
1	-4.045317	0.565325	4.876680
6	-5.497178	3.061932	2.301559
1	-4.104367	2.207492	0.907814
6	-6.002775	3.031317	3.602059
1	-5.865162	2.105908	5.540773
1	-5.899210	3.762932	1.576914
1	-6.801303	3.707051	3.891157
7	-0.734664	-0.081277	1.528224
6	-1.835146	0.740533	1.658785
7	1.672690	1.381581	-1.277166
6	1.161498	2.680573	-1.221807
6	1.923958	3.841411	-1.371395
6	1.290309	5.080237	-1.329159
6	-0.082402	5.200059	-1.151855
6	-0.828568	4.032000	-1.027099
6	-0.226313	2.783487	-1.065094

6	2.128864	6.322153	-1.430675
9	3.181872	6.151975	-2.242508
6	-2.297406	4.120643	-0.746393
9	-2.860105	5.206485	-1.291335
6	2.799113	0.887633	-0.699875
16	4.057410	1.802672	-0.035368
7	2.789146	-0.464438	-0.683646
6	3.838866	-1.286780	-0.130703
6	3.219314	-2.482601	0.619008
6	4.253815	-3.216796	1.500570
6	3.846019	-3.101287	2.977280
6	2.514241	-3.841341	3.158821
6	1.490291	-3.273117	2.157232
7	2.070279	-2.057898	1.497455
6	2.475179	-1.050017	2.523217
6	3.630938	-1.628703	3.380761
6	4.857173	-0.748591	3.318502
6	6.124241	-1.153737	3.287147
6	4.766713	-1.838749	-1.210497
6	6.191048	-1.752306	-1.126260
6	6.941350	-2.373899	-2.168672
7	6.368770	-3.009332	-3.229821
6	5.060089	-3.039940	-3.283483
6	4.218389	-2.474991	-2.295960
6	8.355623	-2.336620	-2.108230
6	9.010977	-1.717300	-1.075209
6	8.261666	-1.086295	-0.048707
6	6.883580	-1.099696	-0.080559
9	1.423851	7.363795	-1.900388
9	2.615950	6.691923	-0.235063
9	-2.544085	4.178965	0.577292
9	-2.969349	3.046402	-1.204121
1	2.756618	-3.150152	-0.111953
1	4.307859	-4.272076	1.218497
1	5.244614	-2.787149	1.336463
1	0.563596	-2.947885	2.626117
1	1.245935	-3.963900	1.348051
1	2.151699	-3.717459	4.183355
1	2.650913	-4.911780	2.985389
1	4.611970	-3.552057	3.613889
1	3.290627	-1.625611	4.424702
1	1.572604	-0.841361	3.100254
1	2.753185	-0.136177	1.991964
1	4.651333	0.322164	3.324397
1	6.938521	-0.436613	3.260404
1	6.405778	-2.203985	3.276577
1	4.406657	-0.669130	0.567774
1	3.138786	-2.550903	-2.406030
1	6.357542	-0.575869	0.708897
1	4.615615	-3.541840	-4.140833
1	8.902292	-2.818694	-2.912118
1	10.094234	-1.706642	-1.056077
1	1.949792	-0.967371	-1.004533
1	0.932046	0.674141	-1.445895
1	2.992687	3.774921	-1.524309
1	-0.805455	1.867789	-0.974161
1	-0.558958	6.173322	-1.123781
8	8.830895	-0.444672	1.003535
6	10.241286	-0.336733	1.034758
1	10.479511	0.240731	1.928238
1	10.720113	-1.320350	1.106768
1	10.623331	0.192229	0.154145
1	1.324065	-1.651020	0.901385

re-re_16-path-A

Number of imaginary frequencies : 1

The smallest frequency is : -344.9900

Electronic energy= -3905.2799411
Zero-point correction= 1.053932
Thermal correction to Energy= 1.119565
Thermal correction to Enthalpy= 1.120509
Thermal correction to Gibbs Free Energy= 0.945873
Sum of electronic and zero-point Energies= -3904.226009
Sum of electronic and thermal Energies= -3904.160376
Sum of electronic and thermal Enthalpies= -3904.159432
Sum of electronic and thermal Free Energies= -3904.334068

Cartesian Coordinates

6	1.358360	-2.013943	3.971096
6	2.267327	-0.788398	3.788653
6	2.840162	-0.932516	2.365043
7	2.034252	-1.993077	1.735184
6	0.853146	-2.308782	2.552825
6	2.509525	-2.842580	0.832143
6	3.650843	-2.654783	0.058498
8	-0.446605	-0.425601	-0.565819
6	-0.335738	-1.397492	2.188043
8	-1.423561	-1.969247	1.910602
8	-0.124611	-0.165691	2.238156
8	0.456127	-2.357531	-1.006970
1	0.568842	-3.349573	2.391896
1	0.540046	-1.830961	4.670736
1	1.934745	-2.873299	4.328209
1	1.678417	0.125195	3.853947
1	3.062838	-0.754257	4.535656
1	2.761174	-0.002113	1.799619
1	3.886560	-1.256723	2.370596
1	1.880926	-3.710174	0.646894
1	4.361621	-1.906930	0.395833
6	4.225347	-3.897917	-0.600104
6	5.041181	-3.731309	-1.882662
1	3.396370	-4.580950	-0.821528
1	4.857501	-4.421203	0.131654
1	5.303149	-4.732787	-2.251822
1	4.426424	-3.295591	-2.678191
6	6.312727	-2.946924	-1.794023
6	6.877188	-2.430952	-0.697710
1	6.838296	-2.783024	-2.734544
1	6.429187	-2.548516	0.283662
6	8.151740	-1.674314	-0.819254
8	8.820054	-1.708557	-1.839714
6	8.619553	-0.857669	0.350094
6	7.766752	-0.459860	1.383929
6	9.957551	-0.452252	0.370403
6	8.247747	0.330033	2.424218
1	6.716883	-0.737099	1.363846
6	10.441105	0.323701	1.415743
1	10.600929	-0.758049	-0.448108
6	9.585560	0.716472	2.444507
1	7.578227	0.647098	3.217480
1	11.483013	0.627609	1.429206
1	9.960267	1.328122	3.259444
6	2.861492	-1.268799	-1.421964
1	2.596553	-2.115070	-2.050473
1	1.829053	0.516162	-0.652593
6	4.092902	-0.518381	-1.778588
6	4.648940	-0.643223	-3.055282
6	4.708377	0.332974	-0.855763
6	5.809189	0.047695	-3.392538
1	4.168509	-1.286191	-3.788578
6	5.868566	1.023022	-1.190417
1	4.274493	0.452415	0.134823
6	6.428910	0.872888	-2.457721
1	6.235093	-0.065874	-4.384480

1	6.337457	1.675015	-0.459856
1	7.345120	1.395125	-2.713241
7	0.558540	-1.119567	-0.822769
6	1.792407	-0.530366	-0.917922
7	-1.710845	1.678559	0.869018
6	-0.912088	2.757438	0.489885
6	-1.379733	3.973279	-0.016673
6	-0.464924	4.978901	-0.319735
6	0.900821	4.820637	-0.124871
6	1.347170	3.610398	0.399205
6	0.463377	2.589863	0.708906
6	-0.971261	6.261445	-0.916318
9	-2.205854	6.562854	-0.491795
6	2.820861	3.381949	0.550898
9	3.463121	4.478550	0.975772
6	-2.852144	1.199492	0.308745
16	-3.812801	1.992659	-0.835810
7	-3.131633	-0.043328	0.762297
6	-4.282623	-0.824906	0.376692
6	-3.863609	-2.296929	0.195613
6	-4.952718	-3.135380	-0.509284
6	-4.413147	-3.661395	-1.847870
6	-3.244675	-4.609864	-1.549166
6	-2.207955	-3.866300	-0.685161
7	-2.588977	-2.418783	-0.601004
6	-2.707495	-1.827225	-1.966694
6	-3.879375	-2.507172	-2.720842
6	-4.909727	-1.496347	-3.165691
6	-6.229406	-1.666223	-3.182240
6	-5.386127	-0.775009	1.430766
6	-6.752112	-0.498515	1.112973
6	-7.688977	-0.543938	2.188463
7	-7.340285	-0.814255	3.478117
6	-6.074130	-1.038822	3.729182
6	-5.063143	-1.034834	2.739131
6	-9.056518	-0.298937	1.914641
6	-9.492806	-0.023596	0.644310
6	-8.557663	0.029511	-0.421253
6	-7.217668	-0.194891	-0.187109
9	-0.175819	7.299667	-0.609801
9	-1.024371	6.199843	-2.257013
9	3.388326	3.028907	-0.615195
9	3.097729	2.393177	1.424259
1	-3.599740	-2.704435	1.174266
1	-5.247193	-3.978130	0.122476
1	-5.843188	-2.522074	-0.665122
1	-1.202640	-3.888712	-1.101598
1	-2.165893	-4.224319	0.345302
1	-2.787332	-4.947167	-2.483805
1	-3.604074	-5.496150	-1.020062
1	-5.200943	-4.198001	-2.382856
1	-3.460080	-2.956074	-3.631055
1	-1.736698	-1.988450	-2.438940
1	-2.846706	-0.749983	-1.841630
1	-4.500036	-0.552236	-3.525853
1	-6.888630	-0.881696	-3.539761
1	-6.707494	-2.579999	-2.837580
1	-4.650911	-0.425133	-0.570035
1	-4.033405	-1.239600	3.023924
1	-6.540355	-0.114112	-1.029317
1	-5.809016	-1.246110	4.764171
1	-9.748068	-0.337928	2.749864
1	-10.545698	0.158540	0.465687
1	-2.451856	-0.524071	1.368575
1	-1.181397	0.976861	1.418384
1	-2.438881	4.132241	-0.164627
1	0.812662	1.649869	1.128929
1	1.595886	5.619095	-0.359838
8	-8.906876	0.294750	-1.706028
6	-10.260889	0.601674	-1.978681

1	-10.312619	0.810925	-3.047326
1	-10.920843	-0.242670	-1.747213
1	-10.591798	1.486923	-1.423792
1	-1.824757	-1.920895	-0.106443

re-re_17-path-A

Number of imaginary frequencies : 1
The smallest frequency is : -263.5058

Electronic energy= -3905.279822
Zero-point correction= 1.051203
Thermal correction to Energy= 1.116934
Thermal correction to Enthalpy= 1.117878
Thermal correction to Gibbs Free Energy= 0.945925
Sum of electronic and zero-point Energies= -3904.228619
Sum of electronic and thermal Energies= -3904.162889
Sum of electronic and thermal Enthalpies= -3904.161944
Sum of electronic and thermal Free Energies= -3904.333897

Cartesian Coordinates

6	2.035907	-3.245619	-4.164222
6	2.284837	-4.674548	-3.651623
6	2.867275	-4.493798	-2.232601
7	2.672725	-3.068553	-1.924691
6	1.747956	-2.453798	-2.879634
6	3.544766	-2.319456	-1.241037
6	4.451644	-2.817413	-0.321180
8	-0.312056	-2.611905	0.397772
6	0.303700	-2.696279	-2.439825
8	-0.438489	-1.617785	-2.487783
8	-0.080524	-3.809475	-2.130127
8	1.377487	-1.243471	0.307533
1	1.940103	-1.381789	-2.948162
1	1.216785	-3.189603	-4.884845
1	2.936288	-2.835032	-4.630301
1	1.344455	-5.222223	-3.596193
1	2.972629	-5.223826	-4.297392
1	2.351831	-5.121202	-1.502008
1	3.939115	-4.711432	-2.195164
1	4.603987	-3.893319	-0.328912
6	3.012043	-3.076356	1.406444
1	3.188528	-2.035072	1.656583
1	1.267432	-4.361717	1.007310
6	3.818394	-4.077225	2.133824
6	4.671891	-3.660053	3.160746
6	3.751625	-5.441823	1.820796
6	5.433098	-4.586218	3.868591
1	4.723429	-2.605130	3.417004
6	4.511530	-6.364662	2.527158
1	3.110539	-5.775932	1.008726
6	5.354562	-5.939488	3.554138
1	6.085108	-4.248869	4.667909
1	4.451280	-7.418578	2.274810
1	5.949199	-6.662071	4.103720
7	0.902486	-2.379327	0.541986
6	1.734996	-3.389587	0.972428
7	-0.224024	1.205252	-0.207871
6	0.515717	2.329484	0.197454
6	0.248346	3.628973	-0.228307
6	1.061824	4.672472	0.214365
6	2.150348	4.448869	1.044408
6	2.419353	3.139790	1.441744
6	1.607962	2.091460	1.039663
6	0.711878	6.075935	-0.190344
9	0.254404	6.140490	-1.450614

6	3.598744	2.888286	2.333974
9	4.757640	3.238894	1.744363
6	-1.579580	1.043787	-0.139791
16	-2.690039	2.304336	0.016485
7	-1.949753	-0.251078	-0.216039
6	-3.314019	-0.707324	-0.021398
6	-3.492750	-2.091859	-0.673391
6	-4.988771	-2.510432	-0.685014
6	-5.445388	-2.693773	-2.140558
6	-4.626738	-3.835093	-2.756776
6	-3.125830	-3.495841	-2.592270
7	-2.946384	-2.129656	-2.051396
6	-3.634036	-1.164647	-2.929674
6	-5.172057	-1.421211	-2.965261
6	-5.955666	-0.198571	-2.556521
6	-7.051423	-0.169282	-1.801312
6	-3.674412	-0.798854	1.462452
6	-4.862344	-0.224025	2.016309
6	-5.113815	-0.451679	3.402155
7	-4.276746	-1.160515	4.212110
6	-3.186417	-1.645509	3.672111
6	-2.845735	-1.495482	2.306724
6	-6.291055	0.081121	3.981257
6	-7.187137	0.808419	3.240659
6	-6.926696	1.045711	1.866930
6	-5.787276	0.545420	1.274815
9	-0.250996	6.590254	0.591829
9	1.765173	6.903748	-0.102102
9	3.713096	1.597684	2.686960
9	3.524973	3.604611	3.466552
1	-2.891756	-2.811674	-0.105348
1	-5.126282	-3.449225	-0.139613
1	-5.599687	-1.755576	-0.183517
1	-2.590364	-3.539712	-3.545753
1	-2.612599	-4.178800	-1.912397
1	-4.886043	-3.953484	-3.814110
1	-4.862650	-4.779117	-2.256190
1	-6.511596	-2.937651	-2.171188
1	-5.447333	-1.641500	-4.006201
1	-3.189743	-1.271814	-3.923832
1	-3.401403	-0.152866	-2.582848
1	-5.569710	0.744464	-2.947420
1	-7.547698	0.767497	-1.567904
1	-7.488833	-1.067886	-1.373461
1	-3.971515	0.014263	-0.509631
1	-1.924785	-1.939149	1.935937
1	-5.618210	0.779707	0.231355
1	-2.521626	-2.204088	4.328969
1	-6.458405	-0.108177	5.036615
1	-8.079441	1.203067	3.711837
1	-1.226180	-0.970760	-0.153802
1	0.328670	0.347451	-0.257559
1	-0.578139	3.821824	-0.899608
1	1.808289	1.077451	1.372260
1	2.781856	5.270456	1.366072
8	-7.756329	1.762984	1.063541
6	-8.896533	2.360159	1.648585
1	-9.394051	2.907877	0.847853
1	-9.587522	1.608928	2.049289
1	-8.619933	3.061621	2.444334
1	-1.431631	-1.841596	-2.220245
1	3.416994	-1.253329	-1.402572
6	5.637793	-2.029219	0.213037
6	5.377696	-0.687854	0.949210
1	6.320537	-1.817674	-0.619684
1	6.189561	-2.681640	0.898347
1	5.006108	-0.883287	1.960955
1	6.333526	-0.164676	1.050445
6	4.384506	0.143135	0.209455
6	4.633803	1.162650	-0.617419

1	3.346983	-0.179358	0.286433
1	5.628877	1.583145	-0.734450
6	3.502282	1.683763	-1.430736
8	2.571002	0.941059	-1.723185
6	3.499127	3.108385	-1.868384
6	4.426521	4.033494	-1.378507
6	2.485623	3.533499	-2.733274
6	4.332101	5.372510	-1.743218
1	5.197771	3.719834	-0.683467
6	2.399102	4.868779	-3.104089
1	1.766406	2.801875	-3.087646
6	3.319257	5.790116	-2.603601
1	5.041457	6.092459	-1.347836
1	1.604784	5.198914	-3.765235
1	3.238595	6.837931	-2.876394

re-re_18-path-A

Number of imaginary frequencies : 1
 The smallest frequency is : -346.9098

Electronic energy= -3905.2799682
 Zero-point correction= 1.053943
 Thermal correction to Energy= 1.119561
 Thermal correction to Enthalpy= 1.120505
 Thermal correction to Gibbs Free Energy= 0.946489
 Sum of electronic and zero-point Energies= -3904.226025
 Sum of electronic and thermal Energies= -3904.160407
 Sum of electronic and thermal Enthalpies= -3904.159463
 Sum of electronic and thermal Free Energies= -3904.333479

 Cartesian Coordinates

6	1.371138	-1.987691	3.967657
6	2.274372	-0.759415	3.778179
6	2.856441	-0.918021	2.360793
7	2.041055	-1.970376	1.729003
6	0.864119	-2.290642	2.551912
6	2.507144	-2.812487	0.814275
6	3.647997	-2.623744	0.039833
8	-0.430603	-0.363782	-0.556764
6	-0.333274	-1.390820	2.185502
8	-1.409778	-1.973823	1.887194
8	-0.140443	-0.157131	2.253687
8	0.466514	-2.292387	-1.021713
1	0.587172	-3.334102	2.395438
1	0.553409	-1.804841	4.667955
1	1.951948	-2.842964	4.327558
1	1.679083	0.150887	3.828973
1	3.065190	-0.711909	4.529403
1	2.798127	0.009742	1.788722
1	3.897942	-1.258345	2.378026
1	1.872679	-3.674346	0.622441
1	4.366838	-1.888094	0.387048
6	4.209605	-3.863123	-0.637005
6	5.025620	-3.686081	-1.918069
1	3.373547	-4.534415	-0.867531
1	4.837320	-4.403320	0.086226
1	5.276126	-4.684712	-2.302648
1	4.414754	-3.231784	-2.706098
6	6.305933	-2.917279	-1.819186
6	6.876993	-2.424804	-0.715454
1	6.832770	-2.745611	-2.757588
1	6.427719	-2.552030	0.264124
6	8.160809	-1.682128	-0.825166
8	8.826823	-1.704977	-1.847442
6	8.642183	-0.896186	0.359596

6	7.796183	-0.504030	1.401145
6	9.987174	-0.515008	0.388024
6	8.290701	0.256329	2.456983
1	6.741712	-0.762619	1.376111
6	10.484061	0.230823	1.448893
1	10.625245	-0.815707	-0.436498
6	9.635252	0.617981	2.485341
1	7.626663	0.569132	3.256506
1	11.531295	0.515498	1.468657
1	10.020706	1.205901	3.312680
6	2.873421	-1.212313	-1.423006
1	2.601442	-2.049396	-2.060780
1	1.854132	0.571338	-0.633612
6	4.111565	-0.469487	-1.772661
6	4.662296	-0.584381	-3.052560
6	4.739944	0.362517	-0.840957
6	5.829885	0.096526	-3.384681
1	4.171675	-1.211619	-3.792721
6	5.908066	1.041843	-1.170109
1	4.309913	0.474340	0.152122
6	6.462736	0.901320	-2.441030
1	6.251284	-0.009421	-4.379381
1	6.388273	1.677429	-0.432464
1	7.384844	1.415134	-2.692409
7	0.572556	-1.056860	-0.822334
6	1.809375	-0.471946	-0.911145
7	-1.742372	1.686093	0.895311
6	-0.946040	2.765497	0.511386
6	-1.417174	3.983604	0.014180
6	-0.503466	4.988124	-0.296244
6	0.864030	4.825862	-0.117289
6	1.313541	3.612663	0.397253
6	0.431055	2.593224	0.713521
6	-1.012098	6.273475	-0.884599
9	-2.245466	6.572672	-0.455131
6	2.787844	3.377858	0.529310
9	3.440940	4.470641	0.947251
6	-2.878722	1.200761	0.330344
16	-3.848635	1.997091	-0.803913
7	-3.143743	-0.050006	0.770429
6	-4.284260	-0.841547	0.374671
6	-3.845117	-2.304251	0.169556
6	-4.922082	-3.143401	-0.552580
6	-4.373556	-3.636617	-1.900224
6	-3.194742	-4.576760	-1.616934
6	-2.169631	-3.837763	-0.735486
7	-2.567055	-2.396095	-0.625739
6	-2.688353	-1.781139	-1.981009
6	-3.851665	-2.459826	-2.749773
6	-4.893019	-1.453293	-3.178079
6	-6.210700	-1.637674	-3.198724
6	-5.386786	-0.822577	1.430704
6	-6.756465	-0.557287	1.119237
6	-7.690565	-0.628224	2.195786
7	-7.336385	-0.913428	3.480703
6	-6.067408	-1.128003	3.726172
6	-5.058408	-1.097989	2.734532
6	-9.061090	-0.393049	1.928383
6	-9.502921	-0.104018	0.663020
6	-8.570833	-0.026905	-0.403738
6	-7.228051	-0.240617	-0.175571
9	-0.215830	7.310323	-0.575337
9	-1.068826	6.218703	-2.225513
9	3.338025	3.023391	-0.644548
9	3.071286	2.386250	1.397598
1	-3.578171	-2.725222	1.141597
1	-5.206622	-4.001849	0.062291
1	-5.820000	-2.538407	-0.698040
1	-1.162924	-3.840919	-1.148778
1	-2.127079	-4.214594	0.288296

1	-2.730704	-4.890494	-2.556483
1	-3.544994	-5.477294	-1.106022
1	-5.153989	-4.171927	-2.447224
1	-3.426048	-2.886800	-3.667515
1	-1.715028	-1.925072	-2.453565
1	-2.838314	-0.707534	-1.838369
1	-4.493493	-0.499357	-3.523398
1	-6.878068	-0.855053	-3.545155
1	-6.678931	-2.561991	-2.868885
1	-4.659267	-0.432971	-0.565556
1	-4.025806	-1.294662	3.014644
1	-6.553503	-0.140678	-1.017977
1	-5.798032	-1.347359	4.757557
1	-9.750521	-0.450480	2.764307
1	-10.557863	0.070661	0.489162
1	-2.456896	-0.530129	1.368987
1	-1.207263	0.984332	1.438624
1	-2.477662	4.144947	-0.121396
1	0.781894	1.649385	1.123409
1	1.558336	5.623366	-0.357800
8	-8.925798	0.251716	-1.684055
6	-10.283197	0.550156	-1.949262
1	-10.339895	0.770917	-3.015341
1	-10.935394	-0.302194	-1.725383
1	-10.619803	1.426425	-1.383621
1	-1.810048	-1.900927	-0.117629

re-re_19-path-A

Number of imaginary frequencies : 1

The smallest frequency is : -303.4645

Electronic energy=	-3905.2777633
Zero-point correction=	1.053035
Thermal correction to Energy=	1.119052
Thermal correction to Enthalpy=	1.119996
Thermal correction to Gibbs Free Energy=	0.945264
Sum of electronic and zero-point Energies=	-3904.224728
Sum of electronic and thermal Energies=	-3904.158711
Sum of electronic and thermal Enthalpies=	-3904.157767
Sum of electronic and thermal Free Energies=	-3904.332499

Cartesian Coordinates

6	1.532749	-2.472233	3.545836
6	2.441110	-1.235886	3.434719
6	2.932514	-1.239755	1.973584
7	2.098833	-2.243379	1.291412
6	0.958029	-2.630848	2.130694
6	2.567404	-3.019394	0.314891
6	3.673308	-2.727935	-0.464616
8	-0.536678	-0.635132	-0.764529
6	-0.234056	-1.675427	1.923945
8	-1.356817	-2.197916	1.703569
8	0.014190	-0.452739	2.038705
8	0.390016	-2.503204	-1.387701
1	0.652949	-3.649646	1.886270
1	0.750696	-2.354255	4.299051
1	2.120526	-3.361747	3.792837
1	1.868762	-0.330362	3.630453
1	3.278362	-1.284911	4.134499
1	2.820506	-0.262908	1.498973
1	3.978955	-1.555770	1.895383
1	1.964153	-3.895199	0.088061
1	4.344699	-1.948440	-0.115113
6	4.290926	-3.839189	-1.290378
6	5.602298	-3.455823	-1.992963

1	3.573515	-4.204200	-2.037376
1	4.501602	-4.694147	-0.634689
1	6.088879	-4.380412	-2.328832
1	5.413065	-2.857634	-2.887614
6	6.544786	-2.702019	-1.098287
6	7.319249	-1.696758	-1.516444
1	6.596480	-3.018890	-0.054605
1	7.316461	-1.394007	-2.561554
6	8.332006	-1.009296	-0.673026
8	9.384143	-0.639341	-1.165243
6	8.054327	-0.760968	0.780511
6	6.761208	-0.521377	1.254339
6	9.138870	-0.667235	1.657017
6	6.556103	-0.189023	2.590902
1	5.926630	-0.552073	0.560716
6	8.929791	-0.369419	2.997995
1	10.138851	-0.828649	1.266937
6	7.638267	-0.125277	3.465227
1	5.553899	0.037804	2.944069
1	9.773085	-0.313221	3.678976
1	7.477483	0.126166	4.509019
6	2.735560	-1.269331	-1.865622
1	2.500481	-2.122946	-2.495999
1	1.656155	0.399401	-0.921245
6	3.899583	-0.439431	-2.256878
6	4.447038	-0.566521	-3.538434
6	4.422990	0.528109	-1.391957
6	5.495629	0.253640	-3.944232
1	4.034370	-1.301837	-4.224630
6	5.480470	1.338896	-1.791226
1	4.002879	0.642725	-0.394911
6	6.020398	1.202869	-3.068990
1	5.905769	0.149129	-4.943887
1	5.879765	2.076330	-1.102662
1	6.847732	1.832629	-3.379758
7	0.465860	-1.281633	-1.129111
6	1.666832	-0.625865	-1.261420
7	-1.452249	1.540572	0.806503
6	-0.602629	2.598363	0.492313
6	-0.977460	3.810708	-0.092771
6	-0.007887	4.787573	-0.317052
6	1.321304	4.609252	0.033997
6	1.676974	3.402929	0.635887
6	0.742607	2.407943	0.863289
6	-0.424505	6.056837	-1.005287
9	-1.653297	6.445538	-0.637282
6	3.103206	3.221354	1.063962
9	3.444912	4.073077	2.040808
6	-2.654233	1.164737	0.296642
16	-3.629007	2.060057	-0.755428
7	-2.995457	-0.074504	0.723044
6	-4.223088	-0.759842	0.389359
6	-3.922753	-2.253641	0.157177
6	-5.107702	-3.009060	-0.483690
6	-4.688827	-3.554032	-1.857649
6	-3.557512	-4.570826	-1.648607
6	-2.420485	-3.897914	-0.854813
7	-2.717674	-2.435901	-0.728330
6	-2.894138	-1.821196	-2.077736
6	-4.152583	-2.420354	-2.756121
6	-5.152015	-1.345068	-3.113183
6	-6.477621	-1.444748	-3.052842
6	-5.260179	-0.649458	1.504207
6	-6.618190	-0.271759	1.265486
6	-7.496194	-0.266930	2.390233
7	-7.098754	-0.580497	3.655550
6	-5.840509	-0.898878	3.833880
6	-4.886843	-0.952327	2.789672
6	-8.855721	0.077390	2.194466
6	-9.339276	0.402201	0.953238

6	-8.461170	0.407023	-0.161052
6	-7.129983	0.084899	-0.003164
9	0.414818	7.069676	-0.736865
9	-0.446174	5.913836	-2.340581
9	3.959017	3.437239	0.050261
9	3.351705	1.979021	1.524853
1	-3.617488	-2.697524	1.107421
1	-5.417352	-3.837144	0.159988
1	-5.963272	-2.336514	-0.580155
1	-1.448924	-3.965630	-1.343415
1	-2.322332	-4.272611	0.165545
1	-3.188412	-4.924058	-2.615697
1	-3.929740	-5.440815	-1.101551
1	-5.539584	-4.040641	-2.341300
1	-3.825083	-2.878492	-3.698730
1	-1.969768	-2.035307	-2.617696
1	-2.957455	-0.738936	-1.936919
1	-4.714692	-0.413285	-3.473707
1	-7.112603	-0.615747	-3.348503
1	-6.983802	-2.341119	-2.702605
1	-4.614148	-0.316359	-0.528521
1	-3.860740	-1.233159	3.016154
1	-6.495258	0.129474	-0.880305
1	-5.535152	-1.140019	4.850249
1	-9.502288	0.073908	3.065845
1	-10.385053	0.659378	0.834666
1	-2.323723	-0.616263	1.282065
1	-0.959484	0.784192	1.317536
1	-2.008493	3.990713	-0.363571
1	1.026735	1.469994	1.334680
1	2.057127	5.386565	-0.140718
8	-8.858079	0.718512	-1.421429
6	-10.201717	1.115600	-1.618429
1	-10.294497	1.346062	-2.679973
1	-10.901999	0.310849	-1.365229
1	-10.447040	2.010430	-1.035249
1	-1.894579	-1.982994	-0.286622

re-re_20-path-A

Number of imaginary frequencies : 1
 The smallest frequency is : -358.0010

Electronic energy= -3905.2716859
 Zero-point correction= 1.054367
 Thermal correction to Energy= 1.119945
 Thermal correction to Enthalpy= 1.120889
 Thermal correction to Gibbs Free Energy= 0.948087
 Sum of electronic and zero-point Energies= -3904.217319
 Sum of electronic and thermal Energies= -3904.151741
 Sum of electronic and thermal Enthalpies= -3904.150797
 Sum of electronic and thermal Free Energies= -3904.323599

 Cartesian Coordinates

6	0.697815	-1.345587	4.916263
6	1.633404	-0.137806	4.763174
6	2.438998	-0.426488	3.482669
7	1.729059	-1.537362	2.823802
6	0.429890	-1.786236	3.472701
6	2.329737	-2.467675	2.093318
6	3.594117	-2.390263	1.511274
8	-0.236149	-0.305857	0.021886
6	-0.686222	-0.943056	2.822619
8	-1.687844	-1.581009	2.398784
8	-0.518036	0.294805	2.803602
8	0.878319	-2.159977	-0.252483

1	0.177371	-2.843417	3.378159
1	-0.223303	-1.099915	5.448780
1	1.200641	-2.158803	5.449158
1	1.048911	0.771108	4.629637
1	2.290898	-0.015739	5.626142
1	2.481420	0.442966	2.824583
1	3.460539	-0.757151	3.702081
1	1.713205	-3.337786	1.878253
1	4.304968	-1.694656	1.948213
6	4.153225	-3.726452	1.015988
6	3.952134	-4.080553	-0.462646
1	3.675881	-4.523213	1.596544
1	5.216392	-3.792793	1.264978
1	4.007377	-5.172248	-0.575375
1	2.932703	-3.812841	-0.773594
6	4.942986	-3.499125	-1.424461
6	6.046090	-2.820264	-1.097863
1	4.763474	-3.677439	-2.484939
1	6.289653	-2.611906	-0.062171
6	6.995156	-2.368774	-2.151541
8	6.786607	-2.587589	-3.333893
6	8.251162	-1.671750	-1.723357
6	8.366777	-1.022626	-0.490630
6	9.326905	-1.650248	-2.616605
6	9.547136	-0.365819	-0.155740
1	7.522208	-0.978040	0.191617
6	10.510605	-1.009542	-2.274035
1	9.212432	-2.144210	-3.576137
6	10.621713	-0.366640	-1.041138
1	9.623041	0.153057	0.794777
1	11.346231	-1.005323	-2.966646
1	11.544166	0.140157	-0.774580
6	3.234406	-0.918966	-0.067943
1	3.199837	-1.740007	-0.775732
1	1.939749	0.779776	0.441350
6	4.443404	-0.047048	-0.131503
6	5.038726	0.170511	-1.382013
6	4.922737	0.661693	0.972155
6	6.068536	1.092870	-1.525122
1	4.675933	-0.376445	-2.248090
6	5.967979	1.573710	0.831987
1	4.465566	0.518003	1.946047
6	6.537090	1.797779	-0.417253
1	6.514442	1.251267	-2.502135
1	6.322115	2.120671	1.700539
1	7.347323	2.511135	-0.529387
7	0.849465	-0.923730	-0.032305
6	2.029878	-0.255963	0.155995
7	-1.879796	1.889991	0.900643
6	-1.041093	2.941371	0.521519
6	-1.435186	4.059766	-0.216750
6	-0.492874	5.041380	-0.516064
6	0.827755	4.949153	-0.098563
6	1.196388	3.840472	0.659507
6	0.280318	2.852421	0.980704
6	-0.916698	6.207674	-1.362578
9	-2.180511	6.577645	-1.111868
6	2.636530	3.670092	1.041209
9	3.211657	4.832000	1.383794
6	-2.859148	1.275703	0.183083
16	-3.575183	1.866407	-1.230733
7	-3.188635	0.083359	0.726835
6	-4.194705	-0.814300	0.208799
6	-3.668797	-2.260636	0.280944
6	-4.546828	-3.253355	-0.511527
6	-3.720877	-3.879823	-1.644848
6	-2.579908	-4.689064	-1.013281
6	-1.779321	-3.770683	-0.069435
7	-2.258362	-2.360527	-0.241224
6	-2.136344	-1.939003	-1.670070

6	-3.098276	-2.788658	-2.539823
6	-4.083872	-1.920391	-3.286248
6	-5.359906	-2.204520	-3.534589
6	-5.492022	-0.743353	1.010624
6	-6.775666	-0.605417	0.397351
6	-7.911838	-0.622535	1.260492
7	-7.823871	-0.739115	2.615665
6	-6.626717	-0.837101	3.138980
6	-5.433531	-0.849880	2.377697
6	-9.204090	-0.515164	0.691413
6	-9.380840	-0.397102	-0.663070
6	-8.248595	-0.369877	-1.517499
6	-6.976298	-0.464024	-0.994924
9	-0.136621	7.281366	-1.160331
9	-0.848635	5.921842	-2.673040
9	3.353891	3.168042	0.022909
9	2.794324	2.824764	2.077552
1	-3.578212	-2.542225	1.332215
1	-4.915535	-4.040691	0.151901
1	-5.419722	-2.732756	-0.911356
1	-0.712624	-3.753301	-0.285970
1	-1.919019	-4.007347	0.987324
1	-1.927642	-5.091443	-1.793771
1	-2.985608	-5.536297	-0.454306
1	-4.352377	-4.537454	-2.247651
1	-2.485886	-3.298212	-3.295353
1	-1.084144	-2.081306	-1.923129
1	-2.351082	-0.867525	-1.714798
1	-3.672978	-0.985938	-3.669541
1	-5.983989	-1.520015	-4.100214
1	-5.836950	-3.116546	-3.184020
1	-4.380699	-0.538794	-0.830838
1	-4.475870	-0.946225	2.884675
1	-6.144832	-0.410529	-1.687786
1	-6.570355	-0.921433	4.222605
1	-10.051621	-0.528668	1.368832
1	-10.381894	-0.315014	-1.068949
1	-2.636081	-0.284290	1.515895
1	-1.451952	1.296813	1.632854
1	-2.458914	4.162926	-0.549007
1	0.560287	1.993478	1.584949
1	1.547913	5.721681	-0.344299
8	-8.337000	-0.249882	-2.866801
6	-9.625063	-0.149246	-3.443519
1	-9.467217	-0.066723	-4.519057
1	-10.229894	-1.039995	-3.236539
1	-10.155836	0.742689	-3.091073
1	-1.637945	-1.744232	0.317290

Conformational Study of First-Michael-addition_path-B [8-9]TS

si-si_1-path-B

Number of imaginary frequencies : 1

The smallest frequency is : -396.6294

Electronic energy= -3905.2863505

Zero-point correction= 1.050351

Thermal correction to Energy= 1.116093

Thermal correction to Enthalpy= 1.117037

Thermal correction to Gibbs Free Energy= 0.944934

Sum of electronic and zero-point Energies= -3904.235999

Sum of electronic and thermal Energies= -3904.170258

Sum of electronic and thermal Enthalpies= -3904.169314

Sum of electronic and thermal Free Energies= -3904.341417

Cartesian Coordinates			
6	3.984730	-2.386204	1.323688
6	4.875075	-2.029028	2.518314
6	5.439801	-0.663739	2.129242
7	4.364225	-0.071834	1.314241
6	3.321527	-1.042713	0.974506
6	4.389045	1.168184	0.856332
6	3.327979	1.834361	0.238977
8	0.217588	1.586948	0.560725
6	2.073168	-0.833284	1.833414
8	0.980033	-1.207451	1.238702
8	2.163068	-0.399211	2.973635
8	-0.650886	3.545894	0.149236
1	3.057843	-0.960407	-0.084360
1	3.248399	-3.163152	1.537957
1	4.592336	-2.715694	0.475754
1	4.268407	-1.933519	3.421774
1	5.661982	-2.763755	2.694328
1	5.655896	-0.019663	2.984810
1	6.344141	-0.760833	1.517285
1	2.464135	1.225289	-0.023119
6	2.310877	2.643746	1.844077
1	1.987729	1.665619	2.181351
1	1.304055	4.521507	1.224133
6	3.356492	3.259512	2.695258
6	3.916963	2.477779	3.715246
6	3.826840	4.561639	2.499523
6	4.923022	2.991336	4.525216
1	3.547453	1.463397	3.855145
6	4.837532	5.072202	3.310649
1	3.407219	5.179646	1.710801
6	5.387187	4.291067	4.323816
1	5.342373	2.380328	5.318953
1	5.194942	6.084853	3.151851
1	6.171333	4.694033	4.956955
7	0.252835	2.844817	0.641619
6	1.311276	3.443857	1.270071
7	0.059835	-1.226439	-1.687738
6	1.211727	-1.924557	-2.009150
6	2.047864	-1.375707	-2.990251
6	3.271533	-1.967861	-3.283385
6	3.688599	-3.125576	-2.641629
6	2.840566	-3.671574	-1.679318
6	1.627608	-3.089193	-1.342839
6	4.172108	-1.285456	-4.271605
9	4.804447	-0.233178	-3.711417
6	3.259047	-4.948043	-1.005914
9	2.612993	-5.151761	0.151731
6	-0.995576	-1.608509	-0.881962
16	-1.596656	-3.183055	-0.798888
7	-1.495899	-0.558678	-0.225309
6	-2.666931	-0.542241	0.627050
6	-2.273350	-0.032300	2.029439
6	-3.487458	-0.028508	2.995420
6	-3.166329	-0.904239	4.213503
6	-1.952247	-0.300170	4.932590
6	-0.794768	-0.159400	3.913544
7	-1.148727	-0.801101	2.623669
6	-1.515136	-2.212511	2.878232
6	-2.788515	-2.327684	3.765290
6	-3.876409	-3.105608	3.065961
6	-5.181732	-2.845359	3.077835
6	-3.732092	0.381736	0.045647
6	-5.077173	-0.044876	-0.193283
6	-5.994228	0.935806	-0.675335
7	-5.648263	2.232539	-0.923520
6	-4.402551	2.574611	-0.706293

6	-3.407141	1.686574	-0.227647
6	-7.338834	0.558341	-0.904383
6	-7.774845	-0.721183	-0.668721
6	-6.860124	-1.693984	-0.193151
6	-5.540611	-1.361503	0.030159
9	5.123525	-2.102108	-4.740691
9	3.493247	-0.804224	-5.321315
9	4.577699	-4.948544	-0.730410
9	3.031252	-6.018825	-1.778455
1	-1.880100	0.981595	1.898323
1	-3.707170	0.992919	3.321351
1	-4.378960	-0.400050	2.484457
1	0.129597	-0.620157	4.265494
1	-0.565630	0.888187	3.696360
1	-1.654893	-0.942939	5.767961
1	-2.212991	0.676386	5.351916
1	-4.026077	-0.937983	4.889714
1	-2.517454	-2.896398	4.665648
1	-0.648176	-2.672917	3.362581
1	-1.647767	-2.711770	1.913980
1	-3.527160	-3.976490	2.508304
1	-5.882531	-3.476129	2.539328
1	-5.602653	-1.994395	3.607383
1	-3.036377	-1.566305	0.689245
1	-2.398671	2.071046	-0.082708
1	-4.880171	-2.146142	0.379265
1	-4.131060	3.609810	-0.910651
1	-8.016491	1.322191	-1.271908
1	-8.811556	-0.977117	-0.852078
1	-0.969598	0.317624	-0.267341
1	0.015914	-0.255045	-1.999186
1	1.736421	-0.480496	-3.522818
1	1.009185	-3.516014	-0.565266
1	4.638477	-3.589902	-2.880435
8	-7.208008	-2.981947	0.068008
6	-8.539813	-3.377140	-0.194628
1	-8.595504	-4.435742	0.060486
1	-9.256112	-2.822208	0.423041
1	-8.796687	-3.249967	-1.252843
1	0.093010	-0.955405	1.807014
6	3.629264	3.001185	-0.673291
1	3.069487	3.887953	-0.346872
1	4.694783	3.252611	-0.636836
1	5.307738	1.715961	1.071040
6	3.215046	2.728507	-2.135021
1	3.827183	1.918129	-2.547535
1	3.395867	3.628292	-2.731697
6	1.771049	2.336432	-2.211095
6	0.747067	3.135496	-2.521922
1	1.524164	1.310811	-1.941207
1	0.899179	4.177955	-2.787756
6	-0.633370	2.585635	-2.553819
8	-0.849127	1.386840	-2.412420
6	-1.768573	3.502098	-2.861262
6	-1.756537	4.847268	-2.482015
6	-2.878070	2.975608	-3.528981
6	-2.849000	5.658399	-2.774327
1	-0.916749	5.241431	-1.918311
6	-3.958096	3.793593	-3.839296
1	-2.880780	1.922112	-3.790372
6	-3.943444	5.135286	-3.461618
1	-2.849028	6.698027	-2.462664
1	-4.818746	3.381505	-4.355813
1	-4.791759	5.771653	-3.693932

Number of imaginary frequencies : 1
The smallest frequency is : -192.6124

Electronic energy= -3905.2830184
Zero-point correction= 1.050350
Thermal correction to Energy= 1.116625
Thermal correction to Enthalpy= 1.117569
Thermal correction to Gibbs Free Energy= 0.941811
Sum of electronic and zero-point Energies= -3904.232668
Sum of electronic and thermal Energies= -3904.166394
Sum of electronic and thermal Enthalpies= -3904.165450
Sum of electronic and thermal Free Energies= -3904.341208

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Cartesian Coordinates
.....

7	-2.612267	0.310611	-0.457748
6	-3.917014	0.797553	-0.654086
6	-4.898182	0.087008	-1.346566
6	-6.158580	0.652271	-1.516988
6	-6.462234	1.918366	-1.035379
6	-5.463766	2.626128	-0.373628
6	-4.204140	2.080178	-0.174881
6	-7.189852	-0.102598	-2.306175
9	-7.079383	-1.427249	-2.141762
6	-5.779605	4.009832	0.115576
9	-6.911563	4.029910	0.838192
6	-2.223416	-0.956528	-0.141859
16	-3.282691	-2.241926	0.155386
7	-0.878402	-1.086134	-0.088261
6	-0.176786	-2.252206	0.413006
6	1.033844	-2.616522	-0.472236
6	1.572802	-4.020930	-0.114348
6	1.418771	-4.950247	-1.327684
6	2.304771	-4.404975	-2.453434
6	1.886652	-2.953102	-2.746773
7	0.680328	-2.594929	-1.931862
6	-0.433682	-3.528670	-2.250356
6	-0.038530	-4.974313	-1.832207
6	-1.050202	-5.563453	-0.878312
6	-0.791772	-6.324433	0.182603
6	0.304988	-2.043777	1.846955
6	-0.019919	-2.947386	2.906764
6	0.548770	-2.680767	4.188614
7	1.342999	-1.604743	4.448429
6	1.584053	-0.779989	3.459949
6	1.094458	-0.960171	2.144361
6	0.277182	-3.570208	5.256609
6	-0.520979	-4.671181	5.083868
6	-1.101315	-4.922340	3.813828
6	-0.859829	-4.073848	2.754465
9	-8.437416	0.246481	-1.957266
9	-7.075894	0.134844	-3.624762
9	-5.967005	4.863021	-0.906043
9	-4.805292	4.517113	0.881086
1	1.813912	-1.854081	-0.374397
1	2.627796	-3.944398	0.157221
1	1.027579	-4.418236	0.745401
1	1.602003	-2.794173	-3.789743
1	2.657450	-2.229202	-2.483944
1	2.205730	-5.026310	-3.348827
1	3.351967	-4.417362	-2.140919
1	1.734122	-5.963473	-1.063577
1	-0.058181	-5.592447	-2.739793
1	-0.609102	-3.443773	-3.325054
1	-1.333430	-3.181776	-1.734844
1	-2.090366	-5.338292	-1.116928
1	-1.595501	-6.709619	0.802297
1	0.219580	-6.585332	0.484201
1	-0.893706	-3.072879	0.383702
1	1.335577	-0.220217	1.383863

1	-1.353047	-4.292506	1.815010
1	2.207030	0.084384	3.687751
1	0.724723	-3.347042	6.219631
1	-0.709940	-5.333709	5.919958
1	-0.334757	-0.243476	-0.254998
1	-1.900060	1.041175	-0.406438
1	-4.684060	-0.898095	-1.739148
1	-3.435247	2.642209	0.343018
1	-7.450943	2.344372	-1.169095
8	-1.910685	-5.981987	3.561205
6	-2.227605	-6.851905	4.631106
1	-2.898567	-7.604782	4.217168
1	-1.333617	-7.347803	5.027332
1	-2.741368	-6.322536	5.441626
1	0.433688	-1.554466	-2.223379
6	1.444930	2.683420	-3.528539
6	1.635438	4.146695	-3.118339
6	2.421754	4.046661	-1.808259
7	2.029867	2.738664	-1.267531
6	1.144724	2.013252	-2.185277
6	2.576055	2.216554	-0.169918
6	3.295046	2.919541	0.773812
8	-1.249562	3.091679	-0.407281
6	1.321304	0.490169	-2.201160
8	2.401931	-0.017842	-1.855203
8	0.280212	-0.128423	-2.583868
8	-0.031916	1.671436	0.693291
1	0.098631	2.208155	-1.911311
1	0.639728	2.531259	-4.248115
1	2.373791	2.271363	-3.941138
1	0.658554	4.603317	-2.930932
1	2.158848	4.745262	-3.865981
1	2.183785	4.847663	-1.101361
1	3.507043	4.051234	-1.975641
1	2.346875	1.174766	0.005301
1	3.649437	3.921490	0.540627
6	4.018761	2.173911	1.860542
6	5.440898	1.742600	1.455583
1	4.093784	2.802770	2.755332
1	3.436056	1.288024	2.144919
1	5.960441	1.334736	2.332823
1	6.008745	2.629167	1.154101
6	5.493511	0.727784	0.342653
6	4.644015	-0.293753	0.189449
1	6.300941	0.838823	-0.379175
1	3.850153	-0.492797	0.908684
6	4.745698	-1.314397	-0.879086
8	4.299415	-2.438616	-0.690016
6	5.416685	-0.987241	-2.177209
6	6.111516	-2.005577	-2.835408
6	5.308209	0.274888	-2.769869
6	6.721952	-1.757504	-4.059623
1	6.171772	-2.984738	-2.370037
6	5.906010	0.514885	-4.003183
1	4.713298	1.038462	-2.279047
6	6.619852	-0.496023	-4.643733
1	7.272903	-2.546767	-4.561211
1	5.808354	1.490342	-4.469709
1	7.090582	-0.303889	-5.603100
6	1.379754	3.653812	1.864218
1	1.368514	2.679634	2.344218
1	0.071109	4.871829	0.583134
6	2.010291	4.754779	2.614878
6	2.420023	4.538267	3.935611
6	2.203364	6.021431	2.045765
6	2.996815	5.566680	4.675872
1	2.268079	3.561178	4.386778
6	2.778487	7.046176	2.784811
1	1.911870	6.198706	1.013761
6	3.176687	6.822137	4.102878

1	3.302044	5.385756	5.701514
1	2.922291	8.022048	2.332029
1	3.628615	7.624102	4.677710
7	-0.324027	2.853327	0.396338
6	0.377981	3.902085	0.945238

si-si_3-path-B

Number of imaginary frequencies : 1

The smallest frequency is : -397.6919

Electronic energy= -3905.2863455
 Zero-point correction= 1.050467
 Thermal correction to Energy= 1.116175
 Thermal correction to Enthalpy= 1.117119
 Thermal correction to Gibbs Free Energy= 0.945292
 Sum of electronic and zero-point Energies= -3904.235878
 Sum of electronic and thermal Energies= -3904.170171
 Sum of electronic and thermal Enthalpies= -3904.169227
 Sum of electronic and thermal Free Energies= -3904.341053

Cartesian Coordinates

6	3.975712	-2.463171	1.253114
6	4.873256	-2.139407	2.451848
6	5.444168	-0.769136	2.091909
7	4.363493	-0.148794	1.305419
6	3.319887	-1.108033	0.935463
6	4.382885	1.107383	0.894183
6	3.318861	1.792365	0.302195
8	0.199484	1.554260	0.604621
6	2.069158	-0.914708	1.794915
8	0.972883	-1.244443	1.180191
8	2.159683	-0.529587	2.952628
8	-0.656565	3.531812	0.261869
1	3.062600	-0.997327	-0.122710
1	3.234544	-3.239010	1.453721
1	4.577652	-2.778912	0.395878
1	4.271079	-2.061392	3.359943
1	5.656509	-2.882697	2.607076
1	5.675985	-0.149110	2.960853
1	6.340017	-0.857829	1.466294
1	2.457280	1.189284	0.018918
6	2.296765	2.550930	1.928755
1	1.966200	1.563752	2.230778
1	1.304085	4.456178	1.372279
6	3.342139	3.129807	2.805950
6	3.890048	2.310063	3.802492
6	3.824579	4.433578	2.655465
6	4.896290	2.787920	4.634001
1	3.511648	1.294727	3.906661
6	4.835847	4.908031	3.487608
1	3.414004	5.080746	1.885577
6	5.373280	4.089111	4.477333
1	5.305758	2.147108	5.409140
1	5.203630	5.921778	3.363536
1	6.157854	4.464022	5.126942
7	0.242348	2.808254	0.729433
6	1.304215	3.377524	1.380031
7	0.042584	-1.184184	-1.737262
6	1.207905	-1.850956	-2.075387
6	2.050074	-1.225544	-3.006713
6	3.290596	-1.769769	-3.310881
6	3.719841	-2.960027	-2.736950
6	2.864990	-3.584814	-1.832277
6	1.633283	-3.048963	-1.480175
6	4.215003	-1.006248	-4.213906

9	4.979849	-0.144686	-3.510714
6	3.291111	-4.899016	-1.240259
9	2.661041	-5.168527	-0.087356
6	-1.005166	-1.595624	-0.936042
16	-1.592743	-3.176273	-0.888711
7	-1.509218	-0.565203	-0.251563
6	-2.678197	-0.572403	0.603652
6	-2.282268	-0.099327	2.018139
6	-3.493619	-0.125705	2.987604
6	-3.164398	-1.032017	4.180522
6	-1.950443	-0.441774	4.911293
6	-0.796946	-0.268037	3.892708
7	-1.151821	-0.877774	2.587595
6	-1.510891	-2.296702	2.806770
6	-2.781599	-2.441218	3.693577
6	-3.867894	-3.204435	2.975731
6	-5.174401	-2.950574	2.997697
6	-3.743158	0.368838	0.049722
6	-5.088704	-0.049722	-0.199707
6	-6.004245	0.943732	-0.658007
7	-5.656919	2.246024	-0.872022
6	-4.411380	2.581632	-0.643761
6	-3.416978	1.680529	-0.188013
6	-7.348837	0.573081	-0.898791
6	-7.786369	-0.711399	-0.695096
6	-6.873581	-1.696103	-0.240754
6	-5.554006	-1.370637	-0.007916
9	5.055656	-1.811485	-4.875118
9	3.551056	-0.275163	-5.118485
9	4.613327	-4.917314	-0.983664
9	3.048820	-5.922842	-2.070210
1	-1.894543	0.919597	1.912903
1	-3.715552	0.885854	3.341637
1	-4.385573	-0.486255	2.469396
1	0.130563	-0.733553	4.229583
1	-0.574191	0.786235	3.702288
1	-1.647029	-1.105886	5.727592
1	-2.214227	0.521720	5.358009
1	-4.021365	-1.087629	4.858821
1	-2.506185	-3.032354	4.578036
1	-0.640397	-2.765479	3.276630
1	-1.644020	-2.771147	1.830215
1	-3.516263	-4.057760	2.393056
1	-5.873580	-3.569312	2.443337
1	-5.598051	-2.116641	3.551638
1	-3.047934	-1.597700	0.638285
1	-2.408196	2.060268	-0.032071
1	-4.895396	-2.164016	0.324763
1	-4.138891	3.621741	-0.819806
1	-8.025056	1.346455	-1.248677
1	-8.822921	-0.961941	-0.886734
1	-0.986517	0.313810	-0.272182
1	-0.007061	-0.201988	-2.011797
1	1.727642	-0.306859	-3.489104
1	1.010055	-3.539656	-0.745105
1	4.684207	-3.388218	-2.986573
8	-7.223371	-2.989219	-0.009669
6	-8.556738	-3.375242	-0.277924
1	-8.614777	-4.438991	-0.045782
1	-9.270236	-2.832015	0.353278
1	-8.815541	-3.224312	-1.332516
1	0.089175	-1.007215	1.758157
6	3.620246	2.989044	-0.571347
1	3.067261	3.867359	-0.212084
1	4.687180	3.233771	-0.532532
1	5.300365	1.649813	1.126820
6	3.198865	2.767759	-2.039433
1	3.804714	1.965981	-2.478270
1	3.385517	3.684070	-2.608461
6	1.752134	2.389515	-2.123730

6	0.735751	3.196894	-2.438145
1	1.494532	1.365955	-1.856623
1	0.895295	4.239994	-2.697131
6	-0.647670	2.655592	-2.482534
8	-0.870338	1.454759	-2.371831
6	-1.777840	3.586928	-2.761393
6	-1.757713	4.918359	-2.336913
6	-2.890466	3.088693	-3.445288
6	-2.845947	5.744723	-2.600753
1	-0.914985	5.287613	-1.760584
6	-3.965971	3.922638	-3.727507
1	-2.899019	2.044338	-3.741034
6	-3.943373	5.250754	-3.304716
1	-2.840451	6.773215	-2.254332
1	-4.829227	3.533593	-4.257415
1	-4.788030	5.899581	-3.515042

si-si_4-path-B

Number of imaginary frequencies : 1
The smallest frequency is : -193.4042

Electronic energy= -3905.2831248
Zero-point correction= 1.050480
Thermal correction to Energy= 1.116697
Thermal correction to Enthalpy= 1.117642
Thermal correction to Gibbs Free Energy= 0.942405
Sum of electronic and zero-point Energies= -3904.232645
Sum of electronic and thermal Energies= -3904.166427
Sum of electronic and thermal Enthalpies= -3904.165483
Sum of electronic and thermal Free Energies= -3904.340720

Cartesian Coordinates

7	-2.617276	0.315012	-0.445380
6	-3.921607	0.803324	-0.639826
6	-4.906030	0.091555	-1.328941
6	-6.165209	0.657099	-1.497643
6	-6.467847	1.926143	-1.018963
6	-5.468117	2.633802	-0.362255
6	-4.207394	2.085979	-0.164131
6	-7.199987	-0.099207	-2.280853
9	-7.085839	-1.423883	-2.119180
6	-5.745970	4.033417	0.103912
9	-7.022088	4.185244	0.489794
6	-2.229045	-0.952655	-0.130518
16	-3.288878	-2.236418	0.171670
7	-0.884161	-1.084147	-0.082474
6	-0.181876	-2.252237	0.412816
6	1.024485	-2.615117	-0.478973
6	1.563697	-4.021280	-0.128420
6	1.403498	-4.946188	-1.344416
6	2.284857	-4.397707	-2.472242
6	1.865899	-2.944837	-2.759190
7	0.664041	-2.588394	-1.936872
6	-0.452453	-3.519996	-2.252950
6	-0.056041	-4.967523	-1.842583
6	-1.063852	-5.560329	-0.886906
6	-0.801104	-6.325024	0.170261
6	0.306262	-2.048961	1.845365
6	-0.010985	-2.958529	2.902418
6	0.565133	-2.697925	4.182175
7	1.358979	-1.621863	4.442949
6	1.591933	-0.791022	3.457624
6	1.094790	-0.964979	2.143979
6	0.301622	-3.593632	5.246993
6	-0.496390	-4.694584	5.073439

6	-1.084921	-4.939239	3.805889
6	-0.850768	-4.085017	2.749520
9	-8.446057	0.246768	-1.923373
9	-7.095299	0.140381	-3.599893
9	-5.529912	4.933696	-0.870632
9	-4.966476	4.384473	1.136424
1	1.805819	-1.853697	-0.382223
1	2.619925	-3.946610	0.138765
1	1.021987	-4.421280	0.732280
1	1.575619	-2.782831	-3.800139
1	2.638395	-2.221965	-2.498613
1	2.181693	-5.016137	-3.369186
1	3.333388	-4.411381	-2.164306
1	1.719282	-5.960558	-1.085271
1	-0.079811	-5.581871	-2.752645
1	-0.633635	-3.430795	-3.326342
1	-1.349141	-3.174548	-1.731092
1	-2.104976	-5.334647	-1.120788
1	-1.602208	-6.712593	0.791849
1	0.211510	-6.586723	0.466921
1	-0.899784	-3.072081	0.383992
1	1.329151	-0.219918	1.386351
1	-1.349771	-4.299223	1.812127
1	2.214239	0.073554	3.686424
1	0.755157	-3.375245	6.208299
1	-0.678872	-5.362200	5.906926
1	-0.339881	-0.243113	-0.254999
1	-1.903987	1.044632	-0.395341
1	-4.693716	-0.895017	-1.718753
1	-3.438751	2.648814	0.354210
1	-7.456940	2.350551	-1.149318
8	-1.895320	-5.998024	3.552851
6	-2.207186	-6.872049	4.620882
1	-2.881680	-7.622192	4.207745
1	-1.311609	-7.370969	5.009642
1	-2.715338	-6.345332	5.436648
1	0.417283	-1.546632	-2.223388
6	1.432962	2.694871	-3.521811
6	1.626568	4.156578	-3.107398
6	2.415676	4.051280	-1.799402
7	2.023475	2.741880	-1.262195
6	1.134697	2.021016	-2.179987
6	2.572264	2.214581	-0.168488
6	3.295059	2.912675	0.776086
8	-1.252303	3.097745	-0.390967
6	1.309133	0.497733	-2.200813
8	2.391984	-0.012370	-1.865192
8	0.264083	-0.118702	-2.576505
8	-0.033835	1.670263	0.699229
1	0.089703	2.216932	-1.902670
1	0.625955	2.546264	-4.240121
1	2.360295	2.282598	-3.937603
1	0.650786	4.614070	-2.916437
1	2.149228	4.756718	-3.854303
1	2.180253	4.850084	-1.089167
1	3.500584	4.055073	-1.969203
1	2.341895	1.172461	0.003388
1	3.650319	3.914990	0.545759
6	4.021783	2.161376	1.856923
6	5.441958	1.730310	1.444962
1	4.100917	2.786243	2.754157
1	3.438999	1.275028	2.139687
1	5.964442	1.318597	2.318661
1	6.009494	2.617540	1.144822
6	5.489798	0.719721	0.328039
6	4.637924	-0.299522	0.172905
1	6.296032	0.831678	-0.394985
1	3.845061	-0.499519	0.892964
6	4.735685	-1.316807	-0.899152
8	4.288240	-2.440987	-0.712569

6	5.404483	-0.986615	-2.197597
6	6.096337	-2.004074	-2.860274
6	5.297268	0.277623	-2.785966
6	6.705157	-1.753168	-4.084693
1	6.155631	-2.984813	-2.398126
6	5.893420	0.520514	-4.019506
1	4.704607	1.040647	-2.291582
6	6.604378	-0.489604	-4.664525
1	7.253880	-2.541802	-4.589694
1	5.796741	1.497628	-4.482752
1	7.073921	-0.295190	-5.624017
6	1.385080	3.644645	1.875074
1	1.373161	2.668424	2.350935
1	0.074566	4.870934	0.603757
6	2.019464	4.741164	2.629052
6	2.433035	4.517757	3.947448
6	2.212418	6.010273	2.065380
6	3.013257	5.541949	4.690870
1	2.281436	3.538638	4.394337
6	2.790878	7.030820	2.807630
1	1.918212	6.192757	1.035043
6	3.192714	6.799982	4.123428
1	3.321349	5.355796	5.714721
1	2.934398	8.008684	2.359075
1	3.647136	7.598701	4.700804
7	-0.324734	2.854106	0.408711
6	0.380823	3.898951	0.960324

si-si_5-path-B

Number of imaginary frequencies : 1
The smallest frequency is : -194.3445

Electronic energy= -3905.2832004
Zero-point correction= 1.050585
Thermal correction to Energy= 1.116744
Thermal correction to Enthalpy= 1.117688
Thermal correction to Gibbs Free Energy= 0.943042
Sum of electronic and zero-point Energies= -3904.232616
Sum of electronic and thermal Energies= -3904.166457
Sum of electronic and thermal Enthalpies= -3904.165513
Sum of electronic and thermal Free Energies= -3904.340158

Cartesian Coordinates

7	-2.614944	0.347267	-0.429919
6	-3.915216	0.842542	-0.632412
6	-4.897045	0.138469	-1.329887
6	-6.153703	0.710225	-1.507224
6	-6.454681	1.978097	-1.029772
6	-5.455205	2.680086	-0.363367
6	-4.199325	2.126828	-0.156584
6	-7.175081	-0.072744	-2.280914
9	-6.845908	-0.161200	-3.581251
6	-5.731109	4.080928	0.099924
9	-5.520689	4.978414	-0.878581
6	-2.237243	-0.923878	-0.115821
16	-3.308434	-2.198289	0.186175
7	-0.893733	-1.066793	-0.067896
6	-0.200886	-2.242475	0.422145
6	0.997032	-2.616345	-0.476562
6	1.524169	-4.027838	-0.129156
6	1.349123	-4.950742	-1.344732
6	2.229685	-4.409979	-2.476879
6	1.821683	-2.953611	-2.762051
7	0.628255	-2.585995	-1.932343
6	-0.498846	-3.506953	-2.242087

6	-0.112851	-4.958629	-1.835983
6	-1.121543	-5.544371	-0.876944
6	-0.860814	-6.309598	0.180342
6	0.296470	-2.046906	1.852488
6	-0.026070	-2.954580	2.909547
6	0.560909	-2.704246	4.186407
7	1.369526	-1.638654	4.444789
6	1.606288	-0.808106	3.460138
6	1.099343	-0.972938	2.149030
6	0.292722	-3.599230	5.250652
6	-0.520541	-4.689415	5.079453
6	-1.120207	-4.923231	3.815042
6	-0.881323	-4.069670	2.759186
9	-7.283358	-1.330811	-1.829807
9	-8.393436	0.483224	-2.220595
9	-4.947150	4.435799	1.127612
9	-7.005659	4.233280	0.491186
1	1.786176	-1.862363	-0.384026
1	2.582317	-3.963708	0.133042
1	0.982426	-4.422491	0.733979
1	1.526050	-2.789900	-3.801231
1	2.601997	-2.237101	-2.507447
1	2.116421	-5.027488	-3.373263
1	3.279596	-4.432708	-2.174278
1	1.656706	-5.968123	-1.087508
1	-0.145808	-5.571170	-2.746992
1	-0.686216	-3.414839	-3.314183
1	-1.389053	-3.154063	-1.713991
1	-2.161848	-5.312392	-1.108247
1	-1.662675	-6.691070	0.804731
1	0.150895	-6.577568	0.474451
1	-0.926881	-3.055174	0.395335
1	1.338391	-0.228986	1.391750
1	-1.388993	-4.274958	1.824446
1	2.240146	0.048500	3.687196
1	0.754928	-3.389093	6.209654
1	-0.706349	-5.356864	5.912383
1	-0.342269	-0.230685	-0.241475
1	-1.896836	1.071944	-0.377349
1	-4.686311	-0.847636	-1.723351
1	-3.431317	2.685623	0.367130
1	-7.439655	2.407733	-1.170324
8	-1.946282	-5.970434	3.564619
6	-2.262449	-6.842978	4.632571
1	-2.949717	-7.582991	4.222301
1	-1.370893	-7.354759	5.013807
1	-2.757878	-6.311543	5.453110
1	0.389482	-1.541881	-2.217267
6	1.433121	2.693932	-3.516612
6	1.641949	4.152811	-3.099670
6	2.438562	4.037057	-1.797184
7	2.037263	2.730156	-1.260469
6	1.137050	2.019204	-2.174748
6	2.587129	2.195046	-0.171249
6	3.322416	2.883889	0.770643
8	-1.230389	3.116398	-0.367380
6	1.299435	0.494556	-2.200594
8	2.381383	-0.024548	-1.876012
8	0.246338	-0.112798	-2.568498
8	-0.017297	1.676187	0.712104
1	0.095435	2.223102	-1.890601
1	0.620670	2.554104	-4.230539
1	2.354434	2.274748	-3.938835
1	0.671391	4.618134	-2.901098
1	2.164921	4.750403	-3.848391
1	2.215575	4.836165	-1.083316
1	3.522320	4.030830	-1.974166
1	2.347282	1.154812	-0.000303
1	3.687036	3.882723	0.539724
6	4.048944	2.123011	1.844937

6	5.462674	1.680787	1.422868
1	4.139776	2.744659	2.743331
1	3.459951	1.241244	2.129190
1	5.987579	1.263450	2.292450
1	6.035427	2.563868	1.120386
6	5.495310	0.671344	0.304431
6	4.633733	-0.340213	0.153028
1	6.299154	0.776605	-0.422252
1	3.842785	-0.533308	0.877062
6	4.717909	-1.359046	-0.918702
8	4.261533	-2.479122	-0.728946
6	5.384015	-1.036150	-2.220297
6	6.064773	-2.060112	-2.884562
6	5.284746	0.228178	-2.809685
6	6.670561	-1.815558	-4.111768
1	6.117893	-3.040757	-2.421463
6	5.877677	0.464762	-4.046022
1	4.700161	0.996360	-2.313789
6	6.577651	-0.551925	-4.692736
1	7.210851	-2.609165	-4.618067
1	5.786888	1.442031	-4.510111
1	7.044695	-0.362567	-5.654457
6	1.427682	3.635034	1.881306
1	1.407768	2.659039	2.357422
1	0.121132	4.875633	0.619459
6	2.078431	4.724738	2.631178
6	2.498908	4.497015	3.946646
6	2.280836	5.991698	2.065996
6	3.095145	5.515124	4.685814
1	2.340467	3.519474	4.394637
6	2.875204	7.006155	2.803994
1	1.981449	6.177043	1.037662
6	3.283839	6.771150	4.116960
1	3.408529	5.325843	5.707480
1	3.025723	7.982439	2.354286
1	3.750688	7.565121	4.690938
7	-0.299383	2.863091	0.425331
6	0.420145	3.900304	0.973073

si-si_6-path-B

Number of imaginary frequencies : 1
The smallest frequency is : -365.0187

Electronic energy= -3905.2896834
Zero-point correction= 1.053483
Thermal correction to Energy= 1.118873
Thermal correction to Enthalpy= 1.119817
Thermal correction to Gibbs Free Energy= 0.950301
Sum of electronic and zero-point Energies= -3904.236200
Sum of electronic and thermal Energies= -3904.170811
Sum of electronic and thermal Enthalpies= -3904.169867
Sum of electronic and thermal Free Energies= -3904.339382

Cartesian Coordinates

6	4.203734	0.436937	-3.051625
6	5.363881	-0.547629	-3.232231
6	5.985173	-0.590327	-1.841329
7	4.815980	-0.454151	-0.956189
6	3.643908	0.096290	-1.662051
6	4.868021	-0.665615	0.346455
6	3.784874	-0.718979	1.230939
8	0.544313	-2.778772	3.266700
6	2.494551	-0.934966	-1.730490
8	1.428581	-0.611231	-1.131063
8	2.708874	-1.993206	-2.350503

8	0.841103	-1.698038	1.397830
1	3.300772	0.980712	-1.119733
1	3.440900	0.340173	-3.825853
1	4.570693	1.468372	-3.052548
1	4.965833	-1.531568	-3.489665
1	6.080006	-0.231289	-3.992748
1	6.513625	-1.519618	-1.617323
1	6.662454	0.257629	-1.680434
1	5.861382	-0.914780	0.723430
1	2.815923	-0.377753	0.862797
6	4.041114	-0.491683	2.698888
6	3.443767	0.833143	3.203339
1	5.115861	-0.516161	2.911357
1	3.578713	-1.300586	3.284811
1	3.708016	0.944881	4.263788
1	3.873969	1.688543	2.669179
6	1.950015	0.852389	3.089415
6	1.232688	1.886705	2.636211
1	1.404711	-0.037393	3.412750
1	1.726445	2.794201	2.301464
6	-0.251808	1.800361	2.586558
8	-0.824869	0.735383	2.766889
6	-1.041909	3.036151	2.286190
6	-0.486511	4.318914	2.322811
6	-2.382043	2.874181	1.918821
6	-1.265586	5.425637	1.997507
1	0.549805	4.467337	2.610101
6	-3.153578	3.979134	1.580048
1	-2.795356	1.869991	1.889278
6	-2.595209	5.256651	1.617903
1	-0.829582	6.419459	2.021323
1	-4.185816	3.842631	1.273287
1	-3.190945	6.119867	1.337726
6	3.267882	-2.725546	1.016876
1	2.711503	-2.473805	0.119662
1	2.806442	-3.666296	2.972654
6	4.522535	-3.478920	0.772857
6	4.912273	-3.730641	-0.548948
6	5.345442	-3.909918	1.820087
6	6.097928	-4.411260	-0.813904
1	4.281081	-3.371641	-1.360628
6	6.531761	-4.584465	1.550689
1	5.064880	-3.703985	2.849535
6	6.911326	-4.838355	0.233629
1	6.385918	-4.608434	-1.842475
1	7.162738	-4.911857	2.371188
1	7.836286	-5.367180	0.026185
7	1.248273	-2.496559	2.285206
6	2.493502	-3.053374	2.141604
7	-0.346756	1.403784	-0.434370
6	-0.049517	2.733312	-0.706403
6	-0.970975	3.730634	-1.055776
6	-0.526923	5.037669	-1.195207
6	0.805266	5.404660	-1.011757
6	1.703197	4.404645	-0.669298
6	1.288284	3.090071	-0.515346
6	-1.509164	6.125019	-1.527503
9	-1.435326	7.137306	-0.642357
6	3.139156	4.707020	-0.367841
9	3.396611	4.588180	0.950757
6	-1.488984	0.662470	-0.587050
16	-2.827348	1.071615	-1.521310
7	-1.373786	-0.502499	0.083032
6	-2.262915	-1.635510	-0.054003
6	-1.421342	-2.923004	-0.148172
6	-2.243224	-4.145329	-0.613048
6	-1.688901	-4.662779	-1.949308
6	-0.247201	-5.141399	-1.722926
6	0.565731	-3.999012	-1.080290
7	-0.260795	-2.749418	-1.091222

6	-0.689125	-2.438392	-2.489450
6	-1.655421	-3.536424	-3.001186
6	-2.998225	-2.958205	-3.381836
6	-4.187154	-3.528144	-3.202203
6	-3.217123	-1.765766	1.126909
6	-4.627884	-1.928913	0.960169
6	-5.403228	-2.097133	2.145229
7	-4.868393	-2.086891	3.399531
6	-3.573239	-1.918649	3.504620
6	-2.701090	-1.763641	2.398870
6	-6.800881	-2.288371	2.025782
6	-7.417895	-2.315700	0.800925
6	-6.644903	-2.138654	-0.374841
6	-5.282816	-1.943339	-0.292806
9	-1.261779	6.662207	-2.733799
9	-2.775073	5.693903	-1.532975
9	3.493273	5.944108	-0.729850
9	3.969282	3.848718	-0.988636
1	-0.959701	-3.095986	0.826736
1	-2.189066	-4.938663	0.137530
1	-3.294611	-3.864259	-0.711863
1	1.480694	-3.754623	-1.623654
1	0.814681	-4.195008	-0.033858
1	0.202461	-5.437283	-2.675360
1	-0.238922	-6.017274	-1.069397
1	-2.301818	-5.492869	-2.310873
1	-1.215204	-3.954897	-3.915896
1	0.238058	-2.372533	-3.063175
1	-1.150991	-1.447382	-2.477198
1	-2.955108	-1.983978	-3.870868
1	-5.098215	-3.035036	-3.526382
1	-4.306097	-4.496126	-2.721775
1	-2.824610	-1.488583	-0.978374
1	-1.633540	-1.649427	2.579756
1	-4.743163	-1.789680	-1.219839
1	-3.158608	-1.908675	4.510599
1	-7.367275	-2.414214	2.942924
1	-8.489233	-2.466145	0.742737
1	-0.652833	-0.575702	0.804711
1	0.480799	0.816619	-0.294861
1	-2.015287	3.489706	-1.192537
1	1.995667	2.330077	-0.193993
1	1.124903	6.435411	-1.118572
8	-7.176490	-2.147625	-1.625900
6	-8.579261	-2.275462	-1.750867
1	-8.792206	-2.224162	-2.818990
1	-8.935124	-3.236689	-1.361699
1	-9.104824	-1.459470	-1.241708
1	0.361986	-1.941121	-0.817862

si-si_7-path-B

Number of imaginary frequencies : 1
The smallest frequency is : -166.3912

Electronic energy= -3905.287757
Zero-point correction= 1.053946
Thermal correction to Energy= 1.119639
Thermal correction to Enthalpy= 1.120584
Thermal correction to Gibbs Free Energy= 0.949262
Sum of electronic and zero-point Energies= -3904.233811
Sum of electronic and thermal Energies= -3904.168118
Sum of electronic and thermal Enthalpies= -3904.167173
Sum of electronic and thermal Free Energies= -3904.338495

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Cartesian Coordinates
.....

8	-0.338049	0.451344	-3.815114
8	-0.522765	-0.368284	-1.811723
6	-3.145020	-1.033726	-2.286143
1	-2.655047	-1.567533	-1.475685
1	-2.655234	-0.057849	-4.184154
6	-4.488402	-1.501564	-2.682464
6	-4.993642	-2.693199	-2.150279
6	-5.275168	-0.781212	-3.592181
6	-6.249139	-3.160869	-2.530108
1	-4.392647	-3.263402	-1.449022
6	-6.526912	-1.247757	-3.968807
1	-4.906914	0.160097	-3.991832
6	-7.018028	-2.441855	-3.439643
1	-6.623517	-4.090584	-2.113660
1	-7.126030	-0.676929	-4.671283
1	-7.997669	-2.804687	-3.733764
7	-1.020672	-0.102394	-2.925860
6	-2.339798	-0.394127	-3.208291
7	0.213269	-0.584886	1.218785
6	-0.794028	-1.464325	1.643359
6	-1.173532	-2.564418	0.869976
6	-2.203313	-3.387043	1.310634
6	-2.877489	-3.130982	2.500463
6	-2.504836	-2.016456	3.244146
6	-1.474026	-1.178925	2.828778
6	-2.593198	-4.578700	0.485838
9	-1.984242	-5.701038	0.887425
6	-3.243797	-1.743889	4.522645
9	-2.816551	-0.631684	5.131590
6	1.411320	-0.926363	0.675171
16	2.037795	-2.499408	0.650209
7	2.060451	0.139841	0.162962
6	3.428789	0.130065	-0.306118
6	3.554107	0.891233	-1.639819
6	4.894387	0.605143	-2.350649
6	4.626049	-0.088952	-3.693663
6	3.847804	0.886201	-4.587600
6	2.593384	1.366746	-3.832981
7	2.433606	0.546395	-2.586472
6	2.387065	-0.910603	-2.919371
6	3.759922	-1.349455	-3.494729
6	4.385453	-2.443999	-2.662117
6	5.680091	-2.593826	-2.392603
6	4.362569	0.796908	0.699485
6	5.559338	0.178098	1.175969
6	6.361071	0.934540	2.082276
7	6.029897	2.183635	2.515587
6	4.916450	2.706705	2.065438
6	4.054166	2.056507	1.150965
6	7.567427	0.369431	2.561793
6	7.977399	-0.878978	2.169172
6	7.175114	-1.630485	1.271926
6	5.989004	-1.113884	0.795257
9	-3.917248	-4.811489	0.549431
9	-2.286914	-4.405877	-0.811519
9	-3.117954	-2.756850	5.391763
9	-4.564744	-1.594710	4.303176
1	3.411767	1.955001	-1.447103
1	5.434586	1.540166	-2.523404
1	5.522126	-0.019288	-1.710806
1	1.674881	1.239357	-4.402140
1	2.657772	2.403941	-3.499083
1	3.562477	0.391666	-5.520669
1	4.474917	1.742638	-4.847999
1	5.571064	-0.357469	-4.173085
1	3.570611	-1.774680	-4.489278
1	1.568896	-1.020675	-3.632166
1	2.121081	-1.447617	-2.004879
1	3.682891	-3.181822	-2.274289
1	6.031312	-3.431721	-1.798626

1	6.437706	-1.896571	-2.741714
1	3.706592	-0.915320	-0.450483
1	3.152517	2.563166	0.810116
1	5.397860	-1.738494	0.134865
1	4.662345	3.702640	2.423171
1	8.158306	0.963366	3.251428
1	8.906627	-1.283621	2.552049
1	1.614238	1.057167	0.224050
1	-0.005154	0.418800	1.252967
1	-0.674458	-2.753857	-0.072509
1	-1.200340	-0.301616	3.408733
1	-3.684845	-3.775446	2.833987
8	7.508261	-2.870732	0.832615
6	8.680868	-3.469094	1.351055
1	8.740460	-4.458018	0.895939
1	9.578157	-2.898660	1.083950
1	8.628260	-3.579187	2.440248
1	1.539975	0.826724	-2.144824
6	-1.367763	4.198992	-1.798494
6	-2.651929	4.172444	-2.633212
6	-3.400944	2.931540	-2.123894
7	-2.368898	2.119375	-1.464796
6	-1.041811	2.709882	-1.669041
6	-2.682648	1.102446	-0.658867
6	-3.906212	0.463860	-0.669181
6	0.038289	2.419755	-0.625374
8	-0.278886	2.110792	0.545916
8	1.212029	2.540156	-1.068280
1	-0.645319	2.344206	-2.627312
1	-0.553952	4.754400	-2.267297
1	-1.554010	4.612695	-0.800895
1	-2.402489	4.051128	-3.691570
1	-3.252174	5.078256	-2.526768
1	-3.888711	2.373668	-2.930879
1	-4.168297	3.185474	-1.381389
1	-1.879350	0.729439	-0.035656
1	-4.714021	0.888089	-1.262597
6	-4.310685	-0.437931	0.456825
6	-4.972449	0.335438	1.635843
1	-5.023677	-1.190130	0.099131
1	-3.432110	-0.972889	0.834928
1	-5.420698	-0.385386	2.324481
1	-5.773601	0.966220	1.234840
6	-3.949141	1.164221	2.346118
6	-3.541879	2.370392	1.938527
1	-3.424960	0.723256	3.192081
1	-4.026949	2.861027	1.098817
6	-2.338946	3.015533	2.529157
8	-1.653456	2.456808	3.368685
6	-1.967055	4.372590	2.013820
6	-0.616776	4.734589	2.007066
6	-2.927454	5.272349	1.544163
6	-0.231621	5.976472	1.517824
1	0.110761	4.010655	2.356959
6	-2.541865	6.526407	1.074691
1	-3.980579	5.006674	1.565055
6	-1.193746	6.874512	1.053213
1	0.819279	6.247432	1.495298
1	-3.291967	7.228598	0.724300
1	-0.890133	7.846122	0.675281

si-si_8-path-B

Number of imaginary frequencies : 1
The smallest frequency is : -243.9946

Electronic energy= -3905.2826392

Zero-point correction=	1.051401
Thermal correction to Energy=	1.117258
Thermal correction to Enthalpy=	1.118202
Thermal correction to Gibbs Free Energy=	0.945044
Sum of electronic and zero-point Energies=	-3904.231238
Sum of electronic and thermal Energies=	-3904.165382
Sum of electronic and thermal Enthalpies=	-3904.164437
Sum of electronic and thermal Free Energies=	-3904.337595

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 Cartesian Coordinates

6	-1.951875	-4.472363	-2.509747
6	-1.741835	-3.054523	-3.049956
6	-1.355435	-2.294459	-1.779585
7	-2.271993	-2.869397	-0.785899
6	-2.627686	-4.250487	-1.148823
6	-2.863192	-2.215073	0.214042
6	-3.551817	-2.845775	1.238027
8	1.017250	-2.974849	0.150073
8	-0.273518	-1.416789	0.951958
1	-3.720449	-4.322400	-1.211108
1	-0.980314	-4.955192	-2.369881
1	-2.556501	-5.103245	-3.163424
1	-0.966123	-2.989082	-3.813853
1	-2.674837	-2.642175	-3.452138
1	-0.328333	-2.572281	-1.506129
1	-2.690384	-1.147593	0.225138
1	-3.772314	-3.905049	1.127306
6	-4.450171	-2.110338	2.202094
6	-4.329171	-0.582644	2.210141
1	-4.276039	-2.488805	3.217431
1	-5.493287	-2.370647	1.975480
1	-4.926939	-0.203250	3.048763
1	-3.292279	-0.274785	2.397382
6	-4.815013	0.048535	0.937065
6	-4.229334	1.097857	0.353929
1	-5.697113	-0.401327	0.480462
1	-3.377185	1.585585	0.826102
6	-4.656116	1.733383	-0.911377
8	-4.298211	2.876977	-1.165665
6	-5.529134	0.994771	-1.879304
6	-5.372698	-0.373408	-2.125049
6	-6.478611	1.725665	-2.599626
6	-6.176960	-1.002683	-3.070639
1	-4.582489	-0.914253	-1.614394
6	-7.291897	1.089311	-3.529548
1	-6.570169	2.791540	-2.414840
6	-7.142174	-0.276773	-3.764730
1	-6.044981	-2.061647	-3.271453
1	-8.039261	1.656453	-4.075353
1	-7.772593	-0.772609	-4.496604
6	-1.661574	-3.214557	2.430100
1	-1.688587	-2.175710	2.748209
1	-0.267520	-4.585682	1.422676
6	-2.219616	-4.206565	3.371151
6	-2.552959	-3.808817	4.670803
6	-2.411747	-5.545058	3.003130
6	-3.050729	-4.730924	5.588016
1	-2.402229	-2.773568	4.965819
6	-2.909764	-6.463471	3.917570
1	-2.181404	-5.861482	1.988506
6	-3.229438	-6.058833	5.214056
1	-3.297441	-4.409826	6.594887
1	-3.055540	-7.496848	3.619337
1	-3.620929	-6.777588	5.926670
7	0.063493	-2.624265	0.879517
6	-0.619268	-3.578459	1.588706
7	2.540639	-0.525270	-0.360602
6	3.764786	-1.185106	-0.558838
6	4.973644	-0.757011	-0.002629

6	6.124931	-1.504656	-0.218716
6	6.106843	-2.684815	-0.954294
6	4.892738	-3.111355	-1.477206
6	3.729621	-2.374570	-1.291217
6	7.432422	-1.004778	0.326491
9	8.268330	-2.015111	0.616073
6	4.835242	-4.355388	-2.315219
9	4.899964	-4.075370	-3.628065
6	2.279103	0.807995	-0.317449
16	3.447791	2.025795	-0.447100
7	0.956501	1.064106	-0.199673
6	0.378334	2.373726	0.028513
6	-0.827116	2.629810	-0.900666
6	-1.261395	4.113094	-0.871192
6	-1.071865	4.726018	-2.266822
6	-2.017499	4.005227	-3.235909
6	-1.724775	2.494895	-3.173336
7	-0.519457	2.246032	-2.319016
6	0.642728	2.997337	-2.866631
6	0.371080	4.525594	-2.772912
6	1.446695	5.228048	-1.979303
6	1.272862	6.239512	-1.131848
6	-0.068761	2.523382	1.479743
6	0.368348	3.600429	2.312704
6	-0.148366	3.647628	3.642252
7	-1.003512	2.715163	4.148368
6	-1.357518	1.729786	3.361582
6	-0.921730	1.592801	2.021370
6	0.243485	4.710868	4.491445
6	1.106131	5.686610	4.063124
6	1.628792	5.629201	2.745582
6	1.270090	4.605119	1.895064
9	8.069372	-0.218805	-0.556474
9	7.270341	-0.284428	1.444522
9	3.694112	-5.034620	-2.123598
9	5.850489	-5.188858	-2.045140
1	-1.649088	1.962923	-0.621279
1	-2.314438	4.177182	-0.586001
1	-0.672079	4.658120	-0.129159
1	-1.496803	2.064673	-4.151540
1	-2.537122	1.922509	-2.726558
1	-1.874673	4.385715	-4.251955
1	-3.056568	4.180757	-2.947261
1	-1.310409	5.792841	-2.240749
1	0.416360	4.927197	-3.794230
1	0.765016	2.662068	-3.898804
1	1.535752	2.701566	-2.310194
1	2.458955	4.860973	-2.153008
1	2.117069	6.690278	-0.619403
1	0.292626	6.652499	-0.906850
1	1.162570	3.097768	-0.194120
1	-1.261924	0.739093	1.437015
1	1.716693	4.594318	0.908127
1	-2.032585	0.986997	3.784587
1	-0.163814	4.724447	5.497129
1	1.387367	6.487958	4.735854
1	0.348844	0.257031	-0.066743
1	1.742779	-1.163701	-0.332920
1	5.009285	0.141230	0.598067
1	2.787592	-2.721252	-1.704351
1	7.011513	-3.263289	-1.102791
8	2.493495	6.547711	2.246291
6	2.922892	7.593574	3.097161
1	3.620154	8.191159	2.509709
1	2.085388	8.227339	3.411543
1	3.440573	7.205732	3.981964
1	-0.343421	1.153908	-2.369181
1	-2.283314	-4.957825	-0.387581
6	-1.356612	-0.772640	-1.936517
8	-2.341060	-0.097520	-1.583685

8 -0.288752 -0.330428 -2.459480

si-si_9-path-B

Number of imaginary frequencies : 1

The smallest frequency is : -198.1795

Electronic energy= -3905.2800675
Zero-point correction= 1.049478
Thermal correction to Energy= 1.115546
Thermal correction to Enthalpy= 1.116490
Thermal correction to Gibbs Free Energy= 0.942602
Sum of electronic and zero-point Energies= -3904.230590
Sum of electronic and thermal Energies= -3904.164521
Sum of electronic and thermal Enthalpies= -3904.163577
Sum of electronic and thermal Free Energies= -3904.337466

Cartesian Coordinates

7 -2.396652 -1.317708 -0.177186
6 -3.710286 -1.786372 0.002932
6 -4.101252 -3.088770 -0.325528
6 -5.424541 -3.467673 -0.147896
6 -6.384084 -2.578585 0.328073
6 -5.987325 -1.281046 0.619546
6 -4.664616 -0.880026 0.467594
6 -5.868104 -4.853247 -0.520953
9 -4.839197 -5.674444 -0.760467
6 -7.013085 -0.280938 1.068467
9 -7.990401 -0.857545 1.784088
6 -1.226496 -1.968146 0.088063
16 -1.119012 -3.508710 0.773865
7 -0.140763 -1.242321 -0.260872
6 1.234707 -1.629756 -0.005072
6 2.146831 -1.319141 -1.219347
6 3.493015 -2.079215 -1.113513
6 3.614939 -3.069072 -2.282397
6 3.680351 -2.250477 -3.576642
6 2.442561 -1.326101 -3.615278
7 1.496598 -1.650098 -2.514839
6 1.133482 -3.080263 -2.584853
6 2.382993 -3.988199 -2.368588
6 2.193328 -4.934306 -1.209242
6 3.109324 -5.284572 -0.308493
6 1.785917 -0.922307 1.233366
6 2.553958 -1.592335 2.238188
6 3.086208 -0.795260 3.296888
7 2.858437 0.542436 3.420005
6 2.103470 1.107168 2.510029
6 1.564522 0.424884 1.394039
6 3.893983 -1.412649 4.283445
6 4.162605 -2.756851 4.247664
6 3.604490 -3.553407 3.214116
6 2.812899 -2.981815 2.240548
9 -6.612945 -5.409402 0.447961
9 -6.632428 -4.842547 -1.627694
9 -7.604559 0.325636 0.025245
9 -6.475696 0.686156 1.825730
1 2.317264 -0.235868 -1.254871
1 4.322694 -1.372867 -1.165186
1 3.572137 -2.595722 -0.154868
1 1.886484 -1.428126 -4.552372
1 2.708772 -0.273034 -3.500230
1 3.699914 -2.915747 -4.445916
1 4.598188 -1.654933 -3.594933
1 4.525642 -3.665568 -2.169652
1 2.498812 -4.611197 -3.266587

1	0.685526	-3.245174	-3.568751
1	0.362885	-3.282831	-1.835023
1	1.199765	-5.378861	-1.137781
1	2.875835	-5.993986	0.479248
1	4.118666	-4.879827	-0.310519
1	1.217104	-2.707851	0.162638
1	0.960275	0.982868	0.683577
1	2.389950	-3.638861	1.489155
1	1.904954	2.170850	2.638197
1	4.288970	-0.780841	5.072333
1	4.782803	-3.202591	5.016229
1	-0.316592	-0.303003	-0.604722
1	-2.335378	-0.325354	-0.409649
1	-3.377682	-3.794427	-0.709175
1	-4.370631	0.137022	0.703355
1	-7.413272	-2.891937	0.469171
8	3.802179	-4.891702	3.117007
6	4.570588	-5.527319	4.120991
1	4.586186	-6.585977	3.861774
1	5.599142	-5.148446	4.142287
1	4.116461	-5.407531	5.111206
1	0.400654	-0.735409	-2.753696
6	-1.235473	2.845251	-4.237800
6	-1.996093	4.132667	-3.904486
6	-1.260952	4.680803	-2.676559
7	-0.638832	3.492232	-2.072940
6	-0.957006	2.285568	-2.839500
6	0.239584	3.570845	-1.071376
6	0.362905	4.663869	-0.237768
8	-3.201694	1.641660	-0.728340
6	0.125330	1.220652	-2.808634
8	1.313668	1.486322	-2.718767
8	-0.379799	0.018871	-2.898973
8	-1.215451	1.522593	0.140219
1	-1.873544	1.829519	-2.441705
1	-1.807752	2.148546	-4.851783
1	-0.284592	3.068912	-4.733536
1	-3.030272	3.888649	-3.643597
1	-2.008588	4.850541	-4.726040
1	-1.932922	5.173825	-1.967237
1	-0.468569	5.388732	-2.948014
1	0.811246	2.673954	-0.867143
1	-0.099155	5.603552	-0.532731
6	1.491071	4.755622	0.752018
6	2.781963	5.339126	0.155455
1	1.178617	5.392178	1.586956
1	1.692091	3.763124	1.173568
1	3.415912	5.723883	0.966411
1	2.531406	6.210627	-0.459084
6	3.625043	4.391831	-0.652140
6	3.791634	3.081823	-0.439540
1	4.216180	4.829011	-1.456074
1	3.268985	2.554282	0.353847
6	4.777679	2.336762	-1.271295
8	5.136848	2.766256	-2.354648
6	5.386933	1.070517	-0.734618
6	6.271775	0.380072	-1.573142
6	5.159670	0.591920	0.560845
6	6.918750	-0.765642	-1.127570
1	6.442738	0.770775	-2.570982
6	5.811010	-0.557509	1.007267
1	4.495677	1.112752	1.243733
6	6.689944	-1.234742	0.166763
1	7.603716	-1.292285	-1.785030
1	5.628265	-0.921667	2.014145
1	7.194789	-2.129575	0.518143
6	-1.381088	4.037954	1.100937
1	-0.689760	3.350694	1.580094
1	-3.309890	3.946515	0.045014
6	-1.591661	5.335577	1.770424

6	-1.037801	5.548107	3.038304
6	-2.344440	6.359491	1.179774
6	-1.244600	6.750565	3.708470
1	-0.456813	4.757303	3.505483
6	-2.549066	7.558887	1.848548
1	-2.761713	6.216824	0.185938
6	-2.000605	7.757382	3.116089
1	-0.815532	6.897561	4.694365
1	-3.132919	8.344682	1.379990
1	-2.160913	8.696507	3.635702
7	-2.265719	2.170233	-0.091411
6	-2.389633	3.466579	0.342964

si-si_10-path-B

Number of imaginary frequencies : 1
The smallest frequency is : -217.7404

Electronic energy= -3905.2755846
Zero-point correction= 1.049531
Thermal correction to Energy= 1.115958
Thermal correction to Enthalpy= 1.116902
Thermal correction to Gibbs Free Energy= 0.938621
Sum of electronic and zero-point Energies= -3904.226054
Sum of electronic and thermal Energies= -3904.159627
Sum of electronic and thermal Enthalpies= -3904.158682
Sum of electronic and thermal Free Energies= -3904.336964

Cartesian Coordinates

7	-3.030964	-0.258620	-0.088751
6	-4.284075	-0.705130	-0.543962
6	-5.477082	-0.031260	-0.266437
6	-6.680597	-0.561664	-0.713410
6	-6.737120	-1.762335	-1.413793
6	-5.546248	-2.432844	-1.658905
6	-4.326153	-1.916064	-1.238329
6	-7.952372	0.198063	-0.466267
9	-8.255761	1.010519	-1.490819
6	-5.571891	-3.764891	-2.350345
9	-6.639991	-3.891794	-3.151043
6	-2.555117	1.018209	-0.041289
16	-3.386785	2.368979	-0.627870
7	-1.331487	1.093290	0.529215
6	-0.510148	2.289065	0.582034
6	0.120981	2.496145	1.978951
6	0.735783	3.918017	2.082260
6	-0.014379	4.708995	3.166142
6	0.233418	4.020743	4.513443
6	-0.174921	2.536572	4.374039
7	-0.857023	2.289505	3.078136
6	-2.008266	3.208486	2.955351
6	-1.533886	4.694562	2.908263
6	-1.988814	5.391173	1.649496
6	-1.291922	6.268789	0.930701
6	0.598918	2.239984	-0.467074
6	0.756883	3.245675	-1.472053
6	1.869512	3.119125	-2.357202
7	2.754223	2.083066	-2.302057
6	2.554910	1.164460	-1.389668
6	1.497755	1.202207	-0.450554
6	2.072111	4.110405	-3.347566
6	1.222208	5.179798	-3.471199
6	0.109562	5.295124	-2.598980
6	-0.117863	4.344278	-1.626803
9	-8.998931	-0.627752	-0.306030
9	-7.874472	0.965495	0.630322

9	-5.622351	-4.781429	-1.472396
9	-4.478264	-3.958700	-3.101626
1	0.886384	1.727385	2.135621
1	1.796972	3.858756	2.343346
1	0.669388	4.428955	1.117676
1	-0.868464	2.229544	5.162867
1	0.683492	1.863386	4.411106
1	-0.348861	4.514327	5.298261
1	1.288681	4.100934	4.790942
1	0.349841	5.740135	3.197380
1	-2.010978	5.219050	3.747690
1	-2.653031	3.023726	3.819111
1	-2.578151	2.943755	2.059885
1	-3.002276	5.144188	1.330313
1	-1.715696	6.727757	0.042814
1	-0.275569	6.556695	1.187815
1	-1.178912	3.123751	0.373224
1	1.406681	0.396615	0.274257
1	-1.000950	4.458373	-1.009466
1	3.265963	0.338668	-1.364759
1	2.923943	3.992788	-4.009706
1	1.402201	5.921884	-4.239959
1	-0.880641	0.207610	0.745102
1	-2.377423	-1.015514	0.120730
1	-5.462544	0.891945	0.296365
1	-3.404580	-2.452612	-1.438673
1	-7.684607	-2.165212	-1.753843
8	-0.782436	6.315426	-2.659471
6	-0.635855	7.270996	-3.692613
1	-1.463761	7.970303	-3.575038
1	0.309646	7.819054	-3.604871
1	-0.698190	6.804760	-4.682589
1	-1.200208	0.863324	3.141913
6	-0.785723	-3.165192	4.241403
6	-0.466441	-4.585877	3.765592
6	0.833367	-4.415755	2.973101
7	0.780994	-3.020360	2.510632
6	-0.418613	-2.340145	3.003530
6	1.775682	-2.438096	1.844452
6	2.791515	-3.110160	1.189932
8	-1.773164	-2.976993	0.242162
6	-0.237487	-0.854166	3.272579
8	0.839428	-0.353983	3.560290
8	-1.366410	-0.210709	3.152200
8	-0.121232	-1.581191	0.012574
1	-1.221841	-2.433871	2.259767
1	-1.828406	-3.025292	4.528881
1	-0.138898	-2.878039	5.077671
1	-1.263344	-4.935915	3.102372
1	-0.356608	-5.301165	4.581939
1	0.910505	-5.102000	2.124186
1	1.723283	-4.543248	3.601821
1	1.705733	-1.362217	1.744218
1	2.971356	-4.158619	1.416072
6	3.934232	-2.318014	0.620677
6	5.152617	-2.201720	1.560002
1	4.276781	-2.766129	-0.320657
1	3.576061	-1.306340	0.382439
1	5.591246	-3.191384	1.724955
1	4.817765	-1.814918	2.529468
6	6.157014	-1.270740	0.954993
6	7.337445	-1.638174	0.447497
1	5.858004	-0.223862	0.898786
1	7.686490	-2.665492	0.534585
6	8.327424	-0.697616	-0.141484
8	9.516131	-0.964848	-0.089245
6	7.867446	0.577444	-0.785457
6	8.746017	1.665192	-0.779603
6	6.634126	0.693965	-1.435483
6	8.380760	2.862449	-1.381968

1	9.710563	1.552422	-0.294775
6	6.270988	1.889853	-2.049662
1	5.967134	-0.161420	-1.479848
6	7.142089	2.976030	-2.013217
1	9.060601	3.708423	-1.362839
1	5.306220	1.975671	-2.542959
1	6.856776	3.912553	-2.482781
6	1.581408	-3.555170	-0.665599
1	1.814526	-2.546140	-0.994341
1	-0.217522	-4.769111	-0.285770
6	2.423232	-4.637831	-1.211678
6	3.333938	-4.346642	-2.233418
6	2.325485	-5.956169	-0.745992
6	4.118978	-5.352933	-2.789427
1	3.409864	-3.328294	-2.605392
6	3.109935	-6.958759	-1.300108
1	1.639686	-6.192084	0.064399
6	4.008241	-6.659724	-2.324907
1	4.814690	-5.114420	-3.587353
1	3.026072	-7.975470	-0.929894
1	4.621642	-7.444398	-2.755881
7	-0.569364	-2.753442	-0.022570
6	0.257086	-3.800396	-0.332761

si-si_11-path-B

Number of imaginary frequencies : 1
The smallest frequency is : -217.1784

Electronic energy=	-3905.2754343
Zero-point correction=	1.049423
Thermal correction to Energy=	1.115870
Thermal correction to Enthalpy=	1.116814
Thermal correction to Gibbs Free Energy=	0.938695
Sum of electronic and zero-point Energies=	-3904.226012
Sum of electronic and thermal Energies=	-3904.159565
Sum of electronic and thermal Enthalpies=	-3904.158620
Sum of electronic and thermal Free Energies=	-3904.336740

Cartesian Coordinates

7	-3.029772	-0.250593	-0.099928
6	-4.279779	-0.698558	-0.562603
6	-5.474684	-0.025347	-0.296305
6	-6.674317	-0.552777	-0.759327
6	-6.724187	-1.749916	-1.464586
6	-5.530623	-2.421324	-1.697911
6	-4.315362	-1.907703	-1.261683
6	-7.951956	0.159205	-0.417992
9	-7.798379	1.489906	-0.409555
6	-5.548686	-3.746063	-2.403603
9	-6.609673	-3.865766	-3.214851
6	-2.553986	1.026136	-0.052022
16	-3.383594	2.376515	-0.642495
7	-1.332181	1.101558	0.522702
6	-0.510441	2.297116	0.575014
6	0.117862	2.507028	1.972733
6	0.732590	3.929047	2.074417
6	-0.019499	4.722237	3.155326
6	0.225639	4.036477	4.504381
6	-0.183012	2.552169	4.367102
7	-0.862453	2.302827	3.070287
6	-2.013270	3.221770	2.943279
6	-1.538517	4.707677	2.894583
6	-1.990942	5.402139	1.633735
6	-1.292498	6.278222	0.914579
6	0.600831	2.245711	-0.471663

6	0.761523	3.249991	-1.477590
6	1.876125	3.121909	-2.360026
7	2.760222	2.085501	-2.301607
6	2.558391	1.168117	-1.388511
6	1.499159	1.207548	-0.451816
6	2.081531	4.112079	-3.350951
6	1.232444	5.181751	-3.477690
6	0.117699	5.298409	-2.608346
6	-0.112442	4.348741	-1.635685
9	-8.933603	-0.130405	-1.285047
9	-8.397888	-0.186080	0.802910
9	-5.605858	-4.771451	-1.536364
9	-4.448431	-3.931678	-3.147251
1	0.882810	1.738486	2.132520
1	1.793269	3.870200	2.337669
1	0.668111	4.438173	1.108748
1	-0.878345	2.247034	5.155094
1	0.675041	1.878663	4.407215
1	-0.357847	4.531720	5.287251
1	1.280440	4.116826	4.783585
1	0.344895	5.753351	3.185322
1	-2.017089	5.233695	3.732206
1	-2.660043	3.038703	3.805906
1	-2.581143	2.955489	2.046981
1	-3.003849	5.154774	1.313091
1	-1.714462	6.735506	0.024966
1	-0.276557	6.566387	1.173037
1	-1.178531	3.131548	0.363054
1	1.406291	0.403061	0.274006
1	-0.996989	4.463801	-1.020633
1	3.269001	0.342035	-1.360768
1	2.934961	3.993421	-4.010852
1	1.414694	5.923062	-4.246667
1	-0.881776	0.216009	0.740100
1	-2.377445	-1.007327	0.113935
1	-5.464235	0.902437	0.259835
1	-3.391449	-2.441766	-1.457832
1	-7.666154	-2.144525	-1.827845
8	-0.773788	6.318982	-2.672198
6	-0.625087	7.272569	-3.706875
1	-1.453492	7.971840	-3.592649
1	0.320030	7.821113	-3.618018
1	-0.684912	6.804334	-4.696073
1	-1.206627	0.877449	3.136272
6	-0.799355	-3.146496	4.246743
6	-0.481964	-4.569611	3.777028
6	0.819605	-4.405061	2.986255
7	0.771061	-3.011287	2.518520
6	-0.428154	-2.326898	3.006460
6	1.768254	-2.433817	1.851841
6	2.783783	-3.110835	1.202071
8	-1.778903	-2.968156	0.244113
6	-0.245316	-0.840347	3.270640
8	0.832221	-0.340048	3.555962
8	-1.373843	-0.196482	3.149319
8	-0.122593	-1.577770	0.013066
1	-1.230175	-2.421925	2.261544
1	-1.842321	-3.003355	4.531567
1	-0.153613	-2.857413	5.083182
1	-1.278374	-4.920661	3.113751
1	-0.375008	-5.281940	4.596340
1	0.896864	-5.094607	2.140032
1	1.708135	-4.532138	3.617021
1	1.700781	-1.358241	1.747083
1	2.960816	-4.158779	1.432782
6	3.929140	-2.323799	0.631071
6	5.146085	-2.205509	1.572038
1	4.272434	-2.777276	-0.307423
1	3.573517	-1.312573	0.387089
1	5.582942	-3.195182	1.741617

1	4.810166	-1.814416	2.539403
6	6.152870	-1.278386	0.965093
6	7.332897	-1.649691	0.459482
1	5.856086	-0.231059	0.905568
1	7.679816	-2.677452	0.549752
6	8.325104	-0.712748	-0.131459
8	9.513225	-0.982400	-0.078228
6	7.868053	0.561817	-0.778496
6	8.748657	1.647910	-0.774195
6	6.635462	0.679320	-1.429743
6	8.386116	2.844624	-1.379289
1	9.712620	1.534341	-0.288398
6	6.275046	1.874632	-2.046653
1	5.966952	-0.174945	-1.472960
6	7.148151	2.959249	-2.011715
1	9.067537	3.689352	-1.361331
1	5.310840	1.961460	-2.540894
1	6.864965	3.895337	-2.483419
6	1.575770	-3.560144	-0.654436
1	1.813479	-2.553386	-0.986833
1	-0.227895	-4.766447	-0.273881
6	2.414884	-4.648469	-1.193416
6	3.329404	-4.365774	-2.214163
6	2.310860	-5.964187	-0.721636
6	4.112011	-5.377809	-2.763156
1	3.410400	-3.349580	-2.590918
6	3.092833	-6.972485	-1.268792
1	1.622099	-6.193525	0.088135
6	3.994985	-6.681914	-2.292662
1	4.810921	-5.145917	-3.560245
1	3.004022	-7.987030	-0.893825
1	4.606491	-7.471015	-2.718207
7	-0.573938	-2.748847	-0.018896
6	0.249940	-3.799465	-0.323615

si-si_12-path-B

Number of imaginary frequencies : 1
 The smallest frequency is : -251.1125

Electronic energy= -3905.2759206
 Zero-point correction= 1.049460
 Thermal correction to Energy= 1.115871
 Thermal correction to Enthalpy= 1.116815
 Thermal correction to Gibbs Free Energy= 0.939951
 Sum of electronic and zero-point Energies= -3904.226460
 Sum of electronic and thermal Energies= -3904.160050
 Sum of electronic and thermal Enthalpies= -3904.159105
 Sum of electronic and thermal Free Energies= -3904.335970

 Cartesian Coordinates

6	2.328296	4.466691	3.638812
6	2.025411	3.042535	4.113633
6	1.387744	2.438905	2.858400
7	0.549304	3.534895	2.370572
6	1.115368	4.833467	2.772952
6	-0.637033	3.422038	1.772395
6	-1.259877	4.473980	1.122831
8	2.675892	2.186816	0.056284
8	0.556574	1.687164	-0.023964
1	0.352416	5.383422	3.335856
1	3.235988	4.461672	3.028614
1	2.469760	5.173931	4.457326
1	2.912136	2.490115	4.426504
1	1.294337	3.045373	4.929472
1	2.180237	2.241685	2.122938

1	-1.043020	2.421147	1.728370
1	-0.885643	5.479074	1.301514
6	-2.690713	4.397658	0.656734
6	-3.197300	2.992667	0.314665
1	-2.798981	5.038777	-0.228141
1	-3.348509	4.839454	1.416604
1	-2.485890	2.509717	-0.374547
1	-3.240306	2.356278	1.206573
6	-4.543096	3.036550	-0.345413
6	-5.511319	2.131301	-0.185230
1	-4.732242	3.861767	-1.033988
1	-5.376538	1.275626	0.472718
6	-6.798845	2.263517	-0.925186
8	-7.185274	3.345228	-1.334570
6	-7.606792	1.025517	-1.154378
6	-7.022238	-0.243474	-1.141891
6	-8.969555	1.159948	-1.437036
6	-7.798433	-1.368912	-1.403365
1	-5.956120	-0.362747	-0.971255
6	-9.745593	0.034093	-1.678366
1	-9.400369	2.155932	-1.461212
6	-9.159678	-1.232105	-1.661531
1	-7.334396	-2.350265	-1.408830
1	-10.805910	0.139811	-1.885092
1	-9.765413	-2.111554	-1.858184
6	-0.086668	4.214669	-0.775488
1	-0.775165	3.424667	-1.056099
1	2.089367	4.454988	-0.529712
6	-0.346825	5.542320	-1.366629
6	-1.357776	5.678088	-2.325225
6	0.397175	6.673090	-1.002796
6	-1.609174	6.911611	-2.920125
1	-1.936604	4.804749	-2.615593
6	0.145991	7.902734	-1.596355
1	1.168845	6.587891	-0.241580
6	-0.857304	8.025177	-2.558242
1	-2.391156	7.000583	-3.667239
1	0.729237	8.770947	-1.306591
1	-1.052226	8.987843	-3.019811
7	1.486096	2.522716	-0.155485
6	1.217449	3.818725	-0.502028
7	2.772608	-0.690113	-0.242590
6	4.055543	-0.698618	-0.817555
6	4.400223	-1.491933	-1.915926
6	5.680686	-1.401200	-2.446818
6	6.629031	-0.522986	-1.930433
6	6.262835	0.276690	-0.856710
6	4.993806	0.193080	-0.294765
6	6.024042	-2.217973	-3.659882
9	7.333804	-2.507816	-3.710467
6	7.255714	1.214083	-0.233892
9	7.716978	0.743221	0.937453
6	1.944571	-1.738555	0.011324
16	2.316564	-3.352326	-0.331508
7	0.795057	-1.350667	0.613942
6	-0.326267	-2.230984	0.894841
6	-0.848870	-2.076620	2.341511
6	-1.839770	-3.222181	2.685207
6	-1.276958	-4.034490	3.861959
6	-1.187742	-3.107133	5.080934
6	-0.338788	-1.876297	4.687564
7	0.251164	-2.046501	3.337265
6	1.048515	-3.289352	3.308556
6	0.145088	-4.538372	3.551561
6	0.255383	-5.531521	2.420829
6	-0.734943	-6.233095	1.873266
6	-1.476983	-1.968868	-0.070312
6	-2.078524	-3.003424	-0.854535
6	-3.206264	-2.644173	-1.652214
7	-3.698480	-1.375579	-1.725337

6	-3.089556	-0.447831	-1.027509
6	-1.986707	-0.698125	-0.177981
6	-3.852959	-3.645681	-2.415910
6	-3.414878	-4.944930	-2.404997
6	-2.285163	-5.296802	-1.621950
6	-1.630013	-4.343823	-0.870845
9	5.352320	-3.375686	-3.692129
9	5.729944	-1.565330	-4.798087
9	6.709266	2.412056	0.027372
9	8.320206	1.419909	-1.021276
1	-1.333618	-1.099262	2.432161
1	-2.817169	-2.812378	2.959098
1	-1.992945	-3.864779	1.814352
1	0.492176	-1.718798	5.381953
1	-0.927385	-0.956466	4.660388
1	-0.733831	-3.639417	5.922988
1	-2.189625	-2.796783	5.392190
1	-1.933470	-4.881602	4.082409
1	0.514894	-5.044808	4.454055
1	1.812210	-3.192432	4.085245
1	1.566031	-3.352765	2.347009
1	1.267504	-5.680414	2.042453
1	-0.544662	-6.934188	1.066555
1	-1.768780	-6.135847	2.195450
1	0.048527	-3.245543	0.760387
1	-1.558200	0.127353	0.388611
1	-0.756801	-4.658757	-0.311264
1	-3.489596	0.561309	-1.110229
1	-4.705755	-3.345388	-3.016214
1	-3.927755	-5.690142	-3.001276
1	0.626802	-0.346748	0.656048
1	2.498217	0.232081	0.104392
1	3.675731	-2.171676	-2.343814
1	4.724734	0.820121	0.549280
1	7.623533	-0.461978	-2.357023
8	-1.785058	-6.556200	-1.560359
6	-2.395271	-7.558250	-2.351055
1	-1.830230	-8.471888	-2.165558
1	-3.440485	-7.720402	-2.062176
1	-2.344209	-7.315839	-3.418687
1	1.026185	-0.825098	3.160657
1	1.388742	5.428204	1.895981
6	0.687074	1.114493	3.093480
8	-0.514731	1.006057	3.294873
8	1.541979	0.130272	3.070543

si-si_13-path-B

Number of imaginary frequencies : 1
 The smallest frequency is : -186.9113

Electronic energy= -3905.2779336
 Zero-point correction= 1.049855
 Thermal correction to Energy= 1.116173
 Thermal correction to Enthalpy= 1.117118
 Thermal correction to Gibbs Free Energy= 0.942132
 Sum of electronic and zero-point Energies= -3904.228078
 Sum of electronic and thermal Energies= -3904.161760
 Sum of electronic and thermal Enthalpies= -3904.160816
 Sum of electronic and thermal Free Energies= -3904.335802

 Cartesian Coordinates

7	2.631735	-0.696673	0.020063
6	4.005942	-0.806347	-0.260760
6	4.767662	-1.915343	0.113194
6	6.128460	-1.938677	-0.171502

6	6.760755	-0.873783	-0.801578
6	5.994391	0.234819	-1.143055
6	4.630361	0.276948	-0.885754
6	6.941596	-3.118830	0.277832
9	6.237053	-4.257811	0.240224
6	6.671276	1.416774	-1.774082
9	7.614911	1.036971	-2.649791
6	1.676556	-1.663528	-0.072878
16	1.950754	-3.221775	-0.673029
7	0.469491	-1.246608	0.371293
6	-0.764497	-2.002844	0.247466
6	-1.601764	-1.970611	1.542781
6	-2.674701	-3.086275	1.549917
6	-2.387823	-4.061573	2.702318
6	-2.548118	-3.288189	4.019036
6	-1.650779	-2.036697	3.962595
7	-0.756703	-2.114428	2.767854
6	0.018607	-3.381177	2.776073
6	-0.943865	-4.594023	2.633313
6	-0.612112	-5.422497	1.414596
6	-1.479265	-6.005530	0.589834
6	-1.631391	-1.455628	-0.882113
6	-2.129681	-2.273732	-1.942508
6	-2.959843	-1.639272	-2.915999
7	-3.266587	-0.311797	-2.892491
6	-2.782343	0.402417	-1.907047
6	-1.975737	-0.125803	-0.871833
6	-3.505251	-2.422464	-3.962472
6	-3.251981	-3.767262	-4.055248
6	-2.414366	-4.391370	-3.094182
6	-1.862793	-3.656861	-2.066172
9	8.033117	-3.292266	-0.481995
9	7.370453	-2.971197	1.543920
9	7.286604	2.184633	-0.858610
9	5.807627	2.205421	-2.427784
1	-2.061508	-0.985022	1.656579
1	-3.660045	-2.639774	1.698108
1	-2.678196	-3.608336	0.588975
1	-0.999385	-1.943590	4.835125
1	-2.217265	-1.109277	3.848787
1	-2.273493	-3.925495	4.865490
1	-3.590804	-2.988377	4.152831
1	-3.093910	-4.896204	2.672492
1	-0.788167	-5.239790	3.508173
1	0.571554	-3.402113	3.718146
1	0.743993	-3.341930	1.958901
1	0.453960	-5.554967	1.227751
1	-1.135803	-6.600579	-0.250675
1	-2.555779	-5.915344	0.711801
1	-0.465750	-3.029781	0.035072
1	-1.630867	0.532855	-0.077068
1	-1.211719	-4.174974	-1.370357
1	-3.038200	1.461369	-1.896905
1	-4.135464	-1.917827	-4.687766
1	-3.685955	-4.340237	-4.866117
1	0.400596	-0.273378	0.659240
1	2.322538	0.258274	0.212306
1	4.298863	-2.754434	0.609827
1	4.045749	1.147166	-1.161957
1	7.820946	-0.908833	-1.026904
8	-2.109441	-5.712920	-3.118444
6	-2.598636	-6.491408	-4.193603
1	-2.209601	-7.497737	-4.037214
1	-3.694390	-6.528399	-4.200244
1	-2.239557	-6.114932	-5.158215
1	-0.080170	-1.203607	2.857341
6	1.079503	2.825192	4.200459
6	1.527368	4.249446	3.862540
6	0.504033	4.711267	2.817886
7	-0.003362	3.461138	2.232201

6	0.663993	2.298843	2.824840
6	-1.043824	3.436888	1.394353
6	-1.503154	4.556334	0.731612
8	2.626655	2.302011	0.347242
6	-0.126939	0.992752	2.879221
8	-1.362609	0.971837	2.795398
8	0.643197	-0.016355	3.023154
8	0.595936	1.749652	-0.184204
1	1.574255	2.077496	2.251016
1	1.863830	2.213487	4.647496
1	0.208607	2.835528	4.865828
1	2.526720	4.220108	3.417378
1	1.555231	4.915682	4.726518
1	0.945477	5.354891	2.050025
1	-0.336679	5.252021	3.270789
1	-1.470191	2.458896	1.205766
1	-1.118717	5.524773	1.040183
6	-2.807585	4.578178	-0.024768
6	-4.047607	4.219222	0.839339
1	-2.937638	5.577515	-0.447794
1	-2.772217	3.893025	-0.884515
1	-4.901753	4.817198	0.500239
1	-3.860378	4.475614	1.885966
6	-4.426975	2.776320	0.709981
6	-4.313348	1.841916	1.662241
1	-4.817045	2.484787	-0.265990
1	-3.860350	2.063216	2.626033
6	-4.683227	0.420122	1.460264
8	-4.245024	-0.440971	2.209482
6	-5.601384	0.030445	0.337594
6	-5.316705	-1.136046	-0.377720
6	-6.754620	0.760257	0.031662
6	-6.155306	-1.554240	-1.403518
1	-4.412914	-1.692250	-0.145739
6	-7.607117	0.326346	-0.979537
1	-6.993842	1.654720	0.598688
6	-7.304254	-0.824676	-1.702955
1	-5.906914	-2.445045	-1.972448
1	-8.507602	0.888971	-1.204411
1	-7.963221	-1.152569	-2.500875
6	0.040572	4.278412	-0.983426
1	-0.591465	3.468954	-1.336837
1	2.108553	4.574415	-0.301477
6	-0.173846	5.600831	-1.598548
6	-1.055528	5.714712	-2.679633
6	0.483815	6.748963	-1.136712
6	-1.265205	6.945164	-3.295626
1	-1.566655	4.828017	-3.045268
6	0.273620	7.975896	-1.752010
1	1.154498	6.680261	-0.283854
6	-0.601199	8.077711	-2.834027
1	-1.946101	7.016424	-4.137729
1	0.789083	8.858066	-1.385684
1	-0.764171	9.038392	-3.311926
7	1.497828	2.611766	-0.091097
6	1.266418	3.918428	-0.462664

si-si_14-path-B

Number of imaginary frequencies : 1
The smallest frequency is : -242.4845

Electronic energy= -3905.2759935
Zero-point correction= 1.049903
Thermal correction to Energy= 1.116077
Thermal correction to Enthalpy= 1.117022
Thermal correction to Gibbs Free Energy= 0.941230

Sum of electronic and zero-point Energies=	-3904.226090
Sum of electronic and thermal Energies=	-3904.159916
Sum of electronic and thermal Enthalpies=	-3904.158972
Sum of electronic and thermal Free Energies=	-3904.334763

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Cartesian Coordinates
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7	-2.952457	-0.035593	-0.133120
6	-4.190208	-0.379813	-0.706005
6	-5.338887	0.399299	-0.571508
6	-6.530654	-0.031550	-1.149182
6	-6.616854	-1.232380	-1.838171
6	-5.469304	-2.014223	-1.936746
6	-4.265513	-1.601514	-1.386097
6	-7.744202	0.835899	-0.975449
9	-7.529438	2.085992	-1.409823
6	-5.563247	-3.344709	-2.625268
9	-6.320420	-3.275408	-3.731212
6	-2.366496	1.193007	-0.059862
16	-3.029410	2.611779	-0.697186
7	-1.178083	1.162571	0.585318
6	-0.268237	2.290041	0.678598
6	0.352450	2.407387	2.090331
6	1.045221	3.787386	2.261074
6	0.331716	4.572368	3.374277
6	0.521003	3.807668	4.689855
6	0.013238	2.363209	4.480314
7	-0.656938	2.216581	3.163436
6	-1.745383	3.209780	3.059973
6	-1.182882	4.664011	3.103277
6	-1.582191	5.456504	1.883187
6	-0.830133	6.331167	1.218477
6	0.843368	2.185405	-0.364592
6	1.157837	3.239316	-1.279478
6	2.250311	3.025639	-2.174812
7	2.972433	1.869107	-2.216042
6	2.626413	0.915419	-1.386807
6	1.582037	1.031051	-0.440433
6	2.603878	4.055593	-3.079480
6	1.923017	5.245538	-3.110181
6	0.829441	5.448795	-2.230132
6	0.453210	4.462489	-1.343381
9	-8.807126	0.357678	-1.637512
9	-8.094717	0.937165	0.318244
9	-6.127838	-4.273266	-1.834038
9	-4.362342	-3.816682	-2.986777
1	1.069796	1.589131	2.228230
1	2.099141	3.656771	2.525842
1	1.016884	4.344994	1.321323
1	-0.717085	2.074227	5.242635
1	0.820983	1.629386	4.506856
1	-0.032047	4.303777	5.493904
1	1.577107	3.803020	4.975497
1	0.759387	5.575682	3.459086
1	-1.637400	5.168186	3.967402
1	-2.426696	3.021269	3.894351
1	-2.302405	3.026124	2.136305
1	-2.605647	5.289364	1.544544
1	-1.221272	6.862483	0.356377
1	0.199770	6.547032	1.492253
1	-0.869587	3.178490	0.483819
1	1.363105	0.187164	0.208656
1	-0.409311	4.653571	-0.715710
1	3.193961	-0.013901	-1.444846
1	3.429121	3.867001	-3.758944
1	2.217900	6.014509	-3.814121
1	-0.818820	0.243873	0.836453
1	-2.395576	-0.845058	0.150456
1	-5.303335	1.333841	-0.026833
1	-3.380232	-2.222021	-1.471596

1	-7.550339	-1.553531	-2.286299
8	0.097186	6.590587	-2.203467
6	0.400687	7.600991	-3.146276
1	-0.323287	8.397875	-2.975818
1	1.411844	7.998950	-3.001039
1	0.295134	7.236118	-4.174400
1	-1.118054	0.816843	3.169249
6	-1.152690	-3.167052	4.432075
6	-1.043074	-4.637017	4.013312
6	0.242098	-4.687561	3.175845
7	0.425694	-3.301854	2.715853
6	-0.686157	-2.455322	3.159045
6	1.550825	-2.870726	2.147298
6	2.489721	-3.695501	1.554202
8	-1.936682	-2.797171	0.312332
6	-0.344879	-0.986807	3.352429
8	0.767892	-0.587964	3.661998
8	-1.392328	-0.231294	3.160940
8	-0.097035	-1.635573	0.269734
1	-1.489146	-2.496666	2.410321
1	-2.162828	-2.872633	4.719719
1	-0.461838	-2.937727	5.250676
1	-1.903979	-4.904479	3.393957
1	-1.003334	-5.323784	4.860078
1	0.165985	-5.374703	2.327624
1	1.117033	-4.973345	3.771052
1	1.645834	-1.797568	2.077518
1	2.429787	-4.765502	1.737164
6	3.838506	-3.175104	1.122361
6	3.912121	-1.654959	1.025564
1	4.609599	-3.531955	1.817158
1	4.090708	-3.621876	0.152411
1	3.812693	-1.205722	2.022862
1	3.044755	-1.278170	0.462814
6	5.142429	-1.092664	0.379743
6	6.129480	-1.792959	-0.189281
1	5.213381	-0.005903	0.401125
1	6.130983	-2.880544	-0.184637
6	7.383867	-1.200203	-0.724338
8	8.392278	-1.885687	-0.763790
6	7.427520	0.228889	-1.177052
6	8.640973	0.911807	-1.045420
6	6.335472	0.875373	-1.763844
6	8.750356	2.232438	-1.461667
1	9.487287	0.390288	-0.609712
6	6.448670	2.195466	-2.190368
1	5.398900	0.348762	-1.913715
6	7.652236	2.876754	-2.031864
1	9.691482	2.760455	-1.344567
1	5.585917	2.676830	-2.639471
1	7.738699	3.908817	-2.357880
6	1.364810	-3.812952	-0.400942
1	1.771559	-2.837673	-0.656044
1	-0.613198	-4.760161	-0.214908
6	2.062300	-4.984402	-0.966461
6	3.096211	-4.790695	-1.890093
6	1.707767	-6.293207	-0.610964
6	3.753091	-5.880332	-2.455846
1	3.374438	-3.779105	-2.175545
6	2.363243	-7.378720	-1.175351
1	0.922216	-6.457153	0.122559
6	3.387918	-7.174899	-2.100488
1	4.547900	-5.715502	-3.175928
1	2.080615	-8.387349	-0.891371
1	3.900210	-8.024772	-2.539727
7	-0.696247	-2.732584	0.140227
6	-0.004536	-3.869517	-0.172367

Number of imaginary frequencies : 1
The smallest frequency is : -209.7626

Electronic energy= -3905.2726963
Zero-point correction= 1.049891
Thermal correction to Energy= 1.116090
Thermal correction to Enthalpy= 1.117034
Thermal correction to Gibbs Free Energy= 0.939014
Sum of electronic and zero-point Energies= -3904.222806
Sum of electronic and thermal Energies= -3904.156607
Sum of electronic and thermal Enthalpies= -3904.155662
Sum of electronic and thermal Free Energies= -3904.333682

Cartesian Coordinates

7	-2.596057	1.482184	-0.236307
6	-3.279319	2.709367	-0.171773
6	-4.468113	2.955050	-0.862658
6	-5.063936	4.207964	-0.773435
6	-4.496912	5.236281	-0.030465
6	-3.298577	4.985063	0.627967
6	-2.691053	3.737983	0.570192
6	-6.312998	4.477343	-1.562888
9	-7.059278	3.376554	-1.717724
6	-2.638186	6.102845	1.381590
9	-3.536753	6.867806	2.020608
6	-3.117668	0.221197	-0.237916
16	-4.761920	-0.132386	-0.061381
7	-2.168677	-0.728053	-0.393471
6	-2.392075	-2.159381	-0.290422
6	-1.689666	-2.933486	-1.429187
6	-2.197056	-4.400061	-1.473515
6	-2.907035	-4.640784	-2.815597
6	-1.865688	-4.493196	-3.932384
6	-1.194488	-3.108009	-3.781855
7	-1.884789	-2.290816	-2.753559
6	-3.316998	-2.186438	-3.096610
6	-4.005326	-3.586015	-3.055850
6	-5.159631	-3.612993	-2.084095
6	-5.493155	-4.612916	-1.270619
6	-1.897126	-2.691551	1.052299
6	-2.744218	-3.385772	1.972466
6	-2.145971	-3.860945	3.178670
7	-0.832898	-3.669662	3.491857
6	-0.096278	-3.015239	2.629537
6	-0.580693	-2.512928	1.398874
6	-2.946153	-4.570529	4.105930
6	-4.274606	-4.811703	3.865762
6	-4.866835	-4.335425	2.667923
6	-4.117708	-3.632076	1.748612
9	-7.080884	5.409164	-0.977644
9	-6.028809	4.930555	-2.796725
9	-1.956688	6.919116	0.559443
9	-1.767619	5.654258	2.296548
1	-0.608094	-2.900300	-1.259623
1	-1.359603	-5.098035	-1.376119
1	-2.874486	-4.593404	-0.637041
1	-1.224467	-2.538868	-4.715977
1	-0.148971	-3.182810	-3.474357
1	-2.348347	-4.589112	-4.910350
1	-1.118486	-5.288850	-3.857885
1	-3.340957	-5.645061	-2.837011
1	-4.427778	-3.775995	-4.052351
1	-3.372682	-1.744714	-4.095469
1	-3.794899	-1.488746	-2.402622
1	-5.776122	-2.713134	-2.080549
1	-6.355824	-4.538277	-0.615651

1	-4.923270	-5.537105	-1.216247
1	-3.468973	-2.304400	-0.375594
1	0.101768	-1.981278	0.739830
1	-4.622892	-3.267814	0.861754
1	0.950976	-2.870016	2.891617
1	-2.468216	-4.918799	5.015846
1	-4.861161	-5.358551	4.594323
1	-1.203807	-0.406372	-0.389887
1	-1.581173	1.573288	-0.164127
1	-4.925506	2.173071	-1.453576
1	-1.758685	3.555671	1.093092
1	-4.977839	6.206070	0.037834
8	-6.171527	-4.532776	2.351321
6	-6.990424	-5.210529	3.284532
1	-7.986363	-5.243849	2.842191
1	-6.642145	-6.235600	3.458197
1	-7.040784	-4.674966	4.239598
1	-1.138505	-1.015014	-2.776352
6	2.068269	1.515779	-3.423283
6	3.037509	2.540208	-2.825738
6	3.633543	1.820698	-1.608028
7	2.644841	0.778312	-1.282789
6	1.474725	0.892399	-2.155768
6	2.912274	-0.220143	-0.436314
6	3.919764	-0.173762	0.506168
8	0.181064	2.612750	0.143903
6	0.692089	-0.385822	-2.399998
8	1.164444	-1.507929	-2.294751
8	-0.537712	-0.115036	-2.747028
8	0.366404	0.496098	0.597778
1	0.768100	1.607592	-1.711484
1	1.300810	1.962089	-4.056880
1	2.604479	0.747149	-3.990261
1	2.478202	3.422302	-2.500964
1	3.810484	2.861468	-3.525409
1	3.787026	2.494379	-0.759537
1	4.588575	1.331550	-1.835627
1	2.238679	-1.067477	-0.476153
1	4.635764	0.643277	0.454646
6	4.368648	-1.409382	1.255854
6	5.819971	-1.301507	1.723308
1	3.746139	-1.574889	2.146028
1	4.246404	-2.301994	0.630983
1	6.066526	-2.152472	2.371429
1	5.933105	-0.412733	2.361349
6	6.855501	-1.229120	0.639978
6	6.642465	-1.384434	-0.671907
1	7.874311	-1.057769	0.986186
1	5.652823	-1.611949	-1.062272
6	7.719231	-1.419485	-1.695373
8	7.560725	-2.072871	-2.712719
6	8.999074	-0.664255	-1.482951
6	10.157172	-1.158072	-2.091318
6	9.054252	0.537801	-0.771220
6	11.361230	-0.477678	-1.961514
1	10.093264	-2.079393	-2.661378
6	10.257992	1.228027	-0.657286
1	8.150924	0.944478	-0.327884
6	11.412572	0.716770	-1.243577
1	12.260210	-0.873180	-2.423427
1	10.293211	2.166374	-0.113007
1	12.352556	1.251357	-1.147420
6	2.605307	0.903383	2.031403
1	2.043139	-0.017503	2.158179
1	2.217539	2.983725	1.417905
6	3.682305	1.141253	3.009020
6	3.789294	0.286377	4.111924
6	4.615823	2.175961	2.858482
6	4.808578	0.457158	5.044548
1	3.059872	-0.508206	4.243189

6	5.633277	2.344772	3.788966
1	4.555560	2.835276	1.995932
6	5.734746	1.483060	4.882550
1	4.876681	-0.211448	5.896547
1	6.354500	3.145553	3.660577
1	6.532987	1.615030	5.605757
7	0.792013	1.672130	0.697435
6	1.933654	1.942050	1.412129

si-si_16-path-B

Number of imaginary frequencies : 1
The smallest frequency is : -244.1164

Electronic energy= -3905.2727943
Zero-point correction= 1.049922
Thermal correction to Energy= 1.116213
Thermal correction to Enthalpy= 1.117157
Thermal correction to Gibbs Free Energy= 0.939460
Sum of electronic and zero-point Energies= -3904.222873
Sum of electronic and thermal Energies= -3904.156581
Sum of electronic and thermal Enthalpies= -3904.155637
Sum of electronic and thermal Free Energies= -3904.333334

Cartesian Coordinates

7	-2.852462	-0.372443	-0.214859
6	-4.042891	-0.954156	-0.692473
6	-5.305698	-0.498971	-0.310586
6	-6.439569	-1.143974	-0.790688
6	-6.349776	-2.249816	-1.628170
6	-5.085251	-2.705535	-1.980748
6	-3.936494	-2.067553	-1.527802
6	-7.783810	-0.656071	-0.331872
9	-7.849408	0.682327	-0.315553
6	-4.948729	-3.931611	-2.836100
9	-6.021532	-4.117311	-3.618853
6	-2.551807	0.950601	-0.128538
16	-3.571551	2.184855	-0.675583
7	-1.342615	1.178106	0.441692
6	-0.692386	2.479314	0.495766
6	-0.161872	2.825663	1.904348
6	0.281298	4.312977	1.959230
6	-0.570790	5.050515	3.003446
6	-0.283615	4.427972	4.376303
6	-0.544822	2.906334	4.279153
7	-1.156500	2.557459	2.973782
6	-2.390443	3.346540	2.788339
6	-2.073250	4.870949	2.709473
6	-2.561023	5.473224	1.414289
6	-1.937107	6.388203	0.675328
6	0.467706	2.545824	-0.491633
6	0.529721	3.506430	-1.550079
6	1.697327	3.495838	-2.371024
7	2.725065	2.616278	-2.203431
6	2.620053	1.739855	-1.235937
6	1.515107	1.668633	-0.354819
6	1.810359	4.447967	-3.412324
6	0.826652	5.375680	-3.640463
6	-0.335267	5.380476	-2.826395
6	-0.480691	4.460308	-1.809522
9	-8.775567	-1.100355	-1.117422
9	-8.059639	-1.069174	0.917756
9	-4.812328	-5.043323	-2.093632
9	-3.872943	-3.867177	-3.634460
1	0.676023	2.161051	2.134586
1	1.338728	4.386714	2.232530

1	0.170104	4.778265	0.976176
1	-1.231830	2.561483	5.057893
1	0.372745	2.318082	4.362722
1	-0.925974	4.884458	5.136274
1	0.753416	4.620009	4.667276
1	-0.316038	6.114469	3.012660
1	-2.626472	5.368257	3.518211
1	-3.041811	3.117669	3.636618
1	-2.896148	2.997718	1.883598
1	-3.535097	5.113053	1.080906
1	-2.380522	6.766043	-0.240805
1	-0.963313	6.790369	0.943516
1	-1.457995	3.205145	0.221734
1	1.514196	0.918481	0.434531
1	-1.398674	4.487459	-1.234095
1	3.451521	1.048327	-1.111944
1	2.707231	4.419033	-4.022429
1	0.943142	6.094141	-4.442952
1	-0.755579	0.359737	0.594740
1	-2.117903	-1.055132	-0.015626
1	-5.397966	0.355170	0.348507
1	-2.955927	-2.427574	-1.819378
1	-7.242189	-2.738936	-2.000985
8	-1.353036	6.263343	-2.987018
6	-1.270764	7.190200	-4.052426
1	-2.190721	7.773764	-4.014842
1	-0.414106	7.864726	-3.936403
1	-1.207991	6.684023	-5.022585
1	-1.396687	1.134498	3.098423
6	-1.041677	-2.717481	4.284521
6	-0.708527	-4.181507	3.991237
6	0.685500	-4.110483	3.363404
7	0.732416	-2.772130	2.752738
6	-0.492869	-2.021073	3.034536
6	1.814955	-2.300117	2.133466
6	2.863379	-3.095920	1.707692
8	-1.562085	-2.952105	0.242575
6	-0.344045	-0.517864	3.189004
8	0.729866	0.064760	3.264517
8	-1.513396	0.055126	3.212863
8	0.144587	-1.620351	0.016479
1	-1.207839	-2.169687	2.210611
1	-2.106640	-2.526742	4.417293
1	-0.501036	-2.365154	5.170208
1	-1.423133	-4.579918	3.264505
1	-0.725213	-4.816474	4.878257
1	0.851011	-4.884816	2.609487
1	1.483212	-4.183456	4.113206
1	1.779622	-1.250250	1.881872
1	2.933150	-4.109417	2.094641
6	4.161283	-2.510970	1.213026
6	4.054277	-1.096205	0.622737
1	4.893819	-2.501940	2.031285
1	4.582683	-3.178915	0.451301
1	3.749774	-0.391265	1.407492
1	3.281767	-1.067870	-0.156868
6	5.372144	-0.663238	0.054314
6	5.643510	-0.602459	-1.253518
1	6.161105	-0.444841	0.774203
1	4.888025	-0.869408	-1.991676
6	6.993603	-0.338476	-1.820490
8	7.318341	-0.876531	-2.864776
6	7.952630	0.559921	-1.099399
6	9.320639	0.347471	-1.296924
6	7.526766	1.625849	-0.301222
6	10.252913	1.169761	-0.677749
1	9.632025	-0.470414	-1.938725
6	8.463024	2.459457	0.304446
1	6.465852	1.819091	-0.177272
6	9.823900	2.226695	0.124793

1	11.313831	0.993134	-0.823736
1	8.129596	3.294376	0.912354
1	10.552241	2.874607	0.602788
6	1.849029	-3.725518	-0.200519
1	2.166791	-2.783034	-0.635195
1	-0.033156	-4.819921	0.118022
6	2.689104	-4.899738	-0.510018
6	3.730245	-4.767727	-1.435879
6	2.469152	-6.148157	0.088195
6	4.524935	-5.861052	-1.770105
1	3.906094	-3.803871	-1.906521
6	3.263108	-7.237744	-0.244378
1	1.678900	-6.261032	0.826758
6	4.292419	-7.097368	-1.175969
1	5.322878	-5.743445	-2.495936
1	3.084509	-8.199319	0.226274
1	4.911465	-7.950647	-1.433599
7	-0.329661	-2.781719	0.081110
6	0.484128	-3.879409	0.001485

si-si_17-path-B

Number of imaginary frequencies : 1
The smallest frequency is : -218.0608

Electronic energy= -3905.2727503
Zero-point correction= 1.049789
Thermal correction to Energy= 1.115999
Thermal correction to Enthalpy= 1.116943
Thermal correction to Gibbs Free Energy= 0.939615
Sum of electronic and zero-point Energies= -3904.222962
Sum of electronic and thermal Energies= -3904.156752
Sum of electronic and thermal Enthalpies= -3904.155808
Sum of electronic and thermal Free Energies= -3904.333136

Cartesian Coordinates

7	-2.660245	1.407561	-0.260283
6	-3.417663	2.591663	-0.266952
6	-4.606898	2.731102	-0.982876
6	-5.276711	3.951147	-0.968661
6	-4.782752	5.048685	-0.278229
6	-3.580863	4.902741	0.407807
6	-2.901576	3.693044	0.425289
6	-6.543219	4.062839	-1.768353
9	-7.394856	3.065322	-1.491584
6	-2.993604	6.097036	1.102208
9	-3.941989	6.855235	1.673723
6	-3.103939	0.118349	-0.217903
16	-4.726032	-0.327100	-0.037326
7	-2.099178	-0.778044	-0.331310
6	-2.245118	-2.216061	-0.189373
6	-1.489642	-2.984301	-1.298321
6	-1.921617	-4.475083	-1.308029
6	-2.598553	-4.789537	-2.651358
6	-1.552101	-4.618929	-3.759701
6	-0.954717	-3.197592	-3.639338
7	-1.699622	-2.388914	-2.642773
6	-3.131384	-2.368357	-3.006444
6	-3.746163	-3.800710	-2.936230
6	-4.913915	-3.861010	-1.982353
6	-5.207048	-4.851562	-1.142317
6	-1.738421	-2.685393	1.171653
6	-2.555832	-3.410867	2.094545
6	-1.945106	-3.833389	3.313829
7	-0.649299	-3.560536	3.638980
6	0.057490	-2.874618	2.776100

6	-0.440027	-2.421958	1.531589
6	-2.713530	-4.575401	4.242619
6	-4.024039	-4.893292	3.993678
6	-4.630570	-4.464238	2.785079
6	-3.911724	-3.734736	1.861990
9	-7.186609	5.216760	-1.539724
9	-6.298168	4.001091	-3.088884
9	-2.333132	6.893299	0.243925
9	-2.123782	5.749723	2.060631
1	-0.413470	-2.890947	-1.117120
1	-1.051813	-5.126812	-1.178719
1	-2.601893	-4.678027	-0.476339
1	-1.000882	-2.656439	-4.589297
1	0.088618	-3.210836	-3.316819
1	-2.016942	-4.765036	-4.740043
1	-0.766273	-5.372807	-3.655345
1	-2.979944	-5.815052	-2.649071
1	-4.141373	-4.039870	-3.933395
1	-3.195843	-1.956379	-4.017399
1	-3.654502	-1.678712	-2.337365
1	-5.578432	-2.996710	-2.017953
1	-6.084069	-4.803759	-0.504206
1	-4.589535	-5.741589	-1.049624
1	-3.311872	-2.420750	-0.280694
1	0.218796	-1.862051	0.871993
1	-4.428487	-3.409250	0.966697
1	1.090250	-2.660897	3.048126
1	-2.225482	-4.884198	5.161416
1	-4.586436	-5.462409	4.724274
1	-1.153453	-0.403211	-0.326924
1	-1.653240	1.565593	-0.188314
1	-5.008976	1.894592	-1.540051
1	-1.966721	3.594916	0.966205
1	-5.317831	5.991219	-0.271416
8	-5.920909	-4.732662	2.461604
6	-6.710785	-5.440331	3.397554
1	-7.701366	-5.527215	2.950670
1	-6.313028	-6.445100	3.582899
1	-6.792314	-4.898945	4.347139
1	-1.017801	-1.085712	-2.690118
6	2.106112	1.544273	-3.394529
6	3.028473	2.626841	-2.826364
6	3.619616	1.983148	-1.564945
7	2.651630	0.932733	-1.206703
6	1.501880	0.962471	-2.112686
6	2.921809	-0.004698	-0.294390
6	3.900490	0.132029	0.670270
8	0.024850	2.683343	0.065283
6	0.778567	-0.357732	-2.312644
8	1.302561	-1.450984	-2.159075
8	-0.457945	-0.156657	-2.680828
8	0.360656	0.625993	0.682350
1	0.756810	1.669318	-1.721695
1	1.340932	1.933743	-4.067078
1	2.680305	0.767421	-3.910748
1	2.435109	3.504543	-2.554217
1	3.806289	2.940286	-3.524232
1	3.740151	2.700755	-0.747782
1	4.590651	1.508698	-1.752214
1	2.273170	-0.871685	-0.296951
1	4.606728	0.953204	0.574777
6	4.345531	-1.029332	1.530490
6	5.825940	-0.935812	1.899568
1	3.779503	-1.055752	2.471808
1	4.142804	-1.981425	1.026079
1	6.074189	-1.708349	2.638911
1	6.008832	0.020698	2.411966
6	6.800072	-1.050901	0.764407
6	6.500104	-1.336375	-0.507880
1	7.845647	-0.910173	1.036507

1	5.476591	-1.537708	-0.816006
6	7.505941	-1.560952	-1.577734
8	7.233053	-2.296908	-2.511143
6	8.853925	-0.903013	-1.516674
6	9.923379	-1.558535	-2.135173
6	9.058597	0.354451	-0.940546
6	11.186281	-0.981349	-2.149364
1	9.743596	-2.522499	-2.600210
6	10.321516	0.939676	-0.970922
1	8.225620	0.884875	-0.490122
6	11.386902	0.269633	-1.566209
1	12.014589	-1.500819	-2.620520
1	10.472103	1.920940	-0.532165
1	12.372638	0.724254	-1.582914
6	2.566300	1.315343	2.079147
1	2.066957	0.384003	2.331059
1	2.036136	3.293963	1.273668
6	3.654467	1.748676	2.976109
6	3.879251	1.064541	4.176063
6	4.489223	2.824261	2.642210
6	4.914033	1.449920	5.025601
1	3.230135	0.237291	4.449906
6	5.519583	3.207554	3.489367
1	4.339547	3.349129	1.701918
6	5.736897	2.518681	4.683610
1	5.074518	0.914767	5.955957
1	6.159001	4.041407	3.217922
1	6.545612	2.816733	5.342996
7	0.700044	1.833122	0.688117
6	1.821487	2.239804	1.367530

si-re_1-path-B

Number of imaginary frequencies : 1
 The smallest frequency is : -296.9468

Electronic energy= -3905.2847095
 Zero-point correction= 1.051058
 Thermal correction to Energy= 1.116507
 Thermal correction to Enthalpy= 1.117451
 Thermal correction to Gibbs Free Energy= 0.947767
 Sum of electronic and zero-point Energies= -3904.233652
 Sum of electronic and thermal Energies= -3904.168203
 Sum of electronic and thermal Enthalpies= -3904.167258
 Sum of electronic and thermal Free Energies= -3904.336942

 Cartesian Coordinates

6	-3.415484	2.903096	1.150013
6	-4.252653	2.843777	2.433054
6	-4.922637	1.462710	2.376407
7	-4.099298	0.686232	1.428311
6	-2.929852	1.451224	0.992363
6	-4.597187	-0.355579	0.760715
6	-3.928962	-1.215976	-0.093775
8	0.053931	-1.340995	2.193892
6	-1.710322	1.224581	1.885821
8	-0.598550	1.239003	1.193771
8	-1.800111	1.116742	3.095459
8	-0.827052	-1.995532	0.318802
1	-2.689982	1.194521	-0.039106
1	-2.587671	3.615359	1.196818
1	-4.039657	3.155882	0.287430
1	-3.601343	2.902732	3.306237
1	-4.988744	3.647408	2.488685
1	-4.941936	0.973574	3.353298
1	-5.946138	1.513699	1.990915

6	-4.752764	-2.099502	-1.008021
1	-5.172219	-1.482477	-1.812739
6	-3.197215	-2.501542	1.525703
1	-2.922856	-3.158853	0.707965
1	-2.150076	-1.483614	3.183423
6	-4.408985	-2.859778	2.290539
6	-5.189282	-3.952705	1.899194
6	-4.807711	-2.106906	3.405049
6	-6.340802	-4.290298	2.607177
1	-4.886068	-4.545955	1.040228
6	-5.957261	-2.442393	4.107373
1	-4.219522	-1.245747	3.710821
6	-6.727687	-3.536412	3.710948
1	-6.932699	-5.145468	2.297043
1	-6.253727	-1.851765	4.968497
1	-7.624126	-3.799297	4.263177
7	-0.934849	-1.732612	1.544185
6	-2.142293	-1.868784	2.176948
7	0.079222	0.313716	-1.490388
6	-0.873480	1.261708	-1.900949
6	-0.798540	2.614945	-1.551009
6	-1.860579	3.459903	-1.843934
6	-3.017587	2.995319	-2.461947
6	-3.080755	1.648731	-2.794985
6	-2.020642	0.785459	-2.540323
6	-1.777070	4.905357	-1.444198
9	-1.008950	5.078679	-0.356252
6	-4.374882	1.103578	-3.318610
9	-4.987793	1.957353	-4.147908
6	1.349559	0.607801	-1.036643
16	2.349697	1.735621	-1.795883
7	1.701455	-0.134855	0.020162
6	2.946260	-0.028847	0.758826
6	2.653821	0.216034	2.257260
6	3.954516	0.552996	3.033523
6	3.794672	1.927976	3.697904
6	2.620175	1.850751	4.684923
6	1.362212	1.371073	3.917986
7	1.638326	1.276042	2.467262
6	2.110503	2.586655	1.976625
6	3.459441	2.996603	2.640320
6	4.526854	3.248015	1.603291
6	5.808833	2.894250	1.667260
6	3.773113	-1.299935	0.621524
6	5.137298	-1.291358	0.190408
6	5.813775	-2.547107	0.152338
7	5.223933	-3.730249	0.490348
6	3.970422	-3.692643	0.868129
6	3.203900	-2.504990	0.948754
6	7.166805	-2.583431	-0.262890
6	7.835842	-1.440341	-0.620198
6	7.161217	-0.193598	-0.580908
6	5.840003	-0.124910	-0.190784
9	-1.262925	5.675256	-2.412612
9	-2.991177	5.403925	-1.152593
9	-5.238847	0.869452	-2.305845
9	-4.223105	-0.058857	-3.968776
1	2.200713	-0.693614	2.657442
1	4.145580	-0.206152	3.798438
1	4.813948	0.551058	2.358361
1	0.514885	2.050048	4.044197
1	1.026606	0.382840	4.243392
1	2.447744	2.833546	5.136097
1	2.860872	1.158609	5.497644
1	4.712228	2.199731	4.228816
1	3.298387	3.946583	3.168779
1	1.319189	3.310126	2.197689
1	2.204471	2.533942	0.887096
1	4.184649	3.793260	0.722158
1	6.495939	3.136025	0.862277

1	6.223941	2.350933	2.512404
1	3.484928	0.824908	0.345759
1	2.164311	-2.561107	1.265887
1	5.367494	0.850867	-0.194174
1	3.508788	-4.643073	1.131199
1	7.657690	-3.551102	-0.285484
1	8.871953	-1.498880	-0.931428
1	0.988962	-0.726855	0.447645
1	-0.341191	-0.509502	-1.056225
1	0.062575	2.989556	-1.013438
1	-2.078878	-0.259667	-2.824426
1	-3.852349	3.658983	-2.660420
8	7.749686	0.983301	-0.914858
6	9.081486	0.951780	-1.389902
1	9.341374	1.984338	-1.624034
1	9.774113	0.572405	-0.629546
1	9.170040	0.345668	-2.299037
1	0.285225	1.129936	1.781453
1	-5.610802	-2.497950	-0.450186
1	-2.910841	-0.983195	-0.403454
1	-5.632340	-0.589737	1.014173
6	-3.999698	-3.269886	-1.672267
1	-4.725191	-3.812290	-2.290628
1	-3.622571	-3.982631	-0.931846
6	-2.876814	-2.798578	-2.542213
6	-1.581970	-3.054204	-2.327398
1	-3.141797	-2.179148	-3.400046
1	-1.268393	-3.642571	-1.470580
6	-0.534703	-2.444439	-3.196269
8	-0.833106	-1.659918	-4.084741
6	0.897430	-2.760451	-2.913961
6	1.293877	-3.981392	-2.359656
6	1.860676	-1.801324	-3.244293
6	2.644734	-4.246523	-2.159409
1	0.553831	-4.737807	-2.115425
6	3.206488	-2.052728	-3.003528
1	1.533757	-0.855201	-3.664793
6	3.599212	-3.280746	-2.472878
1	2.957548	-5.201752	-1.748959
1	3.947396	-1.290616	-3.224559
1	4.650257	-3.483545	-2.289238

si-re_2-path-B

Number of imaginary frequencies : 1

The smallest frequency is : -280.4992

Electronic energy=	-3905.2845125
Zero-point correction=	1.050690
Thermal correction to Energy=	1.116178
Thermal correction to Enthalpy=	1.117122
Thermal correction to Gibbs Free Energy=	0.947822
Sum of electronic and zero-point Energies=	-3904.233822
Sum of electronic and thermal Energies=	-3904.168335
Sum of electronic and thermal Enthalpies=	-3904.167391
Sum of electronic and thermal Free Energies=	-3904.336691

Cartesian Coordinates

6	-3.460269	2.874054	1.248669
6	-4.267187	2.776809	2.550515
6	-4.809861	1.335303	2.563126
7	-4.043230	0.630811	1.519723
6	-2.914318	1.446205	1.069361
6	-4.567698	-0.371740	0.812217
6	-3.918128	-1.185432	-0.099097
8	-0.003136	-1.278375	2.326817

6	-1.675884	1.257913	1.944681
8	-0.574311	1.287994	1.237495
8	-1.747863	1.157733	3.155928
8	-0.770327	-1.903409	0.394822
1	-2.681610	1.207818	0.032350
1	-2.663709	3.622069	1.283887
1	-4.110933	3.102876	0.399098
1	-3.613000	2.931201	3.409306
1	-5.073160	3.511472	2.590737
1	-4.649242	0.857694	3.532909
1	-5.874285	1.279549	2.314868
6	-4.742938	-2.024688	-1.050525
1	-5.163347	-1.374035	-1.827835
6	-3.161070	-2.537406	1.456207
1	-2.796670	-3.111610	0.610823
1	-2.256485	-1.537646	3.210491
6	-4.373490	-3.059434	2.119457
6	-4.973587	-4.222590	1.626107
6	-4.943104	-2.425354	3.232920
6	-6.114311	-4.745491	2.228660
1	-4.532348	-4.730361	0.773339
6	-6.082207	-2.946923	3.833123
1	-4.493643	-1.513914	3.619600
6	-6.671685	-4.108603	3.332570
1	-6.563120	-5.652386	1.836375
1	-6.514136	-2.447771	4.694814
1	-7.561206	-4.513839	3.804055
7	-0.945619	-1.677846	1.622426
6	-2.180419	-1.877643	2.189825
7	0.049975	0.398487	-1.470628
6	-0.898031	1.365854	-1.850317
6	-0.809565	2.708342	-1.466383
6	-1.873062	3.565116	-1.717540
6	-3.043061	3.122459	-2.326495
6	-3.118339	1.785866	-2.695717
6	-2.056937	0.912794	-2.485592
6	-1.775613	4.998164	-1.278830
9	-1.002602	5.134076	-0.189118
6	-4.427315	1.260107	-3.201634
9	-5.041694	2.124451	-4.018685
6	1.326948	0.670629	-1.020092
16	2.334314	1.797303	-1.770380
7	1.674430	-0.092785	0.023399
6	2.929388	-0.029096	0.749099
6	2.662297	0.215968	2.252272
6	3.980704	0.511470	3.015152
6	3.870139	1.889734	3.683158
6	2.706707	1.845246	4.685433
6	1.426043	1.400943	3.934698
7	1.680276	1.303390	2.480022
6	2.182259	2.602106	1.987453
6	3.552375	2.969919	2.632224
6	4.611852	3.191383	1.580191
6	5.883175	2.798112	1.623797
6	3.708879	-1.328020	0.595571
6	5.069651	-1.367472	0.155899
6	5.698558	-2.647085	0.105333
7	5.066565	-3.810404	0.434598
6	3.816822	-3.729039	0.818250
6	3.096927	-2.514085	0.915959
6	7.046123	-2.730693	-0.320914
6	7.753554	-1.611384	-0.679139
6	7.125926	-0.340708	-0.628018
6	5.811751	-0.225429	-0.224867
9	-1.256403	5.788884	-2.227706
9	-2.984064	5.499131	-0.969956
9	-5.278056	1.034247	-2.176130
9	-4.301909	0.097041	-3.856957
1	2.187388	-0.682728	2.651395
1	4.155951	-0.253985	3.777519

1	4.832911	0.484034	2.331469
1	0.598670	2.101709	4.074061
1	1.068278	0.421466	4.262634
1	2.567525	2.832381	5.138504
1	2.938255	1.146296	5.494960
1	4.802420	2.133158	4.202130
1	3.427727	3.923282	3.164306
1	1.415605	3.347017	2.223680
1	2.258665	2.552035	0.896587
1	4.273791	3.750541	0.706263
1	6.565478	3.021441	0.809358
1	6.294108	2.239091	2.460691
1	3.490652	0.808617	0.333276
1	2.058696	-2.534840	1.241844
1	5.375263	0.767127	-0.218689
1	3.320183	-4.663853	1.073236
1	7.500345	-3.715854	-0.353822
1	8.783639	-1.707133	-1.000841
1	0.955519	-0.691820	0.430222
1	-0.379555	-0.416562	-1.030991
1	0.062024	3.063886	-0.932560
1	-2.124083	-0.123963	-2.796181
1	-3.878684	3.795007	-2.488412
8	7.754096	0.814785	-0.963460
6	9.079239	0.736388	-1.452014
1	9.373301	1.759416	-1.687640
1	9.765424	0.331239	-0.699153
1	9.136915	0.128963	-2.362676
1	0.318447	1.180621	1.813094
1	-5.598568	-2.452752	-0.511596
1	-2.901957	-0.936815	-0.402887
1	-5.595053	-0.620061	1.082636
6	-3.980552	-3.161706	-1.759773
1	-4.700171	-3.692786	-2.394138
1	-3.591594	-3.889894	-1.042394
6	-2.860655	-2.654861	-2.612189
6	-1.563611	-2.884095	-2.380063
1	-3.126927	-2.039018	-3.471957
1	-1.248612	-3.473460	-1.523636
6	-0.517403	-2.264196	-3.243503
8	-0.816386	-1.459155	-4.112688
6	0.912012	-2.606705	-2.982335
6	1.294131	-3.846324	-2.460390
6	1.886081	-1.654226	-3.298865
6	2.642391	-4.136112	-2.277146
1	0.544026	-4.596758	-2.228336
6	3.229577	-1.931510	-3.075669
1	1.569099	-0.693411	-3.692916
6	3.608314	-3.177490	-2.577017
1	2.944831	-5.104434	-1.890475
1	3.979992	-1.175590	-3.285203
1	4.658010	-3.400216	-2.410052

si-re_3-path-B

Number of imaginary frequencies : 1

The smallest frequency is : -313.5696

Electronic energy=	-3905.2764903
Zero-point correction=	1.050314
Thermal correction to Energy=	1.116457
Thermal correction to Enthalpy=	1.117401
Thermal correction to Gibbs Free Energy=	0.941640
Sum of electronic and zero-point Energies=	-3904.226176
Sum of electronic and thermal Energies=	-3904.160033
Sum of electronic and thermal Enthalpies=	-3904.159089
Sum of electronic and thermal Free Energies=	-3904.334851

..... Cartesian Coordinates			
6	-0.530803	3.708914	1.190749
6	-0.809576	4.085122	2.655174
6	-1.819295	3.025597	3.148491
7	-1.867983	2.020241	2.067945
6	-0.698689	2.178604	1.207079
6	-3.010636	1.431127	1.720776
6	-3.224297	0.492271	0.724359
8	0.958712	-1.388497	1.490571
6	0.546593	1.564363	1.846227
8	1.512675	1.423490	0.974127
8	0.618556	1.318837	3.035925
8	-0.580391	-1.261960	-0.050973
1	-0.869269	1.744647	0.220507
1	0.458224	4.013912	0.842069
1	-1.282103	4.136944	0.520839
1	0.108731	4.021155	3.242127
1	-1.205837	5.096892	2.751834
1	-1.480660	2.553877	4.072962
1	-2.822291	3.433996	3.294930
6	-4.629550	0.116381	0.302157
1	-4.680857	-0.974982	0.179333
6	-2.539590	-1.259219	1.783553
1	-2.736083	-1.764579	0.841325
1	-0.800835	-1.028997	3.131555
6	-3.562838	-1.434878	2.832906
6	-4.647500	-2.286129	2.600198
6	-3.492950	-0.735231	4.045749
6	-5.658390	-2.419955	3.549116
1	-4.699307	-2.843276	1.668699
6	-4.501537	-0.869148	4.991154
1	-2.656014	-0.064164	4.228207
6	-5.590572	-1.707161	4.742058
1	-6.499780	-3.076079	3.350855
1	-4.444500	-0.316829	5.923866
1	-6.380261	-1.804895	5.480043
7	-0.242362	-1.269818	1.158108
6	-1.195539	-1.149823	2.135188
7	1.290277	0.155512	-1.725768
6	0.484278	1.241885	-2.061877
6	0.882068	2.578709	-1.955336
6	-0.052853	3.585969	-2.165361
6	-1.382393	3.309605	-2.465397
6	-1.761240	1.975134	-2.570297
6	-0.846378	0.947928	-2.388068
6	0.376417	5.020759	-2.042107
9	1.448644	5.158604	-1.247584
6	-3.193544	1.661492	-2.888371
9	-3.517730	1.997522	-4.144001
6	2.643737	0.141879	-1.477841
16	3.774760	1.019026	-2.367647
7	2.935719	-0.692431	-0.470433
6	4.252540	-1.023060	0.033013
6	4.267753	-0.799011	1.560407
6	5.684424	-1.008382	2.158821
6	6.129759	0.287650	2.850308
6	5.147560	0.584301	3.992744
6	3.713641	0.628694	3.409124
7	3.746664	0.540393	1.931745
6	4.600313	1.624852	1.402912
6	6.078739	1.470368	1.864496
6	7.020137	1.384888	0.688097
6	8.096436	0.608546	0.581686
6	4.592367	-2.478881	-0.270464
6	5.827899	-2.876885	-0.871444
6	6.041997	-4.276185	-1.053706
7	5.129990	-5.227586	-0.705770
6	4.002524	-4.819491	-0.178521

6	3.691262	-3.459902	0.062229
6	7.262162	-4.713177	-1.623771
6	8.234673	-3.823042	-2.000764
6	8.014782	-2.432571	-1.827912
6	6.834470	-1.973688	-1.282947
9	0.693721	5.557729	-3.227982
9	-0.602964	5.781988	-1.521603
9	-4.031566	2.339636	-2.081941
9	-3.473151	0.357053	-2.739027
1	3.557543	-1.510785	1.997705
1	5.671977	-1.827085	2.885101
1	6.392780	-1.287463	1.374480
1	3.188360	1.550672	3.669873
1	3.093730	-0.198019	3.765603
1	5.402938	1.538443	4.465569
1	5.224902	-0.190096	4.761910
1	7.142644	0.172409	3.247961
1	6.350339	2.376331	2.423933
1	4.167047	2.563728	1.761570
1	4.515514	1.630050	0.311420
1	6.776781	2.051128	-0.141379
1	8.715126	0.626675	-0.310248
1	8.397332	-0.081908	1.365726
1	4.965865	-0.355150	-0.452873
1	2.731857	-3.208079	0.509502
1	6.712220	-0.901595	-1.185186
1	3.279680	-5.588194	0.088931
1	7.400144	-5.782052	-1.750636
1	9.159379	-4.188199	-2.431502
1	2.152422	-1.008997	0.110181
1	0.759137	-0.578528	-1.252526
1	1.897569	2.821729	-1.671718
1	-1.161939	-0.088003	-2.458613
1	-2.104931	4.107846	-2.599365
8	8.923094	-1.485240	-2.176350
6	10.130536	-1.908119	-2.779972
1	10.694718	-0.999661	-2.991926
1	10.717417	-2.545465	-2.108180
1	9.945577	-2.440956	-3.719877
1	2.367682	0.968768	1.407270
1	-4.827153	0.533329	-0.690828
1	-2.450264	0.342362	-0.027137
1	-3.831555	1.669998	2.394704
6	-5.744504	0.553424	1.249543
1	-5.830790	1.649767	1.249674
1	-5.510270	0.277992	2.287504
6	-7.094602	-0.009830	0.936061
6	-7.418549	-0.789025	-0.100882
1	-7.896039	0.245108	1.629084
1	-6.683161	-1.072606	-0.845507
6	-8.824749	-1.249609	-0.262882
8	-9.713404	-0.837749	0.465229
6	-9.146882	-2.229648	-1.352302
6	-8.171007	-2.967064	-2.029202
6	-10.495106	-2.419356	-1.674409
6	-8.540099	-3.876113	-3.016829
1	-7.120822	-2.856002	-1.781133
6	-10.861774	-3.318101	-2.666553
1	-11.239748	-1.847083	-1.131196
6	-9.882864	-4.048347	-3.340331
1	-7.777023	-4.449189	-3.533586
1	-11.909443	-3.453511	-2.915796
1	-10.168070	-4.752372	-4.116023

si-re_4-path-B

Number of imaginary frequencies : 1

The smallest frequency is : -317.9896

Electronic energy= -3905.2751046
Zero-point correction= 1.050377
Thermal correction to Energy= 1.116465
Thermal correction to Enthalpy= 1.117409
Thermal correction to Gibbs Free Energy= 0.942183
Sum of electronic and zero-point Energies= -3904.224728
Sum of electronic and thermal Energies= -3904.158639
Sum of electronic and thermal Enthalpies= -3904.157695
Sum of electronic and thermal Free Energies= -3904.332921

.....
Cartesian Coordinates

.....
6 1.000552 -4.334960 0.970326
6 1.482410 -4.756564 2.365627
6 2.650966 -3.801963 2.676240
7 2.545753 -2.734230 1.662998
6 1.261206 -2.817464 0.970633
6 3.623967 -2.116352 1.181968
6 3.679080 -1.074986 0.270808
8 -0.204797 0.927328 1.626674
6 0.143345 -2.126551 1.749463
8 -0.851101 -1.794050 0.966780
8 0.183042 -1.989940 2.959147
8 1.236505 0.943137 -0.007474
1 1.342451 -2.395953 -0.032075
1 -0.047900 -4.575430 0.777494
1 1.610583 -4.794129 0.187206
1 0.685934 -4.614352 3.098014
1 1.794987 -5.801420 2.396033
1 2.565610 -3.376052 3.678553
1 3.628242 -4.283064 2.577726
6 5.020313 -0.741604 -0.356051
1 5.523683 -1.663713 -0.666016
6 3.287305 0.497216 1.740126
1 3.551376 1.184868 0.941938
1 1.564527 0.189217 3.080763
6 4.306548 0.308272 2.791481
6 5.520494 0.998252 2.714250
6 4.081004 -0.555882 3.873324
6 6.493024 0.828617 3.697890
1 5.689531 1.682869 1.886717
6 5.053371 -0.727472 4.849069
1 3.141099 -1.099930 3.934819
6 6.263056 -0.035619 4.763257
1 7.428080 1.375568 3.631543
1 4.869513 -1.400045 5.681102
1 7.020545 -0.169275 5.528951
7 0.969236 0.788897 1.210201
6 1.943067 0.449674 2.105548
7 -0.702888 -0.562960 -1.718465
6 -0.110152 -1.750975 -2.151651
6 -0.684232 -3.012141 -1.935453
6 0.024704 -4.152659 -2.279030
6 1.304471 -4.088400 -2.825956
6 1.864064 -2.834892 -3.027757
6 1.171593 -1.670546 -2.704166
6 -0.576159 -5.508754 -2.040148
9 -1.609179 -5.463690 -1.187392
6 3.272419 -2.743286 -3.536271
9 3.586849 -3.767559 -4.338661
6 -2.027341 -0.369410 -1.388368
16 -3.312126 -1.078047 -2.220839
7 -2.156485 0.476932 -0.360901
6 -3.396011 0.924056 0.242305
6 -3.319768 0.679629 1.765299
6 -4.660242 1.015090 2.471746
6 -5.158824 -0.232463 3.214634
6 -4.109129 -0.618613 4.266590

6	-2.748264	-0.817819	3.554231
7	-2.904092	-0.709300	2.086520
6	-3.904294	-1.696381	1.630400
6	-5.310631	-1.413063	2.236897
6	-6.350883	-1.238245	1.157467
6	-7.348385	-0.356883	1.140829
6	-3.617904	2.409056	-0.021480
6	-4.859435	2.933443	-0.500297
6	-4.949790	4.348744	-0.657078
7	-3.919395	5.201655	-0.393454
6	-2.793591	4.678368	0.024669
6	-2.596848	3.291713	0.230069
6	-6.168258	4.910521	-1.108991
6	-7.256054	4.125348	-1.392828
6	-7.161535	2.718144	-1.242053
6	-5.986006	2.138479	-0.814674
9	-1.017977	-6.072419	-3.172672
9	0.332085	-6.355646	-1.519043
9	4.161521	-2.760908	-2.521570
9	3.492650	-1.609902	-4.219221
1	-2.516851	1.313789	2.154973
1	-4.517641	1.834497	3.183074
1	-5.404427	1.348921	1.744290
1	-2.307846	-1.795931	3.763150
1	-2.008695	-0.069554	3.851516
1	-4.415344	-1.536177	4.779887
1	-4.033462	0.167278	5.024253
1	-6.116194	-0.023479	3.701546
1	-5.604992	-2.293305	2.825100
1	-3.531448	-2.680149	1.932224
1	-3.926188	-1.683779	0.535747
1	-6.258399	-1.932186	0.320207
1	-8.047948	-0.319115	0.311556
1	-7.500879	0.368038	1.936638
1	-4.203755	0.333625	-0.193287
1	-1.630888	2.939174	0.585264
1	-5.962734	1.058428	-0.729086
1	-1.976293	5.368404	0.225540
1	-6.209623	5.989025	-1.221533
1	-8.175381	4.584821	-1.735472
1	-1.314499	0.703427	0.178588
1	-0.046919	0.081172	-1.272337
1	-1.657680	-3.089693	-1.470247
1	1.619969	-0.695537	-2.874294
1	1.849658	-4.990368	-3.082239
8	-8.191207	1.870399	-1.500665
6	-9.403943	2.421967	-1.975086
1	-10.080844	1.579855	-2.121512
1	-9.845790	3.113215	-1.247834
1	-9.264149	2.938481	-2.931795
1	-1.626186	-1.263573	1.473724
1	5.675956	-0.267115	0.388413
1	2.782505	-0.797945	-0.281140
1	4.556468	-2.430352	1.653994
6	4.933152	0.171423	-1.593222
1	4.320293	-0.322060	-2.354202
1	5.938497	0.290632	-2.009553
6	4.352698	1.509981	-1.264592
6	5.051368	2.647769	-1.190879
1	3.288028	1.552460	-1.024697
1	6.107734	2.674113	-1.448059
6	4.391475	3.891562	-0.705940
8	3.387103	3.832815	-0.014997
6	4.993511	5.216681	-1.056607
6	5.934215	5.361562	-2.079908
6	4.567457	6.343198	-0.345614
6	6.446584	6.619417	-2.384303
1	6.251211	4.499291	-2.657975
6	5.087365	7.595709	-0.642593
1	3.826370	6.211259	0.435841

6	6.028677	7.734484	-1.662723
1	7.170656	6.729473	-3.185121
1	4.760184	8.466377	-0.083191
1	6.433762	8.714234	-1.896844

si-re_5-path-B

Number of imaginary frequencies : 1

The smallest frequency is : -304.7522

Electronic energy=	-3905.2742147
Zero-point correction=	1.049744
Thermal correction to Energy=	1.115781
Thermal correction to Enthalpy=	1.116725
Thermal correction to Gibbs Free Energy=	0.943301
Sum of electronic and zero-point Energies=	-3904.224470
Sum of electronic and thermal Energies=	-3904.158433
Sum of electronic and thermal Enthalpies=	-3904.157489
Sum of electronic and thermal Free Energies=	-3904.330913

 Cartesian Coordinates

6	3.890154	0.212232	-2.916826
6	2.371805	0.230240	-3.108154
6	1.866413	-0.176216	-1.724072
7	2.841707	-1.189968	-1.307175
6	4.140201	-0.959972	-1.957002
6	2.659675	-2.090274	-0.340811
6	3.678868	-2.794461	0.291903
8	0.681891	-1.142043	3.141755
8	1.461407	-0.277259	1.299553
1	4.444077	-1.877251	-2.474772
1	4.214320	1.144907	-2.447837
1	4.438089	0.095138	-3.853013
1	1.980437	1.202719	-3.406913
1	2.056388	-0.516870	-3.844702
1	1.951036	0.684100	-1.045619
1	1.634699	-2.199697	-0.017983
1	4.680394	-2.723924	-0.127567
6	3.430090	-4.054503	1.088282
6	2.017221	-4.295033	1.646590
1	4.140382	-4.077249	1.925131
1	3.701332	-4.915772	0.461987
1	2.079920	-5.181522	2.291273
1	1.690122	-3.469744	2.286497
6	0.967625	-4.549464	0.604889
6	-0.206337	-3.911318	0.585229
1	1.189374	-5.306993	-0.147586
1	-0.436465	-3.172380	1.353082
6	-1.302308	-4.149243	-0.380746
8	-2.453344	-3.872000	-0.071666
6	-1.020527	-4.735184	-1.731273
6	0.145947	-4.443018	-2.445921
6	-2.009782	-5.531913	-2.316132
6	0.321588	-4.958719	-3.727200
1	0.884960	-3.776780	-2.012013
6	-1.823597	-6.058666	-3.588610
1	-2.917172	-5.733987	-1.755285
6	-0.656017	-5.772471	-4.294744
1	1.220623	-4.719545	-4.286499
1	-2.587651	-6.689045	-4.032323
1	-0.512413	-6.178891	-5.291204
6	3.947914	-1.203192	1.813419
1	3.866876	-0.436756	1.045146
1	2.948595	-1.810923	3.681134
6	5.327668	-1.532946	2.228816
6	6.397715	-0.939711	1.545048

6	5.606885	-2.410145	3.285795
6	7.710558	-1.211394	1.908543
1	6.192162	-0.240803	0.738609
6	6.922376	-2.686198	3.643880
1	4.797834	-2.881501	3.835092
6	7.976803	-2.089766	2.957356
1	8.526996	-0.733705	1.376599
1	7.123184	-3.367444	4.464457
1	9.002165	-2.305143	3.240470
7	1.642126	-0.884710	2.400166
6	2.901014	-1.292377	2.736343
7	0.366761	2.142876	0.472116
6	1.391694	2.975402	0.028559
6	1.263793	4.080179	-0.821384
6	2.410684	4.753410	-1.235121
6	3.688650	4.367702	-0.848544
6	3.797890	3.273683	0.003512
6	2.676853	2.594805	0.450103
6	2.250824	5.975057	-2.097643
9	3.325149	6.173982	-2.877787
6	5.143829	2.725336	0.371736
9	5.489531	1.704018	-0.452996
6	-0.969461	2.068446	0.182131
16	-1.888996	3.312490	-0.480451
7	-1.464209	0.855161	0.511142
6	-2.870170	0.490689	0.505296
6	-3.124706	-0.692739	-0.451751
6	-4.588900	-1.193648	-0.391155
6	-5.106652	-1.414776	-1.818566
6	-4.121306	-2.337431	-2.544547
6	-2.772889	-1.595740	-2.667483
7	-2.770978	-0.347727	-1.857200
6	-3.751477	0.591312	-2.442824
6	-5.156264	-0.073775	-2.572666
6	-6.227012	0.892613	-2.136470
6	-7.206412	0.671158	-1.262909
6	-3.346676	0.163406	1.914953
6	-4.574476	0.687762	2.435591
6	-4.940326	0.297949	3.757654
7	-4.180380	-0.524829	4.536472
6	-3.059232	-0.970160	4.027543
6	-2.603405	-0.657577	2.723534
6	-6.152276	0.784395	4.304475
6	-6.978064	1.614744	3.590966
6	-6.612048	2.003387	2.277223
6	-5.434485	1.552830	1.718979
9	1.182355	5.886558	-2.899933
9	2.096250	7.084161	-1.358504
9	5.166529	2.217774	1.611125
9	6.114757	3.637865	0.279518
1	-2.441709	-1.502071	-0.170418
1	-4.627681	-2.127629	0.176895
1	-5.223989	-0.468149	0.121917
1	-2.566640	-1.294486	-3.699820
1	-1.939625	-2.210616	-2.322462
1	-4.500894	-2.610142	-3.534419
1	-3.984164	-3.256226	-1.966063
1	-6.102275	-1.868216	-1.792060
1	-5.329934	-0.296012	-3.635359
1	-3.362875	0.904895	-3.416421
1	-3.787302	1.486453	-1.816973
1	-6.154890	1.880895	-2.593996
1	-7.912286	1.454678	-1.006576
1	-7.337987	-0.285051	-0.763662
1	-3.398692	1.372403	0.146732
1	-1.646155	-1.060785	2.405069
1	-5.207754	1.881317	0.710433
1	-2.454026	-1.618116	4.658641
1	-6.405378	0.473728	5.312969
1	-7.900022	1.968220	4.037037

1	-0.800732	0.146939	0.824815
1	0.714623	1.355250	1.022072
1	0.288288	4.400686	-1.159501
1	2.784410	1.740188	1.114036
1	4.566089	4.899946	-1.197186
8	-7.371534	2.819167	1.501792
6	-8.560148	3.348198	2.056269
1	-8.991437	3.989437	1.287091
1	-9.277206	2.557154	2.306082
1	-8.354884	3.949522	2.949518
1	-1.404845	0.104552	-2.029289
1	4.908196	-0.722826	-1.211974
6	0.397964	-0.568681	-1.682579
8	-0.020166	-1.587403	-1.146620
8	-0.350426	0.337428	-2.237871

re-si_1-path-B

Number of imaginary frequencies : 1
 The smallest frequency is : -292.4385

Electronic energy= -3905.2785914
 Zero-point correction= 1.050100
 Thermal correction to Energy= 1.116310
 Thermal correction to Enthalpy= 1.117255
 Thermal correction to Gibbs Free Energy= 0.940526
 Sum of electronic and zero-point Energies= -3904.228491
 Sum of electronic and thermal Energies= -3904.162281
 Sum of electronic and thermal Enthalpies= -3904.161337
 Sum of electronic and thermal Free Energies= -3904.338066

 Cartesian Coordinates

6	-1.859095	0.782860	4.582703
6	-2.979153	-0.223773	4.276252
6	-3.571150	0.251317	2.937302
7	-2.554528	1.159006	2.396793
6	-1.330084	1.123613	3.181110
6	-2.679520	1.829759	1.258309
6	-3.672153	1.616049	0.309050
8	0.241308	1.661848	-2.027191
6	-0.426761	-0.017930	2.704278
8	0.805134	0.110643	3.100208
8	-0.880158	-0.975563	2.087075
8	-0.250917	1.105540	0.020281
1	-0.794143	2.073320	3.125710
1	-1.080486	0.378971	5.232446
1	-2.261664	1.690746	5.040161
1	-2.558703	-1.224585	4.157482
1	-3.733989	-0.260511	5.062990
1	-3.750467	-0.578208	2.245760
1	-4.507636	0.807468	3.059477
1	-1.872815	2.526809	1.044232
1	-4.523912	1.009521	0.605850
6	-2.582597	0.026706	-0.704302
1	-2.125877	-0.308007	0.225920
1	-1.917720	0.728218	-2.695063
6	-3.720635	-0.795274	-1.174375
6	-4.075745	-1.925662	-0.426081
6	-4.417484	-0.520304	-2.359259
6	-5.091623	-2.771487	-0.859415
1	-3.521116	-2.153250	0.481679
6	-5.446339	-1.356674	-2.780534
1	-4.147925	0.342345	-2.961503
6	-5.781131	-2.486850	-2.036908
1	-5.339247	-3.657124	-0.282268
1	-5.980446	-1.132237	-3.697995

1	-6.576690	-3.142586	-2.376019
7	-0.539213	1.143125	-1.218204
6	-1.725125	0.608883	-1.639868
7	2.645001	1.504592	0.033838
6	3.342224	2.697835	-0.194903
6	4.604817	2.967149	0.333886
6	5.192754	4.207230	0.098485
6	4.549386	5.196477	-0.631387
6	3.279586	4.919907	-1.131339
6	2.676027	3.688111	-0.928440
6	6.574132	4.448818	0.636501
9	7.511835	3.846552	-0.109967
6	2.548720	6.002696	-1.870917
9	3.338325	6.612130	-2.768542
6	3.115815	0.228121	0.117189
16	4.723571	-0.225081	-0.133937
7	2.133236	-0.651464	0.428075
6	2.247851	-2.095730	0.315782
6	1.622039	-2.805281	1.534877
6	2.041015	-4.297693	1.589536
6	2.836197	-4.543067	2.881670
6	1.902764	-4.279269	4.071217
6	1.320959	-2.853286	3.919566
7	1.978155	-2.129304	2.806970
6	3.439217	-2.118735	3.025840
6	4.021502	-3.564271	2.986346
6	5.081835	-3.707779	1.921827
6	5.277827	-4.755720	1.124288
6	1.549186	-2.586423	-0.948183
6	2.186739	-3.419654	-1.918540
6	1.402482	-3.827751	-3.038893
7	0.105832	-3.450760	-3.227629
6	-0.437832	-2.677335	-2.320531
6	0.240701	-2.228856	-1.162556
6	1.990479	-4.673098	-4.010577
6	3.285641	-5.107988	-3.890556
6	4.062613	-4.698070	-2.776624
6	3.524809	-3.864389	-1.819519
9	6.878162	5.755090	0.672218
9	6.709777	3.972497	1.884695
9	2.113491	6.962566	-1.034543
9	1.476833	5.538043	-2.525023
1	0.536314	-2.706894	1.461280
1	1.156640	-4.942542	1.578302
1	2.638107	-4.558348	0.711797
1	1.466190	-2.257808	4.826182
1	0.249360	-2.866533	3.696473
1	2.457613	-4.372435	5.010402
1	1.098507	-5.020679	4.092155
1	3.198212	-5.575016	2.912741
1	4.515642	-3.749431	3.950320
1	3.611384	-1.644905	3.996597
1	3.900357	-1.484324	2.263270
1	5.755496	-2.854650	1.832230
1	6.087334	-4.762173	0.400900
1	4.646274	-5.640221	1.151737
1	3.315298	-2.316061	0.273554
1	-0.288296	-1.602558	-0.445114
1	4.164832	-3.562850	-0.998018
1	-1.473386	-2.378450	-2.481162
1	1.376344	-4.967396	-4.855259
1	3.705750	-5.757659	-4.649103
1	1.187669	-0.275472	0.492453
1	1.629507	1.587456	-0.051144
1	5.120123	2.221427	0.924443
1	1.697225	3.470556	-1.346739
1	5.019402	6.158730	-0.801807
8	5.348014	-5.087222	-2.579595
6	5.957065	-5.900881	-3.563108
1	6.977637	-6.073400	-3.220458

1	5.446032	-6.865787	-3.663400
1	5.986897	-5.400416	-4.537938
1	1.361751	-0.804367	2.891462
6	-3.888843	2.637145	-0.776030
6	-4.847689	3.765035	-0.382512
1	-4.267186	2.145494	-1.680728
1	-2.920439	3.074564	-1.047392
1	-4.485042	4.256253	0.530193
1	-4.836332	4.545521	-1.156266
6	-6.274306	3.363647	-0.167505
6	-6.824987	2.174699	-0.435375
1	-6.935631	4.127805	0.240311
1	-6.244855	1.358431	-0.856516
6	-8.272778	1.963035	-0.160441
8	-9.013164	2.902897	0.079337
6	-8.818480	0.565570	-0.162161
6	-8.006308	-0.572584	-0.147715
6	-10.209736	0.417078	-0.133193
6	-8.584060	-1.838928	-0.098358
1	-6.922607	-0.490347	-0.157155
6	-10.783379	-0.846114	-0.099077
1	-10.821994	1.312626	-0.135383
6	-9.968558	-1.978109	-0.077966
1	-7.947385	-2.717522	-0.074940
1	-11.863354	-0.952428	-0.083765
1	-10.413597	-2.967831	-0.042958

re-si_2-path-B

Number of imaginary frequencies : 1

The smallest frequency is : -333.0270

Electronic energy=	-3905.2823457
Zero-point correction=	1.050855
Thermal correction to Energy=	1.116691
Thermal correction to Enthalpy=	1.117635
Thermal correction to Gibbs Free Energy=	0.944415
Sum of electronic and zero-point Energies=	-3904.231491
Sum of electronic and thermal Energies=	-3904.165655
Sum of electronic and thermal Enthalpies=	-3904.164711
Sum of electronic and thermal Free Energies=	-3904.337930

Cartesian Coordinates

6	0.708753	2.960472	4.254487
6	-0.125193	4.208947	3.935141
6	0.407905	4.669401	2.572478
7	0.990719	3.455025	1.992268
6	0.855732	2.303103	2.873280
6	1.539109	3.383722	0.786942
6	1.474381	4.378130	-0.185698
8	0.090820	0.921712	-2.635120
6	-0.419971	1.517736	2.552373
8	-0.392239	0.308807	3.032070
8	-1.366819	2.030463	1.967696
8	0.164607	1.379580	-0.505348
1	1.722415	1.642384	2.794702
1	0.237666	2.294034	4.979236
1	1.699598	3.237386	4.625508
1	-1.180340	3.938147	3.846013
1	-0.029486	4.986642	4.694144
1	-0.374721	5.068072	1.921918
1	1.194630	5.427990	2.666641
1	1.994415	2.427995	0.556677
1	1.194452	5.376419	0.142617
6	-0.543532	3.898951	-0.861382
1	-0.801549	3.449383	0.097494

1	-0.513461	3.281173	-2.989166
6	-1.108478	5.245537	-1.109429
6	-2.000690	5.785333	-0.174493
6	-0.808941	5.983094	-2.262051
6	-2.579225	7.032529	-0.383310
1	-2.259715	5.203579	0.707213
6	-1.379368	7.235144	-2.464287
1	-0.128775	5.577987	-3.005527
6	-2.264492	7.763546	-1.526534
1	-3.279709	7.431523	0.343316
1	-1.135965	7.798077	-3.359625
1	-2.711958	8.738793	-1.689320
7	-0.060557	1.730004	-1.708185
6	-0.416766	3.023365	-1.945304
7	0.460408	-1.418557	-0.441767
6	1.642389	-2.041325	-0.840720
6	2.101937	-3.273798	-0.371646
6	3.361312	-3.720420	-0.768969
6	4.187136	-2.969527	-1.594358
6	3.714251	-1.740580	-2.048703
6	2.455138	-1.284129	-1.699616
6	3.837918	-5.054641	-0.267356
9	3.386245	-6.066787	-1.020848
6	4.631332	-0.879215	-2.868507
9	5.033882	-1.497856	-3.987922
6	-0.733835	-1.913697	-0.017654
16	-1.174188	-3.539797	-0.041257
7	-1.540686	-0.916464	0.430184
6	-2.990481	-0.993233	0.503374
6	-3.523553	-0.313051	1.779121
6	-5.021178	-0.645760	2.004197
6	-5.164048	-1.418308	3.325041
6	-4.720974	-0.491019	4.466262
6	-3.294047	0.016368	4.148867
7	-2.732235	-0.690873	2.975553
6	-2.773116	-2.147700	3.216766
6	-4.243153	-2.653700	3.337625
6	-4.557518	-3.710791	2.307237
6	-5.697599	-3.855548	1.634686
6	-3.600196	-0.308054	-0.717149
6	-4.513208	-0.961892	-1.601778
6	-5.002926	-0.202452	-2.706425
7	-4.638782	1.087527	-2.954079
6	-3.794247	1.647266	-2.123976
6	-3.253682	0.993425	-0.991239
6	-5.917775	-0.809406	-3.600348
6	-6.344809	-2.100044	-3.420064
6	-5.858533	-2.850913	-2.319127
6	-4.955876	-2.294349	-1.438029
9	5.176475	-5.135231	-0.259125
9	3.418904	-5.289160	0.989098
9	5.743439	-0.573449	-2.177432
9	4.058331	0.277237	-3.230862
1	-3.372235	0.764719	1.672982
1	-5.613108	0.273619	2.053676
1	-5.409901	-1.231353	1.166545
1	-2.608637	-0.146079	4.986227
1	-3.281241	1.084814	3.910674
1	-4.736013	-1.034247	5.416714
1	-5.414817	0.349657	4.559370
1	-6.203950	-1.723661	3.474420
1	-4.349972	-3.130723	4.321773
1	-2.211727	-2.332826	4.137234
1	-2.241120	-2.649568	2.403027
1	-3.755059	-4.427712	2.128801
1	-5.827700	-4.663466	0.921292
1	-6.539347	-3.178518	1.757356
1	-3.246285	-2.053684	0.519175
1	-2.563182	1.538909	-0.347558
1	-4.600445	-2.916719	-0.624797

1	-3.507376	2.677232	-2.331249
1	-6.269219	-0.212842	-4.435818
1	-7.046351	-2.535322	-4.121638
1	-1.164158	0.028694	0.359278
1	0.460577	-0.407849	-0.610687
1	1.494148	-3.865291	0.300566
1	2.077601	-0.339733	-2.084510
1	5.181251	-3.316394	-1.854663
8	-6.237180	-4.128851	-2.061499
6	-7.116360	-4.761132	-2.971084
1	-7.272541	-5.769067	-2.585935
1	-8.082538	-4.245627	-3.024891
1	-6.680186	-4.824861	-3.974697
1	-1.364111	-0.165278	2.913610
6	2.351396	4.318043	-1.416263
6	3.020778	2.967231	-1.722360
1	3.137925	5.078753	-1.328483
1	1.753419	4.608661	-2.288312
1	2.302047	2.140700	-1.699319
1	3.398771	3.015055	-2.751753
6	4.188059	2.648243	-0.838372
6	4.412333	1.462406	-0.262637
1	4.933490	3.430667	-0.690679
1	3.700837	0.652001	-0.392972
6	5.655805	1.233553	0.522795
8	6.479973	2.124236	0.656343
6	5.897031	-0.107796	1.151743
6	4.947624	-1.134369	1.180840
6	7.146686	-0.315963	1.748651
6	5.245524	-2.344740	1.803603
1	3.966711	-1.009491	0.731423
6	7.445714	-1.525297	2.359168
1	7.870613	0.491364	1.716915
6	6.492333	-2.543004	2.388777
1	4.500863	-3.134096	1.831333
1	8.420034	-1.677673	2.812675
1	6.720757	-3.490760	2.866527

re-si_3-path-B

Number of imaginary frequencies : 1
 The smallest frequency is : -292.1517

Electronic energy= -3905.2785993
 Zero-point correction= 1.050217
 Thermal correction to Energy= 1.116377
 Thermal correction to Enthalpy= 1.117321
 Thermal correction to Gibbs Free Energy= 0.941048
 Sum of electronic and zero-point Energies= -3904.228382
 Sum of electronic and thermal Energies= -3904.162222
 Sum of electronic and thermal Enthalpies= -3904.161278
 Sum of electronic and thermal Free Energies= -3904.337552

 Cartesian Coordinates

6	-1.867436	0.764502	4.590001
6	-2.986443	-0.241523	4.277836
6	-3.576574	0.238511	2.939826
7	-2.559507	1.148725	2.404439
6	-1.336303	1.111141	3.190648
6	-2.682742	1.823134	1.267935
6	-3.673227	1.611813	0.315928
8	0.245193	1.667737	-2.011773
6	-0.431338	-0.027901	2.710944
8	0.800440	0.101560	3.106964
8	-0.883485	-0.984802	2.091665
8	-0.250369	1.105062	0.033182

1	-0.800949	2.061428	3.139796
1	-1.089684	0.358476	5.239458
1	-2.271218	1.670356	5.050419
1	-2.565211	-1.241605	4.155760
1	-3.742502	-0.281768	5.063227
1	-3.754432	-0.588343	2.244737
1	-4.513494	0.793775	3.062719
1	-1.876141	2.521477	1.057724
1	-4.525384	1.004007	0.608945
6	-2.579768	0.026276	-0.699322
1	-2.124359	-0.310455	0.230792
1	-1.911653	0.734626	-2.686603
6	-3.715768	-0.796133	-1.173512
6	-4.070548	-1.928474	-0.428018
6	-4.410834	-0.519950	-2.359166
6	-5.084366	-2.774998	-0.864736
1	-3.517141	-2.156981	0.480252
6	-5.437635	-1.357143	-2.783877
1	-4.141484	0.344232	-2.959325
6	-5.772063	-2.489231	-2.042997
1	-5.331711	-3.662058	-0.289664
1	-5.970411	-1.131850	-3.701903
1	-6.565955	-3.145569	-2.384838
7	-0.536441	1.146039	-1.205800
6	-1.721050	0.612122	-1.631415
7	2.647015	1.507635	0.048466
6	3.340677	2.702347	-0.182684
6	4.612130	2.970079	0.324510
6	5.195371	4.211810	0.083304
6	4.539207	5.204034	-0.629948
6	3.260503	4.928855	-1.108490
6	2.661454	3.696277	-0.900265
6	6.584730	4.447926	0.602579
9	7.498902	3.755277	-0.093212
6	2.517624	6.013013	-1.833925
9	3.294802	6.628173	-2.738502
6	3.118134	0.230804	0.126074
16	4.725135	-0.222463	-0.128978
7	2.135827	-0.649894	0.435139
6	2.250810	-2.093738	0.317771
6	1.622919	-2.807745	1.533124
6	2.042476	-4.300150	1.583306
6	2.835852	-4.549546	2.875756
6	1.900520	-4.290458	4.064829
6	1.317742	-2.864497	3.917060
7	1.976422	-2.136097	2.808247
6	3.437108	-2.125336	3.029593
6	4.020449	-3.570345	2.985546
6	5.082210	-3.709235	1.921825
6	5.280082	-4.754286	1.120974
6	1.554814	-2.580044	-0.949349
6	2.195046	-3.408393	-1.922094
6	1.413190	-3.812774	-3.045472
7	0.116371	-3.436643	-3.234769
6	-0.429798	-2.667713	-2.325355
6	0.246267	-2.223196	-1.164395
6	2.003865	-4.653309	-4.019688
6	3.299321	-5.087200	-3.899220
6	4.073867	-4.681077	-2.782203
6	3.533451	-3.852003	-1.822576
9	6.934159	5.741138	0.537028
9	6.706696	4.064505	1.883707
9	2.090004	6.968224	-0.988395
9	1.438987	5.548312	-2.476920
1	0.537270	-2.709655	1.457998
1	1.158411	-4.945359	1.568641
1	2.640972	-4.557588	0.705567
1	1.460674	-2.272074	4.826039
1	0.246600	-2.877824	3.691782
1	2.454104	-4.386310	5.004484

1	1.096854	-5.032606	4.082130
1	3.198466	-5.581367	2.903806
1	4.513528	-3.758657	3.949457
1	3.607312	-1.655059	4.002416
1	3.899008	-1.487656	2.270185
1	5.755143	-2.855150	1.835918
1	6.090411	-4.757555	0.398487
1	4.649275	-5.639426	1.144848
1	3.318287	-2.313946	0.276699
1	-0.284636	-1.600557	-0.445190
1	4.171653	-3.553121	-0.998691
1	-1.465487	-2.369542	-2.486421
1	1.391543	-4.944795	-4.866655
1	3.721568	-5.733078	-4.659818
1	1.190094	-0.274453	0.500569
1	1.631163	1.589656	-0.032785
1	5.139587	2.221123	0.900304
1	1.676551	3.479428	-1.304352
1	5.006760	6.166315	-0.806024
8	5.359393	-5.069542	-2.584610
6	5.970439	-5.880022	-3.569502
1	6.990540	-6.053014	-3.225690
1	5.460043	-6.844884	-3.673427
1	6.001651	-5.376731	-4.542825
1	1.358480	-0.812126	2.896213
6	-3.887787	2.635654	-0.766971
6	-4.848996	3.761462	-0.373379
1	-4.262866	2.145975	-1.674108
1	-2.919057	3.074844	-1.034261
1	-4.489930	4.250339	0.541997
1	-4.835711	4.544233	-1.144787
6	-6.275981	3.358195	-0.164530
6	-6.824646	2.169384	-0.437191
1	-6.939526	4.120842	0.242497
1	-6.242412	1.354417	-0.857993
6	-8.273383	1.956080	-0.168619
8	-9.015482	2.894813	0.070258
6	-8.818054	0.558256	-0.176119
6	-8.005098	-0.579286	-0.158712
6	-10.209342	0.408690	-0.155963
6	-8.582181	-1.846148	-0.115064
1	-6.921425	-0.496130	-0.161366
6	-10.782226	-0.854991	-0.127738
1	-10.822245	1.303795	-0.160244
6	-9.966677	-1.986400	-0.103580
1	-7.944991	-2.724307	-0.089194
1	-11.862188	-0.962159	-0.119456
1	-10.411152	-2.976534	-0.073276

re-si_4-path-B

Number of imaginary frequencies : 1

The smallest frequency is : -326.0648

Electronic energy=	-3905.2752862
Zero-point correction=	1.049851
Thermal correction to Energy=	1.116249
Thermal correction to Enthalpy=	1.117193
Thermal correction to Gibbs Free Energy=	0.938744
Sum of electronic and zero-point Energies=	-3904.225435
Sum of electronic and thermal Energies=	-3904.159037
Sum of electronic and thermal Enthalpies=	-3904.158093
Sum of electronic and thermal Free Energies=	-3904.336542

Cartesian Coordinates

6	-2.224436	-2.378119	3.649987

6	-2.094770	-3.833119	3.178545
6	-2.607483	-3.801857	1.732432
7	-2.445677	-2.400914	1.329338
6	-1.854001	-1.589696	2.384332
6	-2.770249	-1.914660	0.139381
6	-3.100530	-2.680780	-0.976587
8	0.045845	-0.002340	-2.664808
6	-0.328395	-1.547647	2.248598
8	0.194952	-0.538413	2.881599
8	0.295245	-2.425189	1.664613
8	-0.435946	-0.727353	-0.667090
1	-2.252134	-0.572856	2.368018
1	-1.575070	-2.133659	4.492592
1	-3.257244	-2.146658	3.925541
1	-1.044933	-4.134744	3.189254
1	-2.663188	-4.529536	3.796659
1	-2.043939	-4.462088	1.068069
1	-3.669419	-4.067299	1.659411
1	-2.684671	-0.836959	0.055761
1	-3.361957	-3.721465	-0.799928
6	-1.047327	-3.154337	-1.528856
1	-0.708104	-3.069908	-0.496305
1	-0.551419	-2.241075	-3.485724
6	-1.206012	-4.535627	-2.039403
6	-0.869338	-5.607479	-1.202874
6	-1.663991	-4.808883	-3.334697
6	-0.990887	-6.919781	-1.645536
1	-0.483171	-5.402129	-0.207209
6	-1.795140	-6.122288	-3.772888
1	-1.917784	-3.993825	-4.005789
6	-1.461421	-7.180564	-2.930447
1	-0.714023	-7.739103	-0.989837
1	-2.154236	-6.319547	-4.777928
1	-1.561175	-8.204024	-3.277357
7	-0.306156	-0.925608	-1.917518
6	-0.610653	-2.159526	-2.410927
7	0.595423	1.880553	-0.141748
6	-0.090735	3.051814	-0.466170
6	0.124509	4.303644	0.110620
6	-0.698275	5.368389	-0.256391
6	-1.736948	5.222564	-1.163917
6	-1.942168	3.962681	-1.723992
6	-1.129684	2.892819	-1.396498
6	-0.416501	6.715675	0.346569
9	0.645531	7.304430	-0.225231
6	-3.094176	3.768491	-2.666118
9	-3.135321	4.719573	-3.609617
6	1.851599	1.659348	0.331340
16	3.026777	2.842505	0.575738
7	2.048438	0.340215	0.589990
6	3.348190	-0.298491	0.692737
6	3.357740	-1.355005	1.814314
6	4.802512	-1.827905	2.123935
6	5.144232	-1.458169	3.575798
6	4.195842	-2.235726	4.499633
6	2.743033	-1.927227	4.065743
7	2.713689	-0.849574	3.050729
6	3.407103	0.341811	3.579706
6	4.917498	0.045871	3.827088
6	5.804638	0.979609	3.040527
6	6.941507	0.669780	2.420646
6	3.704992	-0.971542	-0.630538
6	4.921559	-0.706169	-1.331530
6	5.139230	-1.415568	-2.550752
7	4.246197	-2.304129	-3.072433
6	3.136295	-2.508362	-2.406359
6	2.826089	-1.872692	-1.180937
6	6.342755	-1.193378	-3.262611
6	7.296062	-0.321694	-2.801707
6	7.073847	0.384383	-1.591525

6	5.907914	0.200178	-0.880186
9	-1.452996	7.555486	0.208365
9	-0.146186	6.624745	1.658215
9	-4.271566	3.816626	-2.018968
9	-3.046893	2.580069	-3.292072
1	2.728392	-2.191839	1.495735
1	4.886027	-2.911720	1.995179
1	5.510197	-1.367684	1.429236
1	2.128453	-1.597795	4.909088
1	2.253178	-2.796681	3.616396
1	4.360815	-1.938928	5.540446
1	4.396495	-3.308911	4.429999
1	6.182500	-1.722173	3.798186
1	5.124103	0.234878	4.889679
1	2.896491	0.619578	4.506433
1	3.269537	1.165196	2.872165
1	5.461821	2.014626	3.008328
1	7.513044	1.426202	1.891755
1	7.344320	-0.339901	2.405413
1	4.065564	0.489780	0.924553
1	1.884982	-2.111979	-0.686061
1	5.775991	0.778882	0.026971
1	2.427010	-3.216377	-2.832456
1	6.484910	-1.740011	-4.189220
1	8.207779	-0.174897	-3.368502
1	1.274985	-0.283448	0.359826
1	0.114131	1.034116	-0.455466
1	0.912817	4.444784	0.837848
1	-1.267317	1.925402	-1.871776
1	-2.371309	6.061543	-1.426881
8	7.964848	1.263837	-1.066399
6	9.165345	1.500783	-1.775515
1	9.719422	2.236291	-1.191771
1	9.767271	0.588647	-1.865814
1	8.970561	1.910181	-2.773376
1	1.279513	-0.612739	2.873361
6	-3.726478	-2.050606	-2.201991
6	-3.646456	-0.525234	-2.308125
1	-4.780096	-2.352044	-2.263112
1	-3.248916	-2.475287	-3.093270
1	-2.619575	-0.172749	-2.134615
1	-3.859430	-0.226629	-3.342554
6	-4.561187	0.265228	-1.422638
6	-5.455838	-0.218365	-0.554053
1	-4.490499	1.349614	-1.505042
1	-5.578669	-1.287157	-0.407314
6	-6.262630	0.721663	0.272179
8	-6.040377	1.920632	0.266440
6	-7.342704	0.166999	1.153651
6	-7.910025	-1.095784	0.959707
6	-7.806097	0.975814	2.196401
6	-8.925481	-1.542417	1.801198
1	-7.586461	-1.725186	0.137000
6	-8.808023	0.523450	3.044452
1	-7.363278	1.958220	2.323361
6	-9.369462	-0.737969	2.847092
1	-9.372113	-2.518165	1.638579
1	-9.155387	1.152890	3.857550
1	-10.156209	-1.091244	3.506500

re-si_5-path-B

Number of imaginary frequencies : 1
The smallest frequency is : -318.7827

Electronic energy= -3905.2764258
Zero-point correction= 1.049960

Thermal correction to Energy=	1.116190
Thermal correction to Enthalpy=	1.117135
Thermal correction to Gibbs Free Energy=	0.940516
Sum of electronic and zero-point Energies=	-3904.226466
Sum of electronic and thermal Energies=	-3904.160235
Sum of electronic and thermal Enthalpies=	-3904.159291
Sum of electronic and thermal Free Energies=	-3904.335909

Cartesian Coordinates

6	-2.570764	-2.320164	3.426524
6	-2.478636	-3.779953	2.959454
6	-2.898096	-3.730328	1.482821
7	-2.679181	-2.332053	1.098639
6	-2.107553	-1.545862	2.183264
6	-2.930803	-1.825075	-0.102226
6	-3.223321	-2.565126	-1.244555
8	-0.027562	0.241238	-2.620509
6	-0.576786	-1.564936	2.119247
8	-0.042486	-0.564851	2.757955
8	0.035691	-2.477979	1.579805
8	-0.541863	-0.624291	-0.687502
1	-2.466937	-0.514846	2.150693
1	-1.953875	-2.103687	4.300807
1	-3.604553	-2.041841	3.653216
1	-1.446192	-4.128180	3.035333
1	-3.113863	-4.449791	3.541024
1	-2.308358	-4.403133	0.854729
1	-3.959035	-3.972318	1.338152
1	-2.818358	-0.748978	-0.164256
1	-3.482863	-3.611504	-1.100643
6	-1.145722	-2.984101	-1.747022
1	-0.847461	-2.973301	-0.698978
1	-0.593749	-1.924752	-3.612674
6	-1.287194	-4.323840	-2.360362
6	-1.055273	-5.456325	-1.569463
6	-1.625889	-4.500702	-3.708528
6	-1.163589	-6.733574	-2.106847
1	-0.759650	-5.325478	-0.531116
6	-1.743291	-5.779542	-4.242645
1	-1.795190	-3.639861	-4.348553
6	-1.515617	-6.898231	-3.444813
1	-0.966774	-7.600183	-1.483764
1	-2.007711	-5.902400	-5.288013
1	-1.605292	-7.894235	-3.866341
7	-0.391435	-0.733137	-1.947477
6	-0.682680	-1.926441	-2.537309
7	0.591949	1.949554	-0.057909
6	-0.017807	3.159965	-0.390314
6	0.318720	4.413477	0.119774
6	-0.430288	5.525331	-0.268423
6	-1.510639	5.428573	-1.131604
6	-1.839215	4.165787	-1.622909
6	-1.105600	3.048665	-1.271105
6	-0.019685	6.860844	0.284068
9	1.201037	7.218638	-0.141950
6	-3.040091	4.012881	-2.510043
9	-3.125974	4.999830	-3.412156
6	1.840840	1.642150	0.388079
16	3.088199	2.744698	0.655208
7	1.961573	0.307618	0.604510
6	3.217700	-0.407938	0.730812
6	3.124255	-1.489736	1.825539
6	4.528478	-2.042094	2.184914
6	4.828477	-1.711402	3.655914
6	3.806996	-2.457900	4.525563
6	2.389661	-2.071837	4.039468
7	2.453021	-0.976684	3.044744
6	3.179784	0.170814	3.623879
6	4.663112	-0.202075	3.923781

6	5.625731	0.697368	3.187010
6	6.773643	0.337931	2.616152
6	3.579252	-1.068649	-0.597394
6	4.827322	-0.850451	-1.258428
6	5.037649	-1.533706	-2.494021
7	4.114313	-2.360656	-3.062116
6	2.979231	-2.526575	-2.428838
6	2.669646	-1.907203	-1.194982
6	6.266540	-1.351098	-3.172947
6	7.251022	-0.542495	-2.665006
6	7.037861	0.134896	-1.436844
6	5.848606	-0.012445	-0.755910
9	-0.866739	7.838506	-0.068835
9	0.032950	6.843679	1.625937
9	-4.183364	4.035750	-1.802116
9	-3.029415	2.848486	-3.182042
1	2.466887	-2.285378	1.460978
1	4.561526	-3.126721	2.041915
1	5.285952	-1.608786	1.526098
1	1.757712	-1.726530	4.863533
1	1.876827	-2.907802	3.553897
1	3.943069	-2.188330	5.577920
1	3.959291	-3.538089	4.442389
1	5.843184	-2.028051	3.914898
1	4.836806	-0.039149	4.996524
1	2.646766	0.455229	4.535712
1	3.110217	1.012951	2.928609
1	5.333457	1.747644	3.150477
1	7.405589	1.069217	2.121720
1	7.126829	-0.690308	2.611062
1	3.971454	0.329725	1.008665
1	1.703777	-2.107221	-0.731394
1	5.726358	0.542091	0.167493
1	2.246947	-3.187007	-2.891365
1	6.402073	-1.875596	-4.113194
1	8.181051	-0.423488	-3.208060
1	1.156012	-0.264569	0.352649
1	0.056266	1.138126	-0.372801
1	1.148450	4.523333	0.805634
1	-1.339927	2.077167	-1.696579
1	-2.079757	6.306151	-1.415497
8	7.960653	0.949810	-0.864517
6	9.180635	1.159418	-1.548669
1	9.759000	1.845585	-0.929586
1	9.742285	0.225087	-1.667139
1	9.018234	1.614734	-2.532328
1	1.037486	-0.681384	2.806093
6	-3.817233	-1.912093	-2.474659
6	-3.763642	-0.382598	-2.541230
1	-4.863673	-2.228189	-2.573087
1	-3.308201	-2.310199	-3.361004
1	-2.741470	-0.015675	-2.365974
1	-3.988204	-0.063516	-3.567037
6	-4.693346	0.359338	-1.627515
6	-5.535291	-0.194757	-0.749332
1	-4.664572	1.447377	-1.684839
1	-5.601123	-1.272995	-0.640100
6	-6.380477	0.650254	0.133922
8	-6.637527	1.809936	-0.137947
6	-6.905948	0.031650	1.396251
6	-6.345846	-1.122816	1.952378
6	-7.970610	0.661883	2.046763
6	-6.854522	-1.645173	3.138535
1	-5.497341	-1.606201	1.473992
6	-8.484925	0.133376	3.223960
1	-8.381762	1.566146	1.609726
6	-7.927968	-1.022211	3.770604
1	-6.416202	-2.541228	3.567818
1	-9.318036	0.621707	3.719115
1	-8.328833	-1.434835	4.691185

re-si_6-path-B

Number of imaginary frequencies : 1

The smallest frequency is : -316.2106

Electronic energy= -3905.2713821
Zero-point correction= 1.049253
Thermal correction to Energy= 1.115815
Thermal correction to Enthalpy= 1.116759
Thermal correction to Gibbs Free Energy= 0.938032
Sum of electronic and zero-point Energies= -3904.222129
Sum of electronic and thermal Energies= -3904.155567
Sum of electronic and thermal Enthalpies= -3904.154623
Sum of electronic and thermal Free Energies= -3904.333350

Cartesian Coordinates

6	-1.364817	0.226348	4.960223
6	-2.370609	-0.925624	4.808030
6	-3.132707	-0.612894	3.505788
7	-2.316497	0.409863	2.847056
6	-1.025852	0.563992	3.501195
6	-2.661026	1.073324	1.752808
6	-3.714148	0.765171	0.895932
8	0.035496	1.504440	-1.602753
6	-0.033990	-0.470841	2.961478
8	1.203694	-0.157243	3.216152
8	-0.414188	-1.504113	2.425658
8	-0.253235	0.694201	0.396767
1	-0.627248	1.569608	3.355957
1	-0.479900	-0.046550	5.537951
1	-1.832859	1.097454	5.426684
1	-1.838916	-1.873334	4.700447
1	-3.044525	-1.005652	5.662084
1	-3.220123	-1.500600	2.873829
1	-4.134405	-0.204979	3.678872
1	-1.991562	1.888249	1.488113
1	-4.440890	0.026810	1.228372
6	-2.490018	-0.603634	-0.332404
1	-1.954619	-0.932106	0.557825
1	-2.020990	0.394624	-2.255920
6	-3.532162	-1.542484	-0.820348
6	-4.128490	-2.425277	0.089255
6	-3.931253	-1.603233	-2.162617
6	-5.126163	-3.304903	-0.311265
1	-3.805102	-2.413043	1.126236
6	-4.931858	-2.481042	-2.565686
1	-3.462238	-0.965695	-2.905371
6	-5.542528	-3.324287	-1.640788
1	-5.582733	-3.970548	0.413744
1	-5.232924	-2.506664	-3.607901
1	-6.331458	-3.999288	-1.955731
7	-0.624391	0.810932	-0.813643
6	-1.755663	0.172692	-1.234021
7	2.561189	1.724302	0.174924
6	3.025406	3.023872	-0.068930
6	4.265738	3.495135	0.361691
6	4.614309	4.821071	0.114132
6	3.753263	5.695999	-0.531544
6	2.509027	5.215493	-0.932953
6	2.140904	3.897560	-0.715706
6	5.972926	5.290770	0.550120
9	6.940075	4.853969	-0.270512
6	1.578274	6.162518	-1.632728
9	2.084811	6.578806	-2.804342
6	3.241760	0.541747	0.136176

16	4.877962	0.382407	-0.249777
7	2.443084	-0.505408	0.448186
6	2.774563	-1.899706	0.210919
6	2.345625	-2.789127	1.396006
6	2.992886	-4.194175	1.290680
6	3.916403	-4.406643	2.500431
6	3.046951	-4.397180	3.765738
6	2.234131	-3.080545	3.780129
7	2.682749	-2.169375	2.701744
6	4.134497	-1.934191	2.831545
6	4.935121	-3.256895	2.624812
6	5.926613	-3.135446	1.493677
6	6.220888	-4.063855	0.585660
6	2.083804	-2.396589	-1.055785
6	2.789061	-2.996371	-2.144902
6	2.011724	-3.433509	-3.259539
7	0.657774	-3.289776	-3.335935
6	0.051571	-2.723600	-2.322076
6	0.720401	-2.270338	-1.160446
6	2.669904	-4.051655	-4.349942
6	4.028514	-4.239075	-4.351806
6	4.798108	-3.798290	-3.244711
6	4.189845	-3.184244	-2.170662
9	6.055735	6.629598	0.577358
9	6.281029	4.846169	1.778864
9	1.361075	7.267994	-0.899160
9	0.384000	5.613102	-1.887616
1	1.253943	-2.858131	1.395313
1	2.221898	-4.971137	1.280317
1	3.551763	-4.284845	0.355327
1	2.348013	-2.544254	4.727341
1	1.165527	-3.252503	3.620553
1	3.680252	-4.471264	4.655755
1	2.376095	-5.261236	3.768744
1	4.439944	-5.363379	2.412319
1	5.519125	-3.437584	3.538134
1	4.301076	-1.517519	3.829107
1	4.430391	-1.172314	2.104072
1	6.453482	-2.181332	1.449456
1	6.966118	-3.878548	-0.181783
1	5.736039	-5.036660	0.563081
1	3.858317	-1.943600	0.097298
1	0.139436	-1.824128	-0.354206
1	4.824402	-2.843840	-1.360257
1	-1.029798	-2.609521	-2.392095
1	2.057986	-4.373177	-5.186383
1	4.504017	-4.717494	-5.199642
1	1.457414	-0.293987	0.606483
1	1.545104	1.632980	0.147353
1	4.947051	2.838756	0.887155
1	1.178521	3.523627	-1.052506
1	4.035672	6.727725	-0.710540
8	6.145203	-3.947159	-3.166752
6	6.820303	-4.497256	-4.281047
1	7.880076	-4.487948	-4.025431
1	6.508367	-5.530683	-4.473684
1	6.664475	-3.895496	-5.184032
1	1.866177	-0.970111	2.931248
6	-4.197441	1.865167	-0.020737
6	-5.099174	1.431862	-1.190831
1	-3.324162	2.390934	-0.431026
1	-4.753721	2.602944	0.572352
1	-5.473372	2.334057	-1.685019
1	-4.500220	0.884017	-1.924380
6	-6.247312	0.575054	-0.757494
6	-7.521883	0.974455	-0.705933
1	-6.031702	-0.448513	-0.447615
1	-7.799103	1.980626	-1.006903
6	-8.574789	0.048982	-0.205592
8	-8.284710	-1.003522	0.340054

6	-10.014444	0.439246	-0.361227
6	-10.439793	1.421489	-1.260081
6	-10.961002	-0.237967	0.414752
6	-11.793688	1.724026	-1.376010
1	-9.725248	1.937473	-1.892806
6	-12.309676	0.073383	0.308008
1	-10.613126	-1.005859	1.097869
6	-12.727583	1.056705	-0.588478
1	-12.119680	2.480558	-2.082544
1	-13.037903	-0.449336	0.919988
1	-13.782211	1.299438	-0.675207

re-si_7-path-B

Number of imaginary frequencies : 1

The smallest frequency is : -326.5603

Electronic energy=	-3905.2752679
Zero-point correction=	1.050953
Thermal correction to Energy=	1.116567
Thermal correction to Enthalpy=	1.117512
Thermal correction to Gibbs Free Energy=	0.944879
Sum of electronic and zero-point Energies=	-3904.224315
Sum of electronic and thermal Energies=	-3904.158701
Sum of electronic and thermal Enthalpies=	-3904.157756
Sum of electronic and thermal Free Energies=	-3904.330389

Cartesian Coordinates

6	2.409607	3.961156	-4.214716
6	2.789264	4.988844	-3.141275
6	1.454543	5.302801	-2.462793
7	0.688354	4.062510	-2.626615
6	1.351887	3.099736	-3.504094
6	-0.438838	3.772934	-1.997347
6	-1.021897	4.457102	-0.930098
8	-1.464227	0.568779	1.091590
6	2.045166	2.008120	-2.679525
8	2.200492	0.899063	-3.335250
8	2.452033	2.228613	-1.543568
8	-0.315681	1.323300	-0.603726
1	0.640371	2.637809	-4.192230
1	3.253947	3.364622	-4.566353
1	1.950799	4.453887	-5.076740
1	3.472954	4.535132	-2.418846
1	3.259131	5.881710	-3.556165
1	1.552335	5.556645	-1.405650
1	0.919887	6.117626	-2.966348
1	-0.892514	2.834029	-2.306642
1	-0.739770	5.490815	-0.741303
6	0.294769	3.576518	0.598770
1	0.960893	3.188900	-0.167499
1	-0.966660	2.710607	2.213353
6	0.879336	4.704788	1.361040
6	2.187644	5.087639	1.033210
6	0.238909	5.346541	2.428424
6	2.830478	6.103401	1.731738
1	2.702274	4.556437	0.234598
6	0.880423	6.365533	3.124115
1	-0.759171	5.044843	2.729894
6	2.172743	6.752334	2.774026
1	3.846230	6.381394	1.469240
1	0.371094	6.856306	3.947121
1	2.668881	7.548544	3.319570
7	-0.769543	1.464453	0.580443
6	-0.494884	2.617826	1.245788
7	-0.552879	-1.443491	-1.096997

6	-1.809251	-2.025641	-1.279354
6	-2.075629	-3.375357	-1.513000
6	-3.398280	-3.786058	-1.690150
6	-4.462393	-2.900229	-1.656995
6	-4.178749	-1.551934	-1.438945
6	-2.882478	-1.115586	-1.247528
6	-3.646421	-5.254571	-1.889886
9	-3.433253	-5.950598	-0.762137
6	-5.317410	-0.572561	-1.451671
9	-6.331021	-0.979674	-0.677419
6	0.681126	-1.954160	-0.848740
16	1.059994	-3.591617	-0.704965
7	1.618486	-0.967336	-0.743123
6	2.888456	-1.145246	-0.054578
6	4.036776	-0.381154	-0.742833
6	5.411263	-0.873926	-0.219151
6	6.185894	-1.514481	-1.381637
6	6.471193	-0.418719	-2.417815
6	5.126187	0.243598	-2.795558
7	3.984026	-0.508066	-2.221248
6	4.063837	-1.921162	-2.645900
6	5.342601	-2.604596	-2.070923
6	5.000650	-3.800969	-1.216770
6	5.589183	-4.165280	-0.079344
6	2.777500	-0.663634	1.390075
6	3.059567	-1.502781	2.512456
6	2.944769	-0.914802	3.807829
7	2.564827	0.378043	4.016076
6	2.294534	1.106966	2.961778
6	2.393756	0.633252	1.631749
6	3.237643	-1.705983	4.944670
6	3.624033	-3.016209	4.822986
6	3.726699	-3.600415	3.534331
6	3.446213	-2.858649	2.406768
9	-4.905445	-5.506371	-2.276792
9	-2.831026	-5.772956	-2.821482
9	-5.817266	-0.427771	-2.693023
9	-4.947944	0.649610	-1.036709
1	3.902496	0.685390	-0.547592
1	5.989641	-0.036743	0.184525
1	5.272973	-1.589189	0.595982
1	4.979130	0.280207	-3.879079
1	5.052340	1.267784	-2.414665
1	6.949966	-0.853103	-3.301315
1	7.160469	0.323019	-2.003978
1	7.126135	-1.940796	-1.019546
1	5.927471	-2.980943	-2.921682
1	4.065820	-1.924761	-3.739656
1	3.155035	-2.433035	-2.316235
1	4.193583	-4.423101	-1.605242
1	5.273828	-5.058759	0.450869
1	6.397190	-3.595795	0.372961
1	3.104319	-2.213321	-0.082656
1	2.171047	1.311882	0.808710
1	3.512903	-3.356891	1.446063
1	1.986077	2.136661	3.139462
1	3.142458	-1.237041	5.918603
1	3.842350	-3.595431	5.712233
1	1.271235	-0.008345	-0.770445
1	-0.611940	-0.428730	-0.968039
1	-1.270014	-4.094998	-1.553656
1	-2.680618	-0.068410	-1.043794
1	-5.482321	-3.240725	-1.795421
8	4.097495	-4.890357	3.328718
6	4.300062	-5.713067	4.461006
1	4.525315	-6.707133	4.073787
1	5.145114	-5.366408	5.067765
1	3.400602	-5.767421	5.084930
1	2.872463	0.218161	-2.788887
6	-2.424571	4.011567	-0.584329

6	-3.025744	4.663484	0.661695
1	-2.407577	2.923096	-0.463112
1	-3.100227	4.199451	-1.428635
1	-2.267364	4.711522	1.450573
1	-3.293163	5.701670	0.440594
6	-4.224554	3.929696	1.203947
6	-4.323510	2.601614	1.322347
1	-5.073449	4.519738	1.545696
1	-3.516290	1.943269	1.014825
6	-5.572578	1.996334	1.870529
8	-6.520833	2.697582	2.186697
6	-5.662640	0.505593	1.997744
6	-4.561809	-0.340936	1.832350
6	-6.919330	-0.046007	2.270253
6	-4.722853	-1.721014	1.926861
1	-3.570592	0.057120	1.641444
6	-7.077527	-1.421961	2.362450
1	-7.761007	0.626914	2.397021
6	-5.978348	-2.262611	2.186765
1	-3.862648	-2.370315	1.791746
1	-8.057436	-1.843205	2.564993
1	-6.101550	-3.339560	2.252406

re-re_1-path-B

Number of imaginary frequencies : 1

The smallest frequency is : -310.9424

Electronic energy=	-3905.2891753
Zero-point correction=	1.051547
Thermal correction to Energy=	1.116974
Thermal correction to Enthalpy=	1.117918
Thermal correction to Gibbs Free Energy=	0.948099
Sum of electronic and zero-point Energies=	-3904.237628
Sum of electronic and thermal Energies=	-3904.172201
Sum of electronic and thermal Enthalpies=	-3904.171257
Sum of electronic and thermal Free Energies=	-3904.341077

Cartesian Coordinates

6	-3.056878	-0.251953	4.246932
6	-3.662861	-1.650823	4.455442
6	-4.094341	-2.118259	3.048164
7	-3.552876	-1.099097	2.131636
6	-2.525096	-0.307042	2.807318
6	-4.175064	-0.695325	1.024780
6	-5.080269	-1.480563	0.325741
8	-0.263486	-2.306518	0.332829
6	-1.191685	-1.063851	2.780969
8	-0.163161	-0.313638	2.473127
8	-1.141742	-2.244603	3.071698
8	-1.631001	-0.725572	-0.285461
1	-2.427148	0.671111	2.335958
1	-2.276603	-0.012336	4.972633
1	-3.828822	0.521247	4.298882
1	-2.913659	-2.332670	4.855813
1	-4.511024	-1.623303	5.141854
1	-3.686747	-3.102651	2.808426
1	-5.181406	-2.139802	2.933140
1	-3.852142	0.261505	0.625455
1	-5.406330	-2.392793	0.819604
6	-6.112242	-0.910728	-0.625481
6	-5.775409	0.420294	-1.322911
1	-7.047698	-0.780567	-0.067269
1	-6.329408	-1.664551	-1.394329
1	-6.667123	0.734241	-1.878153
1	-5.549179	1.208310	-0.597175

6	-4.634356	0.212717	-2.262334
6	-3.443622	0.813877	-2.221356
1	-4.757178	-0.594883	-2.985861
1	-3.249325	1.640197	-1.543023
6	-2.307996	0.243420	-2.999443
8	-2.406575	-0.848391	-3.541452
6	-1.018894	0.992570	-3.020073
6	-0.979220	2.387087	-2.952868
6	0.171881	0.263518	-3.119863
6	0.245526	3.049346	-2.994233
1	-1.902966	2.956473	-2.881541
6	1.392853	0.923435	-3.132536
1	0.116478	-0.819674	-3.176369
6	1.428648	2.318405	-3.067672
1	0.277314	4.133617	-2.940308
1	2.318809	0.357967	-3.183271
1	2.384261	2.833084	-3.066374
6	-3.557614	-2.534509	-0.844020
1	-3.443177	-1.688187	-1.511957
1	-2.161313	-3.835206	0.270517
6	-4.417318	-3.631036	-1.342142
6	-4.810328	-3.615423	-2.684961
6	-4.823077	-4.692415	-0.523795
6	-5.596147	-4.643301	-3.199817
1	-4.460463	-2.810979	-3.327357
6	-5.609989	-5.714790	-1.038675
1	-4.525735	-4.706868	0.522512
6	-6.000778	-5.691037	-2.377830
1	-5.888009	-4.626086	-4.245065
1	-5.921873	-6.532329	-0.396420
1	-6.617433	-6.489778	-2.777521
7	-1.406462	-1.936733	-0.015770
6	-2.412663	-2.857418	-0.111607
7	0.342867	1.495571	0.101932
6	-0.291340	2.719357	0.261358
6	0.301989	3.984164	0.191734
6	-0.499314	5.116080	0.313081
6	-1.873166	5.047403	0.510677
6	-2.448538	3.782336	0.575261
6	-1.678456	2.638836	0.446875
6	0.151987	6.456792	0.121575
9	-0.572379	7.449768	0.657508
6	-3.932922	3.636846	0.721698
9	-4.550627	3.590613	-0.473853
6	1.648168	1.110404	0.217846
16	2.974203	2.143537	0.388794
7	1.749331	-0.229419	0.182429
6	2.970360	-0.995167	0.321009
6	2.751769	-2.121990	1.351601
6	4.087661	-2.832433	1.694650
6	4.359091	-2.681732	3.198309
6	3.220509	-3.375825	3.958953
6	1.874987	-2.767206	3.490969
7	2.101676	-1.617671	2.586737
6	2.947676	-0.622246	3.275246
6	4.360131	-1.195147	3.602847
6	5.454430	-0.350640	2.997983
6	6.575860	-0.782879	2.425024
6	3.386330	-1.589191	-1.021114
6	4.692473	-1.413702	-1.577692
6	4.949963	-2.031030	-2.839055
7	4.019583	-2.749417	-3.529144
6	2.832883	-2.878852	-2.988143
6	2.472439	-2.323819	-1.737101
6	6.235893	-1.896003	-3.416823
6	7.231066	-1.192451	-2.788962
6	6.970850	-0.575848	-1.538083
6	5.726673	-0.678113	-0.953411
9	1.374200	6.506835	0.665187
9	0.295995	6.740453	-1.185939

9	-4.479357	4.647072	1.404236
9	-4.262616	2.492071	1.357763
1	2.037516	-2.833125	0.924134
1	4.031113	-3.894900	1.437883
1	4.907627	-2.404952	1.111029
1	1.274340	-2.408330	4.331304
1	1.255186	-3.484284	2.947788
1	3.354342	-3.238481	5.037129
1	3.242636	-4.452296	3.763365
1	5.318033	-3.141960	3.455796
1	4.492993	-1.151337	4.692981
1	2.413965	-0.334628	4.186171
1	3.014507	0.271902	2.646959
1	5.288723	0.725880	3.065817
1	7.306080	-0.084576	2.027894
1	6.808151	-1.839579	2.318946
1	3.740080	-0.310833	0.680388
1	1.465888	-2.480656	-1.354786
1	5.575244	-0.176004	-0.005206
1	2.097533	-3.452536	-3.549660
1	6.404592	-2.372466	-4.377011
1	8.205736	-1.107245	-3.254420
1	0.892468	-0.789499	0.156530
1	-0.315367	0.716077	0.038510
1	1.367370	4.078547	0.031694
1	-2.139865	1.655540	0.480558
1	-2.472132	5.945069	0.610794
8	7.900958	0.137166	-0.852104
6	9.181322	0.293306	-1.432482
1	9.757103	0.900089	-0.733275
1	9.683823	-0.671828	-1.567090
1	9.126377	0.813546	-2.395793
1	0.717868	-0.895018	2.450789

re-re_2-path-B

Number of imaginary frequencies : 1

The smallest frequency is : -238.9727

Electronic energy= -3905.2846729
 Zero-point correction= 1.051344
 Thermal correction to Energy= 1.116996
 Thermal correction to Enthalpy= 1.117940
 Thermal correction to Gibbs Free Energy= 0.946168
 Sum of electronic and zero-point Energies= -3904.233329
 Sum of electronic and thermal Energies= -3904.167677
 Sum of electronic and thermal Enthalpies= -3904.166733
 Sum of electronic and thermal Free Energies= -3904.338505

Cartesian Coordinates

6	2.481521	0.329103	3.386565
6	2.906617	1.747609	3.801259
6	3.247136	2.463204	2.478551
7	2.710082	1.583681	1.427705
6	1.854134	0.550356	2.000711
6	3.242310	1.493617	0.208173
6	4.002264	2.480912	-0.388358
8	-0.846299	2.525372	-0.022051
6	0.430369	1.082410	2.180684
8	-0.483095	0.192606	1.890557
8	0.223701	2.203030	2.608157
8	0.715476	1.415331	-1.058764
1	1.847538	-0.333257	1.357965
1	1.782598	-0.129353	4.089805
1	3.348860	-0.328966	3.283111
1	2.079795	2.258302	4.294409

1	3.762942	1.733786	4.477557
1	2.793344	3.455662	2.421047
1	4.327525	2.554892	2.322329
1	2.968007	0.607438	-0.361292
1	4.346943	3.305540	0.232049
6	4.820132	2.169720	-1.610867
6	6.246745	1.697315	-1.265740
1	4.899174	3.061275	-2.243574
1	4.317520	1.394924	-2.201891
1	6.790663	1.527390	-2.203954
1	6.779016	2.484072	-0.719857
6	6.253553	0.427685	-0.470141
6	6.911754	0.254597	0.680793
1	5.700931	-0.410331	-0.895173
1	7.520655	1.052925	1.101413
6	7.040729	-1.051832	1.376351
8	8.040122	-1.288533	2.033752
6	5.958594	-2.085453	1.262671
6	4.604171	-1.745339	1.181094
6	6.327232	-3.431016	1.333821
6	3.632827	-2.742365	1.184122
1	4.318191	-0.697677	1.147247
6	5.357521	-4.426258	1.300151
1	7.380721	-3.678462	1.417065
6	4.008377	-4.083177	1.232696
1	2.577976	-2.482813	1.140774
1	5.651117	-5.470475	1.338480
1	3.246231	-4.856523	1.214895
6	2.263710	3.621187	-1.224838
1	2.302675	2.941063	-2.071582
1	0.739850	4.358660	0.186207
6	2.961954	4.914170	-1.382845
6	3.480316	5.270045	-2.632745
6	3.101041	5.807131	-0.311399
6	4.113759	6.497173	-2.812228
1	3.369067	4.586086	-3.469856
6	3.734942	7.029135	-0.491286
1	2.721746	5.532640	0.669748
6	4.241685	7.378528	-1.743416
1	4.504058	6.763897	-3.789127
1	3.837750	7.711886	0.346088
1	4.736010	8.334680	-1.881891
7	0.301869	2.464613	-0.505382
6	1.120748	3.564157	-0.436567
7	-0.748253	-1.128762	-0.865780
6	0.150426	-2.163864	-1.107193
6	-0.057900	-3.517740	-0.822780
6	0.957414	-4.433760	-1.089903
6	2.184223	-4.055877	-1.616438
6	2.385052	-2.702650	-1.873524
6	1.392510	-1.767827	-1.633889
6	0.745129	-5.868039	-0.694868
9	-0.533700	-6.241492	-0.807790
6	3.710340	-2.255641	-2.415255
9	3.844895	-2.520772	-3.721336
6	-2.077776	-1.116146	-0.546060
16	-3.106022	-2.455584	-0.545359
7	-2.487692	0.127857	-0.238566
6	-3.835966	0.509247	0.129277
6	-3.773838	1.475412	1.329819
6	-5.188666	1.773945	1.896322
6	-5.245442	1.310054	3.360061
6	-4.215285	2.119969	4.159903
6	-2.829204	1.942594	3.492421
7	-2.896151	0.944929	2.402247
6	-3.411486	-0.330114	2.941491
6	-4.867968	-0.179648	3.470752
6	-5.811031	-1.143527	2.793189
6	-7.065323	-0.901535	2.418552
6	-4.563460	1.171190	-1.036963

6	-5.856798	0.748063	-1.478078
6	-6.452984	1.479979	-2.547914
7	-5.845349	2.531386	-3.167901
6	-4.652403	2.873296	-2.747730
6	-3.974239	2.227569	-1.685907
6	-7.741975	1.105597	-2.998577
6	-8.423045	0.060205	-2.429225
6	-7.823498	-0.671641	-1.372739
6	-6.567150	-0.336895	-0.915082
9	1.482713	-6.707893	-1.434853
9	1.098600	-6.074784	0.589995
9	4.734576	-2.851187	-1.789066
9	3.879432	-0.923080	-2.267310
1	-3.290091	2.399587	0.991115
1	-5.401351	2.846096	1.842818
1	-5.952204	1.264778	1.302074
1	-2.072441	1.597647	4.202876
1	-2.452901	2.870949	3.056672
1	-4.193426	1.774074	5.198532
1	-4.500500	3.176256	4.175357
1	-6.247508	1.473702	3.767631
1	-4.862825	-0.438549	4.538768
1	-2.726423	-0.632220	3.739356
1	-3.343675	-1.091114	2.156699
1	-5.399467	-2.139184	2.618399
1	-7.665257	-1.669420	1.939982
1	-7.538410	0.067485	2.557419
1	-4.359307	-0.402444	0.420041
1	-2.985265	2.576290	-1.396046
1	-6.148655	-0.939582	-0.118429
1	-4.175484	3.710134	-3.254704
1	-8.172954	1.678373	-3.813412
1	-9.408724	-0.201618	-2.795012
1	-1.794270	0.880121	-0.210217
1	-0.308710	-0.206384	-0.899963
1	-0.998834	-3.850162	-0.407436
1	1.565248	-0.718359	-1.855678
1	2.967169	-4.783953	-1.798605
8	-8.426542	-1.721683	-0.757219
6	-9.692197	-2.136612	-1.233217
1	-9.972482	-2.999980	-0.629523
1	-10.448122	-1.352370	-1.108779
1	-9.647629	-2.436489	-2.286569
1	-1.456731	0.587092	2.040002

re-re_3-path-B

Number of imaginary frequencies : 1
The smallest frequency is : -259.3024

Electronic energy= -3905.2767362
Zero-point correction= 1.049967
Thermal correction to Energy= 1.116385
Thermal correction to Enthalpy= 1.117329
Thermal correction to Gibbs Free Energy= 0.938576
Sum of electronic and zero-point Energies= -3904.226769
Sum of electronic and thermal Energies= -3904.160352
Sum of electronic and thermal Enthalpies= -3904.159407
Sum of electronic and thermal Free Energies= -3904.338160

Cartesian Coordinates

6	-1.751680	1.073672	3.709212
6	-2.791803	-0.051353	3.838260
6	-3.253221	-0.337397	2.392555
7	-2.318348	0.414599	1.539762
6	-1.152699	0.842504	2.313971

6	-2.686356	1.038458	0.414764
6	-3.790967	0.725386	-0.347470
8	0.290598	-1.741216	-0.111632
6	-0.120073	-0.285981	2.369446
8	1.094817	0.126079	2.108618
8	-0.437426	-1.422875	2.666803
8	-0.554492	0.017800	-1.081029
1	-0.707766	1.733022	1.865918
1	-0.996806	1.048314	4.498460
1	-2.234040	2.055167	3.721312
1	-2.331311	-0.943695	4.261266
1	-3.630436	0.243253	4.471485
1	-3.204183	-1.404265	2.162721
1	-4.267435	0.025795	2.200377
1	-1.990263	1.797069	0.064005
1	-4.574344	0.114671	0.092919
6	-4.181672	1.648107	-1.482917
6	-5.507242	1.263497	-2.162129
1	-3.387269	1.677769	-2.240700
1	-4.272580	2.674877	-1.108635
1	-5.746853	2.036809	-2.901642
1	-5.408455	0.315264	-2.696400
6	-6.619001	1.160450	-1.167615
6	-7.307305	0.042366	-0.915151
1	-6.854575	2.048096	-0.578662
1	-7.091471	-0.871355	-1.463912
6	-8.334209	0.021240	0.161396
8	-8.469688	0.961014	0.928231
6	-9.187563	-1.201406	0.318844
6	-9.353323	-2.143538	-0.700677
6	-9.856399	-1.377806	1.534336
6	-10.173084	-3.251249	-0.501016
1	-8.862517	-2.006996	-1.659021
6	-10.662913	-2.489361	1.737370
1	-9.726835	-0.627592	2.307481
6	-10.821568	-3.428877	0.718476
1	-10.309662	-3.974415	-1.299115
1	-11.170944	-2.625393	2.686783
1	-11.455054	-4.296696	0.874692
6	-2.949790	-1.167841	-1.322007
1	-2.660798	-0.501757	-2.130562
1	-1.983378	-2.623739	0.014381
6	-4.183091	-1.966073	-1.509890
6	-4.690158	-2.153884	-2.800696
6	-4.826313	-2.586881	-0.431849
6	-5.804974	-2.960651	-3.011924
1	-4.195841	-1.676527	-3.642840
6	-5.944394	-3.385900	-0.640938
1	-4.451701	-2.428347	0.576117
6	-6.431828	-3.580848	-1.933128
1	-6.180453	-3.107242	-4.019698
1	-6.442682	-3.852446	0.203013
1	-7.302270	-4.209248	-2.095484
7	-0.685193	-1.123365	-0.581537
6	-1.930204	-1.713107	-0.563227
7	1.867282	1.586206	-0.519455
6	1.506555	2.930468	-0.511528
6	2.266951	3.983511	0.008049
6	1.740198	5.272397	-0.000288
6	0.473065	5.557831	-0.490597
6	-0.273967	4.499921	-0.998570
6	0.229882	3.209374	-1.025719
6	2.607391	6.383712	0.522751
9	3.584149	6.697212	-0.341229
6	-1.682624	4.727469	-1.460886
9	-2.002937	3.949858	-2.507698
6	3.051761	0.945510	-0.280901
16	4.565463	1.683134	-0.162511
7	2.862448	-0.381432	-0.169094
6	3.893657	-1.379327	0.018827

6	3.425714	-2.386757	1.089911
6	4.557855	-3.380333	1.464601
6	4.858450	-3.246040	2.964611
6	3.589167	-3.621484	3.742331
6	2.431042	-2.715368	3.254808
7	2.925093	-1.696412	2.303319
6	3.989414	-0.903571	2.950935
6	5.217743	-1.789342	3.317633
6	6.486491	-1.260482	2.695332
6	7.469619	-1.976745	2.154385
6	4.194066	-2.114114	-1.284147
6	5.520282	-2.267515	-1.798130
6	5.669035	-3.019824	-3.001516
7	4.621276	-3.571773	-3.676920
6	3.421434	-3.388874	-3.184247
6	3.158897	-2.671741	-1.992735
6	6.967199	-3.211361	-3.533389
6	8.076344	-2.691480	-2.916742
6	7.924405	-1.937219	-1.725460
6	6.673504	-1.725866	-1.185669
9	1.906282	7.504965	0.748902
9	3.204513	6.044993	1.674951
9	-1.903588	5.997641	-1.815569
9	-2.567558	4.432006	-0.485705
1	2.558932	-2.923843	0.685799
1	4.252918	-4.407531	1.242123
1	5.454309	-3.175779	0.873106
1	1.951522	-2.183395	4.081462
1	1.645150	-3.277667	2.745115
1	3.757245	-3.492199	4.816500
1	3.347622	-4.675496	3.574924
1	5.679910	-3.912544	3.244424
1	5.352086	-1.739401	4.407215
1	3.544517	-0.449783	3.841590
1	4.268815	-0.084179	2.280209
1	6.586890	-0.173887	2.715433
1	8.347438	-1.496582	1.733167
1	7.436531	-3.061805	2.096147
1	4.787724	-0.860329	0.366410
1	2.131844	-2.568106	-1.649291
1	6.613179	-1.126478	-0.285289
1	2.592988	-3.830264	-3.735473
1	7.051119	-3.786136	-4.450054
1	9.057116	-2.854120	-3.347628
1	1.903842	-0.738126	-0.179635
1	1.073124	0.966700	-0.690892
1	3.251524	3.797539	0.415152
1	-0.357667	2.401645	-1.455231
1	0.080171	6.567145	-0.477693
8	8.968202	-1.386481	-1.053528
6	10.263906	-1.525488	-1.603280
1	10.934735	-0.990788	-0.930222
1	10.571379	-2.576692	-1.653589
1	10.328393	-1.078195	-2.601900
1	1.783752	-0.674378	2.128762

re-re_4-path-B

Number of imaginary frequencies : 1
The smallest frequency is : -311.2179

Electronic energy=	-3905.2749028
Zero-point correction=	1.050409
Thermal correction to Energy=	1.116398
Thermal correction to Enthalpy=	1.117342
Thermal correction to Gibbs Free Energy=	0.942800
Sum of electronic and zero-point Energies=	-3904.224494

Sum of electronic and thermal Energies=	-3904.158505
Sum of electronic and thermal Enthalpies=	-3904.157561
Sum of electronic and thermal Free Energies=	-3904.332103

Cartesian Coordinates			
6	-1.827677	1.037953	3.703838
6	-2.830710	-0.116771	3.870015
6	-3.271163	-0.479423	2.433816
7	-2.392093	0.313604	1.557325
6	-1.230348	0.791319	2.310771
6	-2.798016	0.909098	0.436838
6	-3.886239	0.521069	-0.330265
8	0.289699	-1.766681	-0.063658
6	-0.169067	-0.310384	2.388118
8	1.033838	0.127419	2.123720
8	-0.462580	-1.447269	2.709689
8	-0.588035	-0.014723	-1.024163
1	-0.813217	1.681220	1.836013
1	-1.066671	1.056304	4.487145
1	-2.340389	2.003915	3.695945
1	-2.344823	-0.975680	4.331589
1	-3.683125	0.175327	4.485814
1	-3.140968	-1.545296	2.235660
1	-4.308173	-0.196161	2.230358
1	-2.153074	1.708694	0.081895
1	-4.617192	-0.136265	0.129563
6	-4.393323	1.510936	-1.362691
6	-5.123930	0.957539	-2.586852
1	-3.544652	2.104389	-1.719110
1	-5.061282	2.226569	-0.862253
1	-5.365989	1.800816	-3.248465
1	-4.453775	0.324947	-3.180194
6	-6.390872	0.196184	-2.351093
6	-7.035309	0.028275	-1.191813
1	-6.834650	-0.275113	-3.227791
1	-6.674002	0.472508	-0.270331
6	-8.271278	-0.796509	-1.150918
8	-8.867438	-1.108888	-2.168566
6	-8.782446	-1.255862	0.184482
6	-7.995306	-1.239953	1.340083
6	-10.086438	-1.755456	0.251038
6	-8.507800	-1.712535	2.544914
1	-6.969584	-0.885883	1.299194
6	-10.602093	-2.216595	1.455659
1	-10.678824	-1.771367	-0.657835
6	-9.812352	-2.195576	2.604959
1	-7.888999	-1.705542	3.436638
1	-11.618330	-2.594861	1.501782
1	-10.212985	-2.559185	3.546118
6	-2.957472	-1.242803	-1.299860
1	-2.655265	-0.599637	-2.122257
1	-1.973195	-2.694012	0.035976
6	-4.160119	-2.087051	-1.506059
6	-4.628173	-2.332117	-2.800099
6	-4.840497	-2.654856	-0.422809
6	-5.765772	-3.107786	-3.005536
1	-4.098682	-1.909652	-3.650401
6	-5.980515	-3.424183	-0.626401
1	-4.482058	-2.471270	0.587974
6	-6.451856	-3.644467	-1.919904
1	-6.124225	-3.281316	-4.015235
1	-6.509381	-3.842965	0.224058
1	-7.355267	-4.224127	-2.079073
7	-0.700967	-1.166740	-0.534315
6	-1.927917	-1.774159	-0.527351
7	1.772035	1.626200	-0.481856
6	1.388097	2.963095	-0.460818
6	2.140655	4.029050	0.049251
6	1.590436	5.306281	0.059657

6	0.306193	5.571498	-0.402420
6	-0.429821	4.504277	-0.901531
6	0.098051	3.222383	-0.947361
6	2.438654	6.445122	0.554307
9	1.688592	7.459049	1.014232
6	-1.849117	4.693694	-1.347240
9	-2.099829	4.062367	-2.506914
6	2.968537	1.001869	-0.258358
16	4.471815	1.761977	-0.142527
7	2.799212	-0.328239	-0.158503
6	3.844064	-1.314416	0.015091
6	3.399511	-2.330435	1.088373
6	4.548148	-3.309483	1.449926
6	4.866866	-3.169594	2.945554
6	3.614188	-3.564664	3.739876
6	2.434999	-2.680013	3.264481
7	2.900970	-1.650255	2.309535
6	3.959734	-0.841401	2.946893
6	5.207754	-1.707172	3.293789
6	6.458497	-1.157820	2.652863
6	7.445837	-1.858411	2.099248
6	4.134966	-2.044299	-1.293078
6	5.455216	-2.181817	-1.826453
6	5.595041	-2.930884	-3.032932
7	4.544122	-3.494052	-3.693906
6	3.349661	-3.326246	-3.183059
6	3.096081	-2.613900	-1.986748
6	6.887548	-3.107574	-3.583508
6	7.999703	-2.576769	-2.981798
6	7.856525	-1.825845	-1.787317
6	6.611177	-1.628657	-1.229605
9	3.255245	6.067129	1.547293
9	3.213371	6.944139	-0.420821
9	-2.172358	5.980288	-1.506566
9	-2.714453	4.177445	-0.447493
1	2.535856	-2.877086	0.691266
1	4.252388	-4.340583	1.233217
1	5.434151	-3.095436	0.846144
1	1.953265	-2.158307	4.096336
1	1.655239	-3.255915	2.760619
1	3.793244	-3.429549	4.811564
1	3.388426	-4.622997	3.578039
1	5.702486	-3.822747	3.214618
1	5.357762	-1.655703	4.381262
1	3.518508	-0.399239	3.845275
1	4.215946	-0.014628	2.275973
1	6.541016	-0.069690	2.670409
1	8.309768	-1.364385	1.665503
1	7.429903	-2.943926	2.042406
1	4.736580	-0.786508	0.353216
1	2.073303	-2.523844	-1.626855
1	6.556813	-1.031000	-0.327768
1	2.518522	-3.776994	-3.722450
1	6.964561	-3.680557	-4.501889
1	8.976020	-2.729027	-3.426376
1	1.845849	-0.701403	-0.165295
1	0.987083	0.992465	-0.647667
1	3.135600	3.858200	0.436146
1	-0.485842	2.406004	-1.367235
1	-0.106230	6.572689	-0.371123
8	8.903844	-1.265145	-1.129124
6	10.192283	-1.385759	-1.699899
1	10.866456	-0.842308	-1.037299
1	10.513328	-2.432623	-1.756231
1	10.234423	-0.936830	-2.699007
1	1.745823	-0.659118	2.145751

Number of imaginary frequencies : 1
The smallest frequency is : -285.7071

Electronic energy= -3905.2731716
Zero-point correction= 1.050818
Thermal correction to Energy= 1.116795
Thermal correction to Enthalpy= 1.117739
Thermal correction to Gibbs Free Energy= 0.942478
Sum of electronic and zero-point Energies= -3904.222354
Sum of electronic and thermal Energies= -3904.156376
Sum of electronic and thermal Enthalpies= -3904.155432
Sum of electronic and thermal Free Energies= -3904.330693

Cartesian Coordinates

6	-0.585943	4.324569	1.940397
6	-1.278070	4.058704	3.287289
6	-2.255577	2.898137	3.009986
7	-1.866104	2.387299	1.686255
6	-0.574392	2.938194	1.281887
6	-2.712581	1.816886	0.828656
6	-3.920868	1.253413	1.192700
8	0.379384	-0.837860	1.690374
6	0.555206	2.091856	1.876070
8	1.535896	1.883533	1.034259
8	0.520441	1.710908	3.031553
8	-1.116458	-0.448932	0.152614
1	-0.497025	2.965905	0.194797
1	0.416229	4.745120	2.045891
1	-1.179014	4.999556	1.316335
1	-0.543140	3.749640	4.030585
1	-1.801873	4.941325	3.658433
1	-2.173958	2.109848	3.762806
1	-3.295639	3.235144	2.958441
1	-2.340859	1.722797	-0.187304
1	-4.314145	1.501631	2.174871
6	-4.941776	0.805653	0.178006
6	-4.351626	0.165778	-1.103460
1	-5.595968	1.642708	-0.094728
1	-5.593033	0.076613	0.678119
1	-4.339433	0.901140	-1.913309
1	-3.315188	-0.150466	-0.935599
6	-5.172476	-1.020229	-1.506660
6	-4.705947	-2.272650	-1.564857
1	-6.221159	-0.826734	-1.733937
1	-3.648723	-2.474995	-1.396849
6	-5.497752	-3.454526	-1.994402
8	-4.932627	-4.391610	-2.531709
6	-6.983082	-3.503901	-1.774761
6	-7.619916	-2.844661	-0.718173
6	-7.735810	-4.313884	-2.631341
6	-8.992262	-2.985789	-0.530388
1	-7.042185	-2.236055	-0.029577
6	-9.107295	-4.440278	-2.453237
1	-7.224059	-4.837535	-3.432214
6	-9.737419	-3.775889	-1.401209
1	-9.478815	-2.479562	0.297383
1	-9.687443	-5.060592	-3.128935
1	-10.808501	-3.879890	-1.257441
6	-3.118925	-0.709770	1.910213
1	-3.291996	-1.071527	0.900858
1	-1.425088	-0.678789	3.328518
6	-4.181388	-1.020219	2.885899
6	-5.237055	-1.850541	2.490851
6	-4.162089	-0.522185	4.195130
6	-6.251494	-2.181262	3.384829
1	-5.242211	-2.252491	1.479981
6	-5.175351	-0.852004	5.085967

1	-3.354486	0.134629	4.508949
6	-6.223369	-1.680711	4.683142
1	-7.059311	-2.832967	3.066215
1	-5.151747	-0.460318	6.097895
1	-7.014252	-1.934116	5.381806
7	-0.809168	-0.642695	1.355231
6	-1.790831	-0.650217	2.313555
7	0.977080	0.631035	-1.634559
6	0.494823	1.891430	-1.991709
6	1.228539	3.073240	-1.823930
6	0.614174	4.295715	-2.052302
6	-0.719936	4.392645	-2.441762
6	-1.433142	3.213946	-2.612488
6	-0.839280	1.971706	-2.404334
6	1.366886	5.556858	-1.737860
9	2.687720	5.411706	-1.882548
6	-2.894741	3.276516	-2.945827
9	-3.282623	2.253324	-3.720958
6	2.286841	0.276421	-1.389808
16	3.586786	0.812396	-2.317591
7	2.374140	-0.572883	-0.357397
6	3.580846	-1.193718	0.151865
6	3.672958	-0.927191	1.670130
6	4.998875	-1.463292	2.270482
6	5.747627	-0.301632	2.938354
6	4.863360	0.256342	4.063505
6	3.497100	0.667575	3.458563
7	3.509457	0.512935	1.986782
6	4.609399	1.324509	1.426265
6	5.999565	0.828424	1.922585
6	6.902549	0.476817	0.765747
6	7.744654	-0.551535	0.690995
6	3.565017	-2.696263	-0.104533
6	4.663815	-3.389755	-0.703027
6	4.538432	-4.804154	-0.846508
7	3.433086	-5.504068	-0.463175
6	2.442221	-4.828227	0.063098
6	2.464105	-3.427624	0.266125
6	5.610786	-5.532028	-1.415908
6	6.760235	-4.907681	-1.827139
6	6.879288	-3.500922	-1.690172
6	5.850334	-2.761424	-1.146528
9	0.979027	6.578041	-2.515666
9	1.151847	5.940534	-0.463472
9	-3.224640	4.411522	-3.571566
9	-3.653471	3.215631	-1.828451
1	2.814146	-1.421320	2.139287
1	4.792481	-2.242642	3.010344
1	5.616513	-1.916224	1.490774
1	3.249271	1.710799	3.673301
1	2.669697	0.063744	3.839427
1	5.353663	1.115412	4.533201
1	4.726159	-0.502949	4.839452
1	6.697614	-0.655108	3.350555
1	6.478617	1.657159	2.462184
1	4.421552	2.358388	1.732103
1	4.536615	1.296546	0.334202
1	6.847089	1.163211	-0.080976
1	8.354593	-0.712177	-0.192717
1	7.851922	-1.278620	1.492004
1	4.425266	-0.731073	-0.361148
1	1.599924	-2.942783	0.715157
1	5.989646	-1.689149	-1.074602
1	1.562981	-5.397421	0.358744
1	5.488461	-6.605706	-1.515164
1	7.563603	-5.491961	-2.259606
1	1.550164	-0.664237	0.245524
1	0.280940	0.067991	-1.143282
1	2.252910	3.029888	-1.478131
1	-1.408990	1.057427	-2.550429

1	-1.184163	5.357784	-2.609516
8	7.980046	-2.805641	-2.076155
6	9.060199	-3.525459	-2.638302
1	9.825749	-2.784884	-2.870906
1	9.470919	-4.254852	-1.930390
1	8.766551	-4.038306	-3.561506
1	2.272276	1.247052	1.456066

Stationary Points relevant to Figure S11. Second-Michael-addition [10-11]TS

(2R,3S)_*re-re*-path-A

Number of imaginary frequencies : 1

The smallest frequency is : -371.0329

Electronic energy=	-3905.3066568
Zero-point correction=	1.056381
Thermal correction to Energy=	1.120408
Thermal correction to Enthalpy=	1.121352
Thermal correction to Gibbs Free Energy=	0.951576
Sum of electronic and zero-point Energies=	-3904.250276
Sum of electronic and thermal Energies=	-3904.186249
Sum of electronic and thermal Enthalpies=	-3904.185305
Sum of electronic and thermal Free Energies=	-3904.355080

Cartesian Coordinates

7	-1.772673	-0.082089	-0.030375
6	-3.081658	0.079103	0.273566
6	0.432975	3.024815	2.204321
6	-3.927415	-2.232314	-0.452692
6	-2.816250	1.038541	2.108514
6	-3.456057	-2.050839	-1.753667
6	-3.500925	-3.091461	-2.676777
8	-1.166768	-1.149304	0.301979
6	-4.492583	-4.525501	-1.022161
6	-0.518878	1.860671	2.213686
6	1.800745	2.745385	2.125229
8	-1.149551	0.886304	-0.529329
6	-4.441967	-3.482746	-0.100538
6	2.733733	3.772264	2.034112
6	-5.288837	-0.695293	1.095800
6	-3.890894	-1.137869	0.614225
6	-1.908473	2.082881	1.976341
6	0.018097	4.361281	2.240235
6	-4.018444	-4.333202	-2.316302
6	-5.192604	0.080001	2.417980
6	2.309257	5.099331	2.048553
8	-0.039225	0.730687	2.468141
6	0.951024	5.391088	2.168547
6	-4.278970	1.312560	2.395197
1	-3.520680	0.906524	-0.271011
1	-5.871183	-1.605166	1.283889
1	-4.835406	-0.604233	3.197020
1	3.788634	3.536237	1.929080
1	-3.137755	-2.926483	-3.686722
1	-4.647284	2.075466	1.698456
1	-4.896930	-5.488758	-0.725598
1	-2.257757	3.068655	1.689346
1	-2.405761	0.131533	2.560818
1	-4.799588	-3.647144	0.914502
1	-4.324478	1.777436	3.388083
1	-3.065898	-1.083989	-2.058608

1	-3.412748	-1.604070	1.488243
1	-1.034243	4.606984	2.333575
1	3.035172	5.902418	1.960822
1	0.615586	6.423105	2.188921
1	-6.202618	0.388498	2.711177
1	2.117671	1.707145	2.098402
1	-4.056628	-5.141750	-3.039413
7	1.645974	1.354770	-0.790762
6	1.972296	2.689427	-1.048000
6	0.893807	3.585199	-0.977997
6	1.097179	4.936596	-1.187924
6	2.363721	5.440025	-1.476480
6	3.414909	4.540216	-1.562953
6	3.243038	3.171493	-1.363726
6	-0.062011	5.886446	-1.109356
9	0.270537	7.021239	-0.471012
6	4.804960	5.066906	-1.770116
9	5.398142	5.350504	-0.596035
6	2.392122	0.286763	-0.401488
16	4.061605	0.273165	-0.147787
7	1.607546	-0.795271	-0.177990
6	2.077602	-2.121314	0.163314
6	1.149022	-2.734736	1.229179
6	1.747059	-3.992193	1.896542
6	1.958798	-3.724546	3.394737
6	0.588958	-3.467327	4.042282
6	-0.112755	-2.321488	3.286319
7	0.845350	-1.730787	2.303158
6	2.077903	-1.255077	3.004788
6	2.829320	-2.470328	3.608049
6	4.241953	-2.560524	3.079979
6	4.903912	-3.673072	2.772204
6	2.093081	-3.055242	-1.042787
6	3.241285	-3.827564	-1.401015
6	3.104257	-4.712437	-2.512078
7	1.956470	-4.834407	-3.237404
6	0.933587	-4.095448	-2.885138
6	0.951775	-3.196119	-1.792128
6	4.209833	-5.513811	-2.887478
6	5.398727	-5.455761	-2.206565
6	5.533751	-4.569374	-1.107340
6	4.478977	-3.770700	-0.719676
9	-0.491414	6.249500	-2.330075
9	-1.113905	5.358795	-0.466307
9	4.809871	6.201593	-2.487304
9	5.593565	4.187378	-2.401443
1	0.180037	-2.946346	0.771902
1	1.070309	-4.841261	1.767414
1	2.690442	-4.251961	1.410320
1	-0.425927	-1.499570	3.932184
1	-0.975062	-2.654361	2.704596
1	0.717817	-3.204900	5.096153
1	-0.023707	-4.371239	4.000512
1	2.433077	-4.589309	3.865846
1	2.901400	-2.302096	4.690645
1	1.734642	-0.538109	3.751273
1	2.681971	-0.710795	2.273139
1	4.751404	-1.602402	2.971917
1	5.927795	-3.631965	2.414608
1	4.459742	-4.661811	2.857144
1	3.084390	-2.012152	0.569497
1	0.051425	-2.632975	-1.553059
1	4.643416	-3.094259	0.111093
1	0.022756	-4.201722	-3.471468
1	4.080683	-6.179152	-3.734973
1	6.226777	-6.082117	-2.516062
1	0.594981	-0.711613	-0.302586
1	0.636312	1.190334	-0.746359
1	-0.093052	3.213450	-0.712875
1	4.085390	2.498558	-1.435636

1	2.524359	6.502867	-1.620894
8	6.674856	-4.450337	-0.382009
6	7.808566	-5.187813	-0.798563
1	8.615089	-4.908547	-0.120287
1	7.636851	-6.268116	-0.724538
1	8.098788	-4.933477	-1.824261
1	0.373007	-0.891394	1.907938
6	-9.146062	0.866674	-1.204194
6	-9.294162	-0.656558	-1.166745
6	-7.946535	-1.091654	-0.589526
7	-7.528696	-0.030641	0.345234
6	-8.396467	1.146943	0.101512
6	-6.109090	0.139549	0.097934
1	-7.801225	2.063807	0.074217
1	-10.101073	1.392123	-1.265274
1	-8.538551	1.161840	-2.067356
1	-10.101744	-0.952607	-0.490966
1	-9.465955	-1.112544	-2.143913
1	-7.971331	-2.084801	-0.128116
1	-5.837306	1.197075	0.147729
6	-6.864950	-1.074679	-1.671649
8	-5.859524	-0.275771	-1.261010
8	-6.884533	-1.620483	-2.739164
1	-9.104163	1.234594	0.933294

 (2R,3S)_re-si-path-A

Number of imaginary frequencies : 1
 The smallest frequency is : -297.7691

Electronic energy= -3905.2997636
 Zero-point correction= 1.056785
 Thermal correction to Energy= 1.120821
 Thermal correction to Enthalpy= 1.121765
 Thermal correction to Gibbs Free Energy= 0.950332
 Sum of electronic and zero-point Energies= -3904.242979
 Sum of electronic and thermal Energies= -3904.178943
 Sum of electronic and thermal Enthalpies= -3904.177999
 Sum of electronic and thermal Free Energies= -3904.349431

 Cartesian Coordinates

7	-1.600304	-1.399711	0.254409
6	-2.685865	-0.801237	-0.285366
6	-0.906752	0.030055	3.967968
6	-4.519552	-2.498010	0.251951
6	-2.213697	1.151295	0.588998
6	-3.911407	-3.467072	-0.546170
6	-4.408281	-4.766528	-0.589411
8	-1.639244	-1.814327	1.431957
6	-6.130224	-4.166430	0.976492
6	-0.896849	0.489018	2.542364
6	-1.937645	-0.765465	4.474482
8	-0.498277	-1.413294	-0.398249
6	-5.628868	-2.868490	1.018176
6	-1.885068	-1.219205	5.789921
6	-5.060075	-0.027853	-0.191357
6	-4.026859	-1.053063	0.334815
6	-2.114912	0.938547	1.953302
6	0.174165	0.365621	4.789501
6	-5.520547	-5.121951	0.168229
6	-4.762567	1.392218	0.315061
6	-0.812237	-0.871320	6.608672
8	0.218118	0.502855	1.955064
6	0.216897	-0.075027	6.108374
6	-3.362409	1.913017	-0.034103
1	-2.573025	-0.611308	-1.346494

1	-6.036160	-0.320750	0.213847
1	-4.902920	1.416618	1.401361
1	-2.679095	-1.851517	6.174629
1	-3.928287	-5.502666	-1.227048
1	-3.223029	1.940056	-1.119576
1	-6.994162	-4.431461	1.578624
1	-2.986537	1.026080	2.593452
1	-1.279473	1.170237	0.026955
1	-6.101669	-2.131394	1.664775
1	-3.279729	2.953870	0.304381
1	-3.052688	-3.201426	-1.155971
1	-3.915420	-0.842706	1.406908
1	0.967637	0.985103	4.380978
1	-0.777002	-1.222385	7.635333
1	1.049673	0.203952	6.746524
1	-5.508902	2.072457	-0.109730
1	-2.752482	-1.060482	3.819867
1	-5.909882	-6.134317	0.127613
7	1.459821	1.927420	-0.039666
6	1.397854	3.316715	-0.098260
6	0.380931	3.914009	0.660583
6	0.187609	5.285825	0.615241
6	0.995379	6.103594	-0.168231
6	1.998940	5.498969	-0.915270
6	2.212065	4.124122	-0.899468
6	-0.881817	5.890304	1.478253
9	-0.455096	6.093735	2.734478
6	2.840551	6.338436	-1.835417
9	2.867813	7.624462	-1.455517
6	2.467476	1.048520	-0.341921
16	4.081043	1.426784	-0.615696
7	1.995073	-0.217430	-0.321308
6	2.818987	-1.406698	-0.348312
6	2.132922	-2.521634	0.473504
6	3.096151	-3.673540	0.834190
6	3.298236	-3.719059	2.357740
6	1.954698	-4.074692	3.011197
6	0.880376	-3.092072	2.508594
7	1.555373	-1.981496	1.757917
6	2.590455	-1.333999	2.621852
6	3.735637	-2.342902	2.898244
6	5.066326	-1.836855	2.392809
6	6.041136	-2.574078	1.866573
6	3.046488	-1.929663	-1.764639
6	4.337199	-2.293701	-2.259666
6	4.395950	-2.843278	-3.574620
7	3.300439	-3.008638	-4.368565
6	2.140677	-2.637537	-3.885583
6	1.961622	-2.099441	-2.588062
6	5.651617	-3.242252	-4.093804
6	6.803717	-3.108338	-3.362209
6	6.743523	-2.548587	-2.060359
6	5.537520	-2.145923	-1.528330
9	-1.294735	7.075750	1.008658
9	-1.960433	5.092816	1.564438
9	2.367786	6.313121	-3.093408
9	4.107281	5.906770	-1.889508
1	1.258284	-2.869265	-0.078899
1	2.683615	-4.627176	0.493675
1	4.049071	-3.531027	0.319515
1	0.312651	-2.619858	3.313221
1	0.164247	-3.535087	1.816240
1	2.041029	-4.020187	4.100357
1	1.667202	-5.097190	2.754529
1	4.047483	-4.472901	2.612678
1	3.823512	-2.435708	3.988616
1	2.067963	-1.027382	3.529313
1	2.930786	-0.431187	2.110105
1	5.227308	-0.764337	2.510479
1	6.976817	-2.122591	1.552383

1	5.948187	-3.647239	1.718451
1	3.775128	-1.147026	0.111952
1	0.961888	-1.832685	-2.251515
1	5.549313	-1.699805	-0.541303
1	1.275595	-2.769137	-4.532900
1	5.668668	-3.658172	-5.095922
1	7.749452	-3.423288	-3.786723
1	0.979605	-0.359082	-0.333017
1	0.751269	1.499130	0.571938
1	-0.263800	3.292636	1.279026
1	3.000400	3.685844	-1.497199
1	0.843181	7.175791	-0.199113
8	7.834964	-2.375891	-1.270868
6	9.102301	-2.711339	-1.803101
1	9.828593	-2.466073	-1.027814
1	9.173998	-3.780763	-2.033922
1	9.328195	-2.127914	-2.702904
1	0.834230	-1.268100	1.543672
6	-7.343851	0.389500	-4.340902
6	-8.264607	-0.440924	-3.443472
6	-7.377494	-0.682897	-2.222776
7	-6.543005	0.522924	-2.067489
6	-6.646527	1.301356	-3.326797
6	-5.230269	0.014192	-1.718742
1	-5.658703	1.638137	-3.653203
1	-7.877664	0.945177	-5.114195
1	-6.614749	-0.264930	-4.832419
1	-9.148124	0.134998	-3.153214
1	-8.587533	-1.385102	-3.886795
1	-7.940460	-0.934496	-1.317849
1	-4.449012	0.614095	-2.191897
6	-6.362866	-1.794308	-2.505108
8	-5.123901	-1.308657	-2.288629
8	-6.578977	-2.904135	-2.905438
1	-7.254880	2.191975	-3.134439

(2S,3R)_si-si-path-A

Number of imaginary frequencies : 1
The smallest frequency is : -272.5994

Electronic energy= -3905.2972684
Zero-point correction= 1.056410
Thermal correction to Energy= 1.120615
Thermal correction to Enthalpy= 1.121559
Thermal correction to Gibbs Free Energy= 0.948751
Sum of electronic and zero-point Energies= -3904.240858
Sum of electronic and thermal Energies= -3904.176654
Sum of electronic and thermal Enthalpies= -3904.175710
Sum of electronic and thermal Free Energies= -3904.348517

Cartesian Coordinates

7	0.533277	1.974161	-0.376088
6	-0.058778	3.141998	-0.846833
6	-1.081056	3.672604	-0.046878
6	-1.797245	4.781887	-0.469872
6	-1.512923	5.407469	-1.678550
6	-0.492247	4.876221	-2.458302
6	0.232374	3.753107	-2.071040
6	-2.938085	5.259162	0.380974
9	-3.293517	6.517367	0.092526
6	-0.119510	5.549362	-3.749781
9	0.951696	6.344017	-3.603233
6	1.735289	1.379617	-0.673956
16	3.035034	2.090055	-1.461951
7	1.759454	0.129549	-0.163653

6	2.939424	-0.700173	-0.040956
6	2.816867	-1.571365	1.229472
6	4.162271	-2.179649	1.676793
6	4.542491	-1.619452	3.055130
6	3.487573	-2.081632	4.072893
6	2.088159	-1.671794	3.572834
7	2.252189	-0.776295	2.381579
6	3.100911	0.400025	2.737811
6	4.545669	-0.077090	3.033695
6	5.544610	0.561524	2.096168
6	6.640678	-0.005517	1.598260
6	3.131118	-1.630089	-1.235088
6	4.383377	-1.764433	-1.911189
6	4.450165	-2.721718	-2.966595
7	3.388618	-3.482237	-3.358132
6	2.254875	-3.313962	-2.722842
6	2.076929	-2.404679	-1.651962
6	5.678763	-2.904759	-3.646394
6	6.797083	-2.185829	-3.310044
6	6.724350	-1.227115	-2.267087
6	5.541201	-1.018712	-1.591284
9	-4.033572	4.494501	0.207505
9	-2.642330	5.208182	1.687468
9	-1.114885	6.316543	-4.219653
9	0.186117	4.658781	-4.704204
1	2.064541	-2.339596	1.051142
1	4.077123	-3.268083	1.735242
1	4.933478	-1.953505	0.937018
1	1.515410	-1.103687	4.309594
1	1.467371	-2.505208	3.241028
1	3.687008	-1.630889	5.049479
1	3.534078	-3.166428	4.195899
1	5.527495	-1.989024	3.351703
1	4.795040	0.263588	4.047090
1	2.620344	0.860140	3.602310
1	3.047925	1.108396	1.907970
1	5.334923	1.601658	1.842632
1	7.309610	0.550612	0.949202
1	6.915432	-1.036382	1.807255
1	3.795817	-0.027786	0.051991
1	1.104708	-2.342890	-1.163906
1	5.532826	-0.255468	-0.821977
1	1.412904	-3.925944	-3.040700
1	5.703597	-3.639165	-4.445014
1	7.723715	-2.351404	-3.846407
1	0.868835	-0.297321	0.113405
1	0.151526	1.636324	0.518662
1	-1.312367	3.206953	0.909299
1	1.009460	3.356719	-2.711573
1	-2.070125	6.278083	-2.002646
8	7.781545	-0.471701	-1.872125
6	8.997460	-0.603910	-2.583375
1	9.688218	0.110146	-2.134480
1	9.414474	-1.613254	-2.486636
1	8.871294	-0.360920	-3.644697
1	1.309413	-0.427823	2.130312
7	-1.103681	-1.682254	1.584479
6	-2.315050	-1.584451	1.005487
6	-0.531933	1.022731	4.482791
6	-2.033606	-3.120359	-1.011385
6	-2.470864	0.596874	1.258000
6	-1.915815	-4.242610	-0.192450
6	-1.548095	-5.474761	-0.725698
8	-0.049742	-1.663047	0.853737
6	-1.394937	-4.486735	-2.913239
6	-0.824821	0.970191	3.016147
6	-1.205053	0.205684	5.394397
8	-1.000367	-1.655894	2.831968
6	-1.756258	-3.255111	-2.374333
6	-0.874799	0.252047	6.745961

6	-3.821318	-1.258047	-0.975798
6	-2.431904	-1.744859	-0.480896
6	-2.179922	0.841844	2.583182
6	0.472645	1.883502	4.935958
6	-1.289394	-5.603738	-2.087290
6	-3.962103	0.262201	-0.784740
6	0.119054	1.119954	7.195020
8	0.150656	1.112881	2.230457
6	0.791312	1.938689	6.289100
6	-3.844511	0.767779	0.657297
1	-3.119966	-1.814332	1.689365
1	-3.854194	-1.475181	-2.049025
1	-3.182814	0.750253	-1.384099
1	-1.389017	-0.394970	7.449761
1	-1.467643	-6.338860	-0.073225
1	-4.608985	0.321767	1.304669
1	-1.188088	-4.571659	-3.976146
1	-2.969038	0.851081	3.328509
1	-1.649495	0.708453	0.546981
1	-1.817673	-2.382313	-3.021883
1	-4.049356	1.846492	0.646928
1	-2.118726	-4.157824	0.871612
1	-1.710777	-1.044760	-0.928092
1	0.982199	2.516253	4.214842
1	0.370038	1.157436	8.250593
1	1.558614	2.622280	6.639217
1	-4.922297	0.594318	-1.188751
1	-1.952149	-0.491362	5.027967
1	-1.004672	-6.565631	-2.502016
6	-8.290908	-2.722892	-1.380091
6	-7.573680	-2.233887	-2.640374
6	-6.617969	-1.163069	-2.099432
7	-6.322707	-1.532174	-0.685663
6	-7.157756	-2.702710	-0.364552
6	-4.993331	-1.985774	-0.331762
6	-6.202470	-3.884091	-0.572335
8	-6.481494	-5.046316	-0.686648
8	-4.944663	-3.406712	-0.644682
1	-7.492588	-2.694398	0.679199
1	-8.719313	-3.722425	-1.476286
1	-9.076387	-2.025344	-1.075483
1	-7.007616	-3.060234	-3.084726
1	-8.251336	-1.841142	-3.400764
1	-5.713227	-1.082058	-2.704314
1	-7.102756	-0.180658	-2.097238
1	-4.926316	-1.924341	0.761629

 (2R,3S)_re-re-path-B

Number of imaginary frequencies : 1

The smallest frequency is : -341.4778

Electronic energy= -3905.301538
 Zero-point correction= 1.057013
 Thermal correction to Energy= 1.120892
 Thermal correction to Enthalpy= 1.121837
 Thermal correction to Gibbs Free Energy= 0.953677
 Sum of electronic and zero-point Energies= -3904.244525
 Sum of electronic and thermal Energies= -3904.180646
 Sum of electronic and thermal Enthalpies= -3904.179701
 Sum of electronic and thermal Free Energies= -3904.347861

 Cartesian Coordinates

7	-0.961408	-1.928116	0.757855
6	-2.200186	-1.953963	0.212650
6	1.544476	-4.492880	-1.131468

6	-3.214290	0.082496	1.368409
6	-1.559772	-2.396482	-1.754070
6	-3.198604	-0.539035	2.616316
6	-3.456421	0.192375	3.773708
8	-0.305188	-0.831885	0.803377
6	-3.739907	2.187484	2.456300
6	0.692362	-3.288532	-1.418538
6	2.889451	-4.481834	-1.515737
8	-0.401689	-3.004891	1.055398
6	-3.484638	1.451674	1.303330
6	3.728713	-5.539380	-1.178710
6	-4.227504	-0.891880	-0.800429
6	-2.959838	-0.666421	0.065858
6	-0.697777	-3.478393	-1.670393
6	1.052349	-5.574699	-0.396534
6	-3.727287	1.556885	3.698454
6	-3.820319	-1.268234	-2.237457
6	3.232039	-6.613666	-0.441754
8	1.274462	-2.176872	-1.451634
6	1.894402	-6.628487	-0.050978
6	-2.930154	-2.507696	-2.383671
1	-2.701583	-2.891200	0.414555
1	-4.759405	0.062739	-0.863694
1	-3.295361	-0.404892	-2.667168
1	4.768396	-5.527453	-1.491480
1	-3.444390	-0.306887	4.738039
1	-3.436047	-3.408151	-2.014560
1	-3.933441	3.252906	2.383406
1	-1.086489	-4.490413	-1.721446
1	-1.073963	-1.420639	-1.854867
1	-3.507233	1.945026	0.333015
1	-2.772720	-2.677381	-3.456485
1	-2.996238	-1.604109	2.684763
1	-2.334627	0.006822	-0.538116
1	0.022136	-5.559669	-0.054931
1	3.885901	-7.437012	-0.171248
1	1.508997	-7.458171	0.533684
1	-4.724494	-1.406972	-2.835107
1	3.266320	-3.633445	-2.080898
1	-3.923118	2.125674	4.602120
7	0.201251	1.472127	-0.717080
6	-0.746939	2.501709	-0.839118
6	-1.740491	2.314783	-1.804174
6	-2.789429	3.218228	-1.913379
6	-2.854365	4.340289	-1.094835
6	-1.846007	4.527503	-0.155170
6	-0.802268	3.619430	-0.004259
6	-3.918189	2.908559	-2.850996
9	-4.523027	4.013300	-3.300559
6	-1.926552	5.694359	0.788817
9	-2.511552	5.349072	1.950963
6	1.531799	1.527829	-0.423313
16	2.399417	2.921279	-0.049049
7	2.086650	0.297649	-0.466083
6	3.444473	-0.001304	-0.067970
6	3.487918	-1.412612	0.553138
6	4.792870	-1.680356	1.333522
6	4.476411	-1.857121	2.827367
6	3.628651	-3.124674	2.990804
6	2.415419	-3.033577	2.048505
7	2.330427	-1.639953	1.493700
6	2.299464	-0.642021	2.607246
6	3.652378	-0.669229	3.365284
6	4.344925	0.673137	3.327586
6	5.658138	0.879723	3.268855
6	4.421663	0.040150	-1.240269
6	5.662447	0.747050	-1.188540
6	6.513634	0.648814	-2.329638
7	6.190061	-0.059175	-3.448480
6	5.031145	-0.670671	-3.464082

6	4.115554	-0.654261	-2.384539
6	7.761730	1.317507	-2.310156
6	8.164037	2.050228	-1.223203
6	7.310367	2.154527	-0.094715
6	6.085285	1.523415	-0.085693
9	-3.511475	2.199314	-3.912592
9	-4.863231	2.168848	-2.233991
9	-2.649261	6.700557	0.277243
9	-0.716193	6.174179	1.095142
1	3.325248	-2.142949	-0.241932
1	5.271954	-2.588041	0.954566
1	5.491269	-0.854182	1.179482
1	1.461143	-3.229314	2.535632
1	2.494844	-3.700668	1.187871
1	3.300704	-3.225364	4.029644
1	4.217406	-4.011361	2.742596
1	5.404409	-1.952212	3.396599
1	3.426015	-0.882225	4.418071
1	1.451566	-0.921058	3.235336
1	2.080026	0.333219	2.166790
1	3.681786	1.537599	3.382786
1	6.065490	1.885692	3.268939
1	6.377836	0.066793	3.209099
1	3.732835	0.741410	0.679104
1	3.173673	-1.193325	-2.466485
1	5.456654	1.658810	0.786010
1	4.781275	-1.224569	-4.367106
1	8.389548	1.230561	-3.191043
1	9.124180	2.551945	-1.239819
1	1.548521	-0.473395	-0.873370
1	-0.202130	0.537143	-0.634995
1	-1.679941	1.459093	-2.470723
1	-0.041788	3.770415	0.750988
1	-3.665289	5.053816	-1.190588
8	7.628563	2.863187	1.019023
6	8.864881	3.550876	1.041573
1	8.914021	4.050048	2.009607
1	9.711936	2.860694	0.951803
1	8.921360	4.304420	0.247704
1	1.419638	-1.544916	0.992737
6	-8.023057	-2.004327	1.876985
6	-7.863552	-0.526259	1.513970
6	-6.344580	-0.352682	1.363989
7	-5.787349	-1.705272	1.062675
6	-6.929560	-2.634660	1.030698
6	-5.178888	-1.933450	-0.224890
6	-7.309235	-2.663772	-0.455841
8	-8.334073	-3.047159	-0.951399
8	-6.286703	-2.142723	-1.162676
1	-6.641886	-3.644990	1.345121
1	-9.004899	-2.414129	1.631742
1	-7.816016	-2.179133	2.936439
1	-8.366279	-0.330901	0.560288
1	-8.284044	0.151212	2.259395
1	-6.102422	0.372586	0.585172
1	-5.888007	0.002133	2.293184
1	-4.674699	-2.906430	-0.169159

(2R,3S)_re-re-path-C

Number of imaginary frequencies : 1

The smallest frequency is : -373.8508

Electronic energy= -3905.276557

Zero-point correction= 1.054654

Thermal correction to Energy= 1.119802

Thermal correction to Enthalpy= 1.120746

Thermal correction to Gibbs Free Energy=	0.945832
Sum of electronic and zero-point Energies=	-3904.221903
Sum of electronic and thermal Energies=	-3904.156755
Sum of electronic and thermal Enthalpies=	-3904.155811
Sum of electronic and thermal Free Energies=	-3904.330725

Cartesian Coordinates

7	-1.648076	-0.438522	-0.177417
6	-2.978583	-0.400818	0.068560
6	0.058930	2.915215	2.146175
6	-3.624367	-2.709641	-0.793360
6	-2.975087	0.645985	1.855785
6	-3.323286	-2.339908	-2.105072
6	-3.323854	-3.288367	-3.127065
8	-0.959369	-1.449574	0.172996
6	-3.931481	-4.997049	-1.545581
6	-0.775473	1.666970	2.097949
6	1.450127	2.778164	2.138209
8	-1.098578	0.587523	-0.645567
6	-3.928504	-4.049051	-0.528374
6	2.274775	3.897734	2.114745
6	-5.125858	-1.457439	0.803586
6	-3.667285	-1.704931	0.355353
6	-2.156233	1.761790	1.746659
6	-0.495389	4.200153	2.181364
6	-3.627916	-4.617818	-2.851989
6	-5.223032	-0.552740	2.057021
6	1.713240	5.173187	2.134388
8	-0.221038	0.585498	2.404964
6	0.327963	5.321419	2.184138
6	-4.479586	0.780524	1.964053
1	-3.464183	0.383698	-0.497603
1	-5.558403	-2.430517	1.054709
1	-4.828302	-1.129124	2.903086
1	3.352660	3.774411	2.061968
1	-3.082007	-2.984183	-4.140797
1	-4.889968	1.389182	1.150266
1	-4.161718	-6.033575	-1.318690
1	-2.563541	2.700351	1.387354
1	-2.530382	-0.192428	2.399571
1	-4.152217	-4.352610	0.492869
1	-4.689627	1.335223	2.886613
1	-3.071413	-1.308139	-2.335230
1	-3.155184	-2.167421	1.209113
1	-1.571289	4.332413	2.221690
1	2.353797	6.049824	2.110199
1	-0.113097	6.312541	2.210913
1	-6.279665	-0.349508	2.257643
1	1.872983	1.778080	2.115983
1	-3.623970	-5.355398	-3.648265
7	1.644752	1.428757	-0.810462
6	1.861616	2.794286	-1.027664
6	0.705982	3.592459	-1.003855
6	0.803214	4.959726	-1.177716
6	2.037136	5.577748	-1.381368
6	3.163715	4.774096	-1.428324
6	3.098570	3.389848	-1.266070
6	-0.432595	5.811440	-1.155986
9	-0.252547	6.921831	-0.421392
6	4.523291	5.392828	-1.578412
9	5.187910	5.398221	-0.409547
6	2.464244	0.438429	-0.365826
16	4.106873	0.591554	-0.006417
7	1.777630	-0.715564	-0.179535
6	2.361824	-1.994054	0.171859
6	1.484383	-2.699029	1.224356
6	2.209435	-3.864989	1.930464
6	2.366347	-3.539452	3.424466
6	0.965026	-3.439517	4.048022

6	0.134668	-2.415347	3.248851
7	1.030613	-1.724410	2.271174
6	2.173671	-1.082975	2.993204
6	3.070869	-2.182207	3.618514
6	4.486801	-2.101619	3.097015
6	5.288551	-3.127710	2.822412
6	2.482226	-2.915988	-1.037828
6	3.701898	-3.573760	-1.387739
6	3.663125	-4.448992	-2.514654
7	2.541861	-4.668477	-3.257661
6	1.448832	-4.036156	-2.908645
6	1.368563	-3.153944	-1.804925
6	4.843902	-5.136859	-2.885864
6	6.012007	-4.981841	-2.184730
6	6.048043	-4.107908	-1.067538
6	4.918504	-3.415740	-0.685238
9	-0.769608	6.224064	-2.389833
9	-1.492868	5.164092	-0.654815
9	4.457935	6.664722	-1.998143
9	5.286170	4.719260	-2.451797
1	0.562251	-3.033846	0.745709
1	1.634479	-4.788053	1.816435
1	3.183275	-4.029354	1.463339
1	-0.300373	-1.627649	3.866107
1	-0.661968	-2.874279	2.658893
1	1.041357	-3.133451	5.095201
1	0.473018	-4.415151	4.025190
1	2.935433	-4.329497	3.921005
1	3.115460	-1.987786	4.698122
1	1.721631	-0.417963	3.729614
1	2.715929	-0.464680	2.272213
1	4.869234	-1.089129	2.964740
1	6.301841	-2.964697	2.469085
1	4.974633	-4.162872	2.931547
1	3.346254	-1.789608	0.595375
1	0.416460	-2.680435	-1.571088
1	5.006083	-2.742329	0.159835
1	0.559282	-4.221555	-3.508040
1	4.789965	-5.794818	-3.747001
1	6.898437	-5.524320	-2.491265
1	0.773751	-0.731495	-0.371075
1	0.656775	1.167431	-0.831210
1	-0.258556	3.130432	-0.807155
1	3.999436	2.794111	-1.307735
1	2.110532	6.653437	-1.496135
8	7.160332	-3.899303	-0.319584
6	8.361372	-4.534123	-0.716719
1	9.124244	-4.199725	-0.013421
1	8.277659	-5.625884	-0.662167
1	8.655454	-4.239877	-1.730632
1	0.464331	-0.963011	1.846376
6	-5.941586	-0.842698	-0.285313
7	-7.159959	-1.153921	-0.536274
6	-7.974680	-2.175977	0.162902
6	-9.414540	-1.755769	-0.143402
6	-9.306956	-1.044722	-1.496011
6	-8.006161	-0.276953	-1.346235
6	-8.165226	1.098317	-0.510981
8	-7.163028	1.404274	0.163776
8	-9.249756	1.658200	-0.689079
1	-7.499116	-0.035675	-2.283580
1	-10.121160	-0.342164	-1.669463
1	-9.256468	-1.766823	-2.317664
1	-9.760200	-1.042835	0.610448
1	-10.088030	-2.613890	-0.148400
1	-7.737562	-2.183164	1.227683
1	-7.724655	-3.149070	-0.271958
1	-5.533754	-0.041060	-0.892105

(2R,3S)_re-re-path-D

Number of imaginary frequencies : 1
The smallest frequency is : -354.1392

Electronic energy= -3580.6774843
Zero-point correction= 0.932754
Thermal correction to Energy= 0.991464
Thermal correction to Enthalpy= 0.992408
Thermal correction to Gibbs Free Energy= 0.833986
Sum of electronic and zero-point Energies= -3579.744731
Sum of electronic and thermal Energies= -3579.686020
Sum of electronic and thermal Enthalpies= -3579.685076
Sum of electronic and thermal Free Energies= -3579.843498

Cartesian Coordinates

7	0.169667	2.568087	-0.404651
6	0.465029	3.876014	-0.259798
6	3.067350	0.339701	2.029264
6	-1.717331	4.865293	-1.120363
6	1.466985	3.759677	1.576964
6	-1.420833	4.532623	-2.443245
6	-2.411786	4.573815	-3.421167
8	-0.959363	2.117753	-0.017787
6	-4.014662	5.293018	-1.776597
6	2.019311	1.413893	1.950371
6	2.643111	-0.990743	2.100653
8	1.067670	1.788923	-0.811115
6	-3.023338	5.245148	-0.801063
6	3.565508	-2.031350	2.114245
6	-0.126745	6.218882	0.342058
6	-0.672619	4.824689	-0.009788
6	2.394186	2.730046	1.535022
6	4.440563	0.611609	2.017817
6	-3.710778	4.953759	-3.092751
6	0.722503	6.207791	1.629009
6	4.930450	-1.750696	2.085399
8	0.853218	1.111048	2.292456
6	5.365618	-0.426724	2.052220
6	1.889414	5.214922	1.619402
1	1.319018	4.176296	-0.849924
1	-0.978986	6.890628	0.520626
1	0.062818	5.971597	2.472091
1	3.219550	-3.060836	2.126702
1	-2.165098	4.310681	-4.445339
1	2.581521	5.429238	0.794884
1	-5.025332	5.585382	-1.507996
1	3.395761	2.915598	1.163223
1	0.544133	3.522036	2.113117
1	-3.267674	5.495621	0.229837
1	2.462316	5.359530	2.543571
1	-0.408518	4.244675	-2.709599
1	-1.197363	4.467587	0.887132
1	4.796325	1.635974	1.994013
1	5.651162	-2.563306	2.082411
1	6.427458	-0.202698	2.035610
1	1.110003	7.217171	1.810328
1	1.576724	-1.197091	2.107525
1	-4.481317	4.985172	-3.856919
7	1.197227	-1.058357	-0.832286
6	2.484387	-1.569015	-1.025835
6	3.500477	-0.602394	-1.097444
6	4.818465	-0.990425	-1.252661
6	5.170724	-2.335489	-1.342187
6	4.154329	-3.276461	-1.290880
6	2.815074	-2.919022	-1.147022
6	5.900359	0.046276	-1.337467

9	7.003909	-0.338499	-0.673728
6	4.510174	-4.734068	-1.268510
9	4.691844	-5.167482	-0.007139
6	0.052035	-1.618131	-0.357417
16	-0.154355	-3.231143	0.102091
7	-0.926513	-0.689018	-0.237390
6	-2.293312	-0.945429	0.164912
6	-2.754461	0.135318	1.163540
6	-4.047281	-0.252442	1.914018
6	-3.749943	-0.373969	3.416903
6	-3.315394	1.003558	3.940024
6	-2.130409	1.507909	3.092083
7	-1.684858	0.410088	2.179706
6	-1.323638	-0.804609	2.974155
6	-2.594568	-1.363347	3.667580
6	-2.856501	-2.794138	3.259219
6	-4.042931	-3.352735	3.032809
6	-3.254227	-0.927765	-1.019762
6	-4.184674	-1.983849	-1.265893
6	-5.078534	-1.816576	-2.365163
7	-5.067431	-0.724706	-3.181414
6	-4.185895	0.212191	-2.931044
6	-3.263138	0.159090	-1.858612
6	-6.034756	-2.827963	-2.626816
6	-6.116718	-3.953317	-1.847511
6	-5.220188	-4.119986	-0.760744
6	-4.273062	-3.157797	-0.482785
9	6.279068	0.266897	-2.607711
9	5.519503	1.227942	-0.832833
9	5.650412	-4.984930	-1.929965
9	3.553278	-5.500755	-1.807771
1	-2.869771	1.080023	0.628851
1	-4.816416	0.507780	1.752783
1	-4.434450	-1.194948	1.519244
1	-1.254058	1.782198	3.681109
1	-2.392933	2.348460	2.445786
1	-3.026234	0.930282	4.992245
1	-4.146098	1.710811	3.875908
1	-4.645360	-0.704358	3.949700
1	-2.397810	-1.369812	4.747697
1	-0.550822	-0.481318	3.672365
1	-0.875642	-1.526786	2.285749
1	-1.963079	-3.413182	3.170725
1	-4.121692	-4.400598	2.761142
1	-4.976230	-2.799469	3.101652
1	-2.307897	-1.922032	0.650977
1	-2.578261	0.991755	-1.705874
1	-3.597163	-3.345187	0.343866
1	-4.186839	1.079904	-3.587978
1	-6.704493	-2.678011	-3.467442
1	-6.861007	-4.708157	-2.071358
1	-0.720433	0.286444	-0.470267
1	1.153766	-0.038552	-0.912386
1	3.247728	0.449468	-0.985287
1	2.048976	-3.679884	-1.106473
1	6.208145	-2.636060	-1.438864
8	-5.232969	-5.203189	0.056710
6	-6.146497	-6.245171	-0.229738
1	-5.969344	-7.015269	0.521135
1	-7.185577	-5.903951	-0.152823
1	-5.973956	-6.669399	-1.225437
1	-0.820396	0.756515	1.718442
8	1.026166	6.361663	-1.789018
6	0.669587	6.881589	-0.759008
1	0.939460	7.938372	-0.543696

(2R,3S)_re-re-path-E

Number of imaginary frequencies : 1
The smallest frequency is : -418.5786

Electronic energy= -3905.2946342
Zero-point correction= 1.056743
Thermal correction to Energy= 1.120748
Thermal correction to Enthalpy= 1.121693
Thermal correction to Gibbs Free Energy= 0.955284
Sum of electronic and zero-point Energies= -3904.237891
Sum of electronic and thermal Energies= -3904.173886
Sum of electronic and thermal Enthalpies= -3904.172942
Sum of electronic and thermal Free Energies= -3904.339350

.....
Cartesian Coordinates

.....
6 1.005797 -3.062980 -4.821306
6 1.982430 -4.170652 -4.415211
6 3.263519 -3.403418 -4.089410
7 2.783641 -2.055111 -3.673853
6 1.309371 -1.970721 -3.794058
6 3.578125 -1.141836 -3.249059
6 3.146911 0.175014 -2.722986
8 0.198051 1.891715 0.047528
8 0.326987 0.408084 -1.566286
1 1.013833 -0.968694 -4.105386
1 -0.041490 -3.358393 -4.758061
1 1.216481 -2.708707 -5.835450
1 3.847549 -3.833999 -3.274849
1 3.898442 -3.270547 -4.969267
1 2.134991 0.374194 -3.080962
6 4.084237 1.317380 -3.134477
1 5.121410 1.042900 -2.909178
6 2.989040 0.069259 -1.167908
1 2.348100 -0.801341 -0.993928
1 2.582525 1.810947 0.183671
6 4.301041 -0.189558 -0.448563
6 4.770076 -1.509701 -0.406698
6 5.053809 0.798801 0.190521
6 5.974252 -1.826237 0.213783
1 4.147816 -2.300424 -0.826918
6 6.252424 0.482098 0.829338
1 4.699947 1.824184 0.229042
6 6.722366 -0.826844 0.833414
1 6.308426 -2.858055 0.250089
1 6.809752 1.264961 1.334398
1 7.650952 -1.074422 1.337871
7 0.871470 1.158938 -0.688788
6 2.236885 1.288693 -0.698257
7 0.403743 -1.436358 0.940774
6 1.513270 -1.186713 1.763979
6 1.821252 0.096786 2.228157
6 3.023947 0.306695 2.890212
6 3.922379 -0.731138 3.128610
6 3.593319 -2.000100 2.674293
6 2.403600 -2.234751 1.991071
6 3.376881 1.706918 3.302144
9 2.700312 2.110613 4.384324
6 4.518797 -3.155354 2.918211
9 4.120440 -3.908913 3.955869
6 -0.874467 -0.989191 1.095854
16 -1.464245 -0.250352 2.496024
7 -1.615499 -1.227369 -0.003478
6 -3.028666 -0.961458 -0.154985
6 -3.224816 -0.253547 -1.508722
6 -4.674871 0.190554 -1.798659
6 -4.719548 1.715138 -1.987422
6 -3.849714 2.091755 -3.197352
6 -2.437262 1.501292 -3.009460
7 -2.332469 0.949635 -1.620659

6	-2.648789	2.028528	-0.627722
6	-4.140066	2.423657	-0.747931
6	-4.885214	2.190951	0.544758
6	-6.148844	1.793101	0.671528
6	-3.842160	-2.253430	-0.154128
6	-5.036783	-2.417928	0.616201
6	-5.739568	-3.651131	0.468740
7	-5.317134	-4.666328	-0.336978
6	-4.204005	-4.484085	-1.002320
6	-3.435115	-3.296345	-0.949629
6	-6.942384	-3.844799	1.189300
6	-7.440791	-2.876467	2.022589
6	-6.732226	-1.658372	2.180280
6	-5.553521	-1.441079	1.497937
9	4.683866	1.834241	3.579683
9	3.098224	2.596029	2.324646
9	5.772102	-2.757700	3.182634
9	4.576320	-3.977152	1.853675
1	-2.855026	-0.935167	-2.282306
1	-5.042307	-0.305814	-2.701416
1	-5.325991	-0.110374	-0.974899
1	-1.645698	2.246641	-3.099586
1	-2.235812	0.667426	-3.686312
1	-3.788443	3.180562	-3.287389
1	-4.296663	1.708213	-4.118563
1	-5.750358	2.037800	-2.157731
1	-4.166197	3.504610	-0.941267
1	-1.974290	2.849728	-0.878192
1	-2.374522	1.655035	0.362395
1	-4.310745	2.404279	1.447387
1	-6.600243	1.665852	1.650619
1	-6.777434	1.563318	-0.185532
1	-3.335175	-0.312255	0.667288
1	-2.523425	-3.224634	-1.539601
1	-5.042229	-0.501780	1.668286
1	-3.872572	-5.305607	-1.634993
1	-7.456451	-4.791057	1.055973
1	-8.365751	-3.052735	2.558251
1	-1.152157	-1.632469	-0.831005
1	0.611348	-2.016072	0.114830
1	1.145414	0.920793	2.016688
1	2.170579	-3.225774	1.612935
1	4.868007	-0.546147	3.623931
8	-7.151845	-0.651760	2.989610
6	-8.328921	-0.852198	3.748042
1	-8.466790	0.056924	4.333911
1	-9.204517	-0.998848	3.104517
1	-8.229139	-1.705420	4.428879
1	-1.324152	0.668572	-1.479271
6	0.608484	-2.297929	-2.438715
8	1.330116	-2.668130	-1.487660
8	-0.634193	-2.178497	-2.489258
1	4.015742	1.442137	-4.220356
1	2.148164	-4.910904	-5.198637
1	1.617280	-4.681936	-3.521097
6	3.737560	2.655161	-2.439848
1	3.971172	3.473482	-3.129272
1	4.371365	2.815253	-1.563119
6	2.280666	2.787328	-2.038522
6	1.768994	3.914041	-1.391863
1	1.569484	2.355509	-2.748427
1	2.397716	4.495904	-0.724501
6	0.376066	4.217102	-1.491265
8	-0.389822	3.746813	-2.358385
6	-0.201584	5.207313	-0.512175
6	0.308146	5.354833	0.780661
6	-1.320627	5.953379	-0.892515
6	-0.276289	6.253958	1.668229
1	1.139274	4.734163	1.101924
6	-1.899411	6.859325	-0.009996

1	-1.720671	5.804810	-1.891225
6	-1.374890	7.013786	1.272632
1	0.119489	6.353511	2.674333
1	-2.760953	7.444699	-0.317713
1	-1.827377	7.716713	1.965643
1	4.638590	-1.398961	-3.239799

(2R,3S)_re-re-path-F

Number of imaginary frequencies : 1
The smallest frequency is : -365.5154

Electronic energy=	-3905.3027207
Zero-point correction=	1.057440
Thermal correction to Energy=	1.121291
Thermal correction to Enthalpy=	1.122236
Thermal correction to Gibbs Free Energy=	0.952340
Sum of electronic and zero-point Energies=	-3904.245281
Sum of electronic and thermal Energies=	-3904.181429
Sum of electronic and thermal Enthalpies=	-3904.180485
Sum of electronic and thermal Free Energies=	-3904.350380

Cartesian Coordinates

7	-1.710626	-0.475847	-0.273472
6	-3.041354	-0.485029	-0.040500
6	-0.071489	2.924458	2.141042
6	-3.473272	-2.922863	-0.660167
6	-3.037665	0.580260	1.750645
6	-3.099639	-2.704248	-1.987765
6	-2.933613	-3.774068	-2.865284
8	-0.988966	-1.446660	0.124296
6	-3.504953	-5.309654	-1.104496
6	-0.861003	1.649564	2.039843
6	1.322882	2.830539	2.167334
8	-1.188577	0.549586	-0.775600
6	-3.670966	-4.238616	-0.232409
6	2.112689	3.974887	2.179182
6	-5.179762	-1.553157	0.658896
6	-3.682776	-1.788387	0.338419
6	-2.235243	1.708776	1.655985
6	-0.665638	4.191064	2.184160
6	-3.134500	-5.079961	-2.427620
6	-5.341531	-0.594910	1.857184
6	1.512268	5.232431	2.199352
8	-0.273862	0.583377	2.336409
6	0.122224	5.337208	2.221571
6	-4.541886	0.716601	1.842365
1	-3.575415	0.256708	-0.622881
1	-5.575839	-2.532074	0.952854
1	-5.058534	-1.156632	2.756756
1	3.194800	3.885706	2.150973
1	-2.643754	-3.583001	-3.894265
1	-4.896268	1.380194	1.049812
1	-3.659380	-6.324173	-0.749748
1	-2.657603	2.643089	1.302337
1	-2.587360	-0.258873	2.287779
1	-3.950561	-4.425378	0.802883
1	-4.753660	1.226282	2.791439
1	-2.926765	-1.690619	-2.341072
1	-3.219939	-2.123509	1.277439
1	-1.745752	4.289393	2.200680
1	2.127100	6.127720	2.194948
1	-0.350038	6.313877	2.250364
1	-6.397881	-0.332202	1.976974
1	1.776990	1.844536	2.139200
1	-3.001261	-5.912109	-3.111562

7	1.526971	1.471233	-0.771156
6	1.708573	2.843022	-0.974879
6	0.529585	3.605212	-0.975084
6	0.589571	4.977403	-1.133866
6	1.807674	5.633308	-1.301523
6	2.960480	4.864362	-1.323559
6	2.934192	3.478931	-1.173320
6	-0.671083	5.792053	-1.127298
9	-0.531754	6.906545	-0.389117
6	4.293194	5.549798	-1.401267
9	4.763903	5.839785	-0.174376
6	2.372139	0.492499	-0.349417
16	4.006858	0.682280	0.033834
7	1.719672	-0.686160	-0.210025
6	2.329341	-1.952388	0.140388
6	1.445622	-2.692249	1.163194
6	2.181508	-3.856147	1.861400
6	2.301681	-3.556029	3.364162
6	0.885827	-3.495155	3.959685
6	0.051688	-2.472264	3.162504
7	0.953775	-1.744945	2.217843
6	2.069880	-1.096050	2.975126
6	2.976579	-2.190055	3.595953
6	4.400077	-2.074388	3.102307
6	5.227668	-3.079549	2.826848
6	2.504606	-2.856376	-1.075477
6	3.757344	-3.454908	-1.415454
6	3.772328	-4.320217	-2.550441
7	2.671435	-4.584243	-3.309286
6	1.546968	-4.004503	-2.969174
6	1.412897	-3.136188	-1.859750
6	4.987547	-4.949283	-2.913685
6	6.139059	-4.747651	-2.197207
6	6.121743	-3.883519	-1.071867
6	4.957099	-3.247967	-0.696747
9	-1.007219	6.196760	-2.363807
9	-1.717680	5.114029	-0.637661
9	4.223419	6.710613	-2.071096
9	5.219433	4.791690	-2.002886
1	0.538551	-3.036074	0.662329
1	1.629645	-4.788905	1.717021
1	3.167723	-3.989818	1.410583
1	-0.411742	-1.706438	3.786865
1	-0.723217	-2.935232	2.547101
1	0.934270	-3.208365	5.013992
1	0.414111	-4.479618	3.907228
1	2.875357	-4.344215	3.858396
1	2.998331	-2.014991	4.679552
1	1.590576	-0.456662	3.716733
1	2.612764	-0.451481	2.278172
1	4.764588	-1.052572	2.992527
1	6.243699	-2.889808	2.495163
1	4.933719	-4.122807	2.913214
1	3.297765	-1.729641	0.590253
1	0.437901	-2.706524	-1.635700
1	5.003103	-2.578585	0.154625
1	0.674750	-4.225405	-3.581409
1	4.973450	-5.599797	-3.781964
1	7.052959	-5.245356	-2.499048
1	0.716822	-0.725218	-0.408690
1	0.545887	1.181080	-0.809146
1	-0.425032	3.112273	-0.806834
1	3.853216	2.911597	-1.192044
1	1.852077	6.712056	-1.405119
8	7.215046	-3.630068	-0.309255
6	8.446428	-4.212273	-0.692848
1	9.184090	-3.855402	0.026091
1	8.405589	-5.307080	-0.651058
1	8.745262	-3.895681	-1.698765
1	0.381664	-0.987148	1.793328

6	-9.202989	-0.768297	0.549832
6	-9.443362	-0.519785	-0.941757
6	-8.032810	-0.660735	-1.510976
7	-7.335002	-1.655915	-0.681844
6	-8.167157	-1.894151	0.522234
6	-5.980129	-1.152135	-0.582824
1	-7.570130	-1.955280	1.432116
1	-10.108625	-1.040445	1.095608
1	-8.781197	0.131880	1.014404
1	-10.095959	-1.289811	-1.362985
1	-9.862276	0.462342	-1.169802
1	-8.012734	-0.913349	-2.577392
1	-5.446773	-1.470833	-1.487306
6	-7.226717	0.620332	-1.295033
8	-6.068439	0.301538	-0.686247
8	-7.539585	1.745400	-1.573774
1	-8.669157	-2.860453	0.397640

[12-13]TS-Nitro-H-bond with cinchona-thiourea (Fig. S12)

Number of imaginary frequencies : 1
The smallest frequency is : -894.9844

Electronic energy=	-3905.3051756
Zero-point correction=	1.054449
Thermal correction to Energy=	1.118264
Thermal correction to Enthalpy=	1.119208
Thermal correction to Gibbs Free Energy=	0.949251
Sum of electronic and zero-point Energies=	-3904.250726
Sum of electronic and thermal Energies=	-3904.186912
Sum of electronic and thermal Enthalpies=	-3904.185968
Sum of electronic and thermal Free Energies=	-3904.355924

Cartesian Coordinates

7	-1.488509	-1.747398	-0.542727
6	-2.621459	-1.379448	0.369006
6	0.073250	1.529499	3.256074
6	-4.121446	-2.697625	-1.232361
6	-2.054310	-1.329437	1.796316
6	-4.176173	-1.709775	-2.218962
6	-4.562061	-2.029374	-3.517994
8	-1.012744	-2.860433	-0.437728
6	-4.829192	-4.335403	-2.879103
6	-0.491163	0.130474	3.147568
6	-0.362050	2.575582	2.438757
8	-1.066581	-0.900023	-1.322106
6	-4.437381	-4.013529	-1.583174
6	0.116862	3.869783	2.630326
6	-4.929946	-2.018265	1.148499
6	-3.751733	-2.405190	0.210104
6	-0.863089	-0.372659	1.857932
6	0.991723	1.806322	4.273759
6	-4.896104	-3.339807	-3.850478
6	-4.390172	-1.947675	2.590376
6	1.062703	4.126956	3.619157
8	-0.537268	-0.551749	4.190993
6	1.499666	3.089085	4.442462
6	-3.220118	-0.972370	2.733041
1	-2.904147	-0.377669	0.038913
1	-5.673207	-2.821957	1.087008
1	-4.052185	-2.953066	2.870438
1	-0.243845	4.679030	2.003782
1	-4.605446	-1.249373	-4.271800
1	-3.539848	0.059370	2.532963
1	-5.074139	-5.362584	-3.130565
1	-0.857703	0.375104	1.062991

1	-1.759664	-2.362207	2.034546
1	-4.380123	-4.792641	-0.826248
1	-2.838972	-0.984012	3.756409
1	-3.942072	-0.677600	-1.976408
1	-3.361245	-3.341969	0.625828
1	1.286899	0.997941	4.935962
1	1.450108	5.132708	3.749229
1	2.228096	3.285103	5.223381
1	-5.197789	-1.679174	3.273910
1	-1.107314	2.387559	1.671367
1	-5.197234	-3.584955	-4.864061
7	1.045572	1.515197	-0.844709
6	1.018405	2.908733	-1.040338
6	1.635578	3.807333	-0.164282
6	1.520384	5.169963	-0.401152
6	0.793768	5.672149	-1.477747
6	0.171440	4.767302	-2.325481
6	0.281985	3.395362	-2.119209
6	2.113400	6.139395	0.582261
9	2.651672	7.203393	-0.031313
6	-0.671990	5.253138	-3.468794
9	-1.981371	5.204259	-3.169525
6	2.083229	0.724932	-0.428873
16	3.604084	1.291613	0.011583
7	1.741366	-0.583166	-0.407267
6	2.652031	-1.683341	-0.152918
6	1.987030	-2.715558	0.772745
6	3.003746	-3.781511	1.255356
6	3.176002	-3.670791	2.777204
6	1.836260	-4.020440	3.439447
6	0.731099	-3.154453	2.799732
7	1.348468	-2.076074	1.964399
6	2.335635	-1.319363	2.789741
6	3.533851	-2.227511	3.178401
6	4.846364	-1.706603	2.644363
6	5.868703	-2.439749	2.209643
6	3.063852	-2.364632	-1.455838
6	4.429740	-2.486569	-1.862614
6	4.684832	-3.186920	-3.079812
7	3.701285	-3.707364	-3.866880
6	2.462451	-3.549237	-3.473111
6	2.095021	-2.892764	-2.273361
6	6.024651	-3.355163	-3.504661
6	7.073564	-2.858362	-2.774237
6	6.815688	-2.149257	-1.573363
6	5.521856	-1.964935	-1.133794
9	1.172890	6.621035	1.420540
9	3.061197	5.580529	1.340909
9	-0.502575	4.498084	-4.564446
9	-0.390365	6.518860	-3.800487
1	1.163010	-3.185493	0.229489
1	2.649424	-4.784020	0.998136
1	3.960371	-3.636216	0.746686
1	0.099740	-2.648659	3.533829
1	0.095300	-3.738034	2.127415
1	1.891185	-3.835346	4.516538
1	1.608622	-5.080631	3.299154
1	3.954340	-4.359116	3.117760
1	3.608081	-2.202298	4.273733
1	1.784034	-0.983028	3.668663
1	2.644895	-0.435209	2.223008
1	4.948992	-0.620513	2.654842
1	6.785592	-1.972594	1.863147
1	5.833730	-3.525874	2.171249
1	3.524353	-1.259328	0.344754
1	1.039637	-2.821019	-2.018526
1	5.377842	-1.393083	-0.225554
1	1.686422	-3.962559	-4.114370
1	6.191136	-3.891441	-4.433128
1	8.088483	-3.003411	-3.124596

1	0.839650	-0.836031	-0.802571
1	0.231405	1.027772	-1.206301
1	2.183335	3.445245	0.694339
1	-0.189791	2.702057	-2.810136
1	0.717990	6.740132	-1.650387
8	7.792751	-1.616404	-0.797132
6	9.132825	-1.726328	-1.238765
1	9.737492	-1.208553	-0.494010
1	9.454366	-2.772763	-1.296157
1	9.275512	-1.245894	-2.213356
6	-8.603463	0.171176	-1.010657
6	-8.330622	-1.209450	-1.637151
6	-7.281115	-1.818566	-0.713150
7	-6.403389	-0.664217	-0.436918
6	-7.336619	0.447196	-0.186571
6	-5.630151	-0.710373	0.782462
1	-9.472462	0.156419	-0.347578
1	-8.772634	0.941820	-1.763478
1	-9.227083	-1.827478	-1.713331
1	-7.902226	-1.094721	-2.636709
1	-7.760300	-2.198373	0.205270
1	-6.716300	-2.628879	-1.178032
1	0.447147	-1.299930	1.732427
1	-4.912256	0.119899	0.749658
1	-6.867501	1.413878	-0.406164
6	-7.560818	0.364870	1.325115
8	-8.451562	0.836847	1.976221
8	-6.563613	-0.374156	1.855696

[11-13]_{H2O}TS-Keto-enol (Figure S12)

Number of imaginary frequencies : 1
The smallest frequency is : -1749.8376

Electronic energy= -3981.683788
Zero-point correction= 1.076950
Thermal correction to Energy= 1.143027
Thermal correction to Enthalpy= 1.143971
Thermal correction to Gibbs Free Energy= 0.968012
Sum of electronic and zero-point Energies= -3980.606838
Sum of electronic and thermal Energies= -3980.540761
Sum of electronic and thermal Enthalpies= -3980.539817
Sum of electronic and thermal Free Energies= -3980.715776

Cartesian Coordinates

7	-1.688515	-0.100035	0.547845
6	-3.137185	-0.340370	0.860496
6	-0.357616	2.257906	2.693308
6	-3.138351	-2.162957	-0.967990
6	-3.304520	-0.130241	2.384350
6	-2.835479	-1.254680	-1.984558
6	-2.478680	-1.703670	-3.253235
8	-0.871462	-0.901649	0.956878
6	-2.726235	-3.982081	-2.520621
6	-1.313286	1.205297	3.127948
6	1.005892	1.935389	2.687593
8	-1.404364	0.928609	-0.046466
6	-3.069528	-3.529677	-1.250754
6	1.945995	2.890815	2.316843
6	-5.056473	-1.941725	0.757595
6	-3.549461	-1.750877	0.436340
6	-2.706566	1.207777	2.828276
6	-0.767904	3.540682	2.311211
6	-2.430425	-3.067242	-3.528410
6	-5.298411	-1.691609	2.254834
6	1.537341	4.181869	1.984278

8	-0.841485	0.292515	3.895491
6	0.180650	4.503604	1.982110
6	-4.787854	-0.322757	2.718786
1	-3.657455	0.443737	0.304176
1	-5.298613	-2.987847	0.528457
1	-4.781491	-2.470938	2.827047
1	2.999434	2.627255	2.285984
1	-2.250541	-0.982628	-4.031563
1	-5.368731	0.491626	2.265146
1	-2.683053	-5.048028	-2.721373
1	-3.071602	2.060360	2.259149
1	-2.738738	-0.937132	2.868410
1	-3.284717	-4.248629	-0.462809
1	-4.914663	-0.231288	3.801168
1	-2.896885	-0.185102	-1.807353
1	-3.024454	-2.430617	1.120982
1	-1.821558	3.801955	2.296602
1	2.271775	4.929583	1.698419
1	-0.141543	5.500496	1.700374
1	-6.367041	-1.792225	2.464562
1	1.305021	0.923311	2.948031
1	-2.161785	-3.414572	-4.521073
7	1.364800	1.686765	-0.784169
6	1.370218	3.040070	-1.113969
6	0.113034	3.639728	-1.256881
6	0.006154	5.009009	-1.444885
6	1.133415	5.818789	-1.516807
6	2.376500	5.206723	-1.398945
6	2.516293	3.838301	-1.197641
6	-1.363620	5.619554	-1.465107
9	-2.250680	4.846250	-2.107546
6	3.606869	6.066515	-1.358055
9	3.880105	6.455617	-0.096461
6	2.354264	0.739189	-0.786663
16	3.827736	0.857362	-1.585806
7	1.982840	-0.346881	-0.081209
6	2.776694	-1.550813	0.059471
6	2.229140	-2.322088	1.277590
6	3.114981	-3.534183	1.657897
6	3.191109	-3.594499	3.191161
6	1.763394	-3.521450	3.752451
6	1.188239	-2.119104	3.413801
7	2.035623	-1.427133	2.430975
6	3.325976	-1.110977	3.054081
6	3.970815	-2.366469	3.719198
6	5.447353	-2.440518	3.463941
6	6.378047	-2.477053	4.413572
6	2.694408	-2.434184	-1.177884
6	3.835423	-3.092865	-1.736400
6	3.605055	-3.970889	-2.836730
7	2.373339	-4.191502	-3.378772
6	1.359806	-3.549043	-2.853580
6	1.470466	-2.665679	-1.753765
6	4.704452	-4.653596	-3.410894
6	5.979622	-4.484859	-2.936240
6	6.209426	-3.600858	-1.851415
6	5.159757	-2.920899	-1.271556
9	-1.841512	5.787802	-0.214839
9	-1.375348	6.824369	-2.048858
9	3.462060	7.185704	-2.081946
9	4.691789	5.427978	-1.809675
1	1.223725	-2.669772	1.005006
1	2.692359	-4.460059	1.255634
1	4.119055	-3.436674	1.230519
1	1.135807	-1.480718	4.300833
1	0.174768	-2.179160	3.006099
1	1.768935	-3.689877	4.834223
1	1.152890	-4.312942	3.303006
1	3.690281	-4.513664	3.511618
1	3.818680	-2.318853	4.805494

1	3.169252	-0.322340	3.797871
1	3.989101	-0.693675	2.287484
1	5.760295	-2.456685	2.418068
1	7.435602	-2.528765	4.173882
1	6.112193	-2.454810	5.468126
1	3.816130	-1.259716	0.235198
1	0.578974	-2.173397	-1.372580
1	5.393500	-2.235609	-0.464888
1	0.381101	-3.723793	-3.296705
1	4.499152	-5.314994	-4.246424
1	6.800920	-5.018149	-3.399557
1	1.231835	-0.253489	0.599665
1	0.461730	1.356509	-0.452749
1	-0.784464	3.031618	-1.191539
1	3.497754	3.396937	-1.088165
1	1.046466	6.888824	-1.665823
8	7.439439	-3.367165	-1.327010
6	8.543579	-4.046523	-1.891457
1	9.417775	-3.722208	-1.326317
1	8.439796	-5.133933	-1.796324
1	8.682970	-3.784347	-2.946770
6	-9.164259	-0.635411	-1.218970
6	-9.042534	-2.124419	-1.553388
6	-7.639329	-2.457270	-1.037293
7	-7.396243	-1.576597	0.118312
6	-8.475154	-0.561265	0.145907
6	-6.040887	-1.085438	-0.055063
1	-8.065737	0.426302	0.377102
1	-10.196929	-0.282517	-1.193090
1	-8.616709	-0.038560	-1.957539
1	-9.787333	-2.706540	-1.003080
1	-9.133160	-2.353514	-2.617153
1	-7.510237	-3.519002	-0.803329
1	-5.979267	-0.029452	0.223259
6	-6.576199	-2.037002	-2.052028
8	-5.740503	-1.158004	-1.461069
8	-6.481866	-2.368479	-3.200255
1	-9.180457	-0.823746	0.942301
1	-3.022463	0.962424	4.260884
8	-2.833447	0.246228	5.187520
1	-1.798366	0.062865	4.689825
1	-2.710653	0.764273	5.995685

Stationary Points Relevant to Tables S15-S16: [8-9][‡] and [10-11][‡]

Catalyst-Methyl

1-Michael_si-si-catalyst-Methyl-TS

Number of imaginary frequencies : 1

The smallest frequency is : -312.2527

Electronic energy : =-3039.739024

Zero-point correction= 0.990055

Thermal correction to Energy= 1.046095

Thermal correction to Enthalpy= 1.047039

Thermal correction to Gibbs Free Energy= 0.896620

Sum of electronic and zero-point Energies= -3038.748969

Sum of electronic and thermal Energies= -3038.692929

Sum of electronic and thermal Enthalpies= -3038.691985

Sum of electronic and thermal Free Energies= -3038.842404

Cartesian Coordinates

6	-2.460505	-1.759509	4.013344

6	-2.881619	-3.222007	3.828075
6	-4.048134	-3.137325	2.836098
7	-3.821702	-1.866672	2.128915
6	-2.605270	-1.201579	2.589534
6	-4.708704	-1.341654	1.290894
6	-4.544675	-0.215072	0.499773
8	-1.701558	1.635023	-2.320108
8	-1.610645	0.639164	-0.380744
1	-2.731632	-0.116311	2.562813
1	-1.442389	-1.640795	4.386434
1	-3.149236	-1.239755	4.687049
1	-4.059825	-3.970628	2.128089
1	-5.016987	-3.095775	3.346670
1	-3.688176	0.427419	0.692550
6	-5.770535	0.427596	-0.114664
1	-6.237393	-0.251053	-0.842383
6	-3.413979	-1.184676	-1.104043
1	-2.692916	-1.472766	-0.347232
1	-3.428815	0.040364	-2.946911
6	-4.294358	-2.277121	-1.557540
6	-4.131839	-3.534433	-0.955534
6	-5.269144	-2.113407	-2.547923
6	-4.930207	-4.605007	-1.339621
1	-3.362197	-3.644409	-0.192145
6	-6.071604	-3.187294	-2.925158
1	-5.402457	-1.144961	-3.022803
6	-5.905318	-4.431945	-2.322692
1	-4.791122	-5.577394	-0.877054
1	-6.826292	-3.051970	-3.693412
1	-6.529763	-5.267920	-2.621637
7	-2.068595	0.726621	-1.549185
6	-3.020749	-0.167951	-1.969514
7	-0.191627	-2.400776	-1.633585
6	0.995830	-1.790772	-1.527686
16	1.981745	-1.447808	-2.868903
7	1.317939	-1.448262	-0.252270
6	2.517225	-0.750961	0.157187
6	2.133328	0.407336	1.101939
6	3.261266	1.432548	1.342528
6	2.828806	2.802440	0.795577
6	1.590932	3.281832	1.573928
6	0.503682	2.192098	1.511529
7	0.944430	1.139283	0.547810
6	1.211094	1.748084	-0.792821
6	2.438303	2.687176	-0.690676
6	3.544087	2.257260	-1.625810
6	4.852459	2.335623	-1.394490
6	3.490832	-1.663592	0.893760
6	4.878374	-1.746183	0.559603
6	5.689234	-2.600093	1.366204
7	5.203572	-3.334192	2.407039
6	3.923131	-3.240362	2.668659
6	3.029429	-2.415521	1.945574
6	7.072990	-2.696186	1.082440
6	7.643157	-1.986462	0.057068
6	6.833441	-1.142571	-0.746311
6	5.480901	-1.033414	-0.502908
1	1.768226	-0.019444	2.036971
1	3.470144	1.513206	2.412984
1	4.179515	1.094859	0.855992
1	-0.452813	2.561661	1.136610
1	0.334835	1.682214	2.461640
1	1.212543	4.213491	1.140831
1	1.854340	3.484282	2.615349
1	3.639825	3.525908	0.913932
1	2.106976	3.682528	-1.014531
1	0.290178	2.260362	-1.074683
1	1.364579	0.933407	-1.505839
1	3.205023	1.864788	-2.585166
1	5.571606	2.013195	-2.140918

1	5.259416	2.711880	-0.458982
1	2.981591	-0.355090	-0.747785
1	1.980155	-2.379188	2.232336
1	4.902234	-0.394103	-1.159868
1	3.548573	-3.835133	3.499808
1	7.667919	-3.352814	1.708848
1	8.705193	-2.080886	-0.135566
1	0.657014	-1.680483	0.493666
1	-0.700325	-2.582969	-0.765138
8	7.319210	-0.406690	-1.778908
6	8.692677	-0.525845	-2.094653
1	8.860929	0.122324	-2.955076
1	9.328651	-0.192136	-1.266102
1	8.955974	-1.554809	-2.365300
1	0.165271	0.470101	0.453388
6	-1.351543	-1.584314	1.772731
8	-1.429247	-2.560935	0.988897
8	-0.327112	-0.903137	2.027404
1	-6.524956	0.602245	0.663450
1	-3.174668	-3.707651	4.760374
1	-2.060375	-3.789181	3.382963
6	-5.478978	1.775649	-0.797833
1	-6.437448	2.217907	-1.097724
1	-4.890084	1.631384	-1.707692
6	-4.761288	2.724142	0.111467
6	-3.580957	3.282931	-0.175029
1	-5.224209	2.956028	1.071917
1	-3.100606	3.068940	-1.124448
6	-2.928768	4.211313	0.783323
8	-3.382486	4.396203	1.901796
6	-1.702990	4.962146	0.339907
6	-1.031791	4.691857	-0.858559
6	-1.240703	5.990416	1.169145
6	0.069731	5.462890	-1.227987
1	-1.348084	3.879214	-1.506476
6	-0.142533	6.756865	0.798347
1	-1.770250	6.180393	2.096959
6	0.511531	6.497902	-0.406359
1	0.575600	5.258352	-2.166921
1	0.200452	7.560330	1.442551
1	1.364139	7.100960	-0.703380
1	-5.623460	-1.927794	1.184833
6	-0.761819	-2.840723	-2.888249
1	-0.121730	-3.581985	-3.376135
1	-1.734441	-3.287942	-2.674588
1	-0.896182	-1.999255	-3.573859

1-Michael-*si-re*_path-A-catalyst-Methyl-TS

Number of imaginary frequencies : 1

The smallest frequency is : -313.6403

Electronic energy : =-3039.7327508

Zero-point correction= 0.989287

Thermal correction to Energy= 1.045128

Thermal correction to Enthalpy= 1.046072

Thermal correction to Gibbs Free Energy= 0.896064

Sum of electronic and zero-point Energies= -3038.743463

Sum of electronic and thermal Energies= -3038.687623

Sum of electronic and thermal Enthalpies= -3038.686678

Sum of electronic and thermal Free Energies= -3038.836687

Cartesian Coordinates

6	-2.523777	0.602445	3.529183
6	-3.053411	-0.683507	4.181927
6	-4.079852	-1.234961	3.171525

7	-3.863142	-0.444642	1.949663
6	-2.589782	0.275515	2.027442
6	-4.854379	-0.092681	1.140383
6	-4.705578	0.520702	-0.095765
8	-0.955991	-1.807703	-1.085677
8	-2.074777	-0.094845	-1.815555
1	-2.634683	1.157718	1.388822
1	-1.510896	0.857596	3.849174
1	-3.184595	1.449337	3.745549
1	-2.239710	-1.399937	4.299776
1	-3.503766	-0.499715	5.158931
1	-3.898791	-2.291012	2.961412
1	-5.116862	-1.105346	3.496296
1	-5.844355	-0.439642	1.442454
1	-3.717583	0.879607	-0.376320
6	-5.867141	1.262167	-0.698101
6	-5.918050	2.734608	-0.218322
1	-6.810540	0.770414	-0.433210
1	-5.795568	1.247810	-1.793851
1	-6.815785	3.210488	-0.629329
1	-5.998880	2.748894	0.873994
6	-4.706783	3.495490	-0.658007
6	-3.665309	3.807905	0.120823
1	-4.644446	3.766192	-1.712390
1	-3.665824	3.541705	1.174927
6	-2.481001	4.490877	-0.469295
8	-2.572396	5.102001	-1.521026
6	-1.144293	4.364788	0.205468
6	-0.920429	3.535229	1.307595
6	-0.060374	5.035867	-0.375727
6	0.368616	3.358483	1.805260
1	-1.737156	3.001671	1.779164
6	1.223227	4.871313	0.129023
1	-0.250090	5.669844	-1.235815
6	1.441822	4.021758	1.216426
1	0.533741	2.686292	2.640507
1	2.057277	5.395749	-0.327801
1	2.446335	3.876944	1.604349
6	-4.424329	-1.242318	-1.223556
1	-4.387728	-0.578294	-2.084478
1	-3.065323	-2.723449	-0.288584
6	-5.686626	-1.999649	-1.062906
6	-6.731981	-1.789682	-1.968296
6	-5.870520	-2.920917	-0.023072
6	-7.930257	-2.487838	-1.846323
1	-6.596390	-1.080152	-2.780361
6	-7.066610	-3.617753	0.098804
1	-5.073001	-3.084079	0.697684
6	-8.100405	-3.404486	-0.813330
1	-8.727860	-2.318425	-2.562698
1	-7.194201	-4.332080	0.906130
1	-9.032873	-3.951557	-0.717621
7	-2.040728	-1.223836	-1.271031
6	-3.208565	-1.826364	-0.869590
7	0.607545	-3.551962	0.689433
6	1.668208	-2.911590	0.184891
16	2.890782	-3.689367	-0.711187
7	1.667199	-1.579536	0.436117
6	2.708153	-0.662347	0.046209
6	2.087410	0.660775	-0.448014
6	3.095930	1.542462	-1.216052
6	2.664301	1.661590	-2.687237
6	1.335334	2.425561	-2.732238
6	0.350007	1.753889	-1.760008
7	0.905725	0.421399	-1.348512
6	1.251403	-0.400877	-2.547537
6	2.424749	0.270038	-3.307815
6	3.638903	-0.626685	-3.373885
6	4.910232	-0.234299	-3.344330
6	3.639197	-0.318545	1.207910

6	5.063266	-0.378539	1.111076
6	5.811713	0.042945	2.250850
7	5.236530	0.470295	3.410456
6	3.926935	0.483370	3.466548
6	3.087796	0.104288	2.392440
6	7.226032	0.022177	2.184452
6	7.882305	-0.392188	1.053834
6	7.134585	-0.821421	-0.072960
6	5.756817	-0.821529	-0.038461
1	1.655204	1.186806	0.407356
1	3.132535	2.542190	-0.770996
1	4.096077	1.109302	-1.138507
1	-0.628127	1.561341	-2.195833
1	0.220339	2.319834	-0.835093
1	0.933344	2.421966	-3.750042
1	1.481256	3.468415	-2.438254
1	3.426837	2.198233	-3.257737
1	2.088978	0.428731	-4.341185
1	0.331316	-0.459944	-3.131472
1	1.492300	-1.408041	-2.197245
1	3.422198	-1.690185	-3.478837
1	5.718163	-0.954889	-3.422682
1	5.200048	0.807875	-3.232582
1	3.271579	-1.130395	-0.763434
1	2.006352	0.147184	2.508411
1	5.229433	-1.192170	-0.909564
1	3.481532	0.817958	4.402054
1	7.773194	0.345406	3.064143
1	8.965567	-0.396901	1.033185
1	0.851475	-1.159799	0.904681
1	-0.141679	-2.967652	1.078332
8	7.706311	-1.249501	-1.228009
6	9.116612	-1.339842	-1.281779
1	9.354525	-1.736477	-2.269173
1	9.590281	-0.357547	-1.168055
1	9.506079	-2.023654	-0.518779
1	0.174967	-0.084955	-0.815915
6	-1.363331	-0.566999	1.636346
8	-1.412998	-1.793330	1.847077
8	-0.386265	0.111153	1.205333
6	0.289174	-4.927391	0.384283
1	1.122933	-5.583525	0.643017
1	-0.585002	-5.206706	0.975214
1	0.062689	-5.064346	-0.679315

1-Michael-*re-re*_path-A-Catalyst-Methyl-TS

Number of imaginary frequencies : 1

The smallest frequency is : -341.2404

Electronic energy : =-3039.7343039

Zero-point correction= 0.990362

Thermal correction to Energy= 1.045963

Thermal correction to Enthalpy= 1.046907

Thermal correction to Gibbs Free Energy= 0.897501

Sum of electronic and zero-point Energies= -3038.743942

Sum of electronic and thermal Energies= -3038.688341

Sum of electronic and thermal Enthalpies= -3038.687397

Sum of electronic and thermal Free Energies= -3038.836803

Cartesian Coordinates

6	2.287170	-4.131954	-2.496603
6	3.064196	-4.718843	-1.306318
6	3.869752	-3.533403	-0.736721
7	3.318446	-2.347826	-1.411379
6	2.055965	-2.673517	-2.081777

6	4.007630	-1.246538	-1.669515
6	5.185879	-0.885468	-1.018383
8	0.862450	-0.447677	0.965179
6	0.863250	-2.577559	-1.101139
8	-0.169130	-2.009882	-1.552437
8	1.013616	-3.106599	0.017756
8	2.110601	0.482250	-0.554332
1	1.895941	-1.988987	-2.916064
1	1.350180	-4.658336	-2.691227
1	2.894671	-4.155921	-3.406960
1	2.367320	-5.080124	-0.551558
1	3.719406	-5.538165	-1.608821
1	3.746110	-3.442581	0.344202
1	4.936503	-3.601533	-0.973968
1	3.523716	-0.558197	-2.356720
1	5.707839	-1.682166	-0.495946
6	6.082037	0.224796	-1.534694
6	5.618177	0.929047	-2.817127
1	7.072565	-0.199181	-1.732125
1	6.248688	0.973575	-0.746549
1	6.430326	1.580216	-3.166012
1	5.479145	0.180745	-3.604936
6	4.366537	1.757086	-2.710773
6	3.987693	2.514807	-1.677522
1	3.690778	1.743123	-3.566096
1	4.590422	2.612663	-0.779039
6	2.676453	3.215342	-1.728077
8	2.065189	3.348688	-2.778739
6	2.087353	3.751765	-0.458442
6	2.416579	3.239640	0.800590
6	1.119634	4.756878	-0.559548
6	1.770221	3.711892	1.938736
1	3.143036	2.440013	0.895843
6	0.494612	5.248176	0.581438
1	0.876350	5.146736	-1.543404
6	0.810567	4.716575	1.831123
1	2.009032	3.288295	2.908799
1	-0.246836	6.036816	0.496689
1	0.310067	5.085281	2.721050
6	4.354659	-0.121513	0.786303
1	4.329062	0.839534	0.284577
1	2.918659	-1.335831	1.949519
6	5.504472	-0.346935	1.695423
6	6.372449	0.707345	1.996857
6	5.739223	-1.600339	2.275810
6	7.443767	0.518091	2.866594
1	6.193931	1.688266	1.562887
6	6.806774	-1.788955	3.143701
1	5.082928	-2.432803	2.033952
6	7.663196	-0.729146	3.442555
1	8.103287	1.348803	3.096957
1	6.974150	-2.765412	3.587321
1	8.496696	-0.877795	4.121477
7	1.987435	-0.191414	0.498095
6	3.111235	-0.642503	1.145117
7	-0.719119	-2.436734	2.269718
6	-1.719743	-1.610145	1.938527
16	-2.661732	-0.770892	3.082938
7	-1.902295	-1.487766	0.601360
6	-2.922485	-0.682296	-0.023963
6	-2.332354	0.009380	-1.268506
6	-3.249186	1.111153	-1.842719
6	-2.534745	2.468567	-1.754343
6	-1.277866	2.415619	-2.635638
6	-0.425865	1.202240	-2.221885
7	-0.991314	0.622546	-0.962939
6	-1.058852	1.666627	0.104345
6	-2.087616	2.751159	-0.306472
6	-3.197031	2.878773	0.709903
6	-4.479601	3.128915	0.457366

6	-4.120847	-1.516408	-0.471659
6	-5.472808	-1.165007	-0.167157
6	-6.497664	-2.001962	-0.700758
7	-6.246409	-3.111113	-1.452859
6	-4.992607	-3.411087	-1.687155
6	-3.898538	-2.642606	-1.224016
6	-7.850858	-1.674472	-0.442803
6	-8.190272	-0.576079	0.304837
6	-7.168553	0.246103	0.845200
6	-5.841129	-0.048746	0.619311
1	-2.103033	-0.756289	-2.012362
1	-3.493205	0.890755	-2.885882
1	-4.189451	1.132120	-1.286669
1	0.606901	1.467118	-2.003513
1	-0.433385	0.391908	-2.953599
1	-0.687919	3.330409	-2.521595
1	-1.558156	2.333439	-3.689155
1	-3.199532	3.264791	-2.100188
1	-1.549461	3.707505	-0.314090
1	-0.042386	2.057720	0.197763
1	-1.314023	1.160135	1.039431
1	-2.880024	2.773059	1.748240
1	-5.201095	3.219792	1.263245
1	-4.867560	3.239864	-0.552355
1	-3.241296	0.068582	0.702282
1	-2.883851	-2.950557	-1.466919
1	-5.097504	0.589853	1.081217
1	-4.804793	-4.303546	-2.281535
1	-8.610899	-2.327431	-0.859360
1	-9.234627	-0.351397	0.485639
1	-1.244669	-1.956038	-0.035963
1	-0.093153	-2.715711	1.504586
8	-7.419802	1.346007	1.602640
6	-8.767007	1.651449	1.903677
1	-8.741084	2.537203	2.538829
1	-9.342029	1.878358	0.997967
1	-9.253456	0.834423	2.448874
1	-0.348986	-0.121466	-0.634087
6	-0.193692	-2.535106	3.611489
1	-0.978679	-2.823434	4.313652
1	0.584497	-3.301067	3.610179
1	0.235065	-1.584040	3.948882

1-Michael-*re-si*_path-A-catalyst-methyl-TS

Number of imaginary frequencies : 1

The smallest frequency is : -407.6445

Electronic energy : =-3039.7252189

Zero-point correction= 0.988898

Thermal correction to Energy= 1.044484

Thermal correction to Enthalpy= 1.045428

Thermal correction to Gibbs Free Energy= 0.896504

Sum of electronic and zero-point Energies= -3038.736321

Sum of electronic and thermal Energies= -3038.680735

Sum of electronic and thermal Enthalpies= -3038.679791

Sum of electronic and thermal Free Energies= -3038.828715

Cartesian Coordinates

6	1.419355	-4.382759	-2.539338
6	2.004317	-4.889142	-1.219611
6	3.309236	-4.103894	-1.096059
7	3.011881	-2.839734	-1.781176
6	1.712323	-2.888749	-2.471584
6	3.774531	-1.768920	-1.731058
6	4.995995	-1.652842	-1.051200

8	0.986693	-0.291854	1.286143
6	0.651911	-2.063581	-1.679006
8	0.922411	-0.852591	-1.534439
8	-0.374026	-2.679019	-1.305365
8	1.862035	-2.266770	1.003893
1	1.818529	-2.419557	-3.454656
1	0.348509	-4.561460	-2.623588
1	1.937804	-4.834323	-3.392135
1	1.333138	-4.608488	-0.403260
1	2.169233	-5.967556	-1.196099
1	3.580956	-3.904950	-0.058397
1	4.145827	-4.600275	-1.604201
1	3.339790	-0.903664	-2.227113
1	5.449153	-2.595736	-0.749812
6	6.014953	-0.642046	-1.547192
6	5.469405	0.646996	-2.177786
1	6.655014	-1.132917	-2.291882
1	6.683585	-0.363354	-0.723094
1	6.334491	1.200571	-2.567179
1	4.822106	0.443067	-3.037419
6	4.784438	1.531408	-1.188044
6	3.649286	2.214327	-1.370795
1	5.297872	1.660986	-0.235811
1	3.095514	2.150837	-2.304096
6	3.151568	3.096365	-0.283992
8	3.496268	2.930053	0.878047
6	2.224330	4.224553	-0.626300
6	1.533508	4.850364	0.418241
6	2.070475	4.695186	-1.933890
6	0.699048	5.931387	0.158021
1	1.676687	4.480807	1.428834
6	1.244432	5.786775	-2.191010
1	2.615151	4.233060	-2.750990
6	0.558142	6.403668	-1.147842
1	0.166591	6.413555	0.971806
1	1.140467	6.158399	-3.205262
1	-0.085815	7.253582	-1.351446
6	4.365088	-1.236935	0.985003
1	4.163624	-2.293378	1.122639
1	3.205938	0.641452	1.180717
6	5.671697	-0.798291	1.527104
6	6.703602	-1.737820	1.656425
6	5.908049	0.516381	1.950306
6	7.941882	-1.375577	2.172108
1	6.525919	-2.766087	1.349398
6	7.150485	0.880257	2.461973
1	5.116661	1.258699	1.891763
6	8.171877	-0.059909	2.570863
1	8.725875	-2.120072	2.268791
1	7.315366	1.902955	2.786589
1	9.137923	0.227814	2.973543
7	1.993005	-1.019083	1.120610
6	3.224746	-0.435919	1.114482
7	-0.723704	-2.553532	2.308766
6	-1.777769	-1.779661	2.001684
16	-2.879487	-1.203885	3.164253
7	-1.865484	-1.488590	0.682778
6	-2.858840	-0.621083	0.101425
6	-2.176909	0.309014	-0.925118
6	-3.074612	1.491813	-1.351754
6	-2.444417	2.813849	-0.882015
6	-1.110630	3.004083	-1.615310
6	-0.254425	1.744210	-1.407187
7	-0.896670	0.874070	-0.372502
6	-1.110636	1.646510	0.888249
6	-2.138170	2.779680	0.628570
6	-3.338637	2.666297	1.536545
6	-4.600172	2.941839	1.215198
6	-3.974637	-1.386758	-0.608773
6	-5.361871	-1.110843	-0.392115

6	-6.302397	-1.841656	-1.177787
7	-5.943429	-2.794275	-2.084907
6	-4.664192	-3.040384	-2.225177
6	-3.643166	-2.360977	-1.517721
6	-7.683449	-1.574778	-1.016950
6	-8.131489	-0.635342	-0.123739
6	-7.195608	0.075924	0.669331
6	-5.844408	-0.165197	0.541918
1	-1.850533	-0.295558	-1.777645
1	-3.188431	1.509678	-2.439569
1	-4.072189	1.364380	-0.924450
1	0.748827	1.959856	-1.034984
1	-0.151925	1.126420	-2.298644
1	-0.593254	3.885186	-1.225496
1	-1.280611	3.166163	-2.683345
1	-3.114582	3.647961	-1.106699
1	-1.638112	3.727013	0.874143
1	-0.126606	2.018532	1.178942
1	-1.437579	0.942720	1.658032
1	-3.116306	2.344556	2.554460
1	-5.396652	2.843290	1.945868
1	-4.895048	3.258297	0.217715
1	-3.281084	-0.024217	0.912404
1	-2.601303	-2.618762	-1.696926
1	-5.173454	0.377919	1.196488
1	-4.391191	-3.812011	-2.943213
1	-8.376188	-2.144432	-1.627940
1	-9.194945	-0.453514	-0.023730
1	-1.233456	-1.972582	0.017776
1	0.040323	-2.554669	1.629488
8	-7.554766	1.014974	1.584447
6	-8.933746	1.252610	1.785761
1	-8.998659	2.010614	2.566915
1	-9.415308	1.634121	0.877385
1	-9.453868	0.348073	2.121804
1	-0.225400	0.095555	-0.196059
6	-0.332727	-2.846502	3.670080
1	0.551668	-3.484793	3.629645
1	-0.094249	-1.934610	4.229393
1	-1.132765	-3.370923	4.196159

2R3S_ *re-re*-path-A-catalyst-methyl-TS

Number of imaginary frequencies : 1

The smallest frequency is : -312.3767

Electronic energy : =-3039.7569997

Zero-point correction= 0.993898

Thermal correction to Energy= 1.047664

Thermal correction to Enthalpy= 1.048608

Thermal correction to Gibbs Free Energy= 0.903392

Sum of electronic and zero-point Energies= -3038.763102

Sum of electronic and thermal Energies= -3038.709336

Sum of electronic and thermal Enthalpies= -3038.708392

Sum of electronic and thermal Free Energies= -3038.853607

Cartesian Coordinates

7	-1.440444	0.440827	-0.521025
6	-2.753818	0.456488	-0.207378
6	-0.011315	4.589677	-0.428333
6	-3.107528	-2.020215	0.337873
6	-2.645092	2.237194	0.978519
6	-2.722092	-2.398403	-0.948679
6	-2.578322	-3.742324	-1.280922
8	-0.622981	-0.182581	0.230384
6	-3.196228	-4.367810	0.956300

6	-0.608218	3.415841	0.301641
6	1.196503	5.112193	0.044379
8	-1.027765	1.142553	-1.476144
6	-3.337841	-3.022067	1.284516
6	1.772393	6.224013	-0.559474
6	-4.710294	-0.194762	1.179004
6	-3.269161	-0.561270	0.764399
6	-2.026047	3.235352	0.249003
6	-0.613274	5.176907	-1.545648
6	-2.814042	-4.733217	-0.331017
6	-4.733599	1.102624	1.999981
6	1.157506	6.814401	-1.662905
8	0.158110	2.718404	0.999701
6	-0.029213	6.281387	-2.161055
6	-4.116175	2.331671	1.320873
1	-3.367019	0.835534	-1.015355
1	-5.080116	-1.000839	1.824074
1	-4.205109	0.922828	2.944012
1	2.704957	6.626296	-0.176111
1	-2.290043	-4.016000	-2.291433
1	-4.674935	2.616887	0.421114
1	-3.378090	-5.129489	1.708674
1	-2.627601	3.923499	-0.334908
1	-2.007402	1.714761	1.697089
1	-3.620496	-2.745121	2.298747
1	-4.225992	3.178250	2.011131
1	-2.548707	-1.637582	-1.704381
1	-2.665509	-0.459036	1.677960
1	-1.527340	4.756198	-1.953509
1	1.608156	7.679441	-2.139566
1	-0.500154	6.724551	-3.033180
1	-5.774216	1.326633	2.260963
1	1.667695	4.633387	0.896232
1	-2.703320	-5.780659	-0.593028
7	1.638950	2.306545	-2.172874
6	2.527837	1.592585	-1.472902
16	4.190835	1.945862	-1.461804
7	1.972908	0.583366	-0.752589
6	2.714978	-0.393535	0.011778
6	2.010661	-0.653053	1.358080
6	2.915480	-1.353270	2.393576
6	3.151271	-0.411646	3.584642
6	1.801083	-0.150446	4.270414
6	0.798735	0.373331	3.220554
7	1.531101	0.642823	1.947377
6	2.649190	1.605968	2.192062
6	3.711340	0.943395	3.107354
6	5.062168	0.888272	2.433234
6	5.956474	-0.092166	2.532309
6	2.847328	-1.728352	-0.714795
6	4.106956	-2.372900	-0.920581
6	4.084635	-3.646895	-1.562813
7	2.941217	-4.252454	-1.992081
6	1.810771	-3.619026	-1.797847
6	1.712000	-2.359352	-1.159900
6	5.307494	-4.330269	-1.767964
6	6.502675	-3.794592	-1.361831
6	6.521944	-2.524922	-0.729861
6	5.350140	-1.829122	-0.521918
1	1.098250	-1.222236	1.176075
1	2.441456	-2.274060	2.744626
1	3.862017	-1.633499	1.924937
1	0.324205	1.313675	3.507706
1	0.017252	-0.349225	2.975806
1	1.925612	0.580429	5.074702
1	1.420940	-1.071884	4.718340
1	3.843124	-0.870663	4.295637
1	3.819393	1.582536	3.993713
1	2.187322	2.486901	2.639392
1	3.054605	1.895894	1.219345

1	5.307687	1.759412	1.825342
1	6.910664	-0.029732	2.018665
1	5.778131	-0.991644	3.116403
1	3.702098	0.034760	0.194755
1	0.731255	-1.908147	-1.016740
1	5.422912	-0.847860	-0.066646
1	0.904930	-4.113121	-2.143980
1	5.262819	-5.296669	-2.259714
1	7.422286	-4.341310	-1.533020
1	0.966751	0.433639	-0.832003
1	0.656272	2.083184	-2.035910
8	7.661659	-1.924596	-0.299005
6	8.895481	-2.552343	-0.588172
1	9.668765	-1.885959	-0.205142
1	8.982919	-3.524655	-0.088867
1	9.037758	-2.682682	-1.667252
1	0.860966	1.102892	1.297855
6	-8.890262	-0.586074	-1.052294
6	-8.717751	-1.894674	-0.276702
6	-7.287479	-1.763667	0.247180
7	-7.066536	-0.329494	0.507099
6	-8.166183	0.417770	-0.150210
6	-5.721334	-0.074255	0.027472
1	-7.773695	1.284051	-0.690216
1	-9.934827	-0.321757	-1.228117
1	-8.388854	-0.660556	-2.024218
1	-9.418622	-1.946241	0.561652
1	-8.829190	-2.793354	-0.886877
1	-7.082824	-2.393816	1.119146
1	-5.663820	0.906573	-0.451645
6	-6.278632	-2.095823	-0.854798
8	-5.446604	-1.045536	-1.006033
8	-6.229818	-3.084683	-1.531935
1	-8.845573	0.789256	0.624990
6	1.986491	3.424457	-3.023046
1	2.753915	3.129693	-3.742967
1	1.086131	3.729495	-3.557161
1	2.361875	4.271115	-2.439995

2R3S_ *re-si*-path-A-catalyst-methyl-TS

Number of imaginary frequencies : 1

The smallest frequency is : -286.9903

Electronic energy : =-3039.7524523

Zero-point correction= 0.993968

Thermal correction to Energy= 1.047810

Thermal correction to Enthalpy= 1.048754

Thermal correction to Gibbs Free Energy= 0.902365

Sum of electronic and zero-point Energies= -3038.758485

Sum of electronic and thermal Energies= -3038.704642

Sum of electronic and thermal Enthalpies= -3038.703698

Sum of electronic and thermal Free Energies= -3038.850088

Cartesian Coordinates

7	1.358960	0.166364	-0.197756
6	2.560661	-0.180071	0.314518
6	0.537769	4.061389	0.597524
6	4.080397	0.096699	-1.720902
6	2.283744	1.057372	2.109765
6	3.382719	-0.890115	-2.418163
6	3.676868	-1.162978	-3.751140
8	1.244815	1.228407	-0.848344
6	5.373625	0.538615	-3.730131
6	0.718891	2.749200	1.301909
6	1.399867	4.477166	-0.420303

8	0.327200	-0.522579	0.104224
6	5.073820	0.810280	-2.398163
6	1.153241	5.667654	-1.100229
6	5.001565	0.202761	0.676306
6	3.794386	0.446053	-0.260174
6	2.040219	2.338642	1.654970
6	-0.567790	4.850465	0.929515
6	4.673725	-0.452144	-4.413259
6	4.857331	0.974334	1.998118
6	0.054266	6.454363	-0.759565
8	-0.322300	2.106000	1.585405
6	-0.804328	6.047384	0.260760
6	3.578289	0.663756	2.786415
1	2.563548	-1.180824	0.729842
1	5.890988	0.593555	0.166695
1	4.903008	2.047949	1.784798
1	1.814575	5.977794	-1.903247
1	3.128327	-1.941978	-4.271854
1	3.538385	-0.399470	3.044080
1	6.150821	1.104486	-4.235201
1	2.853177	3.037639	1.486764
1	1.406406	0.465418	2.372642
1	5.614164	1.599774	-1.878842
1	3.623109	1.201151	3.742494
1	2.610640	-1.463615	-1.913200
1	3.621813	1.531281	-0.246736
1	-1.230510	4.511371	1.720565
1	-0.133446	7.383473	-1.288857
1	-1.656199	6.662642	0.533878
1	5.724972	0.742684	2.625349
1	2.233427	3.841235	-0.703620
1	4.905266	-0.670353	-5.451055
7	-1.650004	0.463725	3.491465
6	-2.604948	0.054945	2.630479
16	-4.238450	-0.097232	3.054663
7	-2.133397	-0.202684	1.386378
6	-2.970292	-0.502210	0.244700
6	-2.389843	0.166584	-1.021344
6	-3.419840	0.255856	-2.169169
6	-3.760480	1.729392	-2.446716
6	-2.496174	2.431234	-2.959283
6	-1.350907	2.188092	-1.960296
7	-1.913745	1.566029	-0.714892
6	-3.008220	2.426200	-0.164082
6	-4.201491	2.445291	-1.155057
6	-5.471095	1.928856	-0.520779
6	-6.422570	1.221000	-1.124205
6	-3.111839	-2.000692	-0.014340
6	-4.380727	-2.637622	-0.191927
6	-4.372234	-4.034446	-0.484239
7	-3.232080	-4.775578	-0.578230
6	-2.093509	-4.156784	-0.386954
6	-1.980834	-2.773188	-0.109416
6	-5.605528	-4.699076	-0.689765
6	-6.800342	-4.030612	-0.612409
6	-6.806359	-2.645301	-0.308236
6	-5.623361	-1.970519	-0.096467
1	-1.480556	-0.361938	-1.313077
1	-3.012943	-0.200163	-3.075954
1	-4.317993	-0.305016	-1.898300
1	-0.846714	3.105768	-1.648481
1	-0.589943	1.499017	-2.324479
1	-2.682855	3.503100	-3.074346
1	-2.215794	2.039339	-3.940231
1	-4.552929	1.795874	-3.196577
1	-4.383678	3.496867	-1.413544
1	-2.566780	3.414015	-0.025279
1	-3.280416	2.031581	0.817581
1	-5.608614	2.203026	0.525849
1	-7.314671	0.914592	-0.587325

1	-6.351127	0.908023	-2.163062
1	-3.952866	-0.075479	0.455826
1	-0.995217	-2.333015	0.021831
1	-5.683852	-0.922960	0.171021
1	-1.190452	-4.760380	-0.457964
1	-5.569498	-5.760744	-0.911489
1	-7.728301	-4.565691	-0.774575
1	-1.121468	-0.211485	1.235761
1	-0.844684	0.904605	3.047603
8	-7.944024	-1.908977	-0.204820
6	-9.182856	-2.578962	-0.333319
1	-9.952180	-1.820778	-0.185326
1	-9.303248	-3.019886	-1.329936
1	-9.298888	-3.359949	0.426975
1	-1.157024	1.527300	-0.001800
6	7.640322	-3.628057	1.653747
6	8.408377	-2.877239	0.562606
6	7.419097	-1.775848	0.180771
7	6.686258	-1.425538	1.410356
6	6.965503	-2.482086	2.412992
6	5.307159	-1.270729	0.986328
1	6.045313	-2.778773	2.924198
1	8.281640	-4.239321	2.291634
1	6.888310	-4.282661	1.198324
1	9.322839	-2.433235	0.966720
1	8.666029	-3.488737	-0.304522
1	7.894241	-0.912721	-0.297200
1	4.627488	-1.673335	1.741490
6	6.334104	-2.326930	-0.747455
8	5.130450	-2.088085	-0.191119
8	6.483388	-2.924958	-1.776483
1	7.648126	-2.073748	3.166443
6	-1.936933	0.839934	4.859384
1	-0.988837	1.061656	5.352298
1	-2.590477	1.717682	4.917425
1	-2.428103	0.016917	5.381322

2R3S_si-si-path-A-catalyst-methyl-TS

Number of imaginary frequencies : 1

The smallest frequency is : -315.9435

Electronic energy : =-3039.7493544

Zero-point correction= 0.993365

Thermal correction to Energy= 1.047311

Thermal correction to Enthalpy= 1.048255

Thermal correction to Gibbs Free Energy= 0.902637

Sum of electronic and zero-point Energies= -3038.755989

Sum of electronic and thermal Energies= -3038.702044

Sum of electronic and thermal Enthalpies= -3038.701099

Sum of electronic and thermal Free Energies= -3038.846717

Cartesian Coordinates

7	-1.005314	0.849566	3.222055
6	-2.014917	0.266190	2.538111
16	-3.503131	-0.146067	3.229139
7	-1.721488	0.061471	1.230385
6	-2.684472	-0.364447	0.237422
6	-2.383299	0.308046	-1.121808
6	-3.594987	0.296368	-2.077811
6	-4.069098	1.736916	-2.325506
6	-2.952891	2.488892	-3.065552
6	-1.639320	2.344793	-2.273740
7	-1.948968	1.740887	-0.936137
6	-2.980269	2.561424	-0.230272
6	-4.326483	2.467353	-0.993177

6	-5.420051	1.882357	-0.129933
6	-6.402847	1.081829	-0.535297
6	-2.691458	-1.875922	0.022640
6	-3.893671	-2.650420	0.024151
6	-3.768509	-4.043882	-0.253598
7	-2.576086	-4.657717	-0.497679
6	-1.497728	-3.913627	-0.473478
6	-1.503993	-2.519986	-0.224230
6	-4.937292	-4.843082	-0.283600
6	-6.177787	-4.305696	-0.054519
6	-6.297764	-2.921440	0.230867
6	-5.179049	-2.117784	0.276621
1	-1.511294	-0.174203	-1.563485
1	-3.315115	-0.161782	-3.030620
1	-4.395969	-0.311232	-1.649692
1	-1.143659	3.297885	-2.077283
1	-0.910285	1.683452	-2.742908
1	-3.218830	3.544880	-3.170611
1	-2.824077	2.079754	-4.070596
1	-4.979120	1.733980	-2.930719
1	-4.627795	3.494433	-1.238018
1	-2.581087	3.576218	-0.199509
1	-3.047336	2.192656	0.794896
1	-5.390749	2.182520	0.918205
1	-7.157533	0.729081	0.160492
1	-6.495062	0.738524	-1.562811
1	-3.663479	-0.037523	0.594458
1	-0.563091	-1.972606	-0.244152
1	-5.319792	-1.075578	0.537522
1	-0.549707	-4.410616	-0.671619
1	-4.813725	-5.899942	-0.496917
1	-7.053784	-4.942416	-0.085305
1	-0.751505	0.167156	0.927060
1	-0.405087	1.443984	2.646882
8	-7.487291	-2.309979	0.471716
6	-8.647964	-3.115575	0.534043
1	-9.469929	-2.441451	0.776493
1	-8.856168	-3.600676	-0.427017
1	-8.567264	-3.877895	1.317461
1	-1.078414	1.760169	-0.373903
7	1.444187	0.851158	-0.793576
6	2.666994	0.548536	-0.306231
6	0.429752	4.630200	0.029776
6	2.723331	-1.967175	-0.734325
6	2.483825	1.783140	1.449600
6	2.738464	-1.783923	-2.116418
6	2.564521	-2.864200	-2.977144
8	0.447514	0.110072	-0.496106
6	2.346026	-4.338925	-1.089560
6	0.742973	3.357371	0.760690
6	1.206911	5.051291	-1.053070
8	1.270182	1.931642	-1.399973
6	2.515113	-3.254736	-0.232932
6	0.867477	6.206887	-1.750754
6	4.240451	-0.863617	1.041661
6	2.900564	-0.821466	0.258625
6	2.112784	3.037257	1.002748
6	-0.691717	5.377226	0.402866
6	2.369440	-4.145460	-2.468857
6	4.151176	0.024408	2.295130
6	-0.244350	6.954592	-1.367137
8	-0.228004	2.664487	1.158983
6	-1.022890	6.539855	-0.287554
6	3.849914	1.505362	2.034987
1	3.447881	1.122348	-0.785971
1	4.375070	-1.903467	1.359690
1	3.362772	-0.383687	2.939458
1	1.466127	6.519971	-2.600526
1	2.583308	-2.702987	-4.050660
1	4.628848	1.966053	1.415245

1	2.188452	-5.332129	-0.679122
1	2.872136	3.762962	0.727883
1	1.679413	1.142245	1.822319
1	2.477600	-3.408632	0.843993
1	3.891780	2.026911	2.999968
1	2.891684	-0.789569	-2.526641
1	2.122309	-0.979225	1.018752
1	-1.287394	5.039095	1.246103
1	-0.505628	7.857469	-1.910398
1	-1.885854	7.124498	0.016408
1	5.086567	-0.044234	2.858185
1	2.047447	4.440476	-1.367387
1	2.234283	-4.986152	-3.142003
6	8.873151	-1.377089	0.326552
6	8.163471	-2.359952	1.261043
6	7.063854	-1.497286	1.889931
7	6.733520	-0.439415	0.894879
6	7.696691	-0.572535	-0.211570
6	5.456680	-0.478206	0.211100
6	6.920198	-1.372829	-1.264155
8	7.358394	-1.935599	-2.230039
8	5.618878	-1.385126	-0.916640
1	7.976760	0.399006	-0.634895
1	9.426683	-1.857209	-0.482710
1	9.549543	-0.722110	0.883287
1	7.721225	-3.172930	0.673988
1	8.825028	-2.802925	2.007948
1	6.189165	-2.085625	2.171262
1	7.434552	-1.004422	2.795543
1	5.314583	0.514593	-0.233107
6	-1.111747	1.188220	4.625678
1	-0.145409	1.577106	4.951740
1	-1.886552	1.940404	4.812074
1	-1.355991	0.299314	5.209945

Nitro-Cinchona-thiourea

1-Michael-nitro-cinchona-thiourea-*si-si*_path-A-TS

Number of imaginary frequencies : 1

The smallest frequency is : -252.8042

Electronic energy : = -3435.8459919

Zero-point correction= 1.046269

Thermal correction to Energy= 1.107208

Thermal correction to Enthalpy= 1.108152

Thermal correction to Gibbs Free Energy= 0.948376

Sum of electronic and zero-point Energies= -3434.799723

Sum of electronic and thermal Energies= -3434.738784

Sum of electronic and thermal Enthalpies= -3434.737840

Sum of electronic and thermal Free Energies= -3434.897616

Cartesian Coordinates

6	-1.544899	-0.196419	5.085205
6	-2.390873	-1.461372	5.271700
6	-3.645524	-1.190045	4.428481
7	-3.220942	-0.153974	3.476056
6	-1.796650	0.135534	3.607621
6	-4.088759	0.503960	2.704490
6	-3.826589	1.433833	1.720972
8	-0.730547	1.606939	-1.548974
8	-0.851544	0.848478	0.486621
1	-1.591963	1.179008	3.355639
1	-0.483480	-0.348794	5.284902

1	-1.915518	0.616543	5.717527
1	-3.987222	-2.084809	3.899089
1	-4.472680	-0.804979	5.035503
1	-2.814776	1.819196	1.616138
6	-4.970077	2.258092	1.174018
1	-5.799772	1.599864	0.882579
6	-3.317169	-0.119022	0.083748
1	-2.707801	-0.583009	0.855360
1	-3.017962	0.881965	-1.862142
6	-4.600506	-0.773799	-0.201436
6	-5.020469	-1.802954	0.653709
6	-5.378035	-0.465980	-1.325211
6	-6.174317	-2.524265	0.378390
1	-4.395925	-2.048061	1.511531
6	-6.531729	-1.192856	-1.604552
1	-5.073923	0.326245	-2.003032
6	-6.926245	-2.227923	-0.759958
1	-6.479112	-3.333222	1.034932
1	-7.112006	-0.963282	-2.492239
1	-7.813976	-2.807046	-0.992013
7	-1.369483	1.030317	-0.646955
6	-2.647721	0.608500	-0.886446
7	-0.497745	-2.175440	-0.438595
6	-1.534802	-2.583996	-1.283354
6	-1.770821	-2.012515	-2.544194
6	-2.927802	-2.326568	-3.235951
6	-3.831322	-3.229370	-2.678317
6	-3.597949	-3.841042	-1.455279
6	-2.448418	-3.505607	-0.755979
6	0.778560	-1.808532	-0.738702
16	1.507774	-1.988140	-2.257602
7	1.407807	-1.292199	0.336084
6	2.781075	-0.837848	0.384062
6	2.781120	0.576598	0.995938
6	4.158875	1.272033	1.026039
6	4.106192	2.560585	0.189808
6	3.066323	3.517718	0.798221
6	1.719350	2.779316	0.930856
7	1.827740	1.459707	0.237211
6	2.229926	1.667545	-1.190930
6	3.666183	2.239580	-1.251434
6	4.589643	1.334658	-2.032063
6	5.877328	1.113292	-1.781505
6	3.655798	-1.751089	1.235183
6	4.911670	-2.253417	0.769046
6	5.671863	-3.046800	1.679223
7	5.249549	-3.356626	2.937667
6	4.081296	-2.898119	3.313698
6	3.249428	-2.087407	2.502638
6	6.930641	-3.546542	1.265788
6	7.428147	-3.286044	0.014764
6	6.664212	-2.508667	-0.892261
6	5.432867	-2.011344	-0.522607
1	2.340695	0.503582	1.995082
1	4.430986	1.509774	2.058017
1	4.922478	0.595042	0.635616
1	0.892483	3.307505	0.453044
1	1.445477	2.564031	1.965793
1	2.947703	4.397589	0.157474
1	3.398604	3.864268	1.779925
1	5.088333	3.040721	0.183443
1	3.604165	3.193696	-1.794038
1	1.491791	2.352699	-1.603850
1	2.120258	0.710254	-1.707427
1	4.130504	0.838979	-2.888918
1	6.462206	0.444115	-2.405166
1	6.394089	1.573531	-0.942809
1	3.158118	-0.806685	-0.638791
1	2.293322	-1.740031	2.889966
1	4.882602	-1.444857	-1.263324

1	3.753280	-3.161126	4.317643
1	7.488380	-4.146225	1.977765
1	8.394433	-3.682476	-0.273376
1	0.885742	-1.164484	1.226231
1	-0.765447	-2.136952	0.564161
1	-1.070689	-1.289606	-2.942735
1	-2.255572	-3.938214	0.220713
8	7.079172	-2.208297	-2.150553
6	8.289995	-2.780837	-2.607391
1	8.407014	-2.452126	-3.640323
1	9.149202	-2.432856	-2.021944
1	8.250326	-3.875864	-2.581691
1	0.867443	1.044451	0.260994
6	-0.908448	-0.776333	2.729235
8	-1.456792	-1.736755	2.135322
8	0.315237	-0.489259	2.737226
1	-5.364036	2.918659	1.959315
1	-2.637514	-1.664638	6.315128
1	-1.855848	-2.325433	4.869317
6	-4.597054	3.143381	-0.026813
1	-5.485261	3.728075	-0.298371
1	-4.331646	2.538615	-0.896848
6	-3.489416	4.093854	0.298564
6	-2.338763	4.215829	-0.373677
1	-3.636609	4.746297	1.160960
1	-2.132285	3.590622	-1.236991
6	-1.348057	5.240481	0.054715
8	-1.519596	5.895780	1.070417
6	-0.125583	5.490193	-0.786133
6	0.219713	4.713640	-1.897800
6	0.702675	6.554920	-0.410465
6	1.377249	5.004679	-2.619335
1	-0.389682	3.868001	-2.199522
6	1.848850	6.850494	-1.137288
1	0.420331	7.144534	0.455245
6	2.189069	6.073610	-2.245439
1	1.638116	4.399062	-3.482364
1	2.476620	7.685946	-0.844166
1	3.082791	6.303174	-2.817763
1	-5.125623	0.196499	2.855292
1	-3.151925	-1.862353	-4.188591
1	-4.321763	-4.538613	-1.053145
7	-5.088293	-3.495271	-3.368297
8	-5.812939	-4.372956	-2.927504
8	-5.359567	-2.814661	-4.345414

1-Michael-nitro-cinchona-thiourea-*si-re*_path-A-TS

Number of imaginary frequencies : 1
The smallest frequency is : -300.3471

Electronic energy : =-3435.83837
Zero-point correction= 1.045741
Thermal correction to Energy= 1.107138
Thermal correction to Enthalpy= 1.108083
Thermal correction to Gibbs Free Energy= 0.942474
Sum of electronic and zero-point Energies= -3434.792629
Sum of electronic and thermal Energies= -3434.731231
Sum of electronic and thermal Enthalpies= -3434.730287
Sum of electronic and thermal Free Energies= -3434.895896

Cartesian Coordinates

6	2.288711	-1.625988	3.519808
6	3.291946	-0.549032	3.952027
6	4.355420	-0.558678	2.840947
7	3.709749	-1.255917	1.716270

6	2.290736	-1.491051	1.987227
6	4.404191	-1.895272	0.780966
6	3.888465	-2.441104	-0.383850
8	0.800664	0.622219	-1.278276
8	1.456238	-1.308707	-2.033666
1	1.968854	-2.399805	1.473273
1	1.290944	-1.481339	3.939280
1	2.646078	-2.623670	3.796026
1	2.798867	0.424021	3.977075
1	3.727779	-0.746400	4.932824
1	4.639519	0.453494	2.543654
1	5.258685	-1.109047	3.124296
1	5.485855	-1.883348	0.927057
1	2.808199	-2.464411	-0.510145
6	4.649091	-3.514462	-1.112676
6	4.206013	-4.927006	-0.668128
1	5.726285	-3.403429	-0.942863
1	4.483832	-3.426945	-2.195458
1	4.795888	-5.671662	-1.216877
1	4.408793	-5.057003	0.400339
6	2.754559	-5.149756	-0.949936
6	1.804552	-5.328493	-0.025288
1	2.440533	-5.131834	-1.994666
1	2.053994	-5.359546	1.032410
6	0.391334	-5.543080	-0.434226
8	0.068283	-5.634086	-1.609078
6	-0.653965	-5.661340	0.631905
6	-0.552270	-4.989028	1.852705
6	-1.801494	-6.408107	0.346531
6	-1.599020	-5.047199	2.769609
1	0.326107	-4.390949	2.079423
6	-2.831063	-6.491480	1.274664
1	-1.869873	-6.910912	-0.613160
6	-2.733745	-5.803345	2.484624
1	-1.527266	-4.505000	3.706947
1	-3.714029	-7.082653	1.053890
1	-3.543205	-5.857588	3.205986
6	4.040708	-0.698622	-1.622422
1	3.818349	-1.391765	-2.430126
1	3.108675	1.105583	-0.742494
6	5.450251	-0.267840	-1.509099
6	6.407826	-0.808026	-2.373557
6	5.858681	0.658300	-0.539277
6	7.744216	-0.429424	-2.277348
1	6.096688	-1.519574	-3.133968
6	7.192224	1.035140	-0.443621
1	5.126255	1.074299	0.148196
6	8.139398	0.492239	-1.312790
1	8.474352	-0.850275	-2.961292
1	7.496644	1.756032	0.308743
1	9.179992	0.791337	-1.238199
7	1.719305	-0.187645	-1.542345
6	3.013233	0.170806	-1.270734
7	0.318384	2.955821	0.468391
6	1.147302	4.061974	0.338571
6	0.774046	5.328940	-0.141058
6	1.714697	6.346022	-0.208453
6	3.021212	6.110090	0.198313
6	3.415372	4.866229	0.684897
6	2.481254	3.853689	0.755817
6	-0.978714	2.722009	0.111703
16	-2.034966	3.794892	-0.652951
7	-1.359567	1.468404	0.442347
6	-2.650756	0.909532	0.111932
6	-2.523623	-0.621503	0.013006
6	-3.830328	-1.297260	-0.448378
6	-3.503228	-2.382182	-1.482844
6	-2.420357	-3.293963	-0.891892
6	-1.117579	-2.487803	-0.747402
7	-1.429282	-1.029849	-0.942623

6	-1.796189	-0.778939	-2.367838
6	-2.956564	-1.728383	-2.765679
6	-3.962173	-0.975987	-3.601181
6	-5.277515	-0.914916	-3.412296
6	-3.714230	1.238376	1.156709
6	-5.048210	1.623554	0.811283
6	-5.955582	1.845714	1.889627
7	-5.610884	1.716997	3.202592
6	-4.375418	1.377752	3.473767
6	-3.393945	1.127008	2.485517
6	-7.289810	2.219102	1.597366
6	-7.724015	2.367676	0.305694
6	-6.819724	2.150811	-0.765626
6	-5.511833	1.794135	-0.514383
1	-2.187885	-1.006614	0.980725
1	-4.341416	-1.728962	0.416234
1	-4.500762	-0.554953	-0.885319
1	-0.374874	-2.738635	-1.505714
1	-0.656869	-2.565851	0.238798
1	-2.235016	-4.163189	-1.529165
1	-2.747780	-3.668066	0.084181
1	-4.398453	-2.964872	-1.714904
1	-2.535964	-2.526295	-3.392422
1	-0.882315	-0.940300	-2.942229
1	-2.068559	0.275861	-2.454908
1	-3.529745	-0.426500	-4.438282
1	-5.907433	-0.331134	-4.075652
1	-5.779789	-1.434030	-2.600539
1	-2.961895	1.321368	-0.850813
1	-2.384874	0.856231	2.784500
1	-4.859762	1.660389	-1.370741
1	-4.111813	1.286333	4.525915
1	-7.957590	2.384334	2.436540
1	-8.751173	2.653469	0.113205
1	-0.688140	0.825781	0.898519
1	0.820879	2.127742	0.829923
1	-0.241146	5.509087	-0.459141
1	2.757039	2.877734	1.144735
8	-7.170091	2.272551	-2.070864
6	-8.481588	2.710354	-2.369633
1	-8.537630	2.772882	-3.456598
1	-9.236166	1.999354	-2.013195
1	-8.681974	3.699927	-1.943303
1	-0.566969	-0.476688	-0.758535
6	1.373314	-0.324330	1.583321
8	1.862356	0.824599	1.564070
8	0.170603	-0.645946	1.385357
1	4.439681	4.711375	1.000707
1	1.438300	7.326607	-0.576597
7	4.000353	7.184141	0.120925
8	5.142285	6.946209	0.486329
8	3.633598	8.268528	-0.304035

1-Michael-nitro-cinchona-thiourea-*re-re*_path-A-TS

Number of imaginary frequencies : 1

The smallest frequency is : -255.0547

Electronic energy : =-3435.8372365

Zero-point correction= 1.046126

Thermal correction to Energy= 1.107797

Thermal correction to Enthalpy= 1.108741

Thermal correction to Gibbs Free Energy= 0.941032

Sum of electronic and zero-point Energies= -3434.791111

Sum of electronic and thermal Energies= -3434.729439

Sum of electronic and thermal Enthalpies= -3434.728495

Sum of electronic and thermal Free Energies= -3434.896204

..... Cartesian Coordinates			
6	-2.505491	-0.475510	-3.233271
6	-2.671081	1.034170	-3.469484
6	-3.101584	1.596630	-2.100988
7	-2.836939	0.509174	-1.146066
6	-2.049445	-0.558459	-1.770624
6	-3.542336	0.324118	-0.035033
6	-4.316507	1.290296	0.587200
8	0.421794	1.022099	0.820540
6	-0.540680	-0.270504	-1.645472
8	0.188724	-1.231548	-1.279990
8	-0.161050	0.881383	-1.951709
8	-1.308632	0.035108	1.691513
1	-2.277781	-1.512389	-1.292837
1	-1.789764	-0.935514	-3.918171
1	-3.466056	-0.991287	-3.332069
1	-1.718119	1.471516	-3.764712
1	-3.414960	1.248434	-4.239229
1	-2.537239	2.491660	-1.827033
1	-4.171354	1.829617	-2.068613
1	-3.402655	-0.641015	0.445305
1	-4.572098	2.184118	0.023161
6	-5.278947	0.878597	1.668138
6	-6.689980	0.538238	1.137521
1	-5.382782	1.685178	2.404524
1	-4.876856	0.005255	2.197266
1	-7.340203	0.267254	1.975791
1	-7.109797	1.439533	0.672143
6	-6.658010	-0.562755	0.126763
6	-7.203488	-1.773209	0.277498
1	-6.124602	-0.371768	-0.804308
1	-7.760370	-2.016536	1.176185
6	-7.067142	-2.784730	-0.806511
8	-6.450322	-2.528204	-1.828701
6	-7.707222	-4.131843	-0.640040
6	-8.256953	-4.578615	0.565574
6	-7.735088	-4.974248	-1.757531
6	-8.826005	-5.846437	0.648434
1	-8.237686	-3.955205	1.452498
6	-8.309795	-6.235070	-1.676280
1	-7.300274	-4.614163	-2.683882
6	-8.856825	-6.673596	-0.470641
1	-9.245480	-6.188307	1.589176
1	-8.331658	-6.878039	-2.550338
1	-9.305295	-7.659962	-0.402978
6	-2.714860	2.323165	1.707747
1	-2.911349	1.617288	2.509908
1	-0.959998	3.010259	0.562503
6	-3.363561	3.647209	1.817162
6	-4.065208	3.983966	2.979636
6	-3.285104	4.585733	0.779193
6	-4.665847	5.234171	3.107016
1	-4.121490	3.267525	3.794813
6	-3.882264	5.832604	0.907229
1	-2.760289	4.327250	-0.137330
6	-4.575357	6.160398	2.072973
1	-5.200876	5.484708	4.017473
1	-3.809054	6.551479	0.097379
1	-5.041768	7.135279	2.172179
7	-0.764415	1.051641	1.202281
6	-1.476183	2.222820	1.090820
7	2.281959	1.957069	-1.092084
6	2.205710	3.343449	-1.073794
6	3.271085	4.221317	-0.818196
6	3.059138	5.591466	-0.860034
6	1.797279	6.085653	-1.165196
6	0.729207	5.236257	-1.441998
6	0.937590	3.872156	-1.395992

6	3.137187	1.086896	-0.486217
16	4.536690	1.481388	0.375910
7	2.708314	-0.187552	-0.626073
6	3.385893	-1.352907	-0.105495
6	2.343714	-2.359598	0.420884
6	2.976244	-3.483304	1.270765
6	2.439565	-3.405915	2.708397
6	0.928013	-3.672504	2.670352
6	0.272634	-2.690802	1.679617
7	1.291666	-1.677165	1.256257
6	1.860585	-0.982736	2.450286
6	2.660815	-2.000397	3.303413
6	4.102570	-1.578149	3.460717
6	5.164815	-2.379123	3.490463
6	4.217809	-2.050674	-1.179374
6	5.578157	-2.440257	-0.979419
6	6.216105	-3.137256	-2.049093
7	5.603222	-3.420197	-3.233066
6	4.362812	-3.025922	-3.382538
6	3.627820	-2.344959	-2.383394
6	7.555566	-3.564545	-1.883196
6	8.244124	-3.323878	-0.722090
6	7.610664	-2.620818	0.335195
6	6.310159	-2.183043	0.202491
1	1.783660	-2.755674	-0.428724
1	2.734439	-4.459682	0.841802
1	4.064098	-3.385504	1.258518
1	-0.552150	-2.125062	2.111001
1	-0.075681	-3.168088	0.761757
1	0.499611	-3.546549	3.668876
1	0.735098	-4.701754	2.357246
1	2.932181	-4.156556	3.332000
1	2.216949	-1.999537	4.307733
1	1.001832	-0.558340	2.974154
1	2.472805	-0.153505	2.085516
1	4.254875	-0.505402	3.584720
1	6.162566	-1.975419	3.629451
1	5.091618	-3.457448	3.371433
1	4.029645	-1.025905	0.713172
1	2.596663	-2.058358	-2.578579
1	5.880412	-1.625608	1.026693
1	3.887242	-3.251742	-4.335129
1	8.018900	-4.091131	-2.711119
1	9.267594	-3.665371	-0.624706
1	1.808154	-0.374404	-1.091995
1	1.403173	1.519447	-1.424747
1	4.251803	3.830960	-0.591926
1	0.129231	3.177054	-1.608928
8	8.222636	-2.338966	1.514020
6	9.577672	-2.715897	1.667208
1	9.874103	-2.375955	2.659782
1	9.703747	-3.803413	1.609151
1	10.216689	-2.233915	0.918472
1	0.806951	-0.964608	0.679034
1	-0.240313	5.653265	-1.685707
1	3.870737	6.282049	-0.665735
7	1.585134	7.526060	-1.208786
8	0.471284	7.932302	-1.505156
8	2.528791	8.255163	-0.947837

l-Michael-nitro-cinchona-thiourea-*re-si*_path-A-TS

Number of imaginary frequencies : 1

The smallest frequency is : -272.3281

Electronic energy : =-3435.8402313

Zero-point correction= 1.045231

Thermal correction to Energy=	1.106369
Thermal correction to Enthalpy=	1.107313
Thermal correction to Gibbs Free Energy=	0.945357
Sum of electronic and zero-point Energies=	-3434.795001
Sum of electronic and thermal Energies=	-3434.733862
Sum of electronic and thermal Enthalpies=	-3434.732918
Sum of electronic and thermal Free Energies=	-3434.894874

Cartesian Coordinates

6	-2.117327	1.683864	4.462529
6	-3.523105	1.118345	4.218712
6	-3.958541	1.779839	2.908395
7	-2.697369	2.091297	2.232596
6	-1.520521	1.775595	3.051866
6	-2.598104	2.464366	0.965547
6	-3.625189	2.485870	0.026813
8	-0.415687	0.177735	-2.281645
6	-0.909622	0.426742	2.601294
8	0.339750	0.391555	2.472046
8	-1.714928	-0.519885	2.421066
8	-0.794237	0.689765	-0.200059
1	-0.772230	2.565908	2.949903
1	-1.513651	1.055907	5.120916
1	-2.176180	2.686256	4.898375
1	-3.459733	0.038685	4.076881
1	-4.214008	1.336645	5.035095
1	-4.573684	1.126821	2.284157
1	-4.512818	2.712540	3.074979
1	-1.583921	2.678866	0.638854
1	-4.650730	2.432950	0.382568
6	-3.385007	3.139472	-1.308078
6	-3.274626	4.684103	-1.279727
1	-4.190082	2.855736	-1.995638
1	-2.451379	2.749833	-1.735952
1	-3.138996	5.043436	-2.305294
1	-4.204716	5.112044	-0.891124
6	-2.116557	5.105979	-0.429601
6	-0.880457	5.342615	-0.884848
1	-2.263025	5.148166	0.649134
1	-0.674578	5.333150	-1.950960
6	0.222524	5.607164	0.076741
8	0.014689	5.661055	1.278811
6	1.620261	5.795990	-0.441845
6	2.017755	5.423290	-1.730701
6	2.566445	6.335342	0.437041
6	3.341328	5.593616	-2.131789
1	1.308944	4.986210	-2.426912
6	3.882319	6.519106	0.031207
1	2.244205	6.608125	1.436472
6	4.272696	6.146198	-1.254985
1	3.643014	5.300640	-3.132590
1	4.605616	6.948963	0.716673
1	5.300714	6.286363	-1.574247
6	-3.440381	0.311171	-0.472361
1	-3.034495	0.109153	0.519403
1	-2.824575	-0.000157	-2.569035
6	-4.852506	-0.070939	-0.689160
6	-5.580460	-0.617655	0.374237
6	-5.464561	0.013095	-1.947835
6	-6.869069	-1.103455	0.181785
1	-5.103810	-0.713783	1.346793
6	-6.751789	-0.475127	-2.141611
1	-4.928437	0.449508	-2.785516
6	-7.455108	-1.042794	-1.080421
1	-7.406178	-1.556780	1.008898
1	-7.204342	-0.422462	-3.126605
1	-8.449394	-1.447935	-1.238397
7	-1.214639	0.352868	-1.345363
6	-2.556309	0.206400	-1.544959

7	-1.152599	-2.303213	0.371912
6	-2.327802	-2.881511	-0.108437
6	-2.605289	-3.068386	-1.471665
6	-3.869670	-3.475835	-1.866269
6	-4.841501	-3.719928	-0.899655
6	-4.574309	-3.588215	0.457394
6	-3.317058	-3.160399	0.847225
6	0.129833	-2.416844	-0.073806
16	0.659116	-3.461621	-1.290468
7	0.957310	-1.596460	0.609662
6	2.381602	-1.488775	0.395881
6	2.768285	-0.016924	0.612090
6	4.248902	0.311421	0.356559
6	4.338614	1.699633	-0.298916
6	3.444192	2.681999	0.474563
6	1.972646	2.268596	0.284261
7	1.939251	0.878680	-0.273023
6	2.437491	0.878546	-1.682878
6	3.803113	1.607868	-1.737878
6	4.698378	0.923445	-2.738530
6	5.938167	0.489174	-2.531595
6	3.188375	-2.347829	1.361207
6	4.347833	-3.079372	0.953755
6	5.048112	-3.797078	1.968314
7	4.661944	-3.819332	3.275899
6	3.588689	-3.143048	3.602630
6	2.821204	-2.389458	2.682229
6	6.208718	-4.526700	1.613714
6	6.670818	-4.552357	0.323078
6	5.970650	-3.841599	-0.685496
6	4.833017	-3.127447	-0.373832
1	2.473382	0.259372	1.629021
1	4.790852	0.286188	1.305369
1	4.700999	-0.439126	-0.298194
1	1.448616	2.902416	-0.436589
1	1.403402	2.234946	1.216079
1	3.587693	3.702418	0.107527
1	3.708277	2.670563	1.536173
1	5.370859	2.057993	-0.300790
1	3.625834	2.633483	-2.093056
1	1.665283	1.349864	-2.290729
1	2.508956	-0.164130	-2.001979
1	4.248130	0.773316	-3.720467
1	6.494141	-0.002593	-3.323297
1	6.446454	0.599781	-1.577592
1	2.585163	-1.797467	-0.631515
1	1.944452	-1.846024	3.026983
1	4.325570	-2.620040	-1.186997
1	3.290434	-3.172371	4.648894
1	6.721080	-5.064742	2.404595
1	7.561822	-5.119498	0.082120
1	0.574253	-0.984404	1.352037
1	-1.296502	-1.705092	1.210959
1	-1.842835	-2.845323	-2.206538
1	-3.086199	-3.015210	1.897969
8	6.358685	-3.814572	-1.984958
6	7.482037	-4.586890	-2.362488
1	7.594178	-4.448430	-3.438126
1	8.395140	-4.244505	-1.861129
1	7.327713	-5.651544	-2.152796
1	0.931570	0.579521	-0.267625
1	-5.352469	-3.790899	1.182843
1	-4.120238	-3.579903	-2.914949
7	-6.195692	-4.056912	-1.320205
8	-7.030174	-4.268434	-0.453035
8	-6.433808	-4.095665	-2.516735

Number of imaginary frequencies : 1
The smallest frequency is : -364.6331

Electronic energy : =-3435.8618449
Zero-point correction= 1.049951
Thermal correction to Energy= 1.109053
Thermal correction to Enthalpy= 1.109997
Thermal correction to Gibbs Free Energy= 0.952282
Sum of electronic and zero-point Energies= -3434.811894
Sum of electronic and thermal Energies= -3434.752792
Sum of electronic and thermal Enthalpies= -3434.751848
Sum of electronic and thermal Free Energies= -3434.909563

Cartesian Coordinates

7	-1.610182	0.158450	-0.093956
6	-2.923641	0.188393	0.228428
6	0.240021	3.674781	1.833235
6	-3.516644	-2.246562	-0.323993
6	-2.725318	1.284132	2.000897
6	-3.089626	-2.099024	-1.644297
6	-3.047554	-3.193315	-2.503477
8	-0.884057	-0.811428	0.294544
6	-3.855840	-4.615624	-0.742199
6	-0.544705	2.396012	1.951246
6	1.632235	3.579989	1.744598
8	-1.106332	1.153783	-0.668476
6	-3.893592	-3.518633	0.114948
6	2.414552	4.715606	1.567919
6	-5.006394	-0.777292	1.168444
6	-3.578553	-1.086929	0.670388
6	-1.961010	2.421473	1.775964
6	-0.353080	4.942132	1.785763
6	-3.429701	-4.456016	-2.057374
6	-4.970906	0.083920	2.439900
6	1.813064	5.970696	1.502792
8	0.092832	1.357156	2.239334
6	0.428896	6.081449	1.625095
6	-4.201805	1.405971	2.318685
1	-3.465615	0.925381	-0.351918
1	-5.476305	-1.733369	1.427119
1	-4.523255	-0.506764	3.248177
1	3.491084	4.616241	1.465852
1	-2.724031	-3.054512	-3.530707
1	-4.669537	2.079988	1.590291
1	-4.155540	-5.594493	-0.380066
1	-2.450830	3.337458	1.465750
1	-2.197531	0.457139	2.483641
1	-4.214353	-3.656000	1.146134
1	-4.276434	1.922141	3.284082
1	-2.806015	-1.118099	-2.014568
1	-3.026664	-1.435607	1.555545
1	-1.427776	5.050323	1.887447
1	2.418877	6.860204	1.357030
1	-0.042900	7.058612	1.587391
1	-6.003031	0.296855	2.741397
1	2.088893	2.595735	1.783777
1	-3.400520	-5.306848	-2.730559
7	1.642832	1.904794	-1.005307
6	1.850334	3.220995	-1.418149
6	0.699479	4.031388	-1.419138
6	0.773718	5.361594	-1.778635
6	2.008359	5.881146	-2.158316
6	3.150445	5.093050	-2.201452
6	3.075901	3.756264	-1.837473
6	2.492307	0.933519	-0.567828
16	4.157850	1.092763	-0.341692
7	1.816767	-0.198664	-0.261188

6	2.416276	-1.452357	0.148916
6	1.589344	-2.072893	1.292047
6	2.338272	-3.200730	2.034527
6	2.584529	-2.778806	3.491740
6	1.223904	-2.612302	4.186285
6	0.361900	-1.632515	3.365353
7	1.208966	-1.022125	2.295113
6	2.402268	-0.354176	2.901803
6	3.316469	-1.423119	3.554544
6	4.703952	-1.400193	2.957555
6	5.477730	-2.454943	2.713468
6	2.472829	-2.456642	-0.998451
6	3.672966	-3.142816	-1.362531
6	3.577194	-4.092624	-2.423377
7	2.420527	-4.356420	-3.093840
6	1.346546	-3.697888	-2.734445
6	1.321722	-2.742293	-1.690503
6	4.736740	-4.810414	-2.804954
6	5.938605	-4.614499	-2.174921
6	6.031655	-3.666733	-1.123274
6	4.923776	-2.944518	-0.733324
1	0.637116	-2.423453	0.888921
1	1.745863	-4.119554	2.014368
1	3.281837	-3.413065	1.525812
1	-0.029549	-0.800321	3.953110
1	-0.470507	-2.119813	2.853292
1	1.367018	-2.233322	5.202109
1	0.717881	-3.577772	4.263080
1	3.170990	-3.543532	4.007556
1	3.419998	-1.156562	4.614646
1	2.006415	0.372613	3.611605
1	2.909209	0.197447	2.105671
1	5.090613	-0.404955	2.735578
1	6.472973	-2.332386	2.298203
1	5.156229	-3.474901	2.909043
1	3.422283	-1.225791	0.505440
1	0.382186	-2.250279	-1.443883
1	5.055516	-2.216355	0.058601
1	0.428929	-3.919906	-3.275506
1	4.637366	-5.526212	-3.614303
1	6.807316	-5.181272	-2.487886
1	0.799142	-0.218989	-0.370815
1	0.652737	1.659283	-0.913296
1	-0.245359	3.605801	-1.090626
1	3.959360	3.137114	-1.868066
8	7.180952	-3.413342	-0.447434
6	8.359159	-4.078868	-0.861798
1	9.156908	-3.706296	-0.218906
1	8.275010	-5.164532	-0.734489
1	8.603643	-3.850980	-1.905513
1	0.631665	-0.279137	1.850068
6	-9.066282	0.099876	-1.149963
6	-8.993892	-1.422627	-1.008005
6	-7.588929	-1.618013	-0.439004
7	-7.321509	-0.452948	0.424713
6	-8.346144	0.575202	0.115099
6	-5.940652	-0.105220	0.147239
1	-7.881519	1.559110	0.006151
1	-10.087003	0.479904	-1.224167
1	-8.518639	0.416487	-2.045113
1	-9.738752	-1.784340	-0.293344
1	-9.113097	-1.963550	-1.948954
1	-7.455559	-2.574751	0.077257
1	-5.812060	0.980361	0.147666
6	-6.539587	-1.499871	-1.546791
8	-5.652777	-0.545523	-1.197026
8	-6.499519	-2.091723	-2.588936
1	-9.047741	0.628712	0.954781
1	4.089646	5.527533	-2.521290
1	-0.099580	6.001184	-1.754743

7	2.104350	7.292649	-2.510635
8	3.196681	7.730221	-2.835668
8	1.086892	7.966221	-2.459380

2-Michael-nitro-cinchona-thiourea-2R3S_re-si-path-A-TS

Number of imaginary frequencies : 1

The smallest frequency is : -306.8880

Electronic energy : =-3435.8575718
Zero-point correction= 1.049128
Thermal correction to Energy= 1.108508
Thermal correction to Enthalpy= 1.109452
Thermal correction to Gibbs Free Energy= 0.948691
Sum of electronic and zero-point Energies= -3434.808444
Sum of electronic and thermal Energies= -3434.749064
Sum of electronic and thermal Enthalpies= -3434.748119
Sum of electronic and thermal Free Energies= -3434.908881

Cartesian Coordinates

7	-1.490372	-0.926186	0.307456
6	-2.636116	-0.388079	-0.167674
6	-0.678648	0.529750	3.975980
6	-4.322905	-2.201937	0.459070
6	-2.237100	1.583407	0.685215
6	-3.675873	-3.135404	-0.350717
6	-4.087622	-4.465077	-0.370764
8	-1.441094	-1.344617	1.483426
6	-5.800474	-3.965797	1.239643
6	-0.773511	1.002591	2.557412
6	-1.633958	-0.330802	4.523788
8	-0.429429	-0.879541	-0.405907
6	-5.383438	-2.637945	1.259327
6	-1.481421	-0.804874	5.824113
6	-5.046190	0.223934	0.056801
6	-3.921907	-0.727930	0.522653
6	-2.048559	1.376957	2.041210
6	0.426321	0.911729	4.743355
6	-5.151966	-4.886172	0.421029
6	-4.811884	1.660678	0.547903
6	-0.383627	-0.413429	6.588206
8	0.304939	1.083718	1.910680
6	0.569168	0.449495	6.048088
6	-3.466150	2.268238	0.127250
1	-2.596818	-0.196288	-1.233498
1	-5.977368	-0.130169	0.514187
1	-4.897639	1.680276	1.639928
1	-2.215973	-1.488044	6.238814
1	-3.578556	-5.173367	-1.017273
1	-3.386241	2.303214	-0.964013
1	-6.628243	-4.280936	1.867901
1	-2.887015	1.404187	2.729568
1	-1.335580	1.667548	0.076585
1	-5.885419	-1.928528	1.914801
1	-3.435937	3.313119	0.462065
1	-2.854183	-2.820113	-0.987392
1	-3.767692	-0.510563	1.588063
1	1.160879	1.581097	4.304451
1	-0.269534	-0.782571	7.602691
1	1.421019	0.761640	6.644413
1	-5.619835	2.293451	0.162788
1	-2.466791	-0.660385	3.909559
1	-5.475042	-5.922166	0.398647
7	1.493794	2.498309	-0.154776
6	1.434229	3.878979	-0.292999
6	0.495041	4.543498	0.516829

6	0.315535	5.909856	0.413705
6	1.082600	6.615726	-0.507785
6	2.009504	5.981199	-1.326384
6	2.185813	4.610851	-1.224941
6	2.496327	1.607834	-0.457401
16	4.102467	1.984503	-0.774846
7	2.032865	0.342594	-0.389105
6	2.866409	-0.840447	-0.429539
6	2.237428	-1.945992	0.447628
6	3.237345	-3.074595	0.780325
6	3.523802	-3.081418	2.290631
6	2.224989	-3.443972	3.024387
6	1.107597	-2.489926	2.562530
7	1.719821	-1.384988	1.749510
6	2.789804	-0.702183	2.540398
6	3.964695	-1.686650	2.777023
6	5.258238	-1.169879	2.192406
6	6.216137	-1.902636	1.630237
6	3.036444	-1.389922	-1.844348
6	4.311803	-1.726534	-2.396653
6	4.320874	-2.312619	-3.697163
7	3.192532	-2.533243	-4.429219
6	2.048079	-2.180687	-3.898411
6	1.917646	-1.611935	-2.608085
6	5.559900	-2.690436	-4.269202
6	6.743173	-2.501299	-3.602429
6	6.732282	-1.902037	-2.316948
6	5.543114	-1.519541	-1.734212
1	1.341024	-2.318087	-0.051018
1	2.821618	-4.041983	0.485273
1	4.157821	-2.930144	0.209473
1	0.579334	-2.007828	3.388361
1	0.360623	-2.960074	1.922945
1	2.370726	-3.364681	4.105686
1	1.941502	-4.476168	2.804732
1	4.298834	-3.816943	2.520407
1	4.110696	-1.753609	3.863064
1	2.313892	-0.383990	3.469082
1	3.086900	0.193291	1.990405
1	5.406947	-0.092689	2.279743
1	7.126437	-1.443473	1.258117
1	6.133907	-2.979941	1.508642
1	3.840112	-0.560856	-0.020649
1	0.927811	-1.365950	-2.229380
1	5.592219	-1.038315	-0.765038
1	1.155630	-2.356641	-4.496127
1	5.537256	-3.136245	-5.258336
1	7.675299	-2.801801	-4.065745
1	1.018707	0.191490	-0.357892
1	0.799606	2.096845	0.488797
1	-0.088983	3.968380	1.231290
1	2.898217	4.106685	-1.862272
8	7.857106	-1.670055	-1.592213
6	9.104674	-1.993880	-2.175787
1	9.862109	-1.697425	-1.449746
1	9.194637	-3.069684	-2.367451
1	9.268284	-1.442198	-3.108662
1	0.976423	-0.687468	1.556979
6	-7.564349	0.451460	-3.969705
6	-8.327630	-0.533855	-3.080448
6	-7.372037	-0.697958	-1.897798
7	-6.691275	0.598053	-1.726589
6	-6.960170	1.408696	-2.938583
6	-5.306900	0.255622	-1.459075
1	-6.045484	1.900051	-3.282012
1	-8.199988	0.958269	-4.698402
1	-6.771758	-0.074283	-4.514524
1	-9.271818	-0.099823	-2.738795
1	-8.531562	-1.496646	-3.553436
1	-7.865030	-1.047478	-0.984196

1	-4.636227	0.955297	-1.964320
6	-6.239829	-1.664898	-2.249840
8	-5.062902	-1.035729	-2.058019
8	-6.332226	-2.781640	-2.677590
1	-7.681486	2.191734	-2.679699
1	2.578859	6.562316	-2.041404
1	-0.400913	6.433690	1.034239
7	0.899843	8.057799	-0.622787
8	1.581567	8.659325	-1.436833
8	0.071242	8.588291	0.100728

2-Michael-nitro-cinchona-thiourea-2R3S_si-si-path-A-TS

Number of imaginary frequencies : 1
The smallest frequency is : -293.1146

Electronic energy : =-3435.8545836
Zero-point correction= 1.049057
Thermal correction to Energy= 1.108511
Thermal correction to Enthalpy= 1.109455
Thermal correction to Gibbs Free Energy= 0.948598
Sum of electronic and zero-point Energies= -3434.805526
Sum of electronic and thermal Energies= -3434.746072
Sum of electronic and thermal Enthalpies= -3434.745128
Sum of electronic and thermal Free Energies= -3434.905986

Cartesian Coordinates

7	0.697790	2.126611	-1.155637
6	0.279421	3.185596	-1.950274
6	-0.649207	4.069336	-1.368148
6	-1.171473	5.122230	-2.095384
6	-0.761118	5.290725	-3.414013
6	0.145586	4.424964	-4.014991
6	0.664818	3.366900	-3.287215
6	1.828562	1.344224	-1.224743
16	3.226970	1.682944	-2.089072
7	1.695985	0.274016	-0.414299
6	2.771105	-0.624432	-0.046007
6	2.557829	-1.120318	1.401411
6	3.833879	-1.730736	2.017152
6	4.302194	-0.861444	3.194826
6	3.226573	-0.913289	4.290360
6	1.867720	-0.518120	3.681029
7	2.098360	0.005320	2.294856
6	3.073471	1.138521	2.329583
6	4.466437	0.608030	2.757478
6	5.512267	0.858023	1.695375
6	6.531948	0.060392	1.387945
6	2.852543	-1.842377	-0.961083
6	4.070726	-2.261076	-1.580554
6	4.025017	-3.456675	-2.357326
7	2.889692	-4.188410	-2.542059
6	1.791010	-3.757622	-1.972397
6	1.722254	-2.593356	-1.168983
6	5.215051	-3.918916	-2.970311
6	6.400334	-3.242755	-2.832594
6	6.438925	-2.047641	-2.069695
6	5.297381	-1.568494	-1.464094
1	1.722919	-1.821202	1.412090
1	3.629215	-2.744716	2.371511
1	4.611606	-1.805532	1.253435
1	1.360922	0.277461	4.231666
1	1.166813	-1.347321	3.578107
1	3.489170	-0.232964	5.105762
1	3.163590	-1.920224	4.710194
1	5.248880	-1.240749	3.587356

1	4.767616	1.180959	3.644042
1	2.661861	1.861926	3.034413
1	3.079895	1.600164	1.339654
1	5.412016	1.806221	1.165392
1	7.247965	0.340368	0.621724
1	6.693220	-0.898458	1.874586
1	3.699383	-0.051555	-0.100392
1	0.771464	-2.315349	-0.715745
1	5.373711	-0.635646	-0.918456
1	0.889230	-4.347688	-2.126169
1	5.155290	-4.831346	-3.554601
1	7.294728	-3.621967	-3.312219
1	0.760144	0.038692	-0.066842
1	0.263357	2.088374	-0.222123
1	-0.949197	3.917012	-0.333866
1	1.365713	2.684087	-3.746178
8	7.566569	-1.312545	-1.889187
6	8.746311	-1.729499	-2.549512
1	9.508304	-0.990610	-2.299958
1	9.077527	-2.715406	-2.202604
1	8.612047	-1.750999	-3.637090
1	1.192215	0.367723	1.947601
7	-1.315080	-0.708552	1.694915
6	-2.540561	-0.647510	1.139250
6	-0.410589	2.590542	3.764483
6	-2.497997	-2.714414	-0.354510
6	-2.480867	1.509514	0.781463
6	-2.480209	-3.568864	0.747349
6	-2.246759	-4.931724	0.585372
8	-0.302539	-0.989839	0.961552
6	-2.033617	-4.615995	-1.789589
6	-0.746577	2.185884	2.362189
6	-1.129227	2.102399	4.858986
8	-1.149244	-0.354940	2.884517
6	-2.261957	-3.252893	-1.622247
6	-0.757986	2.461496	6.151800
6	-4.108659	-0.749039	-0.818333
6	-2.745733	-1.212456	-0.235867
6	-2.119664	2.078324	1.985555
6	0.680330	3.438800	3.977310
6	-2.024241	-5.461528	-0.682434
6	-4.104254	0.772325	-1.051890
6	0.323056	3.316451	6.358514
8	0.216480	2.020383	1.566399
6	1.041318	3.807618	5.269524
6	-3.862956	1.638807	0.189276
1	-3.325635	-0.601375	1.881369
1	-4.210459	-1.246198	-1.789391
1	-3.320478	0.996491	-1.786459
1	-1.308791	2.068139	7.000582
1	-2.241445	-5.582000	1.454711
1	-4.627473	1.464926	0.956075
1	-1.856724	-5.016421	-2.783653
1	-2.879812	2.357189	2.708809
1	-1.683506	1.354284	0.050815
1	-2.250477	-2.595316	-2.489488
1	-3.977839	2.688100	-0.113923
1	-2.655693	-3.169411	1.742519
1	-1.986161	-0.746038	-0.880121
1	1.226918	3.811986	3.115825
1	0.606270	3.598449	7.367904
1	1.877640	4.481425	5.428389
1	-5.053066	1.074617	-1.503729
1	-1.945876	1.407731	4.688583
1	-1.843747	-6.524431	-0.808274
6	-8.715296	-1.793936	-0.672438
6	-8.032161	-1.755277	-2.041091
6	-6.940125	-0.693685	-1.853951
7	-6.606366	-0.676581	-0.400752
6	-7.525991	-1.617901	0.260581

6	-5.308012	-1.155008	0.027400
6	-6.699948	-2.906514	0.358976
8	-7.092912	-4.017659	0.587653
8	-5.410291	-2.605206	0.108500
1	-7.794903	-1.288207	1.270815
1	-9.243633	-2.727696	-0.469896
1	-9.409765	-0.957552	-0.552488
1	-7.582097	-2.731262	-2.254596
1	-8.712224	-1.511474	-2.859372
1	-6.066054	-0.898043	-2.474682
1	-7.315964	0.298346	-2.126560
1	-5.178597	-0.813273	1.062055
1	-1.881639	5.813685	-1.659047
1	0.430955	4.581613	-5.047979
7	-1.303596	6.401322	-4.187909
8	-0.915660	6.542202	-5.336392
8	-2.119108	7.131558	-3.646768

Substrate-Nitro

1-Michael-nitrostyrene-Ph-to-Me-*si-si*_path-A-TS

Number of imaginary frequencies : 1

The smallest frequency is : -292.3359

Electronic energy : =-3713.6128748

Zero-point correction= 0.998659

Thermal correction to Energy= 1.061411

Thermal correction to Enthalpy= 1.062355

Thermal correction to Gibbs Free Energy= 0.897185

Sum of electronic and zero-point Energies= -3712.614216

Sum of electronic and thermal Energies= -3712.551464

Sum of electronic and thermal Enthalpies= -3712.550520

Sum of electronic and thermal Free Energies= -3712.715690

Cartesian Coordinates

6	1.965521	0.118386	-5.312974
6	2.936707	-1.066428	-5.245877
6	4.069606	-0.559892	-4.341891
7	3.454387	0.535807	-3.578740
6	2.031306	0.667275	-3.878728
6	4.169278	1.368698	-2.821758
6	3.700216	2.298995	-1.915829
8	0.560460	2.031399	1.321353
8	0.844342	1.347409	-0.715952
1	1.722577	1.712539	-3.798481
1	0.948504	-0.166143	-5.587470
1	2.324891	0.876285	-6.016312
1	4.437340	-1.336171	-3.664678
1	4.914085	-0.166925	-4.920282
1	2.629755	2.497540	-1.885898
6	4.634493	3.392004	-1.449283
1	5.652413	2.993279	-1.353170
6	3.438287	0.774210	-0.262499
1	2.937509	0.169656	-1.015669
1	2.961638	1.733228	1.653396
7	1.299428	1.577320	0.433110
6	2.631996	1.363123	0.693190
7	0.819984	-1.635857	0.232930
6	1.869792	-2.143124	0.994454
6	1.876440	-2.323831	2.380727
6	3.028453	-2.808597	2.998562
6	4.183440	-3.105832	2.290538
6	4.165832	-2.907002	0.910823
6	3.036095	-2.440725	0.264207
6	3.037104	-2.931391	4.496168

9	1.838752	-3.277495	4.982194
6	5.423615	-3.169870	0.135920
9	5.809451	-4.451286	0.218889
6	-0.504223	-1.461493	0.491942
16	-1.309031	-1.846521	1.930742
7	-1.130687	-0.916209	-0.573979
6	-2.550914	-0.675175	-0.693568
6	-2.735187	0.723653	-1.309131
6	-4.204983	1.187685	-1.378137
6	-4.386674	2.448583	-0.521043
6	-3.516010	3.571334	-1.104701
6	-2.061308	3.074778	-1.221794
7	-1.948430	1.750785	-0.530617
6	-2.403084	1.881739	0.892624
6	-3.921101	2.189469	0.924618
6	-4.690638	1.130934	1.678501
6	-5.918102	0.697324	1.403209
6	-3.228034	-1.706502	-1.594003
6	-4.407547	-2.416987	-1.204887
6	-4.974839	-3.308549	-2.164237
7	-4.439462	-3.522468	-3.399868
6	-3.344974	-2.870577	-3.704084
6	-2.704639	-1.949833	-2.839843
6	-6.155611	-4.013561	-1.829222
6	-6.761244	-3.855742	-0.608877
6	-6.188752	-2.978358	0.346970
6	-5.034163	-2.283587	0.055165
9	3.924391	-3.845821	4.918263
9	3.372141	-1.768334	5.083075
9	6.447351	-2.432539	0.606617
9	5.295846	-2.872811	-1.166763
1	-2.260101	0.716371	-2.294844
1	-4.479993	1.401400	-2.414671
1	-4.860136	0.387249	-1.025810
1	-1.345123	3.748177	-0.747486
1	-1.747434	2.911380	-2.255016
1	-3.559822	4.449892	-0.453680
1	-3.887634	3.868454	-2.088579
1	-5.435788	2.755768	-0.526261
1	-4.037229	3.129795	1.480057
1	-1.803823	2.684859	1.324430
1	-2.139078	0.955214	1.410008
1	-4.171664	0.714559	2.543364
1	-6.391950	-0.064385	2.014911
1	-6.491515	1.063889	0.555259
1	-2.983425	-0.706696	0.307473
1	-1.798901	-1.444294	-3.169889
1	-4.624749	-1.646362	0.828851
1	-2.922597	-3.055901	-4.690100
1	-6.565205	-4.685819	-2.576046
1	-7.665010	-4.408360	-0.382050
1	-0.594182	-0.711480	-1.432557
1	1.093300	-1.452974	-0.755743
1	0.997007	-2.094293	2.965876
1	3.040880	-2.282493	-0.810978
1	5.070396	-3.477508	2.792385
8	-6.720240	-2.768684	1.579509
6	-7.866841	-3.512105	1.945688
1	-8.096348	-3.225170	2.972135
1	-8.725010	-3.272325	1.306826
1	-7.674906	-4.590636	1.910696
1	-0.936225	1.485934	-0.534833
6	1.130047	-0.198368	-2.974109
8	1.689490	-1.104627	-2.303030
8	-0.097844	0.041303	-3.039735
1	4.689625	4.168974	-2.225661
1	3.303938	-1.376930	-6.225502
1	2.444567	-1.918619	-4.771794
6	4.240476	4.096564	-0.140523
1	4.936144	4.933756	0.004622

1	4.353821	3.435739	0.723917
6	2.845452	4.636392	-0.195078
6	1.952383	4.596959	0.799587
1	2.526054	5.093114	-1.133492
1	2.206720	4.149781	1.754471
6	0.577905	5.110489	0.572906
8	0.254497	5.575231	-0.512356
6	-0.445966	5.035707	1.669400
6	-0.236286	4.372617	2.882307
6	-1.689915	5.629898	1.421062
6	-1.261061	4.293147	3.821994
1	0.702953	3.872944	3.084532
6	-2.709832	5.556402	2.361825
1	-1.832873	6.147436	0.477483
6	-2.497055	4.880769	3.564168
1	-1.094420	3.763594	4.754287
1	-3.669153	6.024781	2.162234
1	-3.293330	4.813582	4.299293
1	5.248203	1.219265	-2.901211
6	4.855961	0.433612	0.101361
1	5.361844	-0.091423	-0.711211
1	5.432574	1.329347	0.353660
1	4.863236	-0.215172	0.983625

1-Michael-nitrostyrene-Ph-to-Me-si-re_pathA-TS

Number of imaginary frequencies : 1

The smallest frequency is : -294.1953

Electronic energy : =-3713.6099239

Zero-point correction= 0.998799

Thermal correction to Energy= 1.061815

Thermal correction to Enthalpy= 1.062759

Thermal correction to Gibbs Free Energy= 0.895361

Sum of electronic and zero-point Energies= -3712.611125

Sum of electronic and thermal Energies= -3712.548109

Sum of electronic and thermal Enthalpies= -3712.547165

Sum of electronic and thermal Free Energies= -3712.714563

Cartesian Coordinates

6	2.511470	-2.321172	3.317864
6	3.422928	-1.191332	3.820868
6	4.423902	-0.961852	2.671847
7	3.858986	-1.694501	1.527395
6	2.473930	-2.092953	1.795568
6	4.630348	-2.323967	0.639904
6	4.191536	-2.906372	-0.532920
8	1.162109	0.390574	-1.202314
8	1.663523	-1.535156	-2.065752
1	2.246460	-2.994698	1.226664
1	1.514334	-2.296297	3.764711
1	2.959201	-3.300312	3.519332
1	2.837598	-0.286032	3.982459
1	3.929202	-1.453466	4.751717
1	4.520565	0.098815	2.426382
1	5.418460	-1.364560	2.890195
1	5.703037	-2.257699	0.833196
1	3.119035	-2.975504	-0.705529
6	5.033984	-3.938715	-1.230939
6	4.671528	-5.375384	-0.777994
1	6.096550	-3.769883	-1.020539
1	4.905189	-3.865344	-2.319320
1	5.350304	-6.082691	-1.268724
1	4.826166	-5.455356	0.303479
6	3.258622	-5.725652	-1.123872
6	2.243502	-5.780677	-0.254631

1	3.030859	-5.900675	-2.175804
1	2.411420	-5.593764	0.803168
6	0.866464	-6.069189	-0.741267
8	0.683240	-6.624238	-1.811938
6	-0.309603	-5.608720	0.071338
6	-0.181446	-4.741289	1.158797
6	-1.589326	-5.975804	-0.364668
6	-1.313354	-4.228876	1.788367
1	0.795602	-4.427725	1.505687
6	-2.718676	-5.476694	0.271551
1	-1.672166	-6.641391	-1.217799
6	-2.582172	-4.592055	1.344822
1	-1.198211	-3.528166	2.608565
1	-3.707463	-5.767500	-0.070429
1	-3.463868	-4.185849	1.832900
6	4.301605	-1.110847	-1.711853
1	4.007521	-1.769485	-2.524995
1	3.535352	0.679481	-0.701558
7	2.009545	-0.463114	-1.523180
6	3.340752	-0.219688	-1.264790
7	0.348847	2.342432	0.709286
6	1.276609	3.338236	0.407580
6	0.989147	4.635333	-0.034280
6	2.038470	5.516844	-0.277953
6	3.370829	5.164192	-0.091323
6	3.636964	3.879692	0.367156
6	2.614944	2.978296	0.619846
6	1.720717	6.885271	-0.810284
9	2.627975	7.795232	-0.419072
6	5.041884	3.404692	0.586225
9	5.949377	4.367187	0.385588
6	-0.900820	2.105673	0.231868
16	-1.878734	3.203113	-0.605343
7	-1.287328	0.836034	0.496711
6	-2.573577	0.272271	0.160397
6	-2.386757	-1.167134	-0.359139
6	-3.658722	-1.723356	-1.036495
6	-3.389182	-1.956379	-2.532053
6	-2.337246	-3.065061	-2.658652
6	-1.133046	-2.701580	-1.773351
7	-1.255839	-1.266664	-1.347228
6	-1.446687	-0.376369	-2.534165
6	-2.812926	-0.689703	-3.197010
6	-3.724621	0.515018	-3.201973
6	-5.048156	0.499189	-3.064412
6	-3.503056	0.208455	1.370463
6	-4.840694	0.709909	1.351020
6	-5.626767	0.507185	2.524988
7	-5.156156	-0.105689	3.647407
6	-3.913041	-0.520048	3.635457
6	-3.051508	-0.390642	2.520532
6	-6.967096	0.964184	2.537307
6	-7.516485	1.595988	1.451444
6	-6.727018	1.809825	0.292025
6	-5.417817	1.380445	0.248565
9	1.711660	6.906677	-2.154048
9	0.518415	7.317253	-0.406630
9	5.356168	2.385662	-0.242280
9	5.222914	2.934358	1.832979
1	-2.062362	-1.801664	0.470575
1	-3.942723	-2.671782	-0.569233
1	-4.486700	-1.024524	-0.893512
1	-0.174869	-2.795218	-2.280342
1	-1.101654	-3.282139	-0.850103
1	-2.028433	-3.173497	-3.702669
1	-2.747764	-4.024624	-2.333783
1	-4.312260	-2.253708	-3.036298
1	-2.609714	-0.938574	-4.246781
1	-0.591287	-0.574612	-3.182173
1	-1.370356	0.656683	-2.184457

1	-3.225292	1.471682	-3.358706
1	-5.625605	1.417488	-3.102658
1	-5.608095	-0.418402	-2.901292
1	-3.012937	0.892528	-0.623122
1	-2.031965	-0.765684	2.582050
1	-4.846107	1.598919	-0.645236
1	-3.546690	-0.996161	4.543272
1	-7.543292	0.796487	3.441443
1	-8.544484	1.936075	1.490793
1	-0.603812	0.173516	0.890346
1	0.808433	1.506908	1.115624
1	-0.034761	4.949412	-0.180571
1	2.834226	1.978761	0.988668
1	4.169541	5.870157	-0.284878
8	-7.190686	2.433383	-0.820714
6	-8.498286	2.972756	-0.787901
1	-8.647670	3.456679	-1.753317
1	-9.255679	2.190571	-0.659531
1	-8.605438	3.718996	0.007594
1	-0.370429	-0.990401	-0.884227
6	1.435497	-1.011344	1.468732
8	1.759591	0.170660	1.721065
8	0.315788	-1.421767	1.059871
6	5.743317	-0.687778	-1.661075
1	5.963186	-0.133041	-0.745536
1	6.421382	-1.541197	-1.735570
1	5.949552	-0.022729	-2.507112

1-Michael-nitrostyrene-Ph-to-Me-re-re_path-A-TS

Number of imaginary frequencies : 1
The smallest frequency is : -299.0964

Electronic energy : =-3713.6094415
Zero-point correction= 0.998725
Thermal correction to Energy= 1.061970
Thermal correction to Enthalpy= 1.062914
Thermal correction to Gibbs Free Energy= 0.892362
Sum of electronic and zero-point Energies= -3712.610716
Sum of electronic and thermal Energies= -3712.547471
Sum of electronic and thermal Enthalpies= -3712.546527
Sum of electronic and thermal Free Energies= -3712.717079

Cartesian Coordinates

6	2.671608	1.434487	3.182199
6	2.321526	2.884723	2.827161
6	2.879750	3.049446	1.412045
7	2.882643	1.685764	0.855692
6	2.485210	0.678151	1.862972
6	3.593438	1.367936	-0.226787
6	4.142843	2.286581	-1.102759
8	-0.322419	1.028855	-0.954066
6	1.022335	0.236449	1.633328
8	0.837650	-0.883490	1.093644
8	0.134907	1.032475	2.023267
8	1.517895	0.381755	-1.911466
1	3.134402	-0.194785	1.767984
1	2.036037	1.031613	3.972285
1	3.717995	1.358959	3.496107
1	1.239162	3.009380	2.826164
1	2.763319	3.608800	3.514556
1	2.287032	3.723805	0.787202
1	3.915197	3.416113	1.429747
1	3.644433	0.303868	-0.447916
1	4.275097	3.306916	-0.749426
6	5.078246	1.813630	-2.184522

6	6.565960	1.807492	-1.769823
1	4.979771	2.451326	-3.073014
1	4.787639	0.801080	-2.491542
1	7.183154	1.516611	-2.626318
1	6.852125	2.829714	-1.489147
6	6.823947	0.894622	-0.614595
6	7.565352	-0.216490	-0.657749
1	6.348718	1.140145	0.335076
1	8.070970	-0.505642	-1.573730
6	7.719055	-1.052141	0.564873
8	7.267906	-0.683601	1.637646
6	8.443902	-2.362310	0.471165
6	8.758085	-2.977408	-0.744182
6	8.790178	-2.996276	1.669541
6	9.412306	-4.206241	-0.758165
1	8.480513	-2.517993	-1.686563
6	9.450723	-4.216998	1.654799
1	8.529788	-2.509085	2.603281
6	9.763123	-4.824098	0.438695
1	9.646720	-4.681575	-1.705263
1	9.722060	-4.698789	2.588751
1	10.278852	-5.779348	0.424822
6	2.358031	2.877680	-2.262505
1	2.691469	2.122276	-2.967040
1	0.557569	3.323091	-1.085612
7	0.775851	1.290026	-1.478462
6	1.188934	2.602708	-1.583679
7	-2.350965	1.366432	0.937497
6	-2.570332	2.711263	0.645244
6	-3.789986	3.277738	0.265136
6	-3.860923	4.651971	0.046482
6	-2.762585	5.488066	0.204620
6	-1.559314	4.908705	0.596432
6	-1.454070	3.544069	0.813125
6	-5.197361	5.240636	-0.305953
9	-5.990259	5.351173	0.773067
6	-0.320050	5.740514	0.733826
9	-0.585295	7.048201	0.823704
6	-2.851807	0.244479	0.360168
16	-4.247225	0.145998	-0.586911
7	-2.058034	-0.821560	0.622155
6	-2.329573	-2.183093	0.228059
6	-1.030445	-2.844418	-0.271798
6	-1.295958	-4.175443	-1.009645
6	-0.858079	-4.045901	-2.476659
6	0.660085	-3.827396	-2.501758
6	1.004432	-2.621180	-1.608450
7	-0.266050	-1.936914	-1.200498
6	-1.060084	-1.547443	-2.403513
6	-1.525793	-2.827408	-3.146609
6	-3.031756	-2.886637	-3.253969
6	-3.789359	-3.978236	-3.180811
6	-2.862108	-3.014871	1.392847
6	-4.030881	-3.831649	1.296665
6	-4.380038	-4.601997	2.446148
7	-3.673294	-4.575915	3.611193
6	-2.622406	-3.795293	3.664921
6	-2.175946	-3.002113	2.581646
6	-5.518753	-5.441403	2.385282
6	-6.284858	-5.525772	1.251240
6	-5.941375	-4.749753	0.113854
6	-4.842416	-3.917724	0.142259
9	-5.083316	6.469957	-0.832911
9	-5.858649	4.484024	-1.192878
9	0.505442	5.583681	-0.327529
9	0.402436	5.396643	1.813292
1	-0.356472	-2.971821	0.578697
1	-0.741479	-4.988468	-0.532767
1	-2.357853	-4.424460	-0.943177
1	1.603143	-1.867079	-2.115405

1	1.508353	-2.896168	-0.680159
1	0.996223	-3.649277	-3.527524
1	1.175201	-4.720084	-2.137618
1	-1.110932	-4.957120	-3.024755
1	-1.135212	-2.765953	-4.170994
1	-0.395534	-0.920480	-3.000192
1	-1.892741	-0.926736	-2.062575
1	-3.516068	-1.925918	-3.431586
1	-4.867229	-3.916789	-3.292320
1	-3.377434	-4.968242	-3.001219
1	-3.061662	-2.150195	-0.581176
1	-1.287358	-2.385965	2.701929
1	-4.635963	-3.326396	-0.742393
1	-2.071169	-3.777558	4.603098
1	-5.764448	-6.016559	3.272020
1	-7.150572	-6.176983	1.236471
1	-1.150055	-0.652761	1.066418
1	-1.429201	1.215234	1.389138
1	-4.666017	2.654284	0.141317
1	-0.508276	3.092205	1.107835
1	-2.842002	6.554532	0.031342
8	-6.648431	-4.771910	-1.044600
6	-7.821675	-5.560974	-1.095303
1	-8.241954	-5.411879	-2.090085
1	-7.599461	-6.625607	-0.956527
1	-8.554425	-5.240209	-0.345873
1	0.001454	-1.076086	-0.684464
6	2.714418	4.307339	-2.560708
1	2.485129	4.962768	-1.717313
1	3.770842	4.417032	-2.817064
1	2.129057	4.651561	-3.420814

1-Michael-nitrostyrene-Ph-to-Me-re-si-TS

Number of imaginary frequencies : 1

The smallest frequency is : -263.5255

Electronic energy : =-3713.6024827

Zero-point correction= 0.999060

Thermal correction to Energy= 1.062239

Thermal correction to Enthalpy= 1.063184

Thermal correction to Gibbs Free Energy= 0.893563

Sum of electronic and zero-point Energies= -3712.603422

Sum of electronic and thermal Energies= -3712.540243

Sum of electronic and thermal Enthalpies= -3712.539299

Sum of electronic and thermal Free Energies= -3712.708920

Cartesian Coordinates

6	1.155886	-1.392469	4.662711
6	1.986647	-0.109386	4.501763
6	2.818276	-0.340189	3.229433
7	2.163171	-1.463999	2.563262
6	0.917099	-1.858610	3.220946
6	2.517594	-1.927242	1.366820
6	3.515857	-1.436054	0.548411
8	0.139640	-1.887216	-2.425517
6	-0.268281	-1.123773	2.565964
8	-1.296891	-1.784218	2.301852
8	-0.087659	0.109084	2.362702
8	0.041331	-1.528598	-0.285240
1	0.767821	-2.937557	3.133673
1	0.220618	-1.225651	5.201432
1	1.728311	-2.158448	5.194716
1	1.323795	0.743446	4.354089
1	2.619691	0.084611	5.369625
1	2.816777	0.542161	2.578048

1	3.860700	-0.607225	3.442541
1	1.896199	-2.745597	1.004381
1	4.221151	-0.719131	0.961194
6	3.948812	-2.284401	-0.623782
6	4.854693	-1.586605	-1.653288
1	3.054574	-2.650744	-1.147907
1	4.483926	-3.173758	-0.264444
1	5.122503	-2.310942	-2.429228
1	4.295345	-0.782618	-2.144484
6	6.098517	-1.022517	-1.042310
6	7.328413	-1.508815	-1.233967
1	6.002578	-0.160456	-0.381255
1	7.489827	-2.358222	-1.891500
6	8.499496	-0.870910	-0.572941
8	8.392873	0.197086	0.007370
6	9.830231	-1.558263	-0.641588
6	9.967606	-2.910786	-0.966481
6	10.968979	-0.806100	-0.334441
6	11.228509	-3.500048	-0.987847
1	9.094310	-3.517751	-1.181770
6	12.227310	-1.391296	-0.368961
1	10.841197	0.239111	-0.072502
6	12.358335	-2.740722	-0.696487
1	11.328273	-4.552934	-1.231497
1	13.107497	-0.799866	-0.137820
1	13.341604	-3.200349	-0.721854
6	2.128220	0.172242	-0.385436
1	1.507213	0.165323	0.509028
1	2.007813	-0.331919	-2.517064
7	0.558589	-1.305295	-1.410825
6	1.606970	-0.419921	-1.517693
7	-1.092796	1.374272	0.241332
6	-0.330875	2.510104	-0.023708
6	-0.297980	3.216455	-1.231984
6	0.563940	4.302685	-1.361954
6	1.413149	4.707672	-0.337484
6	1.381660	3.984668	0.849830
6	0.527757	2.904984	1.014389
6	0.536302	5.072685	-2.652487
9	-0.503616	5.919039	-2.703912
6	2.304693	4.320096	1.983976
9	1.635798	4.540658	3.125116
6	-2.271664	0.932135	-0.262954
16	-3.166220	1.654196	-1.506528
7	-2.660711	-0.204630	0.361781
6	-3.901073	-0.915365	0.149118
6	-3.560837	-2.413695	0.035352
6	-4.757046	-3.306086	-0.355847
6	-4.469311	-3.992440	-1.699326
6	-3.235400	-4.895238	-1.540152
6	-2.058492	-4.052411	-1.008059
7	-2.467643	-2.613881	-0.984537
6	-2.876017	-2.181226	-2.360833
6	-4.159202	-2.940778	-2.782685
6	-5.286896	-1.989478	-3.106864
6	-6.580608	-2.186404	-2.867455
6	-4.888035	-0.714772	1.296181
6	-6.257517	-0.362008	1.076225
6	-7.097032	-0.272075	2.226594
7	-6.652625	-0.476714	3.498920
6	-5.386003	-0.770320	3.656122
6	-4.466013	-0.908099	2.588246
6	-8.465786	0.044717	2.052625
6	-8.996585	0.265952	0.807710
6	-8.157191	0.189757	-0.332749
6	-6.817939	-0.108859	-0.196700
9	1.646964	5.805629	-2.824545
9	0.424982	4.259010	-3.713514
9	3.047713	5.404823	1.735126
9	3.157697	3.305474	2.237811

1	-3.107116	-2.724355	0.981889
1	-4.927933	-4.060349	0.417033
1	-5.661773	-2.697246	-0.423063
1	-1.166939	-4.098969	-1.635923
1	-1.779162	-4.310098	0.015631
1	-2.975305	-5.344873	-2.502698
1	-3.452720	-5.709795	-0.844719
1	-5.328804	-4.596546	-2.000863
1	-3.920233	-3.483556	-3.706703
1	-2.024718	-2.400709	-3.002614
1	-3.008708	-1.096094	-2.341057
1	-4.981211	-1.067604	-3.603936
1	-7.319970	-1.441556	-3.145460
1	-6.954367	-3.079952	-2.373292
1	-4.336022	-0.552694	-0.783174
1	-3.430696	-1.165964	2.802802
1	-6.217481	-0.129607	-1.097576
1	-5.041792	-0.922581	4.677440
1	-9.081129	0.104310	2.944459
1	-10.048546	0.504542	0.706718
1	-2.078244	-0.588700	1.123201
1	-0.756363	0.850765	1.086663
1	-0.933006	2.919293	-2.055755
1	0.521424	2.341472	1.944493
1	2.083581	5.549130	-0.463472
8	-8.599443	0.398442	-1.600207
6	-9.948427	0.786216	-1.780183
1	-10.077699	0.935808	-2.852330
1	-10.641953	0.007469	-1.441812
1	-10.169767	1.724382	-1.258589
1	-1.621550	-2.075418	-0.692928
6	3.113217	1.297668	-0.530486
1	3.576128	1.562222	0.421216
1	3.896702	1.078824	-1.259086
1	2.568873	2.179171	-0.893117

2-Michael-substrate-enone-Ph-to-Me-2R3S *re-re*-path-A-TS

Number of imaginary frequencies : 1

The smallest frequency is : -351.6241

Electronic energy : =-3713.6274634

Zero-point correction= 1.002815

Thermal correction to Energy= 1.063781

Thermal correction to Enthalpy= 1.064725

Thermal correction to Gibbs Free Energy= 0.900960

Sum of electronic and zero-point Energies= -3712.624648

Sum of electronic and thermal Energies= -3712.563683

Sum of electronic and thermal Enthalpies= -3712.562738

Sum of electronic and thermal Free Energies= -3712.726503

Cartesian Coordinates

7	-1.651023	-0.015789	-0.042106
6	-2.966081	0.057833	0.263351
6	-3.683685	-2.284218	-0.496863
6	-2.708570	0.964264	2.132226
6	-3.252327	-2.043619	-1.801748
6	-3.256029	-3.062201	-2.750067
8	-0.979836	-1.041372	0.291901
6	-4.124015	-4.592681	-1.112327
6	-0.471805	1.959664	2.323212
8	-1.087510	0.989830	-0.540237
6	-4.114074	-3.571661	-0.165414
6	-5.106390	-0.867349	1.111420
6	-3.693590	-1.212167	0.592712
6	-1.872923	2.072183	2.067871

6	-3.692268	-4.340373	-2.411059
6	-5.028576	-0.130369	2.456779
8	0.150129	0.878381	2.394149
6	-4.177643	1.145415	2.460399
1	-3.458815	0.869563	-0.258048
1	-5.634026	-1.813921	1.279267
1	-4.626190	-0.821476	3.207202
1	-2.925927	-2.851558	-3.762855
1	-4.598865	1.910985	1.797484
1	-4.463513	-5.585500	-0.832524
1	-2.294931	3.066351	1.945978
1	-2.238582	0.052430	2.513634
1	-4.437370	-3.781880	0.852743
1	-4.227870	1.573851	3.469229
1	-2.927601	-1.047633	-2.088762
1	-3.169953	-1.666365	1.446812
1	-6.047749	0.118378	2.774104
1	-3.698932	-5.131816	-3.153906
7	1.610632	1.825771	-0.330799
6	1.808317	3.194644	-0.509954
6	0.641197	3.970173	-0.461901
6	0.706273	5.345934	-0.615171
6	1.917259	5.990401	-0.841158
6	3.063474	5.207327	-0.909382
6	3.034139	3.825392	-0.747938
6	-0.575807	6.122798	-0.542368
9	-0.363981	7.439243	-0.418895
6	4.392378	5.882288	-1.103040
9	4.948393	6.228340	0.070050
6	2.457284	0.788126	-0.093305
16	4.123757	0.891868	0.156936
7	1.775816	-0.379222	-0.036661
6	2.351997	-1.686644	0.189197
6	1.453951	-2.475095	1.162360
6	2.142971	-3.735290	1.729942
6	2.297211	-3.592123	3.252225
6	0.896278	-3.514644	3.878193
6	0.111681	-2.370716	3.204349
7	1.036254	-1.605289	2.314158
6	2.203918	-1.095756	3.099411
6	3.049966	-2.293600	3.604218
6	4.474652	-2.210753	3.107798
6	5.239273	-3.227759	2.718179
6	2.477195	-2.489481	-1.101906
6	3.696519	-3.118976	-1.501984
6	3.664182	-3.887756	-2.703599
7	2.549065	-4.027493	-3.475249
6	1.457200	-3.420615	-3.080359
6	1.370451	-2.646098	-1.898369
6	4.844589	-4.546860	-3.124736
6	6.007509	-4.461697	-2.402866
6	6.037798	-3.690903	-1.212475
6	4.908231	-3.030300	-0.778950
9	-1.335365	5.942774	-1.633143
9	-1.323877	5.736444	0.509503
9	4.275338	7.009775	-1.821909
9	5.272260	5.092694	-1.732481
1	0.518759	-2.722162	0.655362
1	1.547436	-4.623161	1.501323
1	3.117554	-3.866889	1.253908
1	-0.295609	-1.651278	3.917156
1	-0.701089	-2.725476	2.566665
1	0.976707	-3.338525	4.954649
1	0.367941	-4.460770	3.737557
1	2.833977	-4.454217	3.656520
1	3.088294	-2.224511	4.699324
1	1.779332	-0.495952	3.904697
1	2.768300	-0.421054	2.451028
1	4.898906	-1.206179	3.101178
1	6.261766	-3.063435	2.393143

1	4.884752	-4.255240	2.699030
1	3.335034	-1.534911	0.637413
1	0.419433	-2.188281	-1.631728
1	4.992359	-2.432964	0.121522
1	0.573855	-3.538895	-3.705260
1	4.795486	-5.124264	-4.042104
1	6.894644	-4.977705	-2.750053
1	0.764146	-0.368689	-0.188589
1	0.620987	1.559748	-0.324805
1	-0.314131	3.481484	-0.273602
1	3.945522	3.247288	-0.805354
1	1.966203	7.066054	-0.962034
8	7.145832	-3.553316	-0.440566
6	8.342484	-4.171280	-0.874313
1	9.099029	-3.915852	-0.131904
1	8.240371	-5.261930	-0.919785
1	8.659663	-3.792604	-1.852745
1	0.510118	-0.769230	1.976723
6	-9.072211	0.534237	-1.099128
6	-9.140254	-0.995101	-1.085021
6	-7.763720	-1.367177	-0.532681
7	-7.390402	-0.300984	0.415190
6	-8.322614	0.832402	0.202587
6	-5.986117	-0.050177	0.150727
1	-7.776692	1.779737	0.183668
1	-10.053669	1.010486	-1.142111
1	-8.489993	0.873629	-1.963614
1	-9.921386	-1.343989	-0.403339
1	-9.301465	-1.444002	-2.067238
1	-7.728436	-2.367722	-0.088607
1	-5.768567	1.018562	0.223605
6	-6.700072	-1.272652	-1.629442
8	-5.738508	-0.419816	-1.222264
8	-6.702667	-1.804437	-2.704172
1	-9.023154	0.868248	1.044235
6	0.287991	3.227476	2.658042
1	0.303444	3.333590	3.749229
1	1.322881	3.143569	2.318492
1	-0.174929	4.122886	2.238734

2-Michael-substrate-enone-Ph-to-Me -2R3S_ *re-si*-path-A-TS

Number of imaginary frequencies : 1

The smallest frequency is : -309.7438

Electronic energy : =-3713.6241535

Zero-point correction= 1.002071

Thermal correction to Energy= 1.063234

Thermal correction to Enthalpy= 1.064178

Thermal correction to Gibbs Free Energy= 0.899122

Sum of electronic and zero-point Energies= -3712.622083

Sum of electronic and thermal Energies= -3712.560919

Sum of electronic and thermal Enthalpies= -3712.559975

Sum of electronic and thermal Free Energies= -3712.725031

Cartesian Coordinates

7	1.557497	-1.527869	-0.721166
6	2.652008	-0.958378	-0.166865
6	4.450030	-2.665437	-0.783896
6	2.206601	1.029614	-0.951329
6	3.818556	-3.657708	-0.033546
6	4.286613	-4.968438	-0.051229
8	1.589104	-1.911264	-1.908678
6	6.027681	-4.332239	-1.581489
6	0.890922	0.473683	-2.949604
8	0.458481	-1.552410	-0.061605

6	5.554779	-3.023144	-1.562622
6	5.038213	-0.226773	-0.239405
6	3.984966	-1.209182	-0.804087
6	2.101014	0.900895	-2.326430
6	5.392962	-5.311859	-0.823089
6	4.760307	1.219256	-0.680204
8	-0.212856	0.388951	-2.351626
6	3.369793	1.745732	-0.299626
1	2.547778	-0.808976	0.901590
1	6.007782	-0.517161	-0.661852
1	4.894952	1.289664	-1.765150
1	3.787664	-5.723928	0.548105
1	3.236705	1.725939	0.786711
1	6.888191	-4.587335	-2.192786
1	2.976205	1.023050	-2.956404
1	1.277245	1.032364	-0.381018
1	6.046234	-2.266730	-2.171664
1	3.303309	2.802570	-0.589038
1	2.963570	-3.402233	0.585866
1	3.870811	-0.953482	-1.866263
1	5.519218	1.868990	-0.230185
1	5.759047	-6.333647	-0.831232
7	-1.329011	1.933668	-0.362688
6	-1.158083	3.309878	-0.254499
6	-0.110766	3.856428	-1.008971
6	0.187175	5.207862	-0.918172
6	-0.542834	6.055442	-0.093366
6	-1.581428	5.501442	0.646797
6	-1.899061	4.148994	0.586145
6	1.355117	5.729580	-1.703811
9	1.386781	5.222629	-2.945344
6	-2.348846	6.375450	1.599040
9	-2.337160	7.660847	1.214607
6	-2.368310	1.113222	-0.008906
16	-3.943218	1.577251	0.344258
7	-1.970614	-0.178009	-0.050956
6	-2.864271	-1.312779	0.017491
6	-2.250643	-2.494080	-0.765864
6	-3.286625	-3.592280	-1.089113
6	-3.473479	-3.691720	-2.610848
6	-2.148300	-4.163345	-3.224613
6	-1.020708	-3.223774	-2.758043
7	-1.629257	-2.040663	-2.065789
6	-2.613404	-1.365356	-2.964562
6	-3.813947	-2.314546	-3.218241
6	-5.114639	-1.700398	-2.755982
6	-6.139677	-2.343325	-2.202316
6	-3.111956	-1.777973	1.450412
6	-4.415269	-2.071590	1.958091
6	-4.492931	-2.572218	3.291400
7	-3.402961	-2.757347	4.088596
6	-2.229571	-2.453886	3.591267
6	-2.032453	-1.967544	2.276331
6	-5.762633	-2.899714	3.826234
6	-6.909978	-2.745327	3.091395
6	-6.830180	-2.236720	1.769645
6	-5.610250	-1.901564	1.222673
9	1.336748	7.064076	-1.811197
9	2.526617	5.398671	-1.127358
9	-1.824396	6.336050	2.836062
9	-3.628709	5.998063	1.708563
1	-1.403933	-2.881967	-0.197274
1	-2.944219	-4.555376	-0.700936
1	-4.233458	-3.362526	-0.595463
1	-0.422644	-2.827807	-3.579816
1	-0.331937	-3.673375	-2.042023
1	-2.218484	-4.161493	-4.316238
1	-1.928782	-5.187006	-2.911643
1	-4.267015	-4.406058	-2.844367
1	-3.893812	-2.449462	-4.304835

1	-2.065474	-1.113066	-3.873999
1	-2.903980	-0.428132	-2.485730
1	-5.205588	-0.628005	-2.933115
1	-7.046487	-1.814579	-1.926707
1	-6.119833	-3.410656	-1.996750
1	-3.807928	-1.011870	-0.444583
1	-1.023840	-1.754968	1.927339
1	-5.606757	-1.494004	0.218708
1	-1.368914	-2.601966	4.240863
1	-5.794230	-3.278124	4.842693
1	-7.866920	-3.003759	3.528739
1	-0.966040	-0.378427	-0.083325
1	-0.672722	1.463910	-1.003702
1	0.473008	3.214053	-1.665982
1	-2.715799	3.751931	1.174365
1	-0.315456	7.113082	-0.035243
8	-7.915371	-2.049809	0.975168
6	-9.191273	-2.348683	1.508618
1	-9.908559	-2.115448	0.721376
1	-9.281036	-3.409418	1.771156
1	-9.414118	-1.734941	2.388808
1	-0.861613	-1.370196	-1.872095
6	7.327481	-0.001610	3.923806
6	8.232057	-0.828935	3.007066
6	7.345344	-1.014773	1.776249
7	6.539869	0.213568	1.652956
6	6.658730	0.955448	2.932401
6	5.215375	-0.251333	1.287447
1	5.678821	1.310240	3.263642
1	7.870838	0.518580	4.714938
1	6.579825	-0.651514	4.393169
1	9.130477	-0.266551	2.736700
1	8.529854	-1.792892	3.424660
1	7.906327	-1.252966	0.866371
1	4.450097	0.347463	1.787475
6	6.304499	-2.110296	2.020833
8	5.078450	-1.592597	1.807165
8	6.493435	-3.235006	2.392844
1	7.291944	1.834043	2.766295
6	0.916845	0.119596	-4.417720
1	1.836559	0.436048	-4.912443
1	0.838561	-0.969256	-4.507157
1	0.055194	0.568401	-4.918837

2-Michael-substrate-enone-Ph-to-Me-2R3S_si-path-A-TS

Number of imaginary frequencies : 1

The smallest frequency is : -281.8117

Electronic energy : =-3713.6219935

Zero-point correction= 1.003109

Thermal correction to Energy= 1.064173

Thermal correction to Enthalpy= 1.065117

Thermal correction to Gibbs Free Energy= 0.901515

Sum of electronic and zero-point Energies= -3712.618884

Sum of electronic and thermal Energies= -3712.557820

Sum of electronic and thermal Enthalpies= -3712.556876

Sum of electronic and thermal Free Energies= -3712.720478

Cartesian Coordinates

7	0.531408	2.042367	0.189259
6	-0.066314	3.241567	-0.186320
6	-1.101237	3.696840	0.642517
6	-1.813995	4.839437	0.309180
6	-1.515040	5.569594	-0.835258
6	-0.483111	5.109569	-1.645704

6	0.237997	3.958067	-1.349372
6	-2.962928	5.240577	1.187823
9	-3.340187	6.508333	0.981398
6	-0.093697	5.903180	-2.861332
9	0.912159	6.751605	-2.596590
6	1.720679	1.464747	-0.181079
16	3.019570	2.230693	-0.917286
7	1.740011	0.170953	0.208695
6	2.924657	-0.659171	0.272702
6	2.818844	-1.600488	1.493093
6	4.172455	-2.220939	1.898449
6	4.556447	-1.734163	3.303518
6	3.509911	-2.261881	4.298060
6	2.106637	-1.828963	3.829328
7	2.257259	-0.870548	2.689110
6	3.101713	0.291958	3.096807
6	4.549106	-0.192872	3.367670
6	5.541563	0.501268	2.463263
6	6.639694	-0.032901	1.934500
6	3.112987	-1.514436	-0.975328
6	4.360827	-1.598043	-1.667833
6	4.422995	-2.483725	-2.784257
7	3.362949	-3.225389	-3.213855
6	2.234548	-3.107337	-2.558089
6	2.060122	-2.268796	-1.430647
6	5.645639	-2.612294	-3.487144
6	6.763155	-1.910682	-3.113901
6	6.696187	-1.026309	-2.006779
6	5.518423	-0.869827	-1.308190
9	-4.045506	4.469712	0.967723
9	-2.663908	5.112690	2.488794
9	-1.114505	6.641656	-3.322939
9	0.317220	5.113085	-3.863218
1	2.070767	-2.364070	1.279544
1	4.096618	-3.311587	1.897729
1	4.936502	-1.949021	1.166722
1	1.539387	-1.302199	4.599352
1	1.483429	-2.644185	3.458381
1	3.713703	-1.870392	5.298871
1	3.561992	-3.351892	4.354518
1	5.545652	-2.112221	3.574175
1	4.798448	0.093291	4.397795
1	2.621307	0.720199	3.977435
1	3.047535	1.033961	2.297272
1	5.323272	1.550791	2.261479
1	7.302263	0.558838	1.310957
1	6.921693	-1.070956	2.092060
1	3.777563	0.012310	0.396377
1	1.092277	-2.245727	-0.930145
1	5.514498	-0.161849	-0.487556
1	1.394640	-3.706175	-2.905125
1	5.666115	-3.290209	-4.334160
1	7.685240	-2.032074	-3.669771
1	0.853030	-0.274816	0.467121
1	0.155937	1.627647	1.054679
1	-1.348343	3.144916	1.547470
1	1.024400	3.621326	-2.011784
1	-2.069253	6.465151	-1.089380
8	7.753732	-0.295237	-1.569830
6	8.967607	-0.382533	-2.291610
1	9.662465	0.295072	-1.794918
1	9.379767	-1.398231	-2.267686
1	8.840347	-0.064388	-3.332792
1	1.307397	-0.516685	2.469127
7	-1.109645	-1.745385	1.870463
6	-2.311722	-1.606953	1.274245
6	-2.024500	-3.101280	-0.770641
6	-2.449217	0.546475	1.600404
6	-2.017892	-4.254511	0.013664
6	-1.676567	-5.486075	-0.537852

8	-0.043713	-1.702305	1.158266
6	-1.330296	-4.437444	-2.674681
6	-0.876077	0.848291	3.450652
8	-1.030035	-1.779693	3.117665
6	-1.665240	-3.206408	-2.116867
6	-3.770943	-1.202612	-0.733119
6	-2.402191	-1.728819	-0.219083
6	-2.207888	0.762383	2.941916
6	-1.334183	-5.584100	-1.883447
6	-3.884345	0.313971	-0.498338
8	0.143967	0.951554	2.719916
6	-3.799892	0.764076	0.962827
1	-3.128296	-1.862353	1.935208
1	-3.782893	-1.387869	-1.812989
1	-3.076507	0.803197	-1.057550
1	-1.682239	-6.374110	0.086723
1	-4.592032	0.308417	1.568942
1	-1.060968	-4.499114	-3.725232
1	-3.029489	0.751620	3.652349
1	-1.604171	0.674564	0.920287
1	-1.644817	-2.311137	-2.735905
1	-3.984925	1.846013	0.988819
1	-2.289780	-4.193570	1.063842
1	-1.658912	-1.033831	-0.636317
1	-4.823975	0.681631	-0.919341
1	-1.071272	-6.545636	-2.313094
6	-8.286071	-2.514279	-1.228373
6	-7.549403	-2.005791	-2.469774
6	-6.547729	-0.996993	-1.892355
7	-6.282848	-1.415980	-0.485930
6	-7.155575	-2.570318	-0.211750
6	-4.972082	-1.923838	-0.136292
6	-6.236337	-3.771818	-0.464489
8	-6.550699	-4.918954	-0.628630
8	-4.963951	-3.330820	-0.511514
1	-7.491706	-2.591362	0.831400
1	-8.748522	-3.494240	-1.361513
1	-9.047463	-1.801639	-0.898747
1	-7.019798	-2.837042	-2.948121
1	-8.210832	-1.555869	-3.212542
1	-5.634585	-0.948608	-2.488331
1	-6.982154	0.008227	-1.869213
1	-4.918800	-1.912368	0.959631
6	-0.687463	0.842748	4.949166
1	0.256034	1.326104	5.210825
1	-1.510457	1.347046	5.461090
1	-0.670549	-0.197079	5.291613

Stationary Points relevant to Scheme S6 and Fig. S15: Epimerization of 2,3-*syn* to 2,3-*anti* product

[14]A

Number of imaginary frequencies : 0

Electronic energy=	-3981.7364677
Zero-point correction=	1.082219
Thermal correction to Energy=	1.150282
Thermal correction to Enthalpy=	1.151226
Thermal correction to Gibbs Free Energy=	0.969239
Sum of electronic and zero-point Energies=	-3980.654248
Sum of electronic and thermal Energies=	-3980.586186
Sum of electronic and thermal Enthalpies=	-3980.585242

Sum of electronic and thermal Free Energies= -3980.767229

Cartesian Coordinates			
7	-4.092113	-0.741096	-0.088625
6	-3.213438	-1.005688	-1.288311
6	-7.474822	-2.454074	-1.256877
6	-1.409345	0.334271	-0.128809
6	-3.618539	-2.350833	-1.915414
6	-1.689638	1.588063	-0.689473
6	-1.394593	2.761162	0.002376
8	-3.728169	-1.157264	0.991590
6	-0.543392	1.461165	1.842727
6	-6.010441	-2.715404	-1.122276
6	-8.080422	-2.227212	-2.495785
8	-5.135646	-0.144039	-0.294811
6	-0.849953	0.288785	1.151872
6	-9.452518	-2.009793	-2.570383
6	-0.798076	-1.305632	-2.027949
6	-1.748734	-0.963376	-0.842457
6	-5.098224	-2.388760	-2.300806
6	-8.249296	-2.449279	-0.092531
6	-0.812409	2.701091	1.268244
6	-1.235756	-2.592670	-2.742756
6	-10.219122	-2.001190	-1.407356
8	-5.550647	-3.191591	-0.103143
6	-9.616438	-2.216707	-0.168428
6	-2.714557	-2.588369	-3.127885
1	-3.461109	-0.191358	-1.976963
1	0.194924	-1.447404	-1.587183
1	-1.047618	-3.438299	-2.071059
1	-9.922967	-1.845056	-3.534368
1	-1.605793	3.721629	-0.457489
1	-2.918455	-1.820673	-3.887156
1	-0.103172	1.400541	2.833697
1	-5.412420	-1.446286	-2.763109
1	-3.436027	-3.131717	-1.166374
1	-0.660457	-0.679835	1.604400
1	-2.976082	-3.549050	-3.582518
1	-2.145533	1.664684	-1.673377
1	-1.614321	-1.778405	-0.122789
1	-7.757425	-2.613582	0.860697
1	-11.288429	-1.822852	-1.465891
1	-10.213516	-2.201100	0.737482
1	-0.610509	-2.751788	-3.628524
1	-7.490323	-2.232183	-3.407322
1	-0.568808	3.616288	1.799463
7	1.896538	1.671859	-0.619422
6	1.974599	3.067648	-0.621360
6	1.254081	3.743664	-1.609845
6	1.189057	5.130668	-1.599430
6	1.852043	5.878697	-0.634091
6	2.578369	5.192633	0.332918
6	2.640614	3.803592	0.361733
6	0.344432	5.797607	-2.645076
9	0.424979	7.131832	-2.593505
6	3.274986	5.944267	1.432018
9	2.673040	5.741009	2.617527
6	2.836319	0.750552	-0.240889
16	4.432012	1.073382	0.144005
7	2.313819	-0.503364	-0.254697
6	3.100264	-1.703995	-0.034024
6	2.114233	-2.882342	0.131161
6	2.817257	-4.167516	0.642670
6	2.175396	-4.572180	1.979258
6	0.691619	-4.878944	1.729062
6	0.045867	-3.628832	1.071579
7	0.991799	-2.504583	1.009278
6	1.465532	-2.210588	2.370207
6	2.250955	-3.411503	2.989507

6	3.637674	-3.011185	3.425672
6	4.762084	-3.706805	3.268317
6	4.025769	-1.977794	-1.213162
6	5.372842	-2.433360	-1.056519
6	6.098395	-2.741630	-2.245494
7	5.581087	-2.607656	-3.499816
6	4.355665	-2.156879	-3.600409
6	3.542658	-1.831863	-2.489254
6	7.430984	-3.207339	-2.132936
6	8.035706	-3.358952	-0.911942
6	7.317603	-3.035991	0.267802
6	6.019567	-2.578228	0.192060
9	0.689633	5.417345	-3.883710
9	-0.955582	5.471593	-2.498156
9	3.282945	7.266691	1.214993
9	4.546971	5.550672	1.575757
1	1.667844	-3.067583	-0.855714
1	2.698579	-4.980050	-0.081139
1	3.890122	-4.001983	0.760995
1	-0.838727	-3.297986	1.627782
1	-0.275483	-3.847598	0.046563
1	0.194380	-5.120441	2.673973
1	0.593776	-5.753085	1.077895
1	2.676674	-5.455988	2.385331
1	1.714782	-3.728867	3.894705
1	0.583839	-1.974006	2.975351
1	2.083455	-1.305817	2.340854
1	3.692090	-2.052034	3.943845
1	5.710535	-3.329265	3.637079
1	4.788427	-4.670498	2.765736
1	3.691802	-1.589607	0.881258
1	2.540118	-1.444837	-2.652258
1	5.522512	-2.328694	1.122096
1	3.957930	-2.038427	-4.606777
1	7.959183	-3.436394	-3.052761
1	9.057388	-3.715433	-0.858196
1	1.322296	-0.598197	-0.041000
1	1.133452	1.291226	-1.178066
1	0.734578	3.174319	-2.376935
1	3.192759	3.296335	1.142925
1	1.803851	6.960648	-0.634318
8	7.842302	-3.151291	1.514727
6	9.192386	-3.556942	1.633247
1	9.413502	-3.559967	2.700729
1	9.347751	-4.565692	1.233040
1	9.868465	-2.856683	1.129085
1	-5.255297	-3.172993	-3.053952
6	-0.640938	-0.169227	-3.007867
8	0.195290	0.700146	-2.882258
1	-1.315110	-0.151914	-3.887970
6	-3.754238	2.038918	4.323673
6	-4.669547	3.119137	3.743300
6	-4.364593	3.040750	2.243996
7	-4.095783	1.608782	1.987754
6	-3.894413	0.928907	3.275498
6	-5.110021	0.045549	3.602886
8	-5.251812	-0.480920	4.682057
8	-5.995278	-0.076414	2.623110
1	-3.025437	0.264607	3.235648
1	-4.037357	1.697707	5.320458
1	-2.718075	2.394210	4.347745
1	-5.717423	2.857641	3.930534
1	-4.491247	4.114800	4.154547
1	-5.195987	3.395161	1.627614
1	-3.482407	3.648574	2.004973
1	-5.614023	0.400576	1.850353
1	-3.282224	1.495407	1.392692

[14-15]A-TS

Number of imaginary frequencies : 1
The smallest frequency is : -1222.1926

Electronic energy= -3981.6993612
Zero-point correction= 1.078334
Thermal correction to Energy= 1.145595
Thermal correction to Enthalpy= 1.146539
Thermal correction to Gibbs Free Energy= 0.966634
Sum of electronic and zero-point Energies= -3980.621027
Sum of electronic and thermal Energies= -3980.553767
Sum of electronic and thermal Enthalpies= -3980.552822
Sum of electronic and thermal Free Energies= -3980.732727

Cartesian Coordinates

7	3.946376	-1.173204	-0.049443
6	2.900150	-1.822250	0.822413
6	7.207864	-2.619281	1.361507
6	1.264485	-0.278236	-0.289539
6	3.366129	-3.254231	1.135079
6	1.632470	0.812125	0.513687
6	1.528349	2.117889	0.041510
8	3.879934	-1.351362	-1.248797
6	0.633353	1.296711	-2.035074
6	5.893688	-3.108256	0.846388
6	7.552534	-2.696731	2.713183
8	4.820993	-0.534531	0.514670
6	0.772700	-0.011327	-1.568024
6	8.800568	-2.252175	3.138706
6	0.476877	-2.466024	0.959381
6	1.531505	-1.723718	0.119672
6	4.733119	-3.266737	1.825059
6	8.109133	-2.077758	0.439879
6	1.023021	2.366588	-1.235625
6	0.938792	-3.893664	1.270263
6	9.695587	-1.710485	2.218802
8	5.748653	-3.385963	-0.327439
6	9.346993	-1.617474	0.871821
6	2.288468	-3.922563	1.988561
1	2.914922	-1.235216	1.744299
1	-0.710916	-2.612914	0.010634
1	1.047738	-4.474939	0.347675
1	9.072968	-2.323959	4.186864
1	1.831988	2.944532	0.677866
1	2.208477	-3.406378	2.956173
1	0.243096	1.474001	-3.032615
1	4.787485	-2.496881	2.602436
1	3.456072	-3.791242	0.182185
1	0.528086	-0.841996	-2.224270
1	2.592954	-4.954692	2.196178
1	2.008486	0.647916	1.518332
1	1.639332	-2.288805	-0.816301
1	7.808483	-2.002103	-0.600332
1	10.664972	-1.354555	2.554097
1	10.040620	-1.183910	0.158616
1	0.183649	-4.407103	1.877802
1	6.857188	-3.116039	3.434752
1	0.923851	3.385737	-1.598248
7	-1.652714	1.558624	0.684274
6	-1.476858	2.947156	0.734462
6	-0.834530	3.453558	1.867480
6	-0.504286	4.799881	1.940134
6	-0.818126	5.676666	0.908249
6	-1.469826	5.160669	-0.205170
6	-1.796350	3.813167	-0.313039
6	0.298988	5.270967	3.116808
9	0.263247	6.601630	3.255856

6	-1.738993	6.036411	-1.394820
9	-0.868415	5.775858	-2.389107
6	-2.619896	0.820323	0.074785
16	-3.915839	1.423088	-0.808613
7	-2.417810	-0.513043	0.270073
6	-3.484096	-1.480777	0.107047
6	-2.933228	-2.926352	0.013165
6	-3.985664	-3.855747	-0.643961
6	-3.495204	-4.272411	-2.042120
6	-2.294787	-5.198719	-1.843844
6	-1.299663	-4.475199	-0.918439
7	-1.654073	-3.029975	-0.757999
6	-1.799155	-2.421228	-2.106520
6	-3.000768	-3.065984	-2.864218
6	-4.055428	-2.056679	-3.245461
6	-5.370095	-2.262690	-3.268831
6	-4.472312	-1.421912	1.276764
6	-5.891782	-1.431266	1.106952
6	-6.689265	-1.473905	2.289453
7	-6.167582	-1.469307	3.548219
6	-4.864293	-1.408090	3.661697
6	-3.978518	-1.387317	2.558179
6	-8.099162	-1.515428	2.162106
6	-8.707364	-1.503273	0.933361
6	-7.912182	-1.432322	-0.239936
6	-6.537718	-1.390233	-0.148933
9	-0.126996	4.728408	4.266292
9	1.592578	4.921783	2.983360
9	-1.624122	7.338675	-1.103757
9	-2.964297	5.837896	-1.896323
1	-2.676421	-3.265308	1.025301
1	-4.135746	-4.754521	-0.038076
1	-4.948398	-3.344355	-0.699581
1	-0.282380	-4.504887	-1.314025
1	-1.287521	-4.908914	0.084093
1	-1.828166	-5.431014	-2.805748
1	-2.605996	-6.143614	-1.390681
1	-4.291713	-4.792094	-2.580463
1	-2.603040	-3.466708	-3.806179
1	-0.857883	-2.599976	-2.633118
1	-1.921216	-1.343351	-1.981750
1	-3.673559	-1.086557	-3.565529
1	-6.050811	-1.482434	-3.594475
1	-5.822531	-3.203485	-2.963981
1	-3.996471	-1.231875	-0.823427
1	-2.908174	-1.323675	2.743745
1	-5.974031	-1.297451	-1.069913
1	-4.459401	-1.383294	4.671545
1	-8.682287	-1.551590	3.076452
1	-9.788421	-1.535300	0.869249
1	-1.703353	-0.732613	0.959178
1	-0.990501	1.028463	1.254126
1	-0.576170	2.784377	2.684040
1	-2.267545	3.433926	-1.210310
1	-0.557161	6.726587	0.967709
8	-8.431546	-1.400705	-1.493417
6	-9.839815	-1.382298	-1.631565
1	-10.035729	-1.324689	-2.702486
1	-10.295866	-2.296315	-1.233559
1	-10.281521	-0.508302	-1.139535
1	4.872635	-4.233142	2.329198
6	-0.135861	-1.837000	2.086904
8	-0.381615	-0.629612	2.278959
1	-0.528558	-2.558162	2.839291
6	4.876301	2.134043	-4.033789
6	5.408471	3.174599	-3.045765
6	4.541221	2.915282	-1.813323
7	4.387718	1.448804	-1.786984
6	4.681972	0.912242	-3.123857
6	5.971920	0.075452	-3.090977

8	6.478717	-0.365350	-4.096150
8	6.499935	-0.099081	-1.886277
1	3.889738	0.246106	-3.477515
1	5.545541	1.917100	-4.867665
1	3.908255	2.456723	-4.431512
1	6.460599	2.969459	-2.816510
1	5.330929	4.202647	-3.405478
1	4.997620	3.274026	-0.885913
1	3.570131	3.415929	-1.929162
1	5.864956	0.303714	-1.248534
1	3.465594	1.171067	-1.467178

[15A]

Number of imaginary frequencies : 0

Electronic energy=	-3981.7136775
Zero-point correction=	1.082618
Thermal correction to Energy=	1.149992
Thermal correction to Enthalpy=	1.150937
Thermal correction to Gibbs Free Energy=	0.971472
Sum of electronic and zero-point Energies=	-3980.631059
Sum of electronic and thermal Energies=	-3980.563685
Sum of electronic and thermal Enthalpies=	-3980.562741
Sum of electronic and thermal Free Energies=	-3980.742206

Cartesian Coordinates

7	4.164339	-1.228304	0.046030
6	3.220461	-1.809629	1.068121
6	7.509157	-2.768496	0.958052
6	1.458923	-0.278287	0.142639
6	3.667452	-3.251619	1.373783
6	1.661908	0.795561	1.020588
6	1.479912	2.106312	0.594319
8	3.913643	-1.386856	-1.132215
6	0.837564	1.316597	-1.589444
6	6.118144	-3.241396	0.686796
6	8.079047	-2.819392	2.232220
8	5.154155	-0.654627	0.474257
6	1.056664	0.002447	-1.163641
6	9.384853	-2.379713	2.427312
6	0.848512	-2.357041	1.568986
6	1.768915	-1.707503	0.551240
6	5.124192	-3.316542	1.842310
6	8.244919	-2.259266	-0.116100
6	1.058047	2.372030	-0.712641
6	1.259312	-3.767862	1.915206
6	10.112965	-1.866884	1.356430
8	5.779913	-3.563665	-0.435304
6	9.540541	-1.801321	0.086493
6	2.706122	-3.833912	2.412776
1	3.370038	-1.185403	1.952940
1	-0.967873	-1.540490	-0.596859
1	1.192277	-4.425306	1.030704
1	9.831949	-2.433191	3.414840
1	1.654881	2.928442	1.282323
1	2.795906	-3.272055	3.351834
1	0.522583	1.510190	-2.610839
1	5.335908	-2.532631	2.577062
1	3.582653	-3.825914	0.442282
1	0.963532	-0.815100	-1.877735
1	2.998986	-4.869514	2.619675
1	1.955223	0.597709	2.047646
1	1.757766	-2.316621	-0.365995
1	7.774185	-2.204181	-1.092555
1	11.127197	-1.512118	1.512477

1	10.103595	-1.388942	-0.744666
1	0.581716	-4.181841	2.669289
1	7.513793	-3.214488	3.071480
1	0.900574	3.396806	-1.036691
7	-1.898929	1.770243	0.749527
6	-1.745619	3.159907	0.758741
6	-1.049655	3.697295	1.847800
6	-0.755052	5.052050	1.894337
6	-1.163345	5.915019	0.883464
6	-1.867784	5.372651	-0.183729
6	-2.153148	4.013095	-0.270889
6	0.085490	5.553633	3.031836
9	0.072870	6.888675	3.122408
6	-2.268912	6.245528	-1.339209
9	-1.471402	6.041480	-2.402963
6	-2.843803	0.976004	0.159539
16	-4.124162	1.513771	-0.805098
7	-2.612047	-0.321112	0.439431
6	-3.525853	-1.388844	0.116733
6	-2.683146	-2.635469	-0.225713
6	-3.468747	-3.752929	-0.940665
6	-2.915897	-3.944702	-2.361272
6	-1.465910	-4.435235	-2.253593
6	-0.664174	-3.440310	-1.392381
7	-1.521570	-2.239773	-1.114666
6	-1.976171	-1.621212	-2.404183
6	-2.914376	-2.614019	-3.140488
6	-4.272970	-2.005156	-3.397069
6	-5.441139	-2.640790	-3.359203
6	-4.451568	-1.724838	1.284916
6	-5.833486	-2.047240	1.106879
6	-6.566418	-2.427152	2.270263
7	-6.023697	-2.469348	3.519425
6	-4.766451	-2.123671	3.644402
6	-3.938863	-1.745790	2.559102
6	-7.932550	-2.774727	2.134711
6	-8.561870	-2.744275	0.916830
6	-7.836626	-2.343012	-0.234583
6	-6.505586	-1.997697	-0.135416
9	-0.317597	5.060720	4.211452
9	1.371780	5.180111	2.881888
9	-2.193373	7.549024	-1.037769
9	-3.520578	5.994541	-1.743975
1	-2.198983	-2.993787	0.689767
1	-3.378956	-4.689958	-0.384969
1	-4.527959	-3.491517	-0.969599
1	0.232005	-3.075880	-1.898746
1	-0.377128	-3.840573	-0.417976
1	-1.020360	-4.518707	-3.248454
1	-1.434860	-5.425873	-1.794162
1	-3.514506	-4.685082	-2.897370
1	-2.461765	-2.812049	-4.120459
1	-1.068153	-1.406910	-2.971830
1	-2.464385	-0.672785	-2.164133
1	-4.260179	-0.949061	-3.667596
1	-6.365974	-2.119901	-3.584618
1	-5.531261	-3.692237	-3.097244
1	-4.116096	-1.089408	-0.752950
1	-2.909100	-1.449824	2.751284
1	-6.005123	-1.668804	-1.038562
1	-4.350010	-2.143080	4.649716
1	-8.466229	-3.062523	3.034610
1	-9.608824	-3.014169	0.847142
1	-1.839625	-0.520217	1.182255
1	-1.225764	1.265524	1.331276
1	-0.729678	3.041742	2.653757
1	-2.682838	3.619338	-1.128029
1	-0.939056	6.973863	0.927359
8	-8.384755	-2.270192	-1.474275
6	-9.759411	-2.577254	-1.614250

1	-9.993755	-2.429969	-2.668701
1	-9.969677	-3.618288	-1.342500
1	-10.384495	-1.908546	-1.011924
1	5.294303	-4.277456	2.347559
6	-0.201385	-1.783617	2.224053
8	-0.724888	-0.596184	2.121735
1	-0.685617	-2.461288	2.955714
6	4.237736	2.464424	-3.620231
6	5.055463	3.391770	-2.718480
6	4.576679	2.993315	-1.320002
7	4.339763	1.538609	-1.410592
6	4.276777	1.152474	-2.826128
6	5.522988	0.338264	-3.213018
8	5.767693	0.043255	-4.360024
8	6.317582	0.006250	-2.204149
1	3.412316	0.510484	-3.023331
1	4.640188	2.344847	-4.627199
1	3.204523	2.822503	-3.688601
1	6.123794	3.172796	-2.829777
1	4.903011	4.452943	-2.925861
1	5.312115	3.218747	-0.542091
1	3.648773	3.526703	-1.073716
1	5.863744	0.303823	-1.382131
1	3.493278	1.272438	-0.918508

[16]A

Number of imaginary frequencies : 0

Electronic energy=	-3981.7339729
Zero-point correction=	1.082176
Thermal correction to Energy=	1.150039
Thermal correction to Enthalpy=	1.150983
Thermal correction to Gibbs Free Energy=	0.970366
Sum of electronic and zero-point Energies=	-3980.651797
Sum of electronic and thermal Energies=	-3980.583934
Sum of electronic and thermal Enthalpies=	-3980.582989
Sum of electronic and thermal Free Energies=	-3980.763607

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Cartesian Coordinates

7	-4.099670	-1.102848	-0.291780
6	-2.637786	-1.273109	-0.615124
6	-4.885008	-4.551738	1.453811
6	-2.746207	0.965457	-1.792103
6	-1.979535	-2.109525	0.498686
6	-3.005705	0.536277	-3.099228
6	-3.722829	1.344218	-3.979798
8	-4.429679	-0.161810	0.399115
6	-3.948593	3.021548	-2.263707
6	-3.925221	-3.407341	1.517195
6	-6.177167	-4.350712	1.948092
8	-4.861747	-1.949449	-0.732707
6	-3.234356	2.208719	-1.385898
6	-7.102521	-5.385884	1.915572
6	-0.514335	-0.116246	-1.107228
6	-1.984619	0.109602	-0.801558
6	-2.658063	-3.470504	0.671290
6	-4.526489	-5.797061	0.931596
6	-4.192467	2.590912	-3.565578
6	0.189153	-0.910795	-0.041057
6	-6.738419	-6.630492	1.402853
8	-4.139359	-2.453728	2.238332
6	-5.450383	-6.837148	0.914771
6	-0.491037	-2.267167	0.167200
1	-2.637870	-1.839168	-1.551003
1	1.862081	-0.570757	-2.101877

1	0.150013	-0.349341	0.904591
1	-8.108677	-5.223829	2.288407
1	-3.917612	0.998093	-4.990187
1	-0.385999	-2.876090	-0.742215
1	-4.310923	3.986486	-1.922806
1	-2.881830	-3.924347	-0.300580
1	-2.082935	-1.547539	1.435302
1	-3.072089	2.530056	-0.361336
1	-0.005984	-2.812186	0.984246
1	-2.637801	-0.429931	-3.435872
1	-2.041649	0.607741	0.176634
1	-3.524023	-5.964571	0.549007
1	-7.461187	-7.440436	1.380706
1	-5.166475	-7.807062	0.519004
1	1.247095	-1.042940	-0.276448
1	-6.438580	-3.372023	2.337615
1	-4.751668	3.218311	-4.252839
7	1.821273	1.830738	0.053991
6	0.849729	2.424532	0.870189
6	-0.000698	3.336627	0.224161
6	-1.011544	3.969334	0.925952
6	-1.224472	3.709751	2.279631
6	-0.388400	2.797272	2.900783
6	0.643763	2.147291	2.222240
6	-1.877689	4.990687	0.243893
9	-1.744987	4.962645	-1.089362
6	-0.588134	2.443745	4.349083
9	-0.939386	1.156774	4.490211
6	2.972365	1.141621	0.324764
16	3.540720	0.733126	1.854319
7	3.615345	0.801896	-0.813153
6	4.764441	-0.077332	-0.924212
6	4.483443	-1.120596	-2.025958
6	5.629415	-2.160703	-2.139677
6	5.044123	-3.562783	-1.921754
6	4.001048	-3.827668	-3.015897
6	2.938230	-2.699357	-2.959169
7	3.177132	-1.791319	-1.817268
6	3.181016	-2.587790	-0.576231
6	4.335427	-3.636607	-0.556326
6	5.224894	-3.458499	0.649561
6	6.548689	-3.590603	0.692381
6	6.032830	0.707867	-1.243232
6	7.240076	0.563496	-0.488883
6	8.368586	1.327879	-0.912872
7	8.341694	2.182242	-1.974478
6	7.214171	2.297487	-2.629932
6	6.038914	1.579682	-2.303028
6	9.587802	1.199993	-0.204643
6	9.704828	0.357312	0.870626
6	8.580492	-0.397436	1.292978
6	7.375711	-0.287342	0.631364
9	-3.180015	4.793635	0.519082
9	-1.584886	6.234400	0.648101
9	-1.542505	3.186728	4.922635
9	0.537785	2.616060	5.055945
1	4.380181	-0.574658	-2.973922
1	6.098268	-2.103071	-3.126688
1	6.409129	-1.956157	-1.401279
1	1.927885	-3.105687	-2.847028
1	2.945758	-2.091825	-3.869108
1	3.536246	-4.806667	-2.860998
1	4.486592	-3.850364	-3.996282
1	5.838303	-4.313391	-1.974900
1	3.879242	-4.632856	-0.473503
1	2.206893	-3.083378	-0.513398
1	3.246931	-1.906586	0.280004
1	4.698934	-3.207892	1.572668
1	7.096996	-3.439630	1.617231
1	7.137963	-3.838382	-0.187085

1	4.873293	-0.578589	0.038255
1	5.146850	1.735775	-2.903904
1	6.547482	-0.875850	1.005805
1	7.204166	2.984820	-3.473769
1	10.429332	1.793782	-0.546183
1	10.652092	0.278001	1.390401
1	3.166454	1.046070	-1.690027
1	1.616034	1.942784	-0.933339
1	0.144012	3.555254	-0.829631
1	1.278573	1.441544	2.740960
1	-2.021165	4.202150	2.825695
8	8.610787	-1.254704	2.344544
6	9.811382	-1.359091	3.086871
1	9.609251	-2.072320	3.886062
1	10.635629	-1.736519	2.470554
1	10.095449	-0.397056	3.528427
6	0.085057	0.340291	-2.213636
1	-1.968585	-4.155098	1.184698
8	1.393805	0.186592	-2.555808
1	-0.447754	0.937181	-2.948949
6	-7.836276	2.379481	-1.339996
6	-8.466086	1.461436	-2.389635
6	-7.258237	0.674562	-2.909696
7	-6.371776	0.521652	-1.736166
6	-6.829565	1.433388	-0.677342
6	-7.517297	0.634051	0.442494
8	-8.138810	1.169912	1.330342
8	-7.396143	-0.683023	0.345461
1	-5.984612	1.956464	-0.218862
1	-8.544800	2.791743	-0.620176
1	-7.302228	3.202275	-1.828190
1	-9.180764	0.783453	-1.908816
1	-8.990377	1.995092	-3.185183
1	-7.538239	-0.302381	-3.315317
1	-6.753582	1.238602	-3.704759
1	-6.806478	-0.845578	-0.426710
1	-5.406337	0.713483	-1.981815

[16-17]A-TS

Number of imaginary frequencies : 1
The smallest frequency is : -1204.2374

Electronic energy=	-3981.6948049
Zero-point correction=	1.077904
Thermal correction to Energy=	1.145541
Thermal correction to Enthalpy=	1.146485
Thermal correction to Gibbs Free Energy=	0.963976
Sum of electronic and zero-point Energies=	-3980.616901
Sum of electronic and thermal Energies=	-3980.549264
Sum of electronic and thermal Enthalpies=	-3980.548320
Sum of electronic and thermal Free Energies=	-3980.730829

Cartesian Coordinates

7	-4.351861	0.067573	0.090073
6	-2.846714	0.082757	0.169365
6	-5.316533	1.575249	3.532082
6	-2.899568	-1.115484	-2.077063
6	-2.424504	1.363276	0.911000
6	-3.452103	-2.280168	-1.532925
6	-4.048323	-3.241939	-2.349639
8	-4.884492	0.705913	-0.791744
6	-3.601686	-1.878843	-4.279056
6	-4.478525	1.897497	2.337563
6	-6.705734	1.573822	3.374424
8	-4.944795	-0.566479	0.952371

6	-3.005702	-0.925555	-3.460727
6	-7.523810	1.286185	4.460401
6	-0.710548	0.002449	-1.156164
6	-2.258395	-0.014626	-1.241611
6	-3.025041	1.432514	2.317911
6	-4.754225	1.289966	4.778991
6	-4.119230	-3.048839	-3.725586
6	-0.245640	1.250746	-0.411541
6	-6.961453	1.016682	5.707507
8	-4.938683	2.522655	1.403700
6	-5.577669	1.022168	5.868085
6	-0.895382	1.407726	0.961148
1	-2.605554	-0.790802	0.782851
1	-0.008199	-1.160628	-0.402228
1	-0.479542	2.143051	-1.014943
1	-8.601471	1.270020	4.333514
1	-4.474194	-4.134453	-1.901148
1	-0.536433	0.618493	1.634508
1	-3.670181	-1.703342	-5.347959
1	-2.934621	0.467043	2.829251
1	-2.798667	2.214227	0.328297
1	-2.618689	-0.007363	-3.896807
1	-0.590619	2.358728	1.410326
1	-3.463459	-2.440409	-0.459055
1	-2.548304	0.928582	-1.729226
1	-3.675868	1.295538	4.910147
1	-7.602775	0.797706	6.555878
1	-5.140522	0.817872	6.840343
1	0.837211	1.234347	-0.283639
1	-7.121981	1.767656	2.390554
1	-4.587261	-3.795033	-4.359979
7	3.163385	1.583725	-0.912619
6	3.484626	2.935743	-0.729444
6	2.672325	3.856092	-1.400396
6	2.933136	5.216762	-1.311568
6	3.994488	5.698086	-0.556508
6	4.801105	4.772108	0.094859
6	4.573154	3.402845	0.014516
6	2.017555	6.159944	-2.038773
9	1.894017	5.824280	-3.332183
6	5.936779	5.259612	0.950829
9	5.565263	5.390515	2.234276
6	3.386667	0.486015	-0.127093
16	4.325380	0.426279	1.265631
7	2.687201	-0.579603	-0.587222
6	2.952449	-1.953786	-0.231689
6	1.671988	-2.800144	-0.385976
6	1.889989	-4.201359	0.245026
6	0.957147	-4.370609	1.453114
6	-0.478762	-4.385427	0.924979
6	-0.686959	-3.106428	0.092874
7	0.461978	-2.169158	0.234208
6	0.686870	-1.885831	1.673287
6	1.086697	-3.187133	2.432002
6	2.423527	-3.053764	3.120296
6	3.343103	-4.006862	3.249264
6	4.038072	-2.551848	-1.130575
6	5.198439	-3.211540	-0.618372
6	6.095516	-3.781940	-1.570953
7	5.912549	-3.698427	-2.918657
6	4.857283	-3.052404	-3.347864
6	3.891991	-2.467823	-2.493193
6	7.240939	-4.470882	-1.103986
6	7.503031	-4.596044	0.236038
6	6.618446	-4.013046	1.179798
6	5.497792	-3.330018	0.757258
9	0.779035	6.141869	-1.519533
9	2.452613	7.424748	-1.988972
9	6.381369	6.460161	0.550025
9	6.977120	4.415740	0.930223

1	1.432508	-2.879929	-1.453519
1	1.683528	-4.987415	-0.487105
1	2.934829	-4.309070	0.546496
1	-1.567850	-2.551680	0.416635
1	-0.803397	-3.308467	-0.976113
1	-1.190546	-4.424456	1.755039
1	-0.647340	-5.269817	0.304980
1	1.176855	-5.308110	1.970306
1	0.339682	-3.340175	3.222302
1	-0.251253	-1.477730	2.059797
1	1.451910	-1.106724	1.751767
1	2.613700	-2.079315	3.572301
1	4.269417	-3.821810	3.783814
1	3.222810	-4.999430	2.822108
1	3.275992	-1.970322	0.810347
1	3.043936	-1.949108	-2.935585
1	4.871037	-2.874540	1.513826
1	4.728939	-2.980874	-4.426114
1	7.907196	-4.895011	-1.847924
1	8.387892	-5.129430	0.561897
1	2.172477	-0.432768	-1.460972
1	2.506605	1.420168	-1.677620
1	1.835711	3.502243	-1.999137
1	5.233895	2.707843	0.513334
1	4.196129	6.760466	-0.489796
8	6.807630	-4.083237	2.521746
6	7.966646	-4.740862	2.999399
1	7.930527	-4.660945	4.085990
1	7.974071	-5.800408	2.718414
1	8.881240	-4.259073	2.635507
6	-0.019006	-0.274242	-2.371044
1	-2.452669	2.155296	2.916100
8	1.106783	0.167536	-2.700443
1	-0.487674	-1.011505	-3.047855
6	-8.790680	-0.922969	-2.745730
6	-8.888653	-2.261259	-2.010983
6	-7.416253	-2.619698	-1.805231
7	-6.766680	-1.326631	-1.516138
6	-7.640933	-0.240894	-1.991389
6	-8.199801	0.563113	-0.806230
8	-9.074285	1.386317	-0.942315
8	-7.664841	0.280482	0.374741
1	-7.093467	0.473682	-2.613235
1	-9.702086	-0.324430	-2.719460
1	-8.505480	-1.087462	-3.790017
1	-9.380796	-2.120433	-1.041531
1	-9.434650	-3.029071	-2.562983
1	-7.261615	-3.325299	-0.982762
1	-7.011402	-3.071960	-2.721221
1	-6.956998	-0.384049	0.217553
1	-5.845449	-1.268765	-1.937091

[17]A

Number of imaginary frequencies : 0

Electronic energy=	-3981.7371047
Zero-point correction=	1.081798
Thermal correction to Energy=	1.150023
Thermal correction to Enthalpy=	1.150967
Thermal correction to Gibbs Free Energy=	0.967656
Sum of electronic and zero-point Energies=	-3980.655307
Sum of electronic and thermal Energies=	-3980.587082
Sum of electronic and thermal Enthalpies=	-3980.586138
Sum of electronic and thermal Free Energies=	-3980.769448

Cartesian Coordinates

7	-4.661210	-0.465433	0.351371
6	-3.180386	-0.516260	0.632049
6	-5.940572	1.704991	3.375703
6	-2.939165	-2.027757	-1.379933
6	-2.737408	0.782795	1.330802
6	-2.933345	-3.275038	-0.745688
6	-3.404627	-4.408700	-1.405012
8	-5.032832	-0.024054	-0.715503
6	-3.902541	-3.069411	-3.346298
6	-4.899147	1.702480	2.305008
6	-7.259244	1.984070	3.004040
8	-5.397873	-0.860722	1.241062
6	-3.429467	-1.937470	-2.685246
6	-8.262252	2.003069	3.964288
6	-0.912736	-0.880871	-0.335816
6	-2.424184	-0.787643	-0.671780
6	-3.544668	1.065310	2.598631
6	-5.634257	1.447843	4.714661
6	-3.889778	-4.308015	-2.708279
6	-0.420299	0.373058	0.378394
6	-7.951522	1.756549	5.301196
8	-5.116409	2.207455	1.221112
6	-6.638608	1.482256	5.676763
6	-1.239744	0.655248	1.634242
1	-3.078999	-1.354586	1.328766
1	-0.770376	-1.761425	0.308857
1	-0.492340	1.226718	-0.307384
1	-9.287079	2.208757	3.672702
1	-3.398322	-5.368651	-0.898344
1	-1.086867	-0.148190	2.369045
1	-4.284900	-2.980527	-4.358467
1	-3.680832	0.155213	3.192945
1	-2.898682	1.608103	0.626788
1	-3.452161	-0.969621	-3.179201
1	-0.894470	1.581889	2.102617
1	-2.563376	-3.365431	0.273523
1	-2.575652	0.076645	-1.328861
1	-4.612247	1.235144	5.014043
1	-8.735741	1.776573	6.051939
1	-6.398249	1.293263	6.718059
1	0.639627	0.253049	0.630640
1	-7.477043	2.168643	1.957084
1	-4.260013	-5.190100	-3.221306
7	2.431188	1.738961	-0.952260
6	2.266841	3.129783	-0.960391
6	1.471275	3.655229	-1.984668
6	1.214274	5.018571	-2.045201
6	1.740727	5.892673	-1.102963
6	2.524101	5.357516	-0.087042
6	2.788743	3.996175	0.006679
6	0.331384	5.525787	-3.149854
9	0.716692	5.056061	-4.346722
6	3.046324	6.260845	0.995281
9	2.228670	6.269634	2.062718
6	3.427110	0.951556	-0.433258
16	4.793625	1.484319	0.382433
7	3.189311	-0.358390	-0.656942
6	4.044499	-1.445431	-0.223059
6	3.251255	-2.757740	-0.412859
6	3.962272	-3.959691	0.264064
6	3.017815	-4.560138	1.316447
6	1.763288	-5.072669	0.596639
6	1.162115	-3.894189	-0.214658
7	1.856925	-2.626622	0.066483
6	1.827746	-2.374052	1.514047
6	2.574474	-3.483445	2.323986
6	3.667607	-2.907144	3.188477
6	4.882901	-3.412898	3.388061
6	5.334565	-1.516906	-1.034311

6	6.613417	-1.760580	-0.441484
6	7.725190	-1.895296	-1.324522
7	7.627757	-1.783252	-2.680021
6	6.443732	-1.533161	-3.180320
6	5.271421	-1.397563	-2.399298
6	9.005463	-2.157251	-0.778922
6	9.195685	-2.281832	0.573236
6	8.090607	-2.134333	1.449791
6	6.833386	-1.869652	0.950423
9	-0.942124	5.134432	-2.978422
9	0.330441	6.862206	-3.221537
9	3.155191	7.529924	0.577500
9	4.250696	5.873438	1.433829
1	3.171785	-2.927195	-1.494145
1	4.211251	-4.722805	-0.480091
1	4.901280	-3.645109	0.724357
1	0.098720	-3.759287	0.016540
1	1.237147	-4.078890	-1.291564
1	1.041735	-5.452744	1.327601
1	2.023621	-5.903885	-0.065573
1	3.512476	-5.383492	1.840234
1	1.846533	-3.948679	3.003572
1	0.774726	-2.319309	1.814286
1	2.265939	-1.388030	1.705623
1	3.398394	-1.988002	3.711973
1	5.594052	-2.922060	4.045062
1	5.223145	-4.325363	2.905023
1	4.284171	-1.302729	0.835831
1	4.323895	-1.190410	-2.889159
1	6.028598	-1.748258	1.665497
1	6.379128	-1.435303	-4.262512
1	9.833077	-2.254688	-1.473862
1	10.187645	-2.480886	0.960728
1	2.290593	-0.640472	-1.032568
1	1.736627	1.241003	-1.504967
1	1.065149	2.992505	-2.745246
1	3.400900	3.613555	0.811363
1	1.550783	6.957545	-1.161459
8	8.190202	-2.239433	2.800562
6	9.465811	-2.497632	3.354972
1	9.320970	-2.542862	4.434625
1	9.870619	-3.455405	3.007435
1	10.176039	-1.695650	3.122760
6	-0.145513	-1.159544	-1.603768
1	-2.988034	1.771488	3.229966
8	0.585095	-0.351429	-2.144294
1	-0.311424	-2.147703	-2.069956
6	-7.880156	-2.872687	-2.965368
6	-8.356849	-3.839709	-1.879702
6	-7.136865	-3.933388	-0.955833
7	-6.496751	-2.600466	-1.024573
6	-7.103723	-1.848292	-2.132360
6	-8.061633	-0.777225	-1.584927
8	-8.845127	-0.190420	-2.293920
8	-7.974287	-0.554457	-0.280403
1	-6.336708	-1.317266	-2.705234
1	-8.684709	-2.408939	-3.537529
1	-7.195592	-3.381683	-3.653219
1	-9.206736	-3.402380	-1.343128
1	-8.666549	-4.814508	-2.262325
1	-7.411007	-4.180355	0.074051
1	-6.447660	-4.707477	-1.317122
1	-7.242846	-1.119145	0.055021
1	-5.496821	-2.693186	-1.168290

Number of imaginary frequencies : 0

Electronic energy = -3580.6989504
Zero-point correction= 0.932924
Thermal correction to Energy= 0.992094
Thermal correction to Enthalpy= 0.993038
Thermal correction to Gibbs Free Energy= 0.830784
Sum of electronic and zero-point Energies= -3579.766027
Sum of electronic and thermal Energies= -3579.706856
Sum of electronic and thermal Enthalpies= -3579.705912
Sum of electronic and thermal Free Energies= -3579.868167

Cartesian Coordinates

7 4.920680 -1.162371 -0.997900
6 4.311506 -1.288289 0.378067
6 8.817498 -1.815852 -0.066896
6 2.185828 -0.404225 -0.522046
6 5.119881 -2.329365 1.167102
6 2.110629 0.860385 0.074789
6 1.649332 1.955631 -0.642438
8 4.567276 -1.943486 -1.857469
6 1.319753 0.556948 -2.572823
6 7.433696 -2.370378 0.074849
6 9.533716 -2.129352 -1.226435
8 5.770650 -0.301049 -1.143222
6 1.800675 -0.539635 -1.853991
6 10.822535 -1.644595 -1.405051
6 2.205771 -1.894512 1.590455
6 2.798995 -1.574728 0.228413
6 6.596165 -1.937678 1.271138
6 9.409928 -1.016798 0.914789
6 1.241541 1.805824 -1.969478
6 3.011457 -2.859083 2.430778
6 11.409265 -0.848312 -0.422041
8 7.001866 -3.175266 -0.726934
6 10.704473 -0.538014 0.738004
6 4.478426 -2.455711 2.549314
1 4.464178 -0.301353 0.822866
1 -0.293805 -1.189309 0.611311
1 2.970737 -3.854637 1.963742
1 11.371621 -1.884840 -2.309766
1 1.605793 2.933687 -0.171180
1 4.563701 -1.498882 3.081745
1 1.020224 0.431633 -3.608941
1 6.701230 -0.857736 1.423030
1 5.045188 -3.289072 0.640902
1 1.900749 -1.506613 -2.341453
1 5.028888 -3.201901 3.131722
1 2.411320 0.976645 1.114127
1 2.724147 -2.474392 -0.398241
1 8.871550 -0.766851 1.823354
1 12.416593 -0.468071 -0.560885
1 11.161501 0.079816 1.504247
1 2.558954 -2.957623 3.422174
1 9.057103 -2.750844 -1.977316
1 0.873601 2.663882 -2.523864
7 -1.513170 1.779644 0.806053
6 -1.194839 3.118411 0.509472
6 -0.592255 3.868271 1.524899
6 -0.146431 5.155191 1.265218
6 -0.297382 5.728496 0.004130
6 -0.902600 4.974694 -0.990751
6 -1.348360 3.675131 -0.758677
6 0.509587 5.969686 2.342982
9 -0.185631 7.085124 2.610384
6 -1.056895 5.525564 -2.380220
9 -0.421628 4.754176 -3.282373
6 -2.608655 1.050993 0.437058
16 -3.822305 1.584101 -0.602222

7	-2.617022	-0.167354	1.017441
6	-3.405543	-1.302619	0.580347
6	-2.472763	-2.521635	0.385091
6	-3.224511	-3.691667	-0.304154
6	-2.541895	-3.996269	-1.646582
6	-1.110479	-4.466752	-1.358384
6	-0.412813	-3.381617	-0.501254
7	-1.248876	-2.166392	-0.377895
6	-1.592721	-1.683051	-1.729039
6	-2.451409	-2.724933	-2.511849
6	-3.769658	-2.144558	-2.960350
6	-4.950529	-2.759421	-2.969023
6	-4.501970	-1.646310	1.582553
6	-5.873246	-1.798871	1.205629
6	-6.790307	-2.191877	2.226052
7	-6.427906	-2.395996	3.523798
6	-5.168784	-2.214796	3.835490
6	-4.172733	-1.846573	2.899962
6	-8.151357	-2.383483	1.886035
6	-8.600992	-2.194733	0.604594
6	-7.690517	-1.786418	-0.403656
6	-6.359064	-1.588667	-0.104745
9	0.633298	5.288875	3.490159
9	1.739948	6.363848	1.976218
9	-0.556142	6.762375	-2.493270
9	-2.340918	5.573551	-2.756213
1	-2.116060	-2.829487	1.377326
1	-3.205348	-4.584942	0.328075
1	-4.275174	-3.430809	-0.457885
1	0.542330	-3.073478	-0.938695
1	-0.208051	-3.741291	0.512752
1	-0.572079	-4.624299	-2.298486
1	-1.126190	-5.423377	-0.827566
1	-3.092180	-4.777192	-2.179604
1	-1.897756	-2.989915	-3.423445
1	-0.649158	-1.484700	-2.241463
1	-2.113834	-0.724625	-1.638459
1	-3.715552	-1.118812	-3.329185
1	-5.843691	-2.254394	-3.323842
1	-5.079650	-3.779307	-2.615111
1	-3.852244	-1.029155	-0.376832
1	-3.147959	-1.727128	3.242935
1	-5.709894	-1.257405	-0.905893
1	-4.893921	-2.371974	4.876944
1	-8.826651	-2.685826	2.679712
1	-9.648237	-2.350881	0.374990
1	-1.838892	-0.386991	1.632270
1	-0.800152	1.280048	1.334200
1	-0.471491	3.436376	2.512864
1	-1.789577	3.091671	-1.557428
1	0.053807	6.735374	-0.194513
8	-8.055345	-1.566845	-1.692314
6	-9.419045	-1.723676	-2.035781
1	-9.491510	-1.481519	-3.096254
1	-9.758567	-2.754454	-1.879863
1	-10.058485	-1.038388	-1.467574
1	7.040519	-2.418201	2.154061
6	1.018896	-1.497543	2.068594
8	0.065199	-0.742062	1.455430
1	0.745010	-1.788071	3.084546

[14-15]B-TS

Number of imaginary frequencies : 1
 The smallest frequency is : -1235.1215

Electronic energy= -3580.67103
 Zero-point correction= 0.929611

Thermal correction to Energy=	0.988073
Thermal correction to Enthalpy=	0.989017
Thermal correction to Gibbs Free Energy=	0.830860
Sum of electronic and zero-point Energies=	-3579.741419
Sum of electronic and thermal Energies=	-3579.682957
Sum of electronic and thermal Enthalpies=	-3579.682013
Sum of electronic and thermal Free Energies=	-3579.840170

 Cartesian Coordinates

7	4.645732	-0.409335	-0.991950
6	3.758537	-1.148985	-0.019905
6	8.297381	-1.576802	0.336489
6	1.790263	-0.018691	-1.148391
6	4.466449	-2.469799	0.332256
6	2.169349	1.235432	-0.653335
6	1.747281	2.405243	-1.279548
8	4.547641	-0.679105	-2.170137
6	0.490786	1.112209	-2.867332
6	6.958618	-2.082977	-0.106112
6	9.268894	-1.353887	-0.644547
8	5.440418	0.388515	-0.519588
6	0.947050	-0.055247	-2.259016
6	10.529739	-0.893683	-0.289397
6	1.500551	-2.133595	0.380463
6	2.354284	-1.333450	-0.620533
6	5.854412	-2.227771	0.932925
6	8.605819	-1.338843	1.678724
6	0.907240	2.350485	-2.389643
6	2.176462	-3.466268	0.716783
6	10.832906	-0.659454	1.051471
8	6.771954	-2.409886	-1.261577
6	9.872289	-0.884424	2.034076
6	3.577524	-3.259707	1.293686
1	3.726986	-0.509809	0.866563
1	0.171210	-2.497534	-0.332635
1	2.267252	-4.090758	-0.180041
1	11.278008	-0.716952	-1.055321
1	2.074123	3.366532	-0.893691
1	3.504507	-2.722007	2.250320
1	-0.163500	1.051862	-3.731969
1	5.845918	-1.349152	1.586862
1	4.582971	-3.036504	-0.600372
1	0.680080	-1.019361	-2.681444
1	4.056962	-4.223409	1.501261
1	2.820457	1.313527	0.212116
1	2.489984	-1.974129	-1.502523
1	7.865892	-1.508578	2.454351
1	11.818666	-0.300254	1.330654
1	10.107697	-0.702551	3.077744
1	1.569088	-4.029870	1.435564
1	9.010503	-1.544534	-1.680899
1	0.573761	3.266200	-2.868830
7	-1.066993	1.619898	0.202774
6	-1.057345	3.021022	0.147220
6	-0.363356	3.685196	1.165667
6	-0.234197	5.064727	1.130309
6	-0.781221	5.814879	0.091864
6	-1.460260	5.140674	-0.912196
6	-1.607194	3.755906	-0.900801
6	0.525347	5.789409	2.203557
9	-0.219893	6.750871	2.769741
6	-1.977284	5.882506	-2.110809
9	-1.219986	5.631676	-3.195570
6	-2.036972	0.744962	-0.172024
16	-3.524987	1.143763	-0.843144
7	-1.660989	-0.544026	0.070005
6	-2.634437	-1.608106	0.215230
6	-1.954724	-2.999127	0.176420
6	-3.002186	-4.097928	-0.136953

6	-2.744377	-4.661114	-1.545629
6	-1.427177	-5.437115	-1.495953
6	-0.363261	-4.506846	-0.885684
7	-0.846680	-3.091818	-0.826548
6	-1.321132	-2.692750	-2.178594
6	-2.564325	-3.540170	-2.588412
6	-3.782140	-2.688975	-2.854950
6	-5.044555	-3.022099	-2.596928
6	-3.398892	-1.488570	1.538525
6	-4.817472	-1.632811	1.641000
6	-5.384513	-1.602631	2.949824
7	-4.650963	-1.407072	4.081419
6	-3.361615	-1.224524	3.940714
6	-2.691813	-1.261884	2.694297
6	-6.783095	-1.774223	3.092919
6	-7.596828	-1.954383	2.004138
6	-7.032978	-1.955457	0.702047
6	-5.675851	-1.789781	0.530251
9	0.936141	4.970660	3.180327
9	1.616058	6.394721	1.705031
9	-1.974856	7.209554	-1.927858
9	-3.227166	5.517669	-2.425257
1	-1.468077	-3.173309	1.145114
1	-2.935630	-4.911490	0.591760
1	-4.008664	-3.682008	-0.059243
1	0.558316	-4.498043	-1.471283
1	-0.112083	-4.795978	0.136711
1	-1.133433	-5.752960	-2.501390
1	-1.530160	-6.336953	-0.883812
1	-3.563343	-5.321426	-1.842092
1	-2.315296	-4.029644	-3.539602
1	-0.486983	-2.861499	-2.864413
1	-1.538658	-1.622524	-2.161100
1	-3.582441	-1.731340	-3.337412
1	-5.862697	-2.357251	-2.855262
1	-5.316951	-3.958038	-2.114966
1	-3.326011	-1.526002	-0.625027
1	-1.617910	-1.087370	2.669633
1	-5.294078	-1.759462	-0.483142
1	-2.789135	-1.045895	4.848930
1	-7.188563	-1.750927	4.099109
1	-8.663523	-2.080419	2.146512
1	-0.818167	-0.628551	0.630855
1	-0.252502	1.208327	0.663669
1	0.074877	3.113655	1.978157
1	-2.118185	3.251859	-1.710746
1	-0.673330	6.893690	0.066132
8	-7.766468	-2.113192	-0.429337
6	-9.170842	-2.229863	-0.301165
1	-9.559389	-2.319327	-1.315815
1	-9.451459	-3.123295	0.268826
1	-9.606942	-1.342592	0.172055
1	6.134574	-3.081564	1.565705
6	0.998367	-1.478990	1.546715
8	0.694507	-0.279857	1.702056
1	0.770186	-2.174621	2.387501

[15]B

Number of imaginary frequencies : 0

Electronic energy=	-3580.7106943
Zero-point correction=	0.933575
Thermal correction to Energy=	0.992724
Thermal correction to Enthalpy=	0.993669
Thermal correction to Gibbs Free Energy=	0.832815
Sum of electronic and zero-point Energies=	-3579.777119

Sum of electronic and thermal Energies=	-3579.717970
Sum of electronic and thermal Enthalpies=	-3579.717026
Sum of electronic and thermal Free Energies=	-3579.877879

 Cartesian Coordinates

7	4.679911	-0.993952	-1.193205
6	3.668483	-1.486458	-0.186082
6	8.086732	-2.171143	0.600403
6	1.773219	-0.422450	-1.561086
6	4.215673	-2.795161	0.421750
6	2.329950	0.851836	-1.415934
6	1.813348	1.937184	-2.121587
8	4.600469	-1.401183	-2.331903
6	0.144630	0.513589	-3.104542
6	6.749744	-2.660439	0.139467
6	9.118722	-2.105897	-0.340848
8	5.542524	-0.237955	-0.775530
6	0.676495	-0.574678	-2.417846
6	10.380211	-1.663825	0.034453
6	1.305271	-2.251121	0.153132
6	2.308087	-1.663716	-0.859389
6	5.570382	-2.579294	1.101601
6	8.333630	-1.795216	1.923574
6	0.716665	1.775828	-2.962370
6	1.822840	-3.570460	0.746797
6	10.622585	-1.292904	1.356718
8	6.612931	-3.145003	-0.966925
6	9.601182	-1.361922	2.300426
6	3.184343	-3.358160	1.406360
1	3.644126	-0.705710	0.578097
1	0.353072	-2.440909	-0.369034
1	1.909197	-4.310490	-0.056703
1	11.175718	-1.604835	-0.701455
1	2.265813	2.915750	-1.991549
1	3.084519	-2.671736	2.260349
1	-0.707471	0.371196	-3.762931
1	5.590360	-1.622574	1.634104
1	4.349728	-3.508513	-0.401066
1	0.236426	-1.560777	-2.548307
1	3.561963	-4.304220	1.806450
1	3.178035	1.020584	-0.757995
1	2.443388	-2.429970	-1.633065
1	7.545785	-1.845439	2.668537
1	11.608904	-0.948213	1.651613
1	9.790648	-1.075909	3.329991
1	1.102647	-3.964921	1.472728
1	8.906244	-2.400436	-1.363232
1	0.309107	2.627257	-3.498001
7	-0.772204	1.590947	0.042084
6	-0.392904	2.940442	0.113818
6	0.850685	3.211835	0.683529
6	1.352719	4.507911	0.674627
6	0.622961	5.557896	0.136757
6	-0.625529	5.273924	-0.410858
6	-1.138152	3.983402	-0.443977
6	2.737525	4.721304	1.210485
9	3.076563	6.015149	1.247890
6	-1.394818	6.385502	-1.067006
9	-0.992455	6.577383	-2.335732
6	-2.006270	1.028925	0.189918
16	-3.420055	1.869985	0.502428
7	-1.959086	-0.329607	0.082167
6	-3.147672	-1.168803	0.149639
6	-2.721381	-2.602760	-0.239493
6	-3.935934	-3.546781	-0.446324
6	-3.888410	-4.094623	-1.881814
6	-2.591016	-4.897750	-2.052537
6	-1.401216	-3.969232	-1.687753
7	-1.853632	-2.593291	-1.431528

6	-2.576965	-2.101581	-2.612905
6	-3.863984	-2.940925	-2.901299
6	-5.098325	-2.075809	-2.941411
6	-6.291570	-2.351864	-2.419227
6	-3.752439	-1.194517	1.548123
6	-5.164883	-1.174349	1.782061
6	-5.603345	-1.318823	3.131420
7	-4.754796	-1.448018	4.191039
6	-3.470749	-1.424397	3.937900
6	-2.927012	-1.305661	2.637183
6	-6.992840	-1.321703	3.404333
6	-7.919925	-1.180330	2.404077
6	-7.481312	-1.016758	1.065715
6	-6.135220	-1.007504	0.767805
9	2.875312	4.230475	2.451449
9	3.647826	4.089147	0.446384
9	-1.221921	7.551814	-0.427609
9	-2.709056	6.135562	-1.108770
1	-2.089151	-2.975394	0.578891
1	-3.898414	-4.377911	0.265007
1	-4.874080	-3.018075	-0.267926
1	-0.657880	-3.935725	-2.492473
1	-0.891936	-4.325269	-0.784524
1	-2.505101	-5.254052	-3.084249
1	-2.605947	-5.779586	-1.404748
1	-4.753428	-4.738846	-2.066632
1	-3.756015	-3.386133	-3.900148
1	-1.882215	-2.148772	-3.458668
1	-2.821663	-1.044305	-2.460361
1	-4.976307	-1.135079	-3.481293
1	-7.120180	-1.657485	-2.515824
1	-6.491350	-3.267894	-1.868898
1	-3.894555	-0.799167	-0.562616
1	-1.849989	-1.282212	2.506431
1	-5.854859	-0.861691	-0.268587
1	-2.800725	-1.509688	4.791723
1	-7.297439	-1.435676	4.439588
1	-8.976277	-1.184399	2.644667
1	-1.217054	-0.725349	-0.496417
1	0.017763	0.950425	0.045245
1	1.429262	2.399618	1.116705
1	-2.099824	3.787354	-0.898761
1	1.013633	6.568946	0.141537
8	-8.329011	-0.862346	0.015721
6	-9.716517	-0.796353	0.284546
1	-10.202378	-0.641483	-0.679097
1	-10.087778	-1.728906	0.725675
1	-9.958285	0.042501	0.947279
1	5.729753	-3.359896	1.858398
6	0.943983	-1.324442	1.288404
8	1.301685	-0.173096	1.407043
1	0.298483	-1.788020	2.064647

[16]B

Number of imaginary frequencies : 0

Electronic energy=	-3580.6784114
Zero-point correction=	0.935138
Thermal correction to Energy=	0.993849
Thermal correction to Enthalpy=	0.994793
Thermal correction to Gibbs Free Energy=	0.834218
Sum of electronic and zero-point Energies=	-3579.743274
Sum of electronic and thermal Energies=	-3579.684563
Sum of electronic and thermal Enthalpies=	-3579.683618
Sum of electronic and thermal Free Energies=	-3579.844193

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Cartesian Coordinates

7	4.636621	-3.265365	0.243296
6	3.537402	-2.269602	-0.047386
6	7.934394	-0.946773	-0.120697
6	1.587031	-3.847616	0.431453
6	4.013940	-0.814459	0.123548
6	1.962815	-4.665772	-0.635989
6	1.217814	-5.800566	-0.968213
8	4.668765	-3.819709	1.319366
6	-0.269146	-5.362820	0.869918
6	6.540865	-1.003118	0.425583
6	8.962677	-1.504276	0.645029
8	5.444625	-3.449863	-0.656630
6	0.466774	-4.226564	1.186179
6	10.272616	-1.474578	0.185192
6	1.398883	-1.330221	0.773057
6	2.304075	-2.551390	0.815773
6	5.396754	-0.527091	-0.454827
6	8.233950	-0.352846	-1.349725
6	0.097658	-6.150940	-0.223295
6	1.528231	-0.498330	-0.474674
6	10.566641	-0.879129	-1.041006
8	6.332862	-1.397406	1.556560
6	9.548242	-0.316759	-1.805939
6	2.959140	0.083358	-0.565579
1	3.346265	-2.433569	-1.112363
1	-0.756775	-1.170816	-1.089586
1	0.796657	0.317827	-0.482891
1	11.066295	-1.915237	0.780053
1	1.526635	-6.414558	-1.808715
1	3.239310	0.229727	-1.616487
1	-1.128068	-5.635808	1.476140
1	5.500557	-0.962730	-1.454795
1	4.030572	-0.604519	1.197340
1	0.165836	-3.605665	2.026134
1	2.988782	1.066219	-0.084483
1	2.845192	-4.442565	-1.229428
1	2.665974	-2.679785	1.842888
1	7.449508	0.091041	-1.954625
1	11.590817	-0.854039	-1.400250
1	9.776407	0.150371	-2.758604
1	1.346881	-1.109514	-1.376939
1	8.709561	-1.960817	1.596251
1	-0.475159	-7.037186	-0.478147
7	-0.883089	2.224295	0.413990
6	-0.414317	3.529645	0.250363
6	0.646693	3.895818	1.093373
6	1.211269	5.158148	1.003938
6	0.747234	6.093613	0.084179
6	-0.298165	5.717854	-0.747890
6	-0.884442	4.457555	-0.685398
6	2.384581	5.501342	1.877100
9	2.429079	6.811275	2.158707
6	-0.770226	6.679036	-1.802334
9	-2.059667	6.497286	-2.114386
6	-1.972953	1.561425	-0.073519
16	-3.195937	2.224130	-1.036794
7	-1.935167	0.257004	0.301167
6	-3.038369	-0.664557	0.138267
6	-2.480476	-2.012364	-0.369036
6	-3.552350	-2.988618	-0.894146
6	-3.337736	-3.234195	-2.396905
6	-1.981635	-3.924474	-2.594441
6	-0.886751	-3.075205	-1.922074
7	-1.491320	-1.770214	-1.486908
6	-2.105817	-1.068724	-2.660600
6	-3.306575	-1.904479	-3.177526
6	-4.588342	-1.105030	-3.156167
6	-5.803416	-1.578846	-2.893154

6	-3.789977	-0.910768	1.445162
6	-5.219259	-0.966474	1.506920
6	-5.801839	-1.304504	2.764624
7	-5.072528	-1.541499	3.891235
6	-3.770700	-1.432943	3.802101
6	-3.082725	-1.124486	2.602981
6	-7.211234	-1.398122	2.864284
6	-8.022884	-1.161968	1.784713
6	-7.442868	-0.801913	0.541603
6	-6.073762	-0.701787	0.412067
9	2.357478	4.836653	3.039844
9	3.548717	5.193152	1.279358
9	-0.070431	6.537753	-2.941994
9	-0.622942	7.954626	-1.415316
1	-1.869821	-2.458839	0.424392
1	-3.486513	-3.938706	-0.356634
1	-4.546005	-2.574711	-0.709590
1	-0.059186	-2.832195	-2.591624
1	-0.486187	-3.545589	-1.025011
1	-1.773259	-4.044260	-3.661189
1	-1.987681	-4.919855	-2.143015
1	-4.135792	-3.871168	-2.785132
1	-3.097907	-2.149441	-4.226822
1	-1.312067	-0.972041	-3.404212
1	-2.400163	-0.066721	-2.338177
1	-4.479905	-0.050237	-3.410108
1	-6.673001	-0.930377	-2.919625
1	-5.985190	-2.618135	-2.629372
1	-3.718135	-0.247435	-0.607603
1	-1.998982	-1.029722	2.626866
1	-5.685850	-0.394967	-0.551775
1	-3.200695	-1.604142	4.713182
1	-7.626174	-1.661182	3.831861
1	-9.097911	-1.240665	1.893465
1	-1.181730	0.045402	1.043607
1	-0.319492	1.648904	1.059437
1	1.016042	3.185562	1.828454
1	-1.703213	4.204964	-1.343215
1	1.181183	7.085262	0.025872
8	-8.171446	-0.537637	-0.573069
6	-9.582902	-0.576543	-0.472903
1	-9.961534	-0.308747	-1.459595
1	-9.941214	-1.579282	-0.212177
1	-9.954297	0.147111	0.261378
6	0.757731	-0.904711	1.894103
1	5.513037	0.559381	-0.574151
8	-0.030041	0.126283	2.032920
1	0.910289	-1.517620	2.800656

[16-17]B-TS

Number of imaginary frequencies : 1
The smallest frequency is : -1169.3504

Electronic energy=	-3580.6603713
Zero-point correction=	0.930262
Thermal correction to Energy=	0.988613
Thermal correction to Enthalpy=	0.989558
Thermal correction to Gibbs Free Energy=	0.830943
Sum of electronic and zero-point Energies=	-3579.730109
Sum of electronic and thermal Energies=	-3579.671758
Sum of electronic and thermal Enthalpies=	-3579.670814
Sum of electronic and thermal Free Energies=	-3579.829428

Cartesian Coordinates

7	-5.181204	-1.760574	-0.990005

6	-3.825608	-1.364807	-0.425724
6	-7.673667	0.419248	1.277180
6	-2.516054	-3.100565	-1.729972
6	-3.934513	0.070833	0.112232
6	-3.338183	-4.087639	-1.171133
6	-3.089680	-5.445756	-1.367641
8	-5.411260	-1.570997	-2.162692
6	-1.205350	-4.900486	-2.737535
6	-6.436203	0.491947	0.436814
6	-8.910037	0.539659	0.635363
8	-5.984141	-2.219986	-0.189471
6	-1.452733	-3.546788	-2.529593
6	-10.087452	0.485758	1.369566
6	-1.422489	-0.795580	-1.192360
6	-2.735261	-1.594754	-1.478159
6	-5.089853	0.240316	1.101414
6	-7.629923	0.250238	2.663845
6	-2.018132	-5.864058	-2.146640
6	-1.476855	0.425080	-0.251352
6	-10.038261	0.318662	2.753232
8	-6.501172	0.782405	-0.741465
6	-8.810357	0.204163	3.399452
6	-2.592746	0.369045	0.778232
1	-3.711019	-2.033029	0.433730
1	-0.453236	-1.581358	-0.276759
1	-1.615874	1.340517	-0.846342
1	-11.044937	0.574432	0.866356
1	-3.747545	-6.175508	-0.905795
1	-2.401529	-0.401559	1.539860
1	-0.367422	-5.198581	-3.360672
1	-5.163382	-0.624290	1.769629
1	-4.087871	0.752632	-0.733118
1	-0.775710	-2.838859	-2.989165
1	-2.648272	1.325663	1.307925
1	-4.187865	-3.833062	-0.548098
1	-3.171029	-1.197315	-2.403875
1	-6.679127	0.160731	3.179575
1	-10.958440	0.278554	3.327939
1	-8.771505	0.076969	4.476502
1	-0.513845	0.552902	0.259060
1	-8.923042	0.671129	-0.441506
1	-1.824843	-6.920759	-2.300583
7	1.589054	1.952360	-0.742814
6	1.557220	3.339670	-0.558455
6	0.459487	4.003642	-1.118293
6	0.354773	5.384709	-1.030016
6	1.327626	6.139840	-0.387871
6	2.419982	5.470243	0.152154
6	2.556737	4.089501	0.072048
6	-0.864673	6.059327	-1.590359
9	-0.614710	7.326741	-1.946369
6	3.465514	6.276099	0.871476
9	4.614736	5.606019	1.016458
6	2.216977	0.966338	-0.043922
16	3.169428	1.186255	1.328915
7	1.916771	-0.261413	-0.548594
6	2.526447	-1.501917	-0.116836
6	1.502650	-2.659352	-0.010088
6	2.093836	-3.802409	0.855008
6	1.333996	-3.880280	2.192753
6	-0.090656	-4.351227	1.894284
6	-0.656728	-3.445397	0.788009
7	0.198054	-2.233214	0.583709
6	0.412005	-1.564718	1.898855
6	1.206843	-2.500759	2.863686
6	2.494279	-1.879467	3.343874
6	3.651575	-2.509202	3.532251
6	3.642783	-1.933131	-1.068079
6	4.991582	-2.132259	-0.636831
6	5.925160	-2.593341	-1.613045

7	5.600267	-2.814904	-2.917715
6	4.363005	-2.587881	-3.281297
6	3.350612	-2.155803	-2.391318
6	7.262816	-2.836428	-1.217922
6	7.673741	-2.634498	0.074539
6	6.747332	-2.159103	1.038469
6	5.438100	-1.908932	0.684975
9	-1.336051	5.419531	-2.670058
9	-1.865165	6.095939	-0.694194
9	3.054668	6.628158	2.101381
9	3.741276	7.416890	0.219328
1	1.248293	-3.011350	-1.016842
1	2.002093	-4.761357	0.336224
1	3.160443	-3.625083	1.017754
1	-1.664807	-3.082376	1.010868
1	-0.695939	-3.967505	-0.167802
1	-0.702791	-4.298303	2.799652
1	-0.095867	-5.389679	1.552510
1	1.832916	-4.580697	2.867640
1	0.582200	-2.639585	3.756525
1	-0.578100	-1.333471	2.297658
1	0.939279	-0.623090	1.731403
1	2.432184	-0.817716	3.580957
1	4.519413	-1.979038	3.912394
1	3.789104	-3.564972	3.312372
1	2.934078	-1.312141	0.876378
1	2.344299	-2.008292	-2.778055
1	4.777534	-1.510436	1.445770
1	4.118726	-2.758661	-4.327884
1	7.952520	-3.189323	-1.977601
1	8.704007	-2.831152	0.345808
1	1.421546	-0.263128	-1.439122
1	0.933495	1.606270	-1.453457
1	-0.307927	3.434420	-1.636168
1	3.429325	3.604724	0.484563
1	1.246178	7.219390	-0.325278
8	7.074129	-1.923649	2.333728
6	8.418970	-2.120536	2.728742
1	8.463939	-1.852951	3.784517
1	8.724913	-3.166734	2.610936
1	9.101789	-1.473987	2.165722
6	-0.775551	-0.443287	-2.419996
1	-4.889230	1.111659	1.739790
8	0.091289	0.440012	-2.583787
1	-1.090594	-0.986029	-3.330138

[17]B

Number of imaginary frequencies : 0

Electronic energy=	-3580.7103959
Zero-point correction=	0.933393
Thermal correction to Energy=	0.993115
Thermal correction to Enthalpy=	0.994059
Thermal correction to Gibbs Free Energy=	0.827736
Sum of electronic and zero-point Energies=	-3579.777003
Sum of electronic and thermal Energies=	-3579.717281
Sum of electronic and thermal Enthalpies=	-3579.716337
Sum of electronic and thermal Free Energies=	-3579.882660

 Cartesian Coordinates

7	-5.174969	-1.907927	-0.640943
6	-3.732203	-1.777167	-0.218583
6	-6.963454	-0.615248	2.772849
6	-3.037233	-2.851681	-2.396159
6	-3.597530	-0.587727	0.747502

6	-2.740210	-4.149602	-1.968406
6	-2.883667	-5.231114	-2.832732
8	-5.544766	-1.283183	-1.612487
6	-3.632965	-3.739506	-4.568859
6	-5.925635	-0.272352	1.750186
6	-8.293005	-0.286915	2.489574
8	-5.884906	-2.616533	0.052466
6	-3.489903	-2.659168	-3.702380
6	-9.296157	-0.582671	3.402671
6	-1.377719	-1.499920	-1.014843
6	-2.851895	-1.665018	-1.467739
6	-4.495472	-0.744983	1.976404
6	-6.648996	-1.236423	3.984728
6	-3.327544	-5.027155	-4.137105
6	-1.205869	-0.329777	-0.056223
6	-8.977219	-1.201983	4.610636
8	-6.210074	0.394052	0.774551
6	-7.654550	-1.525247	4.902277
6	-2.123908	-0.469446	1.153163
1	-3.529803	-2.708721	0.319188
1	-1.076728	-2.434709	-0.518428
1	-1.434862	0.606347	-0.582181
1	-10.327498	-0.332637	3.175314
1	-2.652151	-6.233422	-2.486301
1	-1.837611	-1.355618	1.738206
1	-3.988557	-3.574259	-5.580930
1	-4.501717	-1.784091	2.323418
1	-3.899613	0.316409	0.204787
1	-3.739648	-1.655529	-4.035508
1	-2.007657	0.395816	1.813051
1	-2.397654	-4.322996	-0.950209
1	-3.150689	-0.753826	-1.998928
1	-5.621783	-1.492113	4.225394
1	-9.761223	-1.431979	5.325543
1	-7.406094	-2.004681	5.843621
1	-0.158276	-0.274904	0.260607
1	-8.515740	0.195550	1.543646
1	-3.440198	-5.869289	-4.812328
7	1.126284	1.911599	-0.864651
6	0.488861	3.146625	-0.724364
6	-0.604123	3.348911	-1.587746
6	-1.324622	4.527034	-1.544691
6	-0.994221	5.544248	-0.649819
6	0.081227	5.333431	0.195629
6	0.829750	4.155133	0.178166
6	-2.484781	4.745047	-2.473539
9	-2.283007	5.807388	-3.267535
6	0.478094	6.385992	1.193462
9	1.765981	6.732732	1.058379
6	2.222535	1.349320	-0.265038
16	3.220298	2.060318	0.881133
7	2.423390	0.087782	-0.706872
6	3.487533	-0.795709	-0.273594
6	3.136885	-2.206322	-0.800146
6	4.085272	-3.293372	-0.230397
6	3.240678	-4.346319	0.502150
6	2.278735	-4.983190	-0.509666
6	1.440188	-3.848294	-1.156551
7	1.719774	-2.542320	-0.536866
6	1.468863	-2.632327	0.907580
6	2.392620	-3.685094	1.604530
6	3.162211	-3.075647	2.749028
6	4.443002	-3.275548	3.052373
6	4.843759	-0.369558	-0.825454
6	6.044402	-0.401436	-0.047146
6	7.259468	-0.061127	-0.712822
7	7.323160	0.304943	-2.024771
6	6.198253	0.345992	-2.693682
6	4.939913	0.013280	-2.139053
6	8.473782	-0.099968	0.014487

6	8.504590	-0.452950	1.338791
6	7.293762	-0.776635	2.002208
6	6.094079	-0.742524	1.324180
9	-2.707377	3.688535	-3.267113
9	-3.617216	4.983347	-1.794107
9	0.326444	5.950111	2.454042
9	-0.253580	7.501710	1.068344
1	3.226942	-2.165280	-1.893441
1	4.645946	-3.771588	-1.039689
1	4.817921	-2.852552	0.448269
1	0.366079	-4.047176	-1.059799
1	1.657031	-3.758160	-2.226177
1	1.630990	-5.707491	-0.004730
1	2.842784	-5.528340	-1.272558
1	3.889535	-5.112333	0.937543
1	1.747748	-4.464287	2.035273
1	0.413146	-2.895507	1.041658
1	1.605831	-1.638444	1.348375
1	2.574485	-2.418324	3.392396
1	4.899552	-2.790742	3.909381
1	5.089277	-3.917603	2.459269
1	3.522161	-0.801123	0.821148
1	4.049993	0.072607	-2.759292
1	5.199315	-0.988592	1.883413
1	6.258847	0.649396	-3.737271
1	9.382048	0.162359	-0.518051
1	9.449102	-0.474198	1.869075
1	1.703584	-0.357465	-1.266771
1	0.671378	1.309230	-1.548009
1	-0.878708	2.574991	-2.299190
1	1.665390	4.029578	0.852925
1	-1.560313	6.468281	-0.620120
8	7.232837	-1.131323	3.312175
6	8.440621	-1.171773	4.047601
1	8.167384	-1.474301	5.058838
1	9.142421	-1.904388	3.632096
1	8.921854	-0.187553	4.087223
6	-0.500400	-1.374150	-2.234066
1	-4.091952	-0.144094	2.803099
8	0.074092	-0.350654	-2.555334
1	-0.424005	-2.268922	-2.877536

[14]C

Number of imaginary frequencies : 0

Electronic energy=	-3905.3256321
Zero-point correction=	1.057190
Thermal correction to Energy=	1.122348
Thermal correction to Enthalpy=	1.123292
Thermal correction to Gibbs Free Energy=	0.948236
Sum of electronic and zero-point Energies=	-3904.268442
Sum of electronic and thermal Energies=	-3904.203284
Sum of electronic and thermal Enthalpies=	-3904.202340
Sum of electronic and thermal Free Energies=	-3904.377396

Cartesian Coordinates

6	-1.008485	1.960555	-0.993897
6	-0.360849	3.077206	-0.185440
6	0.216251	2.301385	1.004407
6	-0.825404	1.209898	1.295780
7	-1.640440	1.141334	0.052228
6	-2.639802	0.379880	-0.166716
6	-3.224419	-0.577146	0.819696
6	-4.497521	0.005693	1.501217
6	-5.640203	0.108258	0.491510

6	-5.997783	-1.253588	-0.131933
6	-4.745659	-1.810014	-0.819792
6	-3.544685	-1.911304	0.120712
7	-6.859751	0.669754	1.180231
8	-7.596745	1.363706	0.500729
6	-7.164082	-1.150860	-1.116486
6	-8.531116	-1.231979	-0.447289
8	-8.629705	-1.565563	0.717254
6	-4.174323	1.295461	2.228567
6	-4.130193	2.530765	1.576906
6	-3.707654	3.673466	2.254055
6	-3.325369	3.594017	3.590547
6	-3.385563	2.370229	4.253892
6	-3.809619	1.231618	3.576313
6	0.077361	1.052962	-1.676839
8	-0.008528	-0.173945	-1.455518
8	-7.045372	0.373832	2.340760
6	-9.745015	-0.930861	-1.267113
6	-10.984980	-0.911202	-0.620833
6	-12.143034	-0.643476	-1.338536
6	-12.071463	-0.399843	-2.709807
6	-10.840732	-0.423091	-3.360426
6	-9.678614	-0.684723	-2.641377
8	0.937966	1.679423	-2.323943
6	3.663537	0.142048	-0.311243
7	2.651170	-0.738222	-0.413967
6	2.747766	-2.156333	-0.130586
6	2.970450	-2.947463	-1.417565
6	4.002227	-3.927602	-1.561729
6	4.050998	-4.646360	-2.793487
7	3.192304	-4.422775	-3.828457
6	2.286542	-3.489242	-3.668556
6	2.132676	-2.730128	-2.484399
6	5.041154	-5.644284	-2.963684
6	5.950929	-5.924851	-1.976627
6	5.911523	-5.195541	-0.760572
6	4.961239	-4.216608	-0.563810
8	6.781631	-5.404783	0.262011
6	7.808325	-6.359220	0.076156
7	3.335320	1.354451	-0.859326
6	3.902211	2.624386	-0.741031
6	4.964560	2.982087	0.098336
6	5.377321	4.310581	0.148921
6	4.766891	5.311955	-0.595646
6	3.710419	4.942207	-1.419873
6	3.283436	3.626365	-1.506097
6	6.556814	4.646020	1.017524
9	7.718812	4.344153	0.417224
6	2.954678	5.967905	-2.212204
9	3.499932	7.188105	-2.122999
9	6.602511	5.952857	1.321043
9	6.532449	3.967729	2.174815
9	1.680567	6.071605	-1.784770
9	2.889712	5.650070	-3.513207
16	5.146212	-0.239802	0.406577
6	1.457421	-2.650496	0.559677
6	1.651102	-4.100699	1.091154
6	1.477929	-4.091638	2.618780
6	0.037582	-3.663757	2.928383
6	-0.203594	-2.298580	2.228849
7	1.026575	-1.749417	1.644719
6	2.050415	-1.657801	2.691863
6	2.419527	-3.062004	3.274065
6	3.893720	-3.353790	3.149110
6	4.455240	-4.514817	2.818063
1	-5.438132	0.829585	-0.306413
1	-2.489233	-0.743185	1.612063
1	-3.756932	-2.647688	0.904354
1	-13.102316	-0.622961	-0.831538
1	-3.681699	4.626750	1.735461

1	-4.504133	-1.186800	-1.692032
1	-3.106853	2.303523	5.300691
1	-7.098849	-0.229908	-1.706824
1	-6.290469	-1.920270	0.688634
1	-3.858841	0.277482	4.095493
1	-4.975559	-2.804025	-1.215422
1	-4.421007	2.616758	0.532239
1	-4.801886	-0.737532	2.246269
1	-8.726336	-0.701564	-3.161802
1	-12.976707	-0.190050	-3.271095
1	-10.785308	-0.235826	-4.427833
1	-2.663380	-2.264374	-0.425296
1	-11.015573	-1.104518	0.446291
1	-2.995647	4.484082	4.116540
1	0.654080	-2.615865	-0.187202
1	0.913979	-4.777482	0.646151
1	2.638202	-4.483988	0.819705
1	-0.601778	-1.561024	2.937576
1	-0.930734	-2.403410	1.414439
1	-0.104599	-3.579216	4.011115
1	-0.668033	-4.417174	2.563558
1	1.669560	-5.089051	3.026593
1	2.191629	-3.049986	4.349663
1	1.653512	-1.003938	3.475785
1	2.934026	-1.160412	2.277935
1	4.546100	-2.508727	3.375432
1	5.534290	-4.621099	2.764399
1	3.870055	-5.398360	2.575542
1	3.593978	-2.291964	0.543746
1	1.353356	-1.971673	-2.431071
1	4.986818	-3.671237	0.372240
1	1.616126	-3.309425	-4.507345
1	5.055451	-6.179048	-3.907919
1	6.697106	-6.693707	-2.137287
1	1.751926	-0.439824	-0.804516
1	2.518260	1.344942	-1.483647
1	5.459507	2.234789	0.702573
1	2.449591	3.360073	-2.151665
1	5.096721	6.341532	-0.532140
1	8.403048	-6.343892	0.989719
1	7.401816	-7.367316	-0.068513
1	8.450518	-6.099920	-0.773379
1	0.395665	3.596995	-0.773471
1	-1.116706	3.795841	0.146963
1	1.165923	1.833997	0.722601
1	0.391209	2.927688	1.879616
1	-0.360275	0.228561	1.443770
1	-1.491459	1.462070	2.124317
1	-7.112324	-1.981797	-1.833271
1	-3.067791	0.446632	-1.167204
1	-1.755852	2.281991	-1.722456

[14-15]C-TS

Number of imaginary frequencies : 2
The smallest frequency is : -1290.8492

Electronic energy=	-3905.2710527
Zero-point correction=	1.052219
Thermal correction to Energy=	1.115693
Thermal correction to Enthalpy=	1.116637
Thermal correction to Gibbs Free Energy=	0.949485
Sum of electronic and zero-point Energies=	-3904.218834
Sum of electronic and thermal Energies=	-3904.155360
Sum of electronic and thermal Enthalpies=	-3904.154416
Sum of electronic and thermal Free Energies=	-3904.321568

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Cartesian Coordinates

6	-0.616112	2.370197	-1.381194
6	-0.063387	3.543239	-0.550234
6	-0.341434	3.180257	0.918229
6	-0.407730	1.658257	0.905807
7	-1.068357	1.377977	-0.379619
6	-1.697728	0.305195	-0.784962
6	-2.231775	-0.836165	-0.098384
6	-3.381131	-0.611009	0.930896
6	-4.640110	-0.131032	0.177096
6	-5.143897	-1.092708	-0.911190
6	-4.000293	-1.340167	-1.894601
6	-2.746122	-1.825346	-1.166988
7	-5.764498	0.077569	1.160800
8	-6.493883	1.037940	0.973235
6	-6.379146	-0.536745	-1.625636
6	-7.692445	-0.835201	-0.913939
8	-7.748104	-1.682667	-0.044556
6	-3.096577	0.283226	2.122992
6	-3.343478	1.659303	2.112623
6	-3.031927	2.445682	3.220845
6	-2.464037	1.871825	4.353831
6	-2.244635	0.496058	4.388525
6	-2.576194	-0.287151	3.287722
6	0.445003	1.755118	-2.356296
8	0.450707	0.495832	-2.486621
8	-5.894905	-0.734236	2.052500
6	-8.922496	-0.094927	-1.340404
6	-10.095256	-0.294976	-0.605486
6	-11.265232	0.362492	-0.961550
6	-11.274653	1.220644	-2.060853
6	-10.112364	1.419819	-2.800753
6	-8.937237	0.767484	-2.440399
8	1.210666	2.570115	-2.882785
6	2.701654	0.031509	0.028830
7	1.735452	-0.834451	-0.399127
6	1.930896	-2.271218	-0.273853
6	2.573128	-2.815176	-1.553328
6	3.814213	-3.526043	-1.555721
6	4.281926	-4.013511	-2.812878
7	3.625793	-3.808328	-3.989139
6	2.515730	-3.113930	-3.950107
6	1.949956	-2.599619	-2.758451
6	5.496497	-4.740672	-2.855089
6	6.229211	-4.975766	-1.720355
6	5.770300	-4.474620	-0.474894
6	4.592681	-3.761558	-0.400105
8	6.436497	-4.655531	0.692966
6	7.692425	-5.306541	0.650679
7	2.741425	1.173875	-0.717068
6	3.317950	2.412030	-0.392581
6	3.304835	2.925227	0.903893
6	3.793512	4.206949	1.137656
6	4.297578	4.993672	0.111865
6	4.293103	4.469574	-1.178211
6	3.806609	3.197543	-1.441763
6	3.715311	4.730920	2.541520
9	4.364084	3.940812	3.408373
6	4.765922	5.330091	-2.315166
9	5.768613	6.139102	-1.936127
9	4.227789	5.962551	2.655859
9	2.437780	4.791306	2.967157
9	3.786135	6.121853	-2.778620
9	5.204952	4.600710	-3.348566
16	3.710231	-0.259822	1.343157
6	0.658644	-3.105357	0.010224
6	1.099182	-4.500980	0.539900
6	0.718543	-4.645040	2.025439
6	-0.804411	-4.716097	2.105892

6	-1.349873	-3.522999	1.308746
7	-0.284952	-2.508140	1.011566
6	0.445608	-2.155847	2.260979
6	1.140514	-3.421546	2.858724
6	2.624402	-3.242392	3.051608
6	3.564650	-4.156855	2.825352
1	-4.483304	0.855229	-0.268620
1	-1.007215	-1.588280	0.536258
1	-2.998995	-2.779850	-0.693806
1	-12.171189	0.208642	-0.384030
1	-3.231106	3.512558	3.193222
1	-3.786540	-0.413245	-2.445975
1	-1.832732	0.031952	5.279360
1	-6.280136	0.542864	-1.782001
1	-5.416555	-2.036014	-0.421175
1	-2.445225	-1.365937	3.333476
1	-4.325033	-2.078566	-2.635954
1	-3.769043	2.140469	1.236452
1	-3.640596	-1.597188	1.333198
1	-8.038954	0.933264	-3.026651
1	-12.188893	1.735359	-2.339907
1	-10.119473	2.084707	-3.658309
1	-1.952339	-2.034034	-1.894122
1	-10.064101	-0.966569	0.245997
1	-2.212280	2.486852	5.211540
1	0.076583	-3.198732	-0.912713
1	0.613163	-5.298473	-0.030577
1	2.176255	-4.623689	0.402946
1	-2.150469	-3.000612	1.834953
1	-1.735002	-3.849729	0.342859
1	-1.134550	-4.676851	3.148170
1	-1.178533	-5.648601	1.675191
1	1.166239	-5.551603	2.440492
1	0.719832	-3.567402	3.862970
1	-0.288309	-1.734701	2.950497
1	1.169559	-1.371880	2.022538
1	2.923280	-2.272390	3.445141
1	4.609420	-3.941375	3.026887
1	3.345387	-5.143020	2.423508
1	2.610468	-2.402331	0.568846
1	1.034797	-2.015158	-2.822826
1	4.306194	-3.365206	0.567290
1	2.012177	-2.938479	-4.898585
1	5.829951	-5.100763	-3.822825
1	7.156274	-5.532660	-1.785320
1	1.173896	-0.489405	-1.196216
1	2.390160	1.104574	-1.671248
1	2.911826	2.334770	1.723738
1	3.771819	2.818331	-2.457263
1	4.680086	5.988779	0.307161
1	8.061699	-5.313486	1.676286
1	7.600340	-6.340188	0.296999
1	8.404035	-4.765209	0.016838
1	1.005442	3.639684	-0.746697
1	-0.528990	4.488599	-0.832685
1	0.429436	3.553026	1.596750
1	-1.306909	3.578379	1.244858
1	0.598791	1.224801	0.835463
1	-0.927790	1.210623	1.746694
1	-6.458116	-0.987321	-2.624884
1	-1.755374	0.285190	-1.873729
1	-1.480923	2.668580	-1.980494

[15]C

Number of imaginary frequencies : 1

Electronic energy= -3905.3283764
 Zero-point correction= 1.056031
 Thermal correction to Energy= 1.120731
 Thermal correction to Enthalpy= 1.121675
 Thermal correction to Gibbs Free Energy= 0.947789
 Sum of electronic and zero-point Energies= -3904.272345
 Sum of electronic and thermal Energies= -3904.207645
 Sum of electronic and thermal Enthalpies= -3904.206701
 Sum of electronic and thermal Free Energies= -3904.380587

.....
 Cartesian Coordinates

.....

6	0.584948	1.948128	2.364205
6	0.381185	3.358121	1.808727
6	0.499666	3.151125	0.281267
6	1.191869	1.777481	0.123640
7	1.625915	1.447858	1.477816
6	2.308353	0.282213	1.772813
6	3.467399	-0.154281	1.233477
6	4.314769	0.622419	0.231739
6	5.802212	0.201332	0.314050
6	6.096384	-1.300848	0.429288
6	5.368206	-1.792654	1.679115
6	3.866369	-1.583963	1.526886
7	6.527348	0.733880	-0.902392
8	7.652489	1.166838	-0.723042
6	7.599780	-1.580687	0.504345
6	8.269522	-1.693462	-0.858903
8	7.604357	-1.804791	-1.870203
6	4.302986	2.141659	0.393509
6	4.399938	2.727460	1.658933
6	4.463909	4.108812	1.799402
6	4.432981	4.930837	0.673134
6	4.345772	4.358551	-0.591473
6	4.286014	2.972129	-0.728752
6	-0.719099	1.111602	2.285941
8	-0.604543	-0.120341	1.996383
8	5.979145	0.657569	-1.983669
6	9.765524	-1.709658	-0.924273
6	10.364467	-1.707366	-2.187805
6	11.747381	-1.731060	-2.307016
6	12.544030	-1.764916	-1.162745
6	11.954331	-1.772657	0.098494
6	10.568388	-1.741624	0.219334
8	-1.799449	1.691048	2.522249
6	-3.856012	0.092670	0.092333
7	-3.134578	-0.797466	0.821977
6	-3.093059	-2.223854	0.576736
6	-3.979722	-3.001813	1.545097
6	-4.942917	-3.960888	1.101822
6	-5.663331	-4.668186	2.110645
7	-5.491248	-4.454584	3.445427
6	-4.619384	-3.546833	3.808231
6	-3.837048	-2.800417	2.894861
6	-6.609780	-5.645117	1.716848
6	-6.847048	-5.918037	0.394354
6	-6.141117	-5.201247	-0.606361
6	-5.214479	-4.242235	-0.256710
8	-6.323072	-5.402159	-1.935656
6	-7.335424	-6.304742	-2.341169
7	-3.769843	1.344026	0.610481
6	-4.127902	2.582248	0.057635
6	-5.209691	2.801317	-0.799731
6	-5.449885	4.089058	-1.270530
6	-4.657445	5.171258	-0.905763
6	-3.604042	4.940289	-0.028615
6	-3.338996	3.668460	0.456317
6	-6.570460	4.299506	-2.249477
9	-7.595252	3.465581	-2.025960
6	-2.744160	6.077171	0.442842

9	-2.796075	7.125458	-0.390612
9	-7.049873	5.551820	-2.195456
9	-6.169236	4.092451	-3.514299
9	-1.455585	5.709580	0.549608
9	-3.118044	6.518350	1.654216
16	-4.689459	-0.346434	-1.310877
6	-1.647920	-2.746178	0.712322
6	-1.471896	-4.166891	0.132522
6	-0.509164	-4.114552	-1.065207
6	0.872153	-3.679266	-0.556825
6	0.719992	-2.350526	0.206808
7	-0.672945	-1.831627	0.017140
6	-0.973713	-1.678390	-1.437947
6	-0.978589	-3.080080	-2.108457
6	-2.306809	-3.373500	-2.765576
6	-2.920044	-4.553384	-2.813536
1	6.288511	0.715493	1.147406
1	-0.706077	-0.921134	0.542518
1	3.535069	-2.236283	0.700159
1	12.207150	-1.721884	-3.290117
1	4.531801	4.546967	2.790599
1	5.742289	-1.252400	2.559373
1	4.328041	4.987212	-1.476252
1	8.109775	-0.817660	1.102829
1	5.689570	-1.805766	-0.455875
1	4.224503	2.530084	-1.720161
1	5.587104	-2.854718	1.832197
1	4.402097	2.088694	2.538619
1	3.990247	0.379868	-0.790218
1	10.121336	-1.748073	1.208323
1	13.625530	-1.783989	-1.255284
1	12.573590	-1.799280	0.989241
1	3.334905	-1.929919	2.420586
1	9.724010	-1.682431	-3.063067
1	4.479403	6.009697	0.783432
1	-1.353311	-2.695052	1.764428
1	-1.069414	-4.838830	0.895322
1	-2.444419	-4.563569	-0.168944
1	1.394393	-1.566401	-0.144324
1	0.864002	-2.450138	1.285158
1	1.561098	-3.558423	-1.397636
1	1.290837	-4.441490	0.105101
1	-0.437358	-5.101278	-1.529250
1	-0.224141	-3.057817	-2.905595
1	-0.198250	-1.026089	-1.844962
1	-1.936408	-1.169182	-1.534333
1	-2.773274	-2.520712	-3.259378
1	-3.869225	-4.668228	-3.327191
1	-2.515271	-5.445291	-2.341653
1	-3.436954	-2.380581	-0.446783
1	-3.128765	-2.069885	3.278040
1	-4.724987	-3.703600	-1.059481
1	-4.499376	-3.379523	4.876766
1	-7.141965	-6.169953	2.503338
1	-7.576778	-6.672167	0.124040
1	-2.553057	-0.442919	1.586763
1	-3.138902	1.436423	1.425735
1	-5.852199	1.982745	-1.092108
1	-2.516782	3.496345	1.147152
1	-4.857359	6.165001	-1.289467
1	-7.350525	-6.269563	-3.430607
1	-7.115871	-7.329549	-2.019542
1	-8.317351	-6.003377	-1.959165
1	-0.570080	3.787809	2.121256
1	1.191366	4.000514	2.161995
1	-0.482801	3.144111	-0.199861
1	1.089276	3.946428	-0.180275
1	0.468667	1.021546	-0.236252
1	2.028123	1.798786	-0.575626
1	7.767963	-2.538953	1.015382

1	1.836701	-0.341537	2.534403
1	0.931149	1.946555	3.403335

[16]C

Number of imaginary frequencies : 0

Electronic energy=	-3905.3309318
Zero-point correction=	1.057713
Thermal correction to Energy=	1.122804
Thermal correction to Enthalpy=	1.123748
Thermal correction to Gibbs Free Energy=	0.950260
Sum of electronic and zero-point Energies=	-3904.273219
Sum of electronic and thermal Energies=	-3904.208128
Sum of electronic and thermal Enthalpies=	-3904.207184
Sum of electronic and thermal Free Energies=	-3904.380671

 Cartesian Coordinates

7	4.578392	-1.889231	1.687391
6	3.258204	-1.508831	1.065230
6	6.502357	-3.247237	-1.664989
6	2.442221	-0.810703	3.374364
6	3.484829	-1.074636	-0.395153
6	1.835328	-2.017963	3.731719
6	1.641616	-2.345553	5.071266
8	5.224654	-1.021758	2.236591
6	2.669104	-0.268819	5.725418
6	5.707501	-2.122672	-1.080128
6	7.880603	-3.264319	-1.428999
8	4.921495	-3.052480	1.567889
6	2.863653	0.055106	4.385604
6	8.667706	-4.279057	-1.955916
6	1.240726	-0.079161	1.273662
6	2.604277	-0.416968	1.918413
6	4.191391	-2.150244	-1.221854
6	5.921368	-4.255120	-2.439510
6	2.053873	-1.469073	6.071232
6	1.385772	0.346080	-0.197762
6	8.083920	-5.281324	-2.730196
8	6.261123	-1.189858	-0.531057
6	6.712866	-5.267597	-2.973227
6	2.119748	-0.724787	-0.997212
1	2.680255	-2.438029	1.080491
1	0.644550	-0.999996	1.285160
1	1.927947	1.298979	-0.261462
1	9.735972	-4.291438	-1.765194
1	1.168938	-3.287496	5.331704
1	1.496625	-1.628417	-1.051659
1	3.008695	0.412366	6.499224
1	3.815564	-3.148853	-0.972531
1	4.117383	-0.178434	-0.378646
1	3.372144	0.979752	4.122182
1	2.256180	-0.371532	-2.024283
1	1.507303	-2.714906	2.963282
1	3.277916	0.440621	1.861150
1	4.854428	-4.253321	-2.638853
1	8.699180	-6.074126	-3.144410
1	6.258964	-6.045862	-3.578148
1	0.392260	0.495149	-0.625861
1	8.311799	-2.472239	-0.825827
1	1.903730	-1.724040	7.115259
7	-1.443558	2.304954	-1.077971
6	-0.281835	2.776491	-1.692353
6	0.367649	3.826964	-1.015685
6	1.573210	4.321563	-1.481432
6	2.178118	3.807092	-2.628862

6	1.512583	2.794821	-3.301755
6	0.292214	2.277563	-2.864355
6	2.302312	5.365359	-0.685690
9	2.779912	6.348803	-1.455026
6	2.120012	2.175948	-4.528850
9	3.189289	2.854529	-4.963781
6	-2.101093	1.100663	-1.168138
16	-1.916915	-0.019722	-2.425391
7	-2.899360	0.901889	-0.111053
6	-3.784308	-0.227847	0.102665
6	-3.491080	-0.848823	1.482952
6	-4.432283	-2.049040	1.782792
6	-3.576486	-3.251419	2.202276
6	-2.734492	-2.847658	3.422111
6	-1.860410	-1.625336	3.025978
7	-2.072914	-1.234980	1.624631
6	-1.740213	-2.372241	0.757884
6	-2.615045	-3.631726	1.061916
6	-3.260224	-4.160126	-0.194142
6	-4.520592	-4.560612	-0.347428
6	-5.237125	0.228876	0.041516
6	-6.226297	-0.448846	-0.739385
6	-7.558537	0.057989	-0.682890
7	-7.919000	1.144526	0.057976
6	-6.980947	1.740097	0.751861
6	-5.630010	1.317890	0.779259
6	-8.571282	-0.594419	-1.426719
6	-8.298444	-1.699983	-2.190567
6	-6.972830	-2.200966	-2.246869
6	-5.961657	-1.583274	-1.542106
9	1.531569	5.921431	0.261165
9	3.363582	4.827175	-0.045129
9	1.243708	2.108853	-5.539170
9	2.525991	0.913592	-4.289383
1	-3.645821	-0.056149	2.223243
1	-5.134378	-1.790370	2.581918
1	-5.029908	-2.303933	0.904070
1	-0.794123	-1.845586	3.154612
1	-2.089953	-0.752938	3.647788
1	-2.109292	-3.688596	3.742216
1	-3.393397	-2.596488	4.259336
1	-4.215480	-4.103503	2.454954
1	-1.950291	-4.422733	1.438612
1	-0.680114	-2.607737	0.914451
1	-1.840582	-2.057341	-0.286185
1	-2.595335	-4.207946	-1.058622
1	-4.882961	-4.915396	-1.307237
1	-5.241696	-4.539247	0.465707
1	-3.584509	-0.952896	-0.685863
1	-4.913020	1.867047	1.386182
1	-4.966509	-2.004116	-1.627605
1	-7.280128	2.607256	1.337644
1	-9.575469	-0.187655	-1.366057
1	-9.095743	-2.179792	-2.745469
1	-2.811239	1.517205	0.706504
1	-1.749142	2.903214	-0.299023
1	-0.087013	4.228265	-0.112845
1	-0.199774	1.492069	-3.421084
1	3.127175	4.190963	-2.986098
8	-6.618988	-3.290960	-2.976302
6	-7.617094	-3.923270	-3.753776
1	-7.119569	-4.741953	-4.274062
1	-8.418445	-4.332340	-3.127086
1	-8.046225	-3.237307	-4.493089
6	0.365185	4.352644	3.107562
6	1.856829	4.018283	3.083808
6	1.929568	2.854575	2.105971
7	0.664832	2.112278	2.342185
6	-0.336675	3.003800	3.044592
6	0.379993	0.904348	2.013944

1	0.083429	4.930940	2.223800
1	0.065998	4.910249	3.996110
1	2.476986	4.849747	2.745527
1	2.205063	3.698660	4.070915
1	1.909645	3.200545	1.069552
1	2.788078	2.204365	2.249962
1	3.968494	-1.992213	-2.285947
1	-0.647869	0.592082	2.226675
1	-0.504663	2.559920	4.028196
6	-1.648041	2.953118	2.210025
8	-2.406983	1.992565	2.472640
8	-1.767928	3.802223	1.302033

[16-17]C-TS

Number of imaginary frequencies : 1
The smallest frequency is : -1345.3490

Electronic energy=	-3905.2752234
Zero-point correction=	1.053484
Thermal correction to Energy=	1.117991
Thermal correction to Enthalpy=	1.118936
Thermal correction to Gibbs Free Energy=	0.947618
Sum of electronic and zero-point Energies=	-3904.221740
Sum of electronic and thermal Energies=	-3904.157232
Sum of electronic and thermal Enthalpies=	-3904.156288
Sum of electronic and thermal Free Energies=	-3904.327605

Cartesian Coordinates

7	5.122974	-1.844244	0.028881
6	3.657677	-1.587076	-0.283781
6	6.925515	0.614432	-2.694005
6	2.824368	-3.355621	1.328839
6	3.528127	-0.174637	-0.873739
6	3.588715	-4.297004	0.626245
6	3.559819	-5.652577	0.952820
8	5.540519	-1.600661	1.139359
6	2.015109	-5.192209	2.720476
6	5.866650	0.504623	-1.641099
6	8.214138	0.978209	-2.290434
8	5.807024	-2.257134	-0.895513
6	2.038241	-3.842507	2.384253
6	9.230280	1.108606	-3.227501
6	1.394863	-1.247874	0.899271
6	2.820466	-1.856495	0.975795
6	4.469060	0.065759	-2.055650
6	6.665729	0.385406	-4.048126
6	2.773652	-6.111097	2.001915
6	1.165629	-0.044213	-0.065160
6	8.965318	0.880907	-4.577635
8	6.107404	0.798631	-0.486298
6	7.684086	0.520786	-4.986910
6	2.065773	-0.036373	-1.287600
1	3.439525	-2.302632	-1.082199
1	0.267998	-2.059792	0.356091
1	1.349289	0.901598	0.460987
1	10.229233	1.388653	-2.909004
1	4.164649	-6.346326	0.377368
1	1.809416	-0.840650	-1.989704
1	1.390361	-5.524060	3.544294
1	4.535933	-0.821720	-2.694275
1	3.759467	0.555916	-0.088728
1	1.398395	-3.173819	2.946795
1	1.915933	0.908507	-1.819592
1	4.225534	-4.009298	-0.201812
1	3.380787	-1.347143	1.765629

1	5.671053	0.105982	-4.380406
1	9.758486	0.985363	-5.311495
1	7.477176	0.344983	-6.037586
1	0.118476	-0.021870	-0.375987
1	8.395516	1.152870	-1.235111
1	2.753844	-7.165431	2.257828
7	-1.764948	1.968019	0.907133
6	-1.371206	3.298394	0.685641
6	-0.479326	3.840293	1.618359
6	-0.073738	5.163504	1.502420
6	-0.533810	5.972469	0.470819
6	-1.433311	5.424987	-0.437240
6	-1.867099	4.107297	-0.340631
6	0.926598	5.694934	2.487899
9	0.957778	7.035113	2.500338
6	-1.925272	6.263349	-1.582685
9	-1.904616	7.572368	-1.288672
6	-2.062722	0.996480	0.010232
16	-2.068495	1.194574	-1.672538
7	-2.256181	-0.211120	0.609901
6	-2.862395	-1.356892	-0.049132
6	-2.110635	-2.688451	0.197149
6	-2.885983	-3.836584	-0.518902
6	-2.021634	-4.469316	-1.616858
6	-0.837254	-5.154901	-0.937440
6	-0.164228	-4.120811	-0.018389
7	-0.676824	-2.735913	-0.268725
6	-0.562117	-2.441876	-1.720331
6	-1.456893	-3.394909	-2.564264
6	-2.478397	-2.633121	-3.373399
6	-3.724288	-3.016827	-3.639071
6	-4.303485	-1.502407	0.453334
6	-5.436338	-1.291416	-0.398130
6	-6.728263	-1.488490	0.175855
7	-6.927054	-1.824210	1.482738
6	-5.866177	-1.969221	2.235161
6	-4.536246	-1.827297	1.766857
6	-7.872765	-1.330402	-0.640819
6	-7.764650	-0.998671	-1.967556
6	-6.481183	-0.792401	-2.532087
6	-5.346728	-0.921769	-1.758654
9	0.662913	5.284965	3.736806
9	2.171808	5.276608	2.201928
9	-3.180223	5.948160	-1.932614
9	-1.164764	6.100558	-2.677790
1	-2.057187	-2.861424	1.278092
1	-3.178200	-4.603868	0.204629
1	-3.806435	-3.442517	-0.953622
1	0.916595	-4.089459	-0.167782
1	-0.339809	-4.332239	1.039216
1	-0.128081	-5.527283	-1.683414
1	-1.175375	-6.012844	-0.349976
1	-2.611153	-5.195802	-2.182942
1	-0.800360	-3.906266	-3.281285
1	0.495662	-2.570811	-1.968966
1	-0.822270	-1.390910	-1.882301
1	-2.125079	-1.687001	-3.786491
1	-4.379825	-2.399304	-4.246149
1	-4.144535	-3.944070	-3.257226
1	-2.862668	-1.152226	-1.120154
1	-3.718694	-1.948416	2.471442
1	-4.393776	-0.712782	-2.228607
1	-6.036734	-2.221952	3.279976
1	-8.841935	-1.483776	-0.177574
1	-8.659624	-0.889539	-2.568487
1	-2.389498	-0.205094	1.635086
1	-1.649340	1.683010	1.901569
1	-0.126018	3.218159	2.436850
1	-2.587631	3.716738	-1.045809
1	-0.214805	7.004812	0.387374

8	-6.282161	-0.469690	-3.836811
6	-7.420073	-0.284384	-4.656773
1	-7.039553	-0.022506	-5.644308
1	-8.015743	-1.201648	-4.734123
1	-8.052496	0.531758	-4.288893
6	0.770350	0.086127	5.476141
6	2.114875	-0.643472	5.450032
6	2.363660	-0.891447	3.960525
7	1.002036	-0.926055	3.371369
6	-0.030938	-0.651888	4.419195
6	0.694613	-0.929616	2.093423
1	0.875900	1.127685	5.157764
1	0.283284	0.059126	6.452268
1	2.928928	-0.071892	5.898356
1	2.036787	-1.598339	5.979136
1	2.906399	-0.060316	3.501598
1	2.908298	-1.819839	3.771274
1	4.059337	0.869468	-2.682137
1	-0.330642	-0.623354	1.895671
1	-0.402212	-1.613835	4.788172
6	-1.190212	0.114093	3.748203
8	-2.176669	-0.578771	3.409144
8	-0.974668	1.316439	3.473755

[17]C

Number of imaginary frequencies : 0

Electronic energy=	-3905.3336905
Zero-point correction=	1.056902
Thermal correction to Energy=	1.122058
Thermal correction to Enthalpy=	1.123002
Thermal correction to Gibbs Free Energy=	0.947333
Sum of electronic and zero-point Energies=	-3904.276789
Sum of electronic and thermal Energies=	-3904.211633
Sum of electronic and thermal Enthalpies=	-3904.210689
Sum of electronic and thermal Free Energies=	-3904.386358

Cartesian Coordinates

7	-5.865050	0.272282	-0.940927
6	-4.379015	0.004861	-0.906887
6	-7.264451	-3.466917	-1.520298
6	-3.959944	2.430471	-1.035502
6	-4.160251	-1.385901	-0.292118
6	-4.930567	3.339868	-0.615415
6	-5.269786	4.438924	-1.404431
8	-6.391502	0.733870	0.049908
6	-3.672574	3.732014	-3.060861
6	-6.361490	-2.643547	-0.652569
6	-8.623371	-3.509199	-1.193759
8	-6.455102	-0.044235	-1.961167
6	-3.338504	2.638101	-2.270948
6	-9.504588	-4.261998	-1.958382
6	-2.200082	0.838816	0.011611
6	-3.666517	1.186463	-0.205074
6	-4.907997	-2.472013	-1.070625
6	-6.796355	-4.193369	-2.618475
6	-4.642970	4.637078	-2.629993
6	-1.920537	-0.564172	0.496911
6	-9.032100	-4.986858	-3.051884
8	-6.774063	-2.154687	0.380289
6	-7.679043	-4.954540	-3.378972
6	-2.654123	-1.645374	-0.288141
1	-4.098862	-0.024754	-1.963775
1	2.217442	1.603220	-1.884711
1	-2.238315	-0.631719	1.549843

1	-10.559574	-4.285128	-1.704675
1	-6.028373	5.134248	-1.058818
1	-2.288000	-1.676394	-1.324199
1	-3.176542	3.881377	-4.015301
1	-4.856351	-2.280159	-2.148142
1	-4.533094	-1.367455	0.739433
1	-2.570739	1.941695	-2.601123
1	-2.459821	-2.628273	0.153517
1	-5.429835	3.180588	0.336492
1	-4.148694	1.299244	0.775689
1	-5.743764	-4.177586	-2.882998
1	-9.719037	-5.577657	-3.650032
1	-7.311351	-5.521206	-4.228490
1	-0.840084	-0.748736	0.494644
1	-8.965344	-2.938320	-0.336827
1	-4.907577	5.489736	-3.247592
7	1.912475	0.619802	1.881669
6	0.930156	0.189162	2.786074
6	-0.115452	1.095218	3.007692
6	-1.147079	0.767433	3.874266
6	-1.166981	-0.448312	4.549496
6	-0.105018	-1.320351	4.347242
6	0.945348	-1.022092	3.482488
6	-2.294740	1.724793	3.998973
9	-3.087410	1.437235	5.038437
6	-0.095732	-2.652319	5.042169
9	-0.886997	-2.657156	6.124929
6	2.709455	-0.085040	1.038635
16	2.878599	-1.766776	1.013307
7	3.331449	0.726967	0.143033
6	4.347564	0.289061	-0.793782
6	4.142149	0.939052	-2.177926
6	4.937791	0.214171	-3.286233
6	3.954647	-0.416673	-4.287016
6	3.186512	0.714730	-4.984384
6	2.541034	1.605108	-3.906404
7	2.689967	0.945822	-2.570188
6	2.100000	-0.424211	-2.598357
6	2.926980	-1.314697	-3.567689
6	3.499087	-2.521592	-2.862026
6	4.687408	-3.076923	-3.085763
6	5.754670	0.631067	-0.310111
6	6.797401	-0.343145	-0.223142
6	8.082172	0.120169	0.191665
7	8.343262	1.416678	0.520162
6	7.354084	2.272300	0.449640
6	6.045930	1.927101	0.034320
6	9.150734	-0.805483	0.269087
6	8.974718	-2.128176	-0.046101
6	7.694041	-2.587812	-0.448209
6	6.630603	-1.713566	-0.526781
9	-1.879639	2.991861	4.144175
9	-3.068395	1.700130	2.894966
9	1.136629	-2.997936	5.441675
9	-0.530307	-3.635102	4.235770
1	4.402345	1.999254	-2.112996
1	5.587495	0.920686	-3.809943
1	5.581107	-0.546182	-2.836843
1	1.471000	1.757244	-4.061875
1	3.011570	2.585731	-3.817204
1	2.421187	0.298654	-5.645401
1	3.864448	1.310279	-5.600524
1	4.502440	-1.003107	-5.028758
1	2.233840	-1.690651	-4.331412
1	1.063008	-0.306491	-2.920251
1	2.099429	-0.817145	-1.578289
1	2.841225	-2.973606	-2.119542
1	4.999080	-3.961638	-2.539802
1	5.395237	-2.678797	-3.808633
1	4.238042	-0.792100	-0.889357

1	5.283020	2.701274	-0.007030
1	5.667211	-2.122064	-0.809207
1	7.574632	3.302591	0.721372
1	10.116292	-0.428184	0.589545
1	9.811823	-2.812335	0.022773
1	3.117865	1.727048	0.160833
1	1.840306	1.627076	1.661560
1	-0.109369	2.048892	2.483715
1	1.763182	-1.717843	3.357417
1	-1.977321	-0.700608	5.222895
8	7.432110	-3.878951	-0.770382
6	8.486833	-4.818773	-0.679721
1	8.059068	-5.778333	-0.970813
1	9.307933	-4.570787	-1.362516
1	8.871641	-4.894378	0.343522
6	-0.344848	5.273180	-0.348867
6	-1.772887	5.293036	0.213765
6	-1.881215	3.913762	0.845881
7	-1.230554	3.081977	-0.166310
6	-0.117109	3.802738	-0.775112
6	-1.167547	1.702466	-0.036779
1	0.362078	5.526031	0.447003
1	-0.193675	5.967577	-1.177269
1	-1.932536	6.104149	0.927610
1	-2.509917	5.375833	-0.592545
1	-1.338963	3.880989	1.803415
1	-2.909081	3.590396	1.020844
1	-4.418800	-3.441977	-0.904150
1	-0.163418	1.274490	0.082514
1	-0.143269	3.685269	-1.865965
6	1.244692	3.289289	-0.273341
8	2.128865	3.014791	-1.143479
8	1.394389	3.162732	0.961179

17 (b) Conformational Sampling of Substituent effect (Table S17)

1-Michael-nitro-cinchona-thiourea-*si-si*_conf-1

Number of imaginary frequencies : 1
The smallest frequency is : -285.9676 cm(-1)

Electronic energy : =-3435.8469612
Zero-point correction= 1.045346
Thermal correction to Energy= 1.106272
Thermal correction to Enthalpy= 1.107216
Thermal correction to Gibbs Free Energy= 0.948105
Sum of electronic and zero-point Energies= -3434.801615
Sum of electronic and thermal Energies= -3434.740689
Sum of electronic and thermal Enthalpies= -3434.739745
Sum of electronic and thermal Free Energies= -3434.898856

Cartesian Coordinates

6	-1.676286	-1.031139	5.123148
6	-2.559839	-2.282671	5.039846
6	-3.764984	-1.829974	4.200685
7	-3.285772	-0.632382	3.496399
6	-1.859925	-0.418345	3.727336
6	-4.111282	0.190372	2.851757
6	-3.787103	1.268363	2.048869
8	-0.564267	1.904310	-1.000859
8	-0.824597	0.863289	0.886323
1	-1.623263	0.647396	3.684568
1	-0.627776	-1.251900	5.327151
1	-2.051027	-0.340051	5.884760
1	-2.024308	-3.078087	4.515827
1	-2.863919	-2.659313	6.017917
1	-4.076396	-2.597217	3.485521

1	-4.625216	-1.559937	4.822912
1	-5.162680	-0.093174	2.931752
1	-2.755165	1.613626	2.042879
6	-4.871406	2.265026	1.706454
6	-4.514118	3.256794	0.587356
1	-5.111779	2.857298	2.600892
1	-5.792338	1.733407	1.434156
1	-4.509742	2.765284	-0.389604
1	-5.301801	4.021050	0.555330
6	-3.196132	3.925783	0.827782
6	-2.271772	4.168752	-0.107232
1	-2.963786	4.220594	1.852570
1	-2.450998	3.892626	-1.140623
6	-0.964557	4.758866	0.273019
8	-0.709177	5.021220	1.440941
6	0.075712	5.015970	-0.779707
6	-0.035792	4.573539	-2.101359
6	1.235718	5.692316	-0.380893
6	1.002781	4.793002	-3.002597
1	-0.901892	4.009288	-2.424215
6	2.268519	5.918170	-1.282747
1	1.304155	6.034566	0.647158
6	2.154512	5.462397	-2.596823
1	0.914829	4.430204	-4.021416
1	3.161107	6.449444	-0.965708
1	2.961955	5.629107	-3.303242
6	-3.313258	0.065985	0.201341
1	-2.762254	-0.592193	0.870710
1	-2.867593	1.383470	-1.513107
6	-4.611235	-0.444121	-0.279648
6	-5.172246	-1.562146	0.354426
6	-5.266694	0.091286	-1.395119
6	-6.343293	-2.137249	-0.121416
1	-4.645327	-1.997905	1.201726
6	-6.436272	-0.488527	-1.878492
1	-4.853619	0.950191	-1.914835
6	-6.975672	-1.605410	-1.246105
1	-6.754359	-3.015038	0.367518
1	-6.917270	-0.076106	-2.759357
1	-7.877230	-2.067719	-1.634503
7	-1.275092	1.228580	-0.232024
6	-2.554325	0.914801	-0.593733
7	-0.570164	-1.873486	-0.660794
6	-1.610157	-2.186278	-1.536809
6	-1.852074	-1.507524	-2.742234
6	-3.012584	-1.765333	-3.452404
6	-3.914374	-2.711918	-2.970586
6	-3.676787	-3.421868	-1.801381
6	-2.525155	-3.147072	-1.083175
6	0.704438	-1.462508	-0.905808
16	1.434700	-1.387900	-2.431596
7	1.334715	-1.131038	0.239477
6	2.730095	-0.776957	0.372792
6	2.805433	0.462311	1.283840
6	4.228707	1.029943	1.463911
6	4.282056	2.464908	0.921976
6	3.316317	3.340400	1.736015
6	1.913603	2.700890	1.718362
7	1.919476	1.560341	0.748201
6	2.345967	2.049374	-0.603951
6	3.827198	2.497763	-0.549835
6	4.684515	1.715066	-1.515436
6	5.953761	1.358077	-1.336749
6	3.542188	-1.906664	1.002172
6	4.768221	-2.381784	0.437961
6	5.464322	-3.398042	1.157958
7	5.008336	-3.937921	2.324228
6	3.868046	-3.492796	2.790197
6	3.100158	-2.477113	2.170153
6	6.693545	-3.879033	0.646388

6	7.224236	-3.388478	-0.519491
6	6.523827	-2.387468	-1.239461
6	5.319509	-1.904759	-0.772925
1	2.347894	0.193137	2.241429
1	4.502641	1.020981	2.522430
1	4.945237	0.396386	0.935841
1	1.134487	3.394074	1.393782
1	1.621344	2.283829	2.684555
1	3.273942	4.345120	1.303860
1	3.668376	3.436420	2.766163
1	5.298075	2.858903	1.008477
1	3.847328	3.546096	-0.876418
1	1.673216	2.871471	-0.849122
1	2.157116	1.243735	-1.318816
1	4.192869	1.448668	-2.452541
1	6.489582	0.800207	-2.098761
1	6.501993	1.588611	-0.426410
1	3.115313	-0.542225	-0.620831
1	2.161982	-2.161482	2.622948
1	4.812521	-1.160404	-1.373934
1	3.510787	-3.937955	3.717083
1	7.202222	-4.653011	1.211848
1	8.167872	-3.776459	-0.883989
1	0.821830	-1.185356	1.138889
1	-0.817341	-2.024826	0.337539
1	-1.151281	-0.756846	-3.083301
1	-2.328249	-3.655775	-0.144666
8	6.975007	-1.851395	-2.403692
6	8.170597	-2.368659	-2.955841
1	8.325563	-1.833605	-3.893044
1	9.029298	-2.192640	-2.297103
1	8.085143	-3.440980	-3.165718
1	0.937277	1.207486	0.685576
6	-0.959164	-1.170144	2.720373
8	-1.508185	-1.988230	1.941134
8	0.266388	-0.914227	2.813890
1	-4.398323	-4.150851	-1.454598
1	-3.241108	-1.225465	-4.363227
7	-5.169680	-2.923339	-3.679596
8	-5.905078	-3.817936	-3.292717
8	-5.430441	-2.186039	-4.617936

1-Michael-nitro-cinchona-thiourea-si-si_conf-2

Number of imaginary frequencies : 1

The smallest frequency is : -252.8042 cm(-1)

Electronic energy : =-3435.8459919

Zero-point correction= 1.046269

Thermal correction to Energy= 1.107208

Thermal correction to Enthalpy= 1.108152

Thermal correction to Gibbs Free Energy= 0.948376

Sum of electronic and zero-point Energies= -3434.799723

Sum of electronic and thermal Energies= -3434.738784

Sum of electronic and thermal Enthalpies= -3434.737840

Sum of electronic and thermal Free Energies= -3434.897616

Cartesian Coordinates

6	-1.544899	-0.196419	5.085205
6	-2.390873	-1.461372	5.271700
6	-3.645524	-1.190045	4.428481
7	-3.220942	-0.153974	3.476056
6	-1.796650	0.135534	3.607621
6	-4.088759	0.503960	2.704490
6	-3.826589	1.433833	1.720972
8	-0.730547	1.606939	-1.548974

8	-0.851544	0.848478	0.486621
1	-1.591963	1.179008	3.355639
1	-0.483480	-0.348794	5.284902
1	-1.915518	0.616543	5.717527
1	-3.987222	-2.084809	3.899089
1	-4.472680	-0.804979	5.035503
1	-2.814776	1.819196	1.616138
6	-4.970077	2.258092	1.174018
1	-5.799772	1.599864	0.882579
6	-3.317169	-0.119022	0.083748
1	-2.707801	-0.583009	0.855360
1	-3.017962	0.881965	-1.862142
6	-4.600506	-0.773799	-0.201436
6	-5.020469	-1.802954	0.653709
6	-5.378035	-0.465980	-1.325211
6	-6.174317	-2.524265	0.378390
1	-4.395925	-2.048061	1.511531
6	-6.531729	-1.192856	-1.604552
1	-5.073923	0.326245	-2.003032
6	-6.926245	-2.227923	-0.759958
1	-6.479112	-3.333222	1.034932
1	-7.112006	-0.963282	-2.492239
1	-7.813976	-2.807046	-0.992013
7	-1.369483	1.030317	-0.646955
6	-2.647721	0.608500	-0.886446
7	-0.497745	-2.175440	-0.438595
6	-1.534802	-2.583996	-1.283354
6	-1.770821	-2.012515	-2.544194
6	-2.927802	-2.326568	-3.235951
6	-3.831322	-3.229370	-2.678317
6	-3.597949	-3.841042	-1.455279
6	-2.448418	-3.505607	-0.755979
6	0.778560	-1.808532	-0.738702
16	1.507774	-1.988140	-2.257602
7	1.407807	-1.292199	0.336084
6	2.781075	-0.837848	0.384062
6	2.781120	0.576598	0.995938
6	4.158875	1.272033	1.026039
6	4.106192	2.560585	0.189808
6	3.066323	3.517718	0.798221
6	1.719350	2.779316	0.930856
7	1.827740	1.459707	0.237211
6	2.229926	1.667545	-1.190930
6	3.666183	2.239580	-1.251434
6	4.589643	1.334658	-2.032063
6	5.877328	1.113292	-1.781505
6	3.655798	-1.751089	1.235183
6	4.911670	-2.253417	0.769046
6	5.671863	-3.046800	1.679223
7	5.249549	-3.356626	2.937667
6	4.081296	-2.898119	3.313698
6	3.249428	-2.087407	2.502638
6	6.930641	-3.546542	1.265788
6	7.428147	-3.286044	0.014764
6	6.664212	-2.508667	-0.892261
6	5.432867	-2.011344	-0.522607
1	2.340695	0.503582	1.995082
1	4.430986	1.509774	2.058017
1	4.922478	0.595042	0.635616
1	0.892483	3.307505	0.453044
1	1.445477	2.564031	1.965793
1	2.947703	4.397589	0.157474
1	3.398604	3.864268	1.779925
1	5.088333	3.040721	0.183443
1	3.604165	3.193696	-1.794038
1	1.491791	2.352699	-1.603850
1	2.120258	0.710254	-1.707427
1	4.130504	0.838979	-2.888918
1	6.462206	0.444115	-2.405166
1	6.394089	1.573531	-0.942809

1	3.158118	-0.806685	-0.638791
1	2.293322	-1.740031	2.889966
1	4.882602	-1.444857	-1.263324
1	3.753280	-3.161126	4.317643
1	7.488380	-4.146225	1.977765
1	8.394433	-3.682476	-0.273376
1	0.885742	-1.164484	1.226231
1	-0.765447	-2.136952	0.564161
1	-1.070689	-1.289606	-2.942735
1	-2.255572	-3.938214	0.220713
8	7.079172	-2.208297	-2.150553
6	8.289995	-2.780837	-2.607391
1	8.407014	-2.452126	-3.640323
1	9.149202	-2.432856	-2.021944
1	8.250326	-3.875864	-2.581691
1	0.867443	1.044451	0.260994
6	-0.908448	-0.776333	2.729235
8	-1.456792	-1.736755	2.135322
8	0.315237	-0.489259	2.737226
1	-5.364036	2.918659	1.959315
1	-2.637514	-1.664638	6.315128
1	-1.855848	-2.325433	4.869317
6	-4.597054	3.143381	-0.026813
1	-5.485261	3.728075	-0.298371
1	-4.331646	2.538615	-0.896848
6	-3.489416	4.093854	0.298564
6	-2.338763	4.215829	-0.373677
1	-3.636609	4.746297	1.160960
1	-2.132285	3.590622	-1.236991
6	-1.348057	5.240481	0.054715
8	-1.519596	5.895780	1.070417
6	-0.125583	5.490193	-0.786133
6	0.219713	4.713640	-1.897800
6	0.702675	6.554920	-0.410465
6	1.377249	5.004679	-2.619335
1	-0.389682	3.868001	-2.199522
6	1.848850	6.850494	-1.137288
1	0.420331	7.144534	0.455245
6	2.189069	6.073610	-2.245439
1	1.638116	4.399062	-3.482364
1	2.476620	7.685946	-0.844166
1	3.082791	6.303174	-2.817763
1	-5.125623	0.196499	2.855292
1	-3.151925	-1.862353	-4.188591
1	-4.321763	-4.538613	-1.053145
7	-5.088293	-3.495271	-3.368297
8	-5.812939	-4.372956	-2.927504
8	-5.359567	-2.814661	-4.345414

1-Michael-nitro-cinchona-thiourea-si-si_conf-3

Number of imaginary frequencies : 1

The smallest frequency is : -288.2270 cm(-1)

Electronic energy : =-3435.8451507

Zero-point correction= 1.045534

Thermal correction to Energy= 1.106424

Thermal correction to Enthalpy= 1.107369

Thermal correction to Gibbs Free Energy= 0.947810

Sum of electronic and zero-point Energies= -3434.799617

Sum of electronic and thermal Energies= -3434.738726

Sum of electronic and thermal Enthalpies= -3434.737782

Sum of electronic and thermal Free Energies= -3434.897340

Cartesian Coordinates

6	-1.652171	0.141724	5.106531

6	-2.511955	-1.105417	5.336088
6	-3.757310	-0.842068	4.481974
7	-3.287290	0.094671	3.449228
6	-1.865111	0.403483	3.608403
6	-4.114253	0.668409	2.576703
6	-3.758991	1.457695	1.498148
8	-0.590451	1.230062	-1.724832
8	-0.830866	0.969708	0.422506
1	-1.668994	1.439863	3.321166
1	-0.596369	-0.005770	5.337416
1	-2.030793	0.986548	5.691015
1	-1.987906	-1.987647	4.959764
1	-2.763753	-1.271242	6.384865
1	-4.151439	-1.753631	4.023540
1	-4.557242	-0.367690	5.062166
1	-5.162641	0.394599	2.706991
1	-2.724813	1.787545	1.437126
6	-4.773453	2.263979	0.739265
6	-4.736793	3.775324	1.069324
1	-5.783842	1.875091	0.910047
1	-4.566151	2.165101	-0.336632
1	-5.382726	4.305109	0.360717
1	-5.132954	3.943389	2.074913
6	-3.332437	4.297637	0.984093
6	-2.671573	4.553991	-0.150445
1	-2.772354	4.409291	1.911845
1	-3.149947	4.451265	-1.120899
6	-1.243816	4.956839	-0.080732
8	-0.737325	5.321278	0.971256
6	-0.399496	4.881061	-1.316106
6	-0.745961	4.096676	-2.418344
6	0.819591	5.571865	-1.315432
6	0.120891	3.998791	-3.505590
1	-1.663771	3.518862	-2.417438
6	1.673407	5.489824	-2.407224
1	1.073926	6.172299	-0.447234
6	1.324810	4.696706	-3.503857
1	-0.141975	3.365975	-4.346686
1	2.608872	6.041313	-2.408999
1	1.995432	4.623387	-4.354604
6	-3.248914	-0.141034	0.090784
1	-2.625756	-0.567800	0.872427
1	-2.939101	0.633409	-1.956285
6	-4.509419	-0.859595	-0.171276
6	-4.903590	-1.854384	0.735190
6	-5.280665	-0.644886	-1.318820
6	-6.028338	-2.630208	0.488628
1	-4.279506	-2.030364	1.610648
6	-6.404959	-1.427134	-1.569843
1	-4.995062	0.119658	-2.035024
6	-6.775442	-2.425640	-0.672874
1	-6.313250	-3.411479	1.186636
1	-6.980015	-1.269072	-2.476677
1	-7.639522	-3.047900	-0.882034
7	-1.293744	0.919285	-0.751549
6	-2.589133	0.513144	-0.943366
7	-0.425215	-2.089481	-0.332133
6	-1.421526	-2.583923	-1.179711
6	-1.650099	-2.066314	-2.464734
6	-2.772439	-2.458363	-3.172616
6	-3.648805	-3.380689	-2.603122
6	-3.420474	-3.937674	-1.353501
6	-2.303179	-3.528537	-0.640693
6	0.837977	-1.673565	-0.632067
16	1.610738	-1.906754	-2.119381
7	1.416532	-1.062644	0.420696
6	2.788976	-0.613403	0.480993
6	2.799666	0.790181	1.110047
6	4.188925	1.462498	1.122833
6	4.141235	2.758873	0.301348

6	3.137032	3.720974	0.955029
6	1.778628	3.007122	1.110588
7	1.839301	1.698908	0.386482
6	2.209606	1.927025	-1.047572
6	3.657337	2.466992	-1.132561
6	4.542155	1.552498	-1.946650
6	5.829905	1.297260	-1.730062
6	3.653644	-1.540750	1.329153
6	4.904792	-2.056824	0.866619
6	5.652615	-2.859675	1.778780
7	5.222032	-3.166730	3.035084
6	4.056506	-2.697592	3.406818
6	3.237234	-1.876904	2.593489
6	6.907277	-3.372737	1.369160
6	7.411100	-3.117045	0.119726
6	6.658454	-2.331225	-0.789689
6	5.432079	-1.819491	-0.423559
1	2.377802	0.706752	2.115826
1	4.483992	1.686847	2.151619
1	4.933601	0.776419	0.712734
1	0.953905	3.578026	0.682244
1	1.533479	2.774848	2.149067
1	3.020073	4.613591	0.332464
1	3.501840	4.044432	1.933046
1	5.131951	3.220528	0.275113
1	3.605083	3.426335	-1.665452
1	1.472108	2.631313	-1.437288
1	2.064421	0.981435	-1.576683
1	4.052338	1.081135	-2.800086
1	6.384738	0.626543	-2.379033
1	6.378156	1.729689	-0.896496
1	3.171557	-0.572674	-0.539713
1	2.282498	-1.519980	2.976035
1	4.887005	-1.249579	-1.165745
1	3.721343	-2.959305	4.408759
1	7.456147	-3.979043	2.082423
1	8.373747	-3.524124	-0.165810
1	0.874816	-0.910993	1.291988
1	-0.703665	-2.026546	0.662902
1	-0.977120	-1.316307	-2.861828
1	-2.115413	-3.918105	0.355087
8	7.080429	-2.037022	-2.047099
6	8.283458	-2.627441	-2.501083
1	8.406486	-2.302775	-3.534625
1	9.146934	-2.290410	-1.915441
1	8.228415	-3.721772	-2.473040
1	0.874949	1.283645	0.399540
6	-0.925295	-0.522112	2.796169
8	-1.419841	-1.542167	2.257677
8	0.282799	-0.176256	2.802343
1	-4.125236	-4.650190	-0.943736
1	-2.994925	-2.036726	-4.145244
7	-4.879243	-3.720722	-3.308196
8	-5.582172	-4.605953	-2.847718
8	-5.152326	-3.090116	-4.317974

1-Michael-nitro-cinchona-thiourea-*si-re*_conf-1

Number of imaginary frequencies : 1
The smallest frequency is : -293.8459 cm(-1)

Electronic energy : =-3435.8393943
Zero-point correction= 1.045158
Thermal correction to Energy= 1.106772
Thermal correction to Enthalpy= 1.107717
Thermal correction to Gibbs Free Energy= 0.941445
Sum of electronic and zero-point Energies= -3434.794236

Sum of electronic and thermal Energies=	-3434.732622
Sum of electronic and thermal Enthalpies=	-3434.731678
Sum of electronic and thermal Free Energies=	-3434.897949

Cartesian Coordinates

6	2.133626	-1.621460	3.503335
6	2.879136	-0.412540	4.087412
6	3.998089	-0.123042	3.068003
7	3.628024	-0.902043	1.875281
6	2.254274	-1.396037	1.986217
6	4.531060	-1.444131	1.064141
6	4.254310	-2.083717	-0.133776
8	0.917336	0.740611	-1.251054
8	1.742694	-1.159796	-1.904441
1	2.151653	-2.309460	1.399752
1	1.092872	-1.680145	3.830670
1	2.639008	-2.556353	3.769720
1	2.206404	0.444073	4.142848
1	3.279287	-0.609623	5.083351
1	4.045316	0.939479	2.819358
1	4.983725	-0.452041	3.411762
1	5.570753	-1.255963	1.338384
1	3.213845	-2.277812	-0.383698
6	5.259479	-3.041018	-0.711743
6	5.079875	-4.469491	-0.138504
1	6.278057	-2.696532	-0.497506
1	5.158406	-3.083376	-1.804477
1	5.875738	-5.112756	-0.531069
1	5.184668	-4.430058	0.951149
6	3.749032	-5.043542	-0.512313
6	2.686051	-5.131125	0.295359
1	3.619187	-5.362897	-1.546799
1	2.751385	-4.807133	1.331346
6	1.394266	-5.640842	-0.243749
8	1.366033	-6.322292	-1.255021
6	0.107062	-5.251581	0.427595
6	0.042836	-4.335491	1.480467
6	-1.083129	-5.765282	-0.104468
6	-1.189536	-3.919475	1.979131
1	0.946551	-3.922289	1.911597
6	-2.312246	-5.361942	0.401528
1	-1.017492	-6.470704	-0.926494
6	-2.368037	-4.428078	1.439390
1	-1.226282	-3.187365	2.779192
1	-3.229967	-5.767587	-0.013878
1	-3.327762	-4.098910	1.827879
6	4.259475	-0.352869	-1.382231
1	4.129176	-1.069219	-2.189902
1	3.154472	1.388461	-0.585669
6	5.618420	0.212792	-1.232787
6	6.645435	-0.215999	-2.079787
6	5.909285	1.166779	-0.247636
6	7.932343	0.301066	-1.952765
1	6.428693	-0.951721	-2.849873
6	7.192978	1.682181	-0.121251
1	5.124097	1.498150	0.427670
6	8.209110	1.251050	-0.974276
1	8.716835	-0.036423	-2.622663
1	7.402391	2.423971	0.643037
1	9.210623	1.657159	-0.875359
7	1.896663	-0.012656	-1.426291
6	3.148543	0.429656	-1.078101
7	-0.180218	2.807101	0.463258
6	0.540224	3.985137	0.319252
6	0.057549	5.198997	-0.197429
6	0.901628	6.296909	-0.278359
6	2.216050	6.193893	0.157011
6	2.715042	5.006514	0.686862
6	1.877498	3.913152	0.767714

6	-1.402440	2.405720	0.013816
16	-2.543492	3.350369	-0.802917
7	-1.612500	1.099213	0.288122
6	-2.818911	0.370583	-0.028944
6	-2.461905	-1.073488	-0.439113
6	-3.640861	-1.803379	-1.119427
6	-3.286332	-2.105959	-2.584667
6	-2.120892	-3.103911	-2.594875
6	-0.994151	-2.553902	-1.702943
7	-1.289153	-1.117619	-1.379678
6	-1.522116	-0.329981	-2.628130
6	-2.816137	-0.833841	-3.318789
6	-3.845750	0.262970	-3.452303
6	-5.164270	0.128136	-3.331817
6	-3.762170	0.277633	1.169708
6	-5.156627	0.577417	1.091821
6	-5.935053	0.352628	2.266755
7	-5.410687	-0.101358	3.439911
6	-4.121230	-0.332647	3.477448
6	-3.258886	-0.164174	2.368691
6	-7.326892	0.609277	2.222976
6	-7.933044	1.068873	1.082197
6	-7.153298	1.305360	-0.079702
6	-5.795086	1.069586	-0.069231
1	-2.106685	-1.610986	0.443881
1	-3.846770	-2.743435	-0.597310
1	-4.541089	-1.187553	-1.053140
1	-0.014269	-2.568730	-2.177009
1	-0.928087	-3.067326	-0.741438
1	-1.762328	-3.251837	-3.617861
1	-2.444103	-4.076025	-2.213651
1	-4.151169	-2.534224	-3.098194
1	-2.539183	-1.133070	-4.338236
1	-0.623335	-0.469418	-3.231403
1	-1.573643	0.723934	-2.343233
1	-3.440983	1.244735	-3.700304
1	-5.827658	0.975726	-3.471831
1	-5.637038	-0.819507	-3.085530
1	-3.308179	0.880055	-0.861497
1	-2.198754	-0.389449	2.469338
1	-5.235210	1.296824	-0.968885
1	-3.714645	-0.684547	4.423897
1	-7.896721	0.428554	3.128610
1	-9.000128	1.256356	1.079848
1	-0.868391	0.540805	0.737347
1	0.387660	2.047613	0.876012
1	-0.965147	5.276449	-0.532699
1	2.234473	2.974805	1.183439
8	-7.674535	1.764887	-1.245460
6	-9.049752	2.096860	-1.276346
1	-9.243210	2.483576	-2.277097
1	-9.681793	1.217633	-1.103887
1	-9.292778	2.871219	-0.539648
1	-0.458274	-0.714150	-0.910364
6	1.189223	-0.388150	1.534437
8	1.442639	0.826158	1.680883
8	0.110317	-0.901768	1.127236
1	0.543130	7.238364	-0.676553
1	3.742951	4.956603	1.024071
7	3.092829	7.352586	0.063529
8	4.239543	7.237557	0.470149
8	2.639969	8.380290	-0.415301

1-Michael-nitro-cinchona-thiourea-*si-re*_conf-2

Number of imaginary frequencies : 1
The smallest frequency is : -300.3471 cm(-1)

Electronic energy : =-3435.83837
 Zero-point correction= 1.045741
 Thermal correction to Energy= 1.107138
 Thermal correction to Enthalpy= 1.108083
 Thermal correction to Gibbs Free Energy= 0.942474
 Sum of electronic and zero-point Energies= -3434.792629
 Sum of electronic and thermal Energies= -3434.731231
 Sum of electronic and thermal Enthalpies= -3434.730287
 Sum of electronic and thermal Free Energies= -3434.895896

 Cartesian Coordinates

6	2.288711	-1.625988	3.519808
6	3.291946	-0.549032	3.952027
6	4.355420	-0.558678	2.840947
7	3.709749	-1.255917	1.716270
6	2.290736	-1.491051	1.987227
6	4.404191	-1.895272	0.780966
6	3.888465	-2.441104	-0.383850
8	0.800664	0.622219	-1.278276
8	1.456238	-1.308707	-2.033666
1	1.968854	-2.399805	1.473273
1	1.290944	-1.481339	3.939280
1	2.646078	-2.623670	3.796026
1	2.798867	0.424021	3.977075
1	3.727779	-0.746400	4.932824
1	4.639519	0.453494	2.543654
1	5.258685	-1.109047	3.124296
1	5.485855	-1.883348	0.927057
1	2.808199	-2.464411	-0.510145
6	4.649091	-3.514462	-1.112676
6	4.206013	-4.927006	-0.668128
1	5.726285	-3.403429	-0.942863
1	4.483832	-3.426945	-2.195458
1	4.795888	-5.671662	-1.216877
1	4.408793	-5.057003	0.400339
6	2.754559	-5.149756	-0.949936
6	1.804552	-5.328493	-0.025288
1	2.440533	-5.131834	-1.994666
1	2.053994	-5.359546	1.032410
6	0.391334	-5.543080	-0.434226
8	0.068283	-5.634086	-1.609078
6	-0.653965	-5.661340	0.631905
6	-0.552270	-4.989028	1.852705
6	-1.801494	-6.408107	0.346531
6	-1.599020	-5.047199	2.769609
1	0.326107	-4.390949	2.079423
6	-2.831063	-6.491480	1.274664
1	-1.869873	-6.910912	-0.613160
6	-2.733745	-5.803345	2.484624
1	-1.527266	-4.505000	3.706947
1	-3.714029	-7.082653	1.053890
1	-3.543205	-5.857588	3.205986
6	4.040708	-0.698622	-1.622422
1	3.818349	-1.391765	-2.430126
1	3.108675	1.105583	-0.742494
6	5.450251	-0.267840	-1.509099
6	6.407826	-0.808026	-2.373557
6	5.858681	0.658300	-0.539277
6	7.744216	-0.429424	-2.277348
1	6.096688	-1.519574	-3.133968
6	7.192224	1.035140	-0.443621
1	5.126255	1.074299	0.148196
6	8.139398	0.492239	-1.312790
1	8.474352	-0.850275	-2.961292
1	7.496644	1.756032	0.308743
1	9.179992	0.791337	-1.238199
7	1.719305	-0.187645	-1.542345
6	3.013233	0.170806	-1.270734

7	0.318384	2.955821	0.468391
6	1.147302	4.061974	0.338571
6	0.774046	5.328940	-0.141058
6	1.714697	6.346022	-0.208453
6	3.021212	6.110090	0.198313
6	3.415372	4.866229	0.684897
6	2.481254	3.853689	0.755817
6	-0.978714	2.722009	0.111703
16	-2.034966	3.794892	-0.652951
7	-1.359567	1.468404	0.442347
6	-2.650756	0.909532	0.111932
6	-2.523623	-0.621503	0.013006
6	-3.830328	-1.297260	-0.448378
6	-3.503228	-2.382182	-1.482844
6	-2.420357	-3.293963	-0.891892
6	-1.117579	-2.487803	-0.747402
7	-1.429282	-1.029849	-0.942623
6	-1.796189	-0.778939	-2.367838
6	-2.956564	-1.728383	-2.765679
6	-3.962173	-0.975987	-3.601181
6	-5.277515	-0.914916	-3.412296
6	-3.714230	1.238376	1.156709
6	-5.048210	1.623554	0.811283
6	-5.955582	1.845714	1.889627
7	-5.610884	1.716997	3.202592
6	-4.375418	1.377752	3.473767
6	-3.393945	1.127008	2.485517
6	-7.289810	2.219102	1.597366
6	-7.724015	2.367676	0.305694
6	-6.819724	2.150811	-0.765626
6	-5.511833	1.794135	-0.514383
1	-2.187885	-1.006614	0.980725
1	-4.341416	-1.728962	0.416234
1	-4.500762	-0.554953	-0.885319
1	-0.374874	-2.738635	-1.505714
1	-0.656869	-2.565851	0.238798
1	-2.235016	-4.163189	-1.529165
1	-2.747780	-3.668066	0.084181
1	-4.398453	-2.964872	-1.714904
1	-2.535964	-2.526295	-3.392422
1	-0.882315	-0.940300	-2.942229
1	-2.068559	0.275861	-2.454908
1	-3.529745	-0.426500	-4.438282
1	-5.907433	-0.331134	-4.075652
1	-5.779789	-1.434030	-2.600539
1	-2.961895	1.321368	-0.850813
1	-2.384874	0.856231	2.784500
1	-4.859762	1.660389	-1.370741
1	-4.111813	1.286333	4.525915
1	-7.957590	2.384334	2.436540
1	-8.751173	2.653469	0.113205
1	-0.688140	0.825781	0.898519
1	0.820879	2.127742	0.829923
1	-0.241146	5.509087	-0.459141
1	2.757039	2.877734	1.144735
8	-7.170091	2.272551	-2.070864
6	-8.481588	2.710354	-2.369633
1	-8.537630	2.772882	-3.456598
1	-9.236166	1.999354	-2.013195
1	-8.681974	3.699927	-1.943303
1	-0.566969	-0.476688	-0.758535
6	1.373314	-0.324330	1.583321
8	1.862356	0.824599	1.564070
8	0.170603	-0.645946	1.385357
1	4.439681	4.711375	1.000707
1	1.438300	7.326607	-0.576597
7	4.000353	7.184141	0.120925
8	5.142285	6.946209	0.486329
8	3.633598	8.268528	-0.304035

l-Michael-nitro-cinchona-thiourea-si-re_conf-3

Number of imaginary frequencies : 1
The smallest frequency is : -301.4247 cm(-1)

Electronic energy : =-3435.8395606
Zero-point correction= 1.045803
Thermal correction to Energy= 1.107121
Thermal correction to Enthalpy= 1.108065
Thermal correction to Gibbs Free Energy= 0.944292
Sum of electronic and zero-point Energies= -3434.793757
Sum of electronic and thermal Energies= -3434.732440
Sum of electronic and thermal Enthalpies= -3434.731495
Sum of electronic and thermal Free Energies= -3434.895268

 Cartesian Coordinates

6	2.502339	-0.468895	4.208287
6	3.484686	0.706243	4.292826
6	4.475012	0.452873	3.143159
7	3.798127	-0.530393	2.278893
6	2.404380	-0.709309	2.692313
6	4.476880	-1.377531	1.511919
6	3.955230	-2.242531	0.562619
8	0.607581	0.347473	-0.843302
8	1.353260	-1.679937	-1.079576
1	2.071623	-1.717417	2.435903
1	1.526628	-0.251704	4.647034
1	2.916553	-1.359579	4.691310
1	2.955111	1.644476	4.118913
1	3.990332	0.764948	5.258087
1	4.683834	1.365921	2.580647
1	5.422667	0.026492	3.487945
1	5.561108	-1.279423	1.586121
1	2.876179	-2.372653	0.506861
6	4.787881	-3.390423	0.055889
6	4.363028	-4.742814	0.673425
1	5.847327	-3.212716	0.271787
1	4.702807	-3.476754	-1.037551
1	5.079496	-5.512185	0.362671
1	4.395290	-4.673699	1.765599
6	2.990660	-5.138027	0.219318
6	1.911239	-5.152851	1.009364
1	2.892603	-5.411204	-0.831310
1	2.008076	-4.932894	2.071559
6	0.544314	-5.584732	0.620586
8	-0.213113	-5.989117	1.490402
6	0.064979	-5.513249	-0.800687
6	0.546592	-4.569070	-1.713953
6	-0.982561	-6.363204	-1.176847
6	-0.010214	-4.483333	-2.988699
1	1.321346	-3.868659	-1.422025
6	-1.521066	-6.290028	-2.455553
1	-1.362729	-7.074536	-0.450520
6	-1.036458	-5.346558	-3.363542
1	0.358474	-3.734428	-3.682961
1	-2.325301	-6.959006	-2.744431
1	-1.465366	-5.280785	-4.358791
6	3.910952	-0.837043	-1.079830
1	3.708296	-1.726624	-1.670606
1	2.904157	1.082641	-0.645828
6	5.282530	-0.293937	-1.160039
6	6.242095	-0.929799	-1.953265
6	5.648711	0.849674	-0.435477
6	7.539891	-0.430247	-2.029273
1	5.963721	-1.811101	-2.524634
6	6.943370	1.345971	-0.511106

1	4.912398	1.336788	0.199511
6	7.892831	0.707510	-1.309909
1	8.273443	-0.927115	-2.656192
1	7.214619	2.233611	0.051693
1	8.902929	1.099472	-1.372028
7	1.565694	-0.450118	-0.944970
6	2.843420	0.033948	-0.888103
7	0.094229	3.071063	0.182240
6	0.854688	4.114291	-0.333143
6	0.380487	5.167123	-1.133831
6	1.256317	6.145795	-1.579475
6	2.598551	6.085738	-1.229004
6	3.091595	5.063470	-0.422796
6	2.221909	4.088761	0.022523
6	-1.191917	2.669592	-0.049951
16	-2.304111	3.381650	-1.101089
7	-1.508585	1.574022	0.674831
6	-2.759345	0.861168	0.528050
6	-2.556110	-0.602377	0.958386
6	-3.818122	-1.469820	0.785282
6	-3.410244	-2.866620	0.291733
6	-2.263197	-3.382554	1.170171
6	-1.020088	-2.511011	0.915684
7	-1.445512	-1.268056	0.184830
6	-1.860849	-1.615533	-1.208953
6	-2.888981	-2.772496	-1.152806
6	-3.926911	-2.571223	-2.225988
6	-5.245920	-2.518398	-2.062496
6	-3.876857	1.457938	1.378612
6	-5.220145	1.599236	0.905370
6	-6.180731	2.104154	1.830898
7	-5.878485	2.456227	3.113502
6	-4.633621	2.328118	3.498610
6	-3.600111	1.833291	2.667878
6	-7.524504	2.253224	1.411345
6	-7.918067	1.923146	0.140240
6	-6.960895	1.426660	-0.781576
6	-5.642968	1.276155	-0.405365
1	-2.205402	-0.609116	1.995452
1	-4.348706	-1.530968	1.739100
1	-4.496656	-1.006094	0.064965
1	-0.285095	-2.990330	0.265976
1	-0.525861	-2.169725	1.825038
1	-2.032257	-4.426232	0.939778
1	-2.551750	-3.336750	2.224858
1	-4.260789	-3.551012	0.342193
1	-2.352827	-3.706422	-1.377254
1	-0.944947	-1.876250	-1.742302
1	-2.278961	-0.711720	-1.659072
1	-3.516811	-2.443878	-3.228893
1	-5.906479	-2.353448	-2.907686
1	-5.721312	-2.635388	-1.092400
1	-3.052148	0.904028	-0.523699
1	-2.587404	1.761499	3.054696
1	-4.950889	0.912634	-1.157115
1	-4.404170	2.619244	4.521976
1	-8.233493	2.641591	2.135193
1	-8.953622	2.049996	-0.151330
1	-0.792624	1.137056	1.284701
1	0.659443	2.418028	0.748538
1	-0.661944	5.212267	-1.407281
1	2.576904	3.286955	0.662701
8	-7.266148	1.074196	-2.055813
6	-8.588599	1.293200	-2.507662
1	-8.604084	0.983819	-3.552943
1	-9.313051	0.691397	-1.946077
1	-8.865949	2.351682	-2.443508
1	-0.630169	-0.627417	0.105845
6	1.433626	0.324436	2.091415
8	1.896674	1.417464	1.707492

8	0.221066	-0.021578	2.121824
1	4.141374	5.045403	-0.156933
1	0.901335	6.959506	-2.200179
7	3.509817	7.115068	-1.707775
8	4.681716	7.047165	-1.367442
8	3.059367	7.994098	-2.425580

1-Michael-nitro-cinchona-thiourea-*si-re*_conf-4

Number of imaginary frequencies : 1
The smallest frequency is : -342.2004 cm(-1)

Electronic energy : =-3435.8374068
Zero-point correction= 1.046001
Thermal correction to Energy= 1.107176
Thermal correction to Enthalpy= 1.108120
Thermal correction to Gibbs Free Energy= 0.945631
Sum of electronic and zero-point Energies= -3434.791406
Sum of electronic and thermal Energies= -3434.730231
Sum of electronic and thermal Enthalpies= -3434.729287
Sum of electronic and thermal Free Energies= -3434.891776

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Cartesian Coordinates

6	1.800438	0.147340	4.738770
6	2.373586	1.570897	4.833251
6	3.455384	1.630904	3.733058
7	3.293127	0.375828	2.977172
6	1.962523	-0.180915	3.244365
6	4.345064	-0.334046	2.581206
6	4.343039	-1.501147	1.831156
8	0.616126	-0.033126	-0.417146
8	1.687151	-1.885734	-0.020405
1	1.945210	-1.248253	3.023377
1	0.758628	0.079128	5.057268
1	2.397879	-0.553606	5.329934
1	1.594368	2.305302	4.622900
1	2.788549	1.784235	5.819900
1	3.291904	2.479506	3.066287
1	4.472708	1.674263	4.130755
1	5.305967	0.138403	2.790774
1	3.403024	-2.032058	1.688212
6	5.615454	-2.329389	1.776222
6	5.337436	-3.817550	1.482352
1	6.157701	-2.257532	2.725064
1	6.297897	-1.941338	1.006012
1	6.278284	-4.373175	1.557794
1	4.643038	-4.220774	2.227302
6	4.765847	-3.936972	0.108715
6	3.491816	-4.201608	-0.187251
1	5.422865	-3.662037	-0.717982
1	2.775822	-4.470431	0.584824
6	3.003365	-3.982601	-1.575896
8	3.671856	-3.358622	-2.383992
6	1.660008	-4.513327	-1.969644
6	1.053656	-5.582022	-1.304844
6	1.029251	-3.938441	-3.077487
6	-0.165171	-6.084170	-1.758385
1	1.545516	-6.048466	-0.456233
6	-0.197795	-4.423011	-3.513604
1	1.520477	-3.113359	-3.582902
6	-0.791883	-5.503941	-2.859290
1	-0.621746	-6.932121	-1.257134
1	-0.688175	-3.968181	-4.368769
1	-1.741814	-5.895221	-3.211664
6	4.076759	-0.586055	-0.079627
1	4.088736	-1.596609	-0.482007

1	2.707184	1.142930	-0.154156
6	5.301065	0.212085	-0.308371
6	6.334204	-0.318377	-1.086971
6	5.441878	1.505299	0.215269
6	7.484414	0.425705	-1.339887
1	6.215806	-1.308290	-1.520386
6	6.589775	2.245526	-0.034917
1	4.643681	1.921995	0.826668
6	7.614914	1.706935	-0.814094
1	8.273558	0.005424	-1.955217
1	6.687560	3.246735	0.373116
1	8.508659	2.289206	-1.014220
7	1.686975	-0.642906	-0.191830
6	2.847350	0.074370	-0.119859
7	-0.452371	2.655878	-0.171157
6	0.325703	3.544542	-0.902069
6	-0.071326	4.251316	-2.048795
6	0.823054	5.110118	-2.671141
6	2.102485	5.271706	-2.155559
6	2.515188	4.596576	-1.009982
6	1.625744	3.745183	-0.387538
6	-1.627960	2.020880	-0.437421
16	-2.639562	2.274514	-1.767654
7	-1.907866	1.103159	0.515497
6	-3.093137	0.276790	0.547074
6	-2.719026	-1.120185	1.077821
6	-3.859265	-2.147563	0.913761
6	-3.389333	-3.292396	0.006015
6	-2.210236	-4.000306	0.689270
6	-1.110036	-2.965308	0.997367
7	-1.495440	-1.655905	0.382486
6	-1.685436	-1.819111	-1.089631
6	-2.900405	-2.745303	-1.351207
6	-3.946665	-2.052074	-2.191085
6	-5.267215	-2.165333	-2.070592
6	-4.170424	0.857890	1.460011
6	-5.534151	1.005288	1.058168
6	-6.447792	1.500395	2.036112
7	-6.079083	1.847953	3.301364
6	-4.815109	1.718692	3.620927
6	-3.826289	1.225268	2.736988
6	-7.812715	1.640517	1.686979
6	-8.268452	1.309960	0.436657
6	-7.355744	0.826887	-0.536368
6	-6.018775	0.686253	-0.230986
1	-2.406106	-1.021325	2.119547
1	-4.148068	-2.545909	1.890415
1	-4.739197	-1.659373	0.489355
1	-0.141828	-3.223874	0.566690
1	-0.977113	-2.768451	2.063013
1	-1.813864	-4.780090	0.032572
1	-2.545261	-4.479114	1.613301
1	-4.204861	-4.003276	-0.152071
1	-2.529661	-3.600086	-1.932444
1	-0.743409	-2.227909	-1.463484
1	-1.806936	-0.819274	-1.515131
1	-3.548640	-1.413536	-2.980851
1	-5.936656	-1.630171	-2.736642
1	-5.735711	-2.778544	-1.304758
1	-3.471431	0.195034	-0.473703
1	-2.796940	1.139042	3.077915
1	-5.357734	0.341710	-1.017240
1	-4.533373	2.005771	4.632234
1	-8.487105	2.020530	2.447377
1	-9.319094	1.428459	0.200184
1	-1.225153	0.922222	1.266208
1	0.051756	2.276689	0.648091
1	-1.066385	4.125534	-2.446891
1	1.912556	3.210074	0.513968
8	-7.723796	0.481993	-1.797043

6	-9.075074	0.670868	-2.171529
1	-9.143060	0.364931	-3.215716
1	-9.750854	0.049763	-1.571843
1	-9.373048	1.722206	-2.086533
1	-0.702223	-0.994840	0.506277
6	0.831462	0.516762	2.467339
8	1.044275	1.662513	2.015293
8	-0.251394	-0.126710	2.428003
1	0.532091	5.660724	-3.557500
1	3.517905	4.742953	-0.627651
7	3.032436	6.173033	-2.821357
8	4.145253	6.309164	-2.335241
8	2.655022	6.748037	-3.830208

1-Michael-nitro-cinchona-thiourea-*si-re*_conf-5

Number of imaginary frequencies : 1

The smallest frequency is : -310.2854 cm(-1)

Electronic energy : =-3435.8305447

Zero-point correction= 1.045326

Thermal correction to Energy= 1.107191

Thermal correction to Enthalpy= 1.108135

Thermal correction to Gibbs Free Energy= 0.939367

Sum of electronic and zero-point Energies= -3434.785219

Sum of electronic and thermal Energies= -3434.723354

Sum of electronic and thermal Enthalpies= -3434.722410

Sum of electronic and thermal Free Energies= -3434.891177

Cartesian Coordinates

6	0.220061	0.521909	4.782493
6	0.329670	2.052276	4.836782
6	1.513155	2.385800	3.907258
7	1.780770	1.135501	3.174275
6	0.662040	0.203358	3.343425
6	3.012888	0.787264	2.814337
6	3.384904	-0.300172	2.041587
8	-0.329510	0.050517	-0.561888
8	1.302650	-1.345071	-0.205832
1	1.005856	-0.823195	3.213403
1	-0.786401	0.152551	4.989571
1	0.917799	0.055337	5.484828
1	-0.581710	2.503880	4.442214
1	0.492979	2.423267	5.849993
1	1.252876	3.180014	3.203926
1	2.416696	2.674184	4.452792
1	3.780618	1.516365	3.079577
1	2.641127	-1.058231	1.802797
6	4.835807	-0.727235	2.029082
6	5.118920	-1.889713	1.065090
1	5.145371	-1.045279	3.033534
1	5.475323	0.128504	1.772809
1	4.507054	-2.749517	1.369368
1	4.827843	-1.641796	0.039032
6	6.563300	-2.275258	1.093195
6	7.373002	-2.286044	0.030695
1	6.991892	-2.549024	2.058165
1	6.995387	-2.011400	-0.949870
6	8.810134	-2.644325	0.182828
8	9.308157	-2.796298	1.286311
6	9.651734	-2.794498	-1.048673
6	9.105007	-2.967857	-2.323676
6	11.042010	-2.781453	-0.893774
6	9.938758	-3.120418	-3.427764
1	8.029892	-3.008723	-2.463312
6	11.872782	-2.920900	-1.997264

1	11.449345	-2.657686	0.104273
6	11.321118	-3.090056	-3.267240
1	9.507619	-3.262483	-4.413508
1	12.950471	-2.899581	-1.870622
1	11.970095	-3.200005	-4.130619
6	3.053215	0.696836	0.143458
1	3.456221	-0.214006	-0.286494
1	1.172268	1.843016	-0.008938
6	3.958331	1.864082	0.165771
6	5.260984	1.743387	-0.328717
6	3.541259	3.101892	0.676795
6	6.125704	2.835451	-0.326131
1	5.593922	0.787711	-0.726784
6	4.403278	4.190276	0.679298
1	2.538170	3.201524	1.085263
6	5.698247	4.060779	0.175116
1	7.131354	2.727111	-0.719335
1	4.066651	5.144056	1.073468
1	6.368768	4.914008	0.175476
7	0.868351	-0.173297	-0.275559
6	1.687523	0.896598	-0.030898
7	-2.272181	2.205591	-0.289056
6	-1.828871	3.366255	-0.908526
6	-2.384443	3.958367	-2.054147
6	-1.830800	5.122579	-2.565962
6	-0.733522	5.700629	-1.941163
6	-0.175044	5.144265	-0.793162
6	-0.727378	3.988063	-0.280377
6	-3.151721	1.234323	-0.663530
16	-4.132430	1.223149	-2.039735
7	-3.145818	0.211599	0.221097
6	-3.986654	-0.960873	0.134010
6	-3.193497	-2.189144	0.620253
6	-3.893159	-3.526672	0.295046
6	-3.007968	-4.353781	-0.650821
6	-1.700674	-4.690318	0.082071
6	-1.057781	-3.382084	0.584328
7	-1.816065	-2.223624	0.014619
6	-1.837748	-2.303121	-1.477686
6	-2.654172	-3.545098	-1.915403
6	-3.825484	-3.156979	-2.787804
6	-5.027563	-3.727886	-2.801625
6	-5.237319	-0.830565	1.000197
6	-6.549715	-1.135092	0.522954
6	-7.621652	-1.020732	1.457844
7	-7.451865	-0.627799	2.751648
6	-6.234943	-0.340690	3.142792
6	-5.097541	-0.431170	2.305948
6	-8.935990	-1.330563	1.031928
6	-9.194186	-1.737403	-0.251729
6	-8.127070	-1.843190	-1.180759
6	-6.836935	-1.540885	-0.800495
1	-3.005808	-2.075743	1.690468
1	-4.072206	-4.089423	1.215455
1	-4.867052	-3.332941	-0.160155
1	-0.024450	-3.251152	0.262866
1	-1.101165	-3.265845	1.668810
1	-1.017450	-5.215382	-0.591861
1	-1.903919	-5.354047	0.926370
1	-3.522932	-5.276425	-0.930931
1	-1.991575	-4.169813	-2.528460
1	-0.789821	-2.338543	-1.780038
1	-2.255991	-1.363254	-1.847075
1	-3.629097	-2.338320	-3.481225
1	-5.799850	-3.383838	-3.482266
1	-5.297172	-4.546560	-2.138792
1	-4.269063	-1.089901	-0.912564
1	-4.116744	-0.181576	2.704894
1	-6.060372	-1.615823	-1.552878
1	-6.114520	-0.022062	4.176521

1	-9.733144	-1.232924	1.761676
1	-10.210704	-1.967720	-0.547188
1	-2.480422	0.221528	1.008772
1	-1.709037	1.963378	0.543987
1	-3.237529	3.507555	-2.536857
1	-0.323955	3.537067	0.622591
8	-8.296402	-2.237812	-2.468803
6	-9.612479	-2.493932	-2.920767
1	-9.521464	-2.764768	-3.972924
1	-10.073041	-3.326520	-2.376017
1	-10.247772	-1.604958	-2.833850
1	-1.307127	-1.351689	0.259281
6	-0.517595	0.478039	2.394229
8	-0.664327	1.645034	1.969077
8	-1.284131	-0.503728	2.197441
1	-2.249235	5.586898	-3.450596
1	0.676436	5.619361	-0.321511
7	-0.157928	6.920020	-2.490540
8	0.798835	7.413621	-1.912445
8	-0.659125	7.388810	-3.500290

1-Michael-nitro-cinchona-thiourea-*si-re*_conf-6

Number of imaginary frequencies : 1
The smallest frequency is : -321.4610 cm(-1)

Electronic energy : =-3435.8305938
Zero-point correction= 1.045560
Thermal correction to Energy= 1.107178
Thermal correction to Enthalpy= 1.108122
Thermal correction to Gibbs Free Energy= 0.940948
Sum of electronic and zero-point Energies= -3434.785034
Sum of electronic and thermal Energies= -3434.723416
Sum of electronic and thermal Enthalpies= -3434.722471
Sum of electronic and thermal Free Energies= -3434.889646

Cartesian Coordinates

6	0.861275	-0.662428	4.302935
6	1.113506	0.811505	4.657413
6	2.115125	1.301970	3.591104
7	2.169439	0.214427	2.596916
6	1.018240	-0.676759	2.772263
6	3.305610	-0.128567	2.001133
6	3.480695	-1.075694	1.003594
8	-0.536906	0.181220	-0.792386
8	0.900683	-1.445846	-0.921701
1	1.240163	-1.664198	2.367607
1	-0.122853	-1.018436	4.614189
1	1.625265	-1.307482	4.747885
1	0.186161	1.379603	4.576102
1	1.507734	0.932437	5.667806
1	1.765381	2.218977	3.112891
1	3.120311	1.462995	3.990856
1	4.159210	0.497584	2.266975
1	2.654942	-1.740474	0.756276
6	4.883321	-1.563726	0.717766
6	4.956520	-2.548485	-0.446684
1	5.305575	-2.056586	1.603599
1	5.528365	-0.698706	0.516059
1	4.413178	-3.467383	-0.188034
1	4.432868	-2.158419	-1.330424
6	6.341234	-2.919595	-0.877251
6	7.481452	-2.406418	-0.404520
1	6.424703	-3.670748	-1.662240
1	7.483158	-1.660762	0.383360
6	8.787337	-2.873340	-0.944933

8	8.862478	-3.858112	-1.661049
6	10.026306	-2.109596	-0.583193
6	9.990553	-0.806416	-0.078238
6	11.261254	-2.731307	-0.795392
6	11.176007	-0.138397	0.216041
1	9.043618	-0.295313	0.064145
6	12.442515	-2.068696	-0.489925
1	11.269453	-3.738185	-1.199727
6	12.400605	-0.770299	0.017434
1	11.142712	0.876543	0.598855
1	13.397393	-2.559924	-0.647668
1	13.323389	-0.249825	0.254485
6	2.973555	0.246306	-0.621560
1	3.121538	-0.625456	-1.250982
1	1.309027	1.655565	-0.250577
6	4.068206	1.237978	-0.636592
6	5.221983	0.972773	-1.383194
6	3.994199	2.435556	0.088419
6	6.275767	1.882341	-1.413187
1	5.289612	0.045258	-1.947031
6	5.043819	3.345136	0.055452
1	3.110685	2.648293	0.686110
6	6.187634	3.071518	-0.695552
1	7.161100	1.660817	-2.001054
1	4.972081	4.272151	0.615537
1	7.004720	3.785418	-0.720884
7	0.642116	-0.230585	-0.748224
6	1.648885	0.662512	-0.495973
7	-2.297564	2.224607	0.253746
6	-1.878069	3.480002	-0.166821
6	-2.620462	4.375547	-0.953627
6	-2.080588	5.607380	-1.290916
6	-0.812059	5.952079	-0.842531
6	-0.064021	5.091403	-0.043318
6	-0.600641	3.865315	0.293847
6	-3.287329	1.396782	-0.183557
16	-4.442380	1.735156	-1.370733
7	-3.233266	0.200291	0.443969
6	-4.150757	-0.891550	0.207923
6	-3.388343	-2.227270	0.298229
6	-4.222475	-3.419715	-0.220505
6	-3.528510	-4.039725	-1.442642
6	-2.171767	-4.598332	-0.991540
6	-1.372298	-3.474264	-0.303987
7	-2.103123	-2.178605	-0.485390
6	-2.319964	-1.901837	-1.937231
6	-3.270196	-2.974414	-2.528054
6	-4.505623	-2.346101	-3.128989
6	-5.739013	-2.844887	-3.104332
6	-5.285814	-0.919012	1.228353
6	-6.661481	-1.020571	0.853942
6	-7.617582	-1.099631	1.910107
7	-7.281839	-1.063090	3.230634
6	-6.011665	-0.945144	3.529981
6	-4.978601	-0.874021	2.565074
6	-8.989489	-1.224668	1.582139
6	-9.411190	-1.272640	0.278306
6	-8.458541	-1.184177	-0.769340
6	-7.116288	-1.053193	-0.484057
1	-3.060357	-2.372517	1.330083
1	-4.327155	-4.174950	0.563456
1	-5.228235	-3.079642	-0.478235
1	-0.382509	-3.322995	-0.731318
1	-1.268239	-3.611901	0.773991
1	-1.619465	-4.982957	-1.853788
1	-2.319035	-5.429579	-0.297260
1	-4.144026	-4.844718	-1.852152
1	-2.731671	-3.468795	-3.347181
1	-1.323789	-1.904376	-2.383070
1	-2.717743	-0.887023	-2.018677

1	-4.334380	-1.401075	-3.645854
1	-6.561667	-2.322601	-3.582229
1	-5.984003	-3.779501	-2.605416
1	-4.559090	-0.769248	-0.796851
1	-3.945086	-0.783471	2.892169
1	-6.431866	-0.959383	-1.318415
1	-5.758796	-0.909794	4.587944
1	-9.696583	-1.281725	2.403243
1	-10.467802	-1.369138	0.058831
1	-2.467980	0.004745	1.106369
1	-1.620755	1.773768	0.893801
1	-3.607283	4.104745	-1.295928
1	-0.049275	3.173839	0.925653
8	-8.792548	-1.220372	-2.084731
6	-10.164469	-1.300137	-2.421000
1	-10.208499	-1.292438	-3.510275
1	-10.617356	-2.227436	-2.050850
1	-10.723936	-0.440535	-2.034232
1	-1.504599	-1.417146	-0.113105
6	-0.276915	-0.138030	2.140547
8	-0.389121	1.099719	2.009632
8	-1.149365	-1.012793	1.888175
1	-2.641938	6.306727	-1.898477
1	0.919133	5.392034	0.297483
7	-0.252620	7.246432	-1.207141
8	0.864057	7.525002	-0.796306
8	-0.926544	7.987948	-1.904611

1-Michael-nitro-cinchona-thiourea-*re-si*_conf-1

Number of imaginary frequencies : 1

The smallest frequency is : -272.3281 cm(-1)

Electronic energy : =-3435.8402313

Zero-point correction= 1.045231

Thermal correction to Energy= 1.106369

Thermal correction to Enthalpy= 1.107313

Thermal correction to Gibbs Free Energy= 0.945357

Sum of electronic and zero-point Energies= -3434.795001

Sum of electronic and thermal Energies= -3434.733862

Sum of electronic and thermal Enthalpies= -3434.732918

Sum of electronic and thermal Free Energies= -3434.894874

Cartesian Coordinates

6	-2.117327	1.683864	4.462529
6	-3.523105	1.118345	4.218712
6	-3.958541	1.779839	2.908395
7	-2.697369	2.091297	2.232596
6	-1.520521	1.775595	3.051866
6	-2.598104	2.464366	0.965547
6	-3.625189	2.485870	0.026813
8	-0.415687	0.177735	-2.281645
6	-0.909622	0.426742	2.601294
8	0.339750	0.391555	2.472046
8	-1.714928	-0.519885	2.421066
8	-0.794237	0.689765	-0.200059
1	-0.772230	2.565908	2.949903
1	-1.513651	1.055907	5.120916
1	-2.176180	2.686256	4.898375
1	-3.459733	0.038685	4.076881
1	-4.214008	1.336645	5.035095
1	-4.573684	1.126821	2.284157
1	-4.512818	2.712540	3.074979
1	-1.583921	2.678866	0.638854
1	-4.650730	2.432950	0.382568
6	-3.385007	3.139472	-1.308078

6	-3.274626	4.684103	-1.279727
1	-4.190082	2.855736	-1.995638
1	-2.451379	2.749833	-1.735952
1	-3.138996	5.043436	-2.305294
1	-4.204716	5.112044	-0.891124
6	-2.116557	5.105979	-0.429601
6	-0.880457	5.342615	-0.884848
1	-2.263025	5.148166	0.649134
1	-0.674578	5.333150	-1.950960
6	0.222524	5.607164	0.076741
8	0.014689	5.661055	1.278811
6	1.620261	5.795990	-0.441845
6	2.017755	5.423290	-1.730701
6	2.566445	6.335342	0.437041
6	3.341328	5.593616	-2.131789
1	1.308944	4.986210	-2.426912
6	3.882319	6.519106	0.031207
1	2.244205	6.608125	1.436472
6	4.272696	6.146198	-1.254985
1	3.643014	5.300640	-3.132590
1	4.605616	6.948963	0.716673
1	5.300714	6.286363	-1.574247
6	-3.440381	0.311171	-0.472361
1	-3.034495	0.109153	0.519403
1	-2.824575	-0.000157	-2.569035
6	-4.852506	-0.070939	-0.689160
6	-5.580460	-0.617655	0.374237
6	-5.464561	0.013095	-1.947835
6	-6.869069	-1.103455	0.181785
1	-5.103810	-0.713783	1.346793
6	-6.751789	-0.475127	-2.141611
1	-4.928437	0.449508	-2.785516
6	-7.455108	-1.042794	-1.080421
1	-7.406178	-1.556780	1.008898
1	-7.204342	-0.422462	-3.126605
1	-8.449394	-1.447935	-1.238397
7	-1.214639	0.352868	-1.345363
6	-2.556309	0.206400	-1.544959
7	-1.152599	-2.303213	0.371912
6	-2.327802	-2.881511	-0.108437
6	-2.605289	-3.068386	-1.471665
6	-3.869670	-3.475835	-1.866269
6	-4.841501	-3.719928	-0.899655
6	-4.574309	-3.588215	0.457394
6	-3.317058	-3.160399	0.847225
6	0.129833	-2.416844	-0.073806
16	0.659116	-3.461621	-1.290468
7	0.957310	-1.596460	0.609662
6	2.381602	-1.488775	0.395881
6	2.768285	-0.016924	0.612090
6	4.248902	0.311421	0.356559
6	4.338614	1.699633	-0.298916
6	3.444192	2.681999	0.474563
6	1.972646	2.268596	0.284261
7	1.939251	0.878680	-0.273023
6	2.437491	0.878546	-1.682878
6	3.803113	1.607868	-1.737878
6	4.698378	0.923445	-2.738530
6	5.938167	0.489174	-2.531595
6	3.188375	-2.347829	1.361207
6	4.347833	-3.079372	0.953755
6	5.048112	-3.797078	1.968314
7	4.661944	-3.819332	3.275899
6	3.588689	-3.143048	3.602630
6	2.821204	-2.389458	2.682229
6	6.208718	-4.526700	1.613714
6	6.670818	-4.552357	0.323078
6	5.970650	-3.841599	-0.685496
6	4.833017	-3.127447	-0.373832
1	2.473382	0.259372	1.629021

1	4.790852	0.286188	1.305369
1	4.700999	-0.439126	-0.298194
1	1.448616	2.902416	-0.436589
1	1.403402	2.234946	1.216079
1	3.587693	3.702418	0.107527
1	3.708277	2.670563	1.536173
1	5.370859	2.057993	-0.300790
1	3.625834	2.633483	-2.093056
1	1.665283	1.349864	-2.290729
1	2.508956	-0.164130	-2.001979
1	4.248130	0.773316	-3.720467
1	6.494141	-0.002593	-3.323297
1	6.446454	0.599781	-1.577592
1	2.585163	-1.797467	-0.631515
1	1.944452	-1.846024	3.026983
1	4.325570	-2.620040	-1.186997
1	3.290434	-3.172371	4.648894
1	6.721080	-5.064742	2.404595
1	7.561822	-5.119498	0.082120
1	0.574253	-0.984404	1.352037
1	-1.296502	-1.705092	1.210959
1	-1.842835	-2.845323	-2.206538
1	-3.086199	-3.015210	1.897969
8	6.358685	-3.814572	-1.984958
6	7.482037	-4.586890	-2.362488
1	7.594178	-4.448430	-3.438126
1	8.395140	-4.244505	-1.861129
1	7.327713	-5.651544	-2.152796
1	0.931570	0.579521	-0.267625
1	-5.352469	-3.790899	1.182843
1	-4.120238	-3.579903	-2.914949
7	-6.195692	-4.056912	-1.320205
8	-7.030174	-4.268434	-0.453035
8	-6.433808	-4.095665	-2.516735

1-Michael-nitro-cinchona-thiourea-*re-si*_conf-2

Number of imaginary frequencies : 1
The smallest frequency is : -290.8701 cm(-1)

Electronic energy : =-3435.8357488
Zero-point correction= 1.045729
Thermal correction to Energy= 1.106862
Thermal correction to Enthalpy= 1.107806
Thermal correction to Gibbs Free Energy= 0.945602
Sum of electronic and zero-point Energies= -3434.790020
Sum of electronic and thermal Energies= -3434.728887
Sum of electronic and thermal Enthalpies= -3434.727943
Sum of electronic and thermal Free Energies= -3434.890147

Cartesian Coordinates

6	0.472466	-2.808828	4.173571
6	1.455525	-1.692074	4.557881
6	2.361481	-1.523427	3.323855
7	1.662839	-2.239745	2.257880
6	0.311895	-2.618732	2.661594
6	2.093796	-2.362123	1.010492
6	3.204127	-1.754805	0.436312
8	-0.180877	-1.418681	-2.553433
6	-0.682248	-1.480353	2.348303
8	-1.856788	-1.835016	2.085631
8	-0.240764	-0.305891	2.418977
8	-0.298156	-1.352993	-0.381884
1	-0.002198	-3.523177	2.136026
1	-0.482083	-2.736938	4.698797
1	0.906176	-3.793905	4.371055

1	0.909201	-0.764261	4.731891
1	2.029954	-1.933019	5.453906
1	2.464883	-0.466945	3.059986
1	3.359571	-1.957113	3.452779
1	1.444372	-2.962552	0.374976
1	3.905487	-1.242700	1.090562
6	3.742182	-2.352155	-0.842601
6	4.686548	-1.462538	-1.671483
1	2.893920	-2.639108	-1.479593
1	4.280602	-3.280697	-0.608791
1	5.052720	-2.048006	-2.521203
1	4.123589	-0.616961	-2.079498
6	5.844196	-0.924906	-0.891643
6	7.121619	-1.259754	-1.100480
1	5.635169	-0.201368	-0.102446
1	7.384571	-1.953948	-1.892975
6	8.203222	-0.645558	-0.284773
8	7.963134	0.222925	0.538134
6	9.618371	-1.095672	-0.503096
6	9.946342	-2.286338	-1.157812
6	10.642117	-0.284555	-0.002410
6	11.279597	-2.655759	-1.312892
1	9.169160	-2.944780	-1.531118
6	11.971919	-0.646955	-0.168918
1	10.368961	0.629875	0.513761
6	12.292555	-1.834761	-0.825816
1	11.526486	-3.585333	-1.815728
1	12.760387	-0.006456	0.213354
1	13.331905	-2.120475	-0.955473
6	2.022315	0.059995	-0.224242
1	1.398708	-0.012144	0.667148
1	1.851930	-0.138894	-2.413996
6	3.094080	1.088234	-0.189833
6	3.727920	1.399280	1.021490
6	3.462424	1.813521	-1.330565
6	4.711198	2.376690	1.090136
1	3.443103	0.862425	1.921248
6	4.452293	2.790748	-1.266935
1	2.957008	1.639927	-2.275129
6	5.085045	3.071673	-0.059491
1	5.189748	2.596824	2.038862
1	4.715430	3.346563	-2.160839
1	5.850373	3.839098	-0.008032
7	0.283293	-1.039699	-1.459471
6	1.427582	-0.294747	-1.434310
7	-1.167720	1.494749	0.544904
6	-0.246721	2.522780	0.341817
6	-0.031827	3.164958	-0.887932
6	0.976112	4.108501	-1.003576
6	1.763358	4.409147	0.103545
6	1.568417	3.787903	1.330970
6	0.567456	2.838873	1.442094
6	-2.382131	1.263178	-0.020567
16	-3.145603	2.245850	-1.172831
7	-2.934839	0.129802	0.462024
6	-4.214754	-0.426201	0.081839
6	-3.989661	-1.911356	-0.265239
6	-5.236191	-2.634083	-0.817003
6	-4.952120	-3.138466	-2.239416
6	-3.792914	-4.146548	-2.189014
6	-2.575967	-3.483957	-1.512549
7	-2.881028	-2.037996	-1.281393
6	-3.211463	-1.378809	-2.587663
6	-4.532256	-1.965349	-3.145695
6	-5.576800	-0.891442	-3.341024
6	-6.889569	-1.026110	-3.172170
6	-5.245097	-0.324877	1.202724
6	-6.563772	0.188125	0.985532
6	-7.456881	0.174979	2.098340
7	-7.107896	-0.275803	3.336604

6	-5.884370	-0.714696	3.496335
6	-4.918681	-0.765306	2.461514
6	-8.778021	0.652307	1.922772
6	-9.214063	1.122522	0.710535
6	-8.321947	1.143694	-0.391073
6	-7.026236	0.693522	-0.251257
1	-3.591297	-2.403632	0.626944
1	-5.494906	-3.476185	-0.169445
1	-6.088964	-1.951269	-0.819583
1	-1.670607	-3.502583	-2.121561
1	-2.347342	-3.911126	-0.533606
1	-3.534810	-4.469008	-3.201753
1	-4.092593	-5.034818	-1.627264
1	-5.842307	-3.624388	-2.647002
1	-4.305916	-2.380077	-4.136852
1	-2.357034	-1.568863	-3.234562
1	-3.262206	-0.301006	-2.411147
1	-5.188876	0.072658	-3.673146
1	-7.563167	-0.191925	-3.343094
1	-7.343568	-1.957316	-2.841679
1	-4.565735	0.119647	-0.794762
1	-3.923714	-1.150399	2.674667
1	-6.383564	0.751470	-1.120591
1	-5.616046	-1.064418	4.491575
1	-9.434407	0.632754	2.786584
1	-10.230817	1.482056	0.606649
1	-2.428687	-0.427986	1.173798
1	-0.894074	0.837234	1.304715
1	-0.641984	2.908963	-1.742301
1	0.402165	2.319599	2.381486
8	-8.669419	1.596810	-1.623853
6	-9.977838	2.104753	-1.802893
1	-10.034272	2.429961	-2.841932
1	-10.737723	1.334424	-1.626587
1	-10.169345	2.963049	-1.148843
1	-2.004899	-1.618920	-0.895327
1	1.172439	4.598810	-1.949392
1	2.205496	4.039208	2.169700
7	2.857447	5.361386	-0.037961
8	3.488234	5.664598	0.962442
8	3.096739	5.799602	-1.152478

1-Michael-nitro-cinchona-thiourea-*re-si*_conf-3

Number of imaginary frequencies : 1

The smallest frequency is : -381.7690 cm(-1)

Electronic energy : =-3435.8316842

Zero-point correction= 1.044698

Thermal correction to Energy= 1.105723

Thermal correction to Enthalpy= 1.106668

Thermal correction to Gibbs Free Energy= 0.944825

Sum of electronic and zero-point Energies= -3434.786986

Sum of electronic and thermal Energies= -3434.725961

Sum of electronic and thermal Enthalpies= -3434.725017

Sum of electronic and thermal Free Energies= -3434.886859

Cartesian Coordinates

6	1.391880	1.472405	4.684397
6	1.988912	2.604756	3.847765
6	3.312925	2.013749	3.366264
7	3.021691	0.579999	3.250060
6	1.719718	0.240809	3.848690
6	3.789766	-0.290000	2.625505
6	5.003453	-0.014310	1.985292
8	0.920021	0.159979	-0.663967

6	0.681877	-0.072341	2.730322
8	1.002476	-0.996682	1.953834
8	-0.383713	0.590662	2.740189
8	1.837006	1.637314	0.641543
1	1.830461	-0.671084	4.444463
1	0.315871	1.567279	4.822468
1	1.884755	1.410750	5.660573
1	1.342515	2.794409	2.985969
1	2.130096	3.534166	4.401792
1	3.622874	2.411377	2.398902
1	4.121972	2.158923	4.093849
1	3.364407	-1.289821	2.581002
1	5.451694	0.948924	2.221457
6	6.024153	-1.125294	1.823474
6	5.480865	-2.552629	1.665750
1	6.686862	-1.115213	2.698664
1	6.670698	-0.906996	0.964116
1	6.348987	-3.225233	1.667915
1	4.856892	-2.851943	2.514590
6	4.758732	-2.759471	0.374677
6	3.611897	-3.423881	0.197150
1	5.251812	-2.363596	-0.512349
1	3.082485	-3.866230	1.037339
6	3.068527	-3.586734	-1.175763
8	3.373993	-2.817585	-2.077038
6	2.144300	-4.733187	-1.461724
6	1.432467	-4.727553	-2.667159
6	2.016072	-5.820399	-0.591724
6	0.603848	-5.794522	-2.996739
1	1.555719	-3.884421	-3.339906
6	1.193573	-6.892832	-0.928002
1	2.579562	-5.851114	0.335202
6	0.487564	-6.881025	-2.128254
1	0.055232	-5.785561	-3.933309
1	1.110615	-7.740183	-0.255109
1	-0.151407	-7.718636	-2.389835
6	4.321571	0.750876	0.022988
1	4.147353	1.710056	0.497085
1	3.123732	-0.714561	-1.126355
6	5.611419	0.649175	-0.691672
6	6.665844	1.492816	-0.315448
6	5.811870	-0.239149	-1.757266
6	7.892049	1.439018	-0.966447
1	6.515624	2.198569	0.498285
6	7.042136	-0.295775	-2.405560
1	5.004048	-0.884375	-2.091361
6	8.086270	0.536980	-2.011387
1	8.695308	2.102546	-0.662174
1	7.180134	-0.989784	-3.228614
1	9.043241	0.490740	-2.521429
7	1.945933	0.655682	-0.148310
6	3.163967	0.151830	-0.483020
7	-0.756529	2.665384	-0.230656
6	-0.477188	3.903990	-0.805307
6	-1.467943	4.842090	-1.135930
6	-1.109004	6.075165	-1.653355
6	0.237327	6.375931	-1.829612
6	1.237927	5.472105	-1.490294
6	0.876914	4.238564	-0.978971
6	-1.847975	1.856048	-0.411618
16	-3.012350	2.046523	-1.621644
7	-1.857728	0.831926	0.460795
6	-2.859224	-0.210993	0.467900
6	-2.207730	-1.550904	0.865410
6	-3.132656	-2.754459	0.572171
6	-2.504560	-3.634199	-0.521745
6	-1.201899	-4.230638	0.026226
6	-0.325797	-3.084007	0.554185
7	-0.914195	-1.772789	0.129935
6	-1.086057	-1.744180	-1.353842

6	-2.142137	-2.802450	-1.768892
6	-3.307557	-2.178359	-2.498513
6	-4.580344	-2.558402	-2.419478
6	-3.995372	0.085998	1.445748
6	-5.375127	0.017047	1.074016
6	-6.337558	0.243178	2.102847
7	-6.004221	0.544155	3.390124
6	-4.729204	0.631777	3.678463
6	-3.688589	0.406081	2.745098
6	-7.714126	0.155781	1.783078
6	-8.136503	-0.135281	0.511177
6	-7.177364	-0.341735	-0.513108
6	-5.829776	-0.261346	-0.235115
1	-1.908524	-1.496947	1.916817
1	-3.280482	-3.348902	1.478266
1	-4.114304	-2.390582	0.258836
1	0.690364	-3.097640	0.157237
1	-0.254586	-3.046207	1.640651
1	-0.678775	-4.777487	-0.763105
1	-1.414687	-4.937013	0.833320
1	-3.194344	-4.435493	-0.798931
1	-1.648856	-3.484298	-2.475375
1	-0.096906	-1.941723	-1.770807
1	-1.361442	-0.724918	-1.635463
1	-3.046746	-1.356110	-3.165784
1	-5.350815	-2.058289	-2.997660
1	-4.910494	-3.366389	-1.770888
1	-3.258327	-0.290605	-0.544792
1	-2.651655	0.490032	3.063940
1	-5.137407	-0.391153	-1.057398
1	-4.476929	0.883928	4.706863
1	-8.425488	0.330202	2.583709
1	-9.197096	-0.193529	0.297676
1	-1.201604	0.833171	1.268602
1	0.049076	2.212534	0.217817
1	-2.510550	4.603985	-0.980724
1	1.635584	3.513176	-0.702622
8	-7.509407	-0.621305	-1.800651
6	-8.881096	-0.652237	-2.143610
1	-8.919035	-0.857547	-3.213758
1	-9.413998	-1.447240	-1.608899
1	-9.367661	0.310081	-1.947318
1	-0.218897	-1.051099	0.421280
1	-1.861467	6.810699	-1.909812
1	2.277451	5.737835	-1.637228
7	0.610362	7.676474	-2.371820
8	1.799535	7.923983	-2.501864
8	-0.283751	8.453776	-2.666611

1-Michael-nitro-cinchona-thiourea-*re-re*_conf-1

Number of imaginary frequencies : 1

The smallest frequency is : -316.4881 cm(-1)

Electronic energy : =-3435.8409824

Zero-point correction= 1.045720

Thermal correction to Energy= 1.106767

Thermal correction to Enthalpy= 1.107711

Thermal correction to Gibbs Free Energy= 0.944149

Sum of electronic and zero-point Energies= -3434.795263

Sum of electronic and thermal Energies= -3434.734215

Sum of electronic and thermal Enthalpies= -3434.733271

Sum of electronic and thermal Free Energies= -3434.896834

Cartesian Coordinates

6 2.176328 0.628293 4.800582

6	3.066345	1.786970	4.322288
6	3.820380	1.224923	3.101540
7	3.124688	-0.029616	2.772779
6	1.859202	-0.137089	3.507687
6	3.722505	-1.088157	2.232916
6	4.910199	-1.047698	1.516611
8	0.736916	0.532165	-0.200965
6	0.707717	0.553014	2.747492
8	-0.374271	-0.087228	2.653979
8	0.931765	1.710615	2.331609
8	1.684724	-1.334860	0.378259
1	1.611381	-1.188449	3.662558
1	1.273663	0.971544	5.310746
1	2.728871	-0.030197	5.478309
1	2.447319	2.628608	4.015123
1	3.758174	2.119399	5.098709
1	3.795418	1.912463	2.252636
1	4.864273	0.987791	3.332343
1	3.156876	-2.012489	2.295574
1	5.499530	-0.137523	1.589149
6	5.704866	-2.299014	1.215373
6	5.020798	-3.642542	1.506478
1	6.629251	-2.268500	1.803559
1	6.034414	-2.286332	0.166670
1	5.785139	-4.421527	1.386772
1	4.693256	-3.687715	2.551074
6	3.880786	-4.010777	0.601148
6	2.699135	-4.454026	1.046510
1	4.082593	-3.985311	-0.470641
1	2.517279	-4.526966	2.118422
6	1.602572	-5.043990	0.238625
8	0.787382	-5.763104	0.798224
6	1.478185	-4.798799	-1.234910
6	1.825776	-3.581273	-1.828040
6	0.904844	-5.810142	-2.014422
6	1.610229	-3.384445	-3.191125
1	2.201888	-2.773403	-1.208284
6	0.710689	-5.618160	-3.376587
1	0.617997	-6.740297	-1.533785
6	1.063539	-4.403803	-3.966614
1	1.863279	-2.430474	-3.643790
1	0.278009	-6.410232	-3.979384
1	0.903255	-4.250033	-5.029239
6	4.100013	-0.451672	-0.421277
1	3.903745	-1.505792	-0.602418
1	2.976813	1.437885	-0.562142
6	5.339014	0.093483	-1.020502
6	6.073991	-0.675579	-1.928529
6	5.786939	1.384282	-0.709194
6	7.226298	-0.163177	-2.520138
1	5.726950	-1.672703	-2.188420
6	6.935532	1.894658	-1.298843
1	5.232881	1.984592	0.008793
6	7.659390	1.121028	-2.206582
1	7.782950	-0.768375	-3.228556
1	7.269612	2.896757	-1.049780
1	8.557885	1.520898	-2.665332
7	1.761123	-0.151176	-0.039256
6	2.991567	0.383578	-0.329900
7	-0.647213	2.891203	0.326575
6	0.104917	3.870485	-0.312544
6	-0.394727	4.807178	-1.230680
6	0.455849	5.757367	-1.776070
6	1.793290	5.780527	-1.399871
6	2.307385	4.875979	-0.474299
6	1.461961	3.926623	0.065596
6	-1.741399	2.195465	-0.091730
16	-2.652052	2.497948	-1.483454
7	-2.017696	1.168260	0.742449
6	-3.106740	0.236140	0.556079

6	-2.664444	-1.170146	1.004941
6	-3.654971	-2.270556	0.562713
6	-2.953558	-3.241604	-0.400397
6	-1.822891	-3.943836	0.361420
6	-0.901764	-2.873298	0.974412
7	-1.304231	-1.523618	0.459080
6	-1.261933	-1.506677	-1.033771
6	-2.328297	-2.483702	-1.589822
6	-3.307637	-1.772664	-2.493749
6	-4.611314	-2.018373	-2.598263
6	-4.340181	0.628272	1.367704
6	-5.657889	0.657613	0.813838
6	-6.730400	0.957811	1.705949
7	-6.551622	1.241618	3.026873
6	-5.324719	1.236350	3.486540
6	-4.190141	0.929193	2.698270
6	-8.055177	0.961796	1.205438
6	-8.323233	0.686775	-0.110806
6	-7.252962	0.406207	-0.998668
6	-5.951223	0.401922	-0.545179
1	-2.518013	-1.159593	2.088032
1	-4.017365	-2.821099	1.435186
1	-4.523169	-1.812309	0.083855
1	0.145021	-2.990076	0.697097
1	-0.964673	-2.812812	2.062605
1	-1.250692	-4.591607	-0.309231
1	-2.231415	-4.578310	1.151761
1	-3.668886	-3.982123	-0.767609
1	-1.796111	-3.223484	-2.203998
1	-0.243170	-1.793614	-1.301300
1	-1.416532	-0.473281	-1.354042
1	-2.870593	-0.998958	-3.126385
1	-5.231312	-1.457842	-3.290671
1	-5.116123	-2.771732	-1.998400
1	-3.352297	0.219882	-0.507544
1	-3.203403	0.931836	3.155789
1	-5.167617	0.213026	-1.268948
1	-5.194615	1.473798	4.540728
1	-8.852763	1.190146	1.904904
1	-9.347577	0.695619	-0.463777
1	-1.386219	0.969183	1.532798
1	-0.123708	2.437055	1.096921
1	-1.437845	4.786900	-1.509417
1	1.824710	3.203556	0.791349
8	-7.429195	0.132434	-2.316794
6	-8.744510	0.166870	-2.836397
1	-8.653827	-0.059051	-3.899101
1	-9.385307	-0.586732	-2.363507
1	-9.198340	1.157439	-2.718845
1	-0.609673	-0.842676	0.816089
1	3.353198	4.925724	-0.196670
1	0.086399	6.487692	-2.485510
7	2.680092	6.780924	-1.978819
8	3.848546	6.786825	-1.620395
8	2.213542	7.563137	-2.791514

1-Michael-nitro-cinchona-thiourea-*re-re*_conf-2

Number of imaginary frequencies : 1
The smallest frequency is : -337.2842 cm(-1)

Electronic energy : =-3435.8418922
Zero-point correction= 1.046472
Thermal correction to Energy= 1.107538
Thermal correction to Enthalpy= 1.108482
Thermal correction to Gibbs Free Energy= 0.945360
Sum of electronic and zero-point Energies= -3434.795420

Sum of electronic and thermal Energies=	-3434.734355
Sum of electronic and thermal Enthalpies=	-3434.733410
Sum of electronic and thermal Free Energies=	-3434.896532

Cartesian Coordinates

6	2.455288	0.630810	4.745585
6	3.435391	1.648882	4.143016
6	4.052944	0.922596	2.934418
7	3.176304	-0.237662	2.699694
6	1.963974	-0.161230	3.527407
6	3.588433	-1.370028	2.140768
6	4.752611	-1.496082	1.388846
8	0.798285	0.467890	-0.154178
6	0.838420	0.597270	2.792588
8	-0.278267	0.016408	2.725392
8	1.119549	1.735135	2.360045
8	1.690277	-1.491422	0.168916
1	1.622799	-1.170209	3.764528
1	1.634077	1.105910	5.286347
1	2.974337	-0.049206	5.428583
1	2.890639	2.529479	3.806069
1	4.202957	1.953943	4.856936
1	4.094339	1.556886	2.046302
1	5.061667	0.552951	3.149023
1	2.895935	-2.202658	2.226030
1	5.487585	-0.706090	1.507055
6	5.331524	-2.857334	1.041201
6	4.702608	-4.063585	1.749447
1	6.393844	-2.840759	1.303754
1	5.314474	-3.026060	-0.045574
1	5.391578	-4.916182	1.671159
1	4.628082	-3.857770	2.824610
6	3.367201	-4.543243	1.261014
6	2.792932	-4.272569	0.084727
1	2.822712	-5.214358	1.925817
1	3.270542	-3.634434	-0.649172
6	1.482487	-4.886030	-0.260119
8	0.892682	-5.619381	0.520296
6	0.892191	-4.612228	-1.610948
6	1.213259	-3.474120	-2.357704
6	-0.032244	-5.533246	-2.120223
6	0.604812	-3.255006	-3.592010
1	1.894508	-2.731328	-1.952761
6	-0.616721	-5.327056	-3.363830
1	-0.272379	-6.409529	-1.526154
6	-0.301861	-4.183343	-4.099053
1	0.840294	-2.358594	-4.156688
1	-1.321798	-6.051005	-3.759481
1	-0.766043	-4.015146	-5.065881
6	4.118547	-0.635262	-0.485535
1	3.861763	-1.648441	-0.779298
1	3.077275	1.316904	-0.482825
6	5.417718	-0.126083	-0.978738
6	6.204045	-0.920483	-1.819926
6	5.888570	1.142303	-0.613780
6	7.428859	-0.455792	-2.292212
1	5.843261	-1.900239	-2.121322
6	7.109447	1.606106	-1.086126
1	5.294154	1.766144	0.049162
6	7.884512	0.806926	-1.926528
1	8.024716	-1.080599	-2.949910
1	7.459046	2.592338	-0.797972
1	8.838493	1.170372	-2.294537
7	1.801507	-0.268469	-0.106885
6	3.046351	0.245186	-0.356818
7	-0.438542	2.929784	0.319218
6	0.366714	3.829824	-0.369836
6	-0.077029	4.738530	-1.343041
6	0.827519	5.604391	-1.939660

6	2.163782	5.572833	-1.560599
6	2.623904	4.696704	-0.580968
6	1.724756	3.831400	0.010679
6	-1.580858	2.287169	-0.055948
16	-2.503991	2.596721	-1.437264
7	-1.902397	1.307947	0.818934
6	-3.036083	0.422176	0.671085
6	-2.652164	-0.981515	1.175258
6	-3.705205	-2.051009	0.805407
6	-3.057225	-3.133910	-0.071410
6	-1.952857	-3.812942	0.748193
6	-0.947196	-2.741605	1.209878
7	-1.325400	-1.418959	0.610896
6	-1.336015	-1.500796	-0.878715
6	-2.415199	-2.515901	-1.328753
6	-3.371290	-1.884340	-2.310761
6	-4.691254	-2.047108	-2.358461
6	-4.252466	0.904710	1.456770
6	-5.567344	0.953569	0.896398
6	-6.626780	1.356846	1.763030
7	-6.438496	1.712963	3.065051
6	-5.214390	1.680375	3.530742
6	-4.092531	1.278272	2.767217
6	-7.949015	1.391323	1.256933
6	-8.227245	1.046355	-0.040362
6	-7.169982	0.659635	-0.903538
6	-5.870441	0.623865	-0.444900
1	-2.477964	-0.931125	2.253192
1	-4.108541	-2.506681	1.713853
1	-4.539555	-1.578259	0.283153
1	0.072715	-2.938320	0.880272
1	-0.936920	-2.585784	2.290319
1	-1.438401	-4.572671	0.152963
1	-2.387189	-4.316128	1.616188
1	-3.808085	-3.872593	-0.364724
1	-1.890261	-3.323388	-1.858125
1	-0.327037	-1.800647	-1.159480
1	-1.505130	-0.491337	-1.261674
1	-2.897755	-1.243520	-3.056080
1	-5.288053	-1.548778	-3.115572
1	-5.231736	-2.668700	-1.648899
1	-3.283344	0.372085	-0.390967
1	-3.107273	1.269416	3.227121
1	-5.096597	0.348383	-1.152089
1	-5.076434	1.975456	4.569296
1	-8.736136	1.701255	1.936586
1	-9.249139	1.081426	-0.398582
1	-1.266491	1.097394	1.602653
1	0.067071	2.476878	1.100613
1	-1.118990	4.761585	-1.625383
1	2.044518	3.132719	0.779436
8	-7.357824	0.311092	-2.202260
6	-8.670851	0.368083	-2.725547
1	-8.590939	0.071718	-3.771684
1	-9.342565	-0.326403	-2.207113
1	-9.082570	1.382445	-2.671658
1	-0.596052	-0.737696	0.887250
1	0.500938	6.311751	-2.692147
1	3.670609	4.703307	-0.302045
7	3.106665	6.485252	-2.193616
8	4.273167	6.446087	-1.831253
8	2.685571	7.243519	-3.052537

1-Michael-nitro-cinchona-thiourea-*re-re*_conf-3

Number of imaginary frequencies : 1
The smallest frequency is : -255.0547 cm(-1)

Electronic energy : =-3435.8372365
 Zero-point correction= 1.046126
 Thermal correction to Energy= 1.107797
 Thermal correction to Enthalpy= 1.108741
 Thermal correction to Gibbs Free Energy= 0.941032
 Sum of electronic and zero-point Energies= -3434.791111
 Sum of electronic and thermal Energies= -3434.729439
 Sum of electronic and thermal Enthalpies= -3434.728495
 Sum of electronic and thermal Free Energies= -3434.896204

 Cartesian Coordinates

6	-2.505491	-0.475510	-3.233271
6	-2.671081	1.034170	-3.469484
6	-3.101584	1.596630	-2.100988
7	-2.836939	0.509174	-1.146066
6	-2.049445	-0.558459	-1.770624
6	-3.542336	0.324118	-0.035033
6	-4.316507	1.290296	0.587200
8	0.421794	1.022099	0.820540
6	-0.540680	-0.270504	-1.645472
8	0.188724	-1.231548	-1.279990
8	-0.161050	0.881383	-1.951709
8	-1.308632	0.035108	1.691513
1	-2.277781	-1.512389	-1.292837
1	-1.789764	-0.935514	-3.918171
1	-3.466056	-0.991287	-3.332069
1	-1.718119	1.471516	-3.764712
1	-3.414960	1.248434	-4.239229
1	-2.537239	2.491660	-1.827033
1	-4.171354	1.829617	-2.068613
1	-3.402655	-0.641015	0.445305
1	-4.572098	2.184118	0.023161
6	-5.278947	0.878597	1.668138
6	-6.689980	0.538238	1.137521
1	-5.382782	1.685178	2.404524
1	-4.876856	0.005255	2.197266
1	-7.340203	0.267254	1.975791
1	-7.109797	1.439533	0.672143
6	-6.658010	-0.562755	0.126763
6	-7.203488	-1.773209	0.277498
1	-6.124602	-0.371768	-0.804308
1	-7.760370	-2.016536	1.176185
6	-7.067142	-2.784730	-0.806511
8	-6.450322	-2.528204	-1.828701
6	-7.707222	-4.131843	-0.640040
6	-8.256953	-4.578615	0.565574
6	-7.735088	-4.974248	-1.757531
6	-8.826005	-5.846437	0.648434
1	-8.237686	-3.955205	1.452498
6	-8.309795	-6.235070	-1.676280
1	-7.300274	-4.614163	-2.683882
6	-8.856825	-6.673596	-0.470641
1	-9.245480	-6.188307	1.589176
1	-8.331658	-6.878039	-2.550338
1	-9.305295	-7.659962	-0.402978
6	-2.714860	2.323165	1.707747
1	-2.911349	1.617288	2.509908
1	-0.959998	3.010259	0.562503
6	-3.363561	3.647209	1.817162
6	-4.065208	3.983966	2.979636
6	-3.285104	4.585733	0.779193
6	-4.665847	5.234171	3.107016
1	-4.121490	3.267525	3.794813
6	-3.882264	5.832604	0.907229
1	-2.760289	4.327250	-0.137330
6	-4.575357	6.160398	2.072973
1	-5.200876	5.484708	4.017473
1	-3.809054	6.551479	0.097379

1	-5.041768	7.135279	2.172179
7	-0.764415	1.051641	1.202281
6	-1.476183	2.222820	1.090820
7	2.281959	1.957069	-1.092084
6	2.205710	3.343449	-1.073794
6	3.271085	4.221317	-0.818196
6	3.059138	5.591466	-0.860034
6	1.797279	6.085653	-1.165196
6	0.729207	5.236257	-1.441998
6	0.937590	3.872156	-1.395992
6	3.137187	1.086896	-0.486217
16	4.536690	1.481388	0.375910
7	2.708314	-0.187552	-0.626073
6	3.385893	-1.352907	-0.105495
6	2.343714	-2.359598	0.420884
6	2.976244	-3.483304	1.270765
6	2.439565	-3.405915	2.708397
6	0.928013	-3.672504	2.670352
6	0.272634	-2.690802	1.679617
7	1.291666	-1.677165	1.256257
6	1.860585	-0.982736	2.450286
6	2.660815	-2.000397	3.303413
6	4.102570	-1.578149	3.460717
6	5.164815	-2.379123	3.490463
6	4.217809	-2.050674	-1.179374
6	5.578157	-2.440257	-0.979419
6	6.216105	-3.137256	-2.049093
7	5.603222	-3.420197	-3.233066
6	4.362812	-3.025922	-3.382538
6	3.627820	-2.344959	-2.383394
6	7.555566	-3.564545	-1.883196
6	8.244124	-3.323878	-0.722090
6	7.610664	-2.620818	0.335195
6	6.310159	-2.183043	0.202491
1	1.783660	-2.755674	-0.428724
1	2.734439	-4.459682	0.841802
1	4.064098	-3.385504	1.258518
1	-0.552150	-2.125062	2.111001
1	-0.075681	-3.168088	0.761757
1	0.499611	-3.546549	3.668876
1	0.735098	-4.701754	2.357246
1	2.932181	-4.156556	3.332000
1	2.216949	-1.999537	4.307733
1	1.001832	-0.558340	2.974154
1	2.472805	-0.153505	2.085516
1	4.254875	-0.505402	3.584720
1	6.162566	-1.975419	3.629451
1	5.091618	-3.457448	3.371433
1	4.029645	-1.025905	0.713172
1	2.596663	-2.058358	-2.578579
1	5.880412	-1.625608	1.026693
1	3.887242	-3.251742	-4.335129
1	8.018900	-4.091131	-2.711119
1	9.267594	-3.665371	-0.624706
1	1.808154	-0.374404	-1.091995
1	1.403173	1.519447	-1.424747
1	4.251803	3.830960	-0.591926
1	0.129231	3.177054	-1.608928
8	8.222636	-2.338966	1.514020
6	9.577672	-2.715897	1.667208
1	9.874103	-2.375955	2.659782
1	9.703747	-3.803413	1.609151
1	10.216689	-2.233915	0.918472
1	0.806951	-0.964608	0.679034
1	-0.240313	5.653265	-1.685707
1	3.870737	6.282049	-0.665735
7	1.585134	7.526060	-1.208786
8	0.471284	7.932302	-1.505156
8	2.528791	8.255163	-0.947837

l-Michael-nitro-cinchona-thiourea-re-re_conf-4

Number of imaginary frequencies : 1
The smallest frequency is : -335.5375 cm(-1)

Electronic energy : =-3435.8403076
Zero-point correction= 1.045921
Thermal correction to Energy= 1.107032
Thermal correction to Enthalpy= 1.107977
Thermal correction to Gibbs Free Energy= 0.945237
Sum of electronic and zero-point Energies= -3434.794386
Sum of electronic and thermal Energies= -3434.733275
Sum of electronic and thermal Enthalpies= -3434.732331
Sum of electronic and thermal Free Energies= -3434.895071

Cartesian Coordinates

6	-2.161379	-0.372246	4.780037
6	-3.025101	-1.576395	4.368629
6	-3.763066	-1.115885	3.094770
7	-3.109249	0.149886	2.715779
6	-1.843796	0.308126	3.440551
6	-3.757412	1.171934	2.165359
6	-4.940242	1.038543	1.445816
8	-0.698934	-0.394260	-0.188957
6	-0.691222	-0.438437	2.735058
8	0.408515	0.168449	2.652093
8	-0.933735	-1.606495	2.357917
8	-1.686217	1.486148	0.279136
1	-1.594923	1.367220	3.522326
1	-1.258658	-0.663043	5.321771
1	-2.734560	0.319686	5.405242
1	-2.389298	-2.428978	4.134810
1	-3.727888	-1.861412	5.154021
1	-3.678190	-1.845983	2.286940
1	-4.821545	-0.912157	3.282108
1	-3.239654	2.125474	2.206958
1	-5.447669	0.081733	1.538720
6	-5.884468	2.199064	1.211763
6	-5.270493	3.608490	1.230257
1	-6.672653	2.159131	1.973639
1	-6.397632	2.050741	0.251776
1	-6.096504	4.327933	1.178963
1	-4.741078	3.796461	2.170906
6	-4.364904	3.818631	0.060976
6	-3.067568	4.125060	0.104229
1	-4.810174	3.667170	-0.923793
1	-2.561974	4.306857	1.049681
6	-2.286831	4.181017	-1.161504
8	-2.622570	3.523352	-2.131940
6	-1.103831	5.100567	-1.244787
6	-0.848740	6.066859	-0.266757
6	-0.287617	5.039829	-2.380773
6	0.201613	6.967462	-0.426712
1	-1.486461	6.141847	0.608142
6	0.764231	5.935925	-2.537015
1	-0.509017	4.295372	-3.139646
6	1.006620	6.904495	-1.561349
1	0.383954	7.723676	0.329966
1	1.389734	5.888768	-3.423057
1	1.820775	7.611150	-1.688359
6	-4.084665	0.501722	-0.452197
1	-3.880407	1.542985	-0.690001
1	-2.905640	-1.368007	-0.506854
6	-5.295051	-0.091350	-1.067345
6	-6.023687	0.639551	-2.010806
6	-5.721400	-1.384489	-0.737019

6	-7.149036	0.086758	-2.618156
1	-5.686639	1.635228	-2.287998
6	-6.843280	-1.935311	-1.341777
1	-5.169734	-1.955638	0.006601
6	-7.561584	-1.199437	-2.284711
1	-7.699606	0.661355	-3.356323
1	-7.159078	-2.940047	-1.079336
1	-8.438406	-1.630902	-2.756728
7	-1.742994	0.279620	-0.068042
6	-2.953164	-0.305290	-0.321925
7	0.460934	-2.898269	0.293809
6	-0.368838	-3.822169	-0.327594
6	0.005824	-4.700089	-1.356956
6	-0.924896	-5.586815	-1.878209
6	-2.217683	-5.608559	-1.370549
6	-2.607986	-4.763489	-0.334849
6	-1.683718	-3.877449	0.182223
6	1.591467	-2.267200	-0.130601
16	2.491222	-2.623489	-1.515654
7	1.925814	-1.256841	0.703752
6	3.071252	-0.393641	0.528067
6	2.709154	1.036653	0.968530
6	3.780233	2.070251	0.554368
6	3.158333	3.093150	-0.407363
6	2.056681	3.851424	0.345752
6	1.054209	2.835487	0.924546
7	1.385524	1.474519	0.395670
6	1.368235	1.483769	-1.097892
6	2.513764	2.387128	-1.618030
6	3.465993	1.618303	-2.504047
6	4.784714	1.781571	-2.577490
6	4.265224	-0.860206	1.358084
6	5.576653	-1.023464	0.812952
6	6.608614	-1.418719	1.716207
7	6.397415	-1.654940	3.041976
6	5.176498	-1.513493	3.495473
6	4.080632	-1.115384	2.693878
6	7.925650	-1.578636	1.221765
6	8.224190	-1.363533	-0.099134
6	7.194019	-0.980647	-0.996301
6	5.900473	-0.819838	-0.548196
1	2.536713	1.034589	2.046834
1	4.165573	2.585354	1.438684
1	4.622422	1.558517	0.083431
1	0.024226	3.032135	0.624278
1	1.090761	2.750655	2.012217
1	1.544180	4.536254	-0.333607
1	2.494045	4.447791	1.151225
1	3.921473	3.795981	-0.752378
1	2.051651	3.167786	-2.237788
1	0.374457	1.845111	-1.373770
1	1.450407	0.446067	-1.431137
1	2.994874	0.877079	-3.150844
1	5.384158	1.187564	-3.260072
1	5.321268	2.498271	-1.960443
1	3.330463	-0.396396	-0.532312
1	3.095124	-1.016424	3.143486
1	5.144298	-0.556542	-1.278283
1	5.020109	-1.712733	4.553957
1	8.691675	-1.881050	1.928449
1	9.241337	-1.494344	-0.448734
1	1.312662	-1.027755	1.497090
1	-0.007523	-2.421302	1.084249
1	1.013952	-4.681731	-1.742533
1	-1.951792	-3.201868	0.990558
8	7.403900	-0.753382	-2.318528
6	8.689311	-1.023927	-2.844148
1	8.620671	-0.839309	-3.916452
1	9.449618	-0.360357	-2.415620
1	8.979453	-2.067658	-2.677660

1	0.641472	0.824034	0.710704
1	-3.620770	-4.811539	0.046357
1	-0.651602	-6.267432	-2.675245
7	-3.188249	-6.540774	-1.927387
8	-4.317259	-6.541191	-1.459242
8	-2.827190	-7.274869	-2.833495

1-Michael-nitro-cinchona-thiourea-*re-re*_conf-5

Number of imaginary frequencies : 1
The smallest frequency is : -340.7907 cm(-1)

Electronic energy : =-3435.8422894
Zero-point correction= 1.047022
Thermal correction to Energy= 1.107892
Thermal correction to Enthalpy= 1.108836
Thermal correction to Gibbs Free Energy= 0.947525
Sum of electronic and zero-point Energies= -3434.795267
Sum of electronic and thermal Energies= -3434.734398
Sum of electronic and thermal Enthalpies= -3434.733453
Sum of electronic and thermal Free Energies= -3434.894765

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Cartesian Coordinates

6	2.060895	0.446094	4.907720
6	3.003739	1.559708	4.423951
6	3.758878	0.944130	3.230105
7	3.025510	-0.293323	2.915620
6	1.741740	-0.335480	3.626150
6	3.584892	-1.373434	2.385639
6	4.795796	-1.375328	1.698300
8	0.729059	0.282285	-0.135606
6	0.636241	0.377542	2.819463
8	-0.454910	-0.239800	2.696588
8	0.902876	1.523222	2.395589
8	1.686258	-1.611611	0.340786
1	1.451480	-1.372784	3.799364
1	1.160725	0.834730	5.388761
1	2.572513	-0.216722	5.612722
1	2.423136	2.417555	4.087998
1	3.693151	1.881346	5.206952
1	3.770155	1.609279	2.363384
1	4.789954	0.677638	3.484690
1	2.969837	-2.267699	2.422093
1	5.440449	-0.515266	1.857017
6	5.527879	-2.660909	1.362498
6	4.833973	-3.965100	1.778450
1	6.505910	-2.635947	1.855274
1	5.754503	-2.692811	0.287208
1	5.538629	-4.792446	1.623388
1	4.639953	-3.939777	2.856073
6	3.554163	-4.301652	1.062901
6	3.279283	-4.118744	-0.232127
1	2.760666	-4.755118	1.657508
1	3.997573	-3.687691	-0.924229
6	1.930352	-4.479162	-0.746060
8	1.179343	-5.204034	-0.108307
6	1.480489	-3.924616	-2.062647
6	1.996977	-2.736443	-2.589393
6	0.450954	-4.587524	-2.739451
6	1.476380	-2.208940	-3.767354
1	2.774188	-2.194780	-2.061140
6	-0.050221	-4.073745	-3.930547
1	0.060408	-5.509391	-2.319105
6	0.454563	-2.877147	-4.439162
1	1.862823	-1.272310	-4.155424
1	-0.841372	-4.598096	-4.457569

1	0.052428	-2.466216	-5.359820
6	4.121513	-0.630154	-0.182404
1	3.931564	-1.665777	-0.440300
1	2.969055	1.253847	-0.290854
6	5.389503	-0.054810	-0.688564
6	6.171506	-0.785283	-1.588795
6	5.822669	1.218226	-0.295829
6	7.355261	-0.253372	-2.094206
1	5.837074	-1.767939	-1.912728
6	7.002884	1.749226	-0.799941
1	5.230894	1.788626	0.416599
6	7.773348	1.013861	-1.701013
1	7.947126	-0.829405	-2.798401
1	7.325078	2.738125	-0.489812
1	8.695400	1.429899	-2.093854
7	1.760385	-0.395837	0.032364
6	2.991801	0.186702	-0.128083
7	-0.553568	2.727740	0.282613
6	0.257770	3.650288	-0.364779
6	-0.136232	4.500983	-1.409745
6	0.779174	5.387796	-1.957460
6	2.075744	5.436510	-1.461299
6	2.484689	4.619165	-0.410441
6	1.575663	3.733773	0.133410
6	-1.676794	2.067946	-0.121395
16	-2.597423	2.390572	-1.501679
7	-1.980437	1.062897	0.728194
6	-3.112459	0.174940	0.585783
6	-2.706308	-1.244280	1.027897
6	-3.744544	-2.316514	0.628244
6	-3.108379	-3.304457	-0.362247
6	-1.968331	-4.043620	0.353566
6	-1.016566	-3.005947	0.974726
7	-1.374226	-1.648048	0.450234
6	-1.363511	-1.645545	-1.044866
6	-2.501343	-2.557582	-1.566575
6	-3.479271	-1.795521	-2.428386
6	-4.794812	-1.987144	-2.492469
6	-4.290982	0.618221	1.450559
6	-5.627307	0.721952	0.954449
6	-6.640720	1.081801	1.892628
7	-6.389308	1.347393	3.205835
6	-5.146886	1.264621	3.612986
6	-4.066922	0.898538	2.775347
6	-7.982336	1.169027	1.449106
6	-8.321933	0.916084	0.144857
6	-7.310038	0.571081	-0.787877
6	-5.992894	0.485122	-0.390433
1	-2.528438	-1.230595	2.105197
1	-4.086065	-2.856430	1.515909
1	-4.618729	-1.833671	0.184955
1	0.025538	-3.177920	0.711102
1	-1.096357	-2.936578	2.061507
1	-1.410412	-4.669934	-0.349248
1	-2.367470	-4.696855	1.133823
1	-3.858544	-4.020464	-0.708549
1	-2.029705	-3.310639	-2.210396
1	-0.368629	-1.996091	-1.331457
1	-1.461656	-0.606198	-1.369103
1	-3.029215	-1.038339	-3.071979
1	-5.413861	-1.399262	-3.162766
1	-5.309376	-2.723011	-1.879188
1	-3.399462	0.166765	-0.467363
1	-3.062947	0.839271	3.189668
1	-5.252798	0.248249	-1.145876
1	-4.958445	1.486057	4.661788
1	-8.734301	1.444235	2.181630
1	-9.357812	0.989547	-0.163973
1	-1.354963	0.856095	1.520625
1	-0.071027	2.278987	1.079836

1	-1.147222	4.461855	-1.786049
1	1.858384	3.080979	0.955259
8	-7.559851	0.310446	-2.096916
6	-8.892625	0.423029	-2.557208
1	-8.863090	0.193685	-3.622634
1	-9.554871	-0.292821	-2.056019
1	-9.282440	1.438182	-2.420818
1	-0.646492	-0.984839	0.770702
1	3.500071	4.686523	-0.039148
1	0.490951	6.047984	-2.766347
7	3.029865	6.367538	-2.047348
8	4.160829	6.396716	-1.584879
8	2.654334	7.071928	-2.971065

1-Michael-nitro-cinchona-thiourea-*re-re*_conf-6

Number of imaginary frequencies : 1

The smallest frequency is : -293.8476 cm(-1)

Electronic energy : =-3435.8370908

Zero-point correction= 1.046511

Thermal correction to Energy= 1.107686

Thermal correction to Enthalpy= 1.108630

Thermal correction to Gibbs Free Energy= 0.944154

Sum of electronic and zero-point Energies= -3434.790580

Sum of electronic and thermal Energies= -3434.729405

Sum of electronic and thermal Enthalpies= -3434.728461

Sum of electronic and thermal Free Energies= -3434.892937

Cartesian Coordinates

6	-2.576304	-1.605064	-2.758717
6	-3.097481	-0.202094	-3.108469
6	-3.601743	0.371382	-1.771837
7	-3.056450	-0.528185	-0.742522
6	-2.075435	-1.456559	-1.315348
6	-3.618919	-0.699593	0.448152
6	-4.535823	0.174551	1.019897
8	0.149841	0.949125	0.900279
6	-0.657715	-0.846833	-1.296356
8	0.267715	-1.573235	-0.849779
8	-0.545830	0.305035	-1.772138
8	-1.297341	-0.267316	1.978563
1	-2.077147	-2.389037	-0.745066
1	-1.787883	-1.943171	-3.435018
1	-3.391529	-2.335108	-2.785791
1	-2.284827	0.412524	-3.492310
1	-3.897477	-0.238843	-3.850241
1	-3.256660	1.394541	-1.601900
1	-4.694603	0.349814	-1.698761
1	-3.235405	-1.537981	1.025688
1	-5.011536	0.894685	0.358305
6	-5.339849	-0.235003	2.230324
6	-6.836683	-0.388645	1.941119
1	-5.249166	0.528729	3.013528
1	-4.933203	-1.160611	2.656941
1	-7.383665	-0.492287	2.888583
1	-7.211903	0.544653	1.499217
6	-7.243417	-1.530010	1.061806
6	-6.456475	-2.523027	0.637585
1	-8.288736	-1.560109	0.754384
1	-5.407939	-2.560689	0.908866
6	-7.006623	-3.613931	-0.209069
8	-8.207446	-3.770980	-0.353561
6	-6.037546	-4.534626	-0.889021
6	-4.694147	-4.197858	-1.077846
6	-6.515572	-5.754008	-1.378016

6	-3.838885	-5.071270	-1.743727
1	-4.318205	-3.238159	-0.732921
6	-5.658668	-6.632629	-2.028280
1	-7.564776	-5.992031	-1.236004
6	-4.318633	-6.292230	-2.211548
1	-2.799316	-4.797762	-1.900843
1	-6.033078	-7.582004	-2.397492
1	-3.649511	-6.976675	-2.723722
6	-3.165498	1.648728	1.818399
1	-3.145369	1.059669	2.731616
1	-1.649215	2.537219	0.478392
6	-4.077865	2.814891	1.807555
6	-4.764049	3.179410	2.970793
6	-4.270917	3.573442	0.644982
6	-5.618136	4.280179	2.973733
1	-4.607023	2.611992	3.884179
6	-5.118583	4.672742	0.649008
1	-3.756887	3.289249	-0.269969
6	-5.797176	5.028470	1.815114
1	-6.138326	4.555234	3.885757
1	-5.253428	5.253081	-0.258276
1	-6.460013	5.887662	1.817292
7	-1.005410	0.772099	1.340701
6	-1.959405	1.732177	1.127348
7	1.603515	2.031101	-1.274367
6	1.194819	3.352677	-1.397730
6	2.018767	4.484328	-1.291468
6	1.473887	5.749925	-1.452675
6	0.119624	5.889048	-1.728017
6	-0.714197	4.781990	-1.860848
6	-0.174139	3.521881	-1.697860
6	2.674932	1.462353	-0.655487
16	4.003123	2.267189	0.011663
7	2.543049	0.116818	-0.602289
6	3.506612	-0.787179	-0.016471
6	2.761407	-1.913805	0.725481
6	3.694575	-2.753166	1.626083
6	3.256682	-2.612277	3.092130
6	1.843156	-3.195258	3.229505
6	0.912849	-2.497745	2.218246
7	1.652756	-1.361467	1.583214
6	2.146716	-0.415222	2.627606
6	3.206937	-1.127397	3.507888
6	4.530173	-0.398717	3.476436
6	5.739794	-0.953310	3.488915
6	4.409782	-1.424367	-1.068903
6	5.833746	-1.460138	-0.947966
6	6.553860	-2.142828	-1.973413
7	5.955865	-2.730170	-3.048024
6	4.650683	-2.654004	-3.131782
6	3.835792	-2.017870	-2.165382
6	7.964578	-2.223364	-1.880204
6	8.644757	-1.662027	-0.830359
6	7.926708	-0.972774	0.180918
6	6.553499	-0.870449	0.116627
1	2.239407	-2.528551	-0.010577
1	3.654145	-3.805278	1.330860
1	4.727025	-2.420170	1.497178
1	0.025283	-2.059564	2.673334
1	0.597528	-3.144081	1.397120
1	1.474061	-3.048441	4.248496
1	1.861513	-4.271306	3.038618
1	3.946428	-3.157047	3.741919
1	2.845097	-1.090240	4.543822
1	1.260532	-0.106965	3.185396
1	2.538742	0.465919	2.112488
1	4.454288	0.689135	3.464195
1	6.635238	-0.340127	3.479887
1	5.891127	-2.029896	3.498751
1	4.108366	-0.215401	0.692374

1	2.756387	-2.005335	-2.299581
1	6.054492	-0.310274	0.898432
1	4.186723	-3.121071	-3.998416
1	8.488315	-2.747509	-2.672890
1	9.724351	-1.742271	-0.785937
1	1.678726	-0.321037	-0.947479
1	0.837450	1.363059	-1.474646
1	3.071549	4.369418	-1.083146
1	-0.794203	2.633941	-1.794131
8	8.523180	-0.383583	1.248792
6	9.936226	-0.401104	1.317580
1	10.200308	0.151560	2.219434
1	10.324464	-1.423249	1.398029
1	10.387493	0.093765	0.449980
1	0.980165	-0.840567	0.987702
1	2.095841	6.633228	-1.372788
1	-1.764025	4.923765	-2.086402
7	-0.442683	7.223027	-1.890624
8	-1.634901	7.315293	-2.142438
8	0.303714	8.180869	-1.766504

1-Michael-nitro-cinchona-thiourea-*re-re*_conf-7

Number of imaginary frequencies : 1
The smallest frequency is : -335.6734 cm(-1)

Electronic energy : =-3435.8388221
Zero-point correction= 1.046261
Thermal correction to Energy= 1.107316
Thermal correction to Enthalpy= 1.108260
Thermal correction to Gibbs Free Energy= 0.946102
Sum of electronic and zero-point Energies= -3434.792561
Sum of electronic and thermal Energies= -3434.731507
Sum of electronic and thermal Enthalpies= -3434.730562
Sum of electronic and thermal Free Energies= -3434.892720

Cartesian Coordinates

6	-2.323890	0.648987	4.432327
6	-3.305121	-0.518152	4.231021
6	-3.968201	-0.246659	2.865479
7	-3.172703	0.839092	2.267318
6	-1.915217	1.029647	3.002761
6	-3.680032	1.778179	1.475930
6	-4.863827	1.651247	0.755537
8	-0.901400	-0.629652	-0.346377
6	-0.813604	0.079548	2.484188
8	0.302413	0.593567	2.211695
8	-1.117344	-1.132988	2.426002
8	-1.696716	1.394950	-0.438985
1	-1.580893	2.062901	2.893177
1	-1.464714	0.374900	5.048228
1	-2.827670	1.501489	4.898764
1	-2.758997	-1.459187	4.192499
1	-4.047573	-0.569042	5.029875
1	-3.954214	-1.128251	2.220790
1	-5.000850	0.101260	2.968837
1	-3.041795	2.643586	1.327798
1	-5.532849	0.849738	1.056233
6	-5.548463	2.852649	0.138764
6	-4.802244	4.190307	0.209861
1	-6.516585	2.990312	0.632975
1	-5.792107	2.642963	-0.912101
1	-5.476489	4.951645	-0.205705
1	-4.619509	4.475650	1.252485
6	-3.523439	4.270932	-0.568857
6	-2.435350	4.927388	-0.150057

1	-3.495189	3.818534	-1.561439
1	-2.424635	5.407471	0.825557
6	-1.246188	5.090921	-1.023573
8	-1.222211	4.689932	-2.176452
6	-0.055212	5.801052	-0.453447
6	0.778357	6.507690	-1.325405
6	0.270074	5.722011	0.903526
6	1.916600	7.141637	-0.843526
1	0.517511	6.545754	-2.378569
6	1.427317	6.332481	1.380669
1	-0.360753	5.156772	1.584097
6	2.245234	7.048731	0.509381
1	2.553186	7.703615	-1.519483
1	1.687023	6.254245	2.431529
1	3.139760	7.536049	0.884806
6	-4.164785	0.521226	-0.922260
1	-3.849457	1.451075	-1.389523
1	-3.208144	-1.428199	-0.499989
6	-5.450645	-0.038275	-1.398694
6	-6.091563	0.549005	-2.494266
6	-6.032642	-1.162215	-0.797781
6	-7.282164	0.020886	-2.986812
1	-5.638145	1.410529	-2.977220
6	-7.219745	-1.689784	-1.289589
1	-5.550446	-1.620921	0.062568
6	-7.848171	-1.098861	-2.386203
1	-7.762977	0.483171	-3.842964
1	-7.657495	-2.564100	-0.818571
1	-8.775451	-1.512740	-2.769065
7	-1.869136	0.151281	-0.448404
6	-3.134150	-0.354469	-0.588141
7	0.180796	-2.958547	0.749034
6	-0.727793	-3.930475	0.346663
6	-0.419972	-5.083015	-0.392712
6	-1.424957	-5.984472	-0.711999
6	-2.725870	-5.745647	-0.287453
6	-3.051864	-4.621745	0.467760
6	-2.053047	-3.721939	0.782500
6	1.338703	-2.525321	0.176928
16	2.178334	-3.274620	-1.083873
7	1.751075	-1.361975	0.730765
6	2.936725	-0.636949	0.331491
6	2.643416	0.875703	0.334909
6	3.750382	1.695522	-0.365334
6	3.168788	2.395384	-1.604490
6	2.105952	3.398785	-1.137990
6	1.086132	2.663958	-0.249326
7	1.335859	1.188123	-0.341594
6	1.296639	0.743318	-1.768544
6	2.482934	1.377904	-2.538468
6	3.389508	0.326894	-3.134595
6	4.714286	0.393141	-3.242266
6	4.110085	-0.897875	1.272332
6	5.408390	-1.272643	0.806029
6	6.431375	-1.426540	1.788806
7	6.221491	-1.255051	3.124580
6	5.010983	-0.936089	3.511279
6	3.926108	-0.742353	2.623456
6	7.737309	-1.774661	1.366567
6	8.033306	-1.965599	0.041150
6	7.010543	-1.824247	-0.931896
6	5.727313	-1.491840	-0.553415
1	2.486148	1.197313	1.367042
1	4.153878	2.444791	0.321413
1	4.573944	1.034630	-0.645546
1	0.054608	2.814862	-0.565718
1	1.170938	2.917827	0.809403
1	1.593933	3.842186	-1.997891
1	2.566633	4.216299	-0.575059
1	3.963220	2.917753	-2.143843

1	2.055514	1.943298	-3.376786
1	0.322896	1.064133	-2.143730
1	1.316997	-0.349750	-1.771255
1	2.876765	-0.549652	-3.532572
1	5.277154	-0.409550	-3.708160
1	5.291373	1.235250	-2.867934
1	3.193413	-0.956142	-0.679969
1	2.950397	-0.471693	3.021090
1	4.975157	-1.425594	-1.330576
1	4.855149	-0.810187	4.581125
1	8.497482	-1.886936	2.132716
1	9.042327	-2.231682	-0.250468
1	1.159192	-0.895377	1.431857
1	-0.246891	-2.271713	1.396324
1	0.595197	-5.264557	-0.712180
1	-2.267718	-2.831549	1.367756
8	7.215498	-2.002744	-2.262134
6	8.502589	-2.403165	-2.691743
1	8.435778	-2.518375	-3.773836
1	9.260528	-1.645907	-2.458543
1	8.795103	-3.361613	-2.247566
1	0.565502	0.706510	0.157673
1	-1.204204	-6.877789	-1.283371
1	-4.074013	-4.468604	0.792158
7	-3.775158	-6.695460	-0.631716
8	-4.910196	-6.460551	-0.244012
8	-3.470198	-7.677338	-1.289721

1-Michael-nitro-cinchona-thiourea-*re-re*_conf-8

Number of imaginary frequencies : 1

The smallest frequency is : -341.7296 cm(-1)

Electronic energy : =-3435.83782

Zero-point correction= 1.046324

Thermal correction to Energy= 1.107511

Thermal correction to Enthalpy= 1.108456

Thermal correction to Gibbs Free Energy= 0.945307

Sum of electronic and zero-point Energies= -3434.791496

Sum of electronic and thermal Energies= -3434.730309

Sum of electronic and thermal Enthalpies= -3434.729364

Sum of electronic and thermal Free Energies= -3434.892513

Cartesian Coordinates

6	2.893206	-0.438588	3.921832
6	4.168887	0.091376	3.260505
6	4.513997	-1.011024	2.266931
7	3.198785	-1.497327	1.833228
6	2.125711	-1.085479	2.768548
6	3.030696	-2.351495	0.840999
6	4.061222	-2.764814	-0.009906
8	1.332760	0.805103	-0.924281
6	1.181790	-0.117097	2.020794
8	0.242729	-0.673831	1.389676
8	1.424518	1.105117	2.089858
8	1.686063	-1.290447	-1.389956
1	1.550763	-1.967087	3.060831
1	2.303451	0.350589	4.388666
1	3.140910	-1.193994	4.674358
1	3.939799	1.014749	2.723353
1	4.978733	0.275659	3.968342
1	5.090947	-0.677566	1.404737
1	5.056371	-1.837501	2.746948
1	1.996366	-2.628861	0.645584
1	5.072414	-2.723369	0.388940
6	3.773106	-3.861462	-1.007913

6	3.567739	-5.272152	-0.407383
1	4.600197	-3.916669	-1.724517
1	2.871734	-3.591258	-1.572902
1	3.416598	-5.979370	-1.230046
1	4.470597	-5.574666	0.133393
6	2.383285	-5.296867	0.510229
6	1.128915	-5.553302	0.122330
1	2.532615	-5.011440	1.551271
1	0.913312	-5.826275	-0.907234
6	0.003145	-5.369562	1.077234
8	0.189851	-4.940971	2.204860
6	-1.393417	-5.657164	0.609454
6	-1.673189	-6.471024	-0.491966
6	-2.448706	-5.074892	1.321841
6	-2.993049	-6.700346	-0.874192
1	-0.870107	-6.952384	-1.040605
6	-3.764005	-5.290839	0.929820
1	-2.210899	-4.455828	2.181423
6	-4.037163	-6.106436	-0.170075
1	-3.206017	-7.343617	-1.721885
1	-4.577657	-4.830775	1.481897
1	-5.064637	-6.281262	-0.473907
6	4.293905	-1.051401	-1.298317
1	3.872053	-1.705575	-2.055706
1	3.770258	0.984934	-0.559022
6	5.763522	-0.874988	-1.381365
6	6.496548	-1.706059	-2.238091
6	6.452982	0.104106	-0.653005
6	7.876258	-1.574470	-2.355297
1	5.972239	-2.450481	-2.831332
6	7.831422	0.237533	-0.770554
1	5.909861	0.776943	0.005074
6	8.549295	-0.604175	-1.618188
1	8.425161	-2.225444	-3.028498
1	8.346457	1.006395	-0.203484
1	9.625454	-0.497158	-1.709253
7	2.120057	-0.147014	-1.088416
6	3.469487	0.018784	-0.933956
7	0.297653	3.099228	0.420889
6	1.128122	4.190985	0.218640
6	0.832096	5.330548	-0.546971
6	1.768843	6.347514	-0.657508
6	2.991891	6.235516	-0.009118
6	3.307448	5.117849	0.760376
6	2.377837	4.104714	0.869581
6	-0.930352	2.760850	-0.059109
16	-1.958396	3.714305	-1.001145
7	-1.263288	1.505378	0.317374
6	-2.539553	0.884458	0.053531
6	-2.352470	-0.639413	-0.081077
6	-3.591200	-1.327704	-0.697500
6	-3.216182	-1.941055	-2.055222
6	-2.196736	-3.058475	-1.799135
6	-1.027042	-2.480291	-0.981785
7	-1.156629	-0.986072	-0.930611
6	-1.244424	-0.415192	-2.306626
6	-2.558078	-0.893682	-2.977577
6	-3.438192	0.269269	-3.372032
6	-4.768124	0.299236	-3.338966
6	-3.538389	1.135614	1.183684
6	-4.886388	1.554014	0.958746
6	-5.728554	1.673082	2.104208
7	-5.304140	1.435751	3.377374
6	-4.052709	1.084552	3.542085
6	-3.135952	0.916289	2.477399
6	-7.079192	2.057716	1.921848
6	-7.586965	2.317203	0.674893
6	-6.742693	2.211537	-0.460416
6	-5.421422	1.846129	-0.316396
1	-2.102598	-1.047987	0.901008

1	-3.950380	-2.119192	-0.032755
1	-4.399613	-0.601034	-0.806404
1	-0.050340	-2.687681	-1.415940
1	-1.022731	-2.813135	0.058995
1	-1.834474	-3.463349	-2.749157
1	-2.665098	-3.877661	-1.246769
1	-4.106611	-2.353978	-2.536419
1	-2.277339	-1.410517	-3.904867
1	-0.343354	-0.754685	-2.819819
1	-1.183909	0.671842	-2.211055
1	-2.904647	1.147597	-3.737456
1	-5.315830	1.178591	-3.662644
1	-5.364476	-0.537460	-2.983217
1	-2.924371	1.293171	-0.883719
1	-2.113978	0.612098	2.692328
1	-4.808137	1.810918	-1.208878
1	-3.723178	0.907899	4.564241
1	-7.699098	2.139461	2.808791
1	-8.624588	2.609875	0.568276
1	-0.577698	0.936258	0.828255
1	0.744802	2.351026	0.975244
1	-0.121069	5.413312	-1.046202
1	2.591505	3.221855	1.465885
8	-7.163373	2.454983	-1.728516
6	-8.496573	2.889102	-1.916929
1	-8.613592	3.044739	-2.989650
1	-9.218732	2.133970	-1.584817
1	-8.690144	3.833499	-1.395300
1	-0.297298	-0.621602	-0.475528
1	1.553471	7.231341	-1.245584
1	4.267158	5.059300	1.258705
7	3.968164	7.308024	-0.134328
8	5.035423	7.182893	0.447806
8	3.673989	8.278033	-0.815174

1-Michael-nitro-cinchona-thiourea-re-re_conf-9

Number of imaginary frequencies : 1
The smallest frequency is : -341.3814 cm(-1)

Electronic energy : =-3435.8335966
Zero-point correction= 1.046494
Thermal correction to Energy= 1.107596
Thermal correction to Enthalpy= 1.108540
Thermal correction to Gibbs Free Energy= 0.943686
Sum of electronic and zero-point Energies= -3434.787102
Sum of electronic and thermal Energies= -3434.726001
Sum of electronic and thermal Enthalpies= -3434.725056
Sum of electronic and thermal Free Energies= -3434.889911

Cartesian Coordinates

6	1.296185	-1.707719	3.996637
6	2.239026	-0.505450	3.825226
6	2.811710	-0.651228	2.399849
7	2.015107	-1.721340	1.776965
6	0.807229	-1.988248	2.569367
6	2.508846	-2.602019	0.914051
6	3.657875	-2.426579	0.148989
8	-0.489337	-0.346308	-0.614313
6	-0.335257	-1.022778	2.189806
8	-1.467518	-1.538196	2.000942
8	-0.046145	0.193885	2.148177
8	0.482298	-2.259926	-0.990747
1	0.482012	-3.016565	2.405304
1	0.471789	-1.503397	4.683198
1	1.844774	-2.581230	4.362728

1	1.675876	0.423700	3.899131
1	3.033029	-0.500345	4.574579
1	2.714280	0.274432	1.828581
1	3.861689	-0.961316	2.402754
1	1.885355	-3.476284	0.744443
1	4.355462	-1.659245	0.469141
6	4.255619	-3.674923	-0.476618
6	5.088031	-3.516677	-1.750069
1	3.438428	-4.372058	-0.697958
1	4.883813	-4.176591	0.273371
1	5.377661	-4.519015	-2.095116
1	4.476448	-3.110392	-2.563780
6	6.339371	-2.700255	-1.659608
6	6.878939	-2.152454	-0.566233
1	6.869471	-2.535573	-2.597512
1	6.425907	-2.268807	0.412933
6	8.130612	-1.358399	-0.689199
8	8.812206	-1.394020	-1.700662
6	8.554499	-0.498159	0.465702
6	7.679259	-0.120560	1.488305
6	9.872233	-0.031361	0.484164
6	8.118365	0.708741	2.516327
1	6.643329	-0.446127	1.468266
6	10.314295	0.785521	1.516729
1	10.533464	-0.323110	-0.325169
6	9.436800	1.157029	2.534712
1	7.431734	1.008529	3.301697
1	11.340907	1.137448	1.528628
1	9.779176	1.799698	3.339866
6	2.860338	-1.090792	-1.373667
1	2.636846	-1.954478	-1.994497
1	1.738235	0.665882	-0.650394
6	4.073730	-0.306234	-1.717205
6	4.658042	-0.435393	-2.980272
6	4.649166	0.576218	-0.796147
6	5.805046	0.282930	-3.307098
1	4.211067	-1.104939	-3.710866
6	5.798399	1.289939	-1.118483
1	4.201079	0.684707	0.189645
6	6.384991	1.137922	-2.374154
1	6.252391	0.165794	-4.289095
1	6.242893	1.958659	-0.387934
1	7.292076	1.680043	-2.620111
7	0.543171	-1.017393	-0.832859
6	1.754303	-0.383289	-0.907159
7	-1.478928	2.031299	0.576216
6	-0.636166	3.062521	0.181305
6	-1.004312	4.191301	-0.568347
6	-0.052922	5.153277	-0.874785
6	1.254253	4.999390	-0.431502
6	1.640978	3.897864	0.327696
6	0.695861	2.939131	0.632151
6	-2.673479	1.592417	0.091644
16	-3.628825	2.346595	-1.081446
7	-3.021952	0.413750	0.657208
6	-4.229247	-0.322555	0.357372
6	-3.909513	-1.829452	0.332943
6	-5.061711	-2.679151	-0.246018
6	-4.585383	-3.394329	-1.519735
6	-3.454938	-4.359964	-1.136232
6	-2.355990	-3.573224	-0.394374
7	-2.669409	-2.111171	-0.474742
6	-2.796979	-1.685263	-1.900855
6	-4.025103	-2.382657	-2.539868
6	-5.018447	-1.373739	-3.068177
6	-6.344659	-1.477991	-3.037643
6	-5.320224	-0.084124	1.398281
6	-6.666309	0.244709	1.047583
6	-7.601814	0.372901	2.117460
7	-7.267123	0.220601	3.429928

6	-6.017211	-0.055876	3.708711
6	-5.010522	-0.223396	2.728002
6	-8.952188	0.671404	1.812851
6	-9.373134	0.836515	0.518284
6	-8.438030	0.718729	-0.542176
6	-7.114191	0.438351	-0.279370
1	-3.639152	-2.141185	1.343928
1	-5.387815	-3.420066	0.489217
1	-5.919108	-2.038410	-0.463039
1	-1.364983	-3.691929	-0.831287
1	-2.296557	-3.808672	0.669910
1	-3.044316	-4.832228	-2.033463
1	-3.841923	-5.154923	-0.493634
1	-5.413073	-3.951215	-1.966569
1	-3.660772	-2.956162	-3.402328
1	-1.850398	-1.959229	-2.371026
1	-2.869981	-0.594321	-1.910536
1	-4.574117	-0.492854	-3.533135
1	-6.976510	-0.702038	-3.458035
1	-6.855778	-2.325209	-2.586842
1	-4.577066	-0.002398	-0.626402
1	-3.995581	-0.463587	3.036889
1	-6.435141	0.389539	-1.122111
1	-5.762772	-0.167276	4.761061
1	-9.643661	0.763968	2.643956
1	-10.413361	1.062723	0.316349
1	-2.374950	-0.046535	1.312199
1	-0.997252	1.343679	1.182427
1	-2.022607	4.308504	-0.906342
1	0.960081	2.067193	1.224929
8	-8.771875	0.868605	-1.849975
6	-10.103593	1.232399	-2.159923
1	-10.143671	1.332449	-3.244722
1	-10.816954	0.461539	-1.845268
1	-10.375213	2.190291	-1.701727
1	-1.864544	-1.589342	-0.075202
1	-0.320877	6.029059	-1.453125
1	2.666958	3.807450	0.662953
7	2.244196	6.016774	-0.758403
8	3.378992	5.869266	-0.330154
8	1.891579	6.965293	-1.441177

1-Michael-nitro-cinchona-thiourea-*re-re*_conf-10

Number of imaginary frequencies : 1

The smallest frequency is : -340.8849 cm(-1)

Electronic energy : =-3435.8336486

Zero-point correction= 1.047158

Thermal correction to Energy= 1.108114

Thermal correction to Enthalpy= 1.109059

Thermal correction to Gibbs Free Energy= 0.945710

Sum of electronic and zero-point Energies= -3434.786490

Sum of electronic and thermal Energies= -3434.725534

Sum of electronic and thermal Enthalpies= -3434.724590

Sum of electronic and thermal Free Energies= -3434.887939

Cartesian Coordinates

6	1.267524	-1.854336	3.887725
6	2.217657	-0.651959	3.762134
6	2.805454	-0.758401	2.339398
7	2.013192	-1.808149	1.677589
6	0.794636	-2.090040	2.446865
6	2.513745	-2.664445	0.794222
6	3.669030	-2.463612	0.045553
8	-0.481705	-0.371405	-0.709064

6	-0.335408	-1.103848	2.084777
8	-1.473754	-1.601891	1.886880
8	-0.031867	0.110189	2.066901
8	0.494376	-2.276609	-1.117596
1	0.463794	-3.110502	2.248810
1	0.435899	-1.666442	4.570290
1	1.807927	-2.740695	4.234521
1	1.658539	0.277712	3.857277
1	3.003266	-0.673235	4.520034
1	2.716158	0.183555	1.794094
1	3.854551	-1.071572	2.345123
1	1.892530	-3.533906	0.594216
1	4.357019	-1.699416	0.391862
6	4.284363	-3.688333	-0.609174
6	5.168541	-3.474280	-1.839403
1	3.474191	-4.371022	-0.892983
1	4.880656	-4.225143	0.142525
1	5.485730	-4.459548	-2.208437
1	4.585925	-3.044679	-2.661918
6	6.402595	-2.644224	-1.663459
6	6.889954	-2.150078	-0.521399
1	6.959655	-2.416237	-2.571811
1	6.402133	-2.334009	0.430010
6	8.117813	-1.311108	-0.542998
8	8.864142	-1.295217	-1.507797
6	8.424795	-0.463736	0.657762
6	7.466364	-0.164136	1.630432
6	9.710243	0.073695	0.774550
6	7.790848	0.654983	2.707835
1	6.453663	-0.543978	1.534482
6	10.037921	0.881977	1.856047
1	10.438158	-0.155262	0.002956
6	9.078319	1.172899	2.824787
1	7.039150	0.890052	3.454826
1	11.039834	1.289640	1.945104
1	9.333181	1.806414	3.668668
6	2.877546	-1.092014	-1.448659
1	2.666126	-1.940616	-2.094642
1	1.742339	0.640783	-0.692160
6	4.089678	-0.291321	-1.758395
6	4.691012	-0.389831	-3.015912
6	4.647692	0.575059	-0.811443
6	5.839311	0.339819	-3.311753
1	4.255858	-1.044033	-3.767202
6	5.797566	1.300943	-1.103008
1	4.185513	0.661327	0.170130
6	6.402929	1.176747	-2.352714
1	6.299213	0.246077	-4.290496
1	6.228781	1.955938	-0.352334
1	7.311091	1.727328	-2.574710
7	0.553390	-1.038881	-0.930256
6	1.764250	-0.401595	-0.974461
7	-1.429330	2.003007	0.527343
6	-0.570409	3.022696	0.137934
6	-0.917345	4.156310	-0.614400
6	0.050663	5.102820	-0.917178
6	1.353277	4.928967	-0.467910
6	1.719077	3.822559	0.294664
6	0.757151	2.879817	0.596309
6	-2.632864	1.586286	0.045069
16	-3.584651	2.367904	-1.113440
7	-2.991041	0.405095	0.598592
6	-4.217226	-0.308955	0.322586
6	-3.916793	-1.817853	0.220286
6	-5.092596	-2.623140	-0.373254
6	-4.653760	-3.279930	-1.690853
6	-3.528043	-4.277881	-1.380876
6	-2.403046	-3.543399	-0.624480
7	-2.697881	-2.075795	-0.625129
6	-2.850824	-1.574754	-2.023958

6	-4.098748	-2.227679	-2.672042
6	-5.086515	-1.183696	-3.137271
6	-6.413265	-1.261630	-3.069277
6	-5.251415	-0.111172	1.427948
6	-6.612227	0.237851	1.164759
6	-7.486511	0.325587	2.289099
7	-7.082225	0.117182	3.573811
6	-5.821517	-0.178963	3.771990
6	-4.871241	-0.310986	2.731749
6	-8.849636	0.641670	2.071973
6	-9.340065	0.861940	0.810726
6	-8.465988	0.784636	-0.304174
6	-7.131474	0.487365	-0.126501
1	-3.630036	-2.180248	1.209289
1	-5.411775	-3.396136	0.331483
1	-5.946127	-1.961165	-0.535943
1	-1.421389	-3.653418	-1.084840
1	-2.327334	-3.832479	0.425526
1	-3.143212	-4.707490	-2.310319
1	-3.911002	-5.100574	-0.771786
1	-5.498006	-3.803119	-2.147236
1	-3.756323	-2.764858	-3.566382
1	-1.917712	-1.829764	-2.530056
1	-2.916286	-0.484561	-1.973189
1	-4.637710	-0.298320	-3.588786
1	-7.039638	-0.460466	-3.448424
1	-6.929422	-2.112386	-2.631246
1	-4.607569	0.058869	-0.628340
1	-3.843389	-0.574064	2.973208
1	-6.500025	0.468694	-1.007165
1	-5.511122	-0.336701	4.803191
1	-9.493635	0.700570	2.943326
1	-10.388514	1.099179	0.676382
1	-2.342071	-0.072130	1.239004
1	-0.957126	1.302000	1.125211
1	-1.932130	4.288674	-0.957492
1	1.005304	2.004335	1.191057
8	-8.869853	0.990843	-1.583822
6	-10.213169	1.376676	-1.805005
1	-10.310438	1.524689	-2.880716
1	-10.915498	0.597145	-1.487003
1	-10.451775	2.315054	-1.291419
1	-1.877327	-1.584125	-0.218065
1	2.742098	3.715622	0.634272
1	-0.201002	5.981923	-1.497782
7	2.360682	5.929888	-0.792202
8	3.491265	5.764795	-0.359382
8	2.025771	6.883045	-1.477434

1-Michael-nitrostyrene-Ph-to-Me-si-si_conf-1

Number of imaginary frequencies : 1

The smallest frequency is : -292.3359 cm(-1)

Electronic energy : =-3713.6128748

Zero-point correction= 0.998659

Thermal correction to Energy= 1.061411

Thermal correction to Enthalpy= 1.062355

Thermal correction to Gibbs Free Energy= 0.897185

Sum of electronic and zero-point Energies= -3712.614216

Sum of electronic and thermal Energies= -3712.551464

Sum of electronic and thermal Enthalpies= -3712.550520

Sum of electronic and thermal Free Energies= -3712.715690

Cartesian Coordinates

6	1.965521	0.118386	-5.312974

6	2.936707	-1.066428	-5.245877
6	4.069606	-0.559892	-4.341891
7	3.454387	0.535807	-3.578740
6	2.031306	0.667275	-3.878728
6	4.169278	1.368698	-2.821758
6	3.700216	2.298995	-1.915829
8	0.560460	2.031399	1.321353
8	0.844342	1.347409	-0.715952
1	1.722577	1.712539	-3.798481
1	0.948504	-0.166143	-5.587470
1	2.324891	0.876285	-6.016312
1	4.437340	-1.336171	-3.664678
1	4.914085	-0.166925	-4.920282
1	2.629755	2.497540	-1.885898
6	4.634493	3.392004	-1.449283
1	5.652413	2.993279	-1.353170
6	3.438287	0.774210	-0.262499
1	2.937509	0.169656	-1.015669
1	2.961638	1.733228	1.653396
7	1.299428	1.577320	0.433110
6	2.631996	1.363123	0.693190
7	0.819984	-1.635857	0.232930
6	1.869792	-2.143124	0.994454
6	1.876440	-2.323831	2.380727
6	3.028453	-2.808597	2.998562
6	4.183440	-3.105832	2.290538
6	4.165832	-2.907002	0.910823
6	3.036095	-2.440725	0.264207
6	3.037104	-2.931391	4.496168
9	1.838752	-3.277495	4.982194
6	5.423615	-3.169870	0.135920
9	5.809451	-4.451286	0.218889
6	-0.504223	-1.461493	0.491942
16	-1.309031	-1.846521	1.930742
7	-1.130687	-0.916209	-0.573979
6	-2.550914	-0.675175	-0.693568
6	-2.735187	0.723653	-1.309131
6	-4.204983	1.187685	-1.378137
6	-4.386674	2.448583	-0.521043
6	-3.516010	3.571334	-1.104701
6	-2.061308	3.074778	-1.221794
7	-1.948430	1.750785	-0.530617
6	-2.403084	1.881739	0.892624
6	-3.921101	2.189469	0.924618
6	-4.690638	1.130934	1.678501
6	-5.918102	0.697324	1.403209
6	-3.228034	-1.706502	-1.594003
6	-4.407547	-2.416987	-1.204887
6	-4.974839	-3.308549	-2.164237
7	-4.439462	-3.522468	-3.399868
6	-3.344974	-2.870577	-3.704084
6	-2.704639	-1.949833	-2.839843
6	-6.155611	-4.013561	-1.829222
6	-6.761244	-3.855742	-0.608877
6	-6.188752	-2.978358	0.346970
6	-5.034163	-2.283587	0.055165
9	3.924391	-3.845821	4.918263
9	3.372141	-1.768334	5.083075
9	6.447351	-2.432539	0.606617
9	5.295846	-2.872811	-1.166763
1	-2.260101	0.716371	-2.294844
1	-4.479993	1.401400	-2.414671
1	-4.860136	0.387249	-1.025810
1	-1.345123	3.748177	-0.747486
1	-1.747434	2.911380	-2.255016
1	-3.559822	4.449892	-0.453680
1	-3.887634	3.868454	-2.088579
1	-5.435788	2.755768	-0.526261
1	-4.037229	3.129795	1.480057
1	-1.803823	2.684859	1.324430

1	-2.139078	0.955214	1.410008
1	-4.171664	0.714559	2.543364
1	-6.391950	-0.064385	2.014911
1	-6.491515	1.063889	0.555259
1	-2.983425	-0.706696	0.307473
1	-1.798901	-1.444294	-3.169889
1	-4.624749	-1.646362	0.828851
1	-2.922597	-3.055901	-4.690100
1	-6.565205	-4.685819	-2.576046
1	-7.665010	-4.408360	-0.382050
1	-0.594182	-0.711480	-1.432557
1	1.093300	-1.452974	-0.755743
1	0.997007	-2.094293	2.965876
1	3.040880	-2.282493	-0.810978
1	5.070396	-3.477508	2.792385
8	-6.720240	-2.768684	1.579509
6	-7.866841	-3.512105	1.945688
1	-8.096348	-3.225170	2.972135
1	-8.725010	-3.272325	1.306826
1	-7.674906	-4.590636	1.910696
1	-0.936225	1.485934	-0.534833
6	1.130047	-0.198368	-2.974109
8	1.689490	-1.104627	-2.303030
8	-0.097844	0.041303	-3.039735
1	4.689625	4.168974	-2.225661
1	3.303938	-1.376930	-6.225502
1	2.444567	-1.918619	-4.771794
6	4.240476	4.096564	-0.140523
1	4.936144	4.933756	0.004622
1	4.353821	3.435739	0.723917
6	2.845452	4.636392	-0.195078
6	1.952383	4.596959	0.799587
1	2.526054	5.093114	-1.133492
1	2.206720	4.149781	1.754471
6	0.577905	5.110489	0.572906
8	0.254497	5.575231	-0.512356
6	-0.445966	5.035707	1.669400
6	-0.236286	4.372617	2.882307
6	-1.689915	5.629898	1.421062
6	-1.261061	4.293147	3.821994
1	0.702953	3.872944	3.084532
6	-2.709832	5.556402	2.361825
1	-1.832873	6.147436	0.477483
6	-2.497055	4.880769	3.564168
1	-1.094420	3.763594	4.754287
1	-3.669153	6.024781	2.162234
1	-3.293330	4.813582	4.299293
1	5.248203	1.219265	-2.901211
6	4.855961	0.433612	0.101361
1	5.361844	-0.091423	-0.711211
1	5.432574	1.329347	0.353660
1	4.863236	-0.215172	0.983625

1-Michael-nitrostyrene-Ph-to-Me-si-si_conf-2

Number of imaginary frequencies : 1

The smallest frequency is : -288.8293 cm(-1)

Electronic energy : =-3713.6109281

Zero-point correction= 0.998652

Thermal correction to Energy= 1.061535

Thermal correction to Enthalpy= 1.062479

Thermal correction to Gibbs Free Energy= 0.896112

Sum of electronic and zero-point Energies= -3712.612276

Sum of electronic and thermal Energies= -3712.549393

Sum of electronic and thermal Enthalpies= -3712.548449

Sum of electronic and thermal Free Energies= -3712.714816

Cartesian Coordinates

6	-1.544432	0.612954	5.315118
6	-2.423200	-0.610392	5.596276
6	-3.694392	-0.332778	4.784475
7	-3.244025	0.582721	3.726438
6	-1.813196	0.865271	3.823209
6	-4.089353	1.169935	2.877475
6	-3.753515	1.883196	1.745399
8	-0.876216	1.064106	-1.718728
8	-0.974167	1.077198	0.453447
1	-1.612968	1.897022	3.520466
1	-0.483969	0.443257	5.507068
1	-1.878554	1.473747	5.903276
1	-1.934387	-1.509514	5.213465
1	-2.637734	-0.754195	6.656585
1	-4.115687	-1.242805	4.348688
1	-4.466350	0.159493	5.388169
1	-5.142446	0.974411	3.088279
1	-2.704169	2.123814	1.589549
6	-4.757968	2.731706	1.019956
6	-4.607469	4.245777	1.297373
1	-5.778787	2.422206	1.274288
1	-4.629681	2.584356	-0.063050
1	-5.293500	4.792657	0.641028
1	-4.891775	4.459194	2.331791
6	-3.195821	4.695096	1.053846
6	-2.648953	4.856627	-0.155446
1	-2.542465	4.832000	1.914859
1	-3.231762	4.715079	-1.062243
6	-1.207559	5.193012	-0.271002
8	-0.587162	5.677853	0.664454
6	-0.497061	4.881291	-1.551989
6	-0.985845	3.941908	-2.462245
6	0.736653	5.501195	-1.791648
6	-0.246854	3.619400	-3.599095
1	-1.919410	3.423148	-2.270572
6	1.460238	5.197806	-2.937388
1	1.102750	6.225098	-1.070027
6	0.969849	4.249941	-3.840233
1	-0.617874	2.863757	-4.283213
1	2.406810	5.693927	-3.130100
1	1.541356	4.001873	-4.729330
6	-3.493063	0.137081	0.410629
1	-2.857652	-0.292023	1.182711
1	-3.308162	0.708543	-1.704381
7	-1.520837	0.933211	-0.670831
6	-2.867511	0.632902	-0.719707
7	-0.590115	-1.918296	-0.016249
6	-1.606660	-2.441539	-0.819531
6	-1.771818	-2.080492	-2.161848
6	-2.873965	-2.548711	-2.862150
6	-3.832710	-3.366178	-2.267277
6	-3.662395	-3.702085	-0.931342
6	-2.566193	-3.247296	-0.203833
6	-3.085243	-2.047495	-4.260910
9	-1.947412	-2.013699	-4.964732
6	-4.703119	-4.507110	-0.211227
9	-4.165005	-5.522039	0.480243
6	0.695847	-1.620584	-0.353887
16	1.446657	-2.047131	-1.810586
7	1.318093	-0.949135	0.634008
6	2.696560	-0.514404	0.621714
6	2.732444	0.940375	1.124118
6	4.113522	1.614554	0.992899
6	4.002754	2.831687	0.063405
6	3.031011	3.843803	0.689937
6	1.688369	3.145328	0.981382
7	1.721237	1.775046	0.381331

6	2.002724	1.870403	-1.088112
6	3.437455	2.409915	-1.306542
6	4.283484	1.434225	-2.089942
6	5.584052	1.204114	-1.927170
6	3.571078	-1.366830	1.535593
6	4.823777	-1.913453	1.114351
6	5.571594	-2.642981	2.086452
7	5.142771	-2.850125	3.363758
6	3.979921	-2.349661	3.700179
6	3.160044	-1.597163	2.824955
6	6.826811	-3.184903	1.719185
6	7.333300	-3.023188	0.455168
6	6.583618	-2.305934	-0.511760
6	5.355105	-1.770546	-0.188273
9	-3.962587	-2.799274	-4.941876
9	-3.573338	-0.790279	-4.256932
9	-5.614733	-5.024976	-1.045278
9	-5.371132	-3.750501	0.681185
1	2.371447	0.947002	2.155467
1	4.468858	1.931536	1.977233
1	4.837752	0.897206	0.599991
1	0.841677	3.671240	0.539177
1	1.493877	3.010267	2.047338
1	2.873201	4.681386	0.003588
1	3.448953	4.248009	1.615235
1	4.984695	3.294658	-0.064425
1	3.342814	3.317905	-1.917367
1	1.235215	2.531853	-1.496288
1	1.838866	0.879109	-1.519777
1	3.751975	0.894695	-2.875144
1	6.107582	0.487482	-2.552229
1	6.175624	1.703252	-1.163377
1	3.056324	-0.569804	-0.407428
1	2.209012	-1.205422	3.181072
1	4.814134	-1.251944	-0.970450
1	3.646986	-2.528517	4.720946
1	7.374129	-3.734419	2.478087
1	8.297021	-3.449385	0.203254
1	0.793785	-0.682090	1.487487
1	-0.861766	-1.719879	0.965510
1	-1.062719	-1.404744	-2.625624
1	-2.453797	-3.507556	0.845208
1	-4.689604	-3.720169	-2.827698
8	7.010896	-2.101640	-1.784844
6	8.228647	-2.702060	-2.182465
1	8.358130	-2.451337	-3.235614
1	9.079328	-2.307625	-1.614011
1	8.192537	-3.792304	-2.076112
1	0.768165	1.355835	0.480852
6	-0.920964	-0.078690	2.985794
8	-1.432760	-1.130801	2.534347
8	0.281011	0.281302	2.890089
6	-4.884104	-0.410058	0.263224
1	-5.284786	-0.754197	1.218092
1	-5.564896	0.331929	-0.165807
1	-4.862406	-1.265937	-0.420442

1-Michael-nitrostyrene-Ph-to-Me-si-si_conf-3

Number of imaginary frequencies : 1

The smallest frequency is : -285.1476 cm(-1)

Electronic energy : =-3713.612499

Zero-point correction= 0.999539

Thermal correction to Energy= 1.062135

Thermal correction to Enthalpy= 1.063080

Thermal correction to Gibbs Free Energy= 0.898179

Sum of electronic and zero-point Energies=	-3712.612960
Sum of electronic and thermal Energies=	-3712.550364
Sum of electronic and thermal Enthalpies=	-3712.549419
Sum of electronic and thermal Free Energies=	-3712.714320

Cartesian Coordinates			
6	2.002561	-0.040695	-5.293970
6	2.974357	-1.221771	-5.183147
6	4.093911	-0.692098	-4.275106
7	3.470968	0.429169	-3.556620
6	2.050347	0.546257	-3.874405
6	4.176348	1.286241	-2.817867
6	3.695734	2.246747	-1.950647
8	0.495374	2.069714	1.243730
8	0.823691	1.335352	-0.769138
1	1.735269	1.591329	-3.823991
1	0.989452	-0.334501	-5.573216
1	2.369321	0.698913	-6.012752
1	2.476209	-2.062986	-4.695906
1	3.356107	-1.555683	-6.149432
1	4.445586	-1.448457	-3.567367
1	4.950334	-0.320742	-4.850062
1	5.256043	1.133753	-2.878444
1	2.625123	2.445690	-1.942297
6	4.621953	3.356004	-1.506849
6	4.190049	4.117330	-0.242398
1	4.702359	4.098431	-2.314080
1	5.635144	2.959460	-1.362918
1	4.290529	3.500751	0.655901
1	4.871851	4.969671	-0.121572
6	2.789853	4.634457	-0.355320
6	1.875297	4.633821	0.620392
1	2.485373	5.037008	-1.322931
1	2.114787	4.244210	1.603873
6	0.499987	5.115148	0.337478
8	0.191463	5.508552	-0.779807
6	-0.542022	5.099526	1.419002
6	-0.357399	4.494854	2.666368
6	-1.778373	5.685631	1.119425
6	-1.399549	4.465603	3.589718
1	0.573983	3.997799	2.907934
6	-2.815201	5.662796	2.043838
1	-1.902609	6.156313	0.149018
6	-2.627357	5.045901	3.281540
1	-1.253150	3.980273	4.549105
1	-3.768115	6.125345	1.804107
1	-3.437179	5.018882	4.004372
6	3.413911	0.782448	-0.240871
1	2.940633	0.141041	-0.981655
1	2.891056	1.805999	1.627114
7	1.254441	1.597767	0.381587
6	2.582703	1.400102	0.674162
7	0.859634	-1.576951	0.291983
6	1.921037	-2.030783	1.070312
6	1.983503	-2.007727	2.467437
6	3.143104	-2.444458	3.103863
6	4.255612	-2.890229	2.401562
6	4.185682	-2.886580	1.011168
6	3.043638	-2.468877	0.347534
6	3.162338	-2.438312	4.606441
9	2.405907	-3.420663	5.118090
6	5.357733	-3.348534	0.195696
9	5.214828	-4.613673	-0.226629
6	-0.461784	-1.402892	0.561316
16	-1.234840	-1.710563	2.035226
7	-1.110735	-0.934247	-0.527296
6	-2.536550	-0.735144	-0.651544
6	-2.756250	0.624984	-1.338089
6	-4.236313	1.051390	-1.424884

6	-4.444166	2.350737	-0.634040
6	-3.601487	3.461020	-1.280185
6	-2.136368	2.991579	-1.380437
7	-1.990109	1.709187	-0.619703
6	-2.442706	1.905706	0.796402
6	-3.966771	2.180220	0.820477
6	-4.706091	1.147525	1.637049
6	-5.919750	0.661287	1.389883
6	-3.188352	-1.824962	-1.500769
6	-4.355366	-2.539650	-1.082333
6	-4.900744	-3.485874	-2.001237
7	-4.356320	-3.746670	-3.223797
6	-3.272865	-3.089321	-3.554033
6	-2.654272	-2.117068	-2.731623
6	-6.068340	-4.198541	-1.637635
6	-6.680909	-3.998190	-0.427064
6	-6.129604	-3.067031	0.489587
6	-4.989617	-2.360912	0.168427
9	4.402481	-2.600508	5.093851
9	2.685752	-1.286509	5.105200
9	6.504459	-3.292365	0.888683
9	5.523148	-2.594259	-0.908000
1	-2.284762	0.575726	-2.324385
1	-4.519366	1.204922	-2.470011
1	-4.872121	0.255567	-1.029478
1	-1.432135	3.705252	-0.949007
1	-1.826025	2.779990	-2.405741
1	-3.662177	4.371101	-0.675385
1	-3.984352	3.697559	-2.276129
1	-5.500184	2.633035	-0.650299
1	-4.101600	3.146536	1.324780
1	-1.860309	2.744006	1.180490
1	-2.153856	1.015535	1.361458
1	-4.175028	0.801416	2.525180
1	-6.371262	-0.074429	2.048402
1	-6.503428	0.958472	0.521964
1	-2.965568	-0.727583	0.351643
1	-1.756948	-1.610404	-3.082515
1	-4.596923	-1.679328	0.912655
1	-2.842627	-3.312415	-4.528812
1	-6.462194	-4.911304	-2.354717
1	-7.573750	-4.558677	-0.177673
1	-0.582738	-0.762174	-1.398169
1	1.118608	-1.458631	-0.712119
1	1.141894	-1.647045	3.043879
1	3.011418	-2.449912	-0.739243
1	5.151755	-3.212154	2.918201
8	-6.668114	-2.814523	1.710952
6	-7.791363	-3.574565	2.113951
1	-8.027432	-3.248392	3.127110
1	-8.657559	-3.389285	1.467732
1	-7.567274	-4.647299	2.126838
1	-0.973175	1.465030	-0.611928
6	1.146570	-0.302440	-2.956246
8	1.709656	-1.185332	-2.256600
8	-0.082790	-0.076899	-3.038182
6	4.826758	0.479823	0.170750
1	5.373103	-0.036988	-0.619201
1	5.369129	1.391594	0.440637
1	4.817131	-0.166996	1.055467

1-Michael-nitrostyrene-Ph-to-Me-*si-si*_conf-4

Number of imaginary frequencies : 1
The smallest frequency is : -319.0691 cm(-1)

Electronic energy : =-3713.6134878

Zero-point correction=	0.999590
Thermal correction to Energy=	1.062193
Thermal correction to Enthalpy=	1.063138
Thermal correction to Gibbs Free Energy=	0.899596
Sum of electronic and zero-point Energies=	-3712.613898
Sum of electronic and thermal Energies=	-3712.551294
Sum of electronic and thermal Enthalpies=	-3712.550350
Sum of electronic and thermal Free Energies=	-3712.713892

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

6	-1.529317	0.363369	5.126272
6	-2.424460	-0.831365	5.471956
6	-3.724986	-0.533223	4.717056
7	-3.295331	0.332697	3.609049
6	-1.860777	0.600488	3.643402
6	-4.149646	0.912974	2.770889
6	-3.829546	1.555027	1.586256
8	-1.541192	0.845077	-2.152756
8	-1.249547	0.577100	-0.009843
1	-1.666843	1.627836	3.320929
1	-0.465475	0.171142	5.274177
1	-1.813879	1.242787	5.712686
1	-1.979127	-1.749871	5.082790
1	-2.591275	-0.949265	6.543876
1	-4.199811	-1.438400	4.329672
1	-4.446735	0.006621	5.341716
1	-5.201277	0.772755	3.028392
1	-2.776436	1.741852	1.380569
6	-4.820083	2.482430	0.939536
6	-4.527418	3.971453	1.235763
1	-5.833973	2.251901	1.286616
1	-4.807410	2.334506	-0.150681
1	-5.364489	4.574533	0.864520
1	-4.458133	4.122818	2.317927
6	-3.268995	4.430281	0.566834
6	-2.132629	4.723086	1.211265
1	-3.307026	4.514661	-0.518987
1	-2.090296	4.682808	2.298638
6	-0.893884	5.246202	0.584606
8	-0.062842	5.811634	1.279777
6	-0.639315	5.084545	-0.885154
6	-0.991548	3.925564	-1.583359
6	0.084608	6.089596	-1.537044
6	-0.631578	3.775507	-2.921060
1	-1.506904	3.115079	-1.075484
6	0.422167	5.950269	-2.877364
1	0.376665	6.970855	-0.974495
6	0.065562	4.791924	-3.570073
1	-0.894458	2.857424	-3.436408
1	0.969840	6.739339	-3.382772
1	0.338410	4.679537	-4.614852
6	-3.799843	-0.196366	0.336028
1	-3.076916	-0.650975	1.010747
1	-3.908183	0.393937	-1.784129
7	-1.988514	0.565213	-1.027283
6	-3.321322	0.254493	-0.887673
7	-0.295649	-2.375171	0.076416
6	-1.364607	-2.674807	-0.776701
6	-1.445589	-2.236887	-2.103720
6	-2.616578	-2.446026	-2.816180
6	-3.713164	-3.100113	-2.259515
6	-3.616669	-3.528412	-0.942050
6	-2.461857	-3.316954	-0.197546
6	-2.770788	-1.832636	-4.177617
9	-1.601312	-1.497929	-4.729475
6	-4.770468	-4.237430	-0.295467
9	-4.635946	-5.571369	-0.329989
6	0.994442	-2.086494	-0.241770
16	1.759036	-2.501144	-1.692360

7	1.620406	-1.438663	0.768243
6	2.891411	-0.753053	0.651428
6	2.683486	0.712492	1.097856
6	3.864373	1.647890	0.765230
6	3.382174	2.775918	-0.163252
6	2.305427	3.593468	0.567937
6	1.179884	2.642426	1.016170
7	1.445762	1.279635	0.458681
6	1.532174	1.331961	-1.033644
6	2.753007	2.191974	-1.443342
6	3.689807	1.408592	-2.331974
6	5.020154	1.432792	-2.303631
6	3.971905	-1.379223	1.522261
6	5.298251	-1.625602	1.048275
6	6.232561	-2.156457	1.986949
7	5.915988	-2.446842	3.280833
6	4.684386	-2.225478	3.667607
6	3.680306	-1.689554	2.826679
6	7.562109	-2.399008	1.565633
6	7.964258	-2.136163	0.281369
6	7.030791	-1.617659	-0.652870
6	5.726693	-1.375330	-0.275878
9	-3.397801	-2.663170	-5.028619
9	-3.520012	-0.714759	-4.122784
9	-5.935709	-3.945832	-0.898915
9	-4.898368	-3.895289	0.997859
1	2.452098	0.713869	2.166196
1	4.270499	2.075745	1.685740
1	4.665351	1.076972	0.291017
1	0.195273	2.922972	0.638732
1	1.112122	2.519991	2.098638
1	1.903027	4.369559	-0.090204
1	2.734312	4.095678	1.438403
1	4.222412	3.424311	-0.425099
1	2.367145	3.034375	-2.034827
1	0.578788	1.730881	-1.379932
1	1.601526	0.303538	-1.397007
1	3.194865	0.779066	-3.072598
1	5.604544	0.834720	-2.995535
1	5.580207	2.036122	-1.593384
1	3.188716	-0.782700	-0.398753
1	2.681192	-1.528044	3.224371
1	5.049528	-0.997151	-1.033288
1	4.443495	-2.468509	4.700736
1	8.253233	-2.802698	2.298271
1	8.988731	-2.333410	-0.010365
1	1.038105	-1.128277	1.565623
1	-0.621278	-2.109855	1.024892
1	-0.625262	-1.691787	-2.550008
1	-2.413742	-3.620130	0.844034
1	-4.623197	-3.251226	-2.830300
8	7.346304	-1.333145	-1.941712
6	8.655117	-1.631154	-2.389488
1	8.681097	-1.356940	-3.444249
1	9.410212	-1.047739	-1.849444
1	8.880142	-2.699427	-2.291383
1	0.636639	0.696412	0.721605
6	-1.016654	-0.358961	2.781637
8	-1.522784	-1.439719	2.415219
8	0.173085	0.026346	2.595349
6	-5.219175	-0.696090	0.385679
1	-5.472754	-1.090667	1.371068
1	-5.929054	0.095301	0.124551
1	-5.354252	-1.497462	-0.346914

Number of imaginary frequencies : 1
The smallest frequency is : -193.6946 cm(-1)

Electronic energy : =-3713.6129333
Zero-point correction= 0.999974
Thermal correction to Energy= 1.062452
Thermal correction to Enthalpy= 1.063396
Thermal correction to Gibbs Free Energy= 0.900799
Sum of electronic and zero-point Energies= -3712.612960
Sum of electronic and thermal Energies= -3712.550481
Sum of electronic and thermal Enthalpies= -3712.549537
Sum of electronic and thermal Free Energies= -3712.712134

.....
Cartesian Coordinates

.....
8 0.162574 1.185537 3.902948
8 0.499928 -0.076956 2.170148
6 2.936858 -0.861419 3.181872
1 2.523254 -1.483764 2.394257
1 2.334278 0.559078 4.721680
7 0.876068 0.382937 3.266691
6 2.100413 0.029342 3.809643
7 0.216261 -0.993871 -0.762745
6 1.191619 -2.000987 -0.819316
6 1.409718 -2.880532 0.241832
6 2.444009 -3.807806 0.157414
6 3.265080 -3.881664 -0.961390
6 3.041365 -2.987721 -2.004591
6 2.021215 -2.046207 -1.943014
6 2.759185 -4.631353 1.370679
9 3.523156 -5.692599 1.082802
6 3.940591 -3.056188 -3.205434
9 3.832768 -4.229750 -3.843807
6 -1.063990 -1.112259 -0.327597
16 -1.825565 -2.584320 0.014615
7 -1.667854 0.089394 -0.205310
6 -3.083633 0.296575 0.008588
6 -3.309747 1.393325 1.066756
6 -4.761363 1.423349 1.589834
6 -4.772006 1.073377 3.085140
6 -4.013380 2.175867 3.837959
6 -2.618265 2.346155 3.204890
7 -2.384145 1.220030 2.243841
6 -2.561484 -0.097624 2.928040
6 -4.047705 -0.264304 3.338549
6 -4.673726 -1.474883 2.685664
6 -5.930921 -1.582653 2.262500
6 -3.772984 0.743958 -1.277348
6 -4.939091 0.104201 -1.799040
6 -5.505356 0.660162 -2.984963
7 -4.980137 1.736991 -3.635012
6 -3.899349 2.280946 -3.132705
6 -3.264026 1.825679 -1.953081
6 -6.674932 0.071264 -3.522893
6 -7.267539 -1.013378 -2.928372
6 -6.697004 -1.568379 -1.753751
6 -5.554054 -1.023103 -1.208227
9 3.438945 -3.897563 2.280415
9 1.657079 -5.073769 1.986302
9 5.235252 -2.931778 -2.852859
9 3.678676 -2.087153 -4.090431
1 -3.007640 2.350398 0.640822
1 -5.193045 2.417485 1.444011
1 -5.372271 0.718435 1.020918
1 -1.809142 2.302247 3.931491
1 -2.515330 3.262824 2.621321
1 -3.920323 1.911864 4.895551
1 -4.563069 3.118744 3.781368
1 -5.800755 1.014175 3.449650
1 -4.063007 -0.442895 4.421797

1	-1.883519	-0.075971	3.782151
1	-2.221222	-0.875015	2.238863
1	-4.012300	-2.335977	2.586713
1	-6.295385	-2.507514	1.826469
1	-6.643981	-0.764319	2.327690
1	-3.496196	-0.650007	0.361508
1	-2.376774	2.341823	-1.588904
1	-5.142688	-1.497337	-0.324120
1	-3.486957	3.135953	-3.665131
1	-7.086499	0.510205	-4.425901
1	-8.163042	-1.440321	-3.363809
1	-1.125861	0.925582	-0.431005
1	0.532389	-0.045431	-1.001896
1	0.787681	-2.816319	1.127770
1	1.872520	-1.333203	-2.748939
1	4.070739	-4.606637	-1.012587
8	-7.219545	-2.639266	-1.104010
6	-8.359537	-3.265838	-1.660109
1	-8.590303	-4.106287	-1.005163
1	-9.220502	-2.587657	-1.687464
1	-8.159484	-3.643667	-2.669316
1	-1.412100	1.300495	1.897168
6	1.861062	4.265203	1.294144
6	2.980992	4.351658	2.335992
6	3.659604	2.973539	2.268335
7	2.668319	2.103698	1.622451
6	1.397545	2.814951	1.448594
6	3.003187	0.913983	1.114632
6	4.136188	0.209360	1.459354
6	0.461213	2.355347	0.328215
8	0.910916	1.734209	-0.662272
8	-0.743135	2.674809	0.516607
1	0.820161	2.724450	2.380518
1	1.049278	4.973866	1.465520
1	2.252707	4.412031	0.280850
1	2.549928	4.508701	3.329183
1	3.688638	5.159892	2.141364
1	3.937612	2.591673	3.257122
1	4.565935	2.987191	1.649563
1	2.271250	0.467282	0.452427
1	4.887316	0.686007	2.087778
6	4.595218	-0.934071	0.603061
6	5.485438	-0.474081	-0.590207
1	5.163661	-1.663801	1.190821
1	3.722976	-1.460011	0.201816
1	5.973337	-1.349177	-1.028649
1	6.263374	0.198330	-0.212309
6	4.636849	0.210279	-1.613053
6	4.299285	1.502884	-1.581733
1	4.167279	-0.403485	-2.379740
1	4.727315	2.170475	-0.838514
6	3.232861	2.033529	-2.473768
8	2.605129	1.312703	-3.230727
6	2.915504	3.494258	-2.366904
6	1.601140	3.906248	-2.605122
6	3.887099	4.439958	-2.030432
6	1.259725	5.247567	-2.487030
1	0.859768	3.149465	-2.836399
6	3.548140	5.788262	-1.935395
1	4.915045	4.130462	-1.863611
6	2.233126	6.190344	-2.154139
1	0.233621	5.561581	-2.651137
1	4.309401	6.522228	-1.689836
1	1.965489	7.239038	-2.066438
6	4.124066	-1.388245	3.934473
1	4.921439	-1.723165	3.270774
1	4.525342	-0.637236	4.619814
1	3.810065	-2.255954	4.526255

1-Michael-nitrostyrene-Ph-to-Me-si-re_conf-1

Number of imaginary frequencies : 1

The smallest frequency is : -294.1953 cm(-1)

Electronic energy : =-3713.6099239
Zero-point correction= 0.998799
Thermal correction to Energy= 1.061815
Thermal correction to Enthalpy= 1.062759
Thermal correction to Gibbs Free Energy= 0.895361
Sum of electronic and zero-point Energies= -3712.611125
Sum of electronic and thermal Energies= -3712.548109
Sum of electronic and thermal Enthalpies= -3712.547165
Sum of electronic and thermal Free Energies= -3712.714563

Cartesian Coordinates

6	2.511470	-2.321172	3.317864
6	3.422928	-1.191332	3.820868
6	4.423902	-0.961852	2.671847
7	3.858986	-1.694501	1.527395
6	2.473930	-2.092953	1.795568
6	4.630348	-2.323967	0.639904
6	4.191536	-2.906372	-0.532920
8	1.162109	0.390574	-1.202314
8	1.663523	-1.535156	-2.065752
1	2.246460	-2.994698	1.226664
1	1.514334	-2.296297	3.764711
1	2.959201	-3.300312	3.519332
1	2.837598	-0.286032	3.982459
1	3.929202	-1.453466	4.751717
1	4.520565	0.098815	2.426382
1	5.418460	-1.364560	2.890195
1	5.703037	-2.257699	0.833196
1	3.119035	-2.975504	-0.705529
6	5.033984	-3.938715	-1.230939
6	4.671528	-5.375384	-0.777994
1	6.096550	-3.769883	-1.020539
1	4.905189	-3.865344	-2.319320
1	5.350304	-6.082691	-1.268724
1	4.826166	-5.455356	0.303479
6	3.258622	-5.725652	-1.123872
6	2.243502	-5.780677	-0.254631
1	3.030859	-5.900675	-2.175804
1	2.411420	-5.593764	0.803168
6	0.866464	-6.069189	-0.741267
8	0.683240	-6.624238	-1.811938
6	-0.309603	-5.608720	0.071338
6	-0.181446	-4.741289	1.158797
6	-1.589326	-5.975804	-0.364668
6	-1.313354	-4.228876	1.788367
1	0.795602	-4.427725	1.505687
6	-2.718676	-5.476694	0.271551
1	-1.672166	-6.641391	-1.217799
6	-2.582172	-4.592055	1.344822
1	-1.198211	-3.528166	2.608565
1	-3.707463	-5.767500	-0.070429
1	-3.463868	-4.185849	1.832900
6	4.301605	-1.110847	-1.711853
1	4.007521	-1.769485	-2.524995
1	3.535352	0.679481	-0.701558
7	2.009545	-0.463114	-1.523180
6	3.340752	-0.219688	-1.264790
7	0.348847	2.342432	0.709286
6	1.276609	3.338236	0.407580
6	0.989147	4.635333	-0.034280
6	2.038470	5.516844	-0.277953
6	3.370829	5.164192	-0.091323

6	3.636964	3.879692	0.367156
6	2.614944	2.978296	0.619846
6	1.720717	6.885271	-0.810284
9	2.627975	7.795232	-0.419072
6	5.041884	3.404692	0.586225
9	5.949377	4.367187	0.385588
6	-0.900820	2.105673	0.231868
16	-1.878734	3.203113	-0.605343
7	-1.287328	0.836034	0.496711
6	-2.573577	0.272271	0.160397
6	-2.386757	-1.167134	-0.359139
6	-3.658722	-1.723356	-1.036495
6	-3.389182	-1.956379	-2.532053
6	-2.337246	-3.065061	-2.658652
6	-1.133046	-2.701580	-1.773351
7	-1.255839	-1.266664	-1.347228
6	-1.446687	-0.376369	-2.534165
6	-2.812926	-0.689703	-3.197010
6	-3.724621	0.515018	-3.201973
6	-5.048156	0.499189	-3.064412
6	-3.503056	0.208455	1.370463
6	-4.840694	0.709909	1.351020
6	-5.626767	0.507185	2.524988
7	-5.156156	-0.105689	3.647407
6	-3.913041	-0.520048	3.635457
6	-3.051508	-0.390642	2.520532
6	-6.967096	0.964184	2.537307
6	-7.516485	1.595988	1.451444
6	-6.727018	1.809825	0.292025
6	-5.417817	1.380445	0.248565
9	1.711660	6.906677	-2.154048
9	0.518415	7.317253	-0.406630
9	5.356168	2.385662	-0.242280
9	5.222914	2.934358	1.832979
1	-2.062362	-1.801664	0.470575
1	-3.942723	-2.671782	-0.569233
1	-4.486700	-1.024524	-0.893512
1	-0.174869	-2.795218	-2.280342
1	-1.101654	-3.282139	-0.850103
1	-2.028433	-3.173497	-3.702669
1	-2.747764	-4.024624	-2.333783
1	-4.312260	-2.253708	-3.036298
1	-2.609714	-0.938574	-4.246781
1	-0.591287	-0.574612	-3.182173
1	-1.370356	0.656683	-2.184457
1	-3.225292	1.471682	-3.358706
1	-5.625605	1.417488	-3.102658
1	-5.608095	-0.418402	-2.901292
1	-3.012937	0.892528	-0.623122
1	-2.031965	-0.765684	2.582050
1	-4.846107	1.598919	-0.645236
1	-3.546690	-0.996161	4.543272
1	-7.543292	0.796487	3.441443
1	-8.544484	1.936075	1.490793
1	-0.603812	0.173516	0.890346
1	0.808433	1.506908	1.115624
1	-0.034761	4.949412	-0.180571
1	2.834226	1.978761	0.988668
1	4.169541	5.870157	-0.284878
8	-7.190686	2.433383	-0.820714
6	-8.498286	2.972756	-0.787901
1	-8.647670	3.456679	-1.753317
1	-9.255679	2.190571	-0.659531
1	-8.605438	3.718996	0.007594
1	-0.370429	-0.990401	-0.884227
6	1.435497	-1.011344	1.468732
8	1.759591	0.170660	1.721065
8	0.315788	-1.421767	1.059871
6	5.743317	-0.687778	-1.661075
1	5.963186	-0.133041	-0.745536

1	6.421382	-1.541197	-1.735570
1	5.949552	-0.022729	-2.507112

1-Michael-nitrostyrene-Ph-to-Me-si-re_conf-2

Number of imaginary frequencies : 1

The smallest frequency is : -291.0027 cm(-1)

Electronic energy : =-3713.6092504
Zero-point correction= 1.000223
Thermal correction to Energy= 1.062959
Thermal correction to Enthalpy= 1.063903
Thermal correction to Gibbs Free Energy= 0.898050
Sum of electronic and zero-point Energies= -3712.609027
Sum of electronic and thermal Energies= -3712.546291
Sum of electronic and thermal Enthalpies= -3712.545347
Sum of electronic and thermal Free Energies= -3712.711201

Cartesian Coordinates

6	-2.562219	1.947399	4.102061
6	-3.813791	1.061266	4.175458
6	-4.601737	1.405423	2.896854
7	-3.649823	2.151361	2.057206
6	-2.289344	2.028076	2.588786
6	-4.053330	3.125303	1.238163
6	-3.282931	3.778269	0.298484
8	-0.873388	0.103102	-0.707875
8	-0.895650	2.232281	-1.109628
1	-1.699981	2.901669	2.303159
1	-1.710191	1.537459	4.648862
1	-2.772606	2.951914	4.482693
1	-3.526672	0.009330	4.156541
1	-4.401548	1.247340	5.076185
1	-4.933870	0.506798	2.371384
1	-5.470763	2.041449	3.095399
1	-5.126523	3.323770	1.269349
1	-2.210403	3.592956	0.284683
6	-3.744182	5.065845	-0.331538
6	-2.896092	6.276609	0.119492
1	-4.793835	5.256669	-0.081652
1	-3.689812	5.004183	-1.429429
1	-3.347215	7.191761	-0.281742
1	-2.909878	6.346330	1.211980
6	-1.484004	6.172164	-0.372560
6	-0.426529	5.965152	0.420487
1	-1.339806	6.266680	-1.449010
1	-0.555195	5.920159	1.500955
6	0.996021	5.921606	-0.003897
8	1.861085	6.194749	0.815174
6	1.396620	5.528702	-1.396597
6	0.639044	4.650806	-2.178737
6	2.634524	5.981634	-1.870140
6	1.114139	4.235263	-3.421326
1	-0.295602	4.250789	-1.801487
6	3.094726	5.584292	-3.119426
1	3.222816	6.643462	-1.242359
6	2.335702	4.706813	-3.895943
1	0.528478	3.537173	-4.011626
1	4.048853	5.948464	-3.486552
1	2.702044	4.385513	-4.866136
6	-3.572661	2.275542	-1.261594
1	-3.029199	3.000550	-1.861426
1	-3.318401	0.211128	-0.553740
7	-1.504453	1.154649	-0.913085
6	-2.882347	1.133936	-0.904636
7	-1.043545	-2.456608	0.601615

6	-2.092835	-3.120347	-0.034497
6	-2.000088	-4.293582	-0.789070
6	-3.151030	-4.820396	-1.375239
6	-4.398539	-4.230509	-1.233780
6	-4.479171	-3.078785	-0.454353
6	-3.358234	-2.534153	0.145359
6	-2.997332	-6.046747	-2.229155
9	-2.410831	-5.762740	-3.403389
6	-5.809251	-2.427410	-0.219206
9	-6.448530	-2.943821	0.842459
6	0.293029	-2.444481	0.340430
16	1.125502	-3.499163	-0.682160
7	0.921332	-1.448320	1.008490
6	2.324895	-1.143581	0.839192
6	2.548165	0.360404	1.076827
6	4.002451	0.799561	0.809331
6	4.002818	2.149546	0.077777
6	3.090916	3.115226	0.843605
6	1.641109	2.614245	0.727490
7	1.652444	1.204436	0.203436
6	2.095108	1.196498	-1.224458
6	3.428434	1.977092	-1.339759
6	4.322158	1.294860	-2.342201
6	5.570780	0.878509	-2.148666
6	3.215246	-1.926069	1.799621
6	4.459799	-2.509182	1.399069
6	5.220605	-3.165197	2.411915
7	4.817456	-3.265556	3.710723
6	3.664569	-2.732955	4.029541
6	2.831011	-2.053165	3.109671
6	6.463862	-3.748128	2.066740
6	6.948885	-3.693350	0.785607
6	6.188259	-3.047185	-0.222416
6	4.970288	-2.476195	0.080178
9	-2.234882	-6.976179	-1.633977
9	-4.178352	-6.618771	-2.510766
9	-6.629449	-2.566415	-1.270570
9	-5.684702	-1.105105	0.017639
1	2.234390	0.601851	2.097862
1	4.540173	0.870655	1.758450
1	4.512176	0.048243	0.202580
1	1.049563	3.181079	0.006757
1	1.104195	2.577467	1.675106
1	3.162158	4.128395	0.438930
1	3.396312	3.160791	1.893470
1	5.018028	2.550785	0.024465
1	3.193746	2.979712	-1.727582
1	1.282816	1.647750	-1.795950
1	2.195067	0.152001	-1.529911
1	3.859008	1.127170	-3.315603
1	6.120906	0.382696	-2.942016
1	6.094419	1.010957	-1.205693
1	2.599691	-1.404443	-0.184848
1	1.881259	-1.645715	3.445156
1	4.423703	-2.013545	-0.734423
1	3.350896	-2.826687	5.067566
1	7.019194	-4.241956	2.857383
1	7.903789	-4.148696	0.552027
1	0.360363	-0.767600	1.547466
1	-1.384775	-1.645420	1.145556
1	-1.045591	-4.782708	-0.924604
1	-3.438625	-1.639576	0.755753
1	-5.276330	-4.651835	-1.709183
8	6.592988	-2.947308	-1.513443
6	7.803341	-3.579603	-1.882421
1	7.916565	-3.410440	-2.953533
1	8.663047	-3.144095	-1.359340
1	7.768367	-4.658402	-1.692038
1	0.682975	0.839150	0.237029
6	-1.561312	0.742251	2.157705

8	-2.260518	-0.265930	1.922914
8	-0.301806	0.801875	2.165082
6	-5.057712	2.193810	-1.466589
1	-5.524942	1.527792	-0.736796
1	-5.530095	3.177719	-1.410846
1	-5.257012	1.784870	-2.463544

1-Michael-nitrostyrene-Ph-to-Me-*si-re*_conf-3

Number of imaginary frequencies : 1
The smallest frequency is : -335.7791 cm(-1)

Electronic energy : =-3713.6059432
Zero-point correction= 1.000203
Thermal correction to Energy= 1.063021
Thermal correction to Enthalpy= 1.063965
Thermal correction to Gibbs Free Energy= 0.896617
Sum of electronic and zero-point Energies= -3712.605740
Sum of electronic and thermal Energies= -3712.542922
Sum of electronic and thermal Enthalpies= -3712.541978
Sum of electronic and thermal Free Energies= -3712.709327

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Cartesian Coordinates

6	2.276216	-0.594115	4.745532
6	2.922192	0.794717	4.865471
6	3.983623	0.826255	3.747839
7	3.703759	-0.365062	2.926274
6	2.367955	-0.885244	3.235846
6	4.688585	-1.094246	2.404148
6	4.566807	-2.178879	1.553880
8	0.919949	-0.175971	-0.436133
8	1.853761	-2.134182	-0.331777
1	2.312900	-1.946770	2.993809
1	1.245289	-0.622806	5.104608
1	2.858393	-1.343885	5.290552
1	2.177277	1.570447	4.685789
1	3.366041	0.959640	5.848961
1	3.897833	1.724613	3.133341
1	5.005314	0.754318	4.132800
1	5.687833	-0.702801	2.605075
1	3.580036	-2.611501	1.393691
6	5.753075	-3.106309	1.350259
6	5.324300	-4.515038	0.894634
1	6.330907	-3.198807	2.276079
1	6.447676	-2.707864	0.597349
1	6.209546	-5.159865	0.866065
1	4.617104	-4.941601	1.614083
6	4.704128	-4.418443	-0.460134
6	3.410053	-4.583547	-0.738726
1	5.350868	-4.074988	-1.269547
1	2.707406	-4.917230	0.020814
6	2.889389	-4.197138	-2.078339
8	3.538335	-3.484834	-2.825546
6	1.542424	-4.698253	-2.500235
6	0.990104	-5.864228	-1.964071
6	0.863732	-4.011593	-3.512137
6	-0.221328	-6.351763	-2.451238
1	1.521403	-6.414339	-1.192969
6	-0.358011	-4.483400	-3.978256
1	1.314951	-3.113563	-3.922217
6	-0.897760	-5.659572	-3.453256
1	-0.635203	-7.271559	-2.049837
1	-0.884979	-3.945759	-4.760587
1	-1.844075	-6.036681	-3.829374
6	4.338179	-1.008104	-0.235974
1	4.284615	-1.964990	-0.751904

1	3.108305	0.792506	-0.010422
7	1.942313	-0.884919	-0.324935
6	3.161295	-0.273124	-0.173066
7	-0.133877	2.394467	0.313362
6	0.690553	3.276870	-0.379618
6	0.322304	4.106753	-1.442606
6	1.285484	4.927840	-2.027776
6	2.602887	4.960452	-1.593185
6	2.948342	4.141534	-0.520313
6	2.015703	3.321072	0.087386
6	0.881451	5.757035	-3.213840
9	1.693048	6.812123	-3.388132
6	4.348199	4.175695	0.016412
9	4.539132	5.189552	0.875280
6	-1.320314	1.815069	-0.007774
16	-2.365006	2.276561	-1.255036
7	-1.582339	0.771267	0.811236
6	-2.784667	-0.026414	0.784152
6	-2.421351	-1.503169	1.030343
6	-3.600939	-2.449928	0.721518
6	-3.206593	-3.401297	-0.416871
6	-2.036051	-4.264262	0.071050
6	-0.884527	-3.343798	0.519221
7	-1.240703	-1.925038	0.193804
6	-1.489925	-1.783442	-1.272076
6	-2.741796	-2.611773	-1.658338
6	-3.794459	-1.745364	-2.308050
6	-5.112533	-1.844030	-2.151698
6	-3.776072	0.403372	1.862671
6	-5.157559	0.655188	1.594966
6	-5.978989	1.002113	2.709504
7	-5.509602	1.114839	3.984111
6	-4.233421	0.894002	4.181403
6	-3.330353	0.532470	3.154442
6	-7.357085	1.244723	2.493970
6	-7.911851	1.151152	1.243822
6	-7.091984	0.811188	0.136869
6	-5.744389	0.577142	0.310450
9	0.919864	5.046251	-4.353294
9	-0.368086	6.227471	-3.094733
9	5.255899	4.321273	-0.959807
9	4.656281	3.044513	0.682904
1	-2.063657	-1.609487	2.057045
1	-3.861031	-3.030264	1.611049
1	-4.480360	-1.862259	0.448943
1	0.050949	-3.545360	-0.003852
1	-0.696268	-3.367146	1.594300
1	-1.694313	-4.921653	-0.732853
1	-2.358432	-4.895139	0.903869
1	-4.053482	-4.040069	-0.681266
1	-2.417980	-3.346837	-2.407919
1	-0.574916	-2.131236	-1.757293
1	-1.599076	-0.716200	-1.484537
1	-3.405506	-0.983341	-2.984457
1	-5.787858	-1.178732	-2.680250
1	-5.572258	-2.576756	-1.492946
1	-3.235717	0.081071	-0.204224
1	-2.283705	0.360083	3.395580
1	-5.156202	0.347798	-0.570814
1	-3.870113	0.993866	5.202469
1	-7.958809	1.509777	3.357115
1	-8.969402	1.343815	1.109757
1	-0.860139	0.454909	1.474334
1	0.379037	1.902841	1.065303
1	-0.695512	4.110664	-1.807060
1	2.295160	2.690038	0.927044
1	3.336155	5.600840	-2.069870
8	-7.564423	0.694525	-1.130512
6	-8.923879	1.007201	-1.366281
1	-9.080580	0.878694	-2.437600

1	-9.594649	0.330647	-0.823398
1	-9.151192	2.044051	-1.093216
1	-0.423850	-1.327998	0.426752
6	1.226857	-0.136349	2.528275
8	1.412178	1.068865	2.248001
8	0.161523	-0.793210	2.377201
6	5.614291	-0.222399	-0.367654
1	5.567465	0.707294	0.205015
1	6.493517	-0.788819	-0.053587
1	5.756932	0.042611	-1.421132

1-Michael-nitrostyrene-Ph-to-Me-si-re_conf-4

Number of imaginary frequencies : 1
The smallest frequency is : -296.1533 cm(-1)

Electronic energy : =-3713.601194
Zero-point correction= 1.000165
Thermal correction to Energy= 1.063038
Thermal correction to Enthalpy= 1.063982
Thermal correction to Gibbs Free Energy= 0.895187
Sum of electronic and zero-point Energies= -3712.601029
Sum of electronic and thermal Energies= -3712.538156
Sum of electronic and thermal Enthalpies= -3712.537212
Sum of electronic and thermal Free Energies= -3712.706007

Cartesian Coordinates

6	-2.940732	-2.135601	-1.556663
6	-3.364380	-0.918676	-2.390680
6	-3.844322	0.107972	-1.346982
7	-3.373315	-0.417680	-0.052359
6	-2.398472	-1.492029	-0.267421
6	-4.121081	-0.297933	1.046148
6	-3.782552	-0.693096	2.324648
8	0.530387	0.605403	1.517766
8	-0.558488	-0.513007	3.026194
1	-2.397672	-2.173798	0.583108
1	-2.193128	-2.760104	-2.050776
1	-3.808001	-2.754485	-1.303963
1	-2.505576	-0.518081	-2.930369
1	-4.149285	-1.160990	-3.109422
1	-3.418376	1.097475	-1.524555
1	-4.935510	0.190220	-1.313096
1	-5.039264	0.267190	0.889708
1	-2.873978	-1.275626	2.454834
6	-4.814868	-0.825434	3.425527
6	-6.280183	-0.656648	2.996142
1	-4.606365	-0.118646	4.242209
1	-4.710117	-1.822717	3.869534
1	-6.905701	-0.790386	3.888325
1	-6.480321	0.356677	2.627686
6	-6.687810	-1.669547	1.970023
6	-7.415323	-1.420443	0.876876
1	-6.361399	-2.697739	2.134109
1	-7.765207	-0.413875	0.662369
6	-7.731504	-2.516738	-0.079270
8	-7.119845	-3.572430	-0.050390
6	-8.810248	-2.296507	-1.095560
6	-9.753319	-1.271302	-0.979071
6	-8.883564	-3.179047	-2.178345
6	-10.752804	-1.128010	-1.937239
1	-9.731915	-0.596033	-0.129945
6	-9.874137	-3.028378	-3.139726
1	-8.151401	-3.977104	-2.246302
6	-10.810032	-2.001020	-3.020039
1	-11.488192	-0.336432	-1.836076

1	-9.920879	-3.710815	-3.982311
1	-11.585995	-1.883722	-3.770093
6	-2.696623	1.131129	2.806580
1	-2.551413	0.637921	3.763809
1	-1.489694	1.913701	1.154700
7	-0.500207	0.414701	2.191154
6	-1.586053	1.241371	1.992691
7	1.536061	1.603750	-0.954975
6	1.194635	2.948034	-0.815780
6	2.078453	4.026751	-0.733312
6	1.565612	5.315795	-0.583672
6	0.204524	5.573071	-0.518169
6	-0.663848	4.488377	-0.630334
6	-0.188574	3.199987	-0.789894
6	2.538307	6.450214	-0.428578
9	1.983646	7.631292	-0.743951
6	-2.142462	4.734711	-0.592312
9	-2.591006	5.310827	-1.717995
6	2.651195	0.920648	-0.583039
16	4.151166	1.588603	-0.179127
7	2.414275	-0.411192	-0.553434
6	3.397142	-1.421987	-0.237777
6	2.743791	-2.507055	0.639767
6	3.777058	-3.469665	1.263902
6	3.718460	-3.365923	2.795066
6	2.328246	-3.829104	3.252337
6	1.257639	-2.995441	2.521309
7	1.935451	-1.898919	1.756113
6	2.758069	-1.053211	2.670797
6	3.912668	-1.907104	3.257737
6	5.258884	-1.297784	2.944507
6	6.373437	-1.955064	2.633669
6	3.948008	-2.094001	-1.492789
6	5.346604	-2.281096	-1.721415
6	5.721307	-2.973116	-2.911984
7	4.823170	-3.438336	-3.825499
6	3.552224	-3.228407	-3.586435
6	3.067653	-2.565640	-2.434090
6	7.095781	-3.197329	-3.167826
6	8.064533	-2.766525	-2.298419
6	7.689053	-2.070695	-1.120109
6	6.359782	-1.829315	-0.844967
9	2.981933	6.555022	0.835298
9	3.618937	6.294743	-1.205728
9	-2.485748	5.549488	0.417656
9	-2.842084	3.593745	-0.432320
1	2.000581	-3.036661	0.038695
1	3.564526	-4.498089	0.958714
1	4.776464	-3.223911	0.897658
1	0.556810	-2.503500	3.193807
1	0.688448	-3.565789	1.785027
1	2.229761	-3.706165	4.334721
1	2.192968	-4.890278	3.028188
1	4.486828	-4.002261	3.242024
1	3.801702	-1.894399	4.350082
1	2.062734	-0.681102	3.424902
1	3.110563	-0.195958	2.090759
1	5.294082	-0.209595	3.006253
1	7.299183	-1.423324	2.438208
1	6.411987	-3.038521	2.551891
1	4.206087	-0.935240	0.310739
1	1.995907	-2.433630	-2.303419
1	6.126004	-1.270826	0.053887
1	2.845986	-3.600191	-4.326217
1	7.354721	-3.726188	-4.079199
1	9.107884	-2.955206	-2.521237
1	1.449544	-0.752795	-0.669940
1	0.696159	1.006369	-1.056150
1	3.146243	3.865185	-0.782073
1	-0.874066	2.362153	-0.885234

1	-0.170909	6.582429	-0.390689
8	8.583667	-1.610000	-0.209256
6	9.961804	-1.768077	-0.488262
1	10.491735	-1.299564	0.341270
1	10.244625	-2.825976	-0.542168
1	10.243107	-1.266594	-1.421382
1	1.197181	-1.295086	1.349616
6	-0.970481	-0.982924	-0.522982
8	-0.846066	0.129887	-1.081790
8	-0.041957	-1.780775	-0.219135
6	-3.738464	2.211841	2.741506
1	-3.868927	2.577000	1.719905
1	-4.702290	1.873268	3.130558
1	-3.413822	3.059069	3.356077

1-Michael-nitrostyrene-Ph-to-Me-si-re_conf-5

Number of imaginary frequencies : 1

The smallest frequency is : -296.9743 cm(-1)

Electronic energy : =-3713.6009054

Zero-point correction= 1.000566

Thermal correction to Energy= 1.063487

Thermal correction to Enthalpy= 1.064431

Thermal correction to Gibbs Free Energy= 0.895251

Sum of electronic and zero-point Energies= -3712.600339

Sum of electronic and thermal Energies= -3712.537418

Sum of electronic and thermal Enthalpies= -3712.536474

Sum of electronic and thermal Free Energies= -3712.705655

Cartesian Coordinates

6	0.805625	-0.938161	4.711661
6	0.853254	0.528658	5.165451
6	1.896014	1.186902	4.238973
7	2.160822	0.184016	3.191165
6	1.111678	-0.840206	3.205484
6	3.396843	-0.016598	2.727984
6	3.786574	-0.875811	1.720411
8	-0.157063	0.169908	-0.426011
8	1.416445	-1.318559	-0.577938
1	1.486719	-1.770574	2.778719
1	-0.156063	-1.418799	4.904038
1	1.593439	-1.522181	5.197742
1	-0.118935	0.998966	5.013349
1	1.127549	0.626645	6.217446
1	1.509391	2.101454	3.786207
1	2.835253	1.412295	4.752733
1	4.142096	0.665684	3.140566
1	3.066617	-1.594315	1.332124
6	5.246095	-1.248051	1.593247
6	5.699141	-1.617071	0.170026
1	5.449225	-2.113663	2.239620
1	5.878406	-0.437188	1.976943
1	4.984074	-2.340273	-0.247426
1	5.695194	-0.739384	-0.484148
6	7.064045	-2.227725	0.176899
6	8.122270	-1.749017	-0.483054
1	7.208244	-3.125693	0.779205
1	8.033728	-0.851932	-1.088695
6	9.443607	-2.427047	-0.377547
8	9.634817	-3.310724	0.441822
6	10.551771	-1.994663	-1.290207
6	10.328174	-1.242985	-2.447199
6	11.854449	-2.391578	-0.970004
6	11.394641	-0.888752	-3.268945
1	9.322599	-0.948941	-2.728947

6	12.919044	-2.027306	-1.783549
1	12.008460	-2.984619	-0.074387
6	12.689803	-1.274291	-2.934872
1	11.212138	-0.313491	-4.170929
1	13.928572	-2.329851	-1.524092
1	13.521752	-0.991171	-3.572244
6	3.300386	0.511707	0.100406
1	3.604989	-0.306467	-0.543982
1	1.506463	1.705854	0.469404
7	1.039658	-0.156747	-0.312908
6	1.946947	0.786144	0.121808
7	-2.225136	1.897433	0.563814
6	-1.670005	3.097398	0.117610
6	-2.230818	3.985006	-0.802763
6	-1.524714	5.138512	-1.150191
6	-0.281838	5.440514	-0.615747
6	0.251566	4.555200	0.320640
6	-0.430420	3.414527	0.698745
6	-2.131742	6.047853	-2.180707
9	-1.581821	7.272083	-2.158966
6	1.629123	4.806018	0.857049
9	1.796458	6.073686	1.258242
6	-3.046879	1.014835	-0.066225
16	-4.023890	1.339897	-1.405451
7	-2.980112	-0.206098	0.513331
6	-3.761354	-1.356022	0.120765
6	-2.875395	-2.616639	0.169825
6	-3.528368	-3.829852	-0.527973
6	-2.668039	-4.259015	-1.727165
6	-1.307823	-4.730256	-1.193891
6	-0.698041	-3.612363	-0.326358
7	-1.533055	-2.375933	-0.470566
6	-1.638824	-1.980867	-1.907415
6	-2.419653	-3.074114	-2.682557
6	-3.649953	-2.505535	-3.349390
6	-4.831778	-3.104373	-3.473075
6	-4.951077	-1.579033	1.051490
6	-6.278789	-1.808820	0.574716
6	-7.284197	-2.060468	1.555913
7	-7.040590	-2.071427	2.896675
6	-5.814176	-1.834230	3.291467
6	-4.737324	-1.588226	2.407365
6	-8.609124	-2.315302	1.126674
6	-8.940123	-2.325082	-0.203652
6	-7.940558	-2.064099	-1.176506
6	-6.642205	-1.804593	-0.791796
9	-1.967804	5.569288	-3.424940
9	-3.451428	6.197758	-1.997363
9	2.569396	4.572308	-0.077695
9	1.926368	4.009719	1.901052
1	-2.631052	-2.827321	1.213530
1	-3.617822	-4.663464	0.174193
1	-4.539167	-3.568404	-0.848814
1	0.310423	-3.331038	-0.625838
1	-0.690791	-3.846468	0.739668
1	-0.641328	-4.971178	-2.027148
1	-1.430842	-5.638795	-0.598676
1	-3.159615	-5.073439	-2.265427
1	-1.760747	-3.435242	-3.483086
1	-0.610110	-1.853597	-2.248720
1	-2.125797	-1.002542	-1.942887
1	-3.518243	-1.513912	-3.783436
1	-5.652541	-2.617399	-3.989793
1	-5.034228	-4.090954	-3.063188
1	-4.109925	-1.188304	-0.900197
1	-3.743608	-1.407994	2.811487
1	-5.921556	-1.584998	-1.571343
1	-5.634555	-1.838633	4.364849
1	-9.355372	-2.501417	1.892106
1	-9.963125	-2.524118	-0.499576

1	-2.266752	-0.381338	1.234354
1	-1.647021	1.467782	1.305995
1	-3.198141	3.783326	-1.241676
1	-0.017300	2.737725	1.441179
1	0.252388	6.337626	-0.908039
8	-8.185912	-2.050253	-2.511391
6	-9.510421	-2.285895	-2.949278
1	-9.484670	-2.211756	-4.036614
1	-9.856797	-3.287081	-2.666502
1	-10.204850	-1.534763	-2.556095
1	-1.052620	-1.610001	0.036323
6	-0.174530	-0.417200	2.476725
8	-0.451162	0.802546	2.455166
8	-0.889351	-1.360455	2.040771
6	4.259136	1.653736	0.289093
1	3.875627	2.373393	1.016675
1	5.247762	1.315995	0.609792
1	4.378755	2.181031	-0.664203

1-Michael-nitrostyrene-Ph-to-Me-si-re_conf-6

Number of imaginary frequencies : 1

The smallest frequency is : -301.5295 cm(-1)

Electronic energy : =-3713.5980453

Zero-point correction= 0.996818

Thermal correction to Energy= 1.059868

Thermal correction to Enthalpy= 1.060812

Thermal correction to Gibbs Free Energy= 0.894062

Sum of electronic and zero-point Energies= -3712.601227

Sum of electronic and thermal Energies= -3712.538177

Sum of electronic and thermal Enthalpies= -3712.537233

Sum of electronic and thermal Free Energies= -3712.703983

Cartesian Coordinates

6	-4.599232	1.129288	-2.484215
6	-3.178184	0.670160	-2.818069
6	-2.432128	0.980899	-1.521191
7	-3.026822	2.251434	-1.099668
6	-4.399890	2.373060	-1.607257
6	-2.531397	3.060424	-0.156399
6	-3.277181	3.978746	0.561842
8	-0.702350	1.598324	3.371049
8	-1.597013	0.988988	1.485164
1	-4.489165	3.310401	-2.168491
1	-5.110365	0.354134	-1.905149
1	-5.200484	1.344714	-3.368749
1	-3.109140	-0.386415	-3.077021
1	-2.752730	1.262941	-3.634732
1	-2.687158	0.211417	-0.777933
1	-1.488347	2.889325	0.074509
1	-4.285549	4.200950	0.222026
6	-2.657606	5.032187	1.447137
6	-1.153873	4.909573	1.727188
1	-3.184828	5.041596	2.411223
1	-2.841911	6.019355	1.002843
1	-0.911238	5.657947	2.493599
1	-0.894883	3.938073	2.161882
6	-0.287936	5.185008	0.536068
6	0.784877	4.467334	0.193095
1	-0.532163	6.060558	-0.066977
1	1.057108	3.583262	0.762699
6	1.624048	4.886180	-0.959928
8	1.182289	5.624488	-1.824649
6	3.060726	4.445271	-1.017638
6	3.682216	3.729167	0.011134

6	3.817474	4.844418	-2.126041
6	5.041373	3.428855	-0.065541
1	3.126358	3.423930	0.891307
6	5.170879	4.541657	-2.203173
1	3.320999	5.405313	-2.910955
6	5.786659	3.834656	-1.169722
1	5.518447	2.887582	0.745745
1	5.749014	4.857384	-3.065875
1	6.845980	3.603132	-1.223896
6	-3.859539	2.358280	2.008868
1	-3.906459	1.627379	1.206492
1	-2.789155	2.756844	3.879714
7	-1.670419	1.577104	2.604807
6	-2.833082	2.233558	2.935122
7	-1.467122	-1.659200	0.656700
6	-2.748779	-2.121063	0.369600
6	-3.085151	-3.192092	-0.468356
6	-4.428131	-3.451258	-0.723567
6	-5.458019	-2.679606	-0.192474
6	-5.106126	-1.629987	0.646725
6	-3.779268	-1.361128	0.941294
6	-4.799849	-4.630726	-1.579879
9	-5.816651	-4.333131	-2.405955
6	-6.133595	-0.673221	1.173549
9	-6.095311	0.496162	0.490976
6	-0.220469	-2.012967	0.217363
16	0.189654	-3.504584	-0.442551
7	0.651695	-0.996709	0.401910
6	2.092631	-1.090223	0.275898
6	2.623075	-0.083647	-0.766516
6	4.166898	-0.124757	-0.878173
6	4.560963	-0.059785	-2.359641
6	3.843767	1.139278	-2.990580
6	2.325082	0.861783	-2.962316
7	2.018180	-0.310469	-2.103795
6	2.574429	-1.521335	-2.742574
6	4.087353	-1.337227	-3.073846
6	4.844023	-2.598160	-2.747211
6	5.929414	-2.714130	-1.985223
6	2.766026	-0.872864	1.626057
6	3.832936	-1.714957	2.079523
6	4.416066	-1.403893	3.343408
7	4.003789	-0.366635	4.126614
6	3.010369	0.364679	3.686670
6	2.360956	0.151314	2.445799
6	5.476326	-2.208813	3.826635
6	5.949636	-3.276475	3.108699
6	5.365122	-3.588663	1.854775
6	4.329933	-2.825604	1.357283
9	-3.779958	-5.055741	-2.333667
9	-5.204000	-5.670662	-0.833520
9	-5.916215	-0.353985	2.458642
9	-7.379153	-1.143506	1.071351
1	2.285873	0.917087	-0.464222
1	4.602676	0.715232	-0.329276
1	4.559492	-1.042150	-0.435417
1	1.936519	0.628818	-3.958999
1	1.761003	1.711662	-2.570272
1	4.186825	1.301927	-4.017206
1	4.076009	2.043063	-2.419635
1	5.645319	0.050981	-2.458278
1	4.181480	-1.170062	-4.156446
1	1.986977	-1.717791	-3.644617
1	2.411182	-2.368824	-2.071666
1	4.420505	-3.503438	-3.185301
1	6.381953	-3.683859	-1.804571
1	6.406071	-1.860210	-1.511166
1	2.291919	-2.104378	-0.068062
1	1.521387	0.794283	2.192012
1	3.924269	-3.114307	0.393362

1	2.676911	1.179348	4.326829
1	5.900070	-1.948995	4.791352
1	6.761332	-3.874173	3.505990
1	0.268805	-0.102906	0.707656
1	-1.480936	-0.797263	1.203700
1	-2.311280	-3.799398	-0.916561
1	-3.524703	-0.532101	1.596904
1	-6.495488	-2.890150	-0.426389
8	5.770654	-4.626669	1.081264
6	6.803813	-5.460502	1.569596
1	6.956087	-6.226267	0.808911
1	7.738837	-4.905533	1.710878
1	6.520355	-5.943803	2.511843
1	0.512243	-0.291276	-2.126947
1	-5.118742	2.402777	-0.780414
6	-0.918071	0.917325	-1.622205
8	-0.153850	1.735851	-1.133138
8	-0.544983	-0.176107	-2.233996
6	-5.172058	2.928013	2.466849
1	-5.033125	3.826674	3.074622
1	-5.830516	3.162674	1.629774
1	-5.674653	2.177782	3.087574

1-Michael-nitrostyrene-Ph-to-Me-re-si_conf-1

Number of imaginary frequencies : 1

The smallest frequency is : -263.5255 cm(-1)

Electronic energy : =-3713.6024827

Zero-point correction= 0.999060

Thermal correction to Energy= 1.062239

Thermal correction to Enthalpy= 1.063184

Thermal correction to Gibbs Free Energy= 0.893563

Sum of electronic and zero-point Energies= -3712.603422

Sum of electronic and thermal Energies= -3712.540243

Sum of electronic and thermal Enthalpies= -3712.539299

Sum of electronic and thermal Free Energies= -3712.708920

Cartesian Coordinates

6	1.155886	-1.392469	4.662711
6	1.986647	-0.109386	4.501763
6	2.818276	-0.340189	3.229433
7	2.163171	-1.463999	2.563262
6	0.917099	-1.858610	3.220946
6	2.517594	-1.927242	1.366820
6	3.515857	-1.436054	0.548411
8	0.139640	-1.887216	-2.425517
6	-0.268281	-1.123773	2.565964
8	-1.296891	-1.784218	2.301852
8	-0.087659	0.109084	2.362702
8	0.041331	-1.528598	-0.285240
1	0.767821	-2.937557	3.133673
1	0.220618	-1.225651	5.201432
1	1.728311	-2.158448	5.194716
1	1.323795	0.743446	4.354089
1	2.619691	0.084611	5.369625
1	2.816777	0.542161	2.578048
1	3.860700	-0.607225	3.442541
1	1.896199	-2.745597	1.004381
1	4.221151	-0.719131	0.961194
6	3.948812	-2.284401	-0.623782
6	4.854693	-1.586605	-1.653288
1	3.054574	-2.650744	-1.147907
1	4.483926	-3.173758	-0.264444
1	5.122503	-2.310942	-2.429228
1	4.295345	-0.782618	-2.144484

6	6.098517	-1.022517	-1.042310
6	7.328413	-1.508815	-1.233967
1	6.002578	-0.160456	-0.381255
1	7.489827	-2.358222	-1.891500
6	8.499496	-0.870910	-0.572941
8	8.392873	0.197086	0.007370
6	9.830231	-1.558263	-0.641588
6	9.967606	-2.910786	-0.966481
6	10.968979	-0.806100	-0.334441
6	11.228509	-3.500048	-0.987847
1	9.094310	-3.517751	-1.181770
6	12.227310	-1.391296	-0.368961
1	10.841197	0.239111	-0.072502
6	12.358335	-2.740722	-0.696487
1	11.328273	-4.552934	-1.231497
1	13.107497	-0.799866	-0.137820
1	13.341604	-3.200349	-0.721854
6	2.128220	0.172242	-0.385436
1	1.507213	0.165323	0.509028
1	2.007813	-0.331919	-2.517064
7	0.558589	-1.305295	-1.410825
6	1.606970	-0.419921	-1.517693
7	-1.092796	1.374272	0.241332
6	-0.330875	2.510104	-0.023708
6	-0.297980	3.216455	-1.231984
6	0.563940	4.302685	-1.361954
6	1.413149	4.707672	-0.337484
6	1.381660	3.984668	0.849830
6	0.527757	2.904984	1.014389
6	0.536302	5.072685	-2.652487
9	-0.503616	5.919039	-2.703912
6	2.304693	4.320096	1.983976
9	1.635798	4.540658	3.125116
6	-2.271664	0.932135	-0.262954
16	-3.166220	1.654196	-1.506528
7	-2.660711	-0.204630	0.361781
6	-3.901073	-0.915365	0.149118
6	-3.560837	-2.413695	0.035352
6	-4.757046	-3.306086	-0.355847
6	-4.469311	-3.992440	-1.699326
6	-3.235400	-4.895238	-1.540152
6	-2.058492	-4.052411	-1.008059
7	-2.467643	-2.613881	-0.984537
6	-2.876017	-2.181226	-2.360833
6	-4.159202	-2.940778	-2.782685
6	-5.286896	-1.989478	-3.106864
6	-6.580608	-2.186404	-2.867455
6	-4.888035	-0.714772	1.296181
6	-6.257517	-0.362008	1.076225
6	-7.097032	-0.272075	2.226594
7	-6.652625	-0.476714	3.498920
6	-5.386003	-0.770320	3.656122
6	-4.466013	-0.908099	2.588246
6	-8.465786	0.044717	2.052625
6	-8.996585	0.265952	0.807710
6	-8.157191	0.189757	-0.332749
6	-6.817939	-0.108859	-0.196700
9	1.646964	5.805629	-2.824545
9	0.424982	4.259010	-3.713514
9	3.047713	5.404823	1.735126
9	3.157697	3.305474	2.237811
1	-3.107116	-2.724355	0.981889
1	-4.927933	-4.060349	0.417033
1	-5.661773	-2.697246	-0.423063
1	-1.166939	-4.098969	-1.635923
1	-1.779162	-4.310098	0.015631
1	-2.975305	-5.344873	-2.502698
1	-3.452720	-5.709795	-0.844719
1	-5.328804	-4.596546	-2.000863
1	-3.920233	-3.483556	-3.706703

1	-2.024718	-2.400709	-3.002614
1	-3.008708	-1.096094	-2.341057
1	-4.981211	-1.067604	-3.603936
1	-7.319970	-1.441556	-3.145460
1	-6.954367	-3.079952	-2.373292
1	-4.336022	-0.552694	-0.783174
1	-3.430696	-1.165964	2.802802
1	-6.217481	-0.129607	-1.097576
1	-5.041792	-0.922581	4.677440
1	-9.081129	0.104310	2.944459
1	-10.048546	0.504542	0.706718
1	-2.078244	-0.588700	1.123201
1	-0.756363	0.850765	1.086663
1	-0.933006	2.919293	-2.055755
1	0.521424	2.341472	1.944493
1	2.083581	5.549130	-0.463472
8	-8.599443	0.398442	-1.600207
6	-9.948427	0.786216	-1.780183
1	-10.077699	0.935808	-2.852330
1	-10.641953	0.007469	-1.441812
1	-10.169767	1.724382	-1.258589
1	-1.621550	-2.075418	-0.692928
6	3.113217	1.297668	-0.530486
1	3.576128	1.562222	0.421216
1	3.896702	1.078824	-1.259086
1	2.568873	2.179171	-0.893117

1-Michael-nitrostyrene-Ph-to-Me-re-si_conf-2

Number of imaginary frequencies : 1

The smallest frequency is : -371.0146 cm(-1)

Electronic energy : =-3713.5922066

Zero-point correction= 0.998896

Thermal correction to Energy= 1.061580

Thermal correction to Enthalpy= 1.062524

Thermal correction to Gibbs Free Energy= 0.896060

Sum of electronic and zero-point Energies= -3712.593311

Sum of electronic and thermal Energies= -3712.530626

Sum of electronic and thermal Enthalpies= -3712.529682

Sum of electronic and thermal Free Energies= -3712.696147

Cartesian Coordinates

6	1.555315	1.563146	4.640524
6	1.539432	2.919466	3.933561
6	2.915341	2.982282	3.271679
7	3.225037	1.574405	2.997252
6	2.241818	0.669464	3.614003
6	4.251947	1.161576	2.279028
6	5.183778	1.966295	1.624341
8	0.994909	0.789623	-0.771426
6	1.290801	0.090947	2.529357
8	1.846861	-0.563684	1.621180
8	0.061138	0.300247	2.682757
8	1.425002	2.371518	0.647945
1	2.771106	-0.178883	4.060110
1	0.557299	1.193771	4.871939
1	2.152062	1.609950	5.557755
1	0.766729	2.908221	3.159769
1	1.364922	3.762593	4.603919
1	2.904414	3.552101	2.341577
1	3.683027	3.393418	3.940233
1	4.296101	0.081287	2.162962
1	5.178082	3.019871	1.896965
6	6.575105	1.426087	1.328039
6	6.823536	-0.068914	1.593344

1	7.279719	1.985259	1.955333
1	6.881791	1.640015	0.296858
1	7.910890	-0.216823	1.602815
1	6.459136	-0.357513	2.584746
6	6.271420	-0.985428	0.544900
6	5.429854	-1.998607	0.782810
1	6.651729	-0.828397	-0.464388
1	5.080743	-2.198962	1.794802
6	5.011834	-3.033360	-0.193756
8	4.591593	-4.103162	0.222127
6	5.092334	-2.800579	-1.673866
6	4.899307	-1.540234	-2.247852
6	5.260141	-3.915082	-2.501500
6	4.880652	-1.394362	-3.632057
1	4.731046	-0.683824	-1.603864
6	5.262809	-3.765710	-3.883244
1	5.383289	-4.891162	-2.043256
6	5.070616	-2.505595	-4.449770
1	4.715471	-0.415060	-4.070664
1	5.406750	-4.631712	-4.521437
1	5.062772	-2.391395	-5.529112
6	4.029785	2.491925	-0.214519
1	3.598522	3.316018	0.343069
1	3.301598	0.818454	-1.432682
7	1.807482	1.572522	-0.237449
6	3.106284	1.564702	-0.677686
7	-1.642303	1.752118	0.234793
6	-2.069082	2.984793	-0.274480
6	-3.418821	3.319508	-0.423383
6	-3.762448	4.578751	-0.899855
6	-2.801268	5.531940	-1.219329
6	-1.466304	5.193174	-1.041170
6	-1.092590	3.937050	-0.578716
6	-5.219069	4.931157	-0.997525
9	-5.731638	5.255991	0.202189
6	-0.385100	6.162712	-1.417115
9	0.157383	5.865879	-2.610592
6	-2.139086	0.507595	-0.053003
16	-3.361882	0.195120	-1.181166
7	-1.495380	-0.454078	0.631941
6	-1.759480	-1.869014	0.486907
6	-0.420593	-2.638633	0.480411
6	-0.554971	-4.090438	-0.032028
6	0.213611	-4.242499	-1.357146
6	1.708937	-4.033056	-1.081765
6	1.883505	-2.694661	-0.345157
7	0.590543	-1.939307	-0.383424
6	0.127177	-1.780232	-1.794084
6	-0.229985	-3.173070	-2.375747
6	-1.673699	-3.250208	-2.814012
6	-2.457441	-4.323759	-2.751255
6	-2.630130	-2.410548	1.618235
6	-3.763729	-3.251356	1.385443
6	-4.447530	-3.752932	2.532886
7	-4.091255	-3.447825	3.812771
6	-3.068450	-2.646306	3.979635
6	-2.303637	-2.107857	2.917075
6	-5.557234	-4.612049	2.346682
6	-5.987859	-4.963362	1.092967
6	-5.318436	-4.447057	-0.045817
6	-4.236466	-3.605675	0.101372
9	-5.428040	5.981621	-1.806202
9	-5.951974	3.911667	-1.464556
9	0.623401	6.155177	-0.529699
9	-0.838890	7.422110	-1.497606
1	0.014842	-2.592505	1.483774
1	-0.151685	-4.790538	0.704687
1	-1.611563	-4.333891	-0.168819
1	2.622701	-2.037722	-0.808125
1	2.144633	-2.805353	0.707260

1	2.270247	-4.026500	-2.022076
1	2.112895	-4.841726	-0.469623
1	0.048378	-5.241008	-1.769633
1	0.383057	-3.310501	-3.276363
1	0.948596	-1.296642	-2.324456
1	-0.719468	-1.089229	-1.793508
1	-2.076995	-2.331558	-3.241642
1	-3.480743	-4.290645	-3.111350
1	-2.122314	-5.268929	-2.330927
1	-2.264404	-2.010325	-0.470508
1	-1.467250	-1.448831	3.141474
1	-3.778979	-3.213543	-0.798889
1	-2.802591	-2.399744	5.005907
1	-6.056922	-4.981721	3.236212
1	-6.839940	-5.623569	0.983353
1	-0.856278	-0.161179	1.415245
1	-0.687392	1.754709	0.600103
1	-4.189245	2.601892	-0.171497
1	-0.044738	3.687805	-0.437095
1	-3.086994	6.509453	-1.588819
8	-5.686189	-4.735495	-1.321302
6	-6.829820	-5.544467	-1.516651
1	-6.959762	-5.626683	-2.596044
1	-6.692301	-6.547491	-1.095901
1	-7.725965	-5.086609	-1.082076
1	0.795669	-1.010362	0.037478
6	5.198053	2.830409	-1.094697
1	5.956685	3.418938	-0.576377
1	5.668301	1.937124	-1.517884
1	4.823905	3.430944	-1.931995

1-Michael-nitrostyrene-Ph-to-Me-re-re_conf-1

Number of imaginary frequencies : 1
The smallest frequency is : -299.0964 cm(-1)

Electronic energy : =-3713.6094415
Zero-point correction= 0.998725
Thermal correction to Energy= 1.061970
Thermal correction to Enthalpy= 1.062914
Thermal correction to Gibbs Free Energy= 0.892362
Sum of electronic and zero-point Energies= -3712.610716
Sum of electronic and thermal Energies= -3712.547471
Sum of electronic and thermal Enthalpies= -3712.546527
Sum of electronic and thermal Free Energies= -3712.717079

Cartesian Coordinates

6	2.671608	1.434487	3.182199
6	2.321526	2.884723	2.827161
6	2.879750	3.049446	1.412045
7	2.882643	1.685764	0.855692
6	2.485210	0.678151	1.862972
6	3.593438	1.367936	-0.226787
6	4.142843	2.286581	-1.102759
8	-0.322419	1.028855	-0.954066
6	1.022335	0.236449	1.633328
8	0.837650	-0.883490	1.093644
8	0.134907	1.032475	2.023267
8	1.517895	0.381755	-1.911466
1	3.134402	-0.194785	1.767984
1	2.036037	1.031613	3.972285
1	3.717995	1.358959	3.496107
1	1.239162	3.009380	2.826164
1	2.763319	3.608800	3.514556
1	2.287032	3.723805	0.787202
1	3.915197	3.416113	1.429747

1	3.644433	0.303868	-0.447916
1	4.275097	3.306916	-0.749426
6	5.078246	1.813630	-2.184522
6	6.565960	1.807492	-1.769823
1	4.979771	2.451326	-3.073014
1	4.787639	0.801080	-2.491542
1	7.183154	1.516611	-2.626318
1	6.852125	2.829714	-1.489147
6	6.823947	0.894622	-0.614595
6	7.565352	-0.216490	-0.657749
1	6.348718	1.140145	0.335076
1	8.070970	-0.505642	-1.573730
6	7.719055	-1.052141	0.564873
8	7.267906	-0.683601	1.637646
6	8.443902	-2.362310	0.471165
6	8.758085	-2.977408	-0.744182
6	8.790178	-2.996276	1.669541
6	9.412306	-4.206241	-0.758165
1	8.480513	-2.517993	-1.686563
6	9.450723	-4.216998	1.654799
1	8.529788	-2.509085	2.603281
6	9.763123	-4.824098	0.438695
1	9.646720	-4.681575	-1.705263
1	9.722060	-4.698789	2.588751
1	10.278852	-5.779348	0.424822
6	2.358031	2.877680	-2.262505
1	2.691469	2.122276	-2.967040
1	0.557569	3.323091	-1.085612
7	0.775851	1.290026	-1.478462
6	1.188934	2.602708	-1.583679
7	-2.350965	1.366432	0.937497
6	-2.570332	2.711263	0.645244
6	-3.789986	3.277738	0.265136
6	-3.860923	4.651971	0.046482
6	-2.762585	5.488066	0.204620
6	-1.559314	4.908705	0.596432
6	-1.454070	3.544069	0.813125
6	-5.197361	5.240636	-0.305953
9	-5.990259	5.351173	0.773067
6	-0.320050	5.740514	0.733826
9	-0.585295	7.048201	0.823704
6	-2.851807	0.244479	0.360168
16	-4.247225	0.145998	-0.586911
7	-2.058034	-0.821560	0.622155
6	-2.329573	-2.183093	0.228059
6	-1.030445	-2.844418	-0.271798
6	-1.295958	-4.175443	-1.009645
6	-0.858079	-4.045901	-2.476659
6	0.660085	-3.827396	-2.501758
6	1.004432	-2.621180	-1.608450
7	-0.266050	-1.936914	-1.200498
6	-1.060084	-1.547443	-2.403513
6	-1.525793	-2.827408	-3.146609
6	-3.031756	-2.886637	-3.253969
6	-3.789359	-3.978236	-3.180811
6	-2.862108	-3.014871	1.392847
6	-4.030881	-3.831649	1.296665
6	-4.380038	-4.601997	2.446148
7	-3.673294	-4.575915	3.611193
6	-2.622406	-3.795293	3.664921
6	-2.175946	-3.002113	2.581646
6	-5.518753	-5.441403	2.385282
6	-6.284858	-5.525772	1.251240
6	-5.941375	-4.749753	0.113854
6	-4.842416	-3.917724	0.142259
9	-5.083316	6.469957	-0.832911
9	-5.858649	4.484024	-1.192878
9	0.505442	5.583681	-0.327529
9	0.402436	5.396643	1.813292
1	-0.356472	-2.971821	0.578697

1	-0.741479	-4.988468	-0.532767
1	-2.357853	-4.424460	-0.943177
1	1.603143	-1.867079	-2.115405
1	1.508353	-2.896168	-0.680159
1	0.996223	-3.649277	-3.527524
1	1.175201	-4.720084	-2.137618
1	-1.110932	-4.957120	-3.024755
1	-1.135212	-2.765953	-4.170994
1	-0.395534	-0.920480	-3.000192
1	-1.892741	-0.926736	-2.062575
1	-3.516068	-1.925918	-3.431586
1	-4.867229	-3.916789	-3.292320
1	-3.377434	-4.968242	-3.001219
1	-3.061662	-2.150195	-0.581176
1	-1.287358	-2.385965	2.701929
1	-4.635963	-3.326396	-0.742393
1	-2.071169	-3.777558	4.603098
1	-5.764448	-6.016559	3.272020
1	-7.150572	-6.176983	1.236471
1	-1.150055	-0.652761	1.066418
1	-1.429201	1.215234	1.389138
1	-4.666017	2.654284	0.141317
1	-0.508276	3.092205	1.107835
1	-2.842002	6.554532	0.031342
8	-6.648431	-4.771910	-1.044600
6	-7.821675	-5.560974	-1.095303
1	-8.241954	-5.411879	-2.090085
1	-7.599461	-6.625607	-0.956527
1	-8.554425	-5.240209	-0.345873
1	0.001454	-1.076086	-0.684464
6	2.714418	4.307339	-2.560708
1	2.485129	4.962768	-1.717313
1	3.770842	4.417032	-2.817064
1	2.129057	4.651561	-3.420814

1-Michael-nitrostyrene-Ph-to-Me-re-re_conf-2

Number of imaginary frequencies : 1
The smallest frequency is : -322.6818 cm(-1)

Electronic energy : =-3713.6155425
Zero-point correction= 1.001136
Thermal correction to Energy= 1.063433
Thermal correction to Enthalpy= 1.064377
Thermal correction to Gibbs Free Energy= 0.901319
Sum of electronic and zero-point Energies= -3712.614406
Sum of electronic and thermal Energies= -3712.552110
Sum of electronic and thermal Enthalpies= -3712.551165
Sum of electronic and thermal Free Energies= -3712.714223

Cartesian Coordinates

6	3.204059	-0.303888	4.430680
6	4.160631	0.706207	3.779634
6	4.606624	0.022078	2.478316
7	3.614962	-1.043061	2.246711
6	2.525182	-0.986158	3.235276
6	3.902176	-2.157440	1.571081
6	4.973328	-2.289998	0.703805
8	1.056142	0.117268	-0.220711
6	1.338985	-0.143363	2.721640
8	0.217372	-0.712362	2.657572
8	1.584144	1.052793	2.448316
8	1.764459	-1.936588	-0.210658
1	2.175078	-1.998580	3.445427
1	2.481985	0.170411	5.098501
1	3.763913	-1.053538	4.999420

1	3.629122	1.629099	3.552829
1	5.016272	0.935402	4.418100
1	4.647485	0.711979	1.631808
1	5.590579	-0.449077	2.588325
1	3.171056	-2.955059	1.671007
1	5.756232	-1.541459	0.783554
6	5.420855	-3.639404	0.170603
6	4.775263	-4.868689	0.820055
1	6.501049	-3.719286	0.331934
1	5.292398	-3.696841	-0.921464
1	5.382791	-5.753424	0.583399
1	4.827247	-4.771813	1.911662
6	3.364339	-5.203551	0.436512
6	2.694573	-4.779655	-0.639956
1	2.840840	-5.901185	1.090841
1	3.139413	-4.105401	-1.362203
6	1.315889	-5.274532	-0.894177
8	0.752772	-6.032007	-0.117026
6	0.617908	-4.854041	-2.153580
6	0.931347	-3.677446	-2.841594
6	-0.402923	-5.683301	-2.634430
6	0.221688	-3.332898	-3.990726
1	1.690553	-3.004175	-2.453137
6	-1.091415	-5.351302	-3.794250
1	-0.634498	-6.590449	-2.084955
6	-0.781367	-4.171530	-4.471948
1	0.452674	-2.407925	-4.509472
1	-1.871223	-6.006317	-4.169238
1	-1.324947	-3.904261	-5.372772
6	4.192293	-1.224341	-1.043011
1	3.817893	-2.194245	-1.351859
1	3.380291	0.787065	-0.701014
7	1.971295	-0.709339	-0.369890
6	3.236399	-0.282989	-0.715002
7	0.021388	2.537488	0.699852
6	0.897269	3.359305	-0.011645
6	0.517736	4.400573	-0.864471
6	1.502824	5.169221	-1.478411
6	2.858776	4.947765	-1.264571
6	3.217378	3.920938	-0.398160
6	2.260224	3.133040	0.223458
6	1.084456	6.251166	-2.432706
9	-0.103724	6.777942	-2.108356
6	4.660270	3.591858	-0.162947
9	5.475846	4.613749	-0.446887
6	-1.160694	1.989972	0.308067
16	-2.093207	2.474607	-1.014789
7	-1.510200	0.958212	1.110836
6	-2.712725	0.170710	0.962401
6	-2.392799	-1.306017	1.260783
6	-3.553714	-2.246837	0.868031
6	-3.067929	-3.256239	-0.182906
6	-1.954509	-4.101707	0.449698
6	-0.830623	-3.164567	0.927595
7	-1.155709	-1.755525	0.527010
6	-1.302616	-1.647815	-0.952962
6	-2.486137	-2.534372	-1.414698
6	-3.469778	-1.728500	-2.227347
6	-4.797738	-1.790138	-2.165330
6	-3.821506	0.629160	1.905768
6	-5.163518	0.858803	1.468882
6	-6.114121	1.234012	2.464474
7	-5.799371	1.396899	3.780519
6	-4.553680	1.198754	4.134502
6	-3.532501	0.810179	3.235029
6	-7.458737	1.452972	2.078045
6	-7.859928	1.312503	0.774364
6	-6.909861	0.950900	-0.215174
6	-5.591809	0.735810	0.127122
9	1.974422	7.256899	-2.466670

9	0.976200	5.791646	-3.690915
9	5.062934	2.551465	-0.928384
9	4.894016	3.226687	1.109186
1	-2.124996	-1.402458	2.316341
1	-3.916411	-2.781246	1.750365
1	-4.388004	-1.657513	0.480946
1	0.135416	-3.386471	0.476120
1	-0.705713	-3.142142	2.011569
1	-1.555594	-4.821764	-0.270149
1	-2.351758	-4.669771	1.295183
1	-3.895670	-3.901475	-0.489258
1	-2.067844	-3.305350	-2.077335
1	-0.346599	-1.968822	-1.365363
1	-1.436659	-0.589477	-1.192360
1	-3.012933	-1.038794	-2.938485
1	-5.415861	-1.165296	-2.801990
1	-5.322709	-2.450417	-1.479565
1	-3.047257	0.267103	-0.072117
1	-2.521319	0.662691	3.606456
1	-4.901424	0.489217	-0.671468
1	-4.314525	1.340783	5.186735
1	-8.161447	1.737886	2.854317
1	-8.896088	1.487419	0.510426
1	-0.835320	0.619580	1.809456
1	0.521490	1.987018	1.423125
1	-0.528805	4.610055	-1.037263
1	2.546086	2.332547	0.902519
1	3.608678	5.566522	-1.743735
8	-7.221947	0.797336	-1.527576
6	-8.542526	1.094756	-1.938513
1	-8.560575	0.950421	-3.019027
1	-9.272168	0.419454	-1.476342
1	-8.810042	2.133140	-1.711634
1	-0.353824	-1.168675	0.820635
6	5.490584	-0.764985	-1.647760
1	5.872916	0.125097	-1.142065
1	6.252291	-1.547525	-1.613916
1	5.327049	-0.505997	-2.699860

1-Michael-nitrostyrene-Ph-to-Me-re-re_conf-3

Number of imaginary frequencies : 1
The smallest frequency is : -335.7964 cm(-1)

Electronic energy : =-3713.6089276
Zero-point correction= 1.000093
Thermal correction to Energy= 1.063018
Thermal correction to Enthalpy= 1.063962
Thermal correction to Gibbs Free Energy= 0.895634
Sum of electronic and zero-point Energies= -3712.608834
Sum of electronic and thermal Energies= -3712.545909
Sum of electronic and thermal Enthalpies= -3712.544965
Sum of electronic and thermal Free Energies= -3712.713294

Cartesian Coordinates

6	1.044233	1.587376	4.649563
6	1.315711	2.922163	3.944336
6	2.402259	2.574845	2.923758
7	2.227241	1.134480	2.670042
6	1.181079	0.546897	3.532675
6	3.178071	0.391295	2.102603
6	4.263281	0.908976	1.416330
8	-0.063180	0.580560	-0.261662
6	-0.133973	0.356314	2.743440
8	-0.440092	-0.816924	2.413014
8	-0.798810	1.394716	2.517408

8	1.731886	-0.636511	-0.128907
1	1.519200	-0.429281	3.886079
1	0.058705	1.552584	5.116677
1	1.804455	1.399072	5.414967
1	0.411149	3.259659	3.439897
1	1.652827	3.701808	4.630358
1	2.323357	3.146846	1.995290
1	3.406836	2.730612	3.339184
1	2.983232	-0.676890	2.120598
1	4.520745	1.945984	1.615475
6	5.399557	0.029514	0.945970
6	5.008281	-1.429982	0.732178
1	6.237881	0.083622	1.653074
1	5.785956	0.429817	-0.002464
1	4.748542	-1.897060	1.693050
1	4.086953	-1.483471	0.133331
6	6.051388	-2.286754	0.088241
6	7.292075	-1.922681	-0.250647
1	5.769109	-3.318368	-0.120734
1	7.652074	-0.913563	-0.081636
6	8.196129	-2.908760	-0.903650
8	7.783558	-3.993940	-1.279718
6	9.634868	-2.542116	-1.115585
6	10.262235	-1.497970	-0.429695
6	10.372498	-3.307097	-2.025443
6	11.607833	-1.221477	-0.656147
1	9.716524	-0.910700	0.301508
6	11.710784	-3.022342	-2.260280
1	9.872389	-4.121549	-2.538922
6	12.330266	-1.977208	-1.575335
1	12.092354	-0.415419	-0.114563
1	12.274601	-3.613830	-2.974605
1	13.377267	-1.754735	-1.756745
6	3.328540	1.467264	-0.477382
1	3.681878	0.506121	-0.840283
1	1.416948	2.543851	-0.352094
7	1.178173	0.481072	-0.252393
6	1.957208	1.609184	-0.372658
7	-2.468738	1.845068	0.377526
6	-2.128344	3.054103	-0.227348
6	-2.821705	3.683292	-1.264937
6	-2.363896	4.912009	-1.738858
6	-1.247161	5.545143	-1.208740
6	-0.577246	4.910148	-0.166666
6	-1.000151	3.684577	0.319837
6	-3.158373	5.595961	-2.815094
9	-2.439200	6.535996	-3.448604
6	0.672556	5.504914	0.406881
9	0.767167	6.819893	0.182019
6	-3.006032	0.712757	-0.146196
16	-3.882265	0.595972	-1.585447
7	-2.730235	-0.354623	0.640483
6	-3.214131	-1.697898	0.427095
6	-2.083200	-2.702677	0.718810
6	-2.415291	-4.126261	0.220903
6	-1.423667	-4.528202	-0.882022
6	-0.023720	-4.605114	-0.258463
6	0.277280	-3.271117	0.450273
7	-0.783245	-2.275514	0.086678
6	-0.884579	-2.135205	-1.396939
6	-1.386678	-3.471527	-2.004645
6	-2.677889	-3.286822	-2.766620
6	-3.689013	-4.149547	-2.832151
6	-4.391760	-2.027131	1.342436
6	-5.619866	-2.576027	0.858897
6	-6.620857	-2.879412	1.829775
7	-6.465311	-2.655525	3.165016
6	-5.332900	-2.131126	3.563381
6	-4.267302	-1.805046	2.691287
6	-7.844873	-3.443743	1.395982

6	-8.081820	-3.704570	0.070889
6	-7.087454	-3.394744	-0.892573
6	-5.888856	-2.834701	-0.504689
9	-3.594240	4.732241	-3.742372
9	-4.245449	6.207169	-2.315388
9	1.780995	4.940457	-0.127175
9	0.763312	5.310471	1.733078
1	-1.868523	-2.681931	1.789666
1	-2.349950	-4.839650	1.047220
1	-3.442155	-4.154249	-0.150908
1	1.224634	-2.827387	0.149725
1	0.257787	-3.343756	1.539167
1	0.722285	-4.800216	-1.034348
1	0.025955	-5.427452	0.459828
1	-1.700410	-5.500902	-1.296696
1	-0.632029	-3.798562	-2.732045
1	0.116251	-1.857659	-1.732362
1	-1.554170	-1.295490	-1.601394
1	-2.749080	-2.355083	-3.328751
1	-4.570410	-3.930628	-3.426621
1	-3.689495	-5.095825	-2.296422
1	-3.518491	-1.775065	-0.618673
1	-3.355299	-1.376632	3.100823
1	-5.173852	-2.589517	-1.281238
1	-5.224124	-1.950527	4.631113
1	-8.590866	-3.660665	2.153560
1	-9.029058	-4.135714	-0.230467
1	-2.069161	-0.232200	1.414378
1	-1.894133	1.667603	1.221055
1	-3.698997	3.219048	-1.695444
1	-0.463714	3.183436	1.123567
1	-0.911837	6.501798	-1.590982
8	-7.242401	-3.618466	-2.222470
6	-8.467062	-4.170029	-2.667320
1	-8.381276	-4.258127	-3.750553
1	-8.639950	-5.164648	-2.239780
1	-9.313890	-3.517107	-2.427072
1	-0.497652	-1.359745	0.484615
6	4.156808	2.674591	-0.823271
1	3.820404	3.561958	-0.282142
1	5.216743	2.513240	-0.613839
1	4.060737	2.880536	-1.895207

1-Michael-nitrostyrene-Ph-to-Me-re-re_conf-4

Number of imaginary frequencies : 1
The smallest frequency is : -306.0933 cm(-1)

Electronic energy : =-3713.6103511
Zero-point correction= 0.999929
Thermal correction to Energy= 1.062643
Thermal correction to Enthalpy= 1.063588
Thermal correction to Gibbs Free Energy= 0.897349
Sum of electronic and zero-point Energies= -3712.610422
Sum of electronic and thermal Energies= -3712.547708
Sum of electronic and thermal Enthalpies= -3712.546764
Sum of electronic and thermal Free Energies= -3712.713002

Cartesian Coordinates

6	-3.355561	-0.371558	-2.645288
6	-3.524313	1.149669	-2.525196
6	-3.907866	1.361855	-1.055993
7	-3.430411	0.151935	-0.361869
6	-2.768340	-0.785608	-1.289459
6	-3.927498	-0.226565	0.816237
6	-4.645046	0.598342	1.667592

8	0.004375	0.736526	1.077940
6	-1.231816	-0.616453	-1.263399
8	-0.550965	-1.582207	-0.836198
8	-0.793702	0.469100	-1.710307
8	-1.458625	-0.410775	2.203715
1	-3.010851	-1.811219	-0.997970
1	-2.708479	-0.658495	-3.476708
1	-4.331104	-0.851562	-2.780071
1	-2.579875	1.644647	-2.745664
1	-4.296245	1.535621	-3.193695
1	-3.465108	2.262084	-0.620174
1	-4.996380	1.416082	-0.928052
1	-3.641998	-1.226336	1.138425
1	-5.067121	1.506665	1.242381
6	-5.361949	0.035403	2.872735
6	-6.889668	0.124370	2.783011
1	-5.065595	0.585859	3.776571
1	-5.050940	-1.003439	3.039862
1	-7.326763	-0.101748	3.765482
1	-7.180077	1.164386	2.577874
6	-7.563829	-0.757928	1.778658
6	-6.982067	-1.713625	1.049376
1	-8.635130	-0.609390	1.642629
1	-5.919931	-1.913653	1.132465
6	-7.776185	-2.532996	0.095845
8	-8.992502	-2.594577	0.155369
6	-7.026955	-3.291394	-0.957753
6	-5.729860	-2.935126	-1.337577
6	-7.665046	-4.355890	-1.600489
6	-5.074236	-3.640275	-2.342416
1	-5.241537	-2.083786	-0.869551
6	-7.004868	-5.069471	-2.593149
1	-8.678657	-4.608201	-1.305958
6	-5.708634	-4.712870	-2.964673
1	-4.071373	-3.349478	-2.642568
1	-7.500106	-5.901553	-3.083255
1	-5.195588	-5.266808	-3.744596
6	-3.013873	1.717818	2.573343
1	-3.004235	0.947558	3.338902
1	-1.564361	2.626718	1.190479
7	-1.083794	0.662989	1.679208
6	-1.887629	1.777204	1.773031
7	1.571701	1.688281	-1.039461
6	1.335255	3.050157	-0.858060
6	2.313892	4.033583	-0.677490
6	1.924100	5.364432	-0.556074
6	0.592127	5.759242	-0.622542
6	-0.365091	4.770577	-0.821154
6	-0.009721	3.435219	-0.936888
6	2.984089	6.400052	-0.308306
9	4.129588	6.106602	-0.939150
6	-1.824687	5.104717	-0.883884
9	-2.053761	6.420881	-0.930809
6	2.500863	0.873363	-0.478032
16	3.908884	1.362390	0.317311
7	2.145165	-0.427313	-0.612075
6	2.932931	-1.551509	-0.163301
6	2.001468	-2.614093	0.447881
6	2.776978	-3.716353	1.203609
6	2.380722	-3.698215	2.688099
6	0.888472	-4.042167	2.788337
6	0.090379	-3.064410	1.904389
7	1.013466	-1.995417	1.403197
6	1.673539	-1.297424	2.546501
6	2.592424	-2.296614	3.296412
6	4.022575	-1.811196	3.330179
6	5.116782	-2.562902	3.238582
6	3.718267	-2.195486	-1.304094
6	5.115455	-2.486655	-1.213395
6	5.714536	-3.143512	-2.329837

7	5.031079	-3.478537	-3.460277
6	3.759021	-3.170607	-3.512775
6	3.059786	-2.533857	-2.459760
6	7.091282	-3.469859	-2.273468
6	7.852921	-3.168222	-1.174175
6	7.257725	-2.503797	-0.070976
6	5.921311	-2.166204	-0.096431
9	2.598080	7.618478	-0.721004
9	3.277888	6.509317	0.997980
9	-2.487234	4.629638	0.197331
9	-2.422691	4.549265	-1.950827
1	1.372861	-3.024075	-0.346479
1	2.551091	-4.696637	0.774969
1	3.850989	-3.552394	1.090336
1	-0.704652	-2.547708	2.439058
1	-0.337366	-3.529934	1.014898
1	0.555536	-3.973275	3.828005
1	0.717762	-5.069499	2.456190
1	2.969635	-4.435303	3.240223
1	2.244165	-2.338477	4.336814
1	0.857381	-0.916807	3.162918
1	2.214944	-0.438867	2.139889
1	4.138234	-0.735445	3.467754
1	6.105368	-2.118084	3.291626
1	5.078166	-3.640255	3.097376
1	3.622602	-1.186128	0.599555
1	2.001090	-2.316019	-2.579304
1	5.522235	-1.634655	0.759352
1	3.226827	-3.435338	-4.424436
1	7.522826	-3.967762	-3.135588
1	8.903966	-3.430545	-1.160809
1	1.212619	-0.645086	-0.979126
1	0.715389	1.187795	-1.344455
1	3.360171	3.761832	-0.642229
1	-0.763986	2.665072	-1.088728
1	0.313436	6.802684	-0.536351
8	7.942467	-2.163053	1.050520
6	9.328389	-2.444673	1.096891
1	9.679348	-2.071301	2.059091
1	9.523431	-3.521981	1.037765
1	9.870363	-1.930579	0.295075
1	0.433549	-1.302309	0.892276
6	-3.750548	2.991757	2.885013
1	-3.831855	3.631559	2.003267
1	-4.752716	2.797774	3.275568
1	-3.199737	3.546756	3.652530

1-Michael-nitrostyrene-Ph-to-Me-re-re_conf-5

Number of imaginary frequencies : 1
The smallest frequency is : -321.1147 cm(-1)

Electronic energy : =-3713.6140302
Zero-point correction= 1.001018
Thermal correction to Energy= 1.063190
Thermal correction to Enthalpy= 1.064135
Thermal correction to Gibbs Free Energy= 0.901173
Sum of electronic and zero-point Energies= -3712.613012
Sum of electronic and thermal Energies= -3712.550840
Sum of electronic and thermal Enthalpies= -3712.549896
Sum of electronic and thermal Free Energies= -3712.712858

Cartesian Coordinates

6	3.105249	0.034534	4.430973
6	3.966726	1.119068	3.766635
6	4.515848	0.440651	2.503184

7	3.631142	-0.716145	2.275935
6	2.523268	-0.750279	3.247045
6	4.045428	-1.811424	1.634015
6	5.139642	-1.850825	0.788478
8	1.022619	0.214519	-0.258558
6	1.260121	-0.059429	2.689470
8	0.218095	-0.754870	2.574032
8	1.373099	1.161813	2.433802
8	1.853296	-1.783092	-0.079295
1	2.283326	-1.788761	3.482764
1	2.325683	0.451062	5.072036
1	3.728973	-0.635390	5.031871
1	3.347368	1.972482	3.495751
1	4.777352	1.457136	4.415426
1	4.528297	1.104179	1.634335
1	5.533158	0.062828	2.660831
1	3.396978	-2.676717	1.737387
1	5.833921	-1.016152	0.842516
6	5.745454	-3.149142	0.300278
6	4.991407	-4.442337	0.640341
1	6.754217	-3.235400	0.720077
1	5.889082	-3.114339	-0.790739
1	5.670481	-5.275642	0.415780
1	4.777645	-4.497203	1.713374
6	3.739688	-4.688110	-0.149506
6	2.585483	-5.098404	0.388796
1	3.831105	-4.603329	-1.232973
1	2.503108	-5.234216	1.466576
6	1.391995	-5.582673	-0.348446
8	0.595688	-6.304117	0.234242
6	1.145483	-5.222651	-1.783495
6	1.503369	-3.980795	-2.317073
6	0.439494	-6.137756	-2.572852
6	1.162952	-3.663427	-3.631304
1	1.997272	-3.247031	-1.687010
6	0.121149	-5.826424	-3.889042
1	0.146027	-7.087396	-2.136362
6	0.481864	-4.587340	-4.419678
1	1.427091	-2.690729	-4.035265
1	-0.415014	-6.544486	-4.501286
1	0.225175	-4.341042	-5.445362
6	4.238370	-0.976321	-1.010660
1	3.948804	-1.994391	-1.257982
1	3.297755	0.988766	-0.774401
7	1.986242	-0.563406	-0.338211
6	3.221798	-0.087330	-0.721779
7	-0.190089	2.543761	0.647105
6	0.646407	3.421982	-0.042699
6	0.220638	4.435961	-0.907022
6	1.167448	5.269370	-1.495660
6	2.528814	5.143735	-1.240675
6	2.932118	4.144779	-0.362069
6	2.014434	3.289660	0.230608
6	0.698901	6.315625	-2.466467
9	-0.513300	6.789808	-2.149165
6	4.382325	3.934670	-0.048123
9	5.154679	4.938847	-0.476969
6	-1.323297	1.918734	0.232566
16	-2.264981	2.347447	-1.103483
7	-1.611888	0.857624	1.022951
6	-2.767060	0.004783	0.864246
6	-2.369271	-1.462624	1.113212
6	-3.473843	-2.445864	0.664822
6	-2.935902	-3.347762	-0.455827
6	-1.785873	-4.186095	0.115174
6	-0.728748	-3.237086	0.709483
7	-1.099170	-1.820185	0.386158
6	-1.214258	-1.637967	-1.091411
6	-2.381048	-2.508976	-1.625442
6	-3.395624	-1.669553	-2.364394

6	-4.718423	-1.811718	-2.334251
6	-3.888901	0.367836	1.834032
6	-5.241458	0.561930	1.414231
6	-6.205818	0.825438	2.432290
7	-5.893059	0.924564	3.755157
6	-4.636765	0.770557	4.093762
6	-3.602164	0.485546	3.170954
6	-7.561767	0.995471	2.061390
6	-7.960246	0.914800	0.751793
6	-6.995949	0.669378	-0.259681
6	-5.667119	0.503500	0.067435
9	1.539418	7.362293	-2.516806
9	0.611871	5.830931	-3.716820
9	4.858815	2.804916	-0.622134
9	4.595687	3.791509	1.270536
1	-2.111734	-1.585690	2.168586
1	-3.792940	-3.062983	1.509181
1	-4.346679	-1.883831	0.324672
1	0.267106	-3.377585	0.290544
1	-0.653292	-3.289950	1.797038
1	-1.339441	-4.804934	-0.667996
1	-2.155614	-4.863193	0.889027
1	-3.729798	-4.006593	-0.817266
1	-1.949060	-3.212013	-2.351745
1	-0.245710	-1.934237	-1.498934
1	-1.351966	-0.569754	-1.280056
1	-2.970084	-0.885366	-2.991690
1	-5.362629	-1.160049	-2.915923
1	-5.213843	-2.568731	-1.731436
1	-3.115669	0.113394	-0.164296
1	-2.583996	0.361643	3.532295
1	-4.965378	0.349894	-0.743919
1	-4.399416	0.861600	5.152043
1	-8.276168	1.192353	2.854067
1	-9.005548	1.049147	0.500177
1	-0.923912	0.560129	1.725648
1	0.326290	2.026120	1.384738
1	-0.832841	4.574923	-1.107294
1	2.335438	2.507521	0.916410
1	3.247582	5.813836	-1.697053
8	-7.304252	0.584648	-1.579125
6	-8.642439	0.826489	-1.968486
1	-8.659082	0.742792	-3.055363
1	-9.328364	0.084714	-1.542857
1	-8.969303	1.832791	-1.681955
1	-0.330428	-1.220145	0.739683
6	5.483960	-0.435755	-1.659737
1	5.763739	0.529694	-1.231070
1	6.329033	-1.121192	-1.566789
1	5.297289	-0.285691	-2.728932

1-Michael-nitrostyrene-Ph-to-Me-re-re_conf-6

Number of imaginary frequencies : 1

The smallest frequency is : -333.8892 cm(-1)

Electronic energy : =-3713.6089505

Zero-point correction= 1.000204

Thermal correction to Energy= 1.063088

Thermal correction to Enthalpy= 1.064032

Thermal correction to Gibbs Free Energy= 0.896369

Sum of electronic and zero-point Energies= -3712.608747

Sum of electronic and thermal Energies= -3712.545863

Sum of electronic and thermal Enthalpies= -3712.544919

Sum of electronic and thermal Free Energies= -3712.712581

Cartesian Coordinates

6	0.996969	1.511649	4.716997
6	1.295600	2.850952	4.031491
6	2.388254	2.500567	3.018114
7	2.198872	1.064872	2.747981
6	1.131723	0.483265	3.588667
6	3.150656	0.313555	2.192713
6	4.255065	0.822091	1.531066
8	-0.046514	0.574993	-0.219316
6	-0.176120	0.323391	2.780814
8	-0.496932	-0.841189	2.433396
8	-0.821929	1.374698	2.559296
8	1.725285	-0.674290	-0.068596
1	1.449568	-0.502768	3.933399
1	0.005913	1.485549	5.172866
1	1.745916	1.302874	5.488206
1	0.401711	3.208254	3.521631
1	1.636852	3.616667	4.731000
1	2.325156	3.083508	2.095207
1	3.390251	2.640079	3.445063
1	2.941327	-0.752023	2.199003
1	4.520845	1.854720	1.741761
6	5.389918	-0.067171	1.076373
6	4.989152	-1.521756	0.847561
1	6.215727	-0.025477	1.798694
1	5.797624	0.334135	0.137133
1	4.699861	-1.988372	1.800163
1	4.083476	-1.565589	0.224676
6	6.043101	-2.388153	0.234493
6	7.294275	-2.032285	-0.072781
1	5.762483	-3.420686	0.027776
1	7.658274	-1.028068	0.114278
6	8.226485	-3.038148	-0.651648
8	7.920960	-4.217416	-0.723356
6	9.571412	-2.582867	-1.135369
6	9.871841	-1.242605	-1.396006
6	10.548421	-3.560157	-1.354263
6	11.133694	-0.886703	-1.863813
1	9.121378	-0.470815	-1.261364
6	11.810568	-3.203014	-1.809046
1	10.294224	-4.596499	-1.157551
6	12.105000	-1.863788	-2.064030
1	11.357574	0.154373	-2.073354
1	12.566416	-3.965724	-1.966606
1	13.090671	-1.582441	-2.421664
6	3.362596	1.405508	-0.376224
1	3.707287	0.440907	-0.738207
1	1.466901	2.511935	-0.275573
7	1.192514	0.453297	-0.192572
6	1.992309	1.568858	-0.294122
7	-2.445338	1.870088	0.396380
6	-2.069865	3.074555	-0.196822
6	-2.739902	3.723389	-1.237030
6	-2.251314	4.943654	-1.702656
6	-1.128703	5.551600	-1.157149
6	-0.485269	4.900214	-0.107708
6	-0.936720	3.680576	0.367854
6	-2.966637	5.591636	-2.854041
9	-4.297051	5.583656	-2.682817
6	0.764395	5.473671	0.487340
9	0.874617	6.790602	0.281804
6	-2.989138	0.750680	-0.148700
16	-3.835861	0.661135	-1.607743
7	-2.746756	-0.327904	0.633231
6	-3.248570	-1.660854	0.397428
6	-2.139195	-2.689097	0.690778
6	-2.487779	-4.097890	0.162494
6	-1.486141	-4.497589	-0.932228
6	-0.098288	-4.610605	-0.287127
6	0.215243	-3.294569	0.449413

7	-0.821978	-2.274246	0.087203
6	-0.896166	-2.106037	-1.395183
6	-1.411667	-3.422002	-2.035013
6	-2.685797	-3.199444	-2.815178
6	-3.711285	-4.041986	-2.912950
6	-4.443276	-1.981132	1.293602
6	-5.672854	-2.506281	0.788307
6	-6.692459	-2.801328	1.742176
7	-6.551886	-2.591705	3.081449
6	-5.416624	-2.089790	3.500237
6	-4.333777	-1.773226	2.645919
6	-7.919561	-3.340818	1.285850
6	-8.141656	-3.586129	-0.044836
6	-7.128087	-3.285564	-0.991108
6	-5.926092	-2.749229	-0.581079
9	-2.592635	6.868895	-3.025675
9	-2.723896	4.952862	-4.010142
9	1.872393	4.905274	-0.043347
9	0.840030	5.259879	1.811637
1	-1.942485	-2.690394	1.765347
1	-2.446631	-4.826738	0.976867
1	-3.509495	-4.101990	-0.224422
1	1.174502	-2.862500	0.170347
1	0.178428	-3.385675	1.536497
1	0.657070	-4.806373	-1.053751
1	-0.075915	-5.445822	0.417516
1	-1.773321	-5.457982	-1.368147
1	-0.650643	-3.749916	-2.755370
1	0.115061	-1.841108	-1.708914
1	-1.547027	-1.250830	-1.595493
1	-2.730513	-2.256642	-3.361233
1	-4.578397	-3.796829	-3.518066
1	-3.737911	-4.997447	-2.394651
1	-3.540134	-1.719980	-0.653034
1	-3.420826	-1.362696	3.071423
1	-5.195249	-2.510631	-1.344850
1	-5.319866	-1.920562	4.570983
1	-8.680111	-3.551446	2.030633
1	-9.091830	-3.997798	-0.363568
1	-2.097253	-0.224201	1.419711
1	-1.890579	1.676593	1.249704
1	-3.629069	3.284572	-1.669838
1	-0.421637	3.166978	1.177729
1	-0.773100	6.505711	-1.526736
8	-7.266994	-3.495659	-2.324969
6	-8.493096	-4.024993	-2.792347
1	-8.391811	-4.107939	-3.874649
1	-8.688119	-5.019331	-2.373615
1	-9.333144	-3.360125	-2.561164
1	-0.527607	-1.370869	0.506204
6	4.215617	2.601853	-0.699221
1	3.883490	3.490395	-0.157556
1	5.269043	2.422830	-0.471983
1	4.141773	2.816898	-1.771155

1-Michael-nitrostyrene-Ph-to-Me-re-re_conf-7

Number of imaginary frequencies : 1
The smallest frequency is : -344.9037 cm(-1)

Electronic energy : =-3713.612157
Zero-point correction= 1.000584
Thermal correction to Energy= 1.063077
Thermal correction to Enthalpy= 1.064021
Thermal correction to Gibbs Free Energy= 0.899956
Sum of electronic and zero-point Energies= -3712.611573
Sum of electronic and thermal Energies= -3712.549080

Sum of electronic and thermal Enthalpies= -3712.548136
Sum of electronic and thermal Free Energies= -3712.712201

Cartesian Coordinates			
6	-2.607990	1.992197	3.928068
6	-3.887018	1.246261	3.516809
6	-4.219315	1.801439	2.122720
7	-2.977304	2.447587	1.662033
6	-1.867657	2.213498	2.601900
6	-2.970467	3.459985	0.795654
6	-4.019520	3.765944	-0.057650
8	-1.160798	0.095277	-0.615191
6	-1.053093	0.962734	2.206614
8	0.168408	1.117121	1.955045
8	-1.685882	-0.119308	2.209645
8	-1.124757	2.242318	-0.959930
1	-1.208001	3.083338	2.603491
1	-2.006816	1.430532	4.646077
1	-2.854842	2.964938	4.366151
1	-3.690893	0.176942	3.456525
1	-4.707369	1.420350	4.216065
1	-4.541277	1.025253	1.423999
1	-5.002347	2.567487	2.169927
1	-2.025260	3.990058	0.720190
1	-4.983855	3.324236	0.179466
6	-4.084389	5.074200	-0.817614
6	-2.914800	6.046395	-0.624779
1	-5.000355	5.599106	-0.524499
1	-4.190933	4.883574	-1.896624
1	-3.194118	6.983768	-1.125602
1	-2.782901	6.288930	0.435946
6	-1.607957	5.619702	-1.221519
6	-0.414301	5.866138	-0.669648
1	-1.626045	5.136670	-2.199858
1	-0.343844	6.355577	0.298682
6	0.843491	5.560998	-1.396339
8	0.847318	5.146840	-2.545245
6	2.140968	5.799421	-0.685416
6	3.269898	6.110791	-1.449320
6	2.261913	5.646080	0.698237
6	4.504358	6.279712	-0.835028
1	3.159181	6.211737	-2.524590
6	3.506007	5.783726	1.309347
1	1.393752	5.384212	1.296720
6	4.624673	6.107672	0.544433
1	5.375921	6.537001	-1.428367
1	3.601340	5.642958	2.381255
1	5.591381	6.228691	1.023328
6	-3.711168	2.294315	-1.604839
1	-3.051487	3.014069	-2.081129
1	-3.595579	0.203111	-0.933115
7	-1.748810	1.158736	-0.893812
6	-3.103134	1.142721	-1.136270
7	-1.049812	-2.359372	0.758869
6	-2.232111	-2.916906	0.276939
6	-2.355821	-4.147702	-0.375669
6	-3.618803	-4.582537	-0.772016
6	-4.771328	-3.845841	-0.528664
6	-4.631949	-2.634799	0.142114
6	-3.389204	-2.168132	0.539158
6	-3.713442	-5.880143	-1.523199
9	-2.926764	-6.826648	-0.990524
6	-5.818924	-1.760807	0.410578
9	-6.981341	-2.399873	0.240335
6	0.215859	-2.409994	0.268779
16	0.809411	-3.515500	-0.862219
7	0.975837	-1.420973	0.795972
6	2.373016	-1.205634	0.501667
6	2.640307	0.308810	0.405602

6	4.031946	0.630660	-0.182113
6	3.869318	1.393936	-1.505083
6	3.195166	2.738106	-1.203730
6	1.887014	2.475894	-0.435304
7	1.604515	1.002432	-0.440552
6	1.560045	0.485397	-1.841487
6	2.965661	0.615822	-2.482505
6	3.498015	-0.723626	-2.935068
6	4.765694	-1.125930	-2.888240
6	3.283254	-1.782970	1.583744
6	4.419750	-2.598568	1.288805
6	5.227589	-3.009044	2.391171
7	4.951954	-2.685075	3.686172
6	3.884236	-1.960995	3.914941
6	3.024690	-1.482743	2.897654
6	6.378244	-3.795032	2.139500
6	6.725402	-4.167292	0.866247
6	5.911708	-3.769390	-0.225847
6	4.781841	-3.008854	-0.014545
9	-4.966210	-6.362538	-1.537485
9	-3.334799	-5.740281	-2.804120
9	-5.838649	-0.686949	-0.412863
9	-5.807184	-1.263272	1.659054
1	2.501424	0.747173	1.396819
1	4.605868	1.239652	0.522004
1	4.587675	-0.296722	-0.338116
1	1.018169	2.948180	-0.892133
1	1.934268	2.767480	0.615703
1	2.977840	3.276194	-2.131803
1	3.853985	3.372949	-0.603525
1	4.848686	1.562104	-1.960521
1	2.852137	1.235527	-3.381612
1	0.801132	1.085500	-2.347388
1	1.201048	-0.546439	-1.797129
1	2.751814	-1.396869	-3.358553
1	5.056106	-2.105417	-3.254848
1	5.560730	-0.508993	-2.476351
1	2.585445	-1.680730	-0.458470
1	2.161751	-0.878062	3.166607
1	4.179196	-2.753732	-0.877969
1	3.669942	-1.718128	4.953979
1	6.976122	-4.092898	2.994631
1	7.612434	-4.768369	0.704414
1	0.526130	-0.707824	1.382743
1	-1.232938	-1.523548	1.347618
1	-1.480986	-4.754417	-0.567180
1	-3.287557	-1.217041	1.058889
1	-5.743249	-4.208339	-0.840637
8	6.180972	-4.099855	-1.514985
6	7.295022	-4.933688	-1.769291
1	7.308109	-5.097605	-2.847028
1	8.234772	-4.455195	-1.469026
1	7.198389	-5.900183	-1.261472
1	0.665625	0.865631	-0.021590
6	-5.119598	2.198760	-2.126774
1	-5.738022	1.564143	-1.487794
1	-5.592103	3.179768	-2.213617
1	-5.100982	1.751123	-3.126575

1-Michael-nitrostyrene-Ph-to-Me-re-re_conf-8

Number of imaginary frequencies : 1

The smallest frequency is : -350.7411 cm(-1)

Electronic energy : =-3713.6063599

Zero-point correction= 0.999817

Thermal correction to Energy= 1.062710

Thermal correction to Enthalpy= 1.063654
 Thermal correction to Gibbs Free Energy= 0.894908
 Sum of electronic and zero-point Energies= -3712.606543
 Sum of electronic and thermal Energies= -3712.543650
 Sum of electronic and thermal Enthalpies= -3712.542705
 Sum of electronic and thermal Free Energies= -3712.711452

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 Cartesian Coordinates

6	2.490968	-0.698352	3.445375
6	3.068658	0.604798	2.881745
6	3.649063	0.178889	1.533477
7	2.820432	-0.967270	1.130340
6	1.915484	-1.405666	2.216020
6	3.140122	-1.755602	0.105929
6	4.106898	-1.470532	-0.843086
8	-0.191387	0.178552	-0.836038
6	0.465796	-0.981791	1.890652
8	-0.275991	-1.856763	1.377083
8	0.153356	0.198335	2.173356
8	0.991378	-1.448387	-1.665709
1	1.947456	-2.495080	2.287572
1	1.725698	-0.524711	4.202909
1	3.286972	-1.312206	3.880228
1	2.263948	1.326066	2.738903
1	3.832382	1.048021	3.523678
1	3.614094	0.966695	0.776307
1	4.690597	-0.159801	1.629653
1	2.504138	-2.631491	-0.007259
1	4.893522	-0.770725	-0.572787
6	4.416738	-2.549255	-1.865025
6	5.353958	-2.134007	-2.999990
1	3.466989	-2.880232	-2.304511
1	4.848844	-3.431751	-1.373592
1	5.418022	-2.955550	-3.726784
1	4.936061	-1.294057	-3.568431
6	6.756069	-1.785867	-2.603172
6	7.308233	-1.950484	-1.396519
1	7.396988	-1.379021	-3.385402
1	6.736936	-2.360787	-0.570839
6	8.738799	-1.597014	-1.183398
8	9.460202	-1.294628	-2.119654
6	9.293396	-1.627331	0.209967
6	8.486411	-1.660863	1.351286
6	10.684326	-1.592078	0.354557
6	9.065091	-1.662543	2.617357
1	7.404606	-1.663457	1.264938
6	11.260954	-1.605310	1.617244
1	11.294248	-1.555420	-0.541974
6	10.450368	-1.640811	2.751705
1	8.433507	-1.679010	3.499760
1	12.341077	-1.585590	1.721129
1	10.898969	-1.648340	3.740317
6	3.117378	0.106192	-2.019638
1	2.971813	-0.692831	-2.740596
1	1.853811	1.547317	-0.947292
7	0.881172	-0.256043	-1.299018
6	1.973786	0.573905	-1.398395
7	-1.724542	1.752958	0.910858
6	-1.168814	2.968332	0.512443
6	-1.881113	4.076751	0.044891
6	-1.187767	5.240855	-0.276401
6	0.191487	5.346982	-0.137556
6	0.881933	4.239801	0.344428
6	0.220906	3.064526	0.666172
6	-1.954379	6.407645	-0.831580
9	-3.204877	6.462305	-0.353290
6	2.376159	4.265954	0.459090
9	2.866657	5.508819	0.514659
6	-2.752006	1.044187	0.376910

16	-3.955701	1.646596	-0.643975
7	-2.687016	-0.255511	0.754251
6	-3.657410	-1.268618	0.413254
6	-2.929080	-2.579059	0.060364
6	-3.871877	-3.612004	-0.595664
6	-3.396262	-3.905005	-2.027059
6	-2.010517	-4.557326	-1.942836
6	-1.076593	-3.637389	-1.133239
7	-1.773746	-2.335362	-0.875693
6	-2.198294	-1.705175	-2.161753
6	-3.264548	-2.602870	-2.843017
6	-4.552966	-1.851523	-3.080461
6	-5.786270	-2.338221	-2.967350
6	-4.621132	-1.548746	1.564186
6	-6.041162	-1.553661	1.399965
6	-6.825684	-1.887588	2.544396
7	-6.289978	-2.173513	3.764625
6	-4.985560	-2.132196	3.878443
6	-4.111753	-1.830397	2.806961
6	-8.235557	-1.925708	2.418989
6	-8.855100	-1.646672	1.227932
6	-8.072860	-1.301037	0.095847
6	-6.698086	-1.251682	0.185268
9	-1.360936	7.577015	-0.540957
9	-2.051071	6.346647	-2.169954
9	2.962915	3.664708	-0.601525
9	2.813548	3.606771	1.545332
1	-2.455370	-2.969347	0.964601
1	-3.879823	-4.538281	-0.014637
1	-4.892978	-3.223462	-0.600913
1	-0.157869	-3.386597	-1.660228
1	-0.814585	-4.035867	-0.151406
1	-1.608456	-4.716731	-2.947476
1	-2.084328	-5.534746	-1.458968
1	-4.097278	-4.582496	-2.521539
1	-2.870729	-2.878740	-3.830320
1	-1.283628	-1.601522	-2.747752
1	-2.566317	-0.701914	-1.929636
1	-4.426855	-0.816079	-3.398518
1	-6.651849	-1.718964	-3.180324
1	-5.987816	-3.359763	-2.653980
1	-4.210620	-0.913119	-0.458006
1	-3.038487	-1.820507	2.981896
1	-6.148152	-0.953531	-0.699357
1	-4.571002	-2.352595	4.860399
1	-8.809129	-2.183459	3.303244
1	-9.935981	-1.684088	1.163092
1	-1.846237	-0.577055	1.243410
1	-1.041043	1.162168	1.419879
1	-2.956855	4.030703	-0.056782
1	0.762499	2.196669	1.037020
1	0.708923	6.266958	-0.383630
8	-8.606073	-1.003881	-1.116617
6	-10.015233	-0.939083	-1.227773
1	-10.221911	-0.630997	-2.252932
1	-10.480718	-1.915380	-1.048094
1	-10.439033	-0.199734	-0.538764
1	-1.088528	-1.708804	-0.409701
6	4.236918	1.082312	-2.268318
1	4.333843	1.796346	-1.447347
1	5.200048	0.587586	-2.407761
1	4.019258	1.652790	-3.178843

1-Michael-nitrostyrene-Ph-to-Me-re-re_conf-9

Number of imaginary frequencies : 1
The smallest frequency is : -338.1554 cm(-1)

Electronic energy : =-3713.6115908
 Zero-point correction= 1.001098
 Thermal correction to Energy= 1.063380
 Thermal correction to Enthalpy= 1.064324
 Thermal correction to Gibbs Free Energy= 0.901205
 Sum of electronic and zero-point Energies= -3712.610493
 Sum of electronic and thermal Energies= -3712.548211
 Sum of electronic and thermal Enthalpies= -3712.547267
 Sum of electronic and thermal Free Energies= -3712.710386

 Cartesian Coordinates

6	2.801000	-0.318316	4.603083
6	3.689213	0.866290	4.189685
6	4.330266	0.430383	2.857373
7	3.581608	-0.772465	2.452287
6	2.366181	-0.922560	3.259522
6	4.137307	-1.794132	1.804172
6	5.288084	-1.701294	1.036536
8	1.057333	0.126838	-0.261582
6	1.190982	-0.114252	2.675326
8	0.078097	-0.701189	2.605697
8	1.429271	1.076819	2.375118
8	1.930224	-1.847436	-0.014433
1	2.087306	-1.976122	3.315452
1	1.949649	-0.016599	5.217267
1	3.382067	-1.062966	5.156600
1	3.078804	1.753822	4.030537
1	4.449185	1.087808	4.941803
1	4.261009	1.206046	2.092109
1	5.381817	0.151494	2.981193
1	3.558449	-2.713240	1.816290
1	5.872037	-0.790292	1.149677
6	6.117606	-2.922032	0.689572
6	5.383428	-4.271319	0.615133
1	6.924791	-3.012124	1.427215
1	6.620703	-2.761878	-0.272932
1	6.145476	-5.050143	0.489458
1	4.852501	-4.492044	1.547203
6	4.453548	-4.303438	-0.552955
6	3.145225	-4.564359	-0.538386
1	4.893088	-4.037813	-1.516313
1	2.627850	-4.854861	0.373291
6	2.369786	-4.395753	-1.796905
8	2.756324	-3.635049	-2.668314
6	1.119202	-5.196653	-2.006750
6	0.820202	-6.331323	-1.246419
6	0.277744	-4.832462	-3.063793
6	-0.302699	-7.099255	-1.549617
1	1.478407	-6.636201	-0.438382
6	-0.848305	-5.592655	-3.357862
1	0.538721	-3.960303	-3.655345
6	-1.136395	-6.730906	-2.603041
1	-0.523559	-7.987960	-0.967216
1	-1.495079	-5.307312	-4.181792
1	-2.009382	-7.331153	-2.839652
6	4.362783	-0.957059	-0.787974
1	4.096497	-1.970890	-1.072129
1	3.331953	0.970750	-0.614752
7	2.053310	-0.623857	-0.261846
6	3.294808	-0.105738	-0.539869
7	-0.142399	2.550588	0.594732
6	0.677010	3.440656	-0.100030
6	0.229933	4.474029	-0.929272
6	1.163517	5.303388	-1.544202
6	2.531439	5.150048	-1.352112
6	2.957150	4.133717	-0.503269
6	2.052179	3.289178	0.122125
6	0.672620	6.370820	-2.480299

9	-0.529333	6.842317	-2.121428
6	4.421637	3.879827	-0.312150
9	5.166502	4.963822	-0.560278
6	-1.305616	1.962519	0.206997
16	-2.285654	2.441437	-1.085540
7	-1.593024	0.894433	0.984067
6	-2.759455	0.058060	0.833267
6	-2.369453	-1.414045	1.063441
6	-3.489046	-2.386000	0.629441
6	-2.977089	-3.279289	-0.508361
6	-1.820351	-4.128256	0.034097
6	-0.750744	-3.196140	0.632143
7	-1.110773	-1.776848	0.315763
6	-1.238468	-1.594398	-1.161050
6	-2.438380	-2.429484	-1.677606
6	-3.458321	-1.561418	-2.375101
6	-4.781098	-1.700837	-2.331055
6	-3.858904	0.418985	1.829144
6	-5.218122	0.628949	1.440280
6	-6.159608	0.885230	2.481207
7	-5.818550	0.964663	3.798449
6	-4.556304	0.797703	4.108498
6	-3.542766	0.516860	3.161080
6	-7.521896	1.068283	2.140247
6	-7.947556	1.007223	0.838085
6	-7.005430	0.769846	-0.195833
6	-5.671362	0.591792	0.101880
9	1.515292	7.415889	-2.530765
9	0.551217	5.913524	-3.737688
9	4.866437	2.906509	-1.136725
9	4.707552	3.470193	0.935541
1	-2.095179	-1.545058	2.112530
1	-3.795525	-3.007909	1.475171
1	-4.364491	-1.815621	0.311046
1	0.239515	-3.355613	0.205237
1	-0.676208	-3.250638	1.719969
1	-1.386881	-4.722497	-0.773218
1	-2.185845	-4.820754	0.797341
1	-3.778846	-3.931799	-0.864449
1	-2.042369	-3.129005	-2.426027
1	-0.279361	-1.914610	-1.575676
1	-1.346606	-0.522962	-1.350548
1	-3.038087	-0.761531	-2.985812
1	-5.431310	-1.031424	-2.885250
1	-5.270746	-2.472698	-1.742294
1	-3.125014	0.181380	-0.187729
1	-2.517677	0.377935	3.497757
1	-4.986756	0.445761	-0.725217
1	-4.296510	0.873288	5.162741
1	-8.218589	1.260102	2.949765
1	-8.996837	1.151545	0.609178
1	-0.911938	0.582761	1.690931
1	0.387199	2.006117	1.300310
1	-0.828314	4.628661	-1.086719
1	2.385121	2.495364	0.787787
1	3.242145	5.810370	-1.835393
8	-7.340354	0.705219	-1.509916
6	-8.686376	0.950951	-1.868189
1	-8.726309	0.880039	-2.955360
1	-9.362888	0.203800	-1.436727
1	-9.007695	1.953548	-1.563008
1	-0.331614	-1.176152	0.643496
6	5.585656	-0.347195	-1.421349
1	5.815592	0.625435	-0.979880
1	6.464613	-0.988961	-1.340615
1	5.389642	-0.192400	-2.488219

Number of imaginary frequencies : 1
The smallest frequency is : -348.8564 cm(-1)

Electronic energy : =-3713.6064976
Zero-point correction= 1.000405
Thermal correction to Energy= 1.063107
Thermal correction to Enthalpy= 1.064051
Thermal correction to Gibbs Free Energy= 0.896414
Sum of electronic and zero-point Energies= -3712.606093
Sum of electronic and thermal Energies= -3712.543391
Sum of electronic and thermal Enthalpies= -3712.542447
Sum of electronic and thermal Free Energies= -3712.710083

Cartesian Coordinates

6	2.495739	-0.743969	3.445771
6	3.073704	0.571199	2.910577
6	3.671549	0.168167	1.564180
7	2.844158	-0.966370	1.128928
6	1.933364	-1.430896	2.198393
6	3.165254	-1.715728	0.076645
6	4.131597	-1.386492	-0.859070
8	-0.188598	0.207561	-0.812951
6	0.482455	-1.006051	1.875877
8	-0.257041	-1.877468	1.352870
8	0.166852	0.169688	2.172620
8	1.024950	-1.361753	-1.706972
1	1.969754	-2.521436	2.248633
1	1.723195	-0.586985	4.199489
1	3.290598	-1.362168	3.876571
1	2.267062	1.290447	2.766604
1	3.827039	1.006915	3.569629
1	3.648678	0.967659	0.819937
1	4.710113	-0.177250	1.669171
1	2.532802	-2.588846	-0.072205
1	4.914730	-0.695682	-0.557807
6	4.449277	-2.412891	-1.930484
6	5.396031	-1.936677	-3.032789
1	3.503796	-2.720357	-2.395464
1	4.877634	-3.319549	-1.481513
1	5.459061	-2.711610	-3.809153
1	4.987255	-1.059628	-3.549533
6	6.798192	-1.622626	-2.609466
6	7.341065	-1.849886	-1.408686
1	7.448573	-1.186198	-3.367545
1	6.761675	-2.293429	-0.605818
6	8.775307	-1.525745	-1.173831
8	9.505498	-1.188588	-2.091150
6	9.322981	-1.633674	0.218074
6	8.509114	-1.681235	1.353731
6	10.713406	-1.658587	0.368495
6	9.080501	-1.755243	2.621014
1	7.428552	-1.637455	1.261572
6	11.282296	-1.745616	1.631869
1	11.329065	-1.610746	-0.523608
6	10.464911	-1.794099	2.760935
1	8.444225	-1.781030	3.499814
1	12.361766	-1.773964	1.740528
1	10.907865	-1.860189	3.749868
6	3.132951	0.239522	-1.966456
1	3.007822	-0.523998	-2.728496
1	1.838940	1.607476	-0.842231
7	0.894534	-0.190093	-1.285406
6	1.976367	0.657451	-1.334897
7	-1.755400	1.732480	0.972553
6	-1.220554	2.961029	0.582131
6	-1.956681	4.070488	0.160692
6	-1.282254	5.243437	-0.173412

6	0.100377	5.351357	-0.095969
6	0.816329	4.240559	0.343298
6	0.173989	3.062278	0.685842
6	-2.077779	6.414328	-0.676821
9	-3.306321	6.453862	-0.143573
6	2.314729	4.284949	0.356502
9	2.788848	5.482117	0.720728
6	-2.770881	1.018325	0.421525
16	-3.984855	1.626374	-0.584201
7	-2.683535	-0.289002	0.764955
6	-3.636814	-1.308606	0.395580
6	-2.886954	-2.594620	0.004771
6	-3.813105	-3.627109	-0.675122
6	-3.335653	-3.876564	-2.113843
6	-1.937367	-4.504042	-2.048051
6	-1.018728	-3.586748	-1.217894
7	-1.740132	-2.304618	-0.928260
6	-2.178900	-1.652873	-2.199014
6	-3.231665	-2.552374	-2.898034
6	-4.535313	-1.819439	-3.109576
6	-5.758593	-2.333193	-3.007984
6	-4.594551	-1.635710	1.539219
6	-6.014960	-1.647529	1.378567
6	-6.793657	-2.016863	2.516087
7	-6.252135	-2.333269	3.726124
6	-4.947578	-2.287896	3.836790
6	-4.079213	-1.949531	2.771872
6	-8.203779	-2.059292	2.394597
6	-8.828946	-1.753320	1.213115
6	-8.052380	-1.375437	0.087512
6	-6.677681	-1.319244	0.173862
9	-1.478158	7.582433	-0.394070
9	-2.232624	6.373292	-2.010442
9	2.825620	4.023554	-0.865036
9	2.844740	3.367396	1.186133
1	-2.401846	-3.000489	0.895856
1	-3.803168	-4.567385	-0.117134
1	-4.840715	-3.256309	-0.669033
1	-0.106064	-3.306717	-1.740664
1	-0.747198	-4.003480	-0.246209
1	-1.534352	-4.631865	-3.056812
1	-1.991962	-5.494030	-1.587678
1	-4.024808	-4.555337	-2.623054
1	-2.837718	-2.795782	-3.893695
1	-1.267227	-1.520543	-2.784141
1	-2.562169	-0.660655	-1.943780
1	-4.430617	-0.772531	-3.396348
1	-6.636506	-1.724495	-3.200017
1	-5.939810	-3.367414	-2.725464
1	-4.196871	-0.938019	-0.464763
1	-3.005502	-1.936928	2.943983
1	-6.132821	-0.995355	-0.704897
1	-4.528564	-2.534352	4.810655
1	-8.772969	-2.342120	3.274025
1	-9.909865	-1.794412	1.150876
1	-1.837277	-0.610217	1.245177
1	-1.056404	1.141142	1.458953
1	-3.035404	4.020157	0.102409
1	0.730875	2.194096	1.029781
1	0.604841	6.275248	-0.356901
8	-8.591338	-1.051948	-1.115627
6	-10.001142	-0.992875	-1.221003
1	-10.212592	-0.664030	-2.238726
1	-10.460756	-1.975262	-1.060923
1	-10.426801	-0.270574	-0.515339
1	-1.067464	-1.671495	-0.453062
6	4.234710	1.249607	-2.152434
1	4.291818	1.935892	-1.303849
1	5.212788	0.783172	-2.286394
1	4.024247	1.848316	-3.046414

END
