Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.734539	1.127495	0.097390
2	8	0.734539	1.127495	2.354900
3	6	1.897217	1.127495	2.859435
4	7	3.020604	1.134285	2.094943
5	6	2.949922	1.244776	0.638700
6	6	2.546960	2.477340	0.076617
7	6	3.773504	0.307111	-0.080327
8	7	4.466382	-0.460511	-0.651837
9	1	2.383103	3.327412	0.728748
10	1	2.749850	2.696930	-0.964737
11	1	3.935482	1.091234	2.537465
12	1	2.041837	1.114203	3.942570
13	15	-1.592302	1.046335	-0.129748
14	15	0.643188	-1.336992	-0.246276
15	6	-2.116016	-0.720966	-0.390318
16	6	-1.189728	-1.720537	-0.442425
17	1	0.797741	1.187714	-1.450139
18	1	0.360404	2.677636	0.024794
19	6	-2.509760	1.875284	1.384353
20	6	-2.549985	2.149458	-1.422835
21	6	1.388431	-2.823407	0.816516
22	6	1.575977	-1.961994	-1.856243
23	6	-1.629071	-3.081190	-0.663286
24	6	-3.518549	-1.026476	-0.554502
25	6	-2.945850	0.855951	2.406139
26	6	-1.611173	2.649441	-2.488230
27	6	1.919244	-2.320769	2.131482
28	6	0.710382	-1.838741	-3.084960
29	1	-1.775084	2.536507	1.830778
30	1	-3.318242	1.533316	-1.881939
31	1	0.585462	-3.527212	1.014342
32	1	2.433249	-1.306300	-1.959132
33	6	-3.674501	2.677816	0.757858
34	6	-3.178470	3.280777	-0.573787
35	6	2.483099	-3.461070	-0.076628
36	6	2.030838	-3.406932	-1.550436
37	1	-4.529341	2.031126	0.569450
38	1	-3.988353	3.462829	1.443283
39	1	-2.439571	4.052620	-0.365326
40	1	-4.000099	3.736743	-1.122793
41	1	3.420349	-2.917065	0.022491
42	1	2.654276	-4.488730	0.238315
43	1	1.222280	-4.114925	-1.717577
44	1	2.854194	-3.676211	-2.209501
45	1	-1.168133	1.789201	-3.033424
46	1	-2.167396	3.279320	-3.214274
47	1	-0.793427	3.253772	-2.042933
48	1	-2.070773	0.261726	2.744410
49	1	-3.386119	1.371980	3.285285
50	1	-3.705383	0.167624	1.982563
51	1	1.298457	-2.112215	-3.986320
52	1	-0.170424	-2.510039	-3.020184
53	1	0.357406	-0.791614	-3.195749
54	1	2.304176	-3.171351	2.732860
55	1	2.744010	-1.597850	1.968872
56	1	1.106253	-1.823000	2.700933
57	6	-2.986024	-3.368060	-0.819258
58	6	-3.929297	-2.342755	-0.763739
59	1	-0.914475	-3.888131	-0.725321
60	1	-3.306568	-4.388028	-0.987637
61	1	-4.980860	-2.568114	-0.885684
62	1	-4.259932	-0.240208	-0.512401

DIHY-C:

E(Basis I/Basis I): -849.103529755173

E(Basis II/Basis I): -850.396823884964
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.886860884964

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.543671	-0.575093	0.982607
2	8	0.543671	-0.575093	3.160240
3	6	1.670367	-0.575093	3.736048
4	7	2.837684	-0.361461	3.071905
5	6	2.874407	0.004261	1.665142
6	6	2.317189	1.192615	1.237524
7	6	3.807737	-0.753233	0.866369
8	7	4.603645	-1.351421	0.231414
9	1	1.886517	1.871133	1.960658
10	1	2.481559	1.557373	0.231783
11	1	3.721908	-0.474635	3.561544
12	1	1.744750	-0.758163	4.809893
13	15	0.421908	-0.855834	-1.324083
14	15	-1.311338	1.076211	0.703882
15	6	-0.924793	0.264373	-1.981296
16	6	-1.650979	1.067393	-1.147855
17	1	-0.647002	-1.559336	0.983889
18	1	1.310507	-1.968355	1.012417
19	6	2.094194	-0.639182	-2.332179
20	6	0.106850	-2.622950	-2.110096
21	6	-1.676682	2.909247	1.356196
22	6	-2.926144	0.399720	1.601299
23	6	-2.713310	1.882950	-1.695380
24	6	-1.224031	0.243357	-3.395647
25	6	2.217378	0.733445	-2.945255
26	6	-0.408259	-3.590344	-1.077832
27	6	-0.426448	3.537046	1.908187
28	6	-3.671974	-0.591795	0.742285
29	1	2.883616	-0.779324	-1.603504
30	1	-0.638440	-2.503330	-2.891697
31	1	-2.023110	3.507217	0.518736
32	1	-2.562634	-0.103788	2.491673
33	6	2.105869	-1.788824	-3.366574
34	6	1.474080	-3.031009	-2.706048
35	6	-2.786356	2.749093	2.424521
36	6	-3.761182	1.645196	1.972042
37	1	1.537139	-1.517916	-4.253857
38	1	3.131017	-1.992601	-3.670310
39	1	2.134285	-3.398615	-1.922266
40	1	1.332201	-3.827497	-3.434098
41	1	-2.353316	2.467019	3.382675
42	1	-3.304978	3.697154	2.554832
43	1	-4.339859	1.992551	1.118679
44	1	-4.456498	1.396518	2.771729
45	1	-1.375052	-3.227765	-0.670048
46	1	-0.576328	-4.583321	-1.545888
47	1	0.317891	-3.707981	-0.247475
48	1	2.085197	1.512159	-2.166220
49	1	3.224725	0.851349	-3.397359
50	1	1.456571	0.888324	-3.736545
51	1	-4.523277	-1.016663	1.314886
52	1	-4.069784	-0.105308	-0.172092
53	1	-2.999891	-1.421899	0.442253
54	1	-0.646472	4.565912	2.264035
55	1	0.346334	3.597493	1.113223
56	1	-0.036522	2.941303	2.760060
57	6	-2.985820	1.861829	-3.063395
58	6	-2.241268	1.045077	-3.912302
59	1	-3.324490	2.498191	-1.052018
60	1	-3.783314	2.473557	-3.464974
61	1	-2.458316	1.026680	-4.972482
62	1	-0.662336	-0.392018	-4.066114

DIHY-D:

E(Basis I/Basis I): -849.109823278252
E(Basis II/Basis I): -850.404906114493
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.895694114493

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	1.205473	-0.113352	0.051210
2	8	1.205473	-0.113352	2.323282
3	6	2.383440	-0.113352	2.793294
4	7	3.476405	0.042660	2.002780
5	6	3.347937	0.339534	0.577577
6	6	2.740669	1.547488	0.174765
7	6	4.323127	-0.331318	-0.253661
8	7	5.152619	-0.854724	-0.909812
9	1	2.437798	2.264130	0.928260
10	1	2.930767	1.921741	-0.822110
11	1	4.410188	-0.046243	2.395692
12	1	2.566083	-0.247442	3.862345
13	15	-0.555122	-1.632632	-0.319741
14	15	-0.545603	1.614903	-0.099410
15	6	-2.163314	-0.685329	-0.312741
16	6	-2.164919	0.674203	-0.212852
17	1	1.376286	-0.137727	-1.486591
18	1	1.956200	-1.523728	-0.000016
19	6	-0.381806	-2.703966	-1.946144
20	6	-0.785710	-3.225969	0.793708
21	6	-0.697692	3.017813	-1.463912
22	6	-0.607141	2.943989	1.346824
23	6	-3.421019	1.389055	-0.239094
24	6	-3.414321	-1.398788	-0.431812
25	6	-1.143627	-2.099203	-3.098182
26	6	0.031401	-3.120913	2.053452
27	6	0.228119	2.740495	-2.617650
28	6	-1.502292	2.510738	2.480609
29	1	0.678220	-2.693784	-2.173402
30	1	-1.837100	-3.299763	1.057113
31	1	-1.722170	3.013905	-1.825102
32	1	0.410588	3.009913	1.714252
33	6	-0.854246	-4.121511	-1.551286
34	6	-0.356929	-4.401813	-0.117892
35	6	-0.382804	4.337027	-0.719313
36	6	-1.029245	4.275428	0.681493
37	1	-1.939784	-4.191375	-1.583485
38	1	-0.446841	-4.850591	-2.249122
39	1	0.727564	-4.496699	-0.127604
40	1	-0.776306	-5.330309	0.265015
41	1	0.692827	4.467380	-0.613997
42	1	-0.770321	5.180853	-1.287137
43	1	-2.111233	4.334449	0.586242
44	1	-0.700524	5.112786	1.294279
45	1	-0.333078	-2.270655	2.666933
46	1	-0.072742	-4.052525	2.648942
47	1	1.104598	-2.965762	1.815237
48	1	-0.807665	-1.053776	-3.265359
49	1	-0.954083	-2.685596	-4.021883
50	1	-2.234422	-2.098522	-2.896321
51	1	-1.420567	3.234786	3.318607
52	1	-2.562041	2.463447	2.159510
53	1	-1.191645	1.509251	2.846055
54	1	0.108069	3.525165	-3.394292
55	1	1.283999	2.729271	-2.281686
56	1	-0.016393	1.754803	-3.067452
57	6	-4.625094	0.691817	-0.347468
58	6	-4.621765	-0.699696	-0.443514
59	1	-3.439979	2.467597	-0.175155
60	1	-5.562808	1.232072	-0.361787
61	1	-5.556717	-1.237474	-0.533124
62	1	-3.425717	-2.475897	-0.524266

DIHY-A$\alpha^{\ddagger}$:

E(Basis I/Basis I): -849.094246451291
E(Basis II/Basis I): -850.390405369441
E(Basis II/Basis II): -850.396240391867
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.88515739187

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	-0.031106	1.085805	0.838298
2	8	-0.031106	1.085805	3.021478
3	6	1.102029	1.085805	3.603871
4	7	2.255351	1.221701	2.913938
5	6	2.222352	1.532355	1.489843
6	6	1.578165	2.753196	1.111137
7	6	3.216882	0.875580	0.699586
8	7	4.062943	0.327938	0.078261
9	1	1.319287	3.443582	1.910128
10	1	1.852196	3.232045	0.181080
11	1	3.150702	1.180544	3.394368
12	1	1.163522	0.967859	4.686557
13	15	-0.461229	0.956229	-1.473052
14	15	-0.280085	-1.311033	0.849265
15	6	-0.903709	-0.824196	-1.844001
16	6	-0.788279	-1.783642	-0.883011
17	1	-1.595386	1.138591	0.806651
18	1	-0.105004	2.718117	0.744773
19	6	-1.862327	2.206422	-2.040071
20	6	0.689839	1.495097	-2.979201
21	6	-1.554750	-2.219573	2.031369
22	6	1.202843	-2.423954	1.500393
23	6	-1.095868	-3.159088	-1.201918
24	6	-1.340032	-1.192985	-3.172262
25	6	-3.228739	1.568632	-2.007369
26	6	2.140414	1.562452	-2.590307
27	6	-2.510045	-1.238299	2.657838
28	6	2.077495	-2.910265	0.372265
29	1	-1.825797	3.001682	-1.304449
30	1	0.573757	0.735641	-3.746656
31	1	-2.119087	-2.918867	1.421194
32	1	1.783784	-1.769252	2.140337
33	6	-1.438489	2.718989	-3.436085
34	6	0.100057	2.841218	-3.455676
35	6	-0.676329	-2.971233	3.058920
36	6	0.546255	-3.558449	2.321488
37	1	-1.756575	2.029796	-4.215788
38	1	-1.905167	3.683414	-3.626988
39	1	0.409780	3.649688	-2.795554
40	1	0.459474	3.063404	-4.458864
41	1	-0.336489	-2.290440	3.837439
42	1	-1.259209	-3.760095	3.530765
43	1	0.222504	-4.367486	1.669995
44	1	1.265780	-3.964711	3.029898
45	1	2.460780	0.582758	-2.179332
46	1	2.758069	1.789045	-3.484946
47	1	2.311066	2.353182	-1.837534
48	1	-3.431629	1.156071	-0.996682
49	1	-4.002339	2.330319	-2.240729
50	1	-3.304562	0.749843	-2.751048
51	1	2.959476	-3.443850	0.785083
52	1	1.522406	-3.604073	-0.291248
53	1	2.432693	-2.047861	-0.229658
54	1	-3.250001	-1.782567	3.281990
55	1	-1.971433	-0.514494	3.300692
56	1	-3.056300	-0.684707	1.865257
57	6	-1.511877	-3.505425	-2.487875
58	6	-1.637292	-2.523484	-3.470327
59	1	-1.005808	-3.930208	-0.449530
60	1	-1.741125	-4.536889	-2.722237
61	1	-1.964434	-2.794038	-4.465910

62	1	-1.446234	-0.444016	-3.944513

Frequencies -- -646.6125 16.7600 53.5716

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	-0.051823	1.065437	0.812716
2	8	-0.080979	1.088753	3.019289
3	6	1.038809	1.100629	3.565933
4	7	2.174758	1.203459	2.868676
5	6	2.126467	1.495537	1.451050
6	6	1.478914	2.709280	1.071514
7	6	3.169788	0.880636	0.694165
8	7	4.048375	0.369858	0.126316
9	1	1.228077	3.396267	1.873323
10	1	1.760054	3.198987	0.150381
11	1	3.065854	1.223666	3.351727
12	1	1.129295	1.020425	4.652943
13	15	-0.468817	0.927702	-1.427974
14	15	-0.256952	-1.275835	0.821795
15	6	-0.902207	-0.821777	-1.820787
16	6	-0.756738	-1.776717	-0.874396
17	1	-1.613762	1.061113	0.745734
18	1	-0.236655	2.671464	0.720861
19	6	-1.840436	2.190021	-2.012011
20	6	0.699476	1.447023	-2.917797
21	6	-1.515143	-2.192078	2.002225
22	6	1.236122	-2.346954	1.488711
23	6	-1.033104	-3.158238	-1.193432
24	6	-1.346558	-1.188359	-3.146848
25	6	-3.216176	1.571028	-2.003758
26	6	2.152570	1.469068	-2.533707
27	6	-2.514156	-1.234324	2.596269
28	6	2.120503	-2.839522	0.370611
29	1	-1.807998	2.981137	-1.272357
30	1	0.563238	0.697169	-3.690977
31	1	-2.047774	-2.920923	1.398498
32	1	1.806465	-1.670723	2.115240
33	6	-1.391762	2.711143	-3.397060
34	6	0.148281	2.809234	-3.392276
35	6	-0.631383	-2.899753	3.055167
36	6	0.605128	-3.477912	2.334788
37	1	-1.708294	2.035034	-4.188716
38	1	-1.842574	3.683824	-3.583541
39	1	0.462664	3.605716	-2.719814
40	1	0.527965	3.032782	-4.387578
41	1	-0.310304	-2.193034	3.818420
42	1	-1.201294	-3.688636	3.542408
43	1	0.299521	-4.308458	1.701825
44	1	1.332796	-3.851920	3.052408
45	1	2.444097	0.477858	-2.128805
46	1	2.773135	1.678941	-3.430427
47	1	2.353018	2.252903	-1.781466
48	1	-3.439037	1.150045	-1.000885
49	1	-3.975741	2.346468	-2.238010
50	1	-3.295619	0.762588	-2.757933
51	1	3.018797	-3.335969	0.794458
52	1	1.583855	-3.567520	-0.271000
53	1	2.449013	-1.985300	-0.257412
54	1	-3.247929	-1.794942	3.213230
55	1	-2.014613	-0.485187	3.240639
56	1	-3.063787	-0.710678	1.785971
57	6	-1.457175	-3.508391	-2.476064
58	6	-1.618447	-2.523404	-3.450781
59	1	-0.915650	-3.929969	-0.445379
60	1	-1.664755	-4.543729	-2.713449
61	1	-1.950731	-2.795055	-4.444346
62	1	-1.473481	-0.437283	-3.913889

Frequencies -- -587.2218 19.6941 58.0230

DIHY-Bα‡:

E(Basis I/Basis I): -849.112306441902
E(Basis II/Basis I): -850.407243351664
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.898534351664

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.755518	1.044026	0.105157
2	8	0.790054	1.069220	2.362310
3	6	1.969919	1.109044	2.832818
4	7	3.061366	1.172349	2.029749
5	6	2.907529	1.319112	0.580518
6	6	2.399686	2.584235	0.109021
7	6	3.790027	0.506112	-0.210107
8	7	4.510496	-0.179960	-0.848692
9	1	2.328174	3.395797	0.827741
10	1	2.603199	2.884211	-0.912922
11	1	3.995087	1.160934	2.433112
12	1	2.146608	1.086443	3.910752
13	15	-1.583752	1.040006	-0.121477
14	15	0.607257	-1.360975	-0.239201
15	6	-2.137841	-0.718542	-0.398195
16	6	-1.222255	-1.728337	-0.448513
17	1	0.817241	1.069246	-1.444639
18	1	0.658347	2.671272	0.010278
19	6	-2.500646	1.861919	1.398115
20	6	-2.526824	2.169208	-1.404578
21	6	1.349576	-2.824250	0.850295
22	6	1.573491	-1.986121	-1.826486
23	6	-1.671134	-3.083815	-0.675853
24	6	-3.541858	-1.009442	-0.572719
25	6	-2.938658	0.837081	2.413508
26	6	-1.570630	2.684648	-2.446597
27	6	1.849946	-2.301425	2.168925
28	6	0.727033	-1.884169	-3.070230
29	1	-1.765375	2.519136	1.849941
30	1	-3.291543	1.566092	-1.886245
31	1	0.552942	-3.538582	1.036788
32	1	2.424979	-1.320554	-1.918401
33	6	-3.663422	2.671520	0.777785
34	6	-3.161706	3.289432	-0.544764
35	6	2.470487	-3.450249	-0.017886
36	6	2.036926	-3.422752	-1.497666
37	1	-4.517403	2.026999	0.578737
38	1	-3.980306	3.448878	1.470539
39	1	-2.425236	4.060002	-0.322880
40	1	-3.980861	3.751746	-1.092141
41	1	3.394479	-2.884475	0.087715
42	1	2.658954	-4.469814	0.313112
43	1	1.235192	-4.139179	-1.662788
44	1	2.870050	-3.694228	-2.143368
45	1	-1.133167	1.833180	-3.009825
46	1	-2.109723	3.342041	-3.161111
47	1	-0.748902	3.263362	-1.974527
48	1	-2.064314	0.240199	2.749105
49	1	-3.379430	1.348225	3.295268
50	1	-3.698263	0.151867	1.984914
51	1	1.331715	-2.163410	-3.958727
52	1	-0.149263	-2.561928	-3.010886
53	1	0.367298	-0.841490	-3.199188
54	1	2.239451	-3.139988	2.784072
55	1	2.665520	-1.566522	2.010629
56	1	1.019653	-1.812555	2.720804
57	6	-3.030128	-3.356768	-0.840054
58	6	-3.963832	-2.321773	-0.787609
59	1	-0.961569	-3.896261	-0.732653
60	1	-3.359896	-4.373279	-1.011462

61	1	-5.016829	-2.536746	-0.915531
62	1	-4.275252	-0.215764	-0.532354

Frequencies -- -592.1381 22.0308 47.0424

DIHY-Cβ‡:

E(Basis I/Basis I): -849.077808811202
E(Basis II/Basis I): -850.377945683838
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.870531683838

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.521307	-0.398745	0.945244
2	8	0.423371	-0.444752	3.143588
3	6	1.540971	-0.571535	3.733188
4	7	2.722779	-0.529239	3.070851
5	6	2.748007	-0.200980	1.630068
6	6	2.211130	1.104239	1.273318
7	6	3.965594	-0.655511	0.960199
8	7	4.943532	-0.992757	0.394181
9	1	1.967626	1.769460	2.092811
10	1	2.572673	1.578637	0.369479
11	1	3.600844	-0.679872	3.559065
12	1	1.581997	-0.734497	4.811511
13	15	0.520262	-0.681526	-1.356327
14	15	-1.482876	0.811593	0.661022
15	6	-1.039412	0.102433	-2.012405
16	6	-1.888093	0.739899	-1.159232
17	1	-0.395301	-1.704614	0.898148
18	1	1.931256	-1.332062	1.150039
19	6	2.095866	-0.004140	-2.305002
20	6	0.699296	-2.447343	-2.182015
21	6	-1.887262	2.629702	1.281309
22	6	-2.934035	0.052870	1.724468
23	6	-3.095030	1.347173	-1.669496
24	6	-1.355202	0.029078	-3.419595
25	6	1.882636	1.397716	-2.817385
26	6	0.520835	-3.528110	-1.149582
27	6	-0.622656	3.337897	1.683717
28	6	-3.676322	-1.020663	0.969341
29	1	2.895746	0.000245	-1.572791
30	1	-0.078100	-2.537308	-2.935931
31	1	-2.349993	3.165566	0.456971
32	1	-2.443885	-0.390119	2.586103
33	6	2.382132	-1.043282	-3.412720
34	6	2.107100	-2.443795	-2.826847
35	6	-2.879515	2.439687	2.456069
36	6	-3.814206	1.254375	2.136544
37	1	1.741940	-0.873219	-4.275896
38	1	3.417844	-0.958045	-3.736435
39	1	2.866258	-2.674700	-2.081114
40	1	2.154076	-3.205035	-3.603119
41	1	-2.339791	2.225612	3.377041
42	1	-3.449512	3.354979	2.603767
43	1	-4.494275	1.528526	1.332606
44	1	-4.410476	0.990972	3.008152
45	1	-0.512936	-3.496698	-0.745579
46	1	0.685427	-4.523753	-1.613249
47	1	1.241901	-3.395271	-0.315146
48	1	1.591442	2.066476	-1.980120
49	1	2.823675	1.779421	-3.266552
50	1	1.086326	1.421968	-3.589157
51	1	-4.440269	-1.482661	1.629627
52	1	-4.186023	-0.599214	0.078611
53	1	-2.969169	-1.810325	0.638627
54	1	-0.856868	4.375301	2.003443
55	1	0.077301	3.380476	0.822401
56	1	-0.131605	2.806285	2.525314

57	6	-3.391947	1.276309	-3.031920
58	6	-2.523944	0.618339	-3.905148
59	1	-3.780040	1.851184	-1.002159
60	1	-4.298229	1.730206	-3.411383
61	1	-2.757471	0.564843	-4.960594
62	1	-0.688806	-0.474421	-4.106083

Frequencies -- -740.5681 18.3005 51.2122

DIHY-Dβ‡:

E(Basis I/Basis I): -849.093765805865
E(Basis II/Basis I): -850.389156762642
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.881763762642

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	1.112382	0.245479	0.121933
2	8	1.112382	0.245479	2.411303
3	6	2.279297	0.245479	2.906486
4	7	3.394458	0.357950	2.135862
5	6	3.277154	0.619326	0.692807
6	6	2.573490	1.839288	0.311514
7	6	4.475819	0.238846	-0.047417
8	7	5.451468	-0.039190	-0.647855
9	1	2.324319	2.526579	1.113130
10	1	2.846355	2.295919	-0.631839
11	1	4.320653	0.290780	2.548449
12	1	2.438177	0.139061	3.982436
13	15	-0.244918	-1.684761	-0.256320
14	15	-0.869050	1.501382	-0.204171
15	6	-2.002352	-1.065626	-0.449512
16	6	-2.261989	0.273834	-0.430103
17	1	1.286231	0.247844	-1.415051
18	1	2.504334	-0.676680	0.260501
19	6	0.249755	-2.780117	-1.802944
20	6	-0.296956	-3.255416	0.917427
21	6	-1.101630	2.866052	-1.585018
22	6	-1.263691	2.780994	1.225234
23	6	-3.616816	0.743203	-0.607205
24	6	-3.087191	-2.002047	-0.633567
25	6	-0.483287	-2.353605	-3.049666
26	6	0.406032	-2.960133	2.214812
27	6	-0.010728	2.759283	-2.616197
28	6	-2.164702	2.192012	2.281033
29	1	1.311830	-2.608138	-1.939782
30	1	-1.336620	-3.493895	1.123097
31	1	-2.062771	2.695856	-2.062258
32	1	-0.301530	3.010772	1.669468
33	6	-0.023828	-4.240805	-1.379534
34	6	0.381696	-4.384283	0.102027
35	6	-1.093956	4.210515	-0.817555
36	6	-1.850627	4.023084	0.514910
37	1	-1.076691	-4.488368	-1.497954
38	1	0.554931	-4.919479	-2.003290
39	1	1.465016	-4.310721	0.182169
40	1	0.078867	-5.352423	0.496431
41	1	-0.071863	4.521369	-0.607954
42	1	-1.563881	4.981787	-1.424855
43	1	-2.911962	3.888315	0.316833
44	1	-1.734778	4.899386	1.149981
45	1	-0.132643	-2.155878	2.758547
46	1	0.420221	-3.868648	2.853401
47	1	1.451149	-2.633425	2.027090
48	1	-0.307662	-1.273537	-3.240222
49	1	-0.110289	-2.933274	-3.920257
50	1	-1.574057	-2.528494	-2.949138
51	1	-2.288627	2.916124	3.113728
52	1	-3.165474	1.957003	1.865423
53	1	-1.714555	1.260419	2.684508

54	1	-0.145272	3.543637	-3.390782
55	1	0.986422	2.885093	-2.146055
56	1	-0.053530	1.764259	-3.107842
57	6	-4.658059	-0.169258	-0.783088
58	6	-4.393873	-1.539160	-0.795432
59	1	-3.835158	1.801999	-0.601500
60	1	-5.672020	0.186558	-0.912144
61	1	-5.203091	-2.244096	-0.935526
62	1	-2.895596	-3.065508	-0.658891

Frequencies -- -770.0264 20.3168 45.9823

ALHY-Aα:

E(Basis I/Basis I): -849.141976899636
E(Basis II/Basis I): -850.433077037147
E(Basis II/Basis II): -850.441274348805
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.92713634881

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.779103	-0.134567	0.891471
2	8	0.779103	-0.134567	3.009838
3	6	1.960444	-0.134567	3.516086
4	7	3.041501	-0.235138	2.737558
5	6	2.874397	-0.500442	1.271061
6	6	4.043595	0.105859	0.495590
7	6	2.694705	-1.951258	1.096148
8	7	2.387985	-3.089286	0.962297
9	1	5.015312	-0.262228	0.860490
10	1	3.986063	-0.154528	-0.563914
11	1	3.973898	-0.241965	3.147472
12	1	2.084173	-0.053998	4.596041
13	15	0.662146	0.159852	-1.462000
14	15	-1.617816	0.053498	0.836390
15	6	-1.157558	0.346328	-1.907833
16	6	-2.118036	0.293040	-0.940539
17	1	0.970851	1.375368	0.896661
18	1	4.036216	1.196294	0.585915
19	6	1.651268	1.716493	-2.120223
20	6	1.424898	-0.988938	-2.872017
21	6	-2.573708	1.400397	1.884481
22	6	-2.599606	-1.410024	1.697341
23	6	-3.509180	0.449071	-1.295066
24	6	-1.548809	0.551698	-3.284934
25	6	0.814192	2.969811	-2.069726
26	6	1.917640	-2.292730	-2.304610
27	6	-1.620454	2.455457	2.379874
28	6	-3.028842	-2.461139	0.705240
29	1	2.489403	1.822752	-1.440767
30	1	0.625441	-1.197250	-3.576734
31	1	-3.312594	1.862507	1.235604
32	1	-1.894408	-1.846841	2.397451
33	6	2.134847	1.341700	-3.539709
34	6	2.546543	-0.145563	-3.530430
35	6	-3.254387	0.602692	3.022851
36	6	-3.770303	-0.732399	2.446043
37	1	1.349373	1.504527	-4.273916
38	1	2.981934	1.968078	-3.813522
39	1	3.477608	-0.251149	-2.977265
40	1	2.717764	-0.504879	-4.543545
41	1	-2.541077	0.396991	3.819263
42	1	-4.072110	1.187011	3.440733
43	1	-4.601009	-0.541877	1.769383
44	1	-4.124120	-1.385266	3.241870
45	1	1.103429	-2.791329	-1.737419
46	1	2.238843	-2.963352	-3.129471
47	1	2.782500	-2.123534	-1.633316
48	1	0.440052	3.133907	-1.037032
49	1	1.430368	3.844328	-2.367396

50	1	-0.052788	2.896620	-2.757978
51	1	-3.506770	-3.308673	1.240360
52	1	-3.755686	-2.047174	-0.022987
53	1	-2.143803	-2.842411	0.153179
54	1	-2.172502	3.213869	2.974295
55	1	-0.830825	2.005408	3.016573
56	1	-1.138987	2.962527	1.516887
57	6	-3.874765	0.643552	-2.627096
58	6	-2.896400	0.694894	-3.619973
59	1	-4.275311	0.414243	-0.532588
60	1	-4.918487	0.757388	-2.889884
61	1	-3.182714	0.849371	-4.652218
62	1	-0.806736	0.604466	-4.067284

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.770988	-0.068693	0.845392
2	8	0.830301	0.025957	3.001076
3	6	1.993060	0.014277	3.464531
4	7	3.063701	-0.144181	2.691688
5	6	2.895344	-0.477599	1.274835
6	6	4.133353	-0.139663	0.472787
7	6	2.321462	-1.806699	1.155478
8	7	1.532308	-2.676521	1.083694
9	1	5.030945	-0.624133	0.880893
10	1	4.034171	-0.470277	-0.560752
11	1	3.980660	-0.210171	3.122328
12	1	2.156512	0.132623	4.538947
13	15	0.647474	0.202067	-1.419567
14	15	-1.540038	0.008173	0.801261
15	6	-1.132505	0.402143	-1.884406
16	6	-2.081447	0.284199	-0.928292
17	1	0.840590	1.454925	0.805015
18	1	4.300176	0.939832	0.475263
19	6	1.704275	1.691328	-2.096893
20	6	1.358112	-1.001817	-2.797194
21	6	-2.549109	1.266759	1.892251
22	6	-2.420708	-1.523336	1.624544
23	6	-3.478446	0.403535	-1.271727
24	6	-1.524329	0.652343	-3.253036
25	6	0.919631	2.979336	-2.098675
26	6	1.743212	-2.339390	-2.225072
27	6	-1.663827	2.377672	2.392049
28	6	-2.808829	-2.563685	0.604590
29	1	2.529047	1.782422	-1.399056
30	1	0.560539	-1.152862	-3.518247
31	1	-3.328270	1.691284	1.265612
32	1	-1.680097	-1.944914	2.296473
33	6	2.209187	1.262708	-3.493894
34	6	2.545033	-0.242349	-3.439975
35	6	-3.160427	0.406304	3.023664
36	6	-3.612952	-0.938532	2.416901
37	1	1.453424	1.445020	-4.254324
38	1	3.092608	1.841799	-3.756119
39	1	3.451495	-0.384572	-2.855458
40	1	2.725867	-0.634730	-4.438999
41	1	-2.419743	0.219895	3.799591
42	1	-4.000108	0.933389	3.472715
43	1	-4.467140	-0.775229	1.762650
44	1	-3.912140	-1.634801	3.198016
45	1	0.877808	-2.784858	-1.690611
46	1	2.042762	-3.025092	-3.045684
47	1	2.596418	-2.237393	-1.526146
48	1	0.527190	3.186720	-1.080814
49	1	1.579706	3.819377	-2.401561
50	1	0.067955	2.925684	-2.807176
51	1	-3.232973	-3.452150	1.118212
52	1	-3.567278	-2.165631	-0.100137

53	1	-1.913060	-2.879911	0.028913
54	1	-2.263915	3.096102	2.989590
55	1	-0.848550	1.979508	3.028948
56	1	-1.217430	2.919692	1.531534
57	6	-3.852302	0.643716	-2.594853
58	6	-2.875881	0.770672	-3.584142
59	1	-4.241343	0.307407	-0.511262
60	1	-4.899418	0.733735	-2.853328
61	1	-3.166647	0.958950	-4.609521
62	1	-0.781646	0.751691	-4.030666

ALHY-Bα:

E(Basis I/Basis I): -849.137275969840
E(Basis II/Basis I): -850.429328276664
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.918524276664

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.744693	0.896729	0.306026
2	8	0.744693	0.896729	2.497322
3	6	1.938011	0.896729	2.969571
4	7	3.013055	0.920438	2.166631
5	6	2.841210	1.084478	0.686979
6	6	2.962955	2.584039	0.302970
7	6	3.793059	0.239750	-0.009021
8	7	4.527025	-0.470968	-0.605036
9	1	3.820217	3.057805	0.801641
10	1	3.079153	2.703534	-0.776109
11	1	3.947611	0.899082	2.571934
12	1	2.101013	0.874663	4.049130
13	15	-1.639134	1.046328	0.096860
14	15	0.578386	-1.231097	-0.546417
15	6	-2.169832	-0.573684	-0.652871
16	6	-1.233600	-1.529638	-0.912974
17	1	0.855571	1.145172	-1.233027
18	1	2.069177	3.155171	0.616000
19	6	-2.630857	1.420418	1.743734
20	6	-2.555709	2.481974	-0.866469
21	6	1.207924	-2.810175	0.433654
22	6	1.705283	-1.642113	-2.087878
23	6	-1.645859	-2.798843	-1.467844
24	6	-3.559341	-0.826462	-0.953140
25	6	-3.070265	0.155292	2.436323
26	6	-1.558533	3.282277	-1.661348
27	6	1.554153	-2.457948	1.854991
28	6	0.988313	-1.380404	-3.388280
29	1	-1.928288	1.947323	2.381293
30	1	-3.275622	2.030680	-1.543682
31	1	0.389946	-3.525590	0.433676
32	1	2.551941	-0.970545	-1.999357
33	6	-3.795529	2.343254	1.316830
34	6	-3.264749	3.308139	0.235532
35	6	2.416315	-3.331239	-0.385383
36	6	2.144834	-3.110826	-1.888926
37	1	-4.620915	1.760024	0.913513
38	1	-4.162006	2.896704	2.179484
39	1	-2.566394	4.006921	0.693341
40	1	-4.077594	3.882786	-0.204406
41	1	3.322170	-2.795083	-0.109768
42	1	2.566189	-4.387673	-0.170509
43	1	1.376497	-3.799098	-2.234247
44	1	3.048675	-3.295735	-2.466520
45	1	-1.081610	2.634564	-2.427278
46	1	-2.070996	4.122473	-2.175970
47	1	-0.767349	3.691306	-0.997038
48	1	-2.189365	-0.491738	2.634099
49	1	-3.551578	0.406291	3.405033

50	1	-3.797100	-0.406515	1.814786
51	1	1.684260	-1.544120	-4.237873
52	1	0.119045	-2.058564	-3.507735
53	1	0.631978	-0.329150	-3.419446
54	1	1.854064	-3.373701	2.406824
55	1	2.394097	-1.735422	1.882888
56	1	0.671523	-2.011405	2.359786
57	6	-2.991612	-3.036782	-1.752572
58	6	-3.946307	-2.051519	-1.498055
59	1	-0.919056	-3.572257	-1.669812
60	1	-3.295059	-3.987378	-2.171724
61	1	-4.988893	-2.238990	-1.719958
62	1	-4.308549	-0.073254	-0.751481

ALHY-C/Dβ:

E(Basis I/Basis I): -849.130426713873
E(Basis II/Basis I): -850.416195741229
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.905107741229

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.627744	0.162967	0.805056
2	8	0.627744	0.162967	2.924240
3	6	1.626572	0.162967	3.714364
4	7	2.919372	0.030243	3.374024
5	6	3.451551	-0.164879	1.987548
6	6	2.673403	0.626323	0.905260
7	6	4.881336	0.230370	2.011476
8	7	6.016692	0.547761	1.984441
9	1	2.720273	1.702317	1.145561
10	1	3.215357	0.484098	-0.033716
11	1	3.599424	0.029789	4.129801
12	1	1.434540	0.282343	4.784163
13	15	-1.774960	-0.330156	0.684758
14	15	0.536252	0.259500	-1.525734
15	6	-2.209867	-0.273630	-1.138187
16	6	-1.236592	-0.015832	-2.061415
17	1	0.951181	-1.310732	0.627727
18	1	3.413002	-1.237298	1.752292
19	6	-2.384023	-2.009872	1.489509
20	6	-3.164158	0.690476	1.624702
21	6	1.646082	-0.848998	-2.699980
22	6	1.277356	1.912605	-2.277756
23	6	-1.575014	0.025229	-3.465587
24	6	-3.569966	-0.489151	-1.575222
25	6	-2.391562	-3.141747	0.493546
26	6	-2.575629	1.947505	2.208088
27	6	2.236168	-2.008255	-1.941614
28	6	0.210854	2.950721	-2.518686
29	1	-1.658139	-2.226474	2.266961
30	1	-3.935156	0.957586	0.907489
31	1	1.003983	-1.231276	-3.488471
32	1	1.968141	2.279547	-1.525550
33	6	-3.768809	-1.701073	2.102513
34	6	-3.714738	-0.279339	2.699067
35	6	2.708253	0.119656	-3.274034
36	6	2.035380	1.480044	-3.554498
37	1	-4.547405	-1.751597	1.344240
38	1	-4.001125	-2.432996	2.874004
39	1	-3.064848	-0.284823	3.572490
40	1	-4.703773	0.047281	3.015068
41	1	3.520230	0.259908	-2.562799
42	1	3.128047	-0.299354	-4.186668
43	1	1.350585	1.382934	-4.394448
44	1	2.779709	2.231993	-3.810350
45	1	-2.174889	2.587778	1.393757
46	1	-3.359196	2.514750	2.753707

47	1	-1.749979	1.704478	2.909958
48	1	-1.383877	-3.251198	0.039381
49	1	-2.655228	-4.090661	1.006533
50	1	-3.131018	-2.957704	-0.312338
51	1	0.679879	3.896929	-2.861927
52	1	-0.508133	2.611171	-3.291733
53	1	-0.341479	3.149289	-1.575850
54	1	2.862410	-2.623421	-2.621797
55	1	2.865372	-1.652920	-1.100010
56	1	1.421981	-2.646307	-1.537331
57	6	-2.891436	-0.188026	-3.876800
58	6	-3.886860	-0.444437	-2.933593
59	1	-0.814391	0.224525	-4.207518
60	1	-3.140537	-0.154641	-4.929529
61	1	-4.906675	-0.610081	-3.255954
62	1	-4.350320	-0.692613	-0.855415

ALHY-A$\alpha^{\ddagger}$:

E(Basis I/Basis I): -849.113095189086
E(Basis II/Basis I): -850.403979442768
E(Basis II/Basis II): -850.409877939363
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.89903293936

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.752794	-0.178403	0.856788
2	8	0.676805	-0.233853	2.980586
3	6	1.818675	-0.223061	3.555384
4	7	2.961942	-0.253951	2.847101
5	6	2.933794	-0.458021	1.371314
6	6	4.243953	0.040545	0.729727
7	6	2.691548	-1.885299	1.093942
8	7	2.525161	-3.044351	0.911957
9	1	5.104314	-0.522575	1.114868
10	1	4.215554	-0.109985	-0.352369
11	1	3.861503	-0.245937	3.321426
12	1	1.882783	-0.182516	4.643066
13	15	0.628993	0.156563	-1.485583
14	15	-1.598202	0.055617	0.803478
15	6	-1.190542	0.310424	-1.940876
16	6	-2.136914	0.266589	-0.961975
17	1	2.083315	0.710760	0.888610
18	1	4.397550	1.106012	0.929235
19	6	1.562503	1.759191	-2.120945
20	6	1.440579	-0.937497	-2.908414
21	6	-2.489854	1.448439	1.844626
22	6	-2.576849	-1.361247	1.734232
23	6	-3.532938	0.416054	-1.297072
24	6	-1.597696	0.493406	-3.315898
25	6	0.686345	2.983622	-2.042207
26	6	1.997216	-2.217801	-2.347328
27	6	-1.499639	2.496054	2.279162
28	6	-3.057404	-2.432748	0.788955
29	1	2.405518	1.886587	-1.450582
30	1	0.657734	-1.182725	-3.619368
31	1	-3.241428	1.909182	1.209652
32	1	-1.855666	-1.790157	2.422315
33	6	2.049695	1.428291	-3.549600
34	6	2.524033	-0.040103	-3.560556
35	6	-3.149903	0.696846	3.025763
36	6	-3.709944	-0.642972	2.502378
37	1	1.250002	1.564958	-4.273706
38	1	2.865939	2.094069	-3.824206
39	1	3.459990	-0.110448	-3.009190
40	1	2.711133	-0.378547	-4.577903
41	1	-2.415718	0.497188	3.804503
42	1	-3.942010	1.308555	3.453652
43	1	-4.558254	-0.452857	1.847727

44	1	-4.051036	-1.266486	3.326721
45	1	1.203797	-2.768223	-1.798858
46	1	2.369756	-2.859890	-3.173367
47	1	2.839227	-2.005538	-1.658328
48	1	0.316367	3.116233	-1.003459
49	1	1.271461	3.882960	-2.328522
50	1	-0.183612	2.894343	-2.724952
51	1	-3.530941	-3.255652	1.364898
52	1	-3.801376	-2.027386	0.073397
53	1	-2.198250	-2.846073	0.219373
54	1	-2.016694	3.282888	2.868096
55	1	-0.699191	2.047744	2.903330
56	1	-1.035294	2.967337	1.387085
57	6	-3.916271	0.589229	-2.627682
58	6	-2.950701	0.626966	-3.634924
59	1	-4.287225	0.394747	-0.522201
60	1	-4.963467	0.698112	-2.878433
61	1	-3.251062	0.765958	-4.665400
62	1	-0.864586	0.540306	-4.107154

Frequencies -- -930.4781 23.9484 29.8667

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.751054	-0.196946	0.795129
2	8	0.764663	-0.217548	2.950652
3	6	1.908205	-0.141257	3.446834
4	7	3.014616	-0.130005	2.699709
5	6	2.939363	-0.407024	1.257023
6	6	4.208603	0.055788	0.539935
7	6	2.667686	-1.834742	1.068688
8	7	2.441862	-2.976596	0.981613
9	1	5.085781	-0.474746	0.927092
10	1	4.139001	-0.164263	-0.526044
11	1	3.922025	-0.140096	3.152425
12	1	2.038273	-0.071867	4.530341
13	15	0.551792	0.107166	-1.458839
14	15	-1.526125	0.080485	0.818723
15	6	-1.240899	0.306882	-1.888634
16	6	-2.148366	0.291041	-0.888212
17	1	2.044007	0.717909	0.771511
18	1	4.358184	1.130504	0.668641
19	6	1.529905	1.640495	-2.164722
20	6	1.271172	-1.059025	-2.861630
21	6	-2.323574	1.506884	1.875552
22	6	-2.492261	-1.288745	1.813218
23	6	-3.551356	0.473351	-1.171148
24	6	-1.683991	0.492975	-3.251773
25	6	0.713144	2.906062	-2.097215
26	6	1.785678	-2.349045	-2.282749
27	6	-1.291446	2.541606	2.237824
28	6	-3.047389	-2.361018	0.910486
29	1	2.396428	1.750236	-1.522356
30	1	0.455997	-1.288443	-3.540543
31	1	-3.095761	1.973489	1.270535
32	1	-1.750009	-1.728739	2.471170
33	6	1.967048	1.253348	-3.595580
34	6	2.372471	-0.235258	-3.578048
35	6	-2.942769	0.796881	3.103215
36	6	-3.565876	-0.533152	2.629485
37	1	1.159057	1.410577	-4.305889
38	1	2.806612	1.873483	-3.904307
39	1	3.323139	-0.333861	-3.057074
40	1	2.507706	-0.612091	-4.590022
41	1	-2.175291	0.587831	3.846602
42	1	-3.693810	1.438823	3.559757
43	1	-4.442104	-0.328227	2.017461
44	1	-3.879113	-1.137699	3.478522
45	1	0.993073	-2.836809	-1.676733

46	1	2.080513	-3.037502	-3.102836
47	1	2.673098	-2.162196	-1.645885
48	1	0.377942	3.083386	-1.053459
49	1	1.331058	3.769353	-2.422928
50	1	-0.177892	2.840338	-2.754831
51	1	-3.509534	-3.163928	1.522778
52	1	-3.818389	-1.947786	0.228902
53	1	-2.229639	-2.803615	0.303119
54	1	-1.763678	3.354159	2.829476
55	1	-0.473048	2.091996	2.836460
56	1	-0.858780	2.980698	1.314082
57	6	-3.976098	0.650212	-2.489090
58	6	-3.043372	0.659034	-3.528353
59	1	-4.277564	0.474388	-0.369647
60	1	-5.028154	0.783954	-2.704973
61	1	-3.373692	0.799716	-4.549371
62	1	-0.975769	0.513656	-4.066157

Frequencies -- -950.3232 26.6027 31.2734

PROD-A:

E(Basis I/Basis I): -849.154924087821
E(Basis II/Basis I): -850.445888795353
E(Basis II/Basis II): -850.452197691092
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.93829969109

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.397775	-0.701931	0.734302
2	8	0.397775	-0.701931	2.892572
3	6	1.349436	-0.701931	3.731333
4	7	2.671880	-0.636540	3.446615
5	6	3.286897	-0.551894	2.090237
6	6	4.723676	-1.118200	2.131975
7	6	2.425060	-1.302794	1.126976
8	7	2.106711	-2.269647	0.469374
9	1	4.723674	-2.174221	2.419696
10	1	5.188324	-1.028642	1.145868
11	1	3.319983	-0.652873	4.228568
12	1	1.109776	-0.766786	4.796575
13	15	0.245721	-0.655180	-1.584312
14	15	-1.248469	0.965667	0.714396
15	6	-1.001226	0.657696	-2.056448
16	6	-1.645416	1.347065	-1.072421
17	1	3.312936	0.499668	1.778916
18	1	5.334866	-0.548615	2.842749
19	6	1.910560	-0.500418	-2.596350
20	6	-0.273842	-2.268848	-2.560333
21	6	-0.955327	2.684837	1.601408
22	6	-2.865391	0.630062	1.764125
23	6	-2.615584	2.358163	-1.419646
24	6	-1.314774	0.922031	-3.440830
25	6	2.211726	0.924170	-2.985713
26	6	-0.805790	-3.303919	-1.604921
27	6	0.497565	2.846835	1.961164
28	6	-3.977097	0.053537	0.925081
29	1	2.681135	-0.854037	-1.919983
30	1	-1.054026	-1.998212	-3.266081
31	1	-1.239853	3.473715	0.911226
32	1	-2.564580	-0.102136	2.506661
33	6	1.759937	-1.464474	-3.795424
34	6	1.009811	-2.719320	-3.299315
35	6	-1.893592	2.665499	2.832864
36	6	-3.216680	1.978661	2.432573
37	1	1.196705	-0.994630	-4.599073
38	1	2.741862	-1.730865	-4.182187
39	1	1.657046	-3.278449	-2.625841
40	1	0.746177	-3.367755	-4.132758

41	1	-1.437178	2.107508	3.648706
42	1	-2.072073	3.682680	3.176657
43	1	-3.765902	2.618886	1.745179
44	1	-3.841200	1.807864	3.307537
45	1	-1.707380	-2.910749	-1.088767
46	1	-1.086749	-4.223247	-2.161032
47	1	-0.042436	-3.562791	-0.841459
48	1	2.229124	1.566659	-2.079950
49	1	3.205914	0.976254	-3.477660
50	1	1.448295	1.314634	-3.688631
51	1	-4.840065	-0.205975	1.573989
52	1	-4.315972	0.780274	0.158983
53	1	-3.625614	-0.868769	0.415783
54	1	0.655665	3.823087	2.466373
55	1	0.828212	2.032583	2.638825
56	1	1.118308	2.817953	1.040519
57	6	-2.904928	2.616233	-2.761125
58	6	-2.258118	1.897937	-3.769239
59	1	-3.126233	2.915508	-0.646388
60	1	-3.635754	3.371322	-3.019973
61	1	-2.490151	2.096496	-4.807536
62	1	-0.825260	0.366427	-4.228656

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.374075	-0.678667	0.698972
2	8	0.390926	-0.707617	2.890076
3	6	1.331085	-0.709120	3.700046
4	7	2.642234	-0.633122	3.417553
5	6	3.259765	-0.545972	2.081974
6	6	4.685990	-1.114549	2.124686
7	6	2.407858	-1.296540	1.119755
8	7	2.048460	-2.233463	0.485413
9	1	4.678309	-2.167488	2.414914
10	1	5.150251	-1.024577	1.140866
11	1	3.280950	-0.650140	4.202401
12	1	1.113500	-0.783652	4.772137
13	15	0.232855	-0.622173	-1.535246
14	15	-1.224309	0.925290	0.674448
15	6	-0.999681	0.650720	-2.045049
16	6	-1.650837	1.324022	-1.070733
17	1	3.285361	0.502369	1.764065
18	1	5.291341	-0.544393	2.835925
19	6	1.898214	-0.466258	-2.529046
20	6	-0.269814	-2.235674	-2.504615
21	6	-0.907499	2.635927	1.551810
22	6	-2.813614	0.598157	1.750846
23	6	-2.632429	2.324721	-1.413059
24	6	-1.306396	0.910661	-3.431246
25	6	2.200808	0.957829	-2.919502
26	6	-0.812550	-3.268976	-1.553176
27	6	0.553071	2.796646	1.879578
28	6	-3.943479	0.019108	0.938077
29	1	2.664730	-0.814475	-1.845607
30	1	-1.043377	-1.968755	-3.218706
31	1	-1.203736	3.424355	0.866260
32	1	-2.499933	-0.132768	2.489269
33	6	1.769078	-1.435180	-3.726722
34	6	1.018528	-2.690090	-3.232461
35	6	-1.819538	2.627187	2.802629
36	6	-3.152331	1.945501	2.427972
37	1	1.214259	-0.972166	-4.540042
38	1	2.757323	-1.698078	-4.099285
39	1	1.661462	-3.245674	-2.551969
40	1	0.761297	-3.342139	-4.065004
41	1	-1.350306	2.068828	3.610959
42	1	-1.985525	3.646323	3.146663
43	1	-3.713491	2.588037	1.752548
44	1	-3.760326	1.773727	3.314208

45	1	-1.717139	-2.873259	-1.044199
46	1	-1.092231	-4.187146	-2.111856
47	1	-0.056713	-3.531558	-0.783908
48	1	2.203496	1.603764	-2.015960
49	1	3.201943	1.011098	-3.397052
50	1	1.447004	1.343786	-3.635133
51	1	-4.790541	-0.241509	1.607213
52	1	-4.302416	0.744748	0.180269
53	1	-3.602930	-0.902969	0.420933
54	1	0.724702	3.776114	2.374019
55	1	0.895919	1.986939	2.556187
56	1	1.154205	2.758953	0.946257
57	6	-2.920619	2.584011	-2.755152
58	6	-2.260332	1.876025	-3.762918
59	1	-3.148938	2.874815	-0.638619
60	1	-3.658712	3.331832	-3.014503
61	1	-2.489608	2.074338	-4.801853
62	1	-0.805624	0.362094	-4.216714

MIN:

E(Basis I/Basis I): -847.928885913650
E(Basis II/Basis I): -849.213989934632
E(Basis II/Basis II): -849.219797247572
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -848.727652247572

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.705433	-0.580114	0.876466
2	8	0.705433	-0.580114	3.023457
3	6	1.877826	-0.580114	3.530945
4	7	2.969100	-0.606309	2.745941
5	6	2.810929	-0.698238	1.281694
6	6	2.419166	-1.951948	0.726065
7	6	3.592522	0.280068	0.565248
8	7	4.239876	1.084248	-0.009758
9	1	2.255773	-2.801258	1.383769
10	1	2.692705	-2.194657	-0.293274
11	1	3.904998	-0.598981	3.144127
12	1	2.013330	-0.564838	4.613191
13	15	-1.397382	0.601782	0.921071
14	15	0.447363	-0.484017	-1.475985
15	6	-1.871087	0.986355	-0.838859
16	6	-1.077559	0.544272	-1.855552
17	6	-2.866674	-0.208263	1.929164
18	6	-1.542733	2.273600	1.928972
19	6	0.149588	-2.125421	-2.517093
20	6	1.981593	0.003321	-2.595831
21	6	-1.453802	0.818762	-3.223463
22	6	-3.060184	1.751040	-1.132175
23	6	-3.809068	-0.976046	1.037625
24	6	-0.176997	2.788767	2.298423
25	6	-0.156178	-3.287826	-1.610082
26	6	2.000305	1.473347	-2.929604
27	1	-2.385853	-0.896925	2.616580
28	1	-2.037505	3.003508	1.294489
29	1	-0.706533	-1.946227	-3.160882
30	1	2.851475	-0.225209	-1.991395
31	6	-3.534444	0.956395	2.695759
32	6	-2.420474	1.921076	3.153989
33	6	1.434432	-2.314480	-3.358498
34	6	1.922521	-0.927227	-3.829483
35	1	-4.235675	1.487424	2.055009
36	1	-4.084153	0.568150	3.551263
37	1	-1.821465	1.435301	3.922450
38	1	-2.843320	2.830690	3.576595
39	1	2.214633	-2.787272	-2.764647
40	1	1.223949	-2.959734	-4.209415

41	1	1.240403	-0.535587	-4.580537
42	1	2.910891	-1.000153	-4.279722
43	1	0.417210	2.973255	1.378333
44	1	-0.272729	3.743640	2.857314
45	1	0.363712	2.055703	2.931451
46	1	-3.245137	-1.741980	0.464131
47	1	-4.576337	-1.488299	1.655693
48	1	-4.322175	-0.299092	0.324530
49	1	2.939116	1.722343	-3.467938
50	1	1.141626	1.750482	-3.572812
51	1	1.958130	2.072352	-1.995378
52	1	-0.353902	-4.196975	-2.216405
53	1	0.692512	-3.491862	-0.926650
54	1	-1.058439	-3.062571	-1.002668
55	6	-2.605664	1.557825	-3.499761
56	6	-3.405801	2.025392	-2.456180
57	1	-0.855387	0.447467	-4.042482
58	1	-2.881509	1.764199	-4.525766
59	1	-4.298935	2.596463	-2.674100
60	1	-3.691199	2.110714	-0.330862

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.689801	-0.549093	0.842659
2	8	0.689801	-0.549093	3.010703
3	6	1.844232	-0.549093	3.485356
4	7	2.927517	-0.557200	2.709603
5	6	2.788176	-0.616064	1.257888
6	6	2.462129	-1.848635	0.662766
7	6	3.495472	0.438097	0.579507
8	7	4.075898	1.295922	0.050618
9	1	2.336181	-2.720320	1.296741
10	1	2.757034	-2.047842	-0.358697
11	1	3.854953	-0.573063	3.119476
12	1	2.005259	-0.550460	4.567498
13	15	-1.359663	0.572854	0.878626
14	15	0.426994	-0.496014	-1.422508
15	6	-1.883629	0.914724	-0.843683
16	6	-1.091431	0.474547	-1.847143
17	6	-2.781764	-0.197245	1.962037
18	6	-1.460787	2.269366	1.830929
19	6	0.153012	-2.161779	-2.413806
20	6	1.944707	-0.017107	-2.550362
21	6	-1.478353	0.710066	-3.219054
22	6	-3.093196	1.644691	-1.137780
23	6	-3.757204	-0.997030	1.136527
24	6	-0.081556	2.796958	2.125570
25	6	-0.132285	-3.305814	-1.477032
26	6	1.945313	1.444940	-2.918737
27	1	-2.274252	-0.862298	2.653361
28	1	-1.980480	2.977095	1.191376
29	1	-0.709577	-2.012566	-3.056203
30	1	2.819818	-0.217602	-1.944116
31	6	-3.422034	0.989547	2.718176
32	6	-2.290089	1.965532	3.101680
33	6	1.432908	-2.357867	-3.261482
34	6	1.904526	-0.975965	-3.763348
35	1	-4.147670	1.501480	2.089166
36	1	-3.937960	0.627632	3.605554
37	1	-1.663039	1.504317	3.862893
38	1	-2.693723	2.891195	3.507732
39	1	2.221780	-2.812808	-2.665276
40	1	1.221100	-3.021856	-4.097434
41	1	1.221393	-0.611431	-4.526825
42	1	2.895774	-1.045647	-4.207532
43	1	0.474615	2.947653	1.175927
44	1	-0.155005	3.771374	2.653203
45	1	0.485525	2.087002	2.761644

46	1	-3.214734	-1.779033	0.563990
47	1	-4.494558	-1.492131	1.803108
48	1	-4.304718	-0.345771	0.425302
49	1	2.883800	1.694481	-3.457426
50	1	1.087254	1.695126	-3.573649
51	1	1.888773	2.065692	-1.999576
52	1	-0.328580	-4.230167	-2.060414
53	1	0.726002	-3.487674	-0.799470
54	1	-1.029602	-3.075183	-0.864290
55	6	-2.649777	1.415511	-3.504213
56	6	-3.455091	1.884824	-2.464524
57	1	-0.876069	0.335059	-4.033183
58	1	-2.936513	1.593721	-4.532504
59	1	-4.362537	2.430972	-2.687211
60	1	-3.723230	2.008118	-0.337364

iid-a/b:

E(Basis I/Basis I): -849.105184356823
E(Basis II/Basis I): -850.393492877070
E(Basis II/Basis II): -850.3993041520
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.90082015200

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.674515	-0.621461	0.863728
2	8	0.674515	-0.621461	3.010063
3	6	1.846978	-0.621461	3.516972
4	7	2.937326	-0.645488	2.731072
5	6	2.777318	-0.740667	1.266492
6	6	2.388167	-1.998143	0.715627
7	6	3.562758	0.235719	0.551250
8	7	4.214931	1.039261	-0.019154
9	1	2.230371	-2.845194	1.377308
10	1	2.658544	-2.244893	-0.303576
11	1	3.873734	-0.638175	3.128070
12	1	1.982833	-0.606864	4.599185
13	15	0.428163	-0.501337	-1.489828
14	15	-1.357522	0.678835	0.912518
15	6	-1.063423	0.574622	-1.866798
16	6	-1.831068	1.058458	-0.849203
17	1	-1.218697	-3.634512	1.639126
18	1	-0.833471	-3.003524	1.538780
19	6	1.978304	-0.037069	-2.598403
20	6	0.102232	-2.127911	-2.544850
21	6	-1.393319	2.380031	1.881433
22	6	-2.857571	-0.018948	1.957563
23	6	-2.989511	1.868865	-1.142731
24	6	-1.437047	0.851606	-3.234939
25	6	2.025303	1.434040	-2.924694
26	6	-0.234081	-3.288962	-1.647487
27	6	0.004530	2.815086	2.233253
28	6	-3.846966	-0.765656	1.099959
29	1	2.840797	-0.284717	-1.991169
30	1	-0.744551	-1.927904	-3.194815
31	1	-1.843583	3.124034	1.230345
32	1	-2.405976	-0.708944	2.663018
33	6	1.908289	-0.959565	-3.837440
34	6	1.389865	-2.338970	-3.376590
35	6	-2.285602	2.114736	3.118177
36	6	-3.455315	1.202262	2.692704
37	1	1.238286	-0.550572	-4.590202
38	1	2.897663	-1.049597	-4.282331
39	1	2.155567	-2.829370	-2.778138
40	1	1.173764	-2.976512	-4.231901
41	1	-1.712694	1.618260	3.899576
42	1	-2.653455	3.059343	3.514631
43	1	-4.130089	1.753189	2.040594
44	1	-4.020282	0.870065	3.561771

45	1	-1.152137	-3.058616	-1.066606
46	1	-0.419950	-4.197218	-2.258842
47	1	0.594823	-3.496025	-0.940534
48	1	1.986251	2.029387	-1.988004
49	1	2.972186	1.669309	-3.455009
50	1	1.176144	1.728828	-3.572873
51	1	-4.633738	-1.216379	1.740988
52	1	-4.331075	-0.086873	0.368660
53	1	-3.328866	-1.578697	0.548340
54	1	-0.026626	3.785042	2.773173
55	1	0.501439	2.061091	2.877851
56	1	0.603483	2.942638	1.306571
57	6	-3.332867	2.144186	-2.467166
58	6	-2.559613	1.634427	-3.511221
59	1	-3.597493	2.265396	-0.341123
60	1	-4.202286	2.750894	-2.684871
61	1	-2.832665	1.843674	-4.537444
62	1	-0.857133	0.451848	-4.054012

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.654999	-0.590981	0.825866
2	8	0.633561	-0.630453	2.992780
3	6	1.783421	-0.662455	3.477629
4	7	2.873035	-0.677155	2.711287
5	6	2.744828	-0.712632	1.257240
6	6	2.399276	-1.931238	0.643432
7	6	3.483950	0.334441	0.601838
8	7	4.090743	1.186610	0.093831
9	1	2.252023	-2.808268	1.265184
10	1	2.697657	-2.123557	-0.378203
11	1	3.796422	-0.719826	3.128394
12	1	1.934162	-0.686504	4.560964
13	15	0.420089	-0.481088	-1.441429
14	15	-1.323724	0.651762	0.866022
15	6	-1.049328	0.563505	-1.860703
16	6	-1.821288	1.035782	-0.856006
17	1	-1.338241	-4.006682	1.741401
18	1	-0.975405	-3.364811	1.642114
19	6	1.968034	-0.037349	-2.542863
20	6	0.096552	-2.116149	-2.466980
21	6	-1.328292	2.347252	1.826324
22	6	-2.794360	-0.035991	1.939190
23	6	-2.988413	1.832662	-1.148282
24	6	-1.417363	0.831323	-3.231881
25	6	2.023526	1.429582	-2.887075
26	6	-0.244569	-3.264376	-1.554654
27	6	0.078518	2.781526	2.142114
28	6	-3.804402	-0.785015	1.107895
29	1	2.828274	-0.278104	-1.930165
30	1	-0.750013	-1.923983	-3.119218
31	1	-1.791283	3.089853	1.182758
32	1	-2.329052	-0.725055	2.636524
33	6	1.908828	-0.974211	-3.772144
34	6	1.380938	-2.345786	-3.299174
35	6	-2.192837	2.094284	3.085023
36	6	-3.374953	1.185600	2.687564
37	1	1.248725	-0.572745	-4.537416
38	1	2.902434	-1.072554	-4.205502
39	1	2.143762	-2.838020	-2.698692
40	1	1.157865	-2.988847	-4.148450
41	1	-1.605162	1.598292	3.855720
42	1	-2.546707	3.042831	3.484614
43	1	-4.062846	1.737983	2.050544
44	1	-3.920974	0.854402	3.568918
45	1	-1.154316	-3.018219	-0.967061
46	1	-0.446455	-4.176299	-2.155391
47	1	0.588260	-3.475167	-0.853766

48	1	1.972940	2.037429	-1.958994
49	1	2.978314	1.655795	-3.407086
50	1	1.184980	1.718785	-3.551202
51	1	-4.574269	-1.235236	1.769500
52	1	-4.308134	-0.108355	0.388100
53	1	-3.300129	-1.598966	0.544888
54	1	0.062432	3.755838	2.674776
55	1	0.588608	2.031995	2.781151
56	1	0.656364	2.899901	1.200844
57	6	-3.331497	2.103385	-2.474125
58	6	-2.548368	1.600568	-3.515047
59	1	-3.600733	2.223572	-0.347216
60	1	-4.206998	2.700012	-2.695127
61	1	-2.820385	1.803733	-4.542718
62	1	-0.830691	0.434001	-4.047000

iid-c/d:

E(Basis I/Basis I): -849.104479456437
E(Basis II/Basis I): -850.393496909044
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.896043909044

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.695508	-0.582216	0.856182
2	8	0.695508	-0.582216	3.003157
3	6	1.867517	-0.582216	3.511358
4	7	2.959242	-0.611603	2.727374
5	6	2.802190	-0.698697	1.263352
6	6	2.410467	-1.949580	0.701890
7	6	3.582797	0.282955	0.550615
8	7	4.229017	1.090792	-0.020570
9	1	2.246158	-2.801891	1.355450
10	1	2.685481	-2.187357	-0.318219
11	1	3.894659	-0.602765	3.126471
12	1	2.002481	-0.565330	4.593620
13	15	-1.434545	0.552057	0.897385
14	15	0.438455	-0.488026	-1.496729
15	6	-1.907297	0.938620	-0.862314
16	6	-1.100814	0.517974	-1.877824
17	1	2.762051	3.222551	3.265565
18	1	3.002087	3.078132	2.575702
19	6	-2.891078	-0.301556	1.887753
20	6	-1.628289	2.211868	1.917144
21	6	0.164346	-2.128312	-2.546944
22	6	1.969374	0.023453	-2.610336
23	6	-1.475482	0.794271	-3.245797
24	6	-3.109880	1.681529	-1.156646
25	6	-3.806967	-1.085638	0.982803
26	6	-0.278475	2.756419	2.302359
27	6	-0.132241	-3.299284	-1.647868
28	6	1.970649	1.495029	-2.937467
29	1	-2.399137	-0.983266	2.574219
30	1	-2.134847	2.934923	1.284150
31	1	-0.691219	-1.955247	-3.193123
32	1	2.840255	-0.196743	-2.004281
33	6	-3.593701	0.840682	2.656979
34	6	-2.507661	1.828878	3.131786
35	6	1.454196	-2.297767	-3.384739
36	6	1.926174	-0.902377	-3.848173
37	1	-4.302321	1.359121	2.014051
38	1	-4.140971	0.432726	3.504839
39	1	-1.903555	1.352183	3.901937
40	1	-2.956261	2.724743	3.557200
41	1	2.238374	-2.763283	-2.790388
42	1	1.254624	-2.941882	-4.239143
43	1	1.241697	-0.516219	-4.599910
44	1	2.916903	-0.960815	-4.295337

45	1	0.320632	2.959582	1.389424
46	1	-0.400698	3.705251	2.866286
47	1	0.272526	2.032040	2.936397
48	1	-3.219735	-1.833644	0.409041
49	1	-4.566403	-1.620870	1.591003
50	1	-4.330478	-0.416141	0.270192
51	1	2.906286	1.758247	-3.474555
52	1	1.108759	1.764355	-3.579696
53	1	1.920317	2.089357	-2.000651
54	1	-0.320472	-4.206203	-2.260515
55	1	0.717394	-3.500543	-0.965003
56	1	-1.037212	-3.086487	-1.040035
57	6	-2.640235	1.512354	-3.523222
58	6	-3.454440	1.957411	-2.480695
59	1	-0.867189	0.438075	-4.064222
60	1	-2.915592	1.718802	-4.549382
61	1	-4.357698	2.511950	-2.699651
62	1	-3.752190	2.023218	-0.356467

iid-a‡:

E(Basis I/Basis I): -849.103946617852
E(Basis II/Basis I): -850.392240077422
E(Basis II/Basis II): -850.3978525928
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.89242359283

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.582347	-0.851209	0.848973
2	8	0.556055	-0.969963	2.992656
3	6	1.691857	-0.712881	3.520161
4	7	2.757068	-0.433876	2.751752
5	6	2.641286	-0.563121	1.281257
6	6	2.491285	-1.898191	0.753447
7	6	3.331177	0.501740	0.593880
8	7	3.909227	1.381655	0.057306
9	1	2.535276	-2.737106	1.442750
10	1	2.838438	-2.115499	-0.249826
11	1	3.660288	-0.207606	3.161268
12	1	1.810823	-0.715865	4.604265
13	15	-1.313075	0.662428	0.930700
14	15	0.418813	-0.578609	-1.501653
15	6	-1.806202	1.025398	-0.833545
16	6	-1.078434	0.493928	-1.857501
17	1	-1.278029	-2.873826	1.144322
18	1	-0.527753	-2.850293	1.176512
19	6	-2.847173	0.147272	2.036757
20	6	-1.185641	2.403543	1.822208
21	6	0.228001	-2.163004	-2.648724
22	6	1.970152	0.041480	-2.533587
23	6	-1.467071	0.761896	-3.223435
24	6	-2.932843	1.881734	-1.122128
25	6	-3.919354	-0.550114	1.238478
26	6	0.252318	2.727417	2.128161
27	6	-0.040164	-3.389421	-1.818637
28	6	1.924825	1.527863	-2.784791
29	1	-2.437798	-0.547324	2.763459
30	1	-1.584095	3.154085	1.145269
31	1	-0.614206	-1.993656	-3.313296
32	1	2.831812	-0.182578	-1.916672
33	6	-3.321231	1.444903	2.729814
34	6	-2.069066	2.273490	3.086732
35	6	1.550673	-2.244671	-3.448499
36	6	1.990027	-0.813662	-3.821392
37	1	-3.966018	2.022664	2.070857
38	1	-3.887801	1.199260	3.626178
39	1	-1.522636	1.767750	3.881028
40	1	-2.346981	3.263354	3.444060
41	1	2.328983	-2.714747	-2.849822

42	1	1.402035	-2.849646	-4.341029
43	1	1.313554	-0.406947	-4.569720
44	1	2.993943	-0.816442	-4.242124
45	1	0.837525	2.769941	1.184910
46	1	0.318981	3.713840	2.633861
47	1	0.696111	1.952902	2.787614
48	1	-3.485136	-1.419717	0.701569
49	1	-4.715755	-0.915600	1.920595
50	1	-4.376842	0.136647	0.498221
51	1	2.876477	1.857310	-3.252690
52	1	1.088924	1.794171	-3.462504
53	1	1.794097	2.070546	-1.824871
54	1	-0.088582	-4.285939	-2.472337
55	1	0.760843	-3.535501	-1.064015
56	1	-1.014480	-3.281392	-1.298281
57	6	-2.566321	1.578783	-3.493150
58	6	-3.294984	2.141403	-2.444619
59	1	-0.909048	0.338320	-4.046109
60	1	-2.851006	1.780123	-4.517753
61	1	-4.142619	2.779911	-2.657202
62	1	-3.502217	2.326551	-0.317955

Frequencies -- -144.7806 22.6280 42.3062

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.357020	-0.897245	0.848917
2	8	0.328809	-0.907502	3.021192
3	6	1.483940	-0.931659	3.495839
4	7	2.564157	-0.959657	2.719224
5	6	2.417557	-1.110569	1.269276
6	6	1.966758	-2.372208	0.785619
7	6	3.319697	-0.245002	0.554853
8	7	4.067668	0.463528	0.015901
9	1	1.825138	-3.174098	1.502939
10	1	2.255151	-2.693659	-0.206995
11	1	3.491884	-0.991284	3.128013
12	1	1.643194	-0.928034	4.578067
13	15	-1.061816	0.972652	0.869457
14	15	0.224739	-0.714528	-1.428336
15	6	-1.514359	1.373305	-0.866494
16	6	-0.960631	0.638191	-1.858409
17	1	-1.878990	-2.508295	1.401047
18	1	-1.134255	-2.598148	1.369528
19	6	-2.618858	0.896907	2.040071
20	6	-0.479364	2.659241	1.659145
21	6	-0.364454	-2.261268	-2.471738
22	6	1.851722	-0.549771	-2.496606
23	6	-1.300267	0.920007	-3.234324
24	6	-2.411268	2.458984	-1.183873
25	6	-3.859607	0.440766	1.315021
26	6	1.006141	2.640748	1.902004
27	6	-0.909939	-3.337162	-1.571793
28	6	2.166230	0.886169	-2.834794
29	1	-2.358326	0.158792	2.791855
30	1	-0.713236	3.451428	0.953575
31	1	-1.153056	-1.928619	-3.140026
32	1	2.645719	-0.940996	-1.873018
33	6	-2.741533	2.299055	2.678501
34	6	-1.312730	2.812049	2.954556
35	6	0.878761	-2.711956	-3.276144
36	6	1.647211	-1.455206	-3.733233
37	1	-3.254396	2.986786	2.009367
38	1	-3.313894	2.236540	3.602133
39	1	-0.873493	2.226096	3.760196
40	1	-1.325554	3.855864	3.262620
41	1	1.530300	-3.327081	-2.657920
42	1	0.565767	-3.308593	-4.130903
43	1	1.080148	-0.940133	-4.505219

44	1	2.614838	-1.725480	-4.151969
45	1	1.542942	2.491798	0.940956
46	1	1.329395	3.606593	2.344541
47	1	1.279590	1.817966	2.594186
48	1	-3.668388	-0.531764	0.814120
49	1	-4.689866	0.308905	2.040570
50	1	-4.172444	1.182135	0.552503
51	1	3.165253	0.946878	-3.315845
52	1	1.414802	1.307924	-3.532167
53	1	2.179555	1.500017	-1.909581
54	1	-1.196025	-4.225280	-2.174148
55	1	-0.152888	-3.641056	-0.819128
56	1	-1.814132	-2.962210	-1.048623
57	6	-2.179631	1.961142	-3.538820
58	6	-2.731300	2.732783	-2.514753
59	1	-0.876160	0.334578	-4.037176
60	1	-2.429872	2.173111	-4.570233
61	1	-3.407237	3.543872	-2.752613
62	1	-2.838877	3.065259	-0.397578

Frequencies -- -162.8434 24.6006 46.2124

iid-b‡:

E(Basis I/Basis I): -849.068989390037
E(Basis II/Basis I): -850.362850951617
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.853506951617

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.160683	-1.258728	0.545732
2	8	0.070725	-1.121712	2.817976
3	6	1.198497	-1.169948	3.393305
4	7	2.322571	-1.487477	2.702618
5	6	2.223925	-1.944820	1.327178
6	6	1.368503	-3.037181	1.013248
7	6	3.415317	-1.698551	0.557598
8	7	4.425954	-1.529470	-0.030866
9	1	0.850643	-3.560767	1.810292
10	1	1.554030	-3.601251	0.106356
11	1	3.235313	-1.450262	3.148213
12	1	1.307879	-0.943638	4.456116
13	15	1.100630	0.529658	-0.803806
14	15	-1.880752	-0.000095	0.300897
15	6	-0.289519	1.718153	-1.241975
16	6	-1.546520	1.494804	-0.769660
17	1	-0.413323	-2.279338	-0.816743
18	1	-0.802257	-2.657033	-0.173389
19	6	2.660639	1.558826	-0.188214
20	6	1.962563	0.178052	-2.539600
21	6	-3.089320	0.617362	1.735346
22	6	-3.322609	-1.059219	-0.508478
23	6	-2.616022	2.405972	-1.110598
24	6	-0.043286	2.854934	-2.101517
25	6	2.252225	2.786387	0.586639
26	6	1.829091	-1.278292	-2.897675
27	6	-2.440416	0.537182	3.090690
28	6	-3.300867	-0.980806	-2.014246
29	1	3.196328	0.890555	0.474204
30	1	1.444331	0.769914	-3.288675
31	1	-3.320880	1.656690	1.521478
32	1	-3.128171	-2.081075	-0.202607
33	6	3.506577	1.860214	-1.448031
34	6	3.435582	0.638818	-2.391074
35	6	-4.354240	-0.268626	1.616390
36	6	-4.635466	-0.551989	0.126892
37	1	3.143610	2.748195	-1.959337
38	1	4.538096	2.047267	-1.154999
39	1	4.044507	-0.161012	-1.977181

40	1	3.835619	0.891369	-3.371109
41	1	-4.204455	-1.214865	2.133562
42	1	-5.196558	0.240495	2.081293
43	1	-4.983756	0.353442	-0.364676
44	1	-5.410183	-1.309410	0.022225
45	1	0.755587	-1.540999	-3.006814
46	1	2.342781	-1.480545	-3.861311
47	1	2.273985	-1.919551	-2.108658
48	1	1.587444	2.496767	1.427918
49	1	3.153860	3.283995	1.002098
50	1	1.717524	3.509482	-0.061766
51	1	-4.067211	-1.664570	-2.436489
52	1	-3.516438	0.050319	-2.361716
53	1	-2.303456	-1.287032	-2.394605
54	1	-3.101997	1.006991	3.849042
55	1	-2.273406	-0.519425	3.383526
56	1	-1.473546	1.083248	3.081340
57	6	-2.364512	3.507081	-1.929381
58	6	-1.080797	3.729823	-2.425976
59	1	-3.619398	2.239725	-0.747827
60	1	-3.168237	4.185319	-2.185210
61	1	-0.889583	4.580770	-3.066885
62	1	0.940885	3.038820	-2.503197

Frequencies -- -64.9892 25.0835 55.8436

iid-c‡:

E(Basis I/Basis I): -849.102674371283
E(Basis II/Basis I): -850.389428806102
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.885919806102

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.741488	-0.359543	0.911920
2	8	0.894141	-0.050469	3.032365
3	6	2.054796	-0.288037	3.514752
4	7	3.032170	-0.791170	2.742254
5	6	2.726555	-1.162307	1.352065
6	6	1.780289	-2.218038	1.127231
7	6	3.788856	-0.874749	0.427928
8	7	4.657018	-0.642859	-0.340292
9	1	1.351182	-2.746706	1.975083
10	1	1.870702	-2.796883	0.220410
11	1	3.960405	-0.969320	3.117223
12	1	2.266546	-0.089716	4.565941
13	15	-1.457916	0.631439	0.911541
14	15	0.452785	-0.416276	-1.460863
15	6	-1.946668	0.952756	-0.853978
16	6	-1.107609	0.564924	-1.856030
17	1	2.598205	2.701019	0.910648
18	1	2.229126	2.054172	0.859439
19	6	-2.820796	-0.373160	1.894889
20	6	-1.854876	2.269515	1.913372
21	6	0.255215	-1.968709	-2.671310
22	6	1.997390	0.228640	-2.492352
23	6	-1.463322	0.851309	-3.228537
24	6	-3.183521	1.629625	-1.166401
25	6	-3.649521	-1.235896	0.977624
26	6	-0.589196	2.997871	2.279043
27	6	-0.143175	-3.226573	-1.943613
28	6	1.927300	1.712675	-2.749102
29	1	-2.267210	-1.008607	2.578747
30	1	-2.459125	2.912484	1.280055
31	1	-0.539490	-1.711515	-3.364592
32	1	2.855347	0.024354	-1.863072
33	6	-3.639574	0.686414	2.668381
34	6	-2.667234	1.788485	3.138372
35	6	1.605348	-2.065035	-3.416795

36	6	2.055009	-0.632468	-3.776316
37	1	-4.402447	1.124709	2.027709
38	1	-4.136279	0.220122	3.517285
39	1	-2.002539	1.381708	3.898657
40	1	-3.210090	2.626130	3.572448
41	1	2.360011	-2.533322	-2.787271
42	1	1.487436	-2.671059	-4.313356
43	1	1.401274	-0.229544	-4.546784
44	1	3.071656	-0.634740	-4.165261
45	1	-0.033232	3.269021	1.356971
46	1	-0.837297	3.930021	2.829393
47	1	0.060500	2.369018	2.919903
48	1	-2.989054	-1.923894	0.408407
49	1	-4.363661	-1.841257	1.574827
50	1	-4.223210	-0.613694	0.260187
51	1	2.866555	2.053139	-3.233933
52	1	1.076765	1.965366	-3.413043
53	1	1.807126	2.256488	-1.788519
54	1	-0.515641	-3.974676	-2.675159
55	1	-0.955982	-3.007073	-1.219480
56	1	0.713710	-3.678690	-1.411356
57	6	-2.654923	1.516541	-3.522705
58	6	-3.515806	1.900352	-2.494116
59	1	-0.817201	0.548325	-4.039554
60	1	-2.915718	1.727248	-4.551789
61	1	-4.442484	2.408988	-2.726350
62	1	-3.860549	1.927504	-0.377447

Frequencies -- -28.0117 22.7234 49.1200

iid-d‡:

E(Basis I/Basis I): -849.072995253495
E(Basis II/Basis I): -850.369519290281
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.862266290281

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.894480	-0.117960	0.800986
2	8	0.228996	-1.385031	2.600559
3	6	1.205260	-1.659331	3.367899
4	7	2.482008	-1.371749	3.018792
5	6	2.796793	-0.897055	1.674157
6	6	2.448312	-1.705999	0.555489
7	6	3.928328	-0.000155	1.622401
8	7	4.873058	0.707156	1.586129
9	1	1.981004	-2.666027	0.741330
10	1	3.011285	-1.604363	-0.362798
11	1	3.243929	-1.513597	3.677733
12	1	1.047184	-2.124541	4.343952
13	15	-1.267396	0.857932	0.833144
14	15	0.382079	-0.525049	-1.547121
15	6	-1.874946	1.037040	-0.921481
16	6	-1.171651	0.461871	-1.936465
17	1	1.497808	1.381395	1.418636
18	1	1.613220	1.399101	0.507565
19	6	-2.542022	-0.206324	1.866254
20	6	-1.724971	2.490950	1.825592
21	6	0.146026	-2.191423	-2.584928
22	6	1.847831	0.041790	-2.727906
23	6	-1.658157	0.572394	-3.293236
24	6	-3.104133	1.741830	-1.204989
25	6	-3.280444	-1.188734	0.993369
26	6	-0.481398	3.223156	2.254108
27	6	-0.064223	-3.370807	-1.673926
28	6	1.752888	1.505720	-3.077629
29	1	-1.938848	-0.748508	2.586039
30	1	-2.302534	3.136429	1.170919
31	1	-0.738549	-2.066585	-3.202806
32	1	2.753487	-0.118730	-2.153460

33	6	-3.460372	0.824092	2.560597
34	6	-2.580586	2.003625	3.021986
35	6	1.415539	-2.309461	-3.462113
36	6	1.811246	-0.900674	-3.953555
37	1	-4.225082	1.183050	1.874600
38	1	-3.958235	0.360839	3.410539
39	1	-1.939212	1.669122	3.835760
40	1	-3.192474	2.824716	3.390606
41	1	2.238301	-2.732162	-2.888294
42	1	1.219457	-2.971136	-4.303794
43	1	1.089114	-0.553803	-4.689151
44	1	2.789567	-0.921769	-4.430181
45	1	0.117836	3.503758	1.362292
46	1	-0.759872	4.150936	2.797435
47	1	0.135198	2.589484	2.925929
48	1	-2.555351	-1.847428	0.470950
49	1	-3.946750	-1.819508	1.618794
50	1	-3.896885	-0.660751	0.236328
51	1	2.648599	1.810872	-3.658837
52	1	0.849943	1.713326	-3.686596
53	1	1.708563	2.113519	-2.149241
54	1	-0.279984	-4.277487	-2.277868
55	1	0.838127	-3.562772	-1.061239
56	1	-0.925801	-3.179801	-1.000499
57	6	-2.837094	1.269801	-3.561701
58	6	-3.560312	1.850509	-2.519397
59	1	-1.116343	0.119498	-4.110531
60	1	-3.195868	1.352311	-4.579484
61	1	-4.481096	2.379032	-2.729703
62	1	-3.690500	2.172056	-0.405713

Frequencies -- -89.7654 29.1219 51.0236

molh$_2$-a:

E(Basis I/Basis I): -849.106876497896
E(Basis II/Basis I): -850.398950908566
E(Basis II/Basis II): -850.4054240484
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.89335304841

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.140053	-1.069365	0.898197
2	8	0.140053	-1.069365	3.043719
3	6	1.318066	-1.069365	3.545299
4	7	2.399634	-1.090763	2.752837
5	6	2.219981	-1.293935	1.296373
6	6	1.657885	-2.583839	0.896635
7	6	3.233791	-0.602613	0.539748
8	7	4.079578	-0.032175	-0.057131
9	1	1.525108	-3.340351	1.665673
10	1	1.926311	-2.986186	-0.074020
11	1	3.339317	-1.063378	3.141584
12	1	1.453255	-1.047942	4.627017
13	15	-0.857185	1.170022	0.909437
14	15	0.058587	-0.849476	-1.461032
15	6	-1.331594	1.537526	-0.861567
16	6	-0.959665	0.676285	-1.852600
17	1	-1.736823	-1.627088	0.921197
18	1	-1.322404	-2.297418	0.989731
19	6	-2.359061	1.437745	2.142941
20	6	0.029652	2.797848	1.558927
21	6	-0.640802	-2.320263	-2.563815
22	6	1.724161	-0.793355	-2.502262
23	6	-1.320324	0.965398	-3.222335
24	6	-2.055036	2.742933	-1.193794
25	6	-3.690815	1.155657	1.494307
26	6	1.500475	2.545983	1.753795
27	6	-1.269495	-3.382166	-1.701927
28	6	2.157805	0.622664	-2.789446

29	1	-2.191353	0.714143	2.934632
30	1	-0.104014	3.571712	0.808022
31	1	-1.396074	-1.913102	-3.229655
32	1	2.471647	-1.272064	-1.881552
33	6	-2.214424	2.878669	2.682872
34	6	-0.709272	3.164469	2.868738
35	6	0.579335	-2.837350	-3.364524
36	6	1.451187	-1.632575	-3.771221
37	1	-2.639882	3.598356	1.986721
38	1	-2.743073	2.972777	3.629689
39	1	-0.333338	2.566346	3.697051
40	1	-0.539591	4.213248	3.105285
41	1	1.171419	-3.518980	-2.756167
42	1	0.235631	-3.381800	-4.242069
43	1	0.932483	-1.042774	-4.523797
44	1	2.395426	-1.966788	-4.197309
45	1	1.964422	2.260527	0.785935
46	1	1.996067	3.466448	2.128366
47	1	1.662563	1.725758	2.483845
48	1	-3.690444	0.134435	1.058562
49	1	-4.497726	1.216297	2.254808
50	1	-3.907864	1.888357	0.691429
51	1	3.162828	0.617741	-3.261617
52	1	1.447962	1.126139	-3.476878
53	1	2.211191	1.202995	-1.844367
54	1	-1.590144	-4.239112	-2.331509
55	1	-0.548452	-3.745606	-0.939573
56	1	-2.165692	-2.970106	-1.193139
57	6	-2.036087	2.123173	-3.530667
58	6	-2.399588	3.012037	-2.518873
59	1	-1.026330	0.299479	-4.020859
60	1	-2.300181	2.337301	-4.558183
61	1	-2.945403	3.914292	-2.762567
62	1	-2.332235	3.445505	-0.420573

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.107417	-1.058480	0.856379
2	8	0.107417	-1.058480	3.028516
3	6	1.267717	-1.058480	3.497181
4	7	2.342559	-1.061470	2.716200
5	6	2.189969	-1.266559	1.273473
6	6	1.647902	-2.545380	0.865565
7	6	3.215296	-0.574750	0.540682
8	7	4.064957	-0.010364	-0.017876
9	1	1.534498	-3.307235	1.630331
10	1	1.941402	-2.937977	-0.100781
11	1	3.270855	-1.072138	3.124922
12	1	1.427068	-1.048616	4.578885
13	15	-0.811537	1.132764	0.884657
14	15	0.030672	-0.833331	-1.426050
15	6	-1.316012	1.527598	-0.841478
16	6	-0.968304	0.669411	-1.829224
17	1	-1.630781	-1.592268	0.889629
18	1	-1.191517	-2.287378	0.933993
19	6	-2.282865	1.377812	2.142857
20	6	0.079944	2.747492	1.534973
21	6	-0.656641	-2.294604	-2.534418
22	6	1.693512	-0.765932	-2.451153
23	6	-1.335232	0.963166	-3.196244
24	6	-2.030123	2.742068	-1.158232
25	6	-3.625519	1.098769	1.515307
26	6	1.556462	2.506605	1.694199
27	6	-1.280566	-3.370492	-1.686446
28	6	2.131539	0.652737	-2.719620
29	1	-2.099540	0.644287	2.921713
30	1	-0.074022	3.530075	0.797267
31	1	-1.415478	-1.885986	-3.194957

32	1	2.438461	-1.252312	-1.834025
33	6	-2.137380	2.810401	2.704094
34	6	-0.630323	3.098601	2.864579
35	6	0.562283	-2.800640	-3.344418
36	6	1.432896	-1.589733	-3.732804
37	1	-2.579521	3.539470	2.028443
38	1	-2.648489	2.885488	3.662045
39	1	-0.236219	2.491789	3.678039
40	1	-0.457436	4.144881	3.109309
41	1	1.155188	-3.491151	-2.746929
42	1	0.217326	-3.332196	-4.229228
43	1	0.918420	-0.992834	-4.482565
44	1	2.381386	-1.915881	-4.155482
45	1	1.999628	2.228860	0.714788
46	1	2.053376	3.430041	2.059607
47	1	1.742471	1.687206	2.418622
48	1	-3.630858	0.082481	1.068169
49	1	-4.418473	1.148358	2.291152
50	1	-3.859702	1.840087	0.725123
51	1	3.141830	0.651654	-3.180459
52	1	1.430468	1.163833	-3.410465
53	1	2.174728	1.224386	-1.768980
54	1	-1.605996	-4.215946	-2.329026
55	1	-0.553828	-3.749515	-0.937277
56	1	-2.173861	-2.968025	-1.164925
57	6	-2.042722	2.128686	-3.496399
58	6	-2.387770	3.018630	-2.478611
59	1	-1.053163	0.297518	-3.998966
60	1	-2.314156	2.347657	-4.520983
61	1	-2.928369	3.926268	-2.713787
62	1	-2.292845	3.443477	-0.378941

molh$_2$-b/d:

E(Basis I/Basis I): -849.091828864995
E(Basis II/Basis I): -850.379615835430
E(Basis II/Basis II): -850.388992987402
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.87834898740

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	1.137598	-0.661352	-0.147211
2	8	1.137598	-0.661352	1.936230
3	6	2.313072	-0.661352	2.465911
4	7	3.406299	-0.690784	1.696967
5	6	3.229512	-0.924143	0.251683
6	6	2.594341	-2.205947	-0.104269
7	6	4.233619	-0.299797	-0.566311
8	7	5.042623	0.221258	-1.253171
9	1	2.464213	-2.943163	0.683991
10	1	2.831616	-2.634334	-1.072955
11	1	4.340106	-0.653068	2.099559
12	1	2.410429	-0.630774	3.549991
13	15	0.123399	1.620124	-0.022518
14	15	-1.202748	-1.394114	-0.314426
15	6	-1.741175	1.379495	-0.047776
16	6	-2.288876	0.130623	-0.158568
17	1	1.470554	-0.249426	-1.784941
18	1	1.082266	-1.003066	-1.835220
19	6	0.638435	2.688379	1.548205
20	6	0.501486	3.127149	-1.228979
21	6	-1.976909	-2.772735	0.852764
22	6	-1.706813	-2.405245	-1.924710
23	6	-3.727038	-0.019591	-0.159688
24	6	-2.609929	2.531647	0.045816
25	6	-0.306551	2.491616	2.707325
26	6	1.257264	2.646431	-2.438741
27	6	-1.044614	-3.073229	1.995475
28	6	-2.250661	-1.510176	-3.009670

29	1	1.620787	2.322138	1.825332
30	1	-0.443016	3.558490	-1.548301
31	1	-2.915807	-2.396769	1.249626
32	1	-0.785135	-2.860680	-2.270111
33	6	0.727732	4.150751	1.054516
34	6	1.309188	4.133857	-0.374009
35	6	-2.214542	-3.992692	-0.071271
36	6	-2.697957	-3.490030	-1.447237
37	1	-0.254694	4.617736	1.045525
38	1	1.366648	4.725912	1.722196
39	1	2.356139	3.838586	-0.328928
40	1	1.256896	5.122858	-0.825466
41	1	-1.290614	-4.553492	-0.202235
42	1	-2.950507	-4.655087	0.380721
43	1	-3.704113	-3.085941	-1.358964
44	1	-2.725136	-4.306829	-2.166176
45	1	0.639187	1.915047	-3.001451
46	1	1.488066	3.503330	-3.106512
47	1	2.207897	2.156956	-2.137014
48	1	-0.392006	1.411659	2.949212
49	1	0.081878	3.024798	3.600595
50	1	-1.315237	2.887236	2.472169
51	1	-2.427966	-2.103524	-3.931418
52	1	-3.208184	-1.044641	-2.699476
53	1	-1.517552	-0.707895	-3.238773
54	1	-1.450970	-3.906489	2.607058
55	1	-0.040447	-3.358889	1.616023
56	1	-0.946138	-2.178153	2.644610
57	6	-4.553148	1.099839	-0.061215
58	6	-3.995665	2.373214	0.039459
59	1	-4.176249	-0.998453	-0.246594
60	1	-5.628767	0.979746	-0.066026
61	1	-4.639016	3.240314	0.114417
62	1	-2.194652	3.525664	0.129532

Reopt

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	1.093520	-0.646127	-0.145296
2	8	1.122756	-0.655896	1.959652
3	6	2.288647	-0.643929	2.437457
4	7	3.361105	-0.643911	1.660192
5	6	3.179236	-0.889467	0.233056
6	6	2.566015	-2.169014	-0.112226
7	6	4.164940	-0.251640	-0.591498
8	7	4.948749	0.276363	-1.269530
9	1	2.468119	-2.904703	0.680381
10	1	2.819127	-2.596884	-1.076095
11	1	4.290868	-0.646363	2.066708
12	1	2.428279	-0.625704	3.520018
13	15	0.124769	1.569451	-0.012014
14	15	-1.176259	-1.367494	-0.301446
15	6	-1.717559	1.363124	-0.047675
16	6	-2.264559	0.124775	-0.158101
17	1	1.425441	-0.235574	-1.708620
18	1	1.026011	-1.032380	-1.748174
19	6	0.642359	2.632304	1.549839
20	6	0.523934	3.057037	-1.219369
21	6	-1.949146	-2.742437	0.856288
22	6	-1.656916	-2.376952	-1.907442
23	6	-3.702456	-0.024337	-0.172579
24	6	-2.579704	2.520515	0.036722
25	6	-0.309708	2.453413	2.706473
26	6	1.273781	2.566242	-2.428684
27	6	-1.030007	-3.036804	2.011072
28	6	-2.191594	-1.486798	-3.001261
29	1	1.618315	2.255582	1.834676
30	1	-0.414350	3.499508	-1.541483
31	1	-2.893885	-2.370625	1.242775
32	1	-0.730314	-2.829216	-2.242839

33	6	0.756213	4.092492	1.054403
34	6	1.342710	4.060500	-0.371165
35	6	-2.173481	-3.967468	-0.064268
36	6	-2.646911	-3.469028	-1.444667
37	1	-0.218386	4.575385	1.040378
38	1	1.401483	4.658291	1.723822
39	1	2.385780	3.752420	-0.320990
40	1	1.303761	5.046621	-0.829985
41	1	-1.245802	-4.524253	-0.185766
42	1	-2.910045	-4.631457	0.384223
43	1	-3.657058	-3.072816	-1.367588
44	1	-2.659418	-4.284866	-2.164943
45	1	0.650161	1.836789	-2.987779
46	1	1.507876	3.419088	-3.100510
47	1	2.223248	2.074359	-2.127575
48	1	-0.417347	1.375614	2.948678
49	1	0.086242	2.979051	3.600920
50	1	-1.309954	2.868641	2.469240
51	1	-2.349507	-2.082399	-3.925094
52	1	-3.158090	-1.029484	-2.707187
53	1	-1.461973	-0.678485	-3.220271
54	1	-1.437753	-3.874120	2.616186
55	1	-0.018549	-3.314272	1.645228
56	1	-0.948977	-2.142286	2.663281
57	6	-4.527310	1.097158	-0.084564
58	6	-3.966301	2.368864	0.018711
59	1	-4.153083	-1.002101	-0.263205
60	1	-5.603160	0.980095	-0.100323
61	1	-4.606649	3.238877	0.085422
62	1	-2.160606	3.512717	0.121761

molh$_2$-c:

E(Basis I/Basis I): -849.107999720785
E(Basis II/Basis I): -850.397765504510
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.888376504510

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.710603	0.247656	0.987729
2	8	0.710603	0.247656	3.137641
3	6	1.889165	0.247656	3.650018
4	7	2.977525	0.142965	2.874181
5	6	2.789567	-0.123246	1.436405
6	6	2.041171	-1.348047	1.115708
7	6	3.831397	0.408707	0.605861
8	7	4.667359	0.863392	-0.096726
9	1	1.785283	-2.003686	1.946989
10	1	2.259329	-1.893055	0.208238
11	1	3.913087	0.167598	3.272317
12	1	2.012449	0.334576	4.729519
13	15	-1.543510	-0.572954	0.785193
14	15	0.606106	0.507223	-1.388709
15	6	-2.041447	-0.416569	-1.007747
16	6	-1.147654	0.074399	-1.914447
17	1	-0.107727	2.119262	1.235503
18	1	0.652083	2.259810	1.227325
19	6	-1.770815	-2.417169	1.406967
20	6	-3.074064	0.034499	1.856801
21	6	1.763097	-0.138475	-2.862825
22	6	1.009612	2.377783	-1.856077
23	6	-1.555634	0.250191	-3.291096
24	6	-3.371855	-0.784045	-1.434881
25	6	-1.584750	-3.409757	0.287628
26	6	-2.738388	1.316507	2.571049
27	6	2.570550	-1.347361	-2.477063
28	6	-0.230307	3.237258	-1.857746
29	1	-0.992252	-2.565487	2.147922
30	1	-3.911560	0.212202	1.188204

31	1	1.105144	-0.414716	-3.680853
32	1	1.683306	2.721630	-1.078152
33	6	-3.167732	-2.466287	2.066170
34	6	-3.376207	-1.137697	2.822157
35	6	2.630171	1.082176	-3.247282
36	6	1.734378	2.335883	-3.220818
37	1	-3.945083	-2.586709	1.314404
38	1	-3.224568	-3.311493	2.749644
39	1	-2.704390	-1.105823	3.678331
40	1	-4.397354	-1.056099	3.189860
41	1	3.450284	1.206001	-2.542081
42	1	3.052498	0.928065	-4.238648
43	1	1.017342	2.289349	-4.038032
44	1	2.330109	3.238411	-3.344485
45	1	-2.534951	2.117400	1.829376
46	1	-3.594624	1.631879	3.204197
47	1	-1.843788	1.184884	3.214802
48	1	-0.587527	-3.267028	-0.180452
49	1	-1.644697	-4.443487	0.688716
50	1	-2.367704	-3.283226	-0.488254
51	1	0.049657	4.298182	-2.028521
52	1	-0.930246	2.922945	-2.658745
53	1	-0.750161	3.161298	-0.880538
54	1	3.129776	-1.719455	-3.361516
55	1	1.894425	-2.155189	-2.126583
56	1	3.303057	-1.097258	-1.685632
57	6	-2.845255	-0.101021	-3.692942
58	6	-3.749190	-0.623744	-2.768347
59	1	-0.876257	0.669765	-4.018943
60	1	-3.144831	0.033176	-4.724297
61	1	-4.747033	-0.899133	-3.084390
62	1	-4.083034	-1.188757	-0.728578

molh$_2$-a^t:

E(Basis I/Basis I): -849.095139491569
E(Basis II/Basis I): -850.39325074867
E(Basis II/Basis II): -850.3986013523
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.88783735231

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.065790	-1.124397	0.860469
2	8	0.018187	-1.130249	3.021119
3	6	1.167436	-1.059594	3.577859
4	7	2.299324	-1.017288	2.853325
5	6	2.245612	-1.211873	1.398109
6	6	1.749985	-2.486400	0.936791
7	6	3.220436	-0.442626	0.677103
8	7	4.038493	0.187620	0.100453
9	1	1.576826	-3.269474	1.668175
10	1	2.051481	-2.845348	-0.039778
11	1	3.203499	-0.922184	3.309651
12	1	1.243706	-1.023738	4.665167
13	15	-0.739444	1.195926	0.886284
14	15	-0.016160	-0.909256	-1.479335
15	6	-1.263596	1.549845	-0.871376
16	6	-0.975579	0.654452	-1.859103
17	1	-1.523343	-1.474655	0.768210
18	1	-0.805733	-2.480571	0.805335
19	6	-2.233213	1.416790	2.134852
20	6	0.121452	2.837491	1.544376
21	6	-0.693680	-2.354101	-2.623997
22	6	1.682075	-0.840753	-2.465109
23	6	-1.367020	0.941811	-3.220827
24	6	-1.948849	2.779429	-1.196300
25	6	-3.561469	1.120177	1.485178
26	6	1.598463	2.615772	1.723619
27	6	-1.334941	-3.435660	-1.796390
28	6	2.128249	0.580155	-2.707042

29	1	-2.049228	0.684370	2.914497
30	1	-0.034727	3.618959	0.805655
31	1	-1.440096	-1.931716	-3.290252
32	1	2.411714	-1.338686	-1.837372
33	6	-2.113002	2.854561	2.689497
34	6	-0.612982	3.170844	2.865580
35	6	0.541896	-2.851785	-3.414740
36	6	1.432866	-1.642610	-3.763395
37	1	-2.559195	3.572462	2.004432
38	1	-2.635748	2.927238	3.641402
39	1	-0.216116	2.570994	3.682795
40	1	-0.463984	4.219903	3.114350
41	1	1.116063	-3.557992	-2.817172
42	1	0.213595	-3.364341	-4.316937
43	1	0.935472	-1.025439	-4.508651
44	1	2.383722	-1.971887	-4.178448
45	1	2.060725	2.365260	0.745747
46	1	2.075349	3.538923	2.115495
47	1	1.784680	1.783575	2.434209
48	1	-3.547986	0.102498	1.041594
49	1	-4.368402	1.163823	2.246802
50	1	-3.788731	1.856533	0.687912
51	1	3.148019	0.583095	-3.146434
52	1	1.441152	1.100544	-3.405507
53	1	2.150737	1.140458	-1.749064
54	1	-1.719123	-4.238670	-2.460518
55	1	-0.599302	-3.878518	-1.092197
56	1	-2.188250	-3.016909	-1.222565
57	6	-2.040285	2.126569	-3.522361
58	6	-2.330177	3.043857	-2.512216
59	1	-1.124601	0.256705	-4.020410
60	1	-2.329083	2.338763	-4.543626
61	1	-2.847094	3.964454	-2.750293
62	1	-2.174765	3.500965	-0.423589

Frequencies -- -934.1098 25.8390 55.6025

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.065790	-1.124397	0.860469
2	8	0.018187	-1.130249	3.021119
3	6	1.167436	-1.059594	3.577859
4	7	2.299324	-1.017288	2.853325
5	6	2.245612	-1.211873	1.398109
6	6	1.749985	-2.486400	0.936791
7	6	3.220436	-0.442626	0.677103
8	7	4.038493	0.187620	0.100453
9	1	1.576826	-3.269474	1.668175
10	1	2.051481	-2.845348	-0.039778
11	1	3.203499	-0.922184	3.309651
12	1	1.243706	-1.023738	4.665167
13	15	-0.739444	1.195926	0.886284
14	15	-0.016160	-0.909256	-1.479335
15	6	-1.263596	1.549845	-0.871376
16	6	-0.975579	0.654452	-1.859103
17	1	-1.523343	-1.474655	0.768210
18	1	-0.805733	-2.480571	0.805335
19	6	-2.233213	1.416790	2.134852
20	6	0.121452	2.837491	1.544376
21	6	-0.693680	-2.354101	-2.623997
22	6	1.682075	-0.840753	-2.465109
23	6	-1.367020	0.941811	-3.220827
24	6	-1.948849	2.779429	-1.196300
25	6	-3.561469	1.120177	1.485178
26	6	1.598463	2.615772	1.723619
27	6	-1.334941	-3.435660	-1.796390
28	6	2.128249	0.580155	-2.707042
29	1	-2.049228	0.684370	2.914497
30	1	-0.034727	3.618959	0.805655
31	1	-1.440096	-1.931716	-3.290252

32	1	2.411714	-1.338686	-1.837372
33	6	-2.113002	2.854561	2.689497
34	6	-0.612982	3.170844	2.865580
35	6	0.541896	-2.851785	-3.414740
36	6	1.432866	-1.642610	-3.763395
37	1	-2.559195	3.572462	2.004432
38	1	-2.635748	2.927238	3.641402
39	1	-0.216116	2.570994	3.682795
40	1	-0.463984	4.219903	3.114350
41	1	1.116063	-3.557992	-2.817172
42	1	0.213595	-3.364341	-4.316937
43	1	0.935472	-1.025439	-4.508651
44	1	2.383722	-1.971887	-4.178448
45	1	2.060725	2.365260	0.745747
46	1	2.075349	3.538923	2.115495
47	1	1.784680	1.783575	2.434209
48	1	-3.547986	0.102498	1.041594
49	1	-4.368402	1.163823	2.246802
50	1	-3.788731	1.856533	0.687912
51	1	3.148019	0.583095	-3.146434
52	1	1.441152	1.100544	-3.405507
53	1	2.150737	1.140458	-1.749064
54	1	-1.719123	-4.238670	-2.460518
55	1	-0.599302	-3.878518	-1.092197
56	1	-2.188250	-3.016909	-1.222565
57	6	-2.040285	2.126569	-3.522361
58	6	-2.330177	3.043857	-2.512216
59	1	-1.124601	0.256705	-4.020410
60	1	-2.329083	2.338763	-4.543626
61	1	-2.847094	3.964454	-2.750293
62	1	-2.174765	3.500965	-0.423589

Frequencies -- -934.1098 25.8390 55.6025

molh$_2$-b‡:

E(Basis I/Basis I): -849.086154906411
E(Basis II/Basis I): -850.381328979714
E(Basis II/Basis II): -850.386493184108
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.87818918411

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.985468	-0.895504	-0.176516
2	8	0.985468	-0.895504	1.983088
3	6	2.163565	-0.895504	2.490031
4	7	3.252534	-0.951298	1.705297
5	6	3.077725	-1.202966	0.265239
6	6	2.442167	-2.472573	-0.087958
7	6	4.084742	-0.586715	-0.557463
8	7	4.911730	-0.080634	-1.233088
9	1	2.236056	-3.185298	0.705863
10	1	2.693892	-2.921514	-1.041839
11	1	4.188824	-0.921169	2.102085
12	1	2.294041	-0.840989	3.570909
13	15	0.375735	1.521989	-0.009684
14	15	-1.414171	-1.220905	-0.332135
15	6	-1.498049	1.580535	0.082095
16	6	-2.237739	0.437097	-0.033916
17	1	1.245055	-0.530809	-1.706050
18	1	0.854556	-1.656001	-1.562029
19	6	1.176407	2.532679	1.479177
20	6	0.895805	2.915276	-1.294158
21	6	-2.338191	-2.560031	0.768218
22	6	-2.120437	-2.012716	-1.986842
23	6	-3.679503	0.508362	0.047462
24	6	-2.169254	2.849058	0.255030
25	6	0.306051	2.527876	2.711321
26	6	1.456338	2.289490	-2.542979

27	6	-1.414605	-3.090412	1.831821
28	6	-2.557735	-0.960876	-2.975007
29	1	2.103746	2.014764	1.697732
30	1	0.008843	3.489033	-1.548793
31	1	-3.190828	-2.082287	1.242839
32	1	-1.294023	-2.573501	-2.408483
33	6	1.468470	3.945478	0.923205
34	6	1.925384	3.792809	-0.542210
35	6	-2.797428	-3.648978	-0.233038
36	6	-3.250695	-2.966525	-1.540039
37	1	0.579527	4.570919	0.967088
38	1	2.244118	4.422070	1.519880
39	1	2.908743	3.325981	-0.563340
40	1	2.002532	4.764205	-1.027031
41	1	-1.977037	-4.330115	-0.453085
42	1	-3.608728	-4.227445	0.204944
43	1	-4.175780	-2.420176	-1.368835
44	1	-3.435184	-3.707333	-2.315860
45	1	0.682973	1.654535	-3.025081
46	1	1.761423	3.081650	-3.259080
47	1	2.339989	1.660716	-2.302555
48	1	0.056333	1.485042	2.997085
49	1	0.849385	3.005124	3.553990
50	1	-0.635348	3.086958	2.539010
51	1	-2.857197	-1.444407	-3.928746
52	1	-3.420528	-0.382732	-2.585963
53	1	-1.718081	-0.262828	-3.178531
54	1	-1.908293	-3.917673	2.384474
55	1	-0.472820	-3.468074	1.379369
56	1	-1.173259	-2.283986	2.554968
57	6	-4.314597	1.736924	0.230222
58	6	-3.561060	2.905560	0.330289
59	1	-4.279588	-0.385304	-0.047355
60	1	-5.394456	1.783927	0.286023
61	1	-4.056699	3.858307	0.464553
62	1	-1.599492	3.764296	0.329205

Frequencies -- -835.8535 13.5533 35.8819

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	1.064173	-0.756145	-0.083176
2	8	0.942835	-0.731858	2.080802
3	6	2.059495	-0.540979	2.619832
4	7	3.175996	-0.421188	1.906985
5	6	3.139460	-0.725119	0.482105
6	6	2.737278	-2.072150	0.127556
7	6	4.077883	0.034997	-0.293015
8	7	4.827781	0.669150	-0.915658
9	1	2.620328	-2.796082	0.927641
10	1	3.123374	-2.485943	-0.796194
11	1	4.067314	-0.290193	2.373213
12	1	2.138021	-0.458176	3.706602
13	15	0.175338	1.500604	-0.028480
14	15	-1.190147	-1.380971	-0.355930
15	6	-1.668897	1.345508	-0.004506
16	6	-2.243530	0.121400	-0.118820
17	1	1.344601	-0.483502	-1.611495
18	1	1.121651	-1.575018	-1.419932
19	6	0.794626	2.665032	1.421942
20	6	0.564402	2.875382	-1.362388
21	6	-1.981929	-2.839672	0.677897
22	6	-1.682390	-2.233622	-2.045879
23	6	-3.684031	0.001187	-0.102165
24	6	-2.502534	2.520817	0.104088
25	6	-0.108053	2.615838	2.629993
26	6	1.229265	2.266508	-2.567479
27	6	-1.053274	-3.264033	1.783973
28	6	-2.185666	-1.236604	-3.059442
29	1	1.768631	2.273403	1.693211

30	1	-0.376245	3.327077	-1.665366
31	1	-2.911553	-2.484579	1.113487
32	1	-0.768573	-2.682764	-2.417226
33	6	0.940654	4.075899	0.806439
34	6	1.460194	3.907233	-0.635627
35	6	-2.247233	-3.966309	-0.351961
36	6	-2.707616	-3.329236	-1.678606
37	1	-0.014858	4.595612	0.794208
38	1	1.636208	4.665829	1.400379
39	1	2.491896	3.560494	-0.606617
40	1	1.437181	4.854840	-1.170373
41	1	-1.337907	-4.538428	-0.528847
42	1	-3.003185	-4.645374	0.037752
43	1	-3.703482	-2.907599	-1.560590
44	1	-2.748910	-4.075400	-2.469871
45	1	0.552295	1.519597	-3.033699
46	1	1.453141	3.056409	-3.315372
47	1	2.177288	1.764552	-2.279518
48	1	-0.251232	1.565294	2.957214
49	1	0.353597	3.185656	3.463829
50	1	-1.099120	3.059937	2.409388
51	1	-2.356577	-1.744865	-4.031847
52	1	-3.139964	-0.778397	-2.728497
53	1	-1.431663	-0.434312	-3.205742
54	1	-1.458582	-4.162721	2.295509
55	1	-0.045768	-3.500889	1.380059
56	1	-0.964275	-2.449859	2.532561
57	6	-4.482424	1.138667	0.022672
58	6	-3.892192	2.397941	0.122002
59	1	-4.157532	-0.964612	-0.203655
60	1	-5.560602	1.044520	0.031128
61	1	-4.512272	3.280757	0.208739
62	1	-2.058915	3.503805	0.171653

Frequencies -- -676.3513 18.9736 42.4739

molh$_2$-c‡:

E(Basis I/Basis I): -849.089072547204
E(Basis II/Basis I): -850.386888925347
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.878167925347

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.652935	0.440910	0.998516
2	8	0.652935	0.440910	3.158619
3	6	1.827331	0.440910	3.665389
4	7	2.916349	0.297684	2.891750
5	6	2.744272	-0.028491	1.466599
6	6	2.055375	-1.256777	1.164159
7	6	3.757988	0.552483	0.625328
8	7	4.590943	1.030280	-0.063040
9	1	1.769285	-1.896234	1.993840
10	1	2.243797	-1.776022	0.235616
11	1	3.852940	0.348386	3.284502
12	1	1.958003	0.561785	4.740906
13	15	-1.397295	-0.854578	0.766334
14	15	0.501883	0.744538	-1.353221
15	6	-1.972383	-0.579682	-0.991612
16	6	-1.197569	0.133284	-1.859159
17	1	-0.307142	1.757766	1.039848
18	1	0.943986	2.039006	1.095798
19	6	-1.412367	-2.766691	1.210001
20	6	-2.967211	-0.527924	1.900412
21	6	1.664481	0.138758	-2.836866
22	6	0.807273	2.622776	-1.844661
23	6	-1.671530	0.375109	-3.204166
24	6	-3.249002	-1.097009	-1.429726
25	6	-1.139617	-3.624527	0.000525

26	6	-2.778420	0.716647	2.726378
27	6	2.509207	-1.049150	-2.467356
28	6	-0.471370	3.422520	-1.833203
29	1	-0.607947	-2.895559	1.925451
30	1	-3.824344	-0.389274	1.247470
31	1	0.998985	-0.151437	-3.644532
32	1	1.468753	2.997759	-1.072246
33	6	-2.780578	-3.033761	1.877433
34	6	-3.123296	-1.810249	2.753523
35	6	2.480070	1.389995	-3.231165
36	6	1.526245	2.602423	-3.212682
37	1	-3.555811	-3.177495	1.127862
38	1	-2.726740	-3.936648	2.482853
39	1	-2.447671	-1.782032	3.606689
40	1	-4.141974	-1.876655	3.130973
41	1	3.294112	1.553373	-2.527015
42	1	2.907774	1.247787	-4.222023
43	1	0.810422	2.516306	-4.027559
44	1	2.079137	3.530427	-3.345406
45	1	-2.621697	1.591542	2.060946
46	1	-3.684228	0.899770	3.342336
47	1	-1.905118	0.613003	3.401335
48	1	-0.175380	-3.326131	-0.463174
49	1	-1.073513	-4.690682	0.303835
50	1	-1.948150	-3.518488	-0.751500
51	1	-0.244601	4.492982	-2.022346
52	1	-1.171335	3.066347	-2.615638
53	1	-0.965219	3.335092	-0.842840
54	1	3.078228	-1.393416	-3.356726
55	1	1.857770	-1.880503	-2.125146
56	1	3.231986	-0.789073	-1.672377
57	6	-2.909191	-0.121434	-3.614476
58	6	-3.694320	-0.860358	-2.730404
59	1	-1.074161	0.941119	-3.904768
60	1	-3.257994	0.062687	-4.622378
61	1	-4.651451	-1.249185	-3.053091
62	1	-3.868449	-1.672775	-0.756978

Frequencies -- -944.4023 18.2981 52.0657

molh$_2$-d^1:

E(Basis I/Basis I): -849.085780195916
E(Basis II/Basis I): -850.380324085357
E(Basis II/Basis II): -850.385378765644
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.87717676564

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	1.137807	-0.593722	-0.190485
2	8	1.227164	-0.592986	1.961129
3	6	2.416113	-0.719171	2.425166
4	7	3.465434	-0.855270	1.599744
5	6	3.220483	-1.057171	0.163363
6	6	2.477792	-2.261374	-0.206502
7	6	4.256160	-0.504553	-0.673776
8	7	5.105559	-0.050765	-1.358123
9	1	2.277506	-2.994094	0.570215
10	1	2.653059	-2.683556	-1.189673
11	1	4.417181	-0.893666	1.957861
12	1	2.588172	-0.706903	3.501598
13	15	-1.197625	-1.371623	-0.305748
14	15	0.104908	1.648859	-0.031693
15	6	-2.295057	0.145779	-0.204101
16	6	-1.755875	1.397079	-0.094878
17	1	0.957012	-0.925688	-1.732399
18	1	1.687091	0.084919	-1.502636
19	6	-1.687889	-2.471626	-1.857984
20	6	-1.961664	-2.694426	0.933759
21	6	0.501550	3.209550	-1.162471
22	6	0.576419	2.645649	1.597321

23	6	-2.632013	2.545138	-0.017056
24	6	-3.731921	-0.013063	-0.226620
25	6	-2.245596	-1.641412	-2.986660
26	6	-1.038884	-2.914685	2.101805
27	6	1.287482	2.795595	-2.377992
28	6	-0.398946	2.391929	2.719932
29	1	-0.757621	-2.926281	-2.179556
30	1	-2.910013	-2.308620	1.297834
31	1	-0.440501	3.645346	-1.482563
32	1	1.553303	2.272384	1.883757
33	6	-2.661532	-3.546286	-1.324362
34	6	-2.173718	-3.966848	0.077558
35	6	1.279076	4.182462	-0.242861
36	6	0.664078	4.129231	1.170474
37	1	-3.674988	-3.156326	-1.259138
38	1	-2.672546	-4.400329	-1.999003
39	1	-1.239476	-4.517148	-0.020519
40	1	-2.899594	-4.616871	0.562658
41	1	2.327551	3.894655	-0.186143
42	1	1.227493	5.190413	-0.650292
43	1	-0.322569	4.587372	1.158511
44	1	1.281200	4.679107	1.878705
45	1	-0.951553	-1.978500	2.692044
46	1	-1.446528	-3.709239	2.762051
47	1	-0.029973	-3.218347	1.750930
48	1	-1.525388	-0.840489	-3.257389
49	1	-2.413309	-2.283986	-3.876656
50	1	-3.210496	-1.175997	-2.700543
51	1	-0.038958	2.886090	3.646903
52	1	-1.403150	2.792983	2.473801
53	1	-0.486051	1.301959	2.910542
54	1	1.484795	3.681124	-3.018595
55	1	2.258729	2.344737	-2.083381
56	1	0.707558	2.054035	-2.967348
57	6	-4.016708	2.379294	-0.046933
58	6	-4.565705	1.102428	-0.150795
59	1	-2.224620	3.541385	0.077741
60	1	-4.665866	3.243123	0.014934
61	1	-5.640451	0.976266	-0.171563
62	1	-4.173707	-0.995882	-0.307946

Frequencies -- -675.4361 11.4059 35.6282

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	1.094399	-0.563916	-0.176281
2	8	1.251331	-0.569831	1.984793
3	6	2.427356	-0.751489	2.381210
4	7	3.436058	-0.925853	1.534188
5	6	3.150112	-1.130961	0.121166
6	6	2.352199	-2.289963	-0.218357
7	6	4.188349	-0.631613	-0.740579
8	7	5.034082	-0.225734	-1.427024
9	1	2.160761	-3.012474	0.568199
10	1	2.491959	-2.724160	-1.201252
11	1	4.382417	-1.048266	1.879079
12	1	2.653828	-0.759555	3.450459
13	15	0.117731	1.615764	-0.020499
14	15	-1.178890	-1.317604	-0.290116
15	6	-1.720682	1.414411	-0.154100
16	6	-2.267463	0.177190	-0.265220
17	1	1.676083	0.110171	-1.448429
18	1	0.907767	-0.827023	-1.706809
19	6	0.535999	2.572704	1.634531
20	6	0.588984	3.175611	-1.107007
21	6	-1.982728	-2.582719	0.969459
22	6	-1.623781	-2.466477	-1.806690
23	6	-3.703666	0.031312	-0.337947
24	6	-2.581814	2.575576	-0.116657
25	6	-0.486464	2.314892	2.713716

26	6	1.420386	2.770642	-2.295095
27	6	-1.101084	-2.760300	2.175765
28	6	-2.139656	-1.678705	-2.984892
29	1	1.494530	2.180740	1.955048
30	1	-0.329981	3.631909	-1.462851
31	1	-2.940162	-2.179647	1.287893
32	1	-0.686425	-2.936236	-2.081953
33	6	0.664256	4.062314	1.240451
34	6	1.339999	4.127182	-0.143731
35	6	-2.176875	-3.889057	0.161463
36	6	-2.617449	-3.521401	-1.270250
37	1	-0.313421	4.537191	1.195150
38	1	1.259258	4.588526	1.984564
39	1	2.381281	3.824434	-0.046158
40	1	1.318893	5.140555	-0.540016
41	1	-1.243787	-4.448032	0.114865
42	1	-2.921636	-4.514545	0.650004
43	1	-3.632271	-3.130084	-1.254083
44	1	-2.606005	-4.399023	-1.913735
45	1	0.859333	2.042067	-2.917956
46	1	1.649370	3.662847	-2.915628
47	1	2.376884	2.310509	-1.968238
48	1	-0.600728	1.223101	2.878632
49	1	-0.153650	2.783695	3.663735
50	1	-1.473107	2.739875	2.438124
51	1	-2.276178	-2.354109	-3.855721
52	1	-3.113841	-1.203251	-2.752032
53	1	-1.409479	-0.888395	-3.259996
54	1	-1.539891	-3.519736	2.857035
55	1	-0.085486	-3.091373	1.872339
56	1	-1.021041	-1.799440	2.726266
57	6	-4.527429	1.156558	-0.306639
58	6	-3.966828	2.427871	-0.195918
59	1	-4.153171	-0.947796	-0.419908
60	1	-5.602137	1.042250	-0.364392
61	1	-4.606584	3.300335	-0.165175
62	1	-2.165911	3.567080	-0.011743

Frequencies -- -575.4790 11.7872 41.8823

dihy-a:

E(Basis I/Basis I): -849.103266057062
E(Basis II/Basis I): -850.396911890125
E(Basis II/Basis II): -850.4036530341
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.89180603406

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	-0.129949	-1.110674	0.884528
2	8	-0.129949	-1.110674	3.068038
3	6	0.983852	-1.110674	3.674966
4	7	2.173349	-1.214044	3.028076
5	6	2.240516	-1.482267	1.602841
6	6	1.667850	-2.650993	1.108820
7	6	3.185428	-0.703387	0.851047
8	7	3.996684	-0.092624	0.245253
9	1	1.276997	-3.395641	1.792381
10	1	1.895117	-2.981817	0.105623
11	1	3.041418	-1.137480	3.552143
12	1	1.018642	-1.008735	4.761261
13	15	-0.263333	1.377213	0.827929
14	15	-0.372524	-1.011458	-1.433875
15	6	-0.432241	1.787597	-0.996928
16	6	-0.465368	0.791274	-1.930221
17	1	-1.672309	-0.972693	0.859096
18	1	-0.635192	-2.613529	0.779089
19	6	-1.922146	1.940937	1.726192
20	6	0.740190	2.851281	1.688551

21	6	-1.871585	-1.888624	-2.349930
22	6	0.935162	-1.993994	-2.521463
23	6	-0.628348	1.125486	-3.327468
24	6	-0.568412	3.164051	-1.421191
25	6	-3.107824	1.893176	0.794458
26	6	2.068411	2.368985	2.201853
27	6	-2.937502	-2.302162	-1.370415
28	6	2.068487	-1.113184	-2.983092
29	1	-2.069063	1.220505	2.524741
30	1	0.917434	3.625381	0.948310
31	1	-2.287983	-1.167422	-3.047929
32	1	1.325633	-2.766708	-1.870697
33	6	-1.641320	3.348815	2.296138
34	6	-0.190060	3.366288	2.812862
35	6	-1.235083	-3.081846	-3.100480
36	6	0.125106	-2.633153	-3.672698
37	1	-1.764248	4.109560	1.527838
38	1	-2.340351	3.565679	3.101804
39	1	-0.116421	2.727010	3.690988
40	1	0.109013	4.372350	3.101299
41	1	-1.081346	-3.918001	-2.420331
42	1	-1.901531	-3.409643	-3.896067
43	1	-0.031298	-1.921688	-4.480510
44	1	0.673691	-3.483074	-4.074491
45	1	2.699510	2.044752	1.350686
46	1	2.592190	3.193687	2.730088
47	1	1.931857	1.523003	2.905004
48	1	-3.210716	0.878388	0.357971
49	1	-4.035365	2.131801	1.356437
50	1	-2.995339	2.627730	-0.029444
51	1	2.835417	-1.728996	-3.498487
52	1	1.709503	-0.335362	-3.686654
53	1	2.539571	-0.616383	-2.110619
54	1	-3.767815	-2.805133	-1.909837
55	1	-2.528717	-3.003433	-0.614057
56	1	-3.346689	-1.407202	-0.857144
57	6	-0.739087	2.457359	-3.725289
58	6	-0.712126	3.474700	-2.773476
59	1	-0.668905	0.348414	-4.077033
60	1	-0.857605	2.700449	-4.773275
61	1	-0.814298	4.506776	-3.083062
62	1	-0.589301	3.965536	-0.697750

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	-0.052229	-1.099336	0.814053
2	8	-0.052229	-1.099336	3.023604
3	6	1.078114	-1.099336	3.546334
4	7	2.211437	-1.172992	2.836708
5	6	2.179449	-1.420541	1.412597
6	6	1.585590	-2.615700	0.969646
7	6	3.179741	-0.735368	0.650781
8	7	4.024962	-0.203680	0.053802
9	1	1.307627	-3.358226	1.707774
10	1	1.831741	-3.005661	-0.007824
11	1	3.105363	-1.154111	3.314382
12	1	1.188604	-1.027161	4.632391
13	15	-0.424048	1.269254	0.857873
14	15	-0.282383	-0.928195	-1.436212
15	6	-0.917401	1.720000	-0.858924
16	6	-0.849515	0.783347	-1.833801
17	1	-1.606244	-1.019597	0.737795
18	1	-0.573647	-2.585904	0.732817
19	6	-1.862980	1.683477	2.114329
20	6	0.651787	2.769166	1.521887
21	6	-1.405468	-2.153193	-2.462640
22	6	1.285898	-1.345731	-2.525915
23	6	-1.204144	1.133915	-3.191034
24	6	-1.357391	3.059280	-1.176403