25	6	-3.221587	1.614552	1.461730
26	6	2.097490	2.379697	1.653567
27	6	-2.313182	-2.951862	-1.564779
28	6	2.057996	-0.104245	-2.899432
29	1	-1.798469	0.911797	2.874867
30	1	0.573545	3.582491	0.806329
31	1	-2.015767	-1.552958	-3.130857
32	1	1.915581	-1.977652	-1.911314
33	6	-1.530086	3.072047	2.706629
34	6	0.000222	3.163786	2.867972
35	6	-0.410457	-3.029142	-3.260956
36	6	0.748884	-2.134258	-3.744122
37	1	-1.873863	3.866845	2.047751
38	1	-2.028857	3.190301	3.666696
39	1	0.319183	2.487449	3.659193
40	1	0.303736	4.172210	3.142695
41	1	-0.013972	-3.824059	-2.631226
42	1	-0.923012	-3.489356	-4.103434
43	1	0.388184	-1.455933	-4.514532
44	1	1.549344	-2.734696	-4.172213
45	1	2.498441	2.097055	0.658178
46	1	2.686558	3.238214	2.039911
47	1	2.209379	1.526117	2.352306
48	1	-3.374202	0.618635	0.996685
49	1	-4.011477	1.770558	2.226524
50	1	-3.329151	2.395016	0.681294
51	1	3.016392	-0.390155	-3.381918
52	1	1.482676	0.527201	-3.606819
53	1	2.280230	0.493809	-1.991530
54	1	-3.000212	-3.567196	-2.183497
55	1	-1.730501	-3.633581	-0.912603
56	1	-2.924190	-2.270217	-0.936755
57	6	-1.627514	2.428938	-3.493251
58	6	-1.707568	3.390065	-2.485947
59	1	-1.130583	0.406893	-3.986993
60	1	-1.891216	2.688260	-4.510396
61	1	-2.038525	4.393470	-2.720551
62	1	-1.430176	3.812433	-0.404425

dihy-b:

E(Basis I/Basis I): -849.113211032138
E(Basis II/Basis I): -850.408068071496
E(Basis II/Basis II): -850.412971810967
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.90086381097

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.692754	-1.171608	-0.008203
2	8	0.692754	-1.171608	2.257365
3	6	1.855500	-1.171608	2.760636
4	7	2.974985	-1.202766	1.991414
5	6	2.894648	-1.358104	0.538861
6	6	2.433693	-2.590501	0.013549
7	6	3.799346	-0.501992	-0.186181
8	7	4.577534	0.195719	-0.736632
9	1	2.231019	-3.411552	0.691930
10	1	2.644483	-2.853928	-1.015899
11	1	3.893077	-1.174446	2.428479
12	1	2.002885	-1.136917	3.842915
13	15	0.672844	1.293741	-0.075215
14	15	-1.629934	-0.995959	-0.321145
15	6	-1.143315	1.763138	-0.025791
16	6	-2.103378	0.801631	-0.143395
17	1	0.785827	-1.182934	-1.553400
18	1	0.271119	-2.706755	-0.168427
19	6	1.740826	2.296187	1.233984
20	6	1.379145	2.379320	-1.552960

21	6	-2.863479	-2.067740	0.755862
22	6	-2.323062	-1.741348	-1.991373
23	6	-3.498764	1.176613	-0.160774
24	6	-1.534588	3.151918	0.060730
25	6	0.963451	2.610862	2.487353
26	6	1.718171	1.508535	-2.733156
27	6	-2.161215	-2.659420	1.948693
28	6	-2.503062	-0.679646	-3.046695
29	1	2.559457	1.631019	1.484830
30	1	0.597490	3.077545	-1.839586
31	1	-3.660115	-1.414472	1.100603
32	1	-1.565742	-2.445217	-2.317273
33	6	2.271327	3.542454	0.487211
34	6	2.598508	3.127962	-0.963707
35	6	-3.406789	-3.133879	-0.226183
36	6	-3.629805	-2.468230	-1.600019
37	1	1.529129	4.337522	0.484709
38	1	3.161947	3.917308	0.988239
39	1	3.476437	2.485334	-0.966916
40	1	2.817042	4.002797	-1.573128
41	1	-2.692273	-3.948215	-0.333471
42	1	-4.336423	-3.545874	0.161934
43	1	-4.458696	-1.765876	-1.536075
44	1	-3.874492	-3.213680	-2.354278
45	1	0.799325	1.010337	-3.107765
46	1	2.143748	2.128028	-3.550673
47	1	2.454001	0.728995	-2.449981
48	1	0.544707	1.676789	2.917005
49	1	1.637081	3.075153	3.238157
50	1	0.132208	3.313116	2.278464
51	1	-2.819042	-1.150466	-4.001420
52	1	-3.274808	0.056738	-2.742093
53	1	-1.543278	-0.147022	-3.213957
54	1	-2.859694	-3.315630	2.509879
55	1	-1.281983	-3.258811	1.632657
56	1	-1.826207	-1.847043	2.626504
57	6	-3.865239	2.518826	-0.056848
58	6	-2.884823	3.504822	0.052554
59	1	-4.268326	0.425169	-0.270456
60	1	-4.911310	2.796184	-0.072774
61	1	-3.171339	4.546353	0.120037
62	1	-0.787066	3.929503	0.119245

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.672288	-1.136620	0.000074
2	8	0.703462	-1.170346	2.266075
3	6	1.853300	-1.179210	2.730294
4	7	2.953673	-1.191688	1.958581
5	6	2.863188	-1.339575	0.519277
6	6	2.384997	-2.553590	-0.004716
7	6	3.780063	-0.498579	-0.199652
8	7	4.561660	0.184281	-0.722951
9	1	2.200727	-3.377416	0.673474
10	1	2.598419	-2.815336	-1.033293
11	1	3.869358	-1.206089	2.393806
12	1	2.028932	-1.166834	3.811613
13	15	0.648879	1.259501	-0.067155
14	15	-1.591654	-0.973980	-0.315487
15	6	-1.135843	1.747173	-0.032795
16	6	-2.087649	0.792626	-0.157854
17	1	0.753447	-1.143627	-1.533861
18	1	0.215950	-2.655723	-0.169761
19	6	1.710551	2.252236	1.239334
20	6	1.363654	2.332164	-1.538209
21	6	-2.824368	-2.030814	0.763455
22	6	-2.271591	-1.737013	-1.973242
23	6	-3.483266	1.164515	-0.200048
24	6	-1.523671	3.137324	0.042347

25	6	0.931226	2.570897	2.490702
26	6	1.703549	1.461816	-2.718511
27	6	-2.135312	-2.601939	1.973869
28	6	-2.449616	-0.690981	-3.044658
29	1	2.525014	1.584137	1.494975
30	1	0.586111	3.032671	-1.829793
31	1	-3.625906	-1.374979	1.090823
32	1	-1.510681	-2.441706	-2.287785
33	6	2.254741	3.496801	0.499158
34	6	2.583463	3.081838	-0.950775
35	6	-3.359800	-3.114667	-0.203055
36	6	-3.577255	-2.468251	-1.586338
37	1	1.520256	4.298876	0.495996
38	1	3.146498	3.862163	1.004941
39	1	3.461642	2.439782	-0.953250
40	1	2.801516	3.955836	-1.561414
41	1	-2.642028	-3.928016	-0.294808
42	1	-4.289792	-3.523761	0.187054
43	1	-4.412178	-1.771903	-1.538314
44	1	-3.809146	-3.224060	-2.334191
45	1	0.784358	0.969078	-3.098540
46	1	2.134891	2.081017	-3.533245
47	1	2.435046	0.678755	-2.435157
48	1	0.502328	1.639996	2.917108
49	1	1.606033	3.027501	3.245180
50	1	0.107112	3.281239	2.280838
51	1	-2.751480	-1.177401	-3.996139
52	1	-3.230952	0.042801	-2.759296
53	1	-1.493005	-0.152649	-3.209819
54	1	-2.839388	-3.250723	2.536733
55	1	-1.251612	-3.205208	1.678650
56	1	-1.811469	-1.778338	2.643464
57	6	-3.852499	2.506872	-0.105716
58	6	-2.873194	3.492774	0.014837
59	1	-4.250654	0.412359	-0.318702
60	1	-4.898267	2.783915	-0.137435
61	1	-3.159408	4.534849	0.074945
62	1	-0.776046	3.913988	0.107304

dihy-c:

E(Basis I/Basis I): -849.102064465431
E(Basis II/Basis I): -850.392170733449
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.887010733449

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.431796	0.695722	0.874528
2	8	0.431796	0.695722	3.049518
3	6	1.407532	0.695722	3.844325
4	7	2.677948	0.295836	3.532267
5	6	3.074251	-0.279596	2.276295
6	6	2.398544	-1.301586	1.688459
7	6	4.292406	0.260230	1.722805
8	7	5.299371	0.697105	1.286982
9	1	1.556718	-1.774197	2.179698
10	1	2.747774	-1.723643	0.753173
11	1	3.408793	0.472772	4.217265
12	1	1.274732	1.043722	4.872249
13	15	-1.338138	-1.023629	0.568620
14	15	0.317246	0.993858	-1.412295
15	6	-1.597088	-1.085947	-1.293563
16	6	-0.893007	-0.250569	-2.114249
17	1	-0.612296	1.806884	0.881917
18	1	1.447520	1.928501	0.886737
19	6	-1.220209	-2.836903	1.329664
20	6	-3.140329	-0.787023	1.313897
21	6	1.921487	0.982958	-2.533380

22	6	-0.152013	2.806816	-1.976565
23	6	-1.106986	-0.301597	-3.542719
24	6	-2.573132	-1.986311	-1.864249
25	6	-0.580877	-3.816889	0.378673
26	6	-3.266770	0.576900	1.938789
27	6	3.093205	0.445668	-1.757648
28	6	-1.633387	2.954631	-2.215961
29	1	-0.586257	-2.728582	2.202967
30	1	-3.848913	-0.873480	0.494680
31	1	1.731015	0.338967	-3.387471
32	1	0.142419	3.437738	-1.145265
33	6	-2.655269	-3.212493	1.761608
34	6	-3.320484	-1.941361	2.329249
35	6	2.107979	2.457389	-2.971281
36	6	0.720694	3.084191	-3.221046
37	1	-3.232026	-3.588051	0.919704
38	1	-2.616627	-3.995309	2.517022
39	1	-2.851244	-1.686990	3.278049
40	1	-4.381000	-2.106421	2.510357
41	1	2.617289	3.021064	-2.191451
42	1	2.719336	2.493851	-3.871035
43	1	0.273991	2.650812	-4.113539
44	1	0.807635	4.158320	-3.373796
45	1	-3.133439	1.359796	1.162436
46	1	-4.274448	0.694666	2.390582
47	1	-2.497063	0.718330	2.727050
48	1	0.409584	-3.434202	0.053308
49	1	-0.434106	-4.792047	0.889182
50	1	-1.215019	-3.979719	-0.515423
51	1	-1.871204	4.014745	-2.445305
52	1	-1.963371	2.325677	-3.067899
53	1	-2.195216	2.653030	-1.306572
54	1	4.009219	0.473987	-2.384833
55	1	2.897382	-0.606430	-1.463361
56	1	3.261608	1.051690	-0.843455
57	6	-2.036743	-1.190352	-4.082819
58	6	-2.771459	-2.028238	-3.244758
59	1	-0.559151	0.355748	-4.203159
60	1	-2.195427	-1.222184	-5.152973
61	1	-3.500290	-2.708928	-3.665400
62	1	-3.161020	-2.631269	-1.228121

dihy-d:

E(Basis I/Basis I): -849.110716225148
E(Basis II/Basis I): -850.406139683563
E(Basis II/Basis II): -850.411165253483
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.90010225348

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	1.179896	0.197168	0.106365
2	8	1.179896	0.197168	2.373850
3	6	2.358405	0.197168	2.842773
4	7	3.456921	0.080230	2.052304
5	6	3.346901	-0.148191	0.612458
6	6	2.819855	-1.369763	0.146004
7	6	4.269204	0.633820	-0.181610
8	7	5.058726	1.250051	-0.805809
9	1	2.581861	-2.150511	0.857235
10	1	3.007982	-1.668886	-0.877038
11	1	4.386207	0.167058	2.456699
12	1	2.538479	0.302236	3.915615
13	15	-0.411253	-1.643196	-0.295333
14	15	-0.687777	1.594565	-0.143694
15	6	-2.058478	-0.812423	-0.639020
16	6	-2.170963	0.543644	-0.562481
17	1	1.358216	0.304795	-1.428780
18	1	1.831974	1.654310	0.140921

19	6	0.031226	-2.917011	-1.721924
20	6	-0.842332	-3.107860	0.945295
21	6	-0.680494	3.130131	-1.348641
22	6	-1.018793	2.718501	1.421281
23	6	-3.448290	1.174475	-0.803497
24	6	-3.224220	-1.607212	-0.953667
25	6	-0.533007	-2.490543	-3.053758
26	6	-0.298031	-2.823594	2.319566
27	6	0.447215	3.020421	-2.340357
28	6	-2.049978	2.114372	2.340346
29	1	1.113242	-2.907205	-1.783514
30	1	-1.924290	-3.181992	1.005961
31	1	-1.626962	3.138055	-1.882071
32	1	-0.066444	2.769842	1.937534
33	6	-0.473559	-4.294940	-1.233428
34	6	-0.242873	-4.375526	0.290912
35	6	-0.559831	4.356007	-0.411121
36	6	-1.415259	4.099223	0.847915
37	1	-1.532559	-4.419203	-1.448681
38	1	0.068336	-5.087061	-1.746831
39	1	0.825539	-4.438782	0.489677
40	1	-0.715807	-5.262807	0.707728
41	1	0.477353	4.505906	-0.116163
42	1	-0.896810	5.249394	-0.933306
43	1	-2.470649	4.116471	0.582822
44	1	-1.241294	4.870247	1.596133
45	1	-0.747076	-1.887645	2.714202
46	1	-0.555515	-3.656909	3.006999
47	1	0.804303	-2.709249	2.293245
48	1	-0.194126	-1.460670	-3.294716
49	1	-0.173847	-3.177340	-3.849047
50	1	-1.641356	-2.511920	-3.044443
51	1	-2.149905	2.738852	3.253059
52	1	-3.039257	2.053446	1.842344
53	1	-1.734944	1.092703	2.641322
54	1	0.438191	3.900072	-3.018172
55	1	1.428164	2.978807	-1.822782
56	1	0.322337	2.102208	-2.952413
57	6	-4.565976	0.398360	-1.112084
58	6	-4.453959	-0.990000	-1.187681
59	1	-3.551002	2.248856	-0.736481
60	1	-5.521840	0.873945	-1.289479
61	1	-5.322873	-1.589886	-1.425353
62	1	-3.154792	-2.683909	-1.013148

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	1.142259	0.174777	0.125686
2	8	1.184530	0.189110	2.391385
3	6	2.352028	0.207404	2.812986
4	7	3.426117	0.103422	2.012491
5	6	3.294599	-0.138814	0.589873
6	6	2.777783	-1.364468	0.151750
7	6	4.196332	0.639638	-0.223872
8	7	4.967277	1.242722	-0.848921
9	1	2.591660	-2.141237	0.880999
10	1	2.972444	-1.677921	-0.864841
11	1	4.357008	0.184629	2.405594
12	1	2.566830	0.315949	3.881713
13	15	-0.403632	-1.600417	-0.295122
14	15	-0.665966	1.553390	-0.129758
15	6	-2.033542	-0.799780	-0.648754
16	6	-2.143419	0.545755	-0.565002
17	1	1.310468	0.276257	-1.400021
18	1	1.750097	1.647260	0.173754
19	6	0.055618	-2.867222	-1.708613
20	6	-0.837159	-3.054641	0.940366
21	6	-0.639436	3.080426	-1.332390

22	6	-1.008344	2.675661	1.423362
23	6	-3.415871	1.184029	-0.811599
24	6	-3.195295	-1.593832	-0.978381
25	6	-0.494448	-2.445900	-3.048219
26	6	-0.310265	-2.765091	2.320210
27	6	0.490940	2.966745	-2.320853
28	6	-2.050024	2.078058	2.335109
29	1	1.137642	-2.854041	-1.760673
30	1	-1.919126	-3.133948	0.991118
31	1	-1.582400	3.092372	-1.871504
32	1	-0.061935	2.723761	1.950361
33	6	-0.444008	-4.249490	-1.226739
34	6	-0.228357	-4.325003	0.299691
35	6	-0.520899	4.310468	-0.400327
36	6	-1.390417	4.060441	0.849939
37	1	-1.499430	-4.383027	-1.453378
38	1	0.109997	-5.037095	-1.733948
39	1	0.838153	-4.384949	0.509492
40	1	-0.703626	-5.211228	0.715893
41	1	0.514009	4.456173	-0.095507
42	1	-0.848084	5.203289	-0.929521
43	1	-2.443174	4.086841	0.575566
44	1	-1.217174	4.828323	1.601451
45	1	-0.766101	-1.829240	2.707221
46	1	-0.574292	-3.597072	3.006796
47	1	0.792102	-2.649646	2.307023
48	1	-0.162988	-1.412493	-3.284452
49	1	-0.117254	-3.128518	-3.838763
50	1	-1.602430	-2.479139	-3.055198
51	1	-2.148716	2.700622	3.249280
52	1	-3.037718	2.028281	1.833017
53	1	-1.746122	1.052646	2.634918
54	1	0.484130	3.844645	-3.000987
55	1	1.471218	2.926815	-1.802231
56	1	0.366309	2.047817	-2.931830
57	6	-4.533125	0.413541	-1.136528
58	6	-4.422745	-0.974607	-1.220378
59	1	-3.516451	2.257978	-0.737611
60	1	-5.486088	0.892708	-1.319888
61	1	-5.290091	-1.572037	-1.469718
62	1	-3.126218	-2.670153	-1.042684

dihy-aα‡:

E(Basis I/Basis I): -849.099694514705
E(Basis II/Basis I): -850.396594599060
E(Basis II/Basis II): -850.4021817617
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.89098676166

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	-0.226714	-0.998214	0.885502
2	8	-0.342765	-0.844197	3.062392
3	6	0.747781	-1.016039	3.700787
4	7	1.893420	-1.378257	3.082641
5	6	1.894757	-1.712096	1.664354
6	6	1.112023	-2.843522	1.263470
7	6	3.015003	-1.243241	0.908325
8	7	3.957637	-0.870140	0.296826
9	1	0.744040	-3.501030	2.046955
10	1	1.360798	-3.342581	0.334553
11	1	2.758309	-1.451733	3.612748
12	1	0.780542	-0.862321	4.780435
13	15	-0.318021	1.409883	0.763940
14	15	-0.324668	-0.962769	-1.443645
15	6	-0.609512	1.808516	-1.036591
16	6	-0.607559	0.808979	-1.962810
17	1	-1.780988	-0.854700	0.724484
18	1	-0.559867	-2.592469	0.875838

19	6	-1.765877	2.102916	1.884210
20	6	0.935971	2.763006	1.445442
21	6	-1.586907	-2.084029	-2.433914
22	6	1.210028	-1.717588	-2.406009
23	6	-0.821877	1.122660	-3.356904
24	6	-0.826124	3.173662	-1.457024
25	6	-3.069922	2.179654	1.130808
26	6	2.276331	2.145114	1.734034
27	6	-2.638634	-2.644201	-1.513834
28	6	2.185302	-0.648349	-2.831203
29	1	-1.862500	1.380526	2.688723
30	1	1.054623	3.524779	0.679993
31	1	-2.064941	-1.459513	-3.183378
32	1	1.700434	-2.382203	-1.704026
33	6	-1.268094	3.466765	2.415238
34	6	0.243138	3.344599	2.701179
35	6	-0.706751	-3.171186	-3.095777
36	6	0.600826	-2.513560	-3.584463
37	1	-1.437013	4.252084	1.681194
38	1	-1.811673	3.728554	3.321132
39	1	0.393000	2.688314	3.556754
40	1	0.672964	4.315376	2.940918
41	1	-0.470487	-3.956020	-2.378933
42	1	-1.246382	-3.623313	-3.925704
43	1	0.383933	-1.853618	-4.422017
44	1	1.309833	-3.266866	-3.922881
45	1	2.704387	1.727728	0.798721
46	1	2.971206	2.916312	2.128497
47	1	2.178544	1.332858	2.482910
48	1	-3.326847	1.183459	0.713333
49	1	-3.881884	2.495203	1.819453
50	1	-3.006608	2.911639	0.299885
51	1	3.095133	-1.119785	-3.258970
52	1	1.738513	0.017033	-3.597864
53	1	2.480293	-0.033858	-1.955228
54	1	-3.343171	-3.278823	-2.091969
55	1	-2.177422	-3.261497	-0.715702
56	1	-3.213458	-1.816133	-1.048388
57	6	-1.031406	2.444250	-3.753669
58	6	-1.035020	3.467669	-2.805325
59	1	-0.810768	0.341323	-4.104083
60	1	-1.189709	2.675783	-4.799001
61	1	-1.199362	4.491370	-3.115815
62	1	-0.837154	3.975549	-0.731921

Frequencies -- -610.4339 22.0507 56.2046

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.196037	-1.060592	0.774368
2	8	0.176930	-1.119908	2.983202
3	6	1.291035	-0.944329	3.516304
4	7	2.420496	-0.813414	2.812503
5	6	2.419142	-1.015293	1.380048
6	6	2.055591	-2.313602	0.915702
7	6	3.291502	-0.159726	0.639556
8	7	4.025681	0.526653	0.052177
9	1	2.002699	-3.106661	1.654283
10	1	2.405378	-2.633530	-0.057027
11	1	3.298661	-0.658620	3.294894
12	1	1.382454	-0.884700	4.604714
13	15	-0.739379	1.100197	0.883095
14	15	-0.059070	-0.881627	-1.468582
15	6	-1.312691	1.503354	-0.817074
16	6	-1.012484	0.653984	-1.825553
17	1	-1.323135	-1.422425	0.667311
18	1	0.327719	-2.656756	0.646593
19	6	-2.212346	1.150796	2.158595
20	6	0.016137	2.757678	1.599764
21	6	-0.855885	-2.311461	-2.530106

22	6	1.574292	-0.901009	-2.540068
23	6	-1.426109	0.964844	-3.174907
24	6	-2.050509	2.714702	-1.089517
25	6	-3.531187	0.810319	1.510818
26	6	1.511573	2.657637	1.718714
27	6	-1.559336	-3.313576	-1.653672
28	6	2.042017	0.493394	-2.876442
29	1	-1.970849	0.386122	2.890125
30	1	-0.228592	3.560821	0.910525
31	1	-1.582783	-1.856814	-3.196787
32	1	2.326260	-1.382440	-1.925915
33	6	-2.174531	2.558953	2.795622
34	6	-0.695739	2.966072	2.957589
35	6	0.323093	-2.916259	-3.329323
36	6	1.246322	-1.765735	-3.780349
37	1	-2.684229	3.283537	2.163815
38	1	-2.678189	2.538693	3.760190
39	1	-0.236390	2.348540	3.727582
40	1	-0.609126	4.007036	3.263081
41	1	0.887265	-3.609953	-2.707837
42	1	-0.059635	-3.466105	-4.186881
43	1	0.742851	-1.172746	-4.541117
44	1	2.167944	-2.153538	-4.210171
45	1	1.954813	2.477285	0.717059
46	1	1.922805	3.607160	2.121841
47	1	1.794352	1.828545	2.398290
48	1	-3.466504	-0.178472	1.010403
49	1	-4.326380	0.763201	2.284496
50	1	-3.815338	1.575005	0.759545
51	1	3.038554	0.446675	-3.364075
52	1	1.335086	0.996318	-3.567380
53	1	2.126394	1.099975	-1.950642
54	1	-2.034725	-4.093264	-2.285737
55	1	-0.846124	-3.808420	-0.963771
56	1	-2.353538	-2.810417	-1.063327
57	6	-2.141662	2.135061	-3.434898
58	6	-2.455725	3.008186	-2.392615
59	1	-1.175674	0.306422	-3.994645
60	1	-2.449953	2.367018	-4.446096
61	1	-3.010619	3.915052	-2.595195
62	1	-2.300063	3.398210	-0.289886

Frequencies -- -506.9469 22.3988 55.5119

dihy-bα‡:

E(Basis I/Basis I): -849.111168094574
E(Basis II/Basis I): -850.406183895908
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.897231895908

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.714471	-1.092862	-0.001146
2	8	0.747393	-1.087385	2.259914
3	6	1.926263	-1.142716	2.729903
4	7	3.012488	-1.253113	1.925444
5	6	2.853200	-1.433013	0.479132
6	6	2.292629	-2.686116	0.030947
7	6	3.815685	-0.705065	-0.304592
8	7	4.625950	-0.096161	-0.912295
9	1	2.169477	-3.475686	0.766913
10	1	2.505977	-3.019419	-0.978544
11	1	3.947069	-1.269352	2.326907
12	1	2.106228	-1.096272	3.806534
13	15	0.638744	1.323124	-0.071754
14	15	-1.623250	-0.986721	-0.312542
15	6	-1.176429	1.778308	-0.035957
16	6	-2.126567	0.805644	-0.145825
17	1	0.799908	-1.083416	-1.548209
18	1	0.542021	-2.709554	-0.144362

19	6	1.694236	2.290748	1.270321
20	6	1.390316	2.405917	-1.523447
21	6	-2.834644	-2.068719	0.779996
22	6	-2.323638	-1.749653	-1.972541
23	6	-3.525227	1.166862	-0.160446
24	6	-1.578495	3.163767	0.041901
25	6	0.890599	2.621720	2.502674
26	6	1.719600	1.543165	-2.711937
27	6	-2.102593	-2.657873	1.955872
28	6	-2.513887	-0.698548	-3.036643
29	1	2.489448	1.604500	1.539369
30	1	0.635670	3.134141	-1.808148
31	1	-3.630153	-1.423643	1.142404
32	1	-1.565728	-2.453490	-2.297894
33	6	2.271413	3.525555	0.539674
34	6	2.623882	3.103026	-0.902774
35	6	-3.387298	-3.138519	-0.193627
36	6	-3.624629	-2.479480	-1.568279
37	1	1.544633	4.334839	0.517160
38	1	3.156284	3.881696	1.063887
39	1	3.474331	2.423756	-0.884705
40	1	2.894345	3.969369	-1.503453
41	1	-2.673338	-3.952796	-0.305837
42	1	-4.312226	-3.551073	0.204945
43	1	-4.455257	-1.779676	-1.500267
44	1	-3.873690	-3.229151	-2.316929
45	1	0.792665	1.072455	-3.102151
46	1	2.168126	2.163184	-3.516670
47	1	2.434634	0.743399	-2.431779
48	1	0.437837	1.697412	2.918691
49	1	1.554406	3.068526	3.272581
50	1	0.082611	3.344294	2.272140
51	1	-2.832035	-1.179492	-3.985592
52	1	-3.287879	0.036679	-2.735022
53	1	-1.557416	-0.162708	-3.213111
54	1	-2.779649	-3.330024	2.524417
55	1	-1.218435	-3.238490	1.617500
56	1	-1.767299	-1.845293	2.633431
57	6	-3.903777	2.506826	-0.065521
58	6	-2.932274	3.503451	0.033658
59	1	-4.287404	0.406379	-0.259114
60	1	-4.952475	2.774095	-0.079080
61	1	-3.228745	4.542503	0.095778
62	1	-0.835968	3.947291	0.097887

Frequencies -- -540.6698 30.6305 52.2127

dihy-cβ*:

E(Basis I/Basis I): -849.073157590182
E(Basis II/Basis I): -850.371985816594
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.864232816594

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.656551	0.405483	0.864487
2	8	0.694076	0.546209	3.060613
3	6	1.838677	0.617257	3.603422
4	7	2.980353	0.432487	2.900872
5	6	2.913620	0.009170	1.487596
6	6	2.219066	-1.238142	1.229675
7	6	4.156241	0.302265	0.776812
8	7	5.163858	0.521055	0.204923
9	1	1.892208	-1.810292	2.090640
10	1	2.497204	-1.814886	0.357243
11	1	3.890150	0.552283	3.336630
12	1	1.935362	0.845319	4.666146
13	15	-1.374538	-0.797105	0.786865

14	15	0.380441	0.736866	-1.437222
15	6	-1.994909	-0.693950	-0.967811
16	6	-1.270438	-0.011797	-1.897432
17	1	-0.143398	1.781904	0.832818
18	1	2.174242	1.193201	0.946207
19	6	-1.406333	-2.628156	1.483962
20	6	-2.899149	-0.281052	1.904526
21	6	1.594975	0.180147	-2.884482
22	6	0.520071	2.614567	-1.977883
23	6	-1.771937	0.109154	-3.247446
24	6	-3.257523	-1.290738	-1.336650
25	6	-1.199108	-3.647457	0.392732
26	6	-2.681396	1.074248	2.523593
27	6	2.555552	-0.881604	-2.427404
28	6	-0.825141	3.296453	-1.976349
29	1	-0.573997	-2.674561	2.177075
30	1	-3.769897	-0.238175	1.256198
31	1	0.974760	-0.228540	-3.676891
32	1	1.147693	3.066231	-1.217721
33	6	-2.751535	-2.764419	2.233479
34	6	-3.036485	-1.421778	2.940600
35	6	2.282400	1.486435	-3.344273
36	6	1.224263	2.609729	-3.353904
37	1	-3.558862	-2.992043	1.540556
38	1	-2.689388	-3.575240	2.956822
39	1	-2.323401	-1.284217	3.751656
40	1	-4.039009	-1.411777	3.364271
41	1	3.088239	1.753290	-2.662416
42	1	2.708544	1.345386	-4.335891
43	1	0.510038	2.430434	-4.154963
44	1	1.691043	3.577250	-3.528137
45	1	-2.530670	1.833246	1.727168
46	1	-3.572894	1.361237	3.120384
47	1	-1.796553	1.067229	3.190458
48	1	-0.249098	-3.437579	-0.143184
49	1	-1.140349	-4.664002	0.835696
50	1	-2.035239	-3.625500	-0.335514
51	1	-0.696787	4.377087	-2.197284
52	1	-1.495136	2.856275	-2.742554
53	1	-1.302915	3.192971	-0.979370
54	1	3.196974	-1.199884	-3.276226
55	1	1.992065	-1.764270	-2.058312
56	1	3.203338	-0.494644	-1.619523
57	6	-2.992042	-0.472126	-3.596781
58	6	-3.732313	-1.172870	-2.643789
59	1	-1.211970	0.652688	-3.995495
60	1	-3.364746	-0.378772	-4.608595
61	1	-4.678384	-1.621679	-2.917460
62	1	-3.843937	-1.829625	-0.605611

Frequencies -- -793.3314 18.1505 46.4698

dihy-dβ‡:

E(Basis I/Basis I): -849.094149018128
E(Basis II/Basis I): -850.389886621988
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.882761621988

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	1.089860	-0.248111	0.208975
2	8	0.961673	-0.268443	2.493712
3	6	2.098069	-0.313077	3.053846
4	7	3.254405	-0.428463	2.347008
5	6	3.223030	-0.627980	0.889521
6	6	2.557300	-1.837167	0.416637
7	6	4.457135	-0.202844	0.236165
8	7	5.461695	0.111321	-0.294806
9	1	2.281228	-2.565156	1.171893

10	1	2.881278	-2.245146	-0.533298
11	1	4.154582	-0.400909	2.817895
12	1	2.196587	-0.241627	4.139918
13	15	-0.804049	-1.496295	-0.481484
14	15	-0.282749	1.677222	-0.058579
15	6	-2.154784	-0.260431	-0.870022
16	6	-1.935574	1.074899	-0.695155
17	1	1.370162	-0.163235	-1.311251
18	1	2.463321	0.673399	0.472784
19	6	-0.519253	-2.736311	-1.967863
20	6	-1.631197	-2.894534	0.613559
21	6	0.237959	3.215876	-1.146758
22	6	-0.518214	2.794154	1.533661
23	6	-2.985507	2.019172	-0.999566
24	6	-3.442351	-0.718672	-1.338330
25	6	-0.846547	-2.107166	-3.298538
26	6	-1.114470	-2.831495	2.025572
27	6	1.440493	2.870741	-1.983989
28	6	-1.750555	2.413326	2.314348
29	1	0.539692	-2.966646	-1.937171
30	1	-2.704235	-2.723959	0.618930
31	1	-0.593173	3.467222	-1.799675
32	1	0.359104	2.606262	2.142937
33	6	-1.366009	-3.985757	-1.633160
34	6	-1.284726	-4.219078	-0.109475
35	6	0.508369	4.350495	-0.127684
36	6	-0.525197	4.250422	1.014239
37	1	-2.403689	-3.840655	-1.926246
38	1	-0.980033	-4.847144	-2.174990
39	1	-0.277125	-4.540097	0.149210
40	1	-1.978066	-4.998316	0.201441
41	1	1.509774	4.254714	0.288785
42	1	0.441996	5.315027	-0.627346
43	1	-1.510707	4.521733	0.641394
44	1	-0.271276	4.932161	1.823844
45	1	-1.379888	-1.853090	2.479042
46	1	-1.574118	-3.639787	2.632749
47	1	-0.011125	-2.949671	2.044549
48	1	-0.263318	-1.170803	-3.427164
49	1	-0.580149	-2.806819	-4.118665
50	1	-1.927317	-1.871052	-3.373406
51	1	-1.799029	3.007551	3.251157
52	1	-2.670235	2.605786	1.725064
53	1	-1.711239	1.335297	2.578819
54	1	1.757499	3.756529	-2.574128
55	1	2.284970	2.543474	-1.340742
56	1	1.186267	2.049455	-2.687032
57	6	-4.223081	1.567308	-1.460202
58	6	-4.451646	0.201007	-1.627495
59	1	-2.824284	3.079750	-0.865609
60	1	-5.008128	2.277798	-1.684444
61	1	-5.413567	-0.146376	-1.981631
62	1	-3.633043	-1.774368	-1.471512

Frequencies -- -765.9632 20.7983 50.6269

alhy-$a_{trans}\alpha$:

E(Basis I/Basis I): -849.120923076722
E(Basis II/Basis I): -850.419079667019
E(Basis II/Basis II): -850.425210816012
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.91183381601

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.114756	-0.973146	0.819721
2	8	0.114756	-0.973146	2.975091
3	6	1.286875	-0.973146	3.500919
4	7	2.395308	-1.016000	2.747973

5	6	2.273636	-1.182637	1.284050
6	6	2.015312	-2.655636	0.891092
7	6	3.316724	-0.504271	0.568492
8	7	4.146231	0.072094	-0.051726
9	1	2.393391	-3.358084	1.642780
10	1	2.445924	-2.901827	-0.080355
11	1	3.312105	-0.973308	3.189192
12	1	1.390737	-0.935659	4.585689
13	15	-0.819505	1.115910	0.894944
14	15	-0.036068	-0.823935	-1.507589
15	6	-1.370068	1.532190	-0.828041
16	6	-1.039508	0.705827	-1.855481
17	1	-1.437740	-1.361600	0.700882
18	1	0.912241	-2.920777	0.826927
19	6	-2.221584	1.220803	2.242537
20	6	0.093662	2.700150	1.596313
21	6	-0.785636	-2.299344	-2.551440
22	6	1.613524	-0.813034	-2.567888
23	6	-1.451325	1.031423	-3.200192
24	6	-2.114890	2.741137	-1.085714
25	6	-3.584392	0.965507	1.650384
26	6	1.581759	2.483411	1.644829
27	6	-1.409369	-3.322495	-1.639765
28	6	2.063741	0.591132	-2.884409
29	1	-1.979556	0.429856	2.945775
30	1	-0.129476	3.517931	0.915908
31	1	-1.551641	-1.884636	-3.200914
32	1	2.360972	-1.290225	-1.944186
33	6	-2.060921	2.619871	2.881716
34	6	-0.552076	2.932773	2.983309
35	6	0.407666	-2.851120	-3.370320
36	6	1.294984	-1.669412	-3.815194
37	1	-2.550267	3.378702	2.274125
38	1	-2.522288	2.624988	3.867460
39	1	-0.099389	2.279630	3.727340
40	1	-0.389615	3.963535	3.292816
41	1	0.998870	-3.535447	-2.763897
42	1	0.034000	-3.401070	-4.231931
43	1	0.769490	-1.079557	-4.563448
44	1	2.222022	-2.029205	-4.257864
45	1	1.962207	2.251926	0.627569
46	1	2.084099	3.403022	2.012116
47	1	1.831997	1.644654	2.324430
48	1	-3.599306	-0.022262	1.143580
49	1	-4.347710	0.961630	2.456795
50	1	-3.851103	1.750751	0.914042
51	1	3.050354	0.561636	-3.393033
52	1	1.337789	1.101970	-3.549522
53	1	2.164507	1.177065	-1.946525
54	1	-1.794122	-4.175617	-2.237668
55	1	-0.665168	-3.701770	-0.908653
56	1	-2.259163	-2.868158	-1.088369
57	6	-2.182140	2.196604	-3.443267
58	6	-2.511922	3.050635	-2.388295
59	1	-1.188875	0.384777	-4.026104
60	1	-2.487813	2.441611	-4.452168
61	1	-3.072782	3.955947	-2.581115
62	1	-2.368237	3.411845	-0.275728

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.128910	-0.924112	0.811032
2	8	0.128910	-0.924112	2.988535
3	6	1.282950	-0.924112	3.482089
4	7	2.379885	-0.960891	2.734552
5	6	2.262644	-1.141918	1.286321
6	6	1.998149	-2.609843	0.917924
7	6	3.328523	-0.494832	0.580819
8	7	4.170537	0.045749	-0.015958

9	1	2.374728	-3.307777	1.671957
10	1	2.406168	-2.874119	-0.056379
11	1	3.288877	-0.960253	3.186335
12	1	1.413269	-0.894511	4.567143
13	15	-0.849072	1.072072	0.847488
14	15	-0.014223	-0.804160	-1.447578
15	6	-1.404542	1.480840	-0.845691
16	6	-1.041606	0.661213	-1.853276
17	1	-1.406176	-1.326922	0.701159
18	1	0.895284	-2.866290	0.879796
19	6	-2.245197	1.178820	2.189918
20	6	0.037393	2.674117	1.518405
21	6	-0.719091	-2.307270	-2.470913
22	6	1.634447	-0.773340	-2.490937
23	6	-1.437399	0.963158	-3.208028
24	6	-2.171816	2.671796	-1.118869
25	6	-3.605497	0.888493	1.607671
26	6	1.529039	2.483464	1.567356
27	6	-1.330909	-3.334836	-1.556033
28	6	2.065888	0.634581	-2.817259
29	1	-1.990149	0.405597	2.907988
30	1	-0.198280	3.476929	0.824887
31	1	-1.489611	-1.915464	-3.128895
32	1	2.385623	-1.230122	-1.857163
33	6	-2.110051	2.589551	2.808545
34	6	-0.606591	2.926990	2.902558
35	6	0.486589	-2.845148	-3.280499
36	6	1.350226	-1.649351	-3.732665
37	1	-2.613169	3.331274	2.191289
38	1	-2.570610	2.600184	3.794545
39	1	-0.143605	2.295095	3.658570
40	1	-0.457989	3.965827	3.190964
41	1	1.089318	-3.511511	-2.665467
42	1	0.126379	-3.410956	-4.137487
43	1	0.819786	-1.081183	-4.493915
44	1	2.290439	-1.992052	-4.160698
45	1	1.910747	2.232611	0.555370
46	1	2.016903	3.420587	1.909025
47	1	1.795932	1.667825	2.267909
48	1	-3.604407	-0.106409	1.114889
49	1	-4.364421	0.880671	2.418215
50	1	-3.892677	1.658004	0.862675
51	1	3.058750	0.615878	-3.314132
52	1	1.340380	1.126914	-3.496473
53	1	2.146841	1.231763	-1.884741
54	1	-1.700853	-4.196142	-2.151571
55	1	-0.583962	-3.701609	-0.822253
56	1	-2.189858	-2.891787	-1.009841
57	6	-2.191491	2.109108	-3.472943
58	6	-2.557044	2.963557	-2.429505
59	1	-1.145941	0.316559	-4.023860
60	1	-2.486429	2.339084	-4.488525
61	1	-3.134951	3.854676	-2.637448
62	1	-2.449779	3.342636	-0.317335

alhy-$a_{trans}\alpha^{t}$:

E(Basis I/Basis I): -849.120637306254
E(Basis II/Basis I): -850.418788644361
E(Basis II/Basis II): -850.42499990253
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.91143790253

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.091712	-0.944109	0.836579
2	8	0.108139	-0.912935	2.979958
3	6	1.284443	-1.006222	3.490597

4	7	2.375881	-1.125389	2.725969
5	6	2.231046	-1.273366	1.252538
6	6	2.069125	-2.774884	0.870070
7	6	3.283136	-0.580973	0.553667
8	7	4.111856	0.006666	-0.056858
9	1	2.671083	-3.429774	1.513844
10	1	2.361443	-2.955426	-0.166404
11	1	3.296311	-1.169113	3.160844
12	1	1.401549	-0.988178	4.574632
13	15	-0.864610	1.121846	0.891008
14	15	-0.003594	-0.800511	-1.498622
15	6	-1.392092	1.531500	-0.838113
16	6	-1.034915	0.709967	-1.860567
17	1	-1.486658	-1.249319	0.727407
18	1	1.021663	-3.136953	0.995019
19	6	-2.248372	1.263016	2.252282
20	6	0.099235	2.677663	1.579516
21	6	-0.736108	-2.296040	-2.525030
22	6	1.639376	-0.772038	-2.569321
23	6	-1.436779	1.028663	-3.209937
24	6	-2.143722	2.733707	-1.105641
25	6	-3.623619	1.039140	1.676250
26	6	1.581304	2.418825	1.612982
27	6	-1.326312	-3.325017	-1.597539
28	6	2.071652	0.636072	-2.893398
29	1	-2.015148	0.467631	2.953475
30	1	-0.109002	3.498806	0.898242
31	1	-1.519206	-1.901434	-3.166584
32	1	2.395296	-1.237164	-1.946843
33	6	-2.044384	2.658931	2.885560
34	6	-0.526367	2.930314	2.972183
35	6	0.457193	-2.830427	-3.356042
36	6	1.323361	-1.637029	-3.811301
37	1	-2.518780	3.428763	2.279886
38	1	-2.496047	2.678965	3.875578
39	1	-0.084540	2.265957	3.712827
40	1	-0.332589	3.956876	3.277634
41	1	1.064673	-3.505367	-2.755386
42	1	0.082604	-3.386654	-4.213248
43	1	0.784584	-1.057802	-4.558319
44	1	2.252439	-1.985083	-4.259091
45	1	1.944861	2.180778	0.591140
46	1	2.113021	3.322491	1.978425
47	1	1.814518	1.570378	2.286622
48	1	-3.668288	0.050881	1.172179
49	1	-4.377051	1.055087	2.491746
50	1	-3.880567	1.828924	0.941489
51	1	3.056095	0.616271	-3.406671
52	1	1.337056	1.136069	-3.557005
53	1	2.170254	1.226394	-1.958071
54	1	-1.700902	-4.190818	-2.183549
55	1	-0.563999	-3.681918	-0.873638
56	1	-2.177281	-2.884142	-1.037077
57	6	-2.178557	2.184903	-3.462881
58	6	-2.528375	3.037627	-2.413220
59	1	-1.158934	0.383196	-4.031623
60	1	-2.476399	2.424471	-4.475419
61	1	-3.096069	3.936940	-2.613932
62	1	-2.410881	3.403676	-0.299367

Frequencies -- -102.2316 32.0306 49.2443

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.110381	-0.900156	0.821222
2	8	0.115599	-0.897663	2.987028
3	6	1.272182	-0.969484	3.471706
4	7	2.360289	-1.058328	2.718992

5	6	2.233741	-1.214464	1.261854
6	6	2.075783	-2.707313	0.891470
7	6	3.299954	-0.535277	0.578902
8	7	4.136229	0.028839	-0.003965
9	1	2.668737	-3.362250	1.540258
10	1	2.360868	-2.898508	-0.142807
11	1	3.267330	-1.124199	3.171104
12	1	1.408930	-0.960743	4.556413
13	15	-0.879733	1.076758	0.843678
14	15	0.008008	-0.784140	-1.441760
15	6	-1.420623	1.480800	-0.853318
16	6	-1.040238	0.665181	-1.857817
17	1	-1.446413	-1.223976	0.714818
18	1	1.029016	-3.064831	1.022438
19	6	-2.261761	1.213096	2.196498
20	6	0.046371	2.658621	1.504442
21	6	-0.683372	-2.305918	-2.444749
22	6	1.650436	-0.741521	-2.494387
23	6	-1.432029	0.960853	-3.214993
24	6	-2.194336	2.665958	-1.132349
25	6	-3.632101	0.942453	1.628234
26	6	1.533696	2.433716	1.547371
27	6	-1.265596	-3.334388	-1.511553
28	6	2.065769	0.668342	-2.833118
29	1	-2.011150	0.438811	2.914960
30	1	-0.175457	3.462120	0.806984
31	1	-1.468640	-1.933217	-3.096383
32	1	2.408902	-1.185167	-1.860124
33	6	-2.095923	2.623897	2.806803
34	6	-0.585249	2.931014	2.890579
35	6	0.521661	-2.832232	-3.263539
36	6	1.368297	-1.629136	-3.728409
37	1	-2.587823	3.372037	2.188214
38	1	-2.550249	2.648726	3.795407
39	1	-0.130737	2.293470	3.647016
40	1	-0.413695	3.968166	3.172345
41	1	1.137468	-3.489322	-2.651674
42	1	0.159929	-3.405392	-4.115024
43	1	0.827316	-1.072493	-4.490706
44	1	2.309863	-1.964170	-4.159546
45	1	1.905522	2.178184	0.533035
46	1	2.044222	3.358102	1.890576
47	1	1.784073	1.608926	2.243658
48	1	-3.652644	-0.054917	1.140979
49	1	-4.383372	0.951658	2.445850
50	1	-3.913592	1.712613	0.881920
51	1	3.056606	0.655936	-3.334217
52	1	1.332816	1.148432	-3.512920
53	1	2.145137	1.273046	-1.905406
54	1	-1.623048	-4.210952	-2.092263
55	1	-0.504126	-3.674506	-0.779596
56	1	-2.127813	-2.901677	-0.962179
57	6	-2.196711	2.098584	-3.485617
58	6	-2.574808	2.952106	-2.445670
59	1	-1.131138	0.314647	-4.027676
60	1	-2.489535	2.323397	-4.502976
61	1	-3.159385	3.837737	-2.658318
62	1	-2.480478	3.336471	-0.333364

Frequencies -- -99.4890 36.7240 53.0188

alhy-aα:

E(Basis I/Basis I): -849.144847010076
E(Basis II/Basis I): -850.437390257495
E(Basis II/Basis II): -850.445126704756
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.93163170476

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	45	0.772452	-0.075739	0.902432
2	8	0.772452	-0.075739	3.022504
3	6	1.951866	-0.075739	3.530717
4	7	3.039744	-0.022343	2.755339
5	6	2.901276	0.139777	1.276224
6	6	4.063216	-0.556110	0.568640
7	6	2.747212	1.569104	0.962261
8	7	2.439396	2.683224	0.689467
9	1	5.038205	-0.170817	0.906587
10	1	4.017823	-0.398428	-0.511104
11	1	3.968434	-0.029714	3.173602
12	1	2.072991	-0.119286	4.613216
13	15	-1.619450	-0.001933	0.841228
14	15	0.639628	-0.213292	-1.450978
15	6	-2.133189	-0.034899	-0.947713
16	6	-1.175972	-0.107555	-1.916133
17	1	0.781386	-1.599060	0.899020
18	1	4.036690	-1.632412	0.761954
19	6	-2.556387	-1.335084	1.918035
20	6	-2.577737	1.473602	1.700386
21	6	1.339337	-1.709379	-2.509958
22	6	1.712056	1.083285	-2.456278
23	6	-1.570387	-0.130024	-3.306304
24	6	-3.527336	0.038068	-1.315229
25	6	-2.967339	-2.532350	1.099298
26	6	-1.618923	2.583305	2.041487
27	6	1.704106	-2.866693	-1.619760
28	6	0.932628	2.335564	-2.768499
29	1	-1.834243	-1.644701	2.667212
30	1	-3.322092	1.843877	1.000473
31	1	0.549357	-2.019400	-3.188015
32	1	2.536299	1.337375	-1.799156
33	6	-3.737907	-0.577932	2.566853
34	6	-3.245677	0.835499	2.943061
35	6	2.542037	-1.126880	-3.292178
36	6	2.216808	0.324533	-3.705957
37	1	-4.573511	-0.502204	1.873800
38	1	-4.077631	-1.115246	3.450390
39	1	-2.529625	0.758345	3.759608
40	1	-4.073326	1.459653	3.274807
41	1	3.436835	-1.132326	-2.673507
42	1	2.736964	-1.742429	-4.168414
43	1	1.461961	0.322538	-4.489029
44	1	3.104179	0.818948	-4.097243
45	1	-1.152957	2.976524	1.112985
46	1	-2.162170	3.410663	2.545125
47	1	-0.815761	2.215356	2.714397
48	1	-2.076698	-2.972390	0.602539
49	1	-3.421443	-3.300447	1.760266
50	1	-3.708043	-2.248955	0.323925
51	1	1.598299	3.078779	-3.255928
52	1	0.085434	2.118547	-3.450210
53	1	0.535119	2.776437	-1.829819
54	1	2.115966	-3.698052	-2.230072
55	1	2.461248	-2.561192	-0.870109
56	1	0.799598	-3.231836	-1.088748
57	6	-2.921007	-0.064248	-3.654148
58	6	-3.897502	0.020366	-2.660670
59	1	-0.826880	-0.196874	-4.087228
60	1	-3.211397	-0.078821	-4.696717
61	1	-4.943482	0.071941	-2.933850
62	1	-4.291188	0.104707	-0.552443

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.746570	-0.036445	0.853088
2	8	0.746570	-0.036445	3.009889
3	6	1.897859	-0.036445	3.502440

4	7	2.995568	0.026301	2.754814
5	6	2.900904	0.230516	1.307433
6	6	4.148086	-0.257871	0.599656
7	6	2.446758	1.580074	1.024767
8	7	1.761559	2.509365	0.800032
9	1	5.053115	0.229147	0.988229
10	1	4.102363	-0.042057	-0.467686
11	1	3.901410	0.067784	3.211426
12	1	2.029918	-0.088608	4.586483
13	15	-1.554847	0.037294	0.781467
14	15	0.635972	-0.255872	-1.407126
15	6	-2.093838	-0.141627	-0.961020
16	6	-1.140578	-0.259336	-1.912540
17	1	0.656910	-1.558159	0.892838
18	1	4.261401	-1.336061	0.729912
19	6	-2.439414	-1.222063	1.965980
20	6	-2.525462	1.549079	1.534254
21	6	1.445337	-1.742105	-2.378219
22	6	1.642427	1.058087	-2.434953
23	6	-1.524389	-0.394400	-3.298648
24	6	-3.489431	-0.133992	-1.327187
25	6	-2.824073	-2.493799	1.253491
26	6	-1.585526	2.698918	1.779248
27	6	1.868457	-2.830256	-1.428559
28	6	0.796028	2.248703	-2.808785
29	1	-1.701683	-1.450310	2.728936
30	1	-3.282422	1.851022	0.815367
31	1	0.692126	-2.136657	-3.053949
32	1	2.438568	1.387730	-1.776783
33	6	-3.634701	-0.449702	2.569566
34	6	-3.172665	0.999345	2.829319
35	6	2.624085	-1.122197	-3.168713
36	6	2.217709	0.288016	-3.646705
37	1	-4.479215	-0.448378	1.883250
38	1	-3.950817	-0.926221	3.495591
39	1	-2.450272	1.002686	3.643958
40	1	-4.011419	1.630581	3.116389
41	1	3.507030	-1.047297	-2.537589
42	1	2.870394	-1.760640	-4.014953
43	1	1.478498	0.208181	-4.440607
44	1	3.079048	0.822620	-4.043017
45	1	-1.146354	3.036047	0.816406
46	1	-2.137161	3.548440	2.234519
47	1	-0.763401	2.393927	2.461118
48	1	-1.927314	-2.947571	0.780644
49	1	-3.245944	-3.217934	1.982000
50	1	-3.583595	-2.297112	0.469550
51	1	1.426288	3.014083	-3.308825
52	1	-0.020414	1.956508	-3.500140
53	1	0.350569	2.697136	-1.895566
54	1	2.367610	-3.648562	-1.989417
55	1	2.570961	-2.434312	-0.667549
56	1	0.977703	-3.248448	-0.913845
57	6	-2.875743	-0.393492	-3.652538
58	6	-3.857329	-0.262467	-2.667871
59	1	-0.775071	-0.492261	-4.070854
60	1	-3.162430	-0.492688	-4.691464
61	1	-4.903786	-0.259687	-2.944011
62	1	-4.254589	-0.030268	-0.569950

alhy-bα:

E(Basis I/Basis I): -849.135909241161
E(Basis II/Basis I): -850.427250622911
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.915833622911

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	45	0.762095	-0.956759	0.105610
2	8	0.762095	-0.956759	2.320531
3	6	1.953009	-0.956759	2.786017
4	7	3.024761	-1.000415	1.972635
5	6	2.835079	-1.187213	0.504619
6	6	2.718388	-2.682568	0.124768
7	6	3.856953	-0.450237	-0.210065
8	7	4.671286	0.184585	-0.785652
9	1	3.312150	-3.324046	0.787630
10	1	3.012549	-2.854602	-0.911559
11	1	3.963466	-0.984472	2.367606
12	1	2.126806	-0.915470	3.863467
13	15	0.561191	1.305018	-0.197362
14	15	-1.621248	-1.090937	-0.212078
15	6	-1.265236	1.693771	-0.211759
16	6	-2.189115	0.690399	-0.228301
17	1	-0.877815	-1.010365	-1.448055
18	1	1.666760	-3.058830	0.233985
19	6	1.575635	2.354094	1.106331
20	6	1.331963	2.292733	-1.704190
21	6	-2.832072	-2.098921	0.958325
22	6	-2.289084	-2.017872	-1.804726
23	6	-3.595967	1.013947	-0.278873
24	6	-1.700622	3.070178	-0.261945
25	6	0.737660	2.739317	2.299214
26	6	1.711375	1.361433	-2.824418
27	6	-2.095767	-2.578293	2.180601
28	6	-2.473533	-1.074378	-2.966384
29	1	2.376910	1.696827	1.425499
30	1	0.562565	2.977638	-2.051317
31	1	-3.638330	-1.438474	1.264792
32	1	-1.518225	-2.740032	-2.053354
33	6	2.137113	3.556244	0.310796
34	6	2.530985	3.059682	-1.097157
35	6	-3.364083	-3.255207	0.075593
36	6	-3.587462	-2.725296	-1.355818
37	1	1.391016	4.343994	0.228403
38	1	3.002660	3.962927	0.830593
39	1	3.399624	2.407885	-1.024157
40	1	2.786780	3.897727	-1.742734
41	1	-2.643532	-4.070940	0.045519
42	1	-4.291228	-3.638750	0.497364
43	1	-4.426883	-2.032903	-1.363516
44	1	-3.816508	-3.542584	-2.037198
45	1	0.807164	0.837493	-3.199940
46	1	2.156372	1.940582	-3.660881
47	1	2.446824	0.606964	-2.479603
48	1	0.301289	1.830771	2.764553
49	1	1.372867	3.252649	3.051514
50	1	-0.084651	3.422383	2.005385
51	1	-2.769433	-1.646463	-3.870931
52	1	-3.261384	-0.324549	-2.747808
53	1	-1.520794	-0.544016	-3.176951
54	1	-2.763162	-3.214439	2.799795
55	1	-1.199475	-3.167571	1.891073
56	1	-1.775844	-1.707800	2.790635
57	6	-4.008173	2.347144	-0.313001
58	6	-3.062391	3.373192	-0.305351
59	1	-4.338633	0.228795	-0.304580
60	1	-5.063162	2.585414	-0.353743
61	1	-3.385110	4.405690	-0.340152
62	1	-0.977678	3.874066	-0.270950

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alhy-c/dβ:

E(Basis I/Basis I): -849.130482183392
E(Basis II/Basis I): -850.416366866354
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.905511866354

Center	Atomic	Coordinates (Angstroms)

Number	Number	X	Y	Z
1	45	0.627587	-0.215318	0.795171
2	8	0.627587	-0.215318	2.914659
3	6	1.626252	-0.215318	3.705306
4	7	2.918163	-0.084312	3.362784
5	6	3.445277	0.102422	1.973076
6	6	2.669377	-0.705837	0.899505
7	6	4.877360	-0.283673	1.996897
8	7	6.014612	-0.594274	1.970053
9	1	2.730463	-1.776808	1.153255
10	1	3.206163	-0.564929	-0.042961
11	1	3.600356	-0.081941	4.116605
12	1	1.434441	-0.333430	4.775201
13	15	0.519691	-0.275829	-1.536768
14	15	-1.754840	0.363909	0.694902
15	6	-1.213515	0.200840	-2.061476
16	6	-2.172636	0.474560	-1.128272
17	1	1.011751	1.240418	0.581113
18	1	3.399405	1.172953	1.730284
19	6	1.882261	0.748835	-2.496921
20	6	0.959957	-1.912613	-2.523140
21	6	-2.493524	1.968087	1.543461
22	6	-3.037151	-0.791439	1.632500
23	6	-3.500829	0.848213	-1.556265
24	6	-1.546347	0.257358	-3.466344
25	6	1.389453	2.119134	-2.888015
26	6	1.018807	-3.092881	-1.590178
27	6	-1.377585	2.858832	2.021325
28	6	-3.596515	-1.864442	0.732932
29	1	2.697428	0.855994	-1.790161
30	1	0.173146	-2.075324	-3.254468
31	1	-3.084085	2.501120	0.803667
32	1	-2.464007	-1.257644	2.427816
33	6	2.301681	-0.138226	-3.692051
34	6	2.310119	-1.606871	-3.216645
35	6	-3.386085	1.439841	2.693290
36	6	-4.105219	0.161111	2.215985
37	1	1.606049	-0.025378	-4.520854
38	1	3.289917	0.158369	-4.038725
39	1	3.135628	-1.754328	-2.522444
40	1	2.449973	-2.284962	-4.056526
41	1	-2.778643	1.201822	3.564861
42	1	-4.104712	2.205333	2.980211
43	1	-4.847722	0.416967	1.462991
44	1	-4.617975	-0.323816	3.044746
45	1	0.036617	-3.225592	-1.088796
46	1	1.253797	-4.014956	-2.162751
47	1	1.798527	-2.942804	-0.815796
48	1	1.024136	2.659372	-1.989040
49	1	2.221117	2.701137	-3.338235
50	1	0.565855	2.052276	-3.627034
51	1	-4.241945	-2.548988	1.322805
52	1	-4.202833	-1.423127	-0.084057
53	1	-2.766914	-2.453549	0.287694
54	1	-1.797527	3.753779	2.527403
55	1	-0.720086	2.315532	2.732837
56	1	-0.767522	3.194005	1.155854
57	6	-3.808617	0.911464	-2.915970
58	6	-2.834361	0.613162	-3.868966
59	1	-4.267097	1.073736	-0.827821
60	1	-4.806334	1.187675	-3.231589
61	1	-3.077984	0.657299	-4.922562
62	1	-0.802644	0.025179	-4.215563

alhy-aα^t:

E(Basis I/Basis I): -849.116292425224
E(Basis II/Basis I): -850.407496745827
E(Basis II/Basis II): -850.4132508287

Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.90286382873

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.743843	-0.061274	0.885694
2	8	0.669689	-0.024211	3.007810
3	6	1.815617	-0.081277	3.570867
4	7	2.952761	-0.144876	2.854488
5	6	2.943938	-0.043543	1.370581
6	6	4.185855	-0.753421	0.788328
7	6	2.895669	1.370736	0.958497
8	7	2.905447	2.508834	0.627746
9	1	5.105879	-0.289021	1.168042
10	1	4.202983	-0.661589	-0.300131
11	1	3.850829	-0.202486	3.328734
12	1	1.890525	-0.089591	4.658743
13	15	-1.616793	0.014146	0.816922
14	15	0.603974	-0.181641	-1.467608
15	6	-2.160795	-0.058810	-0.958631
16	6	-1.213967	-0.127393	-1.935323
17	1	1.951349	-1.113350	0.914614
18	1	4.189365	-1.816289	1.049486
19	6	-2.529048	-1.285345	1.952981
20	6	-2.558827	1.512409	1.649590
21	6	1.347357	-1.646946	-2.543192
22	6	1.622041	1.151804	-2.482825
23	6	-1.621606	-0.174505	-3.320790
24	6	-3.560104	-0.013438	-1.308993
25	6	-2.959829	-2.506312	1.181043
26	6	-1.597210	2.636351	1.930308
27	6	1.754430	-2.800782	-1.666365
28	6	0.797919	2.376859	-2.787080
29	1	-1.791641	-1.573776	2.695075
30	1	-3.323264	1.858899	0.959587
31	1	0.569122	-1.981268	-3.222591
32	1	2.442705	1.436250	-1.833852
33	6	-3.695611	-0.509614	2.607193
34	6	-3.195527	0.914936	2.928005
35	6	2.527600	-1.021356	-3.326581
36	6	2.145671	0.416693	-3.738370
37	1	-4.546983	-0.454158	1.931596
38	1	-4.015080	-1.019804	3.514051
39	1	-2.459456	0.862117	3.728514
40	1	-4.015335	1.548182	3.261861
41	1	3.422050	-0.988434	-2.707299
42	1	2.749230	-1.628730	-4.202116
43	1	1.385038	0.384798	-4.515159
44	1	3.010600	0.943295	-4.137733
45	1	-1.153753	2.998048	0.978249
46	1	-2.132227	3.479344	2.416553
47	1	-0.777986	2.295321	2.597741
48	1	-2.081495	-2.964108	0.678571
49	1	-3.401047	-3.252313	1.875248
50	1	-3.716730	-2.244746	0.413710
51	1	1.433238	3.143116	-3.279387
52	1	-0.047241	2.131421	-3.461724
53	1	0.393973	2.802854	-1.844193
54	1	2.126690	-3.637774	-2.294205
55	1	2.557276	-2.498474	-0.964521
56	1	0.880002	-3.156504	-1.081200
57	6	-2.977407	-0.137548	-3.653849
58	6	-3.944617	-0.055957	-2.650192
59	1	-0.884856	-0.235450	-4.108639
60	1	-3.279045	-0.170681	-4.692741
61	1	-4.994181	-0.024487	-2.912428
62	1	-4.315433	0.053892	-0.537738

Frequencies -- -934.4752 20.8367 30.9458

Reopt:

Center	Atomic	Coordinates (Angstroms)

Number	Number	X	Y	Z
1	45	0.756019	-0.016315	0.821773
2	8	0.763593	-0.033068	2.972556
3	6	1.912471	-0.069692	3.460447
4	7	3.014189	-0.076959	2.707384
5	6	2.948052	0.100085	1.251002
6	6	4.202020	-0.477080	0.586856
7	6	2.757568	1.517599	0.929129
8	7	2.625907	2.652281	0.688957
9	1	5.097470	0.035762	0.955863
10	1	4.163209	-0.327824	-0.492362
11	1	3.923450	-0.070629	3.156504
12	1	2.053587	-0.110192	4.544138
13	15	-1.538286	-0.099429	0.832152
14	15	0.539712	-0.117292	-1.443108
15	6	-2.166557	-0.176225	-0.883787
16	6	-1.258236	-0.158307	-1.883368
17	1	1.998202	-1.002603	0.794555
18	1	4.294559	-1.546117	0.792065
19	6	-2.309716	-1.452821	1.992645
20	6	-2.520274	1.328964	1.719986
21	6	1.317680	-1.525708	-2.555652
22	6	1.463392	1.269288	-2.457326
23	6	-1.705222	-0.196908	-3.256690
24	6	-3.577823	-0.216797	-1.179776
25	6	-2.699115	-2.695021	1.232582
26	6	-1.615541	2.507657	1.963309
27	6	1.805135	-2.674083	-1.713176
28	6	0.581093	2.465018	-2.711272
29	1	-1.522159	-1.699687	2.697141
30	1	-3.335822	1.633848	1.070224
31	1	0.533662	-1.887271	-3.213762
32	1	2.290889	1.577451	-1.828400
33	6	-3.489532	-0.758682	2.711600
34	6	-3.061441	0.690950	3.022493
35	6	2.441042	-0.840397	-3.372322
36	6	1.984960	0.586884	-3.743234
37	1	-4.374896	-0.750865	2.078849
38	1	-3.731436	-1.295791	3.626796
39	1	-2.287426	0.677622	3.788113
40	1	-3.900858	1.272955	3.398007
41	1	3.357040	-0.780675	-2.787672
42	1	2.652995	-1.424292	-4.265939
43	1	1.206955	0.538250	-4.501498
44	1	2.814666	1.160560	-4.152168
45	1	-1.239270	2.899132	0.994207
46	1	-2.176834	3.315147	2.479271
47	1	-0.747120	2.214612	2.589890
48	1	-1.819108	-3.093412	0.684393
49	1	-3.057369	-3.471224	1.941310
50	1	-3.507998	-2.478961	0.505168
51	1	1.169645	3.267046	-3.204766
52	1	-0.272759	2.198889	-3.366832
53	1	0.187929	2.854741	-1.748296
54	1	2.171974	-3.491941	-2.368833
55	1	2.633611	-2.354420	-1.050375
56	1	0.973372	-3.064719	-1.089280
57	6	-3.071564	-0.241901	-3.545337
58	6	-4.006999	-0.251350	-2.507996
59	1	-0.993022	-0.191381	-4.068644
60	1	-3.405706	-0.269148	-4.574393
61	1	-5.064971	-0.283560	-2.733749
62	1	-4.306475	-0.217858	-0.380481

Frequencies -- -946.7491 21.7816 31.1001

prod-a:

E(Basis I/Basis I): -849.154456577302
E(Basis II/Basis I): -850.445313761908

E(Basis II/Basis II): -850.4516312338
Sum of electronic and thermal free energies(Basis II/Basis II; 298K): -849.93805323377

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.522000	0.594770	0.707072
2	8	0.522000	0.594770	2.877852
3	6	1.458213	0.594770	3.731828
4	7	2.786019	0.536348	3.468207
5	6	3.418905	0.439437	2.122968
6	6	4.857842	1.000404	2.175761
7	6	2.580877	1.177427	1.134052
8	7	2.268073	2.085786	0.400156
9	1	4.859387	2.059020	2.453820
10	1	5.333344	0.898716	1.196014
11	1	3.422409	0.551726	4.259649
12	1	1.202991	0.654271	4.794022
13	15	-1.375049	-0.780654	0.739439
14	15	0.349818	0.494842	-1.613038
15	6	-1.852369	-1.141265	-1.029688
16	6	-1.119051	-0.588347	-2.036761
17	1	3.445774	-0.614893	1.819646
18	1	5.457376	0.434950	2.899522
19	6	-1.250859	-2.408259	1.816137
20	6	-3.013721	-0.225552	1.652728
21	6	1.809985	-0.088434	-2.782172
22	6	0.235592	2.225978	-2.517132
23	6	-1.481801	-0.844667	-3.411072
24	6	-2.997953	-1.962989	-1.340025
25	6	-0.856370	-3.605888	0.990274
26	6	-2.949595	1.240890	1.987972
27	6	2.889572	-0.771498	-1.985548
28	6	-1.192664	2.649486	-2.747784
29	1	-0.470725	-2.206689	2.542573
30	1	-3.851597	-0.402431	0.984622
31	1	1.403635	-0.794648	-3.500134
32	1	0.708912	2.925398	-1.835980
33	6	-2.622380	-2.550193	2.515151
34	6	-3.103088	-1.135257	2.901867
35	6	2.293294	1.200187	-3.491853
36	6	1.063414	2.075375	-3.813963
37	1	-3.347732	-3.012597	1.848857
38	1	-2.525515	-3.179596	3.397907
39	1	-2.468484	-0.748778	3.697593
40	1	-4.127681	-1.160336	3.268169
41	1	2.966870	1.760313	-2.845529
42	1	2.833539	0.940183	-4.400256
43	1	0.473787	1.602382	-4.596674
44	1	1.373057	3.056081	-4.170431
45	1	-2.857009	1.835958	1.054616
46	1	-3.876935	1.549155	2.515622
47	1	-2.075812	1.457751	2.637626
48	1	0.098091	-3.400723	0.460715
49	1	-0.713782	-4.486696	1.651339
50	1	-1.637870	-3.847775	0.241528
51	1	-1.215243	3.671672	-3.181080
52	1	-1.704918	1.957094	-3.446598
53	1	-1.743441	2.659927	-1.783344
54	1	3.688078	-1.134165	-2.666862
55	1	3.339227	-0.073488	-1.250487
56	1	2.463994	-1.641269	-1.441504
57	6	-2.585644	-1.648305	-3.704291
58	6	-3.342484	-2.205394	-2.671216
59	1	-0.908391	-0.412301	-4.219223
60	1	-2.857443	-1.836803	-4.734791
61	1	-4.199294	-2.824701	-2.902822
62	1	-3.593043	-2.394752	-0.547122

Reopt:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.491272	0.570165	0.675502
2	8	0.529504	0.566185	2.880116
3	6	1.457289	0.574670	3.701852
4	7	2.773451	0.535321	3.431839
5	6	3.396868	0.455560	2.100949
6	6	4.825972	1.017325	2.149857
7	6	2.560616	1.205355	1.129553
8	7	2.188268	2.077504	0.421061
9	1	4.823261	2.068888	2.445271
10	1	5.292442	0.928768	1.166970
11	1	3.406393	0.549533	4.221314
12	1	1.227821	0.625805	4.773141
13	15	-1.335867	-0.763826	0.696642
14	15	0.320341	0.480751	-1.557909
15	6	-1.842485	-1.135065	-1.030443
16	6	-1.120170	-0.575075	-2.025377
17	1	3.419834	-0.590866	1.774550
18	1	5.425173	0.440624	2.860931
19	6	-1.202135	-2.373826	1.781973
20	6	-2.958387	-0.201725	1.616181
21	6	1.782078	-0.111070	-2.707840
22	6	0.235358	2.207946	-2.453554
23	6	-1.481212	-0.816842	-3.402240
24	6	-2.985485	-1.960082	-1.338049
25	6	-0.808679	-3.578748	0.966163
26	6	-2.893260	1.268077	1.936611
27	6	2.845215	-0.814429	-1.906697
28	6	-1.184881	2.652196	-2.695150
29	1	-0.417776	-2.164619	2.501517
30	1	-3.801471	-0.383744	0.956359
31	1	1.374229	-0.808864	-3.432832
32	1	0.709637	2.899522	-1.765450
33	6	-2.565893	-2.515953	2.495796
34	6	-3.043678	-1.098377	2.874834
35	6	2.291558	1.170649	-3.411251
36	6	1.075127	2.060308	-3.742959
37	1	-3.296867	-2.985044	1.840455
38	1	-2.458429	-3.138403	3.382146
39	1	-2.404063	-0.705831	3.663596
40	1	-4.066301	-1.118685	3.246681
41	1	2.965501	1.721605	-2.757416
42	1	2.837709	0.904677	-4.314294
43	1	0.490624	1.599498	-4.536585
44	1	1.398047	3.040838	-4.087722
45	1	-2.805958	1.854174	0.997042
46	1	-3.818186	1.580960	2.465789
47	1	-2.016671	1.492281	2.579768
48	1	0.140657	-3.375323	0.426712
49	1	-0.656894	-4.451768	1.635479
50	1	-1.595022	-3.832475	0.226461
51	1	-1.189300	3.679186	-3.117554
52	1	-1.698822	1.974931	-3.407275
53	1	-1.746184	2.660143	-1.736735
54	1	3.637330	-1.195757	-2.585294
55	1	3.308995	-0.124477	-1.173367
56	1	2.400438	-1.673715	-1.361258
57	6	-2.582545	-1.622965	-3.701257
58	6	-3.334403	-2.193004	-2.670463
59	1	-0.909287	-0.375730	-4.206469
60	1	-2.855462	-1.803656	-4.732865
61	1	-4.189687	-2.813505	-2.904556
62	1	-3.575365	-2.399080	-0.545292

dihy-ab-ts1:

E(Basis I/Basis I): -849.100966579549
E(Basis II/Basis I): -850.389402168883

Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.885336168883

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	-0.198689	-0.956352	0.720213
2	8	0.045805	-0.997138	2.871791
3	6	0.776100	-1.397504	3.813595
4	7	1.987719	-2.012351	3.696636
5	6	2.643057	-2.316992	2.440998
6	6	2.394199	-3.463298	1.772145
7	6	3.570581	-1.319628	1.961481
8	7	4.319475	-0.489994	1.576589
9	1	1.688869	-4.193671	2.156702
10	1	2.900821	-3.685582	0.838385
11	1	2.489255	-2.225993	4.555245
12	1	0.444544	-1.252902	4.846704
13	15	-0.405476	1.513114	0.642593
14	15	-0.495902	-0.895065	-1.561917
15	6	-0.727143	1.893575	-1.169017
16	6	-0.763026	0.881998	-2.086211
17	1	-1.703712	-1.127797	0.815969
18	1	-0.254093	-2.549837	0.623045
19	6	-1.860483	2.235017	1.741337
20	6	0.841771	2.884924	1.295558
21	6	-1.811906	-2.004928	-2.485958
22	6	0.991370	-1.704063	-2.545402
23	6	-1.008249	1.183846	-3.477803
24	6	-0.932191	3.256519	-1.603734
25	6	-3.170374	2.255529	0.994752
26	6	2.159261	2.250668	1.652397
27	6	-2.815830	-2.554113	-1.507721
28	6	2.005095	-0.676464	-2.980564
29	1	-1.942234	1.552078	2.581036
30	1	0.999284	3.608977	0.501246
31	1	-2.323583	-1.379769	-3.212447
32	1	1.454082	-2.390812	-1.844183
33	6	-1.380803	3.628016	2.208397
34	6	0.129176	3.531784	2.509087
35	6	-0.974740	-3.103972	-3.185150
36	6	0.330755	-2.473084	-3.712798
37	1	-1.554963	4.376238	1.438073
38	1	-1.931199	3.926692	3.098760
39	1	0.275014	2.925660	3.401509
40	1	0.551417	4.517057	2.697904
41	1	-0.729482	-3.897124	-2.480867
42	1	-1.552096	-3.538862	-3.998833
43	1	0.106846	-1.800304	-4.538314
44	1	1.010592	-3.241360	-4.076597
45	1	2.613113	1.795562	0.746660
46	1	2.855077	3.018724	2.051458
47	1	2.016128	1.457655	2.417359
48	1	-3.407994	1.236847	0.621321
49	1	-3.984404	2.583442	1.675151
50	1	-3.126421	2.953116	0.133457
51	1	2.867179	-1.182098	-3.464498
52	1	1.561233	0.038105	-3.703691
53	1	2.373514	-0.113031	-2.097089
54	1	-3.546397	-3.199431	-2.039907
55	1	-2.311413	-3.155025	-0.721951
56	1	-3.367725	-1.719363	-1.026037
57	6	-1.206205	2.503566	-3.885247
58	6	-1.169031	3.537704	-2.949983
59	1	-1.031009	0.393201	-4.214879
60	1	-1.387502	2.725304	-4.928970
61	1	-1.324174	4.560251	-3.268946
62	1	-0.912012	4.068068	-0.890330

Frequencies -- -43.7176 18.1162 21.1448

dihy-ab-2:

E(Basis I/Basis I): -849.116817773287
E(Basis II/Basis I): -850.405548929979
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.899875929979

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.423267	-0.894092	0.639117
2	8	0.694805	-0.915919	2.880494
3	6	1.360650	-0.908304	3.938956
4	7	2.629444	-0.396856	4.130038
5	6	3.496088	0.243617	3.192536
6	6	4.714630	0.728400	3.527783
7	6	2.982275	0.333798	1.852463
8	7	2.416477	0.297607	0.821374
9	1	5.106231	0.656643	4.538563
10	1	5.341925	1.205079	2.784609
11	1	3.002381	-0.487727	5.071102
12	1	0.940541	-1.335354	4.857141
13	15	-1.187164	0.978463	0.561045
14	15	0.189048	-1.018930	-1.626889
15	6	-1.576558	1.159080	-1.270610
16	6	-0.998428	0.318064	-2.178552
17	1	-0.775392	-1.855751	0.741487
18	1	1.259610	-2.249604	0.515064
19	6	-2.861425	0.675032	1.536826
20	6	-1.036581	2.800338	1.288288
21	6	-0.310520	-2.669828	-2.540065
22	6	1.893122	-0.913493	-2.577684
23	6	-1.313605	0.451346	-3.582399
24	6	-2.493231	2.178788	-1.728328
25	6	-3.873415	-0.062985	0.697165
26	6	0.369005	3.045903	1.768017
27	6	-0.899877	-3.653788	-1.565117
28	6	2.199302	0.489819	-3.035519
29	1	-2.584499	0.053117	2.382008
30	1	-1.268025	3.508067	0.497680
31	1	-1.052481	-2.421748	-3.294097
32	1	2.634877	-1.223129	-1.849374
33	6	-3.333878	2.068060	2.009494
34	6	-2.085392	2.872757	2.426285
35	6	1.003179	-3.164764	-3.192391
36	6	1.780105	-1.942611	-3.726060
37	1	-3.859012	2.590966	1.213123
38	1	-4.018126	1.960741	2.849177
39	1	-1.680585	2.445949	3.342294
40	1	-2.341150	3.912101	2.623701
41	1	1.615801	-3.685246	-2.458253
42	1	0.772401	-3.859858	-3.997372
43	1	1.252307	-1.515230	-4.576416
44	1	2.775413	-2.233404	-4.056699
45	1	1.075561	2.974500	0.914184
46	1	0.447392	4.062057	2.209257
47	1	0.656833	2.294865	2.534554
48	1	-3.435421	-1.014051	0.326629
49	1	-4.768460	-0.299247	1.310512
50	1	-4.191447	0.549051	-0.171644
51	1	3.210879	0.522059	-3.492351
52	1	1.460085	0.833347	-3.787604
53	1	2.179031	1.182971	-2.168027
54	1	-1.162707	-4.595053	-2.092643
55	1	-0.177224	-3.886458	-0.754889
56	1	-1.823742	-3.231444	-1.116128
57	6	-2.197936	1.441133	-4.012256
58	6	-2.786775	2.302857	-3.087040
59	1	-0.861789	-0.208159	-4.310527
60	1	-2.427982	1.539859	-5.065228
61	1	-3.475010	3.067548	-3.423205
62	1	-2.967783	2.846481	-1.023813

dihy-ab-ts3:

E(Basis I/Basis I): -849.095187477178
E(Basis II/Basis I): -850.381296552169
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.878979552169

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.273026	-0.848085	0.733078
2	8	0.272464	-0.688526	2.888329
3	6	0.789174	-0.980747	3.994518
4	7	2.112632	-1.183382	4.263423
5	6	3.234090	-1.034807	3.377756
6	6	4.317048	-1.840198	3.468886
7	6	3.201139	0.074779	2.456886
8	7	3.205841	0.980860	1.699705
9	1	4.352205	-2.676596	4.161732
10	1	5.188891	-1.664059	2.849897
11	1	2.333993	-1.480789	5.209600
12	1	0.146119	-1.089708	4.875004
13	15	-1.101694	1.275087	0.421518
14	15	0.156365	-1.002951	-1.570429
15	6	-1.276941	1.441662	-1.437774
16	6	-0.749247	0.489573	-2.262710
17	1	1.681214	-1.465473	0.606877
18	1	0.268249	-2.396457	0.825090
19	6	-2.894411	1.201008	1.227088
20	6	-0.792204	3.071138	1.155203
21	6	-0.627380	-2.557745	-2.472397
22	6	1.879911	-1.275519	-2.462145
23	6	-0.915699	0.614661	-3.693457
24	6	-1.984533	2.567145	-2.005268
25	6	-3.905462	0.588625	0.290751
26	6	0.581107	3.146895	1.766037
27	6	-1.442461	-3.380417	-1.510008
28	6	2.484731	0.022751	-2.933237
29	1	-2.789006	0.565031	2.100298
30	1	-0.857169	3.787440	0.341386
31	1	-1.276775	-2.183938	-3.258966
32	1	2.518392	-1.708666	-1.700631
33	6	-3.223363	2.652184	1.643670
34	6	-1.928092	3.290339	2.184961
35	6	0.580943	-3.321884	-3.065625
36	6	1.606069	-2.295001	-3.591724
37	1	-3.588415	3.225191	0.793921
38	1	-3.999122	2.649179	2.407387
39	1	-1.673186	2.824330	3.135155
40	1	-2.062397	4.356697	2.357121
41	1	1.052391	-3.936941	-2.300888
42	1	0.241221	-3.976601	-3.866007
43	1	1.210964	-1.799833	-4.476118
44	1	2.535434	-2.788723	-3.869539
45	1	1.348713	2.989440	0.979417
46	1	0.739829	4.147919	2.220115
47	1	0.703072	2.369407	2.550275
48	1	-3.562319	-0.418242	-0.028746
49	1	-4.881671	0.483564	0.809496
50	1	-4.048621	1.221970	-0.608785
51	1	3.499487	-0.164501	-3.343485
52	1	1.864286	0.488319	-3.725394
53	1	2.571234	0.729598	-2.080940
54	1	-1.931258	-4.217062	-2.052641
55	1	-0.801909	-3.804193	-0.709585
56	1	-2.230416	-2.749126	-1.047136
57	6	-1.596949	1.707336	-4.230471
58	6	-2.130162	2.681896	-3.387962
59	1	-0.513762	-0.134599	-4.360258
60	1	-1.715237	1.796517	-5.302608
61	1	-2.663347	3.525426	-3.807000
62	1	-2.420218	3.321068	-1.365312

Frequencies -- -282.3033 15.1243 22.9957

dihy-ab-4:

E(Basis I/Basis I): -849.103167762324
E(Basis II/Basis I): -850.390026060989
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.887664060989

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.118265	-0.849984	0.842295
2	8	0.124614	-0.437645	2.941760
3	6	0.694838	-0.168118	4.030084
4	7	2.023612	0.047631	4.242213
5	6	3.083710	-0.025223	3.265288
6	6	3.338943	-1.140216	2.546511
7	6	3.849388	1.188979	3.122142
8	7	4.459573	2.195690	3.017392
9	1	2.764396	-2.049428	2.684953
10	1	4.134321	-1.146930	1.808543
11	1	2.287044	0.334265	5.182349
12	1	0.086649	-0.079044	4.936077
13	15	-0.853540	1.327967	0.151752
14	15	-0.138710	-1.480864	-1.354889
15	6	-1.104058	1.149887	-1.702955
16	6	-0.819169	-0.033147	-2.323390
17	1	1.522613	-0.476854	0.395846
18	1	0.765692	-2.291765	1.081259
19	6	-2.527703	1.939538	0.983050
20	6	-0.008821	3.074724	0.442832
21	6	-1.268663	-3.026654	-1.745769
22	6	1.413519	-2.298921	-2.212107
23	6	-1.065800	-0.178004	-3.739342
24	6	-1.612999	2.256696	-2.480455
25	6	-3.742181	1.448072	0.236304
26	6	1.375154	2.883624	1.003469
27	6	-2.077831	-3.395974	-0.530703
28	6	2.196785	-1.308224	-3.035678
29	1	-2.523948	1.503662	1.977066
30	1	0.061370	3.580728	-0.515870
31	1	-1.938095	-2.752268	-2.556662
32	1	2.027234	-2.643585	-1.387435
33	6	-2.416524	3.479128	1.060676
34	6	-0.955323	3.831230	1.408468
35	6	-0.278830	-4.134251	-2.184074
36	6	0.849164	-3.490885	-3.018538
37	1	-2.690038	3.936232	0.112308
38	1	-3.093862	3.858124	1.823933
39	1	-0.757063	3.540482	2.438619
40	1	-0.783432	4.902559	1.322570
41	1	0.155158	-4.619374	-1.311447
42	1	-0.809274	-4.887617	-2.763500
43	1	0.455282	-3.159051	-3.977010
44	1	1.642857	-4.210576	-3.210046
45	1	2.001212	2.320354	0.279329
46	1	1.848977	3.870185	1.191857
47	1	1.332302	2.313953	1.955915
48	1	-3.707622	0.341623	0.146033
49	1	-4.662133	1.731014	0.790169
50	1	-3.791712	1.890494	-0.779396
51	1	3.120421	-1.789947	-3.420224
52	1	1.602438	-0.946499	-3.898714
53	1	2.485201	-0.439450	-2.406806
54	1	-2.702208	-4.288110	-0.748804
55	1	-1.411988	-3.621098	0.329421
56	1	-2.745913	-2.552893	-0.253611
57	6	-1.563321	0.895625	-4.478571
58	6	-1.831842	2.112124	-3.851219

59	1	-0.866566	-1.117225	-4.236365
60	1	-1.741494	0.784105	-5.540252
61	1	-2.217544	2.943300	-4.427246
62	1	-1.838291	3.201231	-2.006553

dihy-ab-ts5:

E(Basis I/Basis I): -849.097312831668
E(Basis II/Basis I): -850.388534963625
Sum of electronic and thermal free energies(Basis II/Basis I; 298K): -849.885670963625

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	45	0.797035	-0.727132	0.431703
2	8	0.721582	-0.697589	2.640126
3	6	1.373823	-0.554536	3.703965
4	7	2.636189	-0.037545	3.783894
5	6	3.379556	0.455442	2.647123
6	6	3.833536	-0.360822	1.668318
7	6	3.562424	1.886899	2.621101
8	7	3.685520	3.062313	2.615719
9	1	3.702761	-1.436494	1.723793
10	1	4.360116	0.044747	0.810225
11	1	3.034476	0.095647	4.709987
12	1	0.936450	-0.841075	4.665196
13	15	-0.401438	1.401974	0.055479
14	15	-0.541090	-1.635132	-1.156999
15	6	-1.666499	0.953343	-1.259918
16	6	-1.721377	-0.317820	-1.755427
17	1	1.633483	-0.483538	-0.835036
18	1	1.517202	-2.159809	0.470230
19	6	-1.260053	2.332201	1.557860
20	6	0.437967	3.064170	-0.563326
21	6	-1.598441	-3.172001	-0.588578
22	6	0.307041	-2.636862	-2.599566
23	6	-2.718412	-0.662171	-2.742164
24	6	-2.583361	1.951489	-1.761428
25	6	-2.686034	1.886734	1.762637
26	6	1.873588	2.807072	-0.936255
27	6	-1.562561	-3.299718	0.911866
28	6	0.420111	-1.823585	-3.864181
29	1	-0.675232	2.049662	2.426839
30	1	-0.104185	3.405687	-1.440758
31	1	-2.622056	-3.006491	-0.914220
32	1	1.299875	-2.860289	-2.225415
33	6	-1.103827	3.841625	1.262415
34	6	0.279548	4.057970	0.613304
35	6	-0.959317	-4.374364	-1.326347
36	6	-0.540360	-3.922135	-2.742129
37	1	-1.884368	4.186836	0.587916
38	1	-1.185702	4.407154	2.188851
39	1	1.056334	3.891498	1.357759
40	1	0.378820	5.077413	0.245254
41	1	-0.079978	-4.723219	-0.787723
42	1	-1.675532	-5.192394	-1.376368
43	1	-1.426172	-3.736645	-3.346432
44	1	0.048924	-4.694434	-3.232813
45	1	1.918747	2.093355	-1.786036
46	1	2.362331	3.756131	-1.242407
47	1	2.428127	2.372872	-0.078079
48	1	-2.722825	0.783060	1.881391
49	1	-3.096573	2.356667	2.681192
50	1	-3.322886	2.177595	0.903055
51	1	0.990929	-2.395335	-4.625928
52	1	-0.580715	-1.586692	-4.278042
53	1	0.957971	-0.874493	-3.655908
54	1	-2.157321	-4.181958	1.229869
55	1	-0.518802	-3.419259	1.271649
56	1	-1.998425	-2.390122	1.377243

57	6	-3.604877	0.307737	-3.211419
58	6	-3.534279	1.613358	-2.725472
59	1	-2.785472	-1.671932	-3.123384
60	1	-4.347671	0.046859	-3.954104
61	1	-4.221069	2.364569	-3.093439
62	1	-2.544003	2.965906	-1.390769
Frequencies --		-55.5441	17.1231	21.2761