Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Electronic Supplementary Information
(Part 2: Optimized geometries)
for:

Deuteration of Pd-activated C(sp^2)–H bonds in the Solid State

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Small molecules

DCl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.000000	0.000000	0.071482
2	1	0	0.000000	0.000000	-1.215200

HF=-460.8338531\ZeroPoint=0.004796\Thermal=0.0071569

AcOD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.090121	0.129012	0.000000
2	8	0	0.627934	1.207124	0.000000
3	8	0	0.789676	-1.036104	0.000000
4	1	0	1.731245	-0.807268	0.000000
5	6	0	-1.392696	-0.123679	0.000000
6	1	0	-1.666523	-0.709147	-0.880628
7	1	0	-1.666526	-0.709131	0.880638
8	1	0	-1.923619	0.825383	-0.000010

HF=-229.1677267\ZeroPoint=0.0580925\Thermal=0.0628231

DMF

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.869154	-0.644204	-0.000103
2	8	0	-1.953477	-0.091650	0.000193
3	7	0	0.342710	-0.021341	-0.000570
4	1	0	-0.768700	-1.745639	-0.000155
5	6	0	1.588230	-0.766462	0.000187
6	1	0	2.183572	-0.529168	0.888850
7	1	0	1.380068	-1.837728	0.000063
8	1	0	2.184620	-0.529184	-0.887761
9	6	0	0.430426	1.430717	0.000052
10	1	0	0.964699	1.780999	0.889673
11	1	0	0.965174	1.781727	-0.888981
12	1	0	-0.577598	1.841275	-0.000055

HF=-248.59639\ZeroPoint=0.101794\Thermal=0.1079407

DMF·DCl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.353994	0.135031	-0.000372
2	8	0	0.373382	-0.857765	-0.000289
3	7	0	-1.699346	0.107534	-0.000009
4	1	0	0.066512	1.152857	-0.000546
5	6	0	-2.489479	1.329787	0.000098
6	1	0	-1.831408	2.199368	-0.000541
7	1	0	-3.127107	1.372741	-0.888281
8	1	0	-3.126157	1.373299	0.889139
9	6	0	-2.423534	-1.158282	0.000387
10	1	0	-1.706015	-1.975846	0.000460
11	1	0	-3.056395	-1.228107	0.890129
12	1	0	-3.056653	-1.228497	-0.889139
13	1	0	1.995418	-0.398771	-0.000007
14	17	0	3.197189	0.176654	0.000029

HF=-709.4467082\ZeroPoint=0.10897\Thermal=0.1178476

Cys^{4D}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	2.528015	-0.336700	0.008567
2	6	0	0.772420	-0.513519	0.511408
3	1	0	0.552331	-1.580206	0.460242
4	1	0	0.650697	-0.187532	1.547710
5	6	0	-0.196059	0.274165	-0.395405
6	1	0	-0.026187	-0.043828	-1.426980
7	7	0	0.052893	1.702765	-0.288631
8	1	0	-0.367197	2.068438	0.561579
9	6	0	-1.627113	-0.116052	-0.012770
10	8	0	-1.938006	-1.360292	-0.445375
11	8	0	-2.388169	0.571785	0.619545
12	1	0	-0.364679	2.205479	-1.063442
13	1	0	-2.836932	-1.564054	-0.144679
14	1	0	2.487395	1.010048	-0.063840

HF=-722.0802521\ZeroPoint=0.0951069\Thermal=0.1040125

Cys^{4D}·DCl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.270414	1.937516	-0.538749
2	6	0	-0.035836	0.830363	0.897616
3	1	0	0.900241	0.720089	1.442251
4	1	0	-0.770025	1.315012	1.538531
5	6	0	-0.560414	-0.566180	0.509326
6	1	0	-0.533498	-1.191314	1.407557
7	7	0	0.311319	-1.198050	-0.506508
8	1	0	1.472820	-1.051093	-0.213092
9	6	0	-1.997839	-0.558992	-0.002204
10	8	0	-2.828212	0.026613	0.877253
11	8	0	-2.344641	-1.034652	-1.052283
12	1	0	0.174514	-0.734485	-1.406904
13	1	0	-3.725677	0.004145	0.510566
14	1	0	0.088279	-2.182957	-0.634105
15	1	0	1.548834	1.530528	-0.721941

16	17	0	3.016825	-0.658275	0.189088

HF=-1182.9346793\ZeroPoint=0.1034239\Thermal=0.1141045

Ala^{3D}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.186639	1.280327	-0.484021
2	1	0	2.202799	1.534071	-0.179328
3	1	0	0.551993	2.163868	-0.399970
4	6	0	0.666112	0.136506	0.401106
5	1	0	0.644859	0.484020	1.438792
6	7	0	1.555091	-1.011854	0.316214
7	1	0	1.533362	-1.399353	-0.623000
8	6	0	-0.779153	-0.178995	0.006955
9	8	0	-1.634696	0.788453	0.421227
10	8	0	-1.139633	-1.149382	-0.610690
11	1	0	1.246751	-1.753431	0.936953
12	1	0	-2.522522	0.545928	0.117236
13	1	0	1.210169	0.968275	-1.532715

HF=-323.8646026\ZeroPoint=0.0975554\Thermal=0.1048899

Ala^{3D}·DCl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.199634	1.400766	0.765979
2	1	0	-0.855537	1.674701	0.730140
3	1	0	0.800688	2.245932	0.431150
4	6	0	0.442338	0.180660	-0.132476
5	1	0	0.175232	0.444549	-1.160774
6	7	0	-0.416943	-0.934668	0.281331
7	1	0	-1.945283	-0.495959	0.034158
8	6	0	1.916727	-0.213165	-0.133176
9	8	0	2.685242	0.748919	-0.686446
10	8	0	2.355623	-1.247238	0.303530
11	1	0	-0.242614	-1.173607	1.255075
12	1	0	3.607448	0.452011	-0.652905
13	1	0	-0.210043	-1.771999	-0.257728
14	17	0	-3.209317	-0.013511	-0.240557
15	1	0	0.467984	1.173724	1.802399

HF=-784.7184437\ZeroPoint=0.1047582\Thermal=0.1144816

1^{D}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.011130	-1.094278	-0.000380
2	6	0	-2.631745	-1.284117	-0.000516
3	6	0	-1.770062	-0.182002	-0.000106
4	6	0	-2.297035	1.119502	0.000379
5	6	0	-3.673136	1.300518	0.000480
6	6	0	-4.534113	0.197515	0.000121
7	1	0	-4.675229	-1.950933	-0.000664
8	1	0	-2.199332	-2.277802	-0.000940
9	1	0	-1.618656	1.962435	0.000665
10	1	0	-4.083272	2.304336	0.000835
11	1	0	-5.607663	0.349016	0.000213
12	7	0	-0.386062	-0.492685	-0.000292
13	7	0	0.386071	0.492721	0.000093
14	6	0	1.770065	0.182021	0.000046
15	6	0	2.297015	-1.119491	0.000537
16	6	0	2.631766	1.284122	-0.000398
17	6	0	3.673113	-1.300534	0.000513
18	1	0	1.618620	-1.962412	0.000944
19	6	0	4.011146	1.094257	-0.000485
20	1	0	2.199373	2.277817	-0.000692
21	6	0	4.534108	-0.197545	-0.000022
22	1	0	4.083230	-2.304359	0.000938
23	1	0	4.675260	1.950900	-0.000880
24	1	0	5.607655	-0.349063	-0.000041

HF=-572.9235904\ZeroPoint=0.1865494\Thermal=0.1976101

1^{2D}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.011130	1.094278	-0.000380
2	6	0	2.631745	1.284117	-0.000516
3	6	0	1.770062	0.182002	-0.000106
4	6	0	2.297035	-1.119502	0.000379
5	6	0	3.673136	-1.300518	0.000480
6	6	0	4.534113	-0.197515	0.000121
7	1	0	4.675229	1.950933	-0.000664
8	1	0	2.199332	2.277802	-0.000940
9	1	0	1.618656	-1.962435	0.000665
10	1	0	4.083272	-2.304336	0.000835
11	1	0	5.607663	-0.349016	0.000213
12	7	0	0.386062	0.492685	-0.000292
13	7	0	-0.386071	-0.492721	0.000093
14	6	0	-1.770065	-0.182021	0.000046
15	6	0	-2.297015	1.119491	0.000537
16	6	0	-2.631766	-1.284122	-0.000398
17	6	0	-3.673113	1.300534	0.000513
18	1	0	-1.618620	1.962412	0.000944
19	6	0	-4.011146	-1.094257	-0.000485
20	1	0	-2.199373	-2.277817	-0.000692
21	6	0	-4.534108	0.197545	-0.000022
22	1	0	-4.083230	2.304359	0.000938
23	1	0	-4.675260	-1.950900	-0.000880
24	1	0	-5.607655	0.349063	-0.000041

HF=-572.9235904\ZeroPoint=0.1832711\Thermal=0.1944739

Trans-Pd(**Cys^{3D}**)$_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	46	0	0.000004	0.000004	-0.439727
2	16	0	1.592048	1.750296	-0.468119
3	6	0	2.946108	0.684622	-1.119354
4	1	0	2.811381	0.499041	-2.188490
5	1	0	3.899734	1.194377	-0.978101
6	6	0	2.964081	-0.651842	-0.383415
7	1	0	3.736200	-1.307670	-0.812357
8	7	0	1.631393	-1.315953	-0.485957
9	1	0	1.524025	-1.975502	0.285298
10	6	0	3.305822	-0.535539	1.099115
11	8	0	4.368940	0.259592	1.304950
12	8	0	2.742297	-1.145752	1.972253
13	1	0	1.556693	-1.836733	-1.355814
14	1	0	4.534192	0.289699	2.259238
15	7	0	-1.631382	1.315966	-0.485906
16	6	0	-2.964073	0.651850	-0.383410
17	1	0	-1.524018	1.975464	0.285393
18	6	0	-2.946088	-0.684598	-1.119376
19	1	0	-3.736182	1.307687	-0.812355
20	6	0	-3.305846	0.535515	1.099110
21	16	0	-1.592036	-1.750284	-0.468142
22	1	0	-2.811343	-0.498995	-2.188506
23	1	0	-3.899716	-1.194357	-0.978150
24	8	0	-4.368966	-0.259622	1.304905
25	8	0	-2.742340	1.145709	1.972273
26	1	0	-4.534239	-0.289750	2.259189
27	1	0	-1.556676	1.836800	-1.355730

HF=-1570.9808775\ZeroPoint=0.1834523\Thermal=0.2010206

Cis-Pd(**Cys^{3D}**)$_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.000005	0.100914	-0.000017
2	16	0	1.597100	1.706910	-0.474935
3	6	0	2.699778	0.623511	-1.475116
4	1	0	2.313123	0.504054	-2.491909
5	1	0	3.679837	1.098582	-1.537837
6	6	0	2.833687	-0.754965	-0.836273
7	1	0	3.474623	-1.395217	-1.461985
8	7	0	1.486430	-1.366096	-0.683898
9	1	0	1.552143	-2.155046	-0.043514
10	6	0	3.488878	-0.743936	0.540121
11	8	0	4.601600	0.006481	0.558849
12	8	0	3.102253	-1.397973	1.477872
13	1	0	1.167219	-1.711156	-1.585687
14	1	0	4.966108	-0.025774	1.455997
15	7	0	-1.486420	-1.366123	0.683823
16	6	0	-2.833668	-0.754991	0.836268
17	1	0	-1.552155	-2.155032	0.043391
18	6	0	-2.699732	0.623464	1.475153
19	1	0	-3.474585	-1.395259	1.461982
20	6	0	-3.488909	-0.743909	-0.540102
21	16	0	-1.597091	1.706892	0.474964
22	1	0	-2.313037	0.503973	2.491926
23	1	0	-3.679788	1.098534	1.537927
24	8	0	-4.601617	0.006532	-0.558769
25	8	0	-3.102335	-1.397931	-1.477884
26	1	0	-4.966158	-0.025692	-1.455904
27	1	0	-1.167187	-1.711239	1.585582

HF=-1570.9773954\ZeroPoint=0.1828109\Thermal=0.2005923

PdCl(**Cys^{3D}**)(**Cys^{4D}**) isomer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.322822	-0.155936	-0.578247
2	7	0	3.273037	0.798289	-0.910414
3	6	0	3.047322	0.224860	0.449147
4	1	0	2.607521	1.594575	-1.061316
5	6	0	2.624565	-1.268474	0.323740
6	1	0	2.226942	0.780905	0.904374
7	6	0	4.310900	0.395774	1.261939
8	16	0	1.526390	-1.522688	-1.119918
9	1	0	2.141067	-1.567785	1.251946
10	1	0	3.507208	-1.897451	0.172530
11	8	0	5.373386	0.750037	0.807326
12	8	0	4.108549	0.069743	2.545276
13	1	0	4.254411	1.043606	-1.059633
14	8	0	-5.604635	0.139918	0.564403
15	6	0	-4.430455	0.780859	0.734736
16	6	0	-3.286135	0.036959	0.061107
17	8	0	-4.309532	1.796143	1.374779
18	7	0	-2.108590	0.919955	-0.096439
19	6	0	-2.877015	-1.186162	0.890152
20	1	0	-3.600680	-0.298236	-0.928508
21	1	0	-2.259805	1.627658	-0.812278
22	1	0	-1.948546	1.435991	0.768832
23	16	0	-1.447736	-2.050985	0.104450
24	1	0	-3.707889	-1.890928	0.951967
25	1	0	-2.621059	-0.865641	1.905098
26	17	0	0.611165	2.091660	-1.138197
27	1	0	4.949033	0.158951	3.020828
28	1	0	2.911299	0.065009	-1.578809
29	1	0	-6.286332	0.629615	1.049918

HF=-2031.8430125\ZeroPoint=0.192275\Thermal=0.2127661

PdCl(**Cys^{3D}**)(**Cys^{4D}**) isomer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.441544	-0.556553	-0.072988
2	7	0	3.105478	-0.652678	0.992513
3	6	0	3.749776	-0.069257	-0.217249
4	1	0	2.537614	-1.503820	0.718442
5	6	0	2.648570	0.410625	-1.195672
6	1	0	4.354070	-0.845493	-0.695855
7	6	0	4.696743	1.022415	0.265140
8	16	0	1.251913	1.200184	-0.301801

9	1	0	2.283352	-0.450002	-1.753201
10	1	0	3.092309	1.121810	-1.890349
11	8	0	4.975174	1.206439	1.424213
12	8	0	5.214541	1.716276	-0.757182
13	1	0	3.764186	-0.818552	1.752288
14	8	0	-5.434523	1.449167	-0.471873
15	6	0	-4.221347	1.673256	0.069676
16	6	0	-3.240727	0.563926	-0.280465
17	8	0	-3.966046	2.620942	0.772118
18	7	0	-1.850720	1.003386	0.005635
19	6	0	-3.530041	-0.705437	0.525588
20	1	0	-3.313556	0.330954	-1.343910
21	1	0	-1.560601	1.733698	-0.642372
22	1	0	-1.824310	1.428660	0.933018
23	16	0	-2.277740	-1.997752	0.136939
24	1	0	-4.519008	-1.088466	0.269239
25	1	0	-3.522359	-0.463612	1.593966
26	17	0	1.032275	-2.437990	-0.198282
27	1	0	5.816348	2.385393	-0.396039
28	1	0	2.382221	0.049817	1.273050
29	1	0	-6.029031	2.157246	-0.179584

HF=-2031.8350277\ZeroPoint=0.1927193\Thermal=0.2130853

Trans-Pd(**Ala^{2D}**)$_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.000000	-0.000003	-0.091869
2	6	0	4.107236	-1.198806	-0.085405
3	1	0	4.209207	-2.238278	0.238691
4	1	0	4.946738	-0.619052	0.298496
5	6	0	2.806598	-0.588132	0.415733
6	1	0	2.753774	-0.657230	1.506632
7	7	0	1.597778	-1.310646	-0.102483
8	1	0	1.398692	-2.153029	0.432099
9	6	0	2.690623	0.929553	0.100057
10	8	0	3.689349	1.619054	0.095827
11	8	0	1.476328	1.376255	-0.093761
12	1	0	1.750127	-1.604640	-1.066277
13	7	0	-1.597775	1.310641	-0.102499
14	6	0	-2.806592	0.588135	0.415731
15	1	0	-1.398685	2.153031	0.432070
16	6	0	-4.107233	1.198816	-0.085392
17	1	0	-2.753756	0.657234	1.506630
18	6	0	-2.690627	-0.929548	0.100055
19	1	0	-4.209192	2.238290	0.238702
20	1	0	-4.946735	0.619070	0.298523
21	8	0	-3.689355	-1.619045	0.095817
22	8	0	-1.476330	-1.376258	-0.093752
23	1	0	-1.750129	1.604622	-1.066297
24	1	0	4.155997	-1.161693	-1.178073
25	1	0	-4.156009	1.161699	-1.178058

HF=-774.5096654\ZeroPoint=0.1838008\Thermal=0.1986061

Cis-Pd(**Ala^{2D}**)$_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.000000	-0.042821	0.000004
2	6	0	4.158249	-1.179268	-0.111328
3	1	0	4.280588	-2.213492	0.224320
4	1	0	4.984716	-0.579378	0.270295
5	6	0	2.847236	-0.584062	0.377967
6	1	0	2.784176	-0.645639	1.468682
7	7	0	1.648012	-1.324684	-0.147699
8	1	0	1.558405	-2.224025	0.318868
9	6	0	2.694268	0.921086	0.033244
10	8	0	3.681995	1.625050	-0.023556
11	8	0	1.469091	1.330960	-0.136403
12	1	0	1.791127	-1.524140	-1.137448
13	7	0	-1.648009	-1.324688	0.147677
14	6	0	-2.847238	-0.584063	-0.377973
15	1	0	-1.558405	-2.224026	-0.318897
16	6	0	-4.158246	-1.179268	0.111338
17	1	0	-2.784193	-0.645640	-1.468689
18	6	0	-2.694268	0.921084	-0.033248
19	1	0	-4.280588	-2.213492	-0.224306
20	1	0	-4.984716	-0.579377	-0.270277
21	8	0	-3.681993	1.625054	0.023505
22	8	0	-1.469098	1.330950	0.136452
23	1	0	-1.791114	-1.524150	1.137427
24	1	0	4.213684	-1.150211	-1.203876
25	1	0	-4.213668	-1.150209	1.203888

HF=-774.4934486\ZeroPoint=0.1835683\Thermal=0.1984247

PdCl(**Ala^{2D}**)(**Ala^{3D}**) isomer 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.274556	-0.515530	-0.443022
2	7	0	-3.444923	-0.488594	-0.040859
3	6	0	-3.065013	0.926559	0.335468
4	1	0	-2.658164	-1.166278	0.224481
5	6	0	-2.798492	1.011931	1.834086
6	1	0	-3.893978	1.576444	0.045683
7	6	0	-1.815573	1.315170	-0.498002
8	1	0	-2.483017	2.028153	2.068361
9	1	0	-1.997922	0.324869	2.118972
10	8	0	-1.421113	0.386999	-1.307990
11	8	0	-1.323374	2.419474	-0.319604
12	1	0	-4.314898	-0.787305	0.399689
13	8	0	4.087851	-0.557528	0.782005
14	6	0	2.979974	-0.315158	0.352131
15	6	0	2.645376	1.115732	-0.135344
16	8	0	1.998883	-1.186606	0.313366
17	7	0	1.437084	1.079309	-1.019010
18	6	0	2.387124	2.019498	1.069714
19	1	0	3.503053	1.486442	-0.700600
20	1	0	0.849249	1.912376	-0.935680
21	1	0	1.690227	0.967579	-1.997382

22	1	0	3.258474	2.001186	1.724826
23	1	0	1.519170	1.666908	1.633237
24	17	0	-1.046040	-2.272310	0.447651
25	1	0	-3.511440	-0.572600	-1.057006
26	1	0	-3.693776	0.779271	2.417543
27	1	0	2.202647	3.050470	0.755358

HF=-1235.362421\ZeroPoint=0.1931396\Thermal=0.2104737

PdCl(**Ala^{2D}**)(**Ala^{3D}**) isomer 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.380333	0.082522	0.095171
2	7	0	3.101391	0.534408	-1.423043
3	6	0	3.535941	-0.602481	-0.516953
4	1	0	2.585272	1.245481	-0.845093
5	6	0	4.476067	-0.095784	0.563001
6	1	0	4.020722	-1.343937	-1.157309
7	6	0	2.216702	-1.214270	0.050746
8	1	0	4.706113	-0.924599	1.231349
9	1	0	3.992322	0.684188	1.155882
10	8	0	1.208793	-0.951319	-0.724978
11	8	0	2.256637	-1.828389	1.093427
12	1	0	3.870277	0.967236	-1.933295
13	8	0	-3.909114	-1.843046	-0.156556
14	6	0	-2.972545	-1.083584	-0.010962
15	6	0	-3.256766	0.408280	0.295325
16	8	0	-1.715174	-1.412621	-0.139042
17	7	0	-2.018750	1.051690	0.850248
18	6	0	-3.691578	1.122916	-0.982074
19	1	0	-4.055537	0.456267	1.038751
20	1	0	-1.978002	2.048928	0.648921
21	1	0	-1.973766	0.944963	1.861619
22	1	0	-4.564441	0.616242	-1.394472
23	1	0	-2.891412	1.097691	-1.726871
24	17	0	1.046886	1.986022	0.380273
25	1	0	2.379246	0.162252	-2.050339
26	1	0	5.409425	0.290731	0.143152
27	1	0	-3.956530	2.166013	-0.782535

HF=-1235.3579978\ZeroPoint=0.1930661\Thermal=0.2106655

Precursor complexes and their isomers

M1-Cl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.735983	0.517349	-0.102632
2	7	0	-4.618837	0.606238	-0.005207
3	7	0	-3.668815	-0.225467	-0.093136
4	6	0	-4.188848	1.921241	-0.020706
5	6	0	-2.797038	2.183908	-0.110477
6	6	0	-2.381024	3.508954	-0.151071
7	1	0	-1.327642	3.749164	-0.218430
8	6	0	-3.328660	4.539555	-0.107205
9	6	0	-4.697400	4.269836	-0.014931
10	1	0	-5.411400	5.083860	0.020307
11	6	0	-5.135870	2.953271	0.028769
12	1	0	-6.187973	2.703492	0.098559
13	6	0	-4.042304	-1.602113	-0.063064
14	6	0	-3.375267	-2.498664	-0.899278
15	6	0	-3.743615	-3.840232	-0.893711
16	1	0	-3.233885	-4.535827	-1.549778
17	6	0	-4.755387	-4.287994	-0.045451
18	6	0	-5.410671	-3.386400	0.795599
19	1	0	-6.191128	-3.733662	1.462754
20	6	0	-5.062487	-2.041166	0.787508
21	1	0	-2.588118	-2.142758	-1.549670
22	17	0	0.384444	1.608393	-0.072457
23	17	0	-0.384436	-1.608360	0.072924
24	46	0	1.735996	-0.517345	0.102805
25	7	0	3.668824	0.225456	0.093005
26	6	0	2.797039	-2.183916	0.110385
27	7	0	4.618830	-0.606251	0.004888
28	6	0	4.042310	1.602107	0.062992
29	6	0	4.188836	-1.921253	0.020405
30	6	0	2.381023	-3.508962	0.150979
31	6	0	3.375387	2.498586	0.899374
32	6	0	5.062366	2.041236	-0.787693
33	6	0	5.135844	-2.953286	-0.029275
34	1	0	1.327651	-3.749170	0.218499
35	6	0	3.328646	-4.539566	0.106908
36	6	0	3.743727	3.840158	0.893865
37	1	0	2.588333	2.142623	1.549850
38	6	0	5.410542	3.386472	-0.795722
39	6	0	4.697372	-4.269852	0.014425
40	1	0	6.187938	-2.703513	-0.099221
41	1	0	3.234087	4.535695	1.550062
42	6	0	4.755376	4.287993	0.045498
43	1	0	6.190900	3.733793	-1.462963
44	1	0	5.411362	-5.083878	-0.020973
45	1	0	-5.558249	-1.328580	1.433671
46	1	0	5.558038	1.328708	-1.433989
47	1	0	5.029493	5.336639	0.034277
48	1	0	-5.029510	-5.336637	-0.034182
49	1	0	2.989069	-5.569347	0.145532
50	1	0	-2.989085	5.569336	-0.145825

HF=-2321.1339726\ZeroPoint=0.3652855\Thermal=0.3942601

D1-Cl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-2.131081	1.135778	-0.251819
2	46	0	2.131151	-1.135811	-0.251932
3	17	0	-3.659434	2.862229	0.115815
4	17	0	3.659541	-2.862246	0.115631
5	7	0	-0.595250	-0.248664	-0.548698
6	7	0	0.595292	0.248606	-0.548738
7	7	0	-5.642084	-1.019674	1.331609
8	7	0	5.641885	1.019819	1.331812
9	8	0	-3.711180	-0.338854	0.350095
10	8	0	3.711204	0.338881	0.349962
11	6	0	-0.626761	-1.641726	-0.645300
12	6	0	0.609799	-2.331947	-0.587976
13	6	0	0.600886	-3.714458	-0.753433
14	1	0	1.529683	-4.265464	-0.702813
15	6	0	-0.601317	-4.385842	-0.991039
16	6	0	-1.811379	-3.690780	-1.066409
17	1	0	-2.733901	-4.221985	-1.270909
18	6	0	-1.832289	-2.314780	-0.893382
19	1	0	-2.754388	-1.758304	-0.952319
20	6	0	0.626801	1.641665	-0.645400
21	6	0	-0.609753	2.331893	-0.588041
22	6	0	-0.600847	3.714394	-0.753585
23	1	0	-1.529640	4.265406	-0.702940
24	6	0	0.601343	4.385760	-0.991305
25	1	0	0.588439	5.462034	-1.127602
26	6	0	1.811400	3.690691	-1.066699
27	1	0	2.733911	4.221883	-1.271282
28	6	0	1.832319	2.314702	-0.893589
29	1	0	2.754415	1.758223	-0.952544
30	6	0	-4.819058	-0.082302	0.844945
31	1	0	-5.181217	0.948743	0.911352
32	6	0	-6.952777	-0.670440	1.863500
33	1	0	-7.036060	-0.989554	2.906485
34	1	0	-7.741418	-1.159051	1.283273
35	1	0	-7.097694	0.408683	1.813213
36	6	0	-5.277647	-2.432919	1.317260
37	1	0	-4.235711	-2.531849	1.021100
38	1	0	-5.910259	-2.981124	0.612138
39	1	0	-5.413892	-2.856864	2.315565
40	6	0	4.818958	0.082377	0.845116
41	1	0	5.181069	-0.948666	0.911804
42	6	0	5.277478	2.433069	1.317105
43	1	0	5.910283	2.981130	0.612044
44	1	0	5.413472	2.857198	2.315366
45	1	0	4.235621	2.531960	1.020653
46	6	0	6.952434	0.670654	1.864101
47	1	0	7.097346	-0.408479	1.814036

48	1	0	7.035452	0.989946	2.907054
49	1	0	7.741232	1.159155	1.283994
50	1	0	-0.588419	-5.462124	-1.127273

HF=-2245.4106195\ZeroPoint=0.3816984\Thermal=0.4136926

M1-OAc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.096767	-0.847878	1.465331
2	46	0	0.096767	-0.847903	-1.465325
3	8	0	-1.524483	-2.326295	1.211509
4	8	0	1.524481	-2.326318	-1.211479
5	8	0	1.428683	-2.344796	1.043173
6	8	0	-1.428686	-2.344812	-1.043143
7	7	0	1.061866	0.853688	1.722792
8	7	0	-1.061865	0.853662	-1.722804
9	6	0	-1.722600	2.888607	2.376427
10	1	0	-1.266052	3.866266	2.478358
11	7	0	0.448514	1.944672	1.930613
12	6	0	3.035069	2.124359	0.999578
13	1	0	2.390303	2.938558	0.700018
14	6	0	-3.086026	2.696180	2.553341
15	1	0	-3.726802	3.535346	2.797087
16	7	0	-0.448513	1.944644	-1.930636
17	6	0	2.469927	0.960491	1.532726
18	6	0	-2.831231	0.313734	2.093947
19	1	0	-3.269535	-0.670369	1.983419
20	6	0	-3.035065	2.124342	-0.999598
21	1	0	-2.390297	2.938544	-0.700047
22	6	0	-3.277248	-0.123468	-1.887196
23	1	0	-2.825940	-1.021622	-2.283528
24	6	0	3.277248	-0.123444	1.887198
25	1	0	2.825938	-1.021594	2.283538
26	6	0	1.722602	2.888572	-2.376460
27	1	0	1.266056	3.866230	-2.478400
28	6	0	-1.462794	0.481877	1.920334
29	6	0	4.655524	-0.032398	1.718746
30	1	0	5.283813	-0.868764	2.002854
31	6	0	3.631429	1.414597	-2.415081
32	6	0	3.086028	2.696142	-2.553374
33	1	0	3.726804	3.535305	-2.797129
34	6	0	-0.918420	1.781784	2.068394
35	6	0	1.866489	-2.748201	-0.062559
36	6	0	5.225816	1.125021	1.190244
37	6	0	4.410339	2.199564	0.830459
38	1	0	4.846308	3.092710	0.398490
39	6	0	-2.469925	0.960469	-1.532736
40	6	0	-3.631428	1.414635	2.415060
41	6	0	-4.410334	2.199552	-0.830477
42	1	0	-4.846301	3.092702	-0.398517
43	6	0	2.831231	0.313701	-2.093957
44	1	0	3.269534	-0.670402	-1.983419
45	6	0	-5.225814	1.125006	-1.190252
46	6	0	1.462794	0.481847	-1.920344
47	6	0	-1.866493	-2.748197	0.062595
48	6	0	0.918421	1.781753	-2.068416
49	6	0	-4.655524	-0.032419	-1.718743
50	1	0	-5.283815	-0.868785	-2.002842
51	6	0	2.943468	-3.812951	-0.042179
52	1	0	3.909325	-3.313658	0.084752
53	1	0	2.959932	-4.366703	-0.979849
54	1	0	2.793376	-4.482800	0.804174
55	6	0	-2.943475	-3.812945	0.042233
56	1	0	-2.793383	-4.482810	-0.804108
57	1	0	-3.909330	-3.313651	-0.084709
58	1	0	-2.959942	-4.366679	0.979913
59	1	0	6.299204	1.187672	1.051334
60	1	0	-6.299201	1.187661	-1.051340
61	1	0	-4.698184	1.272320	2.551311
62	1	0	4.698185	1.272280	-2.551334

HF=-1857.7869146\ZeroPoint=0.4664743\Thermal=0.5017347

D1-OAc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.348311	0.440707	1.074095
2	8	0	-4.324548	0.368062	-1.187760
3	6	0	-4.877576	0.557906	-0.067455
4	6	0	-6.319433	1.016797	-0.097362
5	1	0	-6.818267	0.642498	-0.990230
6	1	0	-6.329002	2.110649	-0.129933
7	1	0	-6.838389	0.696002	0.804832
8	7	0	0.349945	0.588463	1.774387
9	7	0	-0.386910	-0.475474	1.800850
10	6	0	-0.371467	1.782385	1.777641
11	6	0	1.741366	-1.561615	1.824895
12	6	0	-1.777739	1.672770	1.687705
13	6	0	0.333524	-1.666298	1.893593
14	6	0	-2.540869	2.831348	1.734945
15	1	0	-3.619471	2.765827	1.665972
16	6	0	0.262419	3.024393	1.923946
17	1	0	1.339323	3.077696	1.995646
18	6	0	-0.303995	-2.896941	2.105572
19	1	0	-1.382136	-2.946179	2.159775
20	6	0	2.502587	-2.714479	1.960325
21	1	0	3.582416	-2.652891	1.909152
22	6	0	-1.914064	4.072702	1.876679
23	6	0	-0.522570	4.168027	1.970355
24	1	0	-0.050828	5.136667	2.085012
25	6	0	0.479125	-4.034972	2.239224
26	1	0	0.004571	-4.994752	2.405287
27	6	0	1.872259	-3.944865	2.167259
28	46	0	-2.368232	-0.263309	-1.486243
29	46	0	-2.399095	-0.169933	1.452432
30	8	0	-3.106567	-2.196356	1.164955
31	8	0	-3.082150	-2.268416	-1.085997
32	6	0	-3.309304	-2.762540	0.054121
33	6	0	-3.825732	-4.186434	0.093872
34	1	0	-4.420064	-4.354230	0.991422
35	1	0	-2.961211	-4.857902	0.123876

36	1	0	-4.401566	-4.410852	-0.803380
37	8	0	4.348311	-0.440707	-1.074095
38	8	0	4.324548	-0.368062	1.187760
39	6	0	4.877576	-0.557906	0.067455
40	6	0	6.319433	-1.016797	0.097362
41	1	0	6.818267	-0.642498	0.990230
42	1	0	6.329002	-2.110649	0.129933
43	1	0	6.838389	-0.696002	-0.804832
44	7	0	-0.349945	-0.588463	-1.774387
45	7	0	0.386910	0.475474	-1.800850
46	6	0	0.371467	-1.782385	-1.777641
47	6	0	-1.741366	1.561615	-1.824895
48	6	0	1.777739	-1.672770	-1.687705
49	6	0	-0.333524	1.666298	-1.893593
50	6	0	2.540869	-2.831348	-1.734945
51	1	0	3.619471	-2.765827	-1.665972
52	6	0	-0.262419	-3.024393	-1.923946
53	1	0	-1.339323	-3.077696	-1.995646
54	6	0	0.303995	2.896941	-2.105572
55	1	0	1.382136	2.946179	-2.159775
56	6	0	-2.502587	2.714479	-1.960325
57	1	0	-3.582416	2.652891	-1.909152
58	6	0	1.914064	-4.072702	-1.876679
59	6	0	0.522570	-4.168027	-1.970355
60	1	0	0.050828	-5.136667	-2.085012
61	6	0	-0.479125	4.034972	-2.239224
62	1	0	-0.004571	4.994752	-2.405287
63	6	0	-1.872259	3.944865	-2.167259
64	46	0	2.368232	0.263309	1.486243
65	46	0	2.399095	0.169933	-1.452432
66	8	0	3.106567	2.196356	-1.164955
67	8	0	3.082150	2.268416	1.085997
68	6	0	3.309304	2.762540	-0.054121
69	6	0	3.825732	4.186434	-0.093872
70	1	0	4.420064	4.354230	-0.991422
71	1	0	2.961211	4.857902	-0.123876
72	1	0	4.401566	4.410852	0.803380
73	1	0	2.474531	-4.840708	2.275732
74	1	0	-2.474531	4.840708	-2.275732
75	1	0	-2.517822	4.973208	1.916650
76	1	0	2.517822	-4.973208	-1.916650

HF=-2569.700523\ZeroPoint=0.5510627\Thermal=0.5985083

M1-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.249821	-0.621762	-0.130031
2	7	0	-1.119734	1.291359	-0.097665
3	7	0	-2.377661	1.357394	0.057576
4	6	0	-2.989602	0.114047	0.051069
5	6	0	-2.193160	-1.059328	-0.068175
6	6	0	-2.861410	-2.281986	-0.090113
7	1	0	-2.301901	-3.205811	-0.181065
8	6	0	-4.256052	-2.334836	0.000245
9	6	0	-5.022849	-1.170222	0.121451
10	1	0	-6.102252	-1.232675	0.192701
11	6	0	-4.389519	0.062813	0.148604
12	1	0	-4.946230	0.988202	0.240799
13	6	0	-0.423458	2.532430	-0.056070
14	6	0	0.648854	2.722784	-0.932056
15	6	0	1.366859	3.914709	-0.900115
16	1	0	2.187599	4.065991	-1.591636
17	6	0	1.026363	4.911903	0.014140
18	1	0	1.592353	5.835572	0.045963
19	6	0	-0.045700	4.717533	0.886716
20	1	0	-0.311473	5.490166	1.599144
21	6	0	-0.775935	3.533941	0.854109
22	16	0	0.466873	-2.813594	0.021909
23	6	0	2.275111	-2.538024	-0.206248
24	1	0	2.813445	-3.368644	0.251587
25	1	0	2.523767	-2.515100	-1.272598
26	6	0	2.711855	-1.218396	0.444191
27	1	0	2.521508	-1.278460	1.517377
28	7	0	1.906156	-0.109885	-0.113592
29	1	0	2.231141	0.071832	-1.063020
30	6	0	4.196510	-0.976020	0.208331
31	8	0	4.958564	-1.782125	0.974329
32	8	0	4.648092	-0.186191	-0.584923
33	1	0	-4.751761	-3.299959	-0.022896
34	1	0	2.083305	0.752071	0.397805
35	1	0	0.880830	1.951993	-1.656909
36	1	0	5.887776	-1.616998	0.751965
37	1	0	-1.608078	3.366736	1.525695

HF=-1421.8076215\ZeroPoint=0.2722108\Thermal=0.2929132

M1-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.253913	0.114939	-0.106234
2	7	0	-1.810063	0.288378	-0.062777
3	7	0	-2.300886	1.451029	0.057107
4	6	0	-1.355086	2.463967	0.035020
5	6	0	0.016802	2.119495	-0.090223
6	6	0	0.924175	3.177227	-0.151285
7	1	0	1.989059	2.992559	-0.268029
8	6	0	0.492338	4.507083	-0.082457
9	6	0	-0.864172	4.818217	0.052866
10	1	0	-1.183333	5.852142	0.107186
11	6	0	-1.798114	3.792229	0.109608
12	1	0	-2.858657	3.993845	0.206645
13	6	0	-2.759308	-0.778217	-0.019084
14	6	0	-2.583109	-1.878697	-0.859518
15	6	0	-3.514268	-2.912953	-0.835380
16	1	0	-3.379455	-3.765085	-1.491034
17	6	0	-4.605171	-2.858806	0.030070
18	1	0	-5.320466	-3.672970	0.054448
19	6	0	-4.770577	-1.758074	0.873675
20	1	0	-5.611503	-1.717601	1.556527
21	6	0	-3.855243	-0.713431	0.849422
22	1	0	-3.966749	0.145028	1.498679

23	16	0	0.551214	-2.259976	0.017314
24	6	0	2.376118	-2.266210	-0.221812
25	1	0	2.795663	-3.170422	0.220277
26	1	0	2.624170	-2.263234	-1.288958
27	6	0	3.005628	-1.038546	0.445975
28	1	0	2.819756	-1.092122	1.520293
29	7	0	2.355593	0.192439	-0.073667
30	1	0	2.688876	0.362619	-1.023361
31	6	0	4.504434	-0.978055	0.191889
32	8	0	5.163208	-1.921301	0.891643
33	8	0	5.043298	-0.205118	-0.563208
34	1	0	1.221669	5.308857	-0.137874
35	1	0	2.654882	0.998357	0.469907
36	1	0	-1.727820	-1.916661	-1.519870
37	1	0	6.103231	-1.865865	0.660197

36	1	0	7.274374	1.581896	2.562158
37	46	0	-2.234984	0.830891	-0.326459
38	16	0	-3.777938	2.299765	0.558429
39	6	0	-5.181705	1.134553	0.810453
40	1	0	-5.835240	1.542998	1.582095
41	1	0	-5.761462	1.032040	-0.112704
42	6	0	-4.665129	-0.242638	1.243216
43	1	0	-4.143369	-0.137152	2.196121
44	7	0	-3.703882	-0.741962	0.234822
45	6	0	-5.824320	-1.216873	1.408348
46	1	0	-4.234797	-1.050167	-0.579971
47	1	0	-3.233904	-1.575518	0.581512
48	8	0	-6.528433	-0.963231	2.529111
49	8	0	-6.106211	-2.089668	0.624159
50	1	0	-7.274370	-1.581911	2.562154

HF=-1421.7983292\ZeroPoint=0.2723286\Thermal=0.2929422

HF=-2270.6872237\ZeroPoint=0.3540079\Thermal=0.3848609

D1-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	2.234984	-0.830891	-0.326461
2	7	0	0.556613	0.325862	-0.896748
3	7	0	-0.556613	-0.325859	-0.896747
4	6	0	-0.399038	-1.715629	-0.934885
5	6	0	0.890067	-2.252036	-0.698277
6	6	0	1.028558	-3.639250	-0.762932
7	1	0	1.995531	-4.092980	-0.580354
8	6	0	-0.059906	-4.455958	-1.076887
9	6	0	-1.315659	-3.904036	-1.349788
10	1	0	-2.145893	-4.541868	-1.629087
11	6	0	-1.488105	-2.529481	-1.281250
12	1	0	-2.432492	-2.076355	-1.551602
13	6	0	0.399037	1.715632	-0.934885
14	6	0	1.488103	2.529486	-1.281249
15	6	0	1.315655	3.904040	-1.349787
16	1	0	2.145888	4.541873	-1.629085
17	6	0	0.059901	4.455960	-1.076888
18	1	0	-0.076403	5.531004	-1.126492
19	6	0	-1.028562	3.639251	-0.762933
20	1	0	-1.995536	4.092980	-0.580357
21	6	0	-0.890069	2.252037	-0.698277
22	16	0	3.777939	-2.299767	0.558424
23	6	0	5.181706	-1.134554	0.810449
24	1	0	5.835241	-1.542999	1.582091
25	1	0	5.761464	-1.032042	-0.112708
26	6	0	4.665131	0.242637	1.243210
27	1	0	4.143366	0.137150	2.196114
28	7	0	3.703888	0.741964	0.234816
29	1	0	4.234802	1.050158	-0.579982
30	6	0	5.824321	1.216871	1.408352
31	8	0	6.528440	0.963213	2.529108
32	8	0	6.106207	2.089679	0.624175
33	1	0	0.076395	-5.531002	-1.126491
34	1	0	3.233917	1.575525	0.581500
35	1	0	2.432491	2.076361	-1.551599

B1-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.635589	-0.345491	-0.728837
2	46	0	1.551467	0.622908	-0.375047
3	7	0	-1.637085	1.438922	0.268384
4	7	0	-2.483265	1.611639	1.189981
5	6	0	-3.289145	0.499243	1.412632
6	6	0	-3.098849	-0.656105	0.610249
7	6	0	-3.924935	-1.747382	0.862850
8	1	0	-3.836833	-2.661950	0.282009
9	6	0	-4.893610	-1.700019	1.874473
10	6	0	-5.059690	-0.553927	2.654066
11	1	0	-5.812035	-0.529641	3.433427
12	6	0	-4.254428	0.556684	2.423696
13	1	0	-4.357870	1.463762	3.007692
14	6	0	-0.824848	2.557958	-0.085950
15	6	0	0.528313	2.371174	-0.420395
16	6	0	1.247049	3.524863	-0.775628
17	1	0	2.301963	3.439094	-1.003382
18	6	0	0.647936	4.779743	-0.829201
19	1	0	1.235246	5.641678	-1.128117
20	6	0	-0.699576	4.934224	-0.492824
21	1	0	-1.170579	5.909658	-0.532783
22	6	0	-1.433382	3.824819	-0.110664
23	1	0	-2.480044	3.909499	0.153033
24	16	0	2.608164	1.409957	1.572218
25	6	0	4.154248	0.425286	1.414974
26	1	0	4.679161	0.446372	2.370549
27	1	0	4.817301	0.850324	0.654647
28	6	0	3.833070	-1.017447	1.026005
29	1	0	4.766604	-1.598031	0.948600
30	6	0	3.020016	-1.726783	2.098226
31	8	0	3.579912	-1.595730	3.305406
32	8	0	2.036114	-2.415916	1.920813
33	7	0	3.102285	-1.029570	-0.259145
34	1	0	3.747093	-0.742935	-0.992150
35	1	0	2.799486	-1.973734	-0.499329

36	16	0	0.154227	0.102212	-2.313302
37	6	0	0.230370	-1.599736	-3.047546
38	1	0	-0.330447	-1.546757	-3.984358
39	1	0	1.258412	-1.870674	-3.284558
40	6	0	-0.378494	-2.694302	-2.160019
41	1	0	-0.485112	-3.612805	-2.751868
42	7	0	-1.705864	-2.260401	-1.639525
43	1	0	-2.046847	-2.925800	-0.950485
44	6	0	0.589154	-3.030179	-1.032732
45	8	0	1.732064	-3.359231	-1.277422
46	8	0	0.073994	-2.909664	0.177617
47	1	0	-5.521597	-2.566595	2.054178
48	1	0	0.798661	-2.864920	0.851168
49	1	0	-2.379654	-2.232594	-2.401912
50	1	0	3.020100	-2.058315	3.947189

HF=-2270.692385\ZeroPoint=0.3536452\Thermal=0.3836315

36	16	0	0.826430	0.651849	-2.181513
37	6	0	2.243251	1.763677	-1.752490
38	1	0	2.735322	2.041002	-2.683522
39	1	0	1.869515	2.672922	-1.281036
40	6	0	3.252421	1.050739	-0.841789
41	1	0	3.722419	0.242236	-1.410472
42	7	0	2.569361	0.444116	0.324227
43	1	0	2.040221	1.174729	0.822609
44	6	0	4.375358	1.970841	-0.372147
45	8	0	4.958193	2.610407	-1.405821
46	8	0	4.724692	2.094054	0.774386
47	1	0	3.112810	-3.766746	3.642678
48	1	0	3.260405	0.083258	0.976851
49	1	0	5.668728	3.166273	-1.050434
50	1	0	-3.569308	2.078181	4.812815

HF=-2270.6897024\ZeroPoint=0.353837\Thermal=0.3844445

B1-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.040940	-0.885326	-0.237249
2	46	0	-0.969729	1.131623	-0.737532
3	7	0	-0.578594	-2.085078	-0.577505
4	7	0	-0.690823	-3.150275	0.096406
5	6	0	0.345464	-3.329177	1.005156
6	6	0	1.329031	-2.309530	1.135699
7	6	0	2.315996	-2.494931	2.100117
8	1	0	3.089726	-1.749060	2.254136
9	6	0	2.333672	-3.646445	2.897095
10	6	0	1.362635	-4.640009	2.747626
11	1	0	1.390273	-5.526120	3.370505
12	6	0	0.358053	-4.482280	1.800127
13	1	0	-0.415434	-5.229185	1.663917
14	6	0	-1.633967	-1.758494	-1.485442
15	6	0	-1.925834	-0.398502	-1.713754
16	6	0	-2.991254	-0.125347	-2.584473
17	1	0	-3.256091	0.906190	-2.793392
18	6	0	-3.709534	-1.142708	-3.211169
19	1	0	-4.514254	-0.892877	-3.894873
20	6	0	-3.386848	-2.481896	-2.973218
21	1	0	-3.935263	-3.274871	-3.468502
22	6	0	-2.353195	-2.793354	-2.103928
23	1	0	-2.084443	-3.822039	-1.899577
24	16	0	0.104312	2.801273	0.642080
25	6	0	-1.232441	2.965801	1.896876
26	1	0	-1.884169	3.803766	1.627237
27	1	0	-0.794836	3.179802	2.872015
28	6	0	-2.076805	1.684977	1.992936
29	1	0	-1.442398	0.869845	2.347128
30	6	0	-3.231852	1.877869	2.965546
31	8	0	-2.801291	1.918308	4.243007
32	8	0	-4.388107	2.005539	2.645509
33	7	0	-2.585016	1.319518	0.650952
34	1	0	-3.105699	0.446368	0.690234
35	1	0	-3.252386	2.024915	0.340726

B1-Cl-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.287372	0.381165	0.762311
2	46	0	1.253661	-1.024146	0.333528
3	7	0	-2.067076	-1.406829	0.005929
4	7	0	-3.274605	-1.383938	-0.384825
5	6	0	-3.890323	-0.153427	-0.187829
6	6	0	-3.139610	0.942453	0.321785
7	6	0	-3.804705	2.152026	0.533851
8	1	0	-3.270648	2.987680	0.969902
9	6	0	-5.161836	2.280997	0.215622
10	6	0	-5.881210	1.203867	-0.310443
11	1	0	-6.932148	1.315957	-0.549375
12	6	0	-5.248369	-0.017763	-0.508227
13	1	0	-5.784282	-0.877147	-0.893992
14	6	0	-1.339515	-2.612151	-0.175271
15	6	0	0.074119	-2.588067	-0.142335
16	6	0	0.726278	-3.809869	-0.386539
17	1	0	1.808789	-3.835421	-0.402110
18	6	0	0.027029	-4.991572	-0.603533
19	1	0	0.571875	-5.915393	-0.767746
20	6	0	-1.372335	-4.993884	-0.603142
21	1	0	-1.922010	-5.915216	-0.757733
22	6	0	-2.051432	-3.808797	-0.398965
23	1	0	-3.132724	-3.781168	-0.397337
24	16	0	2.495032	-1.163298	-1.665793
25	6	0	3.882055	-0.006830	-1.227626
26	1	0	3.711541	0.951454	-1.719106
27	1	0	4.811297	-0.436196	-1.598966
28	6	0	3.986735	0.209320	0.289788
29	1	0	4.321504	-0.723686	0.752392
30	6	0	5.021700	1.280657	0.616113
31	8	0	6.255651	0.912952	0.198745
32	8	0	4.792791	2.321256	1.175348
33	7	0	2.667505	0.544796	0.847831
34	1	0	2.703445	0.644384	1.859911
35	1	0	2.337606	1.442879	0.491892

36	1	0	-5.662128	3.227664	0.391143
37	1	0	6.868879	1.627860	0.427540
38	1	0	-1.692425	1.345414	-1.174062
39	7	0	-1.618340	2.027745	-1.988551
40	6	0	-0.439603	2.920247	-1.711096
41	6	0	-0.568526	3.552116	-0.317199
42	1	0	-0.442874	3.707438	-2.471772
43	6	0	0.842827	2.096793	-1.897157
44	16	0	-0.315115	2.464979	1.150384
45	1	0	-1.531682	4.071873	-0.265742
46	1	0	0.213362	4.309224	-0.244694
47	8	0	0.605276	0.963184	-2.532866
48	8	0	1.908432	2.506374	-1.507102
49	1	0	-1.475914	1.479274	-2.837887
50	17	0	0.229453	-0.805898	2.490486
51	1	0	-2.500737	2.539675	-2.018228
52	1	0	1.341322	0.244687	-2.376776

HF=-2731.539569\ZeroPoint=0.3623087\Thermal=0.3948098

B1-Cl-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.801379	-1.308974	-0.581247
2	46	0	-1.308894	1.270770	-0.798134
3	7	0	-1.212933	-1.930828	-0.329807
4	7	0	-1.423500	-2.825305	0.536781
5	6	0	-0.277765	-3.220142	1.216958
6	6	0	0.981263	-2.657545	0.872252
7	6	0	2.093404	-3.114651	1.578336
8	1	0	3.078274	-2.743201	1.328363
9	6	0	1.955877	-4.069566	2.592795
10	6	0	0.708742	-4.604747	2.922557
11	1	0	0.620742	-5.347762	3.706361
12	6	0	-0.416048	-4.181873	2.227009
13	1	0	-1.401259	-4.580150	2.440409
14	6	0	-2.343382	-1.551231	-1.115768
15	6	0	-2.521375	-0.201991	-1.449462
16	6	0	-3.648831	0.131138	-2.210320
17	1	0	-3.824761	1.166053	-2.486103
18	6	0	-4.544947	-0.845021	-2.646769
19	1	0	-5.396477	-0.560879	-3.256058
20	6	0	-4.340632	-2.185514	-2.312278
21	1	0	-5.028884	-2.948243	-2.657768
22	6	0	-3.244219	-2.540329	-1.540072
23	1	0	-3.061342	-3.572502	-1.268286
24	16	0	-0.105246	3.211523	0.104144
25	6	0	-1.007222	3.324006	1.709182
26	1	0	-1.672212	4.192246	1.665381
27	1	0	-0.311520	3.479276	2.533080
28	6	0	-1.840581	2.061326	1.993658
29	1	0	-1.166787	1.233571	2.224311
30	6	0	-2.763896	2.288381	3.182952
31	8	0	-2.067398	2.387911	4.333208
32	8	0	-3.963321	2.387307	3.113200
33	7	0	-2.625358	1.682331	0.795792
34	1	0	-3.204006	0.867896	0.990163
35	1	0	-3.272347	2.432835	0.557121
36	1	0	2.840082	-4.404288	3.125802
37	1	0	-2.696398	2.555759	5.051893
38	1	0	2.408985	1.251593	-1.277647
39	7	0	2.650406	2.066303	-0.674062
40	6	0	3.705443	1.631637	0.275785
41	6	0	3.437169	0.187318	0.736505
42	1	0	3.689922	2.310505	1.135837
43	6	0	5.050788	1.831214	-0.417388
44	16	0	3.135477	-0.921897	-0.708962
45	1	0	2.577084	0.181063	1.405463
46	1	0	4.306264	-0.156758	1.296095
47	8	0	6.053680	1.269032	0.270470
48	8	0	5.193620	2.465849	-1.432286
49	1	0	2.985357	2.818593	-1.279854
50	17	0	0.317329	0.494625	-2.352055
51	1	0	1.761425	2.380351	-0.184868
52	1	0	6.879534	1.435993	-0.209391

HF=-2731.5334622\ZeroPoint=0.3624407\Thermal=0.3958952

B1-Cl-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.463896	0.230697	-0.277694
2	46	0	1.841875	0.235168	-0.198102
3	7	0	-0.690423	-0.349759	1.616976
4	7	0	-1.380559	-1.190121	2.265283
5	6	0	-2.463815	-1.676504	1.545819
6	6	0	-2.789366	-1.115553	0.282090
7	6	0	-3.900358	-1.605622	-0.393588
8	1	0	-4.181020	-1.196127	-1.356676
9	6	0	-4.664164	-2.634559	0.167794
10	6	0	-4.339350	-3.181894	1.412696
11	1	0	-4.945619	-3.975376	1.833372
12	6	0	-3.240387	-2.699147	2.109477
13	1	0	-2.964045	-3.091316	3.081273
14	6	0	0.314201	0.347321	2.358511
15	6	0	1.505961	0.745789	1.715004
16	6	0	2.435367	1.469894	2.478496
17	1	0	3.381198	1.750195	2.029761
18	6	0	2.181555	1.814396	3.808187
19	1	0	2.915082	2.386696	4.365763
20	6	0	0.993203	1.414589	4.418505
21	1	0	0.789801	1.678993	5.449798
22	6	0	0.062008	0.678393	3.697326
23	1	0	-0.870863	0.364245	4.148067
24	16	0	3.370364	-1.315892	0.511141
25	6	0	3.956648	-1.821005	-1.168808
26	1	0	4.406539	-2.810723	-1.081663
27	1	0	4.721453	-1.127213	-1.529767
28	6	0	2.811171	-1.859570	-2.178684
29	1	0	3.204937	-2.147880	-3.164700
30	6	0	1.734889	-2.889036	-1.845905
31	8	0	0.551799	-2.673729	-1.902535

32	8	0	2.269529	-4.088073	-1.553074
33	7	0	2.155750	-0.528102	-2.244684
34	1	0	2.714669	0.106614	-2.808094
35	1	0	1.236133	-0.615453	-2.676871
36	16	0	-2.733425	1.078085	-2.030470
37	6	0	-1.746613	2.542204	-2.568415
38	1	0	-0.902609	2.220954	-3.185153
39	1	0	-2.407271	3.149012	-3.188574
40	6	0	-1.231803	3.435672	-1.436158
41	1	0	-2.062088	3.728356	-0.790007
42	7	0	-0.617880	4.654337	-1.977673
43	1	0	-0.320225	5.288196	-1.243873
44	6	0	-0.221558	2.684982	-0.573614
45	8	0	0.299782	1.621692	-0.959481
46	8	0	0.138459	3.288937	0.537597
47	1	0	-5.525510	-3.009510	-0.374978
48	1	0	1.540227	-4.692148	-1.347386
49	1	0	0.181105	4.441367	-2.566713
50	1	0	0.779764	2.729023	1.030525

HF=-2270.6473927\ZeroPoint=0.3521741\Thermal=0.3831045

32	8	0	5.759726	-1.449466	-2.699527
33	7	0	3.232018	-0.792648	-0.164650
34	1	0	2.975688	-1.767800	-0.023603
35	1	0	3.904648	-0.583344	0.574245
36	16	0	-3.201296	2.085982	-0.801988
37	6	0	-2.072158	3.485475	-0.401584
38	1	0	-1.253062	3.522502	-1.123652
39	1	0	-2.658732	4.399270	-0.504009
40	6	0	-1.499762	3.462939	1.017961
41	1	0	-2.306850	3.414749	1.751353
42	7	0	-0.706756	4.672292	1.268156
43	1	0	-0.353631	4.714300	2.217860
44	6	0	-0.602283	2.251064	1.222360
45	8	0	-0.130586	1.636202	0.241980
46	8	0	-0.253220	1.978497	2.456684
47	1	0	-5.870985	-1.906896	-2.847966
48	1	0	6.639122	-1.851518	-2.624744
49	1	0	0.073024	4.749785	0.621963
50	1	0	0.328978	1.184213	2.462606

HF=-2270.6342739\ZeroPoint=0.352536\Thermal=0.3835132

B1-Cl-4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.903617	0.242614	-0.262887
2	46	0	1.558425	0.393594	0.094423
3	7	0	-1.121630	-1.541593	0.586044
4	7	0	-1.781670	-2.599257	0.347564
5	6	0	-2.840522	-2.403581	-0.524036
6	6	0	-3.191536	-1.088847	-0.933639
7	6	0	-4.292124	-0.930547	-1.769272
8	1	0	-4.589234	0.057031	-2.100630
9	6	0	-5.017974	-2.048525	-2.192697
10	6	0	-4.665870	-3.340053	-1.786374
11	1	0	-5.243019	-4.192972	-2.123181
12	6	0	-3.579068	-3.521070	-0.944077
13	1	0	-3.284839	-4.504498	-0.596312
14	6	0	-0.181264	-1.629121	1.661993
15	6	0	0.964854	-0.806395	1.666385
16	6	0	1.812064	-0.916751	2.784445
17	1	0	2.711684	-0.308210	2.833671
18	6	0	1.539537	-1.776760	3.850059
19	1	0	2.211403	-1.817657	4.700680
20	6	0	0.395938	-2.573244	3.816989
21	1	0	0.166196	-3.239427	4.640580
22	6	0	-0.461785	-2.499652	2.727899
23	1	0	-1.361915	-3.099559	2.690658
24	16	0	2.402957	1.705295	-1.707038
25	6	0	4.047839	0.883564	-1.781141
26	1	0	4.740424	1.328973	-1.058557
27	1	0	4.470593	1.010505	-2.778404
28	6	0	3.901982	-0.613551	-1.483604
29	1	0	3.268708	-1.064339	-2.249318
30	6	0	5.256577	-1.306243	-1.460424
31	8	0	5.829538	-1.654596	-0.456228

M1-Ala^{2D}-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.640961	-0.037753	-0.060068
2	7	0	-1.381520	0.548073	-0.014424
3	7	0	-1.600533	1.794884	0.024446
4	6	0	-0.455878	2.572976	0.018417
5	6	0	0.809581	1.933890	-0.021613
6	6	0	1.936213	2.751914	-0.041945
7	1	0	2.934632	2.326863	-0.086622
8	6	0	1.811471	4.147109	-0.015033
9	6	0	0.555363	4.756090	0.031289
10	1	0	0.474206	5.836150	0.052206
11	6	0	-0.588658	3.967401	0.046438
12	1	0	-1.579689	4.404708	0.077450
13	6	0	-2.539737	-0.288054	0.000505
14	6	0	-3.828163	0.259159	0.138612
15	6	0	-4.930646	-0.580506	0.144678
16	1	0	-5.922989	-0.157714	0.253035
17	6	0	-4.768866	-1.964305	0.014701
18	1	0	-5.636204	-2.614730	0.021053
19	6	0	-3.491768	-2.499969	-0.118732
20	1	0	-3.354339	-3.570382	-0.216810
21	6	0	-2.371358	-1.670716	-0.124839
22	1	0	-1.381491	-2.099002	-0.220239
23	6	0	1.698770	-2.786248	0.061250
24	6	0	2.905501	-1.881500	0.446325
25	1	0	2.871591	-1.800841	1.537211
26	7	0	2.679074	-0.491945	-0.073900
27	1	0	2.985579	-0.438135	-1.044679
28	6	0	4.246001	-2.449632	0.002640
29	1	0	2.704881	4.762453	-0.032030
30	1	0	3.236417	0.180747	0.445610
31	1	0	-3.944958	1.328713	0.239474

32	8	0	0.589897	-2.152362	-0.147770
33	8	0	1.859565	-3.993893	0.025957
34	1	0	5.080743	-1.844844	0.369881
35	1	0	4.345010	-3.466512	0.382352
36	1	0	4.300599	-2.503519	-1.089272

HF=-1023.5703307\ZeroPoint=0.2725365\Thermal=0.2916972

M1-Ala^{2D}-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.579164	-0.172982	-0.132905
2	7	0	1.182718	0.899448	-0.097196
3	7	0	1.113361	2.163427	0.009096
4	6	0	-0.189593	2.630114	0.001935
5	6	0	-1.240112	1.682922	-0.082212
6	6	0	-2.551045	2.138278	-0.087578
7	1	0	-3.364071	1.422991	-0.142217
8	6	0	-2.802475	3.514336	-0.020460
9	6	0	-1.758356	4.445307	0.059886
10	1	0	-1.980637	5.504423	0.112585
11	6	0	-0.440529	4.008919	0.073459
12	1	0	0.389903	4.702310	0.137875
13	6	0	2.490937	0.338074	-0.048392
14	6	0	2.767106	-0.780084	-0.840041
15	6	0	4.033789	-1.355462	-0.806290
16	1	0	4.253193	-2.209524	-1.436582
17	6	0	5.019717	-0.829112	0.028366
18	1	0	6.002631	-1.284263	0.061901
19	6	0	4.737465	0.285573	0.819709
20	1	0	5.500516	0.694635	1.471808
21	6	0	3.478740	0.875609	0.783188
22	1	0	3.244397	1.738648	1.392436
23	6	0	-2.542050	-2.269788	0.179545
24	6	0	-1.218112	-3.000667	0.545251
25	1	0	-1.095387	-2.844314	1.622192
26	7	0	-0.060525	-2.312056	-0.104358
27	1	0	0.024176	-2.640572	-1.065022
28	6	0	-1.267877	-4.492473	0.240604
29	1	0	-3.828537	3.867270	-0.029514
30	1	0	0.812082	-2.553125	0.358621
31	1	0	2.000848	-1.160168	-1.504042
32	8	0	-2.433580	-1.001416	-0.101797
33	8	0	-3.591425	-2.884837	0.216602
34	1	0	-0.363697	-4.997625	0.593543
35	1	0	-2.138718	-4.936192	0.722880
36	1	0	-1.369616	-4.662315	-0.835890

HF=-1023.5675103\ZeroPoint=0.2724197\Thermal=0.2915096

D1-Ala^{2D}-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	2.406135	0.314786	0.065837
2	7	0	0.474441	-0.436344	0.096750
3	7	0	-0.474441	0.436344	0.096752
4	6	0	-0.047016	1.767394	0.102664
5	6	0	1.353507	1.987921	0.098845
6	6	0	1.795460	3.305853	0.129434
7	1	0	2.855884	3.537836	0.144686
8	6	0	0.882842	4.368116	0.152226
9	6	0	-0.490768	4.125632	0.146136
10	1	0	-1.191704	4.951294	0.162265
11	6	0	-0.971690	2.821858	0.123654
12	1	0	-2.036813	2.621956	0.122499
13	6	0	0.047016	-1.767394	0.102663
14	6	0	0.971690	-2.821858	0.123650
15	6	0	0.490768	-4.125633	0.146133
16	1	0	1.191704	-4.951294	0.162259
17	6	0	-0.882842	-4.368116	0.152228
18	1	0	-1.251046	-5.388347	0.176056
19	6	0	-1.795460	-3.305853	0.129439
20	1	0	-2.855884	-3.537836	0.144696
21	6	0	-1.353507	-1.987921	0.098849
22	6	0	6.726750	0.522944	-0.195537
23	1	0	7.022089	1.512636	-0.556716
24	1	0	7.392977	-0.227677	-0.620638
25	6	0	5.292880	0.190930	-0.582750
26	1	0	5.169036	0.258131	-1.668031
27	7	0	4.309069	1.163610	0.001776
28	1	0	4.330944	2.043685	-0.506372
29	6	0	4.877788	-1.261569	-0.209391
30	8	0	5.722575	-2.138841	-0.236181
31	8	0	3.619865	-1.415535	0.058779
32	1	0	1.251046	5.388347	0.176053
33	1	0	4.571384	1.375536	0.963938
34	1	0	2.036813	-2.621956	0.122491
35	46	0	-2.406135	-0.314786	0.065846
36	6	0	-6.726751	-0.522946	-0.195570
37	1	0	-7.022080	-1.512639	-0.556755
38	1	0	-7.392970	0.227673	-0.620686
39	6	0	-5.292873	-0.190931	-0.582755
40	1	0	-5.169007	-0.258132	-1.668034
41	7	0	-4.309071	-1.163607	0.001791
42	6	0	-4.877788	1.261568	-0.209388
43	1	0	-4.330951	-2.043691	-0.506341
44	1	0	-4.571391	-1.375513	0.963957
45	8	0	-5.722576	2.138840	-0.236181
46	8	0	-3.619867	1.415536	0.058791
47	1	0	-6.851204	-0.490289	0.891431
48	1	0	6.851181	0.490287	0.891467

HF=-1474.216851\ZeroPoint=0.3548273\Thermal=0.3823989

D1-Ala^{2D}-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	2.396835	0.204846	-0.163885
2	7	0	0.458722	-0.457136	-0.462199
3	7	0	-0.458723	0.457136	-0.462200

4	6	0	0.042509	1.759845	-0.507436
5	6	0	1.439982	1.908065	-0.390456
6	6	0	1.989554	3.183552	-0.427627
7	1	0	3.061446	3.300756	-0.317031
8	6	0	1.157007	4.290664	-0.615077
9	6	0	-0.225215	4.132831	-0.772976
10	1	0	-0.853634	4.998065	-0.947545
11	6	0	-0.791946	2.867129	-0.719079
12	1	0	-1.850240	2.727784	-0.884378
13	6	0	-0.042509	-1.759845	-0.507435
14	6	0	0.791946	-2.867130	-0.719077
15	6	0	0.225215	-4.132832	-0.772974
16	1	0	0.853634	-4.998066	-0.947543
17	6	0	-1.157007	-4.290664	-0.615076
18	1	0	-1.589468	-5.284597	-0.652503
19	6	0	-1.989555	-3.183553	-0.427627
20	1	0	-3.061446	-3.300756	-0.317032
21	6	0	-1.439983	-1.908065	-0.390456
22	6	0	6.044271	-1.883284	1.149962
23	1	0	5.800885	-2.872102	1.549696
24	1	0	6.822039	-1.429891	1.764313
25	6	0	4.817164	-0.981218	1.130766
26	1	0	4.405570	-0.889412	2.141507
27	7	0	3.708434	-1.523836	0.284781
28	1	0	3.270780	-2.314327	0.750596
29	6	0	5.147504	0.471092	0.696988
30	8	0	6.253288	0.928349	0.910261
31	8	0	4.162759	1.138986	0.158365
32	1	0	1.589468	5.284597	-0.652504
33	1	0	4.102113	-1.881615	-0.584639
34	1	0	1.850239	-2.727784	-0.884376
35	46	0	-2.396835	-0.204846	-0.163886
36	6	0	-6.044269	1.883285	1.149966
37	1	0	-5.800881	2.872102	1.549700
38	1	0	-6.822036	1.429892	1.764317
39	6	0	-4.817162	0.981218	1.130767
40	1	0	-4.405568	0.889410	2.141507
41	7	0	-3.708433	1.523836	0.284781
42	6	0	-5.147504	-0.471091	0.696988
43	1	0	-3.270779	2.314327	0.750597
44	1	0	-4.102113	1.881615	-0.584639
45	8	0	-6.253288	-0.928349	0.910260
46	8	0	-4.162760	-1.138986	0.158363
47	1	0	-6.452308	2.000468	0.141227
48	1	0	6.452309	-2.000466	0.141223
6	6	0	-2.784088	-0.487126	0.630704
7	6	0	-3.608578	-1.524997	1.049983
8	1	0	-3.348530	-2.556477	0.836079
9	6	0	-4.787412	-1.255089	1.757514
10	6	0	-5.162847	0.056379	2.058431
11	1	0	-6.078092	0.247523	2.605653
12	6	0	-4.354386	1.114571	1.658504
13	1	0	-4.613110	2.142707	1.883008
14	6	0	-0.352837	2.490036	-0.425915
15	6	0	1.011083	2.124308	-0.487536
16	6	0	1.926127	3.135062	-0.807717
17	1	0	2.983215	2.897739	-0.870425
18	6	0	1.511917	4.437319	-1.085691
19	1	0	2.245351	5.189635	-1.355702
20	6	0	0.156471	4.770061	-1.033950
21	1	0	-0.170254	5.778052	-1.261154
22	6	0	-0.775420	3.800113	-0.697940
23	1	0	-1.831380	4.033707	-0.648380
24	6	0	3.623315	-0.516390	3.619906
25	1	0	4.204341	0.367130	3.900817
26	1	0	2.694817	-0.530435	4.198483
27	6	0	3.326879	-0.532988	2.127981
28	1	0	4.258101	-0.497020	1.554173
29	6	0	2.606693	-1.837496	1.658114
30	8	0	1.986531	-1.734233	0.523852
31	8	0	2.698402	-2.846875	2.335460
32	7	0	2.539133	0.676873	1.700864
33	1	0	1.806110	0.868341	2.382212
34	1	0	3.127583	1.506333	1.671874
35	6	0	-1.064069	-2.956859	-3.046012
36	1	0	-1.714993	-2.080710	-3.106927
37	1	0	-1.679526	-3.833567	-2.822310
38	6	0	0.010466	-2.761257	-1.976502
39	1	0	0.656925	-3.640742	-1.929555
40	7	0	-0.612878	-2.529273	-0.637478
41	6	0	0.914661	-1.568113	-2.343733
42	8	0	0.558727	-0.412230	-1.777078
43	8	0	1.818802	-1.694435	-3.129809
44	1	0	-5.416722	-2.078825	2.077519
45	1	0	-1.327356	-3.227072	-0.449659
46	1	0	0.125275	-2.616478	0.072869
47	1	0	4.182743	-1.412857	3.886851
48	1	0	-0.590065	-3.109759	-4.016374

HF=-1474.2066117\ZeroPoint=0.3544037\Thermal=0.3820808

HF=-1474.2054708\ZeroPoint=0.3540788\Thermal=0.3815395

B1-Ala^{2D}-1-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.134035	-0.492583	-0.447849
2	46	0	1.613655	0.258406	-0.096411
3	7	0	-1.328084	1.508545	-0.060528
4	7	0	-2.340605	1.893584	0.592460
5	6	0	-3.177910	0.842299	0.950579

B1-Ala^{2D}-1-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.615159	-0.635727	0.143517
2	46	0	-1.799369	0.073641	0.078883
3	7	0	1.416769	1.399607	0.011318
4	7	0	2.355035	2.039416	-0.549412
5	6	0	3.381174	1.221060	-1.005712
6	6	0	3.313817	-0.169916	-0.737318
7	6	0	4.368144	-0.970450	-1.158795

8	1	0	4.363067	-2.041162	-0.976566
9	6	0	5.456085	-0.407635	-1.841925
10	6	0	5.505526	0.962001	-2.104020
11	1	0	6.352474	1.383242	-2.632127
12	6	0	4.466677	1.786680	-1.681632
13	1	0	4.481775	2.855305	-1.860227
14	6	0	0.430569	2.163720	0.699260
15	6	0	-0.904444	1.720631	0.816902
16	6	0	-1.787397	2.581917	1.492744
17	1	0	-2.836476	2.318375	1.543235
18	6	0	-1.368419	3.775344	2.067947
19	1	0	-2.083962	4.397363	2.595160
20	6	0	-0.031989	4.176112	1.965503
21	1	0	0.305022	5.100291	2.420580
22	6	0	0.859533	3.380558	1.274379
23	1	0	1.897744	3.668227	1.174198
24	6	0	-5.280801	-1.584862	-1.953260
25	1	0	-5.103223	-2.615192	-2.275790
26	1	0	-5.859424	-1.603691	-1.024549
27	6	0	-3.966284	-0.841144	-1.747701
28	1	0	-3.386796	-0.849251	-2.677282
29	6	0	-4.179073	0.664710	-1.430010
30	8	0	-3.261934	1.239752	-0.700383
31	8	0	-5.141745	1.244819	-1.898333
32	7	0	-3.099100	-1.466721	-0.712927
33	1	0	-3.644649	-1.783278	0.086415
34	1	0	-2.631574	-2.298819	-1.058832
35	6	0	1.279698	-3.040932	2.782703
36	1	0	1.469520	-1.984812	2.987051
37	1	0	2.190559	-3.612205	2.985905
38	6	0	0.827089	-3.235554	1.335680
39	1	0	0.637534	-4.292989	1.140401
40	7	0	1.878022	-2.723032	0.394888
41	6	0	-0.494345	-2.476900	1.091891
42	8	0	-0.318171	-1.194721	0.878053
43	8	0	-1.561452	-3.057138	1.136348
44	1	0	6.267357	-1.047423	-2.172384
45	1	0	2.807412	-2.949973	0.740993
46	1	0	1.785679	-3.165338	-0.517141
47	1	0	-5.881207	-1.069928	-2.703282
48	1	0	0.500827	-3.391388	3.461473

HF=-1474.2024886\ZeroPoint=0.3539997\Thermal=0.381698

B1-Ala^{2D}-2-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.160794	-0.670456	-0.597479
2	46	0	1.425131	0.581933	-0.050104
3	7	0	-1.772778	1.195816	-0.111204
4	7	0	-2.859944	1.335234	0.523280
5	6	0	-3.484315	0.126480	0.793664
6	6	0	-2.813910	-1.071385	0.425449
7	6	0	-3.415918	-2.281338	0.754551
8	1	0	-2.929138	-3.216066	0.496659
9	6	0	-4.646682	-2.297834	1.421879
10	6	0	-5.297115	-1.109071	1.772062
11	1	0	-6.249457	-1.143715	2.287747
12	6	0	-4.715716	0.114351	1.463017
13	1	0	-5.190329	1.052068	1.727766
14	6	0	-0.999064	2.372261	-0.376581
15	6	0	0.411303	2.286904	-0.380646
16	6	0	1.104886	3.491152	-0.591637
17	1	0	2.190379	3.483080	-0.599151
18	6	0	0.445334	4.697569	-0.819926
19	1	0	1.018811	5.600520	-1.001962
20	6	0	-0.951062	4.743212	-0.827919
21	1	0	-1.469928	5.676435	-1.013921
22	6	0	-1.674008	3.583178	-0.597529
23	1	0	-2.756481	3.593850	-0.585178
24	6	0	3.646947	0.081465	3.628642
25	1	0	3.907207	1.060245	4.043156
26	1	0	2.772756	-0.305988	4.161149
27	6	0	3.367595	0.169451	2.134317
28	1	0	4.238782	0.581340	1.614420
29	6	0	3.134317	-1.227908	1.475286
30	8	0	2.412534	-1.218778	0.401644
31	8	0	3.677770	-2.205296	1.965669
32	7	0	2.230755	1.098152	1.823946
33	1	0	1.483120	0.961955	2.502540
34	1	0	2.518603	2.069813	1.908281
35	6	0	2.638681	-1.289877	-2.714195
36	1	0	3.221650	-1.224559	-1.797380
37	1	0	2.816324	-0.399833	-3.321744
38	6	0	1.146264	-1.371200	-2.383852
39	1	0	0.596449	-1.554695	-3.322901
40	7	0	0.563300	-0.175592	-1.754880
41	6	0	0.751532	-2.569909	-1.543818
42	8	0	-0.292711	-2.604257	-0.884398
43	8	0	1.536385	-3.625499	-1.632820
44	1	0	-5.103325	-3.249173	1.675004
45	1	0	0.436925	0.545476	-2.456455
46	1	0	4.467907	-0.613574	3.803874
47	1	0	2.959116	-2.168491	-3.278200
48	1	0	1.215550	-4.306289	-1.020199

HF=-1474.1928959\ZeroPoint=0.3537219\Thermal=0.3810965

B1-Ala^{2D}-2-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.261471	-0.617879	-0.522182
2	46	0	1.568664	0.344716	-0.136561
3	7	0	-1.563482	1.347109	-0.165218
4	7	0	-2.594432	1.698169	0.477038
5	6	0	-3.379378	0.623109	0.870022
6	6	0	-2.922625	-0.687134	0.566956
7	6	0	-3.692365	-1.761315	0.998252
8	1	0	-3.375264	-2.777551	0.786961
9	6	0	-4.878586	-1.538981	1.710316
10	6	0	-5.314994	-0.242533	1.999146

11	1	0	-6.234635	-0.090157	2.551429
12	6	0	-4.564009	0.850441	1.580852
13	1	0	-4.872931	1.867037	1.793974
14	6	0	-0.656523	2.364505	-0.593459
15	6	0	0.725836	2.092099	-0.636539
16	6	0	1.571584	3.159990	-0.970266
17	1	0	2.644472	3.009320	-0.949278
18	6	0	1.067662	4.413104	-1.306449
19	1	0	1.749800	5.211976	-1.577339
20	6	0	-0.311348	4.647598	-1.290482
21	1	0	-0.706098	5.621555	-1.555757
22	6	0	-1.173693	3.630801	-0.918696
23	1	0	-2.242739	3.793265	-0.869081
24	6	0	3.660265	-1.930829	2.978496
25	1	0	3.356264	-2.981566	2.927656
26	1	0	4.671861	-1.835453	2.571930
27	6	0	2.689184	-1.037573	2.218161
28	1	0	1.676457	-1.158566	2.616812
29	6	0	3.018595	0.478245	2.365692
30	8	0	2.577603	1.241291	1.415544
31	8	0	3.629041	0.855340	3.352484
32	7	0	2.600084	-1.382625	0.763221
33	1	0	3.544414	-1.441755	0.384999
34	1	0	2.190596	-2.307017	0.654366
35	6	0	2.300960	-1.965404	-2.702138
36	1	0	2.900783	-2.005238	-1.793672
37	1	0	2.656602	-1.124769	-3.299312
38	6	0	0.819774	-1.739708	-2.374295
39	1	0	0.261626	-1.799202	-3.324979
40	7	0	0.493299	-0.466620	-1.727687
41	6	0	0.182095	-2.860270	-1.578427
42	8	0	-0.786677	-2.700783	-0.836837
43	8	0	0.700131	-4.071506	-1.762155
44	1	0	-5.466852	-2.387019	2.045487
45	1	0	0.432001	0.249672	-2.442854
46	1	0	3.701132	-1.619934	4.022366
47	1	0	2.449086	-2.889351	-3.264433
48	1	0	0.168886	-4.713600	-1.263724

HF=-1474.1756308\ZeroPoint=0.3530994\Thermal=0.3807895

B1-Ala^{2D}-2-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.812931	-0.449448	-0.876549
2	46	0	1.647984	0.613453	0.310423
3	7	0	-1.481414	1.368612	-0.289259
4	7	0	-2.664858	1.477813	0.156266
5	6	0	-3.346392	0.267531	0.151649
6	6	0	-2.635813	-0.900642	-0.235954
7	6	0	-3.300157	-2.121573	-0.166913
8	1	0	-2.778364	-3.030056	-0.448209
9	6	0	-4.630206	-2.174007	0.264597
10	6	0	-5.319936	-1.012299	0.636026
11	1	0	-6.350448	-1.075861	0.965322
12	6	0	-4.679082	0.218825	0.586519
13	1	0	-5.183057	1.134071	0.875359
14	6	0	-0.644661	2.523822	-0.233375
15	6	0	0.735015	2.361587	0.003075
16	6	0	1.514817	3.524503	0.087629
17	1	0	2.580521	3.444278	0.273761
18	6	0	0.955698	4.790688	-0.081543
19	1	0	1.590151	5.669187	-0.032832
20	6	0	-0.412552	4.926544	-0.325624
21	1	0	-0.850075	5.908237	-0.465255
22	6	0	-1.213245	3.796505	-0.392446
23	1	0	-2.278623	3.874371	-0.568329
24	6	0	-0.104388	-1.149897	2.924367
25	1	0	-0.485366	-0.589271	3.781932
26	1	0	-0.616393	-0.816229	2.019453
27	6	0	1.407297	-0.956599	2.793484
28	1	0	1.898670	-1.293177	3.714470
29	6	0	1.996164	-1.781007	1.640225
30	8	0	2.745030	-1.248646	0.818639
31	8	0	1.643522	-3.031493	1.580910
32	7	0	1.740604	0.480266	2.515327
33	1	0	1.092860	1.089595	3.006040
34	1	0	2.678119	0.705197	2.837755
35	6	0	3.260564	-1.135758	-2.309443
36	1	0	3.740686	-1.065555	-1.334902
37	1	0	3.562332	-0.280496	-2.921055
38	6	0	1.743093	-1.164606	-2.169286
39	1	0	1.301316	-1.278141	-3.170538
40	7	0	1.134944	0.065860	-1.595916
41	6	0	1.202129	-2.384152	-1.378521
42	8	0	-0.053639	-2.348203	-1.088987
43	8	0	1.945709	-3.313243	-1.027276
44	1	0	-5.137893	-3.132031	0.314257
45	1	0	1.195766	0.829240	-2.261795
46	1	0	-0.329225	-2.205823	3.070667
47	1	0	3.607834	-2.052667	-2.790133
48	1	0	1.828780	-3.371066	0.637830

HF=-1474.1910832\ZeroPoint=0.3533511\Thermal=0.3802815

B1-Ala^{2D}-2-4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.099688	-0.576921	-0.788127
2	46	0	1.521657	0.622365	-0.079421
3	7	0	-1.705920	1.198005	-0.033469
4	7	0	-2.783241	1.247044	0.634144
5	6	0	-3.403773	0.007457	0.733673
6	6	0	-2.747904	-1.122526	0.173121
7	6	0	-3.352141	-2.367084	0.324216
8	1	0	-2.871436	-3.247417	-0.088993
9	6	0	-4.569607	-2.480485	1.005067
10	6	0	-5.205609	-1.356564	1.547814
11	1	0	-6.149001	-1.466550	2.069804
12	6	0	-4.622735	-0.102353	1.418337
13	1	0	-5.087055	0.785613	1.831949
14	6	0	-0.940202	2.399384	-0.150729

15	6	0	0.465953	2.322306	-0.223920	33	1	0	3.734003	-0.978010	0.250427
16	6	0	1.173638	3.528817	-0.308365	34	1	0	2.544246	-2.013024	-0.195381
17	1	0	2.257468	3.512161	-0.354056	35	6	0	2.617154	-0.916337	-3.043719
18	6	0	0.517910	4.758972	-0.343255	36	1	0	3.291432	-0.779899	-2.196389
19	1	0	1.093970	5.674302	-0.427964	37	1	0	2.718635	-0.044581	-3.696454
20	6	0	-0.876034	4.811074	-0.280750	38	6	0	1.170516	-1.062608	-2.585488
21	1	0	-1.391429	5.763998	-0.315719	39	1	0	0.535132	-1.168083	-3.476963
22	6	0	-1.603927	3.635382	-0.176040	40	7	0	0.634569	0.087009	-1.828747
23	1	0	-2.684613	3.650091	-0.114247	41	6	0	0.884533	-2.340038	-1.750707
24	6	0	3.513270	-2.494099	2.413311	42	8	0	-0.315897	-2.428008	-1.280816
25	1	0	3.508360	-3.414184	1.826634	43	8	0	1.778896	-3.165522	-1.543911
26	1	0	4.522824	-2.073352	2.394940	44	1	0	-5.030295	-3.457037	1.116071
27	6	0	2.502898	-1.514679	1.810275	45	1	0	0.520100	0.892715	-2.434936
28	1	0	1.497969	-1.952353	1.861029	46	1	0	3.260031	-2.734397	3.446294
29	6	0	2.392410	-0.199470	2.569197	47	1	0	2.934663	-1.807907	-3.587350
30	8	0	2.176688	0.879563	2.034818	48	1	0	2.366246	0.559578	4.287222
31	8	0	2.518343	-0.312258	3.887793	---					
32	7	0	2.748282	-1.192800	0.390357	HF=-1474.1850125\ZeroPoint=0.3537154\Thermal=0.3810576					

Structures from Table S3

Table S3. B3LYP-D3/6-311+G**/SDD(Pd)/gas phase free energies for the pre- (R) and postreaction (P) complexes and the transition states (TS) for **the D-transfer to the monopalladated complexes M1-1 and M1-2** using various D-sources. Free energies relative to **M1-1** (in kcal mol^{-1}).

D-source→	**Cys^{4D}**·DCl	**Cys^{4D}**·DCl	**Cys^{4D}** (neutral)		**Cys^{4D}** (zwitter)		DCl	AcOD
Donor group→	COOD	ND_3^+	COOD	COOD	ND_3^+	ND_3^+	DCl	AcOD
M1-1								
Prereaction complex (R)	**-12.0**	-4.3	**0.7**	-7.8	-2.7	-6.6**	-0.8	-5.3
Transition state (TS)	**9.8**	11.1	**17.5**	18.9*	25.0	24.1*	23.6	28.8
Postreaction complex (P, **1^D** coordinated *via* N(azo) to Pd)	**5.4**	5.6	**14.9**	18.6*	21.7	22.8*	13.5	22.6
M1-2								
Prereaction complex (R)	**2.7**	0.9	**5.7**	-	11.0	3.0**	2.8	1.7
Transition state (TS)	**9.8**	14.6	**18.3**	-	27.0	23.3*	17.7	20.8
Postreaction complex (P, **1^D** coordinated *via* N(azo) to Pd)	**2.0**	8.6	**13.7**	-	19.9	18.9*	-13.1	-1.8

* Species in which the intermolecular D-transfer from the coordinated **Cys^{3D}** to the non-coordinated outer **Cys^{4D}** occurred. ** Intermolecular D-transfer occurs spontaneously in the examined geometry.

G = -12.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.069261	-0.722411	-0.930167
2	16	0	0.257557	0.935631	-2.537773
3	6	0	-1.356315	1.826275	-2.334964
4	1	0	-1.586127	2.335311	-3.269144
5	1	0	-1.287484	2.572827	-1.538285
6	6	0	-2.461691	0.830613	-1.983387
7	1	0	-2.543536	0.106728	-2.802043
8	7	0	-2.085028	0.102331	-0.756398
9	1	0	-2.047966	0.772233	0.026872
10	6	0	-3.847565	1.456782	-1.833774
11	8	0	-4.100549	2.366972	-2.800112
12	8	0	-4.646128	1.145935	-0.988807
13	1	0	-2.805559	-0.573391	-0.512243
14	1	0	-5.003838	2.693036	-2.666403
15	6	0	1.735106	-1.556959	-1.126815
16	6	0	1.888671	-2.673501	-0.256378
17	6	0	2.813307	-1.247716	-1.953128
18	7	0	0.850322	-3.014036	0.606555
19	6	0	3.066200	-3.436036	-0.213260
20	1	0	2.751478	-0.410058	-2.638729
21	6	0	3.990953	-2.001598	-1.909426
22	7	0	-0.143204	-2.235404	0.514282
23	6	0	4.122569	-3.092358	-1.045444
24	1	0	3.127127	-4.277154	0.467653
25	1	0	4.819322	-1.728153	-2.554236
26	6	0	-1.247923	-2.518671	1.370334
27	1	0	5.042862	-3.663495	-1.023965
28	6	0	-1.883991	-1.448125	2.004128
29	6	0	-1.692523	-3.831170	1.556593
30	6	0	-2.973277	-1.698923	2.833356
31	1	0	-1.508893	-0.438186	1.884725
32	6	0	-2.790996	-4.065934	2.376729
33	1	0	-1.183149	-4.641695	1.051090
34	1	0	-3.457796	-0.869216	3.334209
35	6	0	-3.433717	-3.003144	3.014841
36	1	0	-3.149674	-5.079578	2.514365
37	1	0	-4.291260	-3.192178	3.650279
38	1	0	2.415686	-0.648238	1.320320
39	1	0	0.996164	3.568573	-0.192482
40	7	0	1.181520	2.591883	0.044764
41	6	0	2.437769	2.532749	0.850189
42	1	0	0.317355	2.290033	0.615138
43	6	0	2.170043	3.066643	2.267656
44	1	0	3.190105	3.136810	0.344378
45	6	0	2.980878	1.104979	0.890896
46	1	0	3.115235	3.118124	2.808790
47	1	0	1.495529	2.394581	2.797261
48	16	0	1.436988	4.754501	2.281752
49	8	0	2.088326	0.260804	1.425031
50	8	0	4.080474	0.803754	0.510148
51	1	0	0.151813	4.324127	2.229885
52	1	0	1.179147	2.029829	-0.842079
53	17	0	-1.339440	2.245373	1.576193

HF=-2604.78612\ZeroPoint= 0.379323\Thermal=0.4122324

G = 9.8 kcal mol^{-1}

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	46	0	0.714081	0.144120	0.632864
2	16	0	-0.237499	-0.994138	2.420977
3	6	0	-1.595335	0.197585	2.827065
4	1	0	-1.810433	0.122037	3.891721
5	1	0	-2.496544	-0.047877	2.260930
6	6	0	-1.148651	1.610280	2.469686
7	1	0	-0.285637	1.874517	3.090518
8	7	0	-0.722538	1.618310	1.051252
9	1	0	-1.536262	1.351546	0.462800
10	6	0	-2.192450	2.701024	2.699013
11	8	0	-2.871339	2.518085	3.849094
12	8	0	-2.355771	3.642543	1.966500
13	1	0	-0.447425	2.556111	0.764719
14	1	0	-3.490644	3.257795	3.948071
15	6	0	2.458502	-1.088890	0.323947
16	6	0	3.382049	-0.228462	-0.338411
17	6	0	2.976373	-2.075874	1.171039
18	7	0	2.923759	0.816422	-1.143447
19	6	0	4.761429	-0.392176	-0.201555
20	1	0	2.287988	-2.767306	1.639767
21	6	0	4.353718	-2.214038	1.340212
22	7	0	1.708182	1.101358	-0.951874
23	6	0	5.241289	-1.382918	0.650932
24	1	0	5.431983	0.268280	-0.737884
25	1	0	4.739622	-2.988937	1.992766
26	6	0	1.161172	2.153420	-1.738313
27	1	0	6.310260	-1.511264	0.776416
28	6	0	-0.200038	2.088122	-2.051829
29	6	0	1.948454	3.227820	-2.171704
30	6	0	-0.774726	3.103584	-2.809241
31	1	0	-0.800317	1.244015	-1.732927
32	6	0	1.358290	4.240648	-2.916647
33	1	0	2.998385	3.258116	-1.911679
34	1	0	-1.828298	3.046188	-3.054444
35	6	0	-0.001098	4.181731	-3.237007
36	1	0	1.956828	5.082846	-3.244051
37	1	0	-0.454603	4.978678	-3.814958
38	1	0	1.501025	-1.520642	-0.384062
39	1	0	-3.148456	-2.953867	0.350966
40	7	0	-2.233159	-2.540490	0.174757
41	6	0	-1.511456	-3.280650	-0.928559
42	1	0	-2.417680	-1.524449	-0.090176
43	6	0	-1.964393	-2.772935	-2.288321
44	1	0	-1.743445	-4.337857	-0.799177
45	6	0	-0.002910	-3.081812	-0.604048
46	1	0	-1.482935	-3.372308	-3.060796
47	1	0	-1.658511	-1.737756	-2.427360
48	16	0	-3.787710	-2.903255	-2.556622
49	8	0	0.592484	-2.179859	-1.282743
50	8	0	0.431362	-3.726633	0.350138
51	1	0	-4.076149	-1.674817	-2.067445
52	1	0	-1.665640	-2.527024	1.039032
53	17	0	-3.055084	0.278336	-0.587674

HF=-2604.7506011\ZeroPoint=0.3758715\Thermal=0.4080361

G = 5.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.836403	0.084554	-0.506387
2	16	0	-0.225861	-0.646042	-2.608168
3	6	0	0.870142	0.752616	-3.122194
4	1	0	0.783292	0.881914	-4.200055
5	1	0	1.906362	0.526288	-2.865941
6	6	0	0.428832	2.014388	-2.393918
7	1	0	-0.578881	2.284245	-2.727529
8	7	0	0.373759	1.709139	-0.942334
9	1	0	1.326744	1.412895	-0.634218
10	6	0	1.300332	3.248483	-2.614307
11	8	0	1.722238	3.349893	-3.888811
12	8	0	1.537219	4.063517	-1.759769
13	1	0	0.131541	2.542554	-0.408318
14	1	0	2.243013	4.164504	-3.965376
15	6	0	-2.549920	-1.353843	0.020520
16	6	0	-3.348232	-0.428943	0.740704
17	6	0	-3.144575	-2.178705	-0.936204
18	7	0	-2.757682	0.447595	1.667330
19	6	0	-4.725689	-0.371393	0.538123
20	1	0	-2.512823	-2.899725	-1.440829
21	6	0	-4.513878	-2.083387	-1.175196
22	7	0	-1.560458	0.722588	1.382833
23	6	0	-5.296664	-1.192622	-0.433439
24	1	0	-5.323776	0.325762	1.112010
25	1	0	-4.981124	-2.719215	-1.917960
26	6	0	-0.850072	1.571822	2.273352
27	1	0	-6.364541	-1.139423	-0.612568
28	6	0	0.546697	1.492223	2.254859
29	6	0	-1.507810	2.466184	3.128894
30	6	0	1.289729	2.310601	3.098549
31	1	0	1.049293	0.783510	1.607750
32	6	0	-0.753259	3.282937	3.959576
33	1	0	-2.588660	2.513334	3.123027
34	1	0	2.370631	2.243587	3.081318
35	6	0	0.643338	3.207735	3.947233
36	1	0	-1.252193	3.986274	4.616046
37	1	0	1.223790	3.852935	4.596534
38	1	0	-1.583365	-1.690935	0.466510
39	1	0	3.251820	-2.883126	-1.154176
40	7	0	2.368191	-2.497072	-0.823910
41	6	0	1.930963	-3.122357	0.477225
42	1	0	2.514252	-1.455987	-0.709546
43	6	0	2.646827	-2.504349	1.664849
44	1	0	2.158486	-4.187512	0.398877
45	6	0	0.372775	-2.967744	0.486966
46	1	0	2.345789	-3.042489	2.561871
47	1	0	2.358459	-1.463191	1.791087
48	16	0	4.489981	-2.593139	1.555094
49	8	0	-0.149902	-2.475446	1.507495
50	8	0	-0.166514	-3.312022	-0.589897
51	1	0	4.634438	-1.402926	0.929080
52	1	0	1.603946	-2.661290	-1.498401
53	17	0	3.116701	0.436486	-0.272900

HF=-2604.7537109\ZeroPoint=0.3749492\Thermal=0.4081827

G = 2.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.997505	-0.578017	0.759958
2	7	0	-2.552593	0.252378	-0.296513
3	7	0	-3.222164	-0.498690	-1.071044
4	6	0	-2.719127	-1.790195	-1.157422
5	6	0	-1.493196	-2.098919	-0.501860
6	6	0	-1.011375	-3.403020	-0.645792
7	1	0	-0.075513	-3.693755	-0.177807
8	6	0	-1.702736	-4.348948	-1.409137
9	6	0	-2.903845	-4.017973	-2.045815
10	1	0	-3.430472	-4.761344	-2.632619
11	6	0	-3.416949	-2.732965	-1.925173
12	1	0	-4.346574	-2.446327	-2.403186
13	6	0	-2.965092	1.615043	-0.225718
14	6	0	-4.320428	1.956658	-0.318390
15	6	0	-4.690949	3.293040	-0.256428
16	1	0	-5.740089	3.561128	-0.307477
17	6	0	-3.718598	4.288192	-0.119145
18	1	0	-4.014388	5.330012	-0.068471
19	6	0	-2.372584	3.939712	-0.036586
20	1	0	-1.612009	4.703628	0.072435
21	6	0	-1.985303	2.602565	-0.078590
22	1	0	-0.938583	2.335485	-0.007931
23	6	0	1.544658	-0.451893	2.283546
24	7	0	0.682273	-1.468994	1.627735
25	1	0	0.414271	-2.176123	2.311231
26	6	0	0.718550	0.334219	3.306120
27	1	0	-1.300258	-5.351303	-1.512817
28	1	0	1.217499	-1.942940	0.899831
29	1	0	-5.059272	1.172951	-0.422093
30	1	0	-0.060761	-1.071764	-1.486983
31	6	0	4.123233	0.200264	-1.677759
32	1	0	4.697800	-0.723589	-1.704161
33	1	0	3.873538	0.424576	-0.643816
34	6	0	2.835089	0.001406	-2.495674
35	1	0	3.060194	-0.513072	-3.434988
36	7	0	2.187972	1.306230	-2.822868
37	1	0	2.017067	1.847787	-1.824117
38	6	0	1.837373	-0.863664	-1.718333
39	8	0	0.591015	-0.639559	-2.108483
40	8	0	2.188172	-1.656122	-0.875422
41	1	0	1.290654	1.170453	-3.285873
42	1	0	2.813883	1.872592	-3.397618
43	17	0	1.961157	2.397965	-0.187862
44	16	0	-0.816886	0.989510	2.522124
45	1	0	0.462071	-0.311097	4.153472
46	1	0	1.310683	1.170189	3.678382
47	6	0	2.732816	-1.134516	2.939383
48	8	0	2.816740	-2.320837	3.150217
49	8	0	3.684194	-0.246813	3.289529
50	1	0	4.393082	-0.732239	3.738550
51	1	0	1.896654	0.241728	1.515760
52	16	0	5.203933	1.550414	-2.302510
53	1	0	4.624712	2.513729	-1.549185

HF=-2604.7605911\ZeroPoint=0.3776242\Thermal=0.4104873

G = 9.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.844881	-0.508711	0.677360
2	7	0	-2.490693	0.277465	-0.270672
3	7	0	-3.223229	-0.513047	-0.938376
4	6	0	-2.721711	-1.808298	-1.020710
5	6	0	-1.358533	-2.066168	-0.694577
6	6	0	-0.926092	-3.397492	-0.751582
7	1	0	0.117608	-3.618901	-0.552561
8	6	0	-1.794911	-4.420856	-1.128047
9	6	0	-3.121615	-4.136536	-1.472627
10	1	0	-3.785992	-4.937599	-1.775041
11	6	0	-3.588096	-2.828299	-1.431897
12	1	0	-4.613596	-2.584886	-1.683361
13	6	0	-2.903767	1.638872	-0.209163
14	6	0	-4.259425	1.985007	-0.297615
15	6	0	-4.622252	3.322900	-0.242556
16	1	0	-5.670018	3.596297	-0.291431
17	6	0	-3.643841	4.314601	-0.116044
18	1	0	-3.935101	5.357990	-0.072373
19	6	0	-2.299114	3.961517	-0.035740
20	1	0	-1.533804	4.721856	0.063609
21	6	0	-1.918495	2.622434	-0.069223
22	1	0	-0.871108	2.354277	-0.003593
23	6	0	1.648051	-0.341050	2.265812
24	7	0	0.868705	-1.349997	1.504360
25	1	0	0.637007	-2.132664	2.115094
26	6	0	0.741471	0.297752	3.320133
27	1	0	-1.435437	-5.443035	-1.175767
28	1	0	1.429932	-1.727594	0.732129
29	1	0	-5.002717	1.204932	-0.393745
30	1	0	-0.390231	-1.264597	-1.312246
31	6	0	3.938900	0.134162	-1.760142
32	1	0	4.524066	-0.782339	-1.796562
33	1	0	3.689015	0.343865	-0.723175
34	6	0	2.658423	-0.071452	-2.578179
35	1	0	2.894045	-0.529331	-3.543060
36	7	0	1.965715	1.227492	-2.849471
37	1	0	1.856603	1.761774	-1.882260
38	6	0	1.656277	-0.988132	-1.843133
39	8	0	0.428876	-0.755120	-2.152394
40	8	0	2.077211	-1.824646	-1.047570
41	1	0	1.031166	1.043001	-3.217376
42	1	0	2.514000	1.810950	-3.481600
43	17	0	1.884335	2.406295	-0.189546
44	16	0	-0.820171	0.891045	2.534151
45	1	0	0.510375	-0.426206	4.108324
46	1	0	1.246813	1.152231	3.770193
47	6	0	2.854810	-1.002477	2.910244

48	8	0	3.001939	-2.194508	3.032015
49	8	0	3.735396	-0.089979	3.363381
50	1	0	4.464049	-0.564661	3.791918
51	1	0	1.975950	0.432706	1.565881
52	16	0	5.004333	1.508433	-2.366768
53	1	0	4.400257	2.455706	-1.611448

HF=-2604.7489444\ZeroPoint=0.3749956\Thermal=0.4071548

G = 2.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.817079	-0.422522	0.548523
2	7	0	-2.572339	0.362073	-0.242582
3	7	0	-3.439587	-0.435489	-0.695020
4	6	0	-3.025782	-1.775374	-0.742216
5	6	0	-1.671321	-2.118264	-0.959496
6	6	0	-1.283796	-3.457688	-0.936700
7	1	0	-0.240652	-3.689594	-1.121798
8	6	0	-2.236598	-4.449129	-0.710075
9	6	0	-3.582378	-4.106208	-0.538603
10	1	0	-4.320349	-4.883999	-0.379821
11	6	0	-3.986807	-2.774869	-0.569791
12	1	0	-5.023516	-2.495899	-0.426605
13	6	0	-2.901598	1.748155	-0.240490
14	6	0	-4.236918	2.177812	-0.254963
15	6	0	-4.507644	3.537497	-0.258454
16	1	0	-5.536181	3.879132	-0.252209
17	6	0	-3.460128	4.466035	-0.262980
18	1	0	-3.681258	5.527397	-0.265688
19	6	0	-2.138024	4.029548	-0.254434
20	1	0	-1.318930	4.738358	-0.257101
21	6	0	-1.847756	2.668247	-0.231134
22	1	0	-0.814806	2.339903	-0.222801
23	6	0	1.733865	-0.256901	2.026525
24	7	0	0.925331	-1.257689	1.286671
25	1	0	0.722851	-2.050728	1.895082
26	6	0	0.870136	0.348738	3.132138
27	1	0	-1.940576	-5.491602	-0.691888
28	1	0	1.431646	-1.634610	0.463333
29	1	0	-5.034018	1.446719	-0.250479
30	1	0	-0.962813	-1.397029	-1.413521
31	6	0	3.895422	-0.163556	-1.331010
32	1	0	4.368823	-1.133629	-1.195882
33	1	0	3.414374	0.118328	-0.398467
34	6	0	2.861320	-0.280883	-2.447719
35	1	0	3.311290	-0.744798	-3.329520
36	7	0	2.332208	1.056846	-2.867401
37	1	0	2.121001	1.649332	-1.982475
38	6	0	1.612824	-1.125508	-2.042747
39	8	0	0.539276	-0.770766	-2.581046
40	8	0	1.805197	-2.050240	-1.220776
41	1	0	1.432056	0.870297	-3.328848
42	1	0	2.984199	1.568366	-3.459060
43	17	0	1.854003	2.462141	-0.303467
44	16	0	-0.732008	0.919960	2.408427
45	1	0	0.680374	-0.386948	3.919425
46	1	0	1.369224	1.215086	3.566402
47	6	0	2.979637	-0.914522	2.595323
48	8	0	3.138901	-2.105807	2.700342
49	8	0	3.878715	0.003213	2.996395
50	1	0	4.642451	-0.465025	3.367254
51	1	0	2.012536	0.540500	1.330962
52	16	0	5.222906	1.076001	-1.651300
53	1	0	4.532767	2.114515	-1.123499

HF=-2604.762957\ZeroPoint=0.3787629\Thermal=0.4115772

G = -4.3 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.477306	2.794905	0.553510
2	7	0	0.381953	2.172518	0.454513
3	6	0	-0.695119	2.637875	1.263442
4	6	0	-0.917507	4.007662	1.444741
5	6	0	-2.008070	4.420960	2.201194
6	1	0	-2.198239	5.480124	2.332066
7	6	0	-2.863890	3.479005	2.778257
8	6	0	-2.624985	2.116057	2.603688
9	1	0	-3.278560	1.371338	3.041601
10	6	0	-1.541371	1.689301	1.843488
11	1	0	-1.338305	0.631888	1.740576
12	6	0	2.472474	2.284196	-0.281892
13	6	0	3.730490	2.899169	-0.265967
14	6	0	4.737956	2.408711	-1.089129
15	1	0	5.715906	2.875215	-1.090117
16	6	0	4.477455	1.319064	-1.923855
17	1	0	5.258263	0.946112	-2.578749
18	6	0	3.216694	0.709060	-1.937911
19	1	0	3.037595	-0.121151	-2.614551
20	6	0	2.186369	1.165792	-1.112475
21	1	0	-3.718629	3.809551	3.357266
22	1	0	3.893480	3.751300	0.383623
23	46	0	0.258962	0.617305	-0.950996
24	16	0	0.370672	-1.150548	-2.443752
25	6	0	-1.369695	-1.764887	-2.244103
26	1	0	-1.624827	-2.341420	-3.132603
27	1	0	-1.449833	-2.417344	-1.373277
28	6	0	-2.302304	-0.572853	-2.091807
29	1	0	-2.205865	0.065211	-2.976007
30	7	0	-1.876911	0.228859	-0.913357
31	6	0	-3.796347	-0.886737	-1.967908
32	1	0	-2.161329	-0.299503	-0.068084
33	1	0	-2.429634	1.084044	-0.874602
34	8	0	-4.100948	-2.168722	-2.238756
35	8	0	-4.612425	-0.043101	-1.697688
36	1	0	-5.051208	-2.281732	-2.081816
37	1	0	1.968419	-0.725270	-0.015739
38	7	0	2.448670	-1.512376	0.483382
39	6	0	1.523544	-2.688135	0.546231
40	1	0	3.315389	-1.717024	-0.013981
41	6	0	2.168799	-3.895384	1.226747

42	1	0	1.250246	-2.920638	-0.485148
43	6	0	0.268249	-2.191262	1.277159
44	16	0	2.893885	-3.549677	2.885074
45	1	0	2.999737	-4.275944	0.628098
46	1	0	1.420143	-4.683718	1.298351
47	8	0	-0.736581	-2.992853	1.095878
48	8	0	0.310535	-1.159226	1.920455
49	1	0	1.736940	-3.222707	3.498371
50	1	0	-1.660330	-2.524775	1.344734
51	1	0	2.662137	-1.192060	1.433862
52	17	0	-3.171416	-1.582813	1.390990
53	1	0	-0.250817	4.722207	0.979114

HF=-2604.7738134\ZeroPoint=0.3785083\Thermal=0.411363

G = 11.1 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.453670	2.663404	0.592141
2	7	0	0.391397	1.976160	0.607214
3	6	0	-0.621964	2.388953	1.515583
4	6	0	-0.790013	3.743238	1.840414
5	6	0	-1.824805	4.110899	2.689249
6	1	0	-1.973353	5.156992	2.931011
7	6	0	-2.682657	3.140724	3.217732
8	6	0	-2.501444	1.795970	2.898340
9	1	0	-3.157679	1.031792	3.296551
10	6	0	-1.473322	1.413273	2.044033
11	1	0	-1.313811	0.364681	1.835286
12	6	0	2.377134	2.249361	-0.371200
13	6	0	3.422049	3.123542	-0.683455
14	6	0	4.301538	2.796246	-1.710455
15	1	0	5.105892	3.475495	-1.967487
16	6	0	4.142922	1.601502	-2.419658
17	1	0	4.823351	1.359772	-3.228291
18	6	0	3.120899	0.715853	-2.084641
19	1	0	3.021851	-0.223022	-2.619462
20	6	0	2.226522	1.001798	-1.043263
21	1	0	-3.494953	3.437886	3.871158
22	1	0	3.508199	4.057527	-0.141304
23	46	0	0.185189	0.472556	-0.863672
24	16	0	0.161124	-1.129137	-2.518695
25	6	0	-1.602433	-1.656063	-2.331516
26	1	0	-1.907295	-2.150270	-3.253217
27	1	0	-1.701519	-2.356221	-1.501402
28	6	0	-2.438098	-0.413314	-2.076148
29	1	0	-2.318486	0.275838	-2.918542
30	7	0	-1.911098	0.261413	-0.857515
31	6	0	-3.946383	-0.611769	-1.909111
32	1	0	-2.189790	-0.340065	-0.047686
33	1	0	-2.399309	1.145160	-0.717791
34	8	0	-4.381055	-1.791154	-2.383173
35	8	0	-4.664147	0.242849	-1.455531
36	1	0	-5.333013	-1.845710	-2.206574
37	1	0	2.114729	-0.070680	-0.273920
38	7	0	2.660361	-1.184816	0.586954
39	6	0	1.843824	-2.404971	0.500909
40	1	0	3.624875	-1.360209	0.317350
41	6	0	2.504188	-3.662817	1.093156
42	1	0	1.621966	-2.594688	-0.553294
43	6	0	0.511601	-2.110659	1.191237
44	16	0	3.088347	-3.497059	2.831290
45	1	0	3.401936	-3.912288	0.522424
46	1	0	1.811075	-4.500165	1.009338
47	8	0	-0.423019	-2.960087	0.838960
48	8	0	0.399200	-1.187988	1.975558
49	1	0	1.879200	-3.269266	3.385159
50	1	0	-1.352583	-2.627629	1.125660
51	1	0	2.652074	-0.841680	1.547439
52	17	0	-3.048965	-1.775655	1.201761
53	1	0	-0.126687	4.481763	1.409770

HF=-2604.7474071\ZeroPoint=0.3747354\Thermal=0.4070148

G = 5.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.370383	3.032190	0.993107
2	7	0	-0.330348	1.985892	0.923083
3	6	0	-1.386676	1.847394	1.862067
4	6	0	-2.054699	2.966475	2.380919
5	6	0	-3.112177	2.769597	3.257258
6	1	0	-3.648937	3.625034	3.650673
7	6	0	-3.497315	1.473629	3.619372
8	6	0	-2.819718	0.368824	3.106613
9	1	0	-3.111038	-0.640632	3.369174
10	6	0	-1.760953	0.549316	2.223611
11	1	0	-1.211455	-0.306720	1.854387
12	6	0	1.376886	3.099516	0.014074
13	6	0	1.814270	4.365073	-0.379716
14	6	0	2.738639	4.479007	-1.414744
15	1	0	3.063477	5.462564	-1.733798
16	6	0	3.247169	3.340604	-2.046779
17	1	0	3.965995	3.443891	-2.850812
18	6	0	2.850746	2.075193	-1.623671
19	1	0	3.269038	1.179293	-2.065148
20	6	0	1.921193	1.939416	-0.591171
21	1	0	-4.332987	1.330293	4.294809
22	1	0	1.400370	5.239850	0.106404
23	46	0	0.002680	0.687728	-0.723093
24	16	0	0.516258	-0.607197	-2.549166
25	6	0	-1.016116	-1.640955	-2.585100
26	1	0	-1.131066	-2.042520	-3.591314
27	1	0	-0.934548	-2.465549	-1.876356
28	6	0	-2.184273	-0.743872	-2.217998
29	1	0	-2.261359	0.064866	-2.951807
30	7	0	-1.894022	-0.132025	-0.889746
31	6	0	-3.569598	-1.390079	-2.152217
32	1	0	-1.959916	-0.911379	-0.184058
33	1	0	-2.628599	0.531681	-0.645872
34	8	0	-3.645551	-2.542174	-2.837076
35	8	0	-4.500272	-0.868620	-1.592407

36	1	0	-4.541609	-2.895261	-2.723022
37	1	0	1.907820	0.947417	-0.075853
38	7	0	3.447114	-0.782166	0.356070
39	6	0	2.784784	-2.066066	0.150477
40	1	0	4.400853	-0.824390	0.009834
41	6	0	3.535892	-3.309638	0.678711
42	1	0	2.639878	-2.209975	-0.926076
43	6	0	1.381679	-2.007747	0.749043
44	16	0	3.906735	-3.279792	2.483023
45	1	0	4.514547	-3.371742	0.197161
46	1	0	2.979150	-4.214699	0.436246
47	8	0	0.661862	-3.058527	0.404662
48	8	0	1.003786	-1.094495	1.458813
49	1	0	2.631467	-3.400463	2.906647
50	1	0	-0.307891	-2.956048	0.681829
51	1	0	3.499547	-0.586769	1.352963
52	17	0	-2.244149	-2.665471	0.804366
53	1	0	-1.752232	3.959802	2.076284

HF=-2604.7548239\ZeroPoint=0.3770313\Thermal=0.4104443

G = 0.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.466104	1.406796	-0.610100
2	7	0	-2.027793	0.217884	-0.517442
3	6	0	-2.965793	-0.750623	-0.050327
4	6	0	-4.333288	-0.614515	-0.322011
5	6	0	-5.223540	-1.559185	0.171193
6	1	0	-6.280074	-1.466723	-0.052579
7	6	0	-4.762069	-2.629394	0.941720
8	6	0	-3.400822	-2.756940	1.209300
9	1	0	-3.035908	-3.585143	1.804533
10	6	0	-2.497494	-1.826164	0.707573
11	1	0	-1.438867	-1.926431	0.904904
12	6	0	-1.512565	2.327310	-1.014764
13	6	0	-1.902927	3.664496	-1.183138
14	6	0	-0.945379	4.605087	-1.537616
15	1	0	-1.224807	5.643118	-1.673364
16	6	0	0.385037	4.206661	-1.712929
17	1	0	1.136104	4.946267	-1.969955
18	6	0	0.767728	2.870371	-1.548754
19	1	0	1.816424	2.610567	-1.648381
20	6	0	-0.169009	1.897499	-1.192388
21	1	0	-5.461622	-3.364299	1.322809
22	1	0	-2.942018	3.938457	-1.040470
23	46	0	-0.082436	-0.134524	-1.120356
24	16	0	-0.229857	-2.453421	-1.592480
25	6	0	1.277526	-2.501237	-2.659334
26	1	0	1.044201	-2.103694	-3.650682
27	1	0	1.606418	-3.534934	-2.772478
28	6	0	2.400227	-1.678584	-2.032954
29	1	0	3.255101	-1.625427	-2.717847
30	7	0	1.913848	-0.290405	-1.753572
31	6	0	2.935943	-2.398034	-0.799810
32	1	0	2.533837	0.198676	-1.084256
33	1	0	1.966821	0.243629	-2.618798
34	8	0	2.750546	-1.720172	0.341138
35	8	0	3.487793	-3.465152	-0.872883
36	1	0	3.175617	-2.196989	1.073206
37	1	0	0.546020	1.377421	0.730283
38	7	0	0.999490	1.742262	1.595531
39	6	0	0.582301	0.954554	2.791475
40	1	0	0.721898	2.720959	1.661162
41	6	0	1.201487	-0.443857	2.774607
42	1	0	0.922300	1.495030	3.679408
43	6	0	-0.948976	0.884462	2.872480
44	16	0	2.956208	-0.497395	3.310267
45	1	0	0.654552	-1.061674	3.485149
46	1	0	1.093764	-0.888633	1.783564
47	8	0	-1.520020	1.935695	2.249171
48	8	0	-1.554829	0.021389	3.443082
49	1	0	3.474425	0.157231	2.234061
50	1	0	2.051215	1.703969	1.339056
51	1	0	-4.674717	0.215667	-0.925774
52	1	0	-2.484452	1.828956	2.263177
53	17	0	3.655288	1.579640	0.303184

HF=-2604.7671278\ZeroPoint=0.3791684\Thermal=0.4116516

G = 14.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.383259	1.380537	-0.605904
2	7	0	-1.916831	0.205072	-0.505734
3	6	0	-2.850183	-0.816164	-0.165968
4	6	0	-4.214723	-0.673651	-0.453373
5	6	0	-5.094803	-1.682005	-0.088080
6	1	0	-6.148356	-1.583844	-0.322621
7	6	0	-4.627219	-2.823638	0.569320
8	6	0	-3.270214	-2.957716	0.852306
9	1	0	-2.902630	-3.838904	1.363687
10	6	0	-2.375717	-1.961455	0.478159
11	1	0	-1.321901	-2.058969	0.698323
12	6	0	-1.434755	2.348776	-0.909915
13	6	0	-1.887932	3.584788	-1.384975
14	6	0	-0.958267	4.544356	-1.767465
15	1	0	-1.295790	5.499673	-2.151932
16	6	0	0.411862	4.279086	-1.656263
17	1	0	1.130790	5.037550	-1.945891
18	6	0	0.863314	3.061683	-1.147447
19	1	0	1.924773	2.891991	-0.990444
20	6	0	-0.046198	2.069806	-0.749944
21	1	0	-5.320548	-3.607183	0.852222
22	1	0	-2.953148	3.759306	-1.479822
23	46	0	0.075985	-0.061371	-0.992615
24	16	0	-0.127664	-2.172000	-1.945126
25	6	0	1.500955	-2.200235	-2.818051
26	1	0	1.418520	-1.680645	-3.775965
27	1	0	1.775212	-3.239013	-3.006528
28	6	0	2.558775	-1.527094	-1.952665
29	1	0	3.498791	-1.428808	-2.509099

30	7	0	2.076161	-0.169929	-1.564483
31	6	0	2.902275	-2.411568	-0.755981
32	1	0	2.676412	0.266389	-0.824435
33	1	0	2.163630	0.441409	-2.374803
34	8	0	2.625145	-1.834946	0.417100
35	8	0	3.390054	-3.504099	-0.889247
36	1	0	2.938941	-2.388412	1.151284
37	1	0	0.333607	1.585627	0.434160
38	7	0	0.803461	1.755104	1.805749
39	6	0	0.274437	0.857516	2.844885
40	1	0	0.593597	2.727327	2.012996
41	6	0	0.876068	-0.545198	2.739318
42	1	0	0.500199	1.255082	3.844010
43	6	0	-1.253575	0.802979	2.772697
44	16	0	2.587829	-0.679570	3.392718
45	1	0	0.274984	-1.228642	3.337076
46	1	0	0.854049	-0.886575	1.703789
47	8	0	-1.772330	1.976462	2.342050
48	8	0	-1.929982	-0.138287	3.093287
49	1	0	3.199702	0.023587	2.398143
50	1	0	1.826019	1.670410	1.665514
51	1	0	-4.560864	0.212090	-0.968426
52	1	0	-2.736827	1.882816	2.306425
53	17	0	3.674616	1.485046	0.531112

HF=-2604.7431944\ZeroPoint=0.3752452\Thermal=0.4072524

G = 8.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.151534	1.866070	-0.046122
2	7	0	-1.683138	0.793720	-0.514109
3	6	0	-2.641153	-0.200908	-0.877120
4	6	0	-3.988000	0.129006	-1.090107
5	6	0	-4.890540	-0.875895	-1.404697
6	1	0	-5.929601	-0.624652	-1.583308
7	6	0	-4.465969	-2.205960	-1.497464
8	6	0	-3.129031	-2.525695	-1.283916
9	1	0	-2.795642	-3.554273	-1.337710
10	6	0	-2.210629	-1.524751	-0.984662
11	1	0	-1.172885	-1.771565	-0.810040
12	6	0	-1.206613	2.807155	0.374168
13	6	0	-1.566479	4.157397	0.322980
14	6	0	-0.629594	5.123789	0.675000
15	1	0	-0.895368	6.172825	0.615670
16	6	0	0.646483	4.751099	1.109228
17	1	0	1.361679	5.513631	1.395285
18	6	0	0.994516	3.403689	1.209099
19	1	0	1.957290	3.082522	1.592217
20	6	0	0.070612	2.425213	0.845983
21	1	0	-5.179200	-2.986196	-1.736065
22	1	0	-2.557036	4.428503	-0.021066
23	46	0	0.380765	0.653094	-0.800451
24	16	0	0.311585	-0.367239	-2.856474
25	6	0	2.079873	-0.122408	-3.342202
26	1	0	2.209328	0.863373	-3.794475
27	1	0	2.334831	-0.887421	-4.077111
28	6	0	2.958538	-0.254029	-2.106803
29	1	0	3.993869	0.020311	-2.344052
30	7	0	2.435261	0.663837	-1.056130
31	6	0	3.030377	-1.711414	-1.647696
32	1	0	2.835464	0.501150	-0.094848
33	1	0	2.688463	1.620208	-1.300601
34	8	0	2.622696	-1.863349	-0.388282
35	8	0	3.442895	-2.587296	-2.363320
36	1	0	2.769394	-2.768464	-0.062800
37	1	0	0.238048	1.385371	1.195029
38	7	0	-0.059966	-0.159106	2.698755
39	6	0	-0.496680	-1.548267	2.767222
40	1	0	-0.535683	0.409235	3.391137
41	6	0	0.376841	-2.439731	1.873374
42	1	0	-0.460642	-1.968841	3.785898
43	6	0	-1.961602	-1.704893	2.356252
44	16	0	2.034337	-2.826491	2.568050
45	1	0	-0.115569	-3.401373	1.736192
46	1	0	0.505413	-1.963539	0.899836
47	8	0	-2.651029	-0.540737	2.380973
48	8	0	-2.480059	-2.757122	2.074056
49	1	0	2.590707	-1.596447	2.372439
50	1	0	0.944483	-0.072881	2.855595
51	1	0	-4.302956	1.160487	-1.013430
52	1	0	-3.563544	-0.745757	2.125157
53	17	0	3.114301	0.704538	1.920621

HF=-2604.7524933\ZeroPoint=0.3780734\Thermal=0.411019

G = 0.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.325758	0.276084	-0.837691
2	7	0	2.284223	0.281440	-0.166661
3	7	0	2.822030	1.401229	0.083047
4	6	0	1.957150	2.480285	-0.044539
5	6	0	0.601738	2.239801	-0.398656
6	6	0	-0.230911	3.356275	-0.493327
7	1	0	-1.279619	3.241411	-0.750291
8	6	0	0.256867	4.644645	-0.242852
9	6	0	1.595026	4.852515	0.103427
10	1	0	1.958570	5.855352	0.293263
11	6	0	2.455009	3.766007	0.205583
12	1	0	3.498591	3.890420	0.470417
13	6	0	3.143054	-0.852119	-0.035022
14	6	0	4.480375	-0.779960	-0.439840
15	6	0	5.297626	-1.894135	-0.295380
16	1	0	6.329622	-1.847219	-0.623561
17	6	0	4.792540	-3.070933	0.261768
18	1	0	5.433730	-3.938141	0.370036
19	6	0	3.461171	-3.131873	0.669536
20	1	0	3.062327	-4.041710	1.101988
21	6	0	2.628916	-2.027720	0.515100
22	1	0	1.593722	-2.070648	0.824416
23	16	0	0.095603	-1.982618	-1.544298

24	6	0	-1.558940	-1.802338	-2.339675
25	1	0	-2.066554	-2.767293	-2.331720
26	1	0	-1.434191	-1.490294	-3.381440
27	6	0	-2.407780	-0.772253	-1.589533
28	1	0	-2.624154	-1.142054	-0.585950
29	7	0	-1.659567	0.502718	-1.448881
30	1	0	-1.704749	1.017698	-2.327953
31	6	0	-3.719298	-0.516592	-2.315796
32	8	0	-3.967386	0.473761	-2.960425
33	8	0	-4.566765	-1.555054	-2.186981
34	1	0	-0.415241	5.493338	-0.315742
35	1	0	-5.365900	-1.354214	-2.697922
36	1	0	-2.120643	1.067887	-0.732837
37	1	0	4.854912	0.138605	-0.872140
38	1	0	-0.323922	1.440602	1.428861
39	1	0	-3.482875	-0.383221	3.079712
40	6	0	-2.435235	-0.158640	3.284278
41	6	0	-1.642849	-1.470491	3.385059
42	7	0	-2.348758	0.546780	4.566345
43	6	0	-1.939865	0.681901	2.111069
44	1	0	-0.593195	-1.261361	3.596155
45	1	0	-2.047872	-2.044759	4.218784
46	16	0	-1.759164	-2.567520	1.912694
47	1	0	-1.404055	0.880964	4.731174
48	1	0	-2.970718	1.348157	4.588155
49	8	0	-0.645592	0.997300	2.243015
50	8	0	-2.629641	1.034755	1.175571
51	1	0	-0.883667	-1.928699	1.102443

HF=-2143.9082694\ZeroPoint=0.3689063\Thermal=0.4000296

G = 17.5 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.224945	0.191040	-0.714280
2	7	0	2.209019	0.351238	-0.149863
3	7	0	2.683820	1.517663	-0.037440
4	6	0	1.745590	2.540157	-0.177102
5	6	0	0.354877	2.272265	-0.052564
6	6	0	-0.534656	3.329631	-0.273881
7	1	0	-1.595374	3.150511	-0.129428
8	6	0	-0.065148	4.603067	-0.592805
9	6	0	1.309245	4.851563	-0.676307
10	1	0	1.665779	5.848231	-0.908748
11	6	0	2.221647	3.825343	-0.456502
12	1	0	3.289684	3.992931	-0.526990
13	6	0	3.133883	-0.721244	0.018727
14	6	0	4.478843	-0.572964	-0.342847
15	6	0	5.352256	-1.635985	-0.159826
16	1	0	6.390400	-1.532524	-0.453360
17	6	0	4.896952	-2.835980	0.393346
18	1	0	5.584441	-3.662057	0.534022
19	6	0	3.558819	-2.972973	0.756002
20	1	0	3.199802	-3.899409	1.187660
21	6	0	2.668179	-1.922034	0.560160
22	1	0	1.629386	-2.025339	0.841184
23	16	0	0.301789	-1.865217	-1.780271
24	6	0	-1.407350	-1.863697	-2.480344
25	1	0	-1.734303	-2.898538	-2.588116
26	1	0	-1.399852	-1.396706	-3.469548
27	6	0	-2.350889	-1.099934	-1.549330
28	1	0	-2.456961	-1.637373	-0.605257
29	7	0	-1.775735	0.233055	-1.252642
30	1	0	-1.915400	0.846338	-2.055704
31	6	0	-3.719526	-0.937682	-2.194494
32	8	0	-4.106468	0.068872	-2.734840
33	8	0	-4.432535	-2.078094	-2.131974
34	1	0	-0.767902	5.413476	-0.751556
35	1	0	-5.276242	-1.930076	-2.586435
36	1	0	-2.254697	0.662266	-0.435580
37	1	0	4.814642	0.362044	-0.770739
38	1	0	-0.077335	1.528135	0.895418
39	1	0	-3.359918	-0.330139	3.077040
40	6	0	-2.329140	-0.044859	3.295026
41	6	0	-1.472818	-1.301112	3.488535
42	7	0	-2.312427	0.714729	4.553844
43	6	0	-1.815271	0.779235	2.101338
44	1	0	-0.463033	-1.016906	3.786306
45	1	0	-1.907296	-1.916069	4.277558
46	16	0	-1.353531	-2.392576	2.007047
47	1	0	-1.398076	1.142000	4.677930
48	1	0	-2.992793	1.467502	4.519302
49	8	0	-0.563743	1.046228	2.134674
50	8	0	-2.606205	1.119661	1.197375
51	1	0	-0.608649	-1.558353	1.251514

HF=-2143.8808618\ZeroPoint=0.3653626\Thermal=0.3955837

G = 14.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.340571	0.384158	-0.549785
2	7	0	2.315396	0.242208	0.080349
3	7	0	2.886125	1.309400	0.435095
4	6	0	2.039974	2.427064	0.513604
5	6	0	0.658399	2.292665	0.786106
6	6	0	-0.154788	3.426175	0.788875
7	1	0	-1.207234	3.297304	1.020336
8	6	0	0.399500	4.680168	0.536655
9	6	0	1.773552	4.808559	0.307393
10	1	0	2.200579	5.788415	0.127950
11	6	0	2.601941	3.689705	0.308724
12	1	0	3.665418	3.774265	0.121511
13	6	0	3.129647	-0.927341	0.035231
14	6	0	4.503017	-0.843502	-0.226415
15	6	0	5.257856	-2.007455	-0.257293
16	1	0	6.317863	-1.952785	-0.475935
17	6	0	4.655798	-3.245495	-0.014015
18	1	0	5.252200	-4.150204	-0.038533
19	6	0	3.290198	-3.318667	0.252140
20	1	0	2.818924	-4.274647	0.445123
21	6	0	2.517554	-2.161876	0.266137

22	1	0	1.458039	-2.210902	0.476313
23	16	0	0.351130	-1.268963	-2.141432
24	6	0	-1.308791	-0.949725	-2.889439
25	1	0	-1.682324	-1.891918	-3.292660
26	1	0	-1.209447	-0.231465	-3.707876
27	6	0	-2.253030	-0.403371	-1.818631
28	1	0	-2.460602	-1.174678	-1.074331
29	7	0	-1.602507	0.734591	-1.129159
30	1	0	-1.651133	1.561333	-1.725241
31	6	0	-3.558886	0.058373	-2.448703
32	8	0	-3.821330	1.205202	-2.714058
33	8	0	-4.368741	-0.981092	-2.723661
34	1	0	-0.229863	5.562566	0.541951
35	1	0	-5.167457	-0.634675	-3.150706
36	1	0	-2.098109	0.951865	-0.221242
37	1	0	4.952282	0.122537	-0.413409
38	1	0	0.234308	1.382473	1.291788
39	1	0	-3.815156	-0.947871	2.288906
40	6	0	-2.851970	-0.885537	2.799657
41	6	0	-2.167168	-2.253025	2.780946
42	7	0	-3.105793	-0.526106	4.206957
43	6	0	-1.997238	0.181634	2.081582
44	1	0	-1.242285	-2.212427	3.356841
45	1	0	-2.825649	-3.000661	3.225260
46	16	0	-1.758200	-2.876452	1.092911
47	1	0	-2.222625	-0.293263	4.655073
48	1	0	-3.685794	0.306628	4.248637
49	8	0	-0.759703	0.162057	2.307895
50	8	0	-2.600731	1.001566	1.326226
51	1	0	-0.816948	-1.949146	0.827421

HF=-2143.8840857\ZeroPoint=0.3675981\Thermal=0.3986411

G = 5.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.881283	-0.202947	-0.888704
2	7	0	2.091125	1.028399	0.241837
3	7	0	1.978318	2.281526	0.086208
4	6	0	0.967780	2.647467	-0.790641
5	6	0	0.142316	1.636782	-1.357506
6	6	0	-0.850427	2.066156	-2.242638
7	1	0	-1.529820	1.349736	-2.690899
8	6	0	-1.026340	3.424147	-2.531385
9	6	0	-0.207407	4.396820	-1.949801
10	1	0	-0.356015	5.444728	-2.182029
11	6	0	0.797228	4.010208	-1.072392
12	1	0	1.456722	4.734719	-0.608773
13	6	0	3.110846	0.613499	1.151243
14	6	0	4.318795	1.316015	1.233343
15	6	0	5.290806	0.898949	2.133448
16	1	0	6.233922	1.430611	2.187397
17	6	0	5.060259	-0.204137	2.958887
18	1	0	5.823301	-0.527216	3.657758
19	6	0	3.852844	-0.894455	2.874769
20	1	0	3.669469	-1.753200	3.509605
21	6	0	2.876614	-0.495998	1.966305
22	1	0	1.941281	-1.033133	1.886293
23	16	0	2.039556	-2.271105	-0.630093
24	6	0	1.018907	-3.262558	-1.806297
25	1	0	1.424539	-3.178166	-2.819595
26	1	0	1.051693	-4.313523	-1.515617
27	6	0	-0.432557	-2.789077	-1.810835
28	1	0	-0.991984	-3.307417	-2.599597
29	7	0	-0.459110	-1.314980	-2.071445
30	1	0	-1.401841	-0.939221	-1.948285
31	6	0	-1.144887	-3.166263	-0.508719
32	8	0	-1.416649	-2.110357	0.252836
33	8	0	-1.436006	-4.308127	-0.251435
34	1	0	-1.815934	3.726438	-3.211736
35	1	0	-0.193482	-1.152013	-3.040916
36	1	0	4.482531	2.166518	0.584910
37	1	0	-1.335934	0.939033	0.081285
38	16	0	-4.401255	1.601534	2.860748
39	6	0	-5.038943	0.524457	1.513662
40	1	0	-5.901571	0.024797	1.960653
41	1	0	-5.408045	1.137421	0.688663
42	6	0	-4.070333	-0.557833	0.974784
43	1	0	-4.659359	-1.221971	0.338281
44	7	0	-3.403703	-1.385171	1.991649
45	6	0	-3.026865	0.048842	0.036074
46	8	0	-2.070032	0.700677	0.694316
47	8	0	-3.085252	-0.054516	-1.171057
48	1	0	-4.093633	-1.931792	2.499023
49	1	0	-3.395374	2.160945	2.159606
50	1	0	-2.943784	-0.782530	2.671644
51	1	0	-2.023224	-2.294046	1.013364

HF=-2143.9025326\ZeroPoint=0.3692364\Thermal=0.3995489

G = 18.3 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.735128	-0.086902	-0.961054
2	7	0	1.976722	0.864948	0.377416
3	7	0	1.973748	2.131009	0.389942
4	6	0	1.030117	2.704891	-0.456152
5	6	0	-0.052877	1.929599	-0.961154
6	6	0	-0.924757	2.558829	-1.859835
7	1	0	-1.789036	2.007809	-2.214837
8	6	0	-0.743595	3.891629	-2.226306
9	6	0	0.308136	4.641157	-1.687609
10	1	0	0.431573	5.681232	-1.966052
11	6	0	1.192226	4.054575	-0.790612
12	1	0	2.021345	4.609295	-0.367768
13	6	0	2.882539	0.227820	1.274238
14	6	0	4.088968	0.841255	1.636138
15	6	0	4.941317	0.194678	2.520017
16	1	0	5.883651	0.656824	2.790441
17	6	0	4.591704	-1.048682	3.054829
18	1	0	5.261877	-1.548338	3.744930
19	6	0	3.387920	-1.649161	2.693625

20	1	0	3.114235	-2.613792	3.104050
21	6	0	2.531458	-1.021967	1.793106
22	1	0	1.599041	-1.483597	1.497823
23	16	0	1.977295	-2.027652	-1.318034
24	6	0	0.737078	-2.998894	-2.296703
25	1	0	1.020935	-2.972791	-3.352734
26	1	0	0.775327	-4.039481	-1.968612
27	6	0	-0.685157	-2.451113	-2.160448
28	1	0	-1.311216	-2.849775	-2.964403
29	7	0	-0.626075	-0.959602	-2.277560
30	1	0	-1.547674	-0.538664	-2.081264
31	6	0	-1.415768	-2.859925	-0.869456
32	8	0	-0.965506	-2.243467	0.212446
33	8	0	-2.325720	-3.657821	-0.890489
34	1	0	-1.438799	4.359976	-2.914520
35	1	0	-0.352838	-0.709665	-3.225822
36	1	0	4.343623	1.803755	1.213232
37	1	0	-0.783686	1.173400	-0.123323
38	16	0	-3.973366	1.322745	3.133257
39	6	0	-4.635980	0.255259	1.785336
40	1	0	-5.400180	-0.353930	2.274618
41	1	0	-5.135352	0.872543	1.035855
42	6	0	-3.614720	-0.669182	1.089674
43	1	0	-4.176084	-1.342997	0.438483
44	7	0	-2.799325	-1.500911	1.994915
45	6	0	-2.683169	0.133258	0.161596
46	8	0	-1.724826	0.750518	0.748644
47	8	0	-2.902811	0.121382	-1.059899
48	1	0	-3.398415	-2.109950	2.545838
49	1	0	-2.980287	1.877941	2.408120
50	1	0	-2.305474	-0.892849	2.646157
51	1	0	-1.648537	-2.228112	0.964392

HF=-2143.8804983\ZeroPoint=0.3653791\Thermal=0.3948417

G = 13.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.764751	0.131514	-0.833800
2	7	0	2.171810	0.464808	0.648588
3	7	0	2.470023	1.659358	0.927533
4	6	0	1.681542	2.618354	0.278500
5	6	0	0.348844	2.338558	-0.106704
6	6	0	-0.384831	3.302528	-0.798809
7	1	0	-1.413154	3.067864	-1.053291
8	6	0	0.197834	4.532126	-1.100490
9	6	0	1.503824	4.815120	-0.685098
10	1	0	1.943621	5.780179	-0.908685
11	6	0	2.245029	3.870560	0.018173
12	1	0	3.259699	4.072745	0.338650
13	6	0	2.889545	-0.553064	1.340492
14	6	0	4.172278	-0.317857	1.853176
15	6	0	4.828315	-1.336934	2.527934
16	1	0	5.826937	-1.168234	2.913569
17	6	0	4.208647	-2.577787	2.706451
18	1	0	4.726961	-3.368780	3.236193
19	6	0	2.931420	-2.801066	2.197578
20	1	0	2.448995	-3.761392	2.333641
21	6	0	2.267989	-1.795359	1.500936
22	1	0	1.278251	-1.959956	1.095386
23	16	0	1.737049	-1.714091	-1.808812
24	6	0	0.428762	-2.133043	-3.057372
25	1	0	0.751314	-1.772195	-4.037696
26	1	0	0.344426	-3.220311	-3.108127
27	6	0	-0.917419	-1.499939	-2.710959
28	1	0	-1.567275	-1.511694	-3.590928
29	7	0	-0.673274	-0.081280	-2.302796
30	1	0	-1.536193	0.362413	-1.909800
31	6	0	-1.722479	-2.239233	-1.626377
32	8	0	-1.254391	-2.070309	-0.405709
33	8	0	-2.708207	-2.880511	-1.921637
34	1	0	-0.371103	5.284390	-1.634681
35	1	0	-0.377373	0.455409	-3.116032
36	1	0	4.636090	0.648240	1.706893
37	1	0	-0.248323	1.528358	0.382771
38	16	0	-4.570503	0.613219	3.105213
39	6	0	-4.934693	0.082262	1.375488
40	1	0	-5.768565	-0.617913	1.473769
41	1	0	-5.282568	0.937394	0.793088
42	6	0	-3.769524	-0.591712	0.627378
43	1	0	-4.163749	-0.962222	-0.321724
44	7	0	-3.154018	-1.735216	1.332630
45	6	0	-2.664089	0.441950	0.294817
46	8	0	-1.810095	0.657814	1.184631
47	8	0	-2.716719	0.974019	-0.850904
48	1	0	-3.858768	-2.421337	1.589824
49	1	0	-3.398491	1.222189	2.822193
50	1	0	-2.726391	-1.390470	2.190571
51	1	0	-2.000046	-2.174933	0.313402

HF=-2143.888605\ZeroPoint=0.3677448\Thermal=0.3978432

G = -7.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.489601	-0.138135	1.310823
2	7	0	-2.060045	-0.755032	0.084552
3	7	0	-2.033801	-1.936408	-0.369123
4	6	0	-0.988680	-2.685753	0.161521
5	6	0	-0.069698	-2.068985	1.055664
6	6	0	0.975183	-2.858543	1.536368
7	1	0	1.705581	-2.433689	2.215484
8	6	0	1.105082	-4.193228	1.142598
9	6	0	0.196253	-4.779978	0.253705
10	1	0	0.314192	-5.815302	-0.043391
11	6	0	-0.861042	-4.025889	-0.239986
12	1	0	-1.589526	-4.444182	-0.925426
13	6	0	-3.031744	0.112261	-0.488941
14	6	0	-3.762116	0.949839	0.357396
15	6	0	-4.695839	1.828732	-0.184127
16	1	0	-5.281181	2.464023	0.470762
17	6	0	-4.880514	1.886906	-1.566326

18	1	0	-5.599697	2.579591	-1.987956
19	6	0	-4.135315	1.056437	-2.404682
20	1	0	-4.269913	1.110437	-3.478998
21	6	0	-3.209576	0.163677	-1.873387
22	1	0	-2.596452	-0.467715	-2.502476
23	16	0	1.460398	0.376796	2.436486
24	6	0	1.201929	2.196532	2.667424
25	1	0	0.722604	2.384371	3.632675
26	1	0	2.177385	2.682990	2.662910
27	6	0	0.342463	2.785336	1.550581
28	1	0	0.145191	3.845842	1.762071
29	7	0	-0.931082	2.020988	1.465154
30	1	0	-1.471667	2.314020	0.654693
31	6	0	1.089059	2.746453	0.212579
32	8	0	2.231498	3.144549	0.116912
33	8	0	0.359431	2.264645	-0.777004
34	1	0	1.929833	-4.783214	1.528483
35	1	0	-1.491628	2.206174	2.293762
36	1	0	-3.612815	0.878382	1.428758
37	1	0	0.741613	-2.754457	-1.696869
38	16	0	4.617692	1.088229	-1.202404
39	6	0	3.145047	-0.010595	-1.097961
40	1	0	3.515038	-1.013722	-0.894534
41	1	0	2.539339	0.292951	-0.243111
42	6	0	2.319330	-0.042115	-2.397098
43	1	0	2.953291	-0.466781	-3.188036
44	7	0	1.830760	1.297702	-2.762112
45	6	0	1.127599	-0.983657	-2.264214
46	8	0	1.523879	-2.203196	-1.870792
47	8	0	-0.015913	-0.684785	-2.508938
48	1	0	2.629071	1.888767	-2.982401
49	1	0	3.998464	2.189281	-0.725099
50	1	0	0.942610	1.990148	-1.578668
51	1	0	1.234361	1.240857	-3.583197

HF=-2143.9259807\ZeroPoint=0.3692752\Thermal=0.3993144

G = 18.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.655278	-0.469634	0.935626
2	7	0	-2.055951	0.726490	-0.097430
3	7	0	-2.941740	0.171807	-0.801991
4	6	0	-2.920678	-1.224916	-0.709906
5	6	0	-1.751442	-1.897661	-0.260627
6	6	0	-1.822742	-3.284339	-0.078688
7	1	0	-0.935953	-3.816965	0.243844
8	6	0	-3.000700	-3.978193	-0.352356
9	6	0	-4.122521	-3.299958	-0.835744
10	1	0	-5.028706	-3.849134	-1.063938
11	6	0	-4.086265	-1.919799	-1.026794
12	1	0	-4.950342	-1.374415	-1.386529
13	6	0	-1.997362	2.150290	-0.192239
14	6	0	-2.031268	2.900006	0.984053
15	6	0	-1.960069	4.288264	0.912864
16	1	0	-2.007294	4.877582	1.821170
17	6	0	-1.832398	4.916428	-0.326124
18	1	0	-1.762903	5.996686	-0.379926
19	6	0	-1.791705	4.154644	-1.494572
20	1	0	-1.685050	4.643204	-2.456316
21	6	0	-1.878721	2.767109	-1.437881
22	1	0	-1.806612	2.148508	-2.321296
23	16	0	0.896255	-1.920028	1.805232
24	6	0	1.712417	-0.803514	3.036463
25	1	0	1.218506	-0.908116	4.006270
26	1	0	2.753252	-1.114318	3.128116
27	6	0	1.662837	0.634959	2.559430
28	1	0	1.987553	1.308779	3.364077
29	7	0	0.257768	0.984086	2.171064
30	1	0	0.305972	1.836568	1.609564
31	6	0	2.596435	0.918112	1.351575
32	8	0	3.728522	0.431824	1.376651
33	8	0	2.078388	1.658831	0.449638
34	1	0	-3.040506	-5.052006	-0.209616
35	1	0	-0.309285	1.155663	2.997776
36	1	0	-2.157300	2.396980	1.935511
37	1	0	-0.696815	-1.570651	-0.828608
38	16	0	4.949750	-0.773460	-1.470136
39	6	0	3.146422	-1.172598	-1.473513
40	1	0	3.020734	-2.183406	-1.855086
41	1	0	2.796085	-1.172421	-0.442635
42	6	0	2.313637	-0.231935	-2.340743
43	1	0	2.553250	-0.386955	-3.397125
44	7	0	2.600522	1.206665	-2.032651
45	6	0	0.780192	-0.422899	-2.162011
46	8	0	0.426598	-1.585512	-1.807706
47	8	0	0.067848	0.573653	-2.353038
48	1	0	3.553525	1.450290	-2.303612
49	1	0	4.896915	-0.092185	-0.297969
50	1	0	2.468946	1.416395	-0.959339
51	1	0	1.901306	1.771208	-2.521105

HF=-2143.881752\ZeroPoint=0.3657141\Thermal=0.3948113

G = 18.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.680630	-0.515261	0.857325
2	7	0	-1.998157	0.872667	-0.067692
3	7	0	-2.956952	0.445668	-0.760691
4	6	0	-3.080288	-0.953116	-0.738367
5	6	0	-1.961324	-1.783407	-0.482158
6	6	0	-2.157501	-3.160919	-0.352928
7	1	0	-1.299330	-3.798989	-0.181774
8	6	0	-3.434888	-3.702435	-0.484319
9	6	0	-4.521280	-2.874936	-0.779041
10	1	0	-5.508799	-3.304856	-0.900546
11	6	0	-4.349398	-1.498528	-0.919248
12	1	0	-5.184116	-0.842478	-1.133570
13	6	0	-1.807505	2.289127	-0.089819
14	6	0	-1.739451	2.970403	1.125615
15	6	0	-1.543812	4.348456	1.126916

16	1	0	-1.510757	4.887284	2.066556
17	6	0	-1.394723	5.030958	-0.080336
18	1	0	-1.227547	6.101810	-0.078523
19	6	0	-1.457904	4.335953	-1.288806
20	1	0	-1.333671	4.866065	-2.226046
21	6	0	-1.669814	2.961064	-1.304256
22	1	0	-1.673468	2.388628	-2.220850
23	16	0	0.745870	-2.146544	1.597079
24	6	0	1.595095	-1.230640	2.962328
25	1	0	1.057357	-1.393015	3.899952
26	1	0	2.604879	-1.632293	3.050616
27	6	0	1.673507	0.244003	2.627909
28	1	0	1.992582	0.816730	3.509134
29	7	0	0.321486	0.739176	2.201473
30	1	0	0.488806	1.608768	1.686185
31	6	0	2.689348	0.581228	1.499204
32	8	0	3.771114	-0.007721	1.511982
33	8	0	2.278621	1.468757	0.680990
34	1	0	-3.582473	-4.771212	-0.383150
35	1	0	-0.268386	0.923294	3.009036
36	1	0	-1.887230	2.430062	2.052999
37	1	0	-0.941111	-1.470010	-0.908045
38	16	0	4.928865	-0.909334	-1.481634
39	6	0	3.105646	-1.202921	-1.555454
40	1	0	2.930811	-2.164278	-2.032985
41	1	0	2.733298	-1.278845	-0.535003
42	6	0	2.347326	-0.141557	-2.344013
43	1	0	2.619130	-0.197121	-3.402314
44	7	0	2.680782	1.246833	-1.883365
45	6	0	0.796047	-0.284290	-2.241421
46	8	0	0.368119	-1.452409	-2.114474
47	8	0	0.153191	0.788901	-2.277587
48	1	0	3.616678	1.523545	-2.176777
49	1	0	4.896497	-0.366499	-0.238664
50	1	0	2.612934	1.334506	-0.805064
51	1	0	1.944177	1.853679	-2.261444

HF=-2143.8826956\ZeroPoint=0.3679127\Thermal=0.3977636

G = -2.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.429200	0.128699	-0.714054
2	7	0	1.666967	1.093774	0.674548
3	7	0	1.840683	2.339410	0.541024
4	6	0	1.078100	2.888369	-0.485362
5	6	0	0.244965	2.040653	-1.266077
6	6	0	-0.505087	2.645631	-2.273878
7	1	0	-1.139359	2.044591	-2.916697
8	6	0	-0.439565	4.027886	-2.487225
9	6	0	0.384096	4.842622	-1.705361
10	1	0	0.427081	5.909979	-1.886624
11	6	0	1.152034	4.271548	-0.698934
12	1	0	1.808121	4.868242	-0.075861
13	6	0	2.428693	0.458028	1.699051
14	6	0	3.778357	0.771218	1.884916
15	6	0	4.498128	0.114130	2.876887
16	1	0	5.548756	0.341643	3.016223
17	6	0	3.874711	-0.838116	3.685458
18	1	0	4.440955	-1.347796	4.456580
19	6	0	2.524237	-1.134174	3.499222
20	1	0	2.030524	-1.861652	4.132989
21	6	0	1.794566	-0.496169	2.499362
22	1	0	0.738940	-0.707905	2.367751
23	16	0	-0.987493	-0.714044	-2.352441
24	6	0	-1.031311	-2.486477	-1.800000
25	1	0	-1.823840	-2.627888	-1.063983
26	1	0	-1.244918	-3.104115	-2.671379
27	6	0	0.301734	-2.900442	-1.177112
28	1	0	0.191225	-3.920990	-0.781557
29	7	0	0.674435	-1.962226	-0.096287
30	1	0	1.634905	-2.132008	0.193837
31	6	0	1.455982	-2.968654	-2.169966
32	8	0	1.111146	-3.621869	-3.297045
33	8	0	2.564374	-2.545821	-1.958295
34	1	0	-1.033913	4.471935	-3.279328
35	1	0	0.061844	-2.097269	0.717572
36	1	0	4.245212	1.509167	1.245283
37	1	0	1.890683	-3.644640	-3.872033
38	1	0	-2.590482	0.057004	-1.059270
39	16	0	-5.019006	0.408799	2.365223
40	6	0	-3.248676	0.887014	2.163647
41	1	0	-3.268404	1.967276	1.996787
42	1	0	-2.700468	0.699982	3.087322
43	6	0	-2.510026	0.173904	1.034823
44	1	0	-1.539846	0.646034	0.868545
45	7	0	-3.264331	0.216051	-0.261812
46	1	0	-3.870400	-0.625214	-0.218580
47	6	0	-2.293426	-1.347902	1.333515
48	8	0	-1.289727	-1.623366	2.018892
49	8	0	-3.157271	-2.099375	0.826686
50	1	0	-3.812880	1.063085	-0.402155
51	1	0	-4.810453	-0.925702	2.384550

HF=-2143.9168844\ZeroPoint=0.3699717\Thermal=0.4001879

G = 25.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.357157	0.382893	0.574147
2	7	0	0.883483	-1.656884	0.282875
3	7	0	0.657414	-2.441587	1.250460
4	6	0	-0.066171	-1.865622	2.298440
5	6	0	-0.688997	-0.593521	2.157016
6	6	0	-1.304517	-0.038317	3.286987
7	1	0	-1.786358	0.929053	3.196655
8	6	0	-1.327591	-0.724286	4.499557
9	6	0	-0.744488	-1.990643	4.604091
10	1	0	-0.776192	-2.524241	5.546892
11	6	0	-0.113837	-2.567340	3.505466
12	1	0	0.367825	-3.535345	3.573450
13	6	0	1.687048	-2.190050	-0.765165

14	6	0	2.736303	-3.074840	-0.482516
15	6	0	3.516304	-3.556421	-1.525372
16	1	0	4.340986	-4.226874	-1.313027
17	6	0	3.245712	-3.173060	-2.841757
18	1	0	3.858174	-3.552765	-3.651601
19	6	0	2.193010	-2.299680	-3.112245
20	1	0	1.971400	-2.008952	-4.132476
21	6	0	1.412687	-1.791085	-2.076836
22	1	0	0.577978	-1.127373	-2.289328
23	16	0	-0.121740	2.515533	1.262958
24	6	0	0.208203	3.352819	-0.343833
25	1	0	-0.640225	3.174838	-1.007558
26	1	0	0.322280	4.420819	-0.157769
27	6	0	1.471929	2.769253	-0.965859
28	1	0	1.622562	3.208747	-1.962461
29	7	0	1.314732	1.301228	-1.087919
30	1	0	2.213366	0.865547	-1.285932
31	6	0	2.746240	3.054302	-0.182371
32	8	0	2.845880	4.353679	0.155610
33	8	0	3.599223	2.235482	0.054738
34	1	0	-1.808323	-0.278827	5.362992
35	1	0	0.643708	1.079188	-1.851305
36	1	0	2.935219	-3.355091	0.543480
37	1	0	3.680346	4.469444	0.634160
38	1	0	-1.415043	-0.392852	1.122400
39	16	0	-5.109097	-0.082285	-1.970605
40	6	0	-3.621018	-1.168955	-2.052379
41	1	0	-3.967703	-2.141054	-1.690158
42	1	0	-3.306536	-1.292046	-3.090408
43	6	0	-2.411790	-0.697345	-1.224869
44	1	0	-1.673658	-1.503588	-1.246725
45	7	0	-2.727289	-0.390133	0.184758
46	1	0	-3.068930	0.573170	0.211203
47	6	0	-1.764177	0.566433	-1.870154
48	8	0	-0.783354	0.354727	-2.637529
49	8	0	-2.271065	1.659722	-1.557169
50	1	0	-3.461831	-0.993576	0.547472
51	1	0	-4.437815	1.079602	-2.133989

HF=-2143.870873\ZeroPoint=0.3656013\Thermal=0.3952249

G = 21.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.794455	-0.338918	0.162524
2	7	0	-0.646393	1.697624	0.877388
3	7	0	-1.167663	1.754898	2.021616
4	6	0	-1.408897	0.446100	2.528356
5	6	0	-0.416910	-0.566322	2.423127
6	6	0	-0.725686	-1.852298	2.910359
7	1	0	0.024308	-2.628754	2.828431
8	6	0	-1.961703	-2.115725	3.477653
9	6	0	-2.905949	-1.087738	3.612560
10	1	0	-3.864871	-1.297063	4.072536
11	6	0	-2.634771	0.193623	3.155382
12	1	0	-3.361807	0.991572	3.239539
13	6	0	-0.369956	2.929890	0.226090
14	6	0	-1.037834	4.112339	0.578625
15	6	0	-0.738436	5.283430	-0.101299
16	1	0	-1.258307	6.199740	0.153016
17	6	0	0.224445	5.282877	-1.116665
18	1	0	0.452319	6.202745	-1.643175
19	6	0	0.884581	4.103489	-1.454810
20	1	0	1.636756	4.099388	-2.234773
21	6	0	0.585440	2.914265	-0.793887
22	1	0	1.120738	2.001073	-1.044595
23	16	0	-1.375493	-2.509894	-0.288595
24	6	0	-0.657718	-2.581663	-1.980250
25	1	0	0.427172	-2.652456	-1.890198
26	1	0	-1.060201	-3.457940	-2.489270
27	6	0	-1.011959	-1.297360	-2.716708
28	1	0	-0.508805	-1.280853	-3.694475
29	7	0	-0.546238	-0.145134	-1.911835
30	1	0	-1.012462	0.705523	-2.224407
31	6	0	-2.497963	-1.125616	-3.003101
32	8	0	-3.035558	-2.236054	-3.541679
33	8	0	-3.112461	-0.101871	-2.832402
34	1	0	-2.194799	-3.111880	3.833520
35	1	0	0.500030	-0.022803	-1.998020
36	1	0	-1.783539	4.092811	1.362112
37	1	0	-3.971152	-2.054776	-3.716574
38	1	0	0.627443	-0.331415	2.184452
39	16	0	5.468838	-1.603779	0.129134
40	6	0	4.706311	0.076553	0.138125
41	1	0	5.259453	0.623342	0.907088
42	1	0	4.885661	0.567986	-0.820226
43	6	0	3.193549	0.115805	0.452781
44	1	0	2.924897	1.175136	0.521502
45	7	0	2.786378	-0.557029	1.690962
46	1	0	2.776296	-1.557192	1.498602
47	6	0	2.406766	-0.481521	-0.739053
48	8	0	2.079222	0.336556	-1.656402
49	8	0	2.152489	-1.699419	-0.709107
50	1	0	3.478705	-0.404845	2.419625
51	1	0	4.501583	-2.197293	-0.603346

HF=-2143.8750606\ZeroPoint=0.3679486\Thermal=0.3986843

G = 11.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.735942	0.388686	1.401214
2	7	0	2.256614	-0.189618	0.373784
3	6	0	3.208572	-0.454144	-0.658041
4	6	0	4.513229	-0.844157	-0.330944
5	6	0	5.429125	-1.089133	-1.346253
6	1	0	6.434813	-1.405775	-1.094800
7	6	0	5.055883	-0.939099	-2.683650
8	6	0	3.756278	-0.549282	-3.001867
9	1	0	3.457413	-0.438114	-4.037480
10	6	0	2.827002	-0.311979	-1.993449
11	1	0	1.810925	-0.031732	-2.235454

12	6	0	1.812352	0.597677	2.412481
13	6	0	2.218151	1.319643	3.547450
14	6	0	1.287668	1.584737	4.541588
15	1	0	1.575773	2.139629	5.426410
16	6	0	-0.030445	1.136076	4.390577
17	1	0	-0.760257	1.354559	5.163361
18	6	0	-0.423231	0.411703	3.260243
19	1	0	-1.460655	0.101480	3.181704
20	6	0	0.488660	0.109059	2.246383
21	1	0	5.773000	-1.135334	-3.472364
22	1	0	3.244882	1.658996	3.623640
23	46	0	0.274221	-0.830506	0.471722
24	16	0	-0.070058	-1.800984	-1.680117
25	6	0	-1.888132	-2.086017	-1.512284
26	1	0	-2.176767	-2.901678	-2.173671
27	1	0	-2.445303	-1.192756	-1.805103
28	6	0	-2.208263	-2.459431	-0.067752
29	1	0	-1.681448	-3.389849	0.169367
30	7	0	-1.697242	-1.405000	0.843372
31	6	0	-3.686729	-2.703272	0.217505
32	1	0	-2.246081	-0.537388	0.719579
33	1	0	-1.830257	-1.693834	1.809064
34	8	0	-4.252533	-3.499823	-0.711339
35	8	0	-4.276357	-2.273885	1.177130
36	1	0	-5.182053	-3.624582	-0.465671
37	1	0	0.524314	2.112658	0.198909
38	7	0	-0.415477	2.457875	0.011744
39	6	0	-0.982913	2.047660	-1.320403
40	1	0	-0.481417	3.473460	0.134100
41	6	0	-1.021137	3.174209	-2.340509
42	1	0	-0.384967	1.212765	-1.694829
43	6	0	-2.393777	1.441333	-0.983373
44	16	0	-1.807403	4.717657	-1.706997
45	1	0	-0.019584	3.470878	-2.659258
46	1	0	-1.573493	2.813133	-3.206391
47	8	0	-3.133958	1.204601	-1.930762
48	8	0	-2.551409	1.229492	0.263210
49	1	0	-3.028893	4.178276	-1.508031
50	1	0	-1.128921	1.974452	0.649118
51	1	0	4.785623	-0.962923	0.709472

HF=-2143.8962547\ZeroPoint=0.3732051\Thermal=0.4036364

G = 27.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.642224	0.948821	-1.048706
2	7	0	-2.050027	-0.066146	-0.569349
3	6	0	-2.860449	-1.011684	0.119802
4	6	0	-4.216488	-1.166945	-0.204025
5	6	0	-4.980729	-2.086253	0.498618
6	1	0	-6.024107	-2.225368	0.240344
7	6	0	-4.407270	-2.836063	1.531270
8	6	0	-3.062162	-2.670370	1.850526
9	1	0	-2.612230	-3.247855	2.649059
10	6	0	-2.272214	-1.769759	1.139853
11	1	0	-1.225697	-1.647263	1.393632
12	6	0	-1.781508	1.879573	-1.628064
13	6	0	-2.318955	2.819307	-2.514544
14	6	0	-1.469713	3.729518	-3.132738
15	1	0	-1.871159	4.450561	-3.835101
16	6	0	-0.098505	3.719857	-2.849453
17	1	0	0.554523	4.439766	-3.330197
18	6	0	0.424754	2.806796	-1.936551
19	1	0	1.481173	2.847351	-1.687438
20	6	0	-0.395398	1.865905	-1.296269
21	1	0	-5.010726	-3.552058	2.077618
22	1	0	-3.381211	2.802729	-2.727666
23	46	0	-0.022039	-0.230632	-0.897223
24	16	0	0.134142	-2.537713	-1.042074
25	6	0	1.910003	-2.630788	-0.561829
26	1	0	2.281498	-3.628685	-0.792186
27	1	0	2.000180	-2.438364	0.510655
28	6	0	2.660627	-1.574937	-1.363052
29	1	0	2.517686	-1.786637	-2.428756
30	7	0	2.062988	-0.247984	-1.070297
31	6	0	4.168362	-1.511786	-1.139780
32	1	0	2.335608	0.053380	-0.104300
33	1	0	2.429627	0.448422	-1.713698
34	8	0	4.716188	-2.738033	-1.021215
35	8	0	4.808102	-0.490751	-1.124870
36	1	0	5.672928	-2.623821	-0.912829
37	1	0	-0.120509	1.792432	0.003210
38	7	0	0.105419	2.227313	1.378066
39	6	0	0.007527	1.114418	2.344475
40	1	0	-0.502342	3.005998	1.624421
41	6	0	0.087890	1.555539	3.814073
42	1	0	-0.956085	0.620684	2.198583
43	6	0	1.128174	0.079557	2.026128
44	16	0	1.556655	2.588004	4.239470
45	1	0	-0.772306	2.177284	4.077739
46	1	0	0.066919	0.663106	4.440960
47	8	0	0.886419	-1.102384	2.300839
48	8	0	2.179039	0.579494	1.516981
49	1	0	2.473369	1.784269	3.657339
50	1	0	1.072477	2.554959	1.384983
51	1	0	-4.643320	-0.578434	-1.004981

HF=-2143.866579\ZeroPoint=0.3654842\Thermal=0.3953186

G = 19.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.818675	-0.655998	1.093174
2	7	0	2.190137	-0.239954	0.082572
3	6	0	2.886244	0.628129	-0.806520
4	6	0	4.284284	0.595600	-0.902608
5	6	0	4.921215	1.470172	-1.770152
6	1	0	6.000233	1.440468	-1.866428
7	6	0	4.174189	2.383639	-2.521841
8	6	0	2.786022	2.412870	-2.411691
9	1	0	2.204356	3.120060	-2.990534

10	6	0	2.126381	1.526048	-1.564859
11	1	0	1.045096	1.551694	-1.479483
12	6	0	2.012100	-1.411614	1.969796
13	6	0	2.561953	-2.528619	2.600487
14	6	0	1.751685	-3.311095	3.417675
15	1	0	2.164971	-4.195201	3.889154
16	6	0	0.412910	-2.968922	3.636210
17	1	0	-0.202074	-3.584141	4.282432
18	6	0	-0.117646	-1.821974	3.051453
19	1	0	-1.137897	-1.516341	3.253946
20	6	0	0.672123	-1.028843	2.214521
21	1	0	4.678861	3.066045	-3.196355
22	1	0	3.596938	-2.789209	2.416302
23	46	0	0.255127	-0.935176	-0.191420
24	16	0	0.294846	-1.180453	-2.474309
25	6	0	-1.515508	-0.945452	-2.714398
26	1	0	-1.763719	-1.238328	-3.734527
27	1	0	-1.758813	0.105874	-2.547489
28	6	0	-2.227540	-1.826798	-1.697092
29	1	0	-1.946388	-2.869202	-1.886216
30	7	0	-1.754601	-1.456922	-0.340943
31	6	0	-3.751858	-1.785444	-1.735506
32	1	0	-2.163107	-0.531122	-0.020987
33	1	0	-2.050837	-2.155101	0.336731
34	8	0	-4.224423	-1.732850	-2.998339
35	8	0	-4.456648	-1.847085	-0.761132
36	1	0	-5.192844	-1.739264	-2.950515
37	1	0	0.335178	-0.008150	1.964307
38	7	0	-0.266788	2.074456	2.305808
39	6	0	-0.634122	2.739223	1.051237
40	1	0	0.198683	2.728967	2.929450
41	6	0	-1.440873	4.048855	1.198548
42	1	0	0.285620	3.000021	0.518753
43	6	0	-1.409489	1.754522	0.144686
44	16	0	-2.981499	3.915015	2.206949
45	1	0	-0.840289	4.801111	1.717576
46	1	0	-1.684730	4.433638	0.206455
47	8	0	-1.216308	1.829004	-1.083178
48	8	0	-2.183958	0.943667	0.746745
49	1	0	-3.450896	2.799550	1.606848
50	1	0	-1.125918	1.785465	2.768443
51	1	0	4.844535	-0.116461	-0.311494
9	6	0	0.384096	4.842622	-1.705361
10	1	0	0.427081	5.909979	-1.886624
11	6	0	1.152034	4.271548	-0.698934
12	1	0	1.808121	4.868242	-0.075861
13	6	0	2.428693	0.458028	1.699051
14	6	0	3.778357	0.771218	1.884916
15	6	0	4.498128	0.114130	2.876887
16	1	0	5.548756	0.341643	3.016223
17	6	0	3.874711	-0.838116	3.685458
18	1	0	4.440955	-1.347796	4.456580
19	6	0	2.524237	-1.134174	3.499222
20	1	0	2.030524	-1.861652	4.132989
21	6	0	1.794566	-0.496169	2.499362
22	1	0	0.738940	-0.707905	2.367751
23	16	0	-0.987493	-0.714044	-2.352441
24	6	0	-1.031311	-2.486477	-1.800000
25	1	0	-1.823840	-2.627888	-1.063983
26	1	0	-1.244918	-3.104115	-2.671379
27	6	0	0.301734	-2.900442	-1.177112
28	1	0	0.191225	-3.920990	-0.781557
29	7	0	0.674435	-1.962226	-0.096287
30	1	0	1.634905	-2.132008	0.193837
31	6	0	1.455982	-2.968654	-2.169966
32	8	0	1.111146	-3.621869	-3.297045
33	8	0	2.564374	-2.545821	-1.958295
34	1	0	-1.033913	4.471935	-3.279328
35	1	0	0.061844	-2.097269	0.717572
36	1	0	4.245212	1.509167	1.245283
37	1	0	1.890683	-3.644640	-3.872033
38	1	0	-2.590482	0.057004	-1.059270
39	16	0	-5.019006	0.408799	2.365223
40	6	0	-3.248676	0.887014	2.163647
41	1	0	-3.268404	1.967276	1.996787
42	1	0	-2.700468	0.699982	3.087322
43	6	0	-2.510026	0.173904	1.034823
44	1	0	-1.539846	0.646034	0.868545
45	7	0	-3.264331	0.216051	-0.261812
46	1	0	-3.870400	-0.625214	-0.218580
47	6	0	-2.293426	-1.347902	1.333515
48	8	0	-1.289727	-1.623366	2.018892
49	8	0	-3.157271	-2.099375	0.826686
50	1	0	-3.812880	1.063085	-0.402155
51	1	0	-4.810453	-0.925702	2.384550

HF=-2143.8764616\ZeroPoint=0.3679541\Thermal=0.398797

HF=-2143.9168844\ZeroPoint=0.3699717\Thermal=0.4001879

G = -2.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.429200	0.128699	-0.714054
2	7	0	1.666967	1.093774	0.674548
3	7	0	1.840683	2.339410	0.541024
4	6	0	1.078100	2.888369	-0.485362
5	6	0	0.244965	2.040653	-1.266077
6	6	0	-0.505087	2.645631	-2.273878
7	1	0	-1.139359	2.044591	-2.916697
8	6	0	-0.439565	4.027886	-2.487225

G = 25.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.357157	0.382893	0.574147
2	7	0	0.883483	-1.656884	0.282875
3	7	0	0.657414	-2.441587	1.250460
4	6	0	-0.066171	-1.865622	2.298440
5	6	0	-0.688997	-0.593521	2.157016
6	6	0	-1.304517	-0.038317	3.286987
7	1	0	-1.786358	0.929053	3.196655

8	6	0	-1.327591	-0.724286	4.499557
9	6	0	-0.744488	-1.990643	4.604091
10	1	0	-0.776192	-2.524241	5.546892
11	6	0	-0.113837	-2.567340	3.505466
12	1	0	0.367825	-3.535345	3.573450
13	6	0	1.687048	-2.190050	-0.765165
14	6	0	2.736303	-3.074840	-0.482516
15	6	0	3.516304	-3.556421	-1.525372
16	1	0	4.340986	-4.226874	-1.313027
17	6	0	3.245712	-3.173060	-2.841757
18	1	0	3.858174	-3.552765	-3.651601
19	6	0	2.193010	-2.299680	-3.112245
20	1	0	1.971400	-2.008952	-4.132476
21	6	0	1.412687	-1.791085	-2.076836
22	1	0	0.577978	-1.127373	-2.289328
23	16	0	-0.121740	2.515533	1.262958
24	6	0	0.208203	3.352819	-0.343833
25	1	0	-0.640225	3.174838	-1.007558
26	1	0	0.322280	4.420819	-0.157769
27	6	0	1.471929	2.769253	-0.965859
28	1	0	1.622562	3.208747	-1.962461
29	7	0	1.314732	1.301228	-1.087919
30	1	0	2.213366	0.865547	-1.285932
31	6	0	2.746240	3.054302	-0.182371
32	8	0	2.845880	4.353679	0.155610
33	8	0	3.599223	2.235482	0.054738
34	1	0	-1.808323	-0.278827	5.362992
35	1	0	0.643708	1.079188	-1.851305
36	1	0	2.935219	-3.355091	0.543480
37	1	0	3.680346	4.469444	0.634160
38	1	0	-1.415043	-0.392852	1.122400
39	16	0	-5.109097	-0.082285	-1.970605
40	6	0	-3.621018	-1.168955	-2.052379
41	1	0	-3.967703	-2.141054	-1.690158
42	1	0	-3.306536	-1.292046	-3.090408
43	6	0	-2.411790	-0.697345	-1.224869
44	1	0	-1.673658	-1.503588	-1.246725
45	7	0	-2.727289	-0.390133	0.184758
46	1	0	-3.068930	0.573170	0.211203
47	6	0	-1.764177	0.566433	-1.870154
48	8	0	-0.783354	0.354727	-2.637529
49	8	0	-2.271065	1.659722	-1.557169
50	1	0	-3.461831	-0.993576	0.547472
51	1	0	-4.437815	1.079602	-2.133989

HF=-2143.870873\ZeroPoint=0.3656013\Thermal=0.3952249

G = 21.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.794455	-0.338918	0.162524
2	7	0	-0.646393	1.697624	0.877388
3	7	0	-1.167663	1.754898	2.021616
4	6	0	-1.408897	0.446100	2.528356
5	6	0	-0.416910	-0.566322	2.423127
6	6	0	-0.725686	-1.852298	2.910359
7	1	0	0.024308	-2.628754	2.828431
8	6	0	-1.961703	-2.115725	3.477653
9	6	0	-2.905949	-1.087738	3.612560
10	1	0	-3.864871	-1.297063	4.072536
11	6	0	-2.634771	0.193623	3.155382
12	1	0	-3.361807	0.991572	3.239539
13	6	0	-0.369956	2.929890	0.226090
14	6	0	-1.037834	4.112339	0.578625
15	6	0	-0.738436	5.283430	-0.101299
16	1	0	-1.258307	6.199740	0.153016
17	6	0	0.224445	5.282877	-1.116665
18	1	0	0.452319	6.202745	-1.643175
19	6	0	0.884581	4.103489	-1.454810
20	1	0	1.636756	4.099388	-2.234773
21	6	0	0.585440	2.914265	-0.793887
22	1	0	1.120738	2.001073	-1.044595
23	16	0	-1.375493	-2.509894	-0.288595
24	6	0	-0.657718	-2.581663	-1.980250
25	1	0	0.427172	-2.652456	-1.890198
26	1	0	-1.060201	-3.457940	-2.489270
27	6	0	-1.011959	-1.297360	-2.716708
28	1	0	-0.508805	-1.280853	-3.694475
29	7	0	-0.546238	-0.145134	-1.911835
30	1	0	-1.012462	0.705523	-2.224407
31	6	0	-2.497963	-1.125616	-3.003101
32	8	0	-3.035558	-2.236054	-3.541679
33	8	0	-3.112461	-0.101871	-2.832402
34	1	0	-2.194799	-3.111880	3.833520
35	1	0	0.500030	-0.022803	-1.998020
36	1	0	-1.783539	4.092811	1.362112
37	1	0	-3.971152	-2.054776	-3.716574
38	1	0	0.627443	-0.331415	2.184452
39	16	0	5.468838	-1.603779	0.129134
40	6	0	4.706311	0.076553	0.138125
41	1	0	5.259453	0.623342	0.907088
42	1	0	4.885661	0.567986	-0.820226
43	6	0	3.193549	0.115805	0.452781
44	1	0	2.924897	1.175136	0.521502
45	7	0	2.786378	-0.557029	1.690962
46	1	0	2.776296	-1.557192	1.498602
47	6	0	2.406766	-0.481521	-0.739053
48	8	0	2.079222	0.336556	-1.656402
49	8	0	2.152489	-1.699419	-0.709107
50	1	0	3.478705	-0.404845	2.419625
51	1	0	4.501583	-2.197293	-0.603346

HF=-2143.8750606\ZeroPoint=0.3679486\Thermal=0.3986843

G = 11.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.735942	0.388686	1.401214
2	7	0	2.256614	-0.189618	0.373784
3	6	0	3.208572	-0.454144	-0.658041
4	6	0	4.513229	-0.844157	-0.330944
5	6	0	5.429125	-1.089133	-1.346253

6	1	0	6.434813	-1.405775	-1.094800
7	6	0	5.055883	-0.939099	-2.683650
8	6	0	3.756278	-0.549282	-3.001867
9	1	0	3.457413	-0.438114	-4.037480
10	6	0	2.827002	-0.311979	-1.993449
11	1	0	1.810925	-0.031732	-2.235454
12	6	0	1.812352	0.597677	2.412481
13	6	0	2.218151	1.319643	3.547450
14	6	0	1.287668	1.584737	4.541588
15	1	0	1.575773	2.139629	5.426410
16	6	0	-0.030445	1.136076	4.390577
17	1	0	-0.760257	1.354559	5.163361
18	6	0	-0.423231	0.411703	3.260243
19	1	0	-1.460655	0.101480	3.181704
20	6	0	0.488660	0.109059	2.246383
21	1	0	5.773000	-1.135334	-3.472364
22	1	0	3.244882	1.658996	3.623640
23	46	0	0.274221	-0.830506	0.471722
24	16	0	-0.070058	-1.800984	-1.680117
25	6	0	-1.888132	-2.086017	-1.512284
26	1	0	-2.176767	-2.901678	-2.173671
27	1	0	-2.445303	-1.192756	-1.805103
28	6	0	-2.208263	-2.459431	-0.067752
29	1	0	-1.681448	-3.389849	0.169367
30	7	0	-1.697242	-1.405000	0.843372
31	6	0	-3.686729	-2.703272	0.217505
32	1	0	-2.246081	-0.537388	0.719579
33	1	0	-1.830257	-1.693834	1.809064
34	8	0	-4.252533	-3.499823	-0.711339
35	8	0	-4.276357	-2.273885	1.177130
36	1	0	-5.182053	-3.624582	-0.465671
37	1	0	0.524314	2.112658	0.198909
38	7	0	-0.415477	2.457875	0.011744
39	6	0	-0.982913	2.047660	-1.320403
40	1	0	-0.481417	3.473460	0.134100
41	6	0	-1.021137	3.174209	-2.340509
42	1	0	-0.384967	1.212765	-1.694829
43	6	0	-2.393777	1.441333	-0.983373
44	16	0	-1.807403	4.717657	-1.706997
45	1	0	-0.019584	3.470878	-2.659258
46	1	0	-1.573493	2.813133	-3.206391
47	8	0	-3.133958	1.204601	-1.930762
48	8	0	-2.551409	1.229492	0.263210
49	1	0	-3.028893	4.178276	-1.508031
50	1	0	-1.128921	1.974452	0.649118
51	1	0	4.785623	-0.962923	0.709472

HF=-2143.8962547\ZeroPoint=0.3732051\Thermal=0.4036364

G = 27.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.642224	0.948821	-1.048706
2	7	0	-2.050027	-0.066146	-0.569349
3	6	0	-2.860449	-1.011684	0.119802
4	6	0	-4.216488	-1.166945	-0.204025
5	6	0	-4.980729	-2.086253	0.498618
6	1	0	-6.024107	-2.225368	0.240344
7	6	0	-4.407270	-2.836063	1.531270
8	6	0	-3.062162	-2.670370	1.850526
9	1	0	-2.612230	-3.247855	2.649059
10	6	0	-2.272214	-1.769759	1.139853
11	1	0	-1.225697	-1.647263	1.393632
12	6	0	-1.781508	1.879573	-1.628064
13	6	0	-2.318955	2.819307	-2.514544
14	6	0	-1.469713	3.729518	-3.132738
15	1	0	-1.871159	4.450561	-3.835101
16	6	0	-0.098505	3.719857	-2.849453
17	1	0	0.554523	4.439766	-3.330197
18	6	0	0.424754	2.806796	-1.936551
19	1	0	1.481173	2.847351	-1.687438
20	6	0	-0.395398	1.865905	-1.296269
21	1	0	-5.010726	-3.552058	2.077618
22	1	0	-3.381211	2.802729	-2.727666
23	46	0	-0.022039	-0.230632	-0.897223
24	16	0	0.134142	-2.537713	-1.042074
25	6	0	1.910003	-2.630788	-0.561829
26	1	0	2.281498	-3.628685	-0.792186
27	1	0	2.000180	-2.438364	0.510655
28	6	0	2.660627	-1.574937	-1.363052
29	1	0	2.517686	-1.786637	-2.428756
30	7	0	2.062988	-0.247984	-1.070297
31	6	0	4.168362	-1.511786	-1.139780
32	1	0	2.335608	0.053380	-0.104300
33	1	0	2.429627	0.448422	-1.713698
34	8	0	4.716188	-2.738033	-1.021215
35	8	0	4.808102	-0.490751	-1.124870
36	1	0	5.672928	-2.623821	-0.912829
37	1	0	-0.120509	1.792432	0.003210
38	7	0	0.105419	2.227313	1.378066
39	6	0	0.007527	1.114418	2.344475
40	1	0	-0.502342	3.005998	1.624421
41	6	0	0.087890	1.555539	3.814073
42	1	0	-0.956085	0.620684	2.198583
43	6	0	1.128174	0.079557	2.026128
44	16	0	1.556655	2.588004	4.239470
45	1	0	-0.772306	2.177284	4.077739
46	1	0	0.066919	0.663106	4.440960
47	8	0	0.886419	-1.102384	2.300839
48	8	0	2.179039	0.579494	1.516981
49	1	0	2.473369	1.784269	3.657339
50	1	0	1.072477	2.554959	1.384983
51	1	0	-4.643320	-0.578434	-1.004981

HF=-2143.866579\ZeroPoint=0.3654842\Thermal=0.3953186

G = 19.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.818675	-0.655998	1.093174
2	7	0	2.190137	-0.239954	0.082572
3	6	0	2.886244	0.628129	-0.806520

4	6	0	4.284284	0.595600	-0.902608
5	6	0	4.921215	1.470172	-1.770152
6	1	0	6.000233	1.440468	-1.866428
7	6	0	4.174189	2.383639	-2.521841
8	6	0	2.786022	2.412870	-2.411691
9	1	0	2.204356	3.120060	-2.990534
10	6	0	2.126381	1.526048	-1.564859
11	1	0	1.045096	1.551694	-1.479483
12	6	0	2.012100	-1.411614	1.969796
13	6	0	2.561953	-2.528619	2.600487
14	6	0	1.751685	-3.311095	3.417675
15	1	0	2.164971	-4.195201	3.889154
16	6	0	0.412910	-2.968922	3.636210
17	1	0	-0.202074	-3.584141	4.282432
18	6	0	-0.117646	-1.821974	3.051453
19	1	0	-1.137897	-1.516341	3.253946
20	6	0	0.672123	-1.028843	2.214521
21	1	0	4.678861	3.066045	-3.196355
22	1	0	3.596938	-2.789209	2.416302
23	46	0	0.255127	-0.935176	-0.191420
24	16	0	0.294846	-1.180453	-2.474309
25	6	0	-1.515508	-0.945452	-2.714398
26	1	0	-1.763719	-1.238328	-3.734527
27	1	0	-1.758813	0.105874	-2.547489
28	6	0	-2.227540	-1.826798	-1.697092
29	1	0	-1.946388	-2.869202	-1.886216
30	7	0	-1.754601	-1.456922	-0.340943
31	6	0	-3.751858	-1.785444	-1.735506
32	1	0	-2.163107	-0.531122	-0.020987
33	1	0	-2.050837	-2.155101	0.336731
34	8	0	-4.224423	-1.732850	-2.998339
35	8	0	-4.456648	-1.847085	-0.761132
36	1	0	-5.192844	-1.739264	-2.950515
37	1	0	0.335178	-0.008150	1.964307
38	7	0	-0.266788	2.074456	2.305808
39	6	0	-0.634122	2.739223	1.051237
40	1	0	0.198683	2.728967	2.929450
41	6	0	-1.440873	4.048855	1.198548
42	1	0	0.285620	3.000021	0.518753
43	6	0	-1.409489	1.754522	0.144686
44	16	0	-2.981499	3.915015	2.206949
45	1	0	-0.840289	4.801111	1.717576
46	1	0	-1.684730	4.433638	0.206455
47	8	0	-1.216308	1.829004	-1.083178
48	8	0	-2.183958	0.943667	0.746745
49	1	0	-3.450896	2.799550	1.606848
50	1	0	-1.125918	1.785465	2.768443
51	1	0	4.844535	-0.116461	-0.311494

HF=-2143.8764616\ZeroPoint=0.3679541\Thermal=0.398797

G = -6.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.856044	0.105736	-1.170549
2	7	0	-2.064180	1.153863	0.193953
3	7	0	-1.644120	2.282230	0.592887
4	6	0	-0.510987	2.712515	-0.086170
5	6	0	0.067023	1.878839	-1.084752
6	6	0	1.183535	2.374363	-1.757528
7	1	0	1.652320	1.782575	-2.536208
8	6	0	1.710679	3.631823	-1.442783
9	6	0	1.138199	4.427736	-0.445700
10	1	0	1.566035	5.393988	-0.207712
11	6	0	0.018524	3.971729	0.234960
12	1	0	-0.456385	4.562776	1.009305
13	6	0	-3.200556	0.632042	0.873706
14	6	0	-3.382211	0.822982	2.246810
15	6	0	-4.493127	0.268504	2.872434
16	1	0	-4.628468	0.402272	3.939400
17	6	0	-5.426454	-0.463766	2.136892
18	1	0	-6.288994	-0.895048	2.631224
19	6	0	-5.245746	-0.642523	0.765303
20	1	0	-5.975571	-1.198010	0.187867
21	6	0	-4.128821	-0.104961	0.133372
22	1	0	-3.982521	-0.217167	-0.934305
23	16	0	0.777013	-0.900238	-2.450536
24	6	0	0.130966	-2.639860	-2.442582
25	1	0	-0.496502	-2.787853	-3.325635
26	1	0	0.983865	-3.315198	-2.496816
27	6	0	-0.664595	-2.934851	-1.176217
28	1	0	-1.099831	-3.941172	-1.244884
29	7	0	-1.739968	-1.912681	-1.023157
30	1	0	-2.139226	-1.997031	-0.089760
31	6	0	0.225268	-2.906096	0.086481
32	8	0	1.350140	-3.452844	-0.008503
33	8	0	-0.221271	-2.294225	1.093606
34	1	0	2.581527	3.992601	-1.979956
35	1	0	-2.478087	-2.078822	-1.702953
36	1	0	-2.648422	1.390422	2.804096
37	1	0	2.352335	-3.135853	1.115532
38	1	0	1.022809	0.109075	0.369544
39	16	0	3.784643	1.787916	1.469822
40	6	0	3.714290	0.453784	0.201072
41	1	0	3.262163	0.917479	-0.676278
42	1	0	4.726326	0.142829	-0.051559
43	6	0	2.897298	-0.777711	0.591934
44	1	0	2.679116	-1.357393	-0.308473
45	7	0	1.558498	-0.355466	1.124692
46	1	0	0.936990	-1.172831	1.400004
47	6	0	3.595861	-1.687034	1.634673
48	8	0	4.555878	-1.289129	2.256939
49	8	0	3.073568	-2.881529	1.799221
50	1	0	1.688509	0.319820	1.884820
51	1	0	4.520562	1.076963	2.349288

HF=-2143.9248513\ZeroPoint=0.3699996\Thermal=0.3994154

G = 24.1 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.694301	0.314211	-1.201695

2	7	0	-1.703335	1.345292	0.351760
3	7	0	-1.162085	2.364891	0.869086
4	6	0	0.011435	2.757327	0.217654
5	6	0	0.711172	1.834570	-0.608882
6	6	0	1.815331	2.305478	-1.329081
7	1	0	2.361347	1.620424	-1.966989
8	6	0	2.231648	3.629772	-1.206260
9	6	0	1.564274	4.500554	-0.341096
10	1	0	1.910889	5.521368	-0.231285
11	6	0	0.453028	4.068942	0.380907
12	1	0	-0.087878	4.736143	1.040886
13	6	0	-2.867373	0.860560	1.015392
14	6	0	-2.888745	0.714649	2.403225
15	6	0	-4.024753	0.193994	3.012385
16	1	0	-4.039244	0.054470	4.086732
17	6	0	-5.135893	-0.159502	2.246396
18	1	0	-6.017216	-0.566956	2.727438
19	6	0	-5.111793	0.004716	0.860921
20	1	0	-5.979850	-0.254855	0.266439
21	6	0	-3.971294	0.501984	0.238902
22	1	0	-3.939028	0.653010	-0.833892
23	16	0	0.686461	-0.772862	-2.682175
24	6	0	-0.197575	-2.403830	-2.787251
25	1	0	-0.706435	-2.461777	-3.753076
26	1	0	0.544595	-3.197941	-2.719665
27	6	0	-1.184104	-2.553529	-1.640762
28	1	0	-1.835852	-3.419781	-1.817002
29	7	0	-2.016378	-1.312196	-1.547536
30	1	0	-2.593367	-1.387877	-0.709660
31	6	0	-0.501640	-2.767043	-0.253819
32	8	0	0.495911	-3.527229	-0.256397
33	8	0	-0.999380	-2.145572	0.710349
34	1	0	3.090542	3.979842	-1.766581
35	1	0	-2.612561	-1.205097	-2.364824
36	1	0	-2.012300	0.980081	2.979798
37	1	0	1.436775	-3.436115	1.027819
38	1	0	0.876863	0.737831	-0.053691
39	16	0	4.162066	0.977681	1.456075
40	6	0	3.688974	-0.369393	0.290311
41	1	0	3.474404	0.135433	-0.650839
42	1	0	4.552107	-1.015364	0.133359
43	6	0	2.476990	-1.219335	0.685797
44	1	0	2.140744	-1.741258	-0.213123
45	7	0	1.351172	-0.375294	1.129265
46	1	0	0.524532	-0.950416	1.320470
47	6	0	2.830777	-2.265391	1.771098
48	8	0	3.710223	-2.059344	2.582713
49	8	0	2.099804	-3.364505	1.790491
50	1	0	1.617241	0.146177	1.962399
51	1	0	4.514249	0.149054	2.460577

HF=-2143.8732197\ZeroPoint=0.3662323\Thermal=0.39537

G = 22.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.667271	0.510375	1.165390
2	7	0	1.677262	1.279170	-0.545497
3	7	0	1.202925	2.277848	-1.152598
4	6	0	0.097790	2.849719	-0.500745
5	6	0	-0.739782	2.062020	0.326955
6	6	0	-1.763094	2.684874	1.045894
7	1	0	-2.410921	2.085191	1.674028
8	6	0	-1.961970	4.059134	0.930080
9	6	0	-1.160880	4.812759	0.068599
10	1	0	-1.337556	5.876882	-0.035853
11	6	0	-0.133131	4.213685	-0.659284
12	1	0	0.504680	4.790393	-1.317701
13	6	0	2.747224	0.605035	-1.204738
14	6	0	2.632305	0.240430	-2.546159
15	6	0	3.667558	-0.469325	-3.144153
16	1	0	3.575271	-0.780802	-4.177672
17	6	0	4.812641	-0.791740	-2.416080
18	1	0	5.614042	-1.348263	-2.887298
19	6	0	4.925689	-0.405850	-1.079839
20	1	0	5.821816	-0.642608	-0.518528
21	6	0	3.885087	0.281149	-0.463934
22	1	0	3.960869	0.604570	0.567875
23	16	0	-0.718765	-0.308953	2.795039
24	6	0	0.133235	-1.915704	3.171264
25	1	0	0.620522	-1.828645	4.145630
26	1	0	-0.622906	-2.698978	3.208913
27	6	0	1.134651	-2.254122	2.082712
28	1	0	1.806967	-3.054216	2.420628
29	7	0	1.949313	-1.038432	1.757699
30	1	0	2.496200	-1.269345	0.925006
31	6	0	0.495894	-2.737323	0.740337
32	8	0	-0.529592	-3.446543	0.852692
33	8	0	1.073104	-2.350930	-0.298710
34	1	0	-2.755602	4.540407	1.488774
35	1	0	2.563807	-0.777875	2.525370
36	1	0	1.728824	0.485306	-3.089403
37	1	0	-1.460204	-3.597789	-0.472528
38	1	0	-0.877373	0.970965	0.015897
39	16	0	-4.047400	0.696715	-1.832930
40	6	0	-3.597146	-0.372894	-0.399825
41	1	0	-3.347088	0.324960	0.399827
42	1	0	-4.480263	-0.932031	-0.091137
43	6	0	-2.418965	-1.331299	-0.602383
44	1	0	-2.118722	-1.674182	0.391049
45	7	0	-1.257888	-0.633633	-1.180119
46	1	0	-0.449508	-1.256634	-1.218189
47	6	0	-2.813012	-2.564871	-1.446355
48	8	0	-3.687190	-2.515010	-2.288015
49	8	0	-2.110717	-3.668411	-1.237633
50	1	0	-1.483814	-0.316274	-2.119443
51	1	0	-4.415561	-0.324051	-2.634060

HF=-2143.8741488\ZeroPoint=0.3678762\Thermal=0.3980567

G = 3.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	7	0	-3.173726	0.793979	-0.964090
2	7	0	-2.178153	1.020152	-0.214765
3	6	0	-1.950618	2.398418	0.088960
4	6	0	-3.024998	3.253931	0.350664
5	6	0	-2.778812	4.592239	0.635457
6	1	0	-3.609006	5.253961	0.853615
7	6	0	-1.472123	5.082699	0.645653
8	6	0	-0.406086	4.225700	0.375547
9	1	0	0.610463	4.600649	0.374957
10	6	0	-0.642533	2.881905	0.109206
11	1	0	0.178644	2.212094	-0.100201
12	6	0	-3.387522	-0.551118	-1.224226
13	6	0	-4.440904	-0.905659	-2.078631
14	6	0	-4.652498	-2.248433	-2.363356
15	1	0	-5.458573	-2.547095	-3.022529
16	6	0	-3.815417	-3.212615	-1.795124
17	1	0	-3.976947	-4.261193	-2.022697
18	6	0	-2.767960	-2.848221	-0.939064
19	1	0	-2.144566	-3.636183	-0.526822
20	6	0	-2.525084	-1.511601	-0.633429
21	1	0	-1.285946	6.126904	0.867962
22	1	0	-5.068240	-0.128943	-2.500200
23	46	0	-1.182517	-0.620542	0.578868
24	16	0	0.374517	0.421331	2.101322
25	6	0	0.758088	-1.130707	3.041788
26	1	0	-0.022363	-1.259657	3.795159
27	1	0	1.716308	-1.013942	3.546303
28	6	0	0.826049	-2.355734	2.137938
29	1	0	0.886151	-3.260713	2.755424
30	7	0	-0.390812	-2.440677	1.267296
31	6	0	2.098486	-2.349967	1.255694
32	1	0	-0.116023	-2.961261	0.432240
33	1	0	-1.137754	-2.945649	1.737552
34	8	0	1.909892	-2.566644	0.000770
35	8	0	3.170940	-2.103722	1.804291
36	1	0	3.175719	-2.298417	-0.964609
37	1	0	1.648482	0.352772	0.395388
38	7	0	2.117621	0.087623	-0.526122
39	6	0	3.612567	0.077780	-0.394577
40	1	0	1.838504	0.744550	-1.262146
41	6	0	4.129564	1.510924	-0.306894
42	1	0	3.826789	-0.453774	0.538881
43	6	0	4.251176	-0.742779	-1.540773
44	16	0	3.551934	2.618410	-1.663643
45	1	0	3.774139	1.971549	0.616812
46	1	0	5.217161	1.497713	-0.293480
47	8	0	3.827215	-1.986249	-1.675771
48	8	0	5.099352	-0.255989	-2.251150
49	1	0	4.246039	1.994409	-2.637702
50	1	0	1.754042	-0.865058	-0.703607
51	1	0	-4.032417	2.859056	0.338565

HF=-2143.9093055\ZeroPoint=0.3700928\Thermal=0.399472

G = 23.3 kcal mol^{-1}

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	7	0	2.222928	1.253193	0.618010
2	7	0	1.818650	0.125511	0.198679
3	6	0	2.574061	-0.453437	-0.860393
4	6	0	3.942191	-0.177167	-0.999412
5	6	0	4.643067	-0.734354	-2.058034
6	1	0	5.703750	-0.537464	-2.160623
7	6	0	3.988623	-1.550062	-2.986969
8	6	0	2.629461	-1.816506	-2.845963
9	1	0	2.117252	-2.448126	-3.561458
10	6	0	1.916531	-1.281226	-1.776935
11	1	0	0.864301	-1.495719	-1.658399
12	6	0	1.423105	1.820325	1.603131
13	6	0	1.961214	2.864890	2.363958
14	6	0	1.206290	3.412598	3.393333
15	1	0	1.617469	4.212017	3.998119
16	6	0	-0.085318	2.936919	3.648842
17	1	0	-0.670841	3.374896	4.449390
18	6	0	-0.630388	1.923926	2.863155
19	1	0	-1.654001	1.607572	3.042010
20	6	0	0.098252	1.343285	1.815260
21	1	0	4.542517	-1.979743	-3.813567
22	1	0	2.966800	3.209245	2.154595
23	46	0	0.187326	-0.714066	1.154706
24	16	0	0.647257	-2.942724	0.761631
25	6	0	-1.007365	-3.679784	1.157666
26	1	0	-0.910627	-4.286344	2.061593
27	1	0	-1.292502	-4.317847	0.321181
28	6	0	-2.070279	-2.610738	1.333359
29	1	0	-2.934617	-3.019327	1.873819
30	7	0	-1.506271	-1.466589	2.122709
31	6	0	-2.627051	-2.008445	0.006246
32	1	0	-2.232921	-0.751946	2.157203
33	1	0	-1.268811	-1.749746	3.071112
34	8	0	-3.197913	-0.869494	0.181164
35	8	0	-2.492711	-2.629687	-1.039532
36	1	0	-3.635069	-0.168991	-1.194868
37	1	0	-0.676293	1.191050	0.750917
38	7	0	-1.728633	1.490427	-0.244859
39	6	0	-1.493722	0.970562	-1.611233
40	1	0	-1.895849	2.495478	-0.280729
41	6	0	-0.310630	1.681417	-2.267315
42	1	0	-1.246124	-0.091533	-1.506600
43	6	0	-2.780068	1.042762	-2.478445
44	16	0	-0.406856	3.521946	-2.272857
45	1	0	0.605147	1.449669	-1.725604
46	1	0	-0.200043	1.332314	-3.291957
47	8	0	-3.836481	0.410029	-2.001699
48	8	0	-2.804004	1.661493	-3.519047
49	1	0	-1.435187	3.588628	-3.142966
50	1	0	-2.526664	1.001787	0.163697
51	1	0	4.433216	0.457285	-0.274102

HF=-2143.8727405\ZeroPoint=0.3658799\Thermal=0.3951661

G = 18.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.634044	0.876277	0.367667
2	7	0	1.665185	0.784707	-0.436532
3	6	0	1.452333	1.908001	-1.289787
4	6	0	2.498034	2.793079	-1.591618
5	6	0	2.245612	3.888192	-2.402961
6	1	0	3.052423	4.567420	-2.651559
7	6	0	0.958948	4.115886	-2.902785
8	6	0	-0.075017	3.234918	-2.597817
9	1	0	-1.073172	3.405054	-2.982071
10	6	0	0.167767	2.121250	-1.800158
11	1	0	-0.631228	1.432180	-1.569279
12	6	0	2.792999	-0.205511	1.242565
13	6	0	4.088424	-0.496690	1.681309
14	6	0	4.299978	-1.597448	2.504168
15	1	0	5.305555	-1.838693	2.827763
16	6	0	3.225064	-2.387313	2.923509
17	1	0	3.399566	-3.232182	3.579227
18	6	0	1.927653	-2.066124	2.529882
19	1	0	1.084246	-2.636755	2.901772
20	6	0	1.695799	-0.977384	1.688869
21	1	0	0.769072	4.976493	-3.533555
22	1	0	4.910201	0.124536	1.347235
23	46	0	0.601759	-1.009461	-0.491266
24	16	0	0.229042	-1.031238	-2.742327
25	6	0	-0.819267	-2.548663	-2.901000
26	1	0	-0.200132	-3.366286	-3.277643
27	1	0	-1.607106	-2.317991	-3.619192
28	6	0	-1.457968	-2.899431	-1.574929
29	1	0	-1.853291	-3.923182	-1.603733
30	7	0	-0.431611	-2.816762	-0.480064
31	6	0	-2.658630	-1.982700	-1.164666
32	1	0	-0.970597	-2.853721	0.389907
33	1	0	0.220595	-3.597632	-0.516407
34	8	0	-2.805906	-1.904074	0.104086
35	8	0	-3.326324	-1.474643	-2.055288
36	1	0	-3.793057	-0.754830	0.705527
37	1	0	0.650677	-0.600208	1.619182
38	7	0	-1.428557	-0.252721	2.050139
39	6	0	-2.018546	0.844886	1.262995
40	1	0	-1.520032	-0.038635	3.040364
41	6	0	-1.248902	2.147673	1.484371
42	1	0	-1.906699	0.568776	0.208097
43	6	0	-3.539525	1.017201	1.501351
44	16	0	-1.074246	2.684448	3.239629
45	1	0	-0.224740	2.023464	1.132056
46	1	0	-1.709941	2.955694	0.918337
47	8	0	-4.295504	-0.022328	1.179629
48	8	0	-4.010573	2.031668	1.970061
49	1	0	-2.384580	2.948665	3.417153
50	1	0	-1.937841	-1.108252	1.848593
51	1	0	3.486934	2.605528	-1.196531

HF=-2143.8806268\ZeroPoint=0.3686977\Thermal=0.3989058

G = -0.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.531445	0.151092	0.052878
2	7	0	-0.728859	-1.519551	-0.146403
3	7	0	-0.185174	-2.624827	-0.439403
4	6	0	1.201832	-2.564281	-0.438483
5	6	0	1.852176	-1.328414	-0.167605
6	6	0	3.243894	-1.329762	-0.141931
7	1	0	3.785298	-0.414494	0.066273
8	6	0	3.958559	-2.509626	-0.378045
9	6	0	3.303570	-3.714980	-0.649941
10	1	0	3.875016	-4.617329	-0.831936
11	6	0	1.916949	-3.746635	-0.681381
12	1	0	1.371632	-4.660721	-0.885362
13	6	0	-2.152503	-1.495278	-0.148732
14	6	0	-2.803230	-0.807942	0.879502
15	6	0	-4.193734	-0.749896	0.893619
16	1	0	-4.700976	-0.237456	1.702976
17	6	0	-4.931352	-1.357534	-0.123037
18	1	0	-6.013654	-1.301247	-0.116266
19	6	0	-4.273776	-2.040350	-1.147263
20	1	0	-4.844805	-2.510922	-1.939332
21	6	0	-2.884828	-2.117699	-1.162977
22	1	0	-2.358163	-2.639680	-1.951494
23	16	0	2.098576	1.840755	0.100550
24	6	0	0.980527	3.207163	0.634824
25	1	0	0.842208	3.171276	1.718753
26	1	0	1.450242	4.156348	0.376716
27	6	0	-0.384683	3.097696	-0.040735
28	1	0	-1.037748	3.902172	0.329279
29	7	0	-0.977934	1.769674	0.251161
30	1	0	-1.760871	1.590226	-0.374969
31	6	0	-0.340414	3.268227	-1.554549
32	8	0	0.385491	4.341362	-1.913953
33	8	0	-0.938740	2.569830	-2.333730
34	1	0	5.043002	-2.485796	-0.349156
35	1	0	-1.330155	1.760687	1.205502
36	1	0	-2.218176	-0.372316	1.680768
37	1	0	0.372721	4.395994	-2.881298
38	17	0	-0.017664	0.590484	3.393532
39	1	0	0.512841	0.291981	2.202704

HF=-1882.6588947\ZeroPoint=0.2784074\Thermal=0.301907

G = 23.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.488889	0.220963	0.213241
2	7	0	-0.877604	-1.290468	-0.324874
3	7	0	-0.420445	-2.335523	-0.859757
4	6	0	0.978794	-2.404741	-0.798672
5	6	0	1.698396	-1.581349	0.115034
6	6	0	3.096438	-1.657814	0.123995
7	1	0	3.648678	-1.047039	0.828185

8	6	0	3.758593	-2.527825	-0.738393
9	6	0	3.032353	-3.350173	-1.605909
10	1	0	3.556773	-4.035352	-2.261893
11	6	0	1.639879	-3.301799	-1.634406
12	1	0	1.065227	-3.930283	-2.303760
13	6	0	-2.291843	-1.140448	-0.288558
14	6	0	-2.852321	-0.672374	0.904289
15	6	0	-4.229439	-0.485166	0.970841
16	1	0	-4.680096	-0.155993	1.899969
17	6	0	-5.029280	-0.737205	-0.145678
18	1	0	-6.100198	-0.578854	-0.091239
19	6	0	-4.454756	-1.201735	-1.329983
20	1	0	-5.076966	-1.397721	-2.195451
21	6	0	-3.081956	-1.415781	-1.406373
22	1	0	-2.615089	-1.776042	-2.314274
23	16	0	2.169847	1.766209	0.529949
24	6	0	1.092838	3.118344	1.160688
25	1	0	0.826494	2.930728	2.203928
26	1	0	1.644099	4.057529	1.106584
27	6	0	-0.179110	3.200207	0.323701
28	1	0	-0.856084	3.960923	0.738428
29	7	0	-0.850604	1.872343	0.320800
30	1	0	-1.519434	1.821371	-0.447190
31	6	0	0.054621	3.599422	-1.129642
32	8	0	0.867962	4.662971	-1.227979
33	8	0	-0.484306	3.070617	-2.069179
34	1	0	4.841038	-2.581355	-0.727003
35	1	0	-1.358010	1.731081	1.191922
36	1	0	-2.205967	-0.549797	1.768939
37	1	0	0.969968	4.874502	-2.168252
38	17	0	0.120466	-1.564526	2.859306
39	1	0	1.177271	-1.392949	1.173125

HF=-1882.6219682\ZeroPoint=0.279069\Thermal=0.3014516

G = 13.5 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.558288	-0.080069	0.376168
2	7	0	-1.023807	-1.517383	0.003999
3	7	0	-0.576791	-2.671989	-0.231605
4	6	0	0.815428	-2.744629	0.035707
5	6	0	1.359580	-2.158653	1.208303
6	6	0	2.750230	-2.183522	1.401886
7	1	0	3.165531	-1.732336	2.294349
8	6	0	3.575437	-2.778901	0.457590
9	6	0	3.018199	-3.395234	-0.668422
10	1	0	3.666556	-3.872454	-1.394126
11	6	0	1.643844	-3.392867	-0.880887
12	1	0	1.207094	-3.846305	-1.761766
13	6	0	-2.406490	-1.288042	-0.206535
14	6	0	-2.974819	-0.194392	0.453858
15	6	0	-4.327712	0.078903	0.277949
16	1	0	-4.756943	0.928369	0.795220
17	6	0	-5.098138	-0.726061	-0.558037
18	1	0	-6.149238	-0.504894	-0.704902
19	6	0	-4.519822	-1.817143	-1.219930
20	1	0	-5.121962	-2.432732	-1.877962
21	6	0	-3.175945	-2.108944	-1.046908
22	1	0	-2.710107	-2.941131	-1.557765
23	16	0	2.436100	1.199346	0.657176
24	6	0	1.627811	2.856551	0.542538
25	1	0	1.144526	3.102092	1.488884
26	1	0	2.395180	3.596169	0.314733
27	6	0	0.565238	2.799911	-0.542783
28	1	0	-0.018545	3.731867	-0.536429
29	7	0	-0.351096	1.680105	-0.224689
30	1	0	-0.943697	1.479758	-1.030093
31	6	0	1.106263	2.627678	-1.953888
32	8	0	2.106998	3.490175	-2.213695
33	8	0	0.660538	1.856932	-2.767385
34	1	0	4.648961	-2.781772	0.600236
35	1	0	-0.971092	2.011475	0.590871
36	1	0	-2.394317	0.435566	1.120452
37	1	0	2.387403	3.348954	-3.130337
38	17	0	-1.949768	2.775714	2.008940
39	1	0	0.704828	-1.876027	2.030167

HF=-1882.6373031\ZeroPoint=0.2806629\Thermal=0.3037865

G = 2.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.126564	0.268871	-0.024902
2	7	0	1.934967	0.359694	-0.099497
3	7	0	2.478701	1.501502	-0.126484
4	6	0	1.576026	2.547317	0.008074
5	6	0	0.196086	2.246529	0.156073
6	6	0	-0.667230	3.323879	0.335862
7	1	0	-1.733363	3.169737	0.474897
8	6	0	-0.183400	4.638544	0.362967
9	6	0	1.177985	4.909829	0.205205
10	1	0	1.536040	5.932025	0.226912
11	6	0	2.068972	3.858491	0.028985
12	1	0	3.132876	4.028234	-0.088614
13	6	0	2.821569	-0.753091	-0.222343
14	6	0	2.590863	-1.883022	0.563968
15	6	0	3.455236	-2.968849	0.469111
16	1	0	3.282568	-3.842581	1.086050
17	6	0	4.530957	-2.934994	-0.417184
18	1	0	5.193601	-3.788858	-0.498708
19	6	0	4.750710	-1.803311	-1.204764
20	1	0	5.581581	-1.777978	-1.900376
21	6	0	3.903120	-0.706130	-1.107209
22	1	0	4.057359	0.178790	-1.710809
23	16	0	-0.538593	-2.098816	-0.442244
24	6	0	-2.375263	-2.015752	-0.631383
25	1	0	-2.681259	-2.665220	-1.449740
26	1	0	-2.849343	-2.376667	0.286392
27	6	0	-2.840861	-0.583547	-0.918444
28	1	0	-2.504651	-0.295360	-1.917844
29	7	0	-2.221127	0.348590	0.055061

30	1	0	-2.476244	0.065615	1.004472
31	6	0	-4.357792	-0.449532	-0.878121
32	8	0	-4.946621	-1.250077	-1.787178
33	8	0	-4.961855	0.283532	-0.135612
34	1	0	-0.878175	5.458382	0.513211
35	1	0	-2.600333	1.283303	-0.072883
36	1	0	1.757402	-1.897762	1.253919
37	1	0	-5.906292	-1.130427	-1.716668
38	17	0	-1.386167	-1.843790	2.781151
39	1	0	-0.869327	-2.078133	1.525584

HF=-1882.653039\ZeroPoint=0.2787244\Thermal=0.3020037

G = 17.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.183335	-0.002669	-0.104621
2	7	0	1.867002	0.212164	-0.074544
3	7	0	2.334816	1.374219	-0.245796
4	6	0	1.380290	2.380213	-0.338234
5	6	0	0.027504	2.143017	0.032254
6	6	0	-0.882152	3.186932	-0.173438
7	1	0	-1.907314	3.066643	0.161253
8	6	0	-0.474069	4.408707	-0.704818
9	6	0	0.869237	4.630036	-1.026430
10	1	0	1.182407	5.589715	-1.420023
11	6	0	1.802854	3.620261	-0.833941
12	1	0	2.847813	3.759413	-1.083789
13	6	0	2.832074	-0.832853	0.042016
14	6	0	2.558010	-1.905056	0.893910
15	6	0	3.502518	-2.916576	1.040123
16	1	0	3.298280	-3.742579	1.710708
17	6	0	4.696851	-2.872335	0.324060
18	1	0	5.422582	-3.670463	0.429931
19	6	0	4.956794	-1.803010	-0.536997
20	1	0	5.880265	-1.773058	-1.103471
21	6	0	4.032833	-0.776342	-0.676161
22	1	0	4.218403	0.059745	-1.337131
23	16	0	-0.333500	-2.243392	-0.723585
24	6	0	-2.113279	-2.476505	-0.305951
25	1	0	-2.490610	-3.340409	-0.852831
26	1	0	-2.228424	-2.664938	0.765553
27	6	0	-2.897167	-1.224429	-0.697573
28	1	0	-2.811266	-1.088414	-1.778643
29	7	0	-2.281682	-0.048014	-0.037877
30	1	0	-2.487153	-0.031957	0.967481
31	6	0	-4.376023	-1.317527	-0.343283
32	8	0	-4.973449	-2.326802	-1.009305
33	8	0	-4.946454	-0.590182	0.428287
34	1	0	-1.198189	5.204121	-0.841617
35	1	0	-2.680240	0.813547	-0.403509
36	1	0	1.626022	-1.930793	1.440601
37	1	0	-5.905889	-2.350183	-0.744204
38	17	0	-1.073181	1.391008	2.720912
39	1	0	-0.332560	1.569604	1.206535

HF=-1882.6288302\ZeroPoint=0.2771222\Thermal=0.2999654

G = -13.1 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.244975	-0.339307	0.413650
2	7	0	1.723115	0.161024	0.014093
3	7	0	2.196143	1.286723	-0.247101
4	6	0	1.402247	2.434696	-0.052175
5	6	0	0.595318	2.630358	1.077809
6	6	0	-0.112812	3.820357	1.202182
7	1	0	-0.723375	3.984770	2.082521
8	6	0	-0.036038	4.798527	0.209818
9	6	0	0.786731	4.605430	-0.901073
10	1	0	0.858292	5.369570	-1.666059
11	6	0	1.531037	3.438119	-1.019488
12	1	0	2.190101	3.274766	-1.863432
13	6	0	2.626009	-0.938285	-0.211632
14	6	0	2.545283	-2.056481	0.620281
15	6	0	3.414810	-3.122254	0.406507
16	1	0	3.369741	-3.984209	1.061676
17	6	0	4.333657	-3.084699	-0.641134
18	1	0	4.997409	-3.924596	-0.811625
19	6	0	4.393598	-1.967542	-1.476388
20	1	0	5.096640	-1.941250	-2.300834
21	6	0	3.547823	-0.886564	-1.261329
22	1	0	3.575781	-0.016243	-1.902863
23	16	0	-0.773742	-0.009085	-1.835652
24	6	0	-2.423025	-0.826498	-1.782044
25	1	0	-3.020773	-0.456694	-2.616132
26	1	0	-2.317598	-1.910925	-1.886549
27	6	0	-3.121354	-0.508427	-0.455203
28	1	0	-3.281749	0.568749	-0.388974
29	7	0	-2.231605	-0.917414	0.659167
30	1	0	-2.253752	-1.933176	0.759037
31	6	0	-4.456784	-1.232135	-0.356494
32	8	0	-5.391820	-0.646404	-1.130066
33	8	0	-4.652399	-2.224598	0.299621
34	1	0	-0.600713	5.718333	0.311230
35	1	0	-2.546014	-0.549449	1.556054
36	1	0	1.835082	-2.070169	1.437053
37	1	0	-6.205999	-1.169412	-1.066137
38	17	0	0.029306	-0.615363	2.781222
39	1	0	0.558636	1.882647	1.859409

HF=-1882.6805004\ZeroPoint=0.2817838\Thermal=0.3052053

G = -5.3 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.429856	0.159011	-0.243985
2	7	0	1.463374	1.033893	-0.175799
3	7	0	1.541512	2.291229	-0.307149
4	6	0	0.296925	2.901012	-0.391025

5	6	0	-0.877289	2.100002	-0.323526
6	6	0	-2.101737	2.761780	-0.382142
7	1	0	-3.027663	2.199563	-0.339304
8	6	0	-2.155902	4.155232	-0.497018
9	6	0	-0.990022	4.925341	-0.564598
10	1	0	-1.052679	6.003161	-0.656533
11	6	0	0.246294	4.297802	-0.510968
12	1	0	1.172663	4.858473	-0.558625
13	6	0	2.698104	0.332331	-0.066226
14	6	0	2.785104	-0.708306	0.863448
15	6	0	3.975752	-1.419034	0.986508
16	1	0	4.050576	-2.214035	1.719566
17	6	0	5.067364	-1.106951	0.175627
18	1	0	5.989106	-1.670078	0.265404
19	6	0	4.970606	-0.068450	-0.751924
20	1	0	5.815921	0.173173	-1.386037
21	6	0	3.790815	0.658363	-0.873907
22	1	0	3.696902	1.464696	-1.589797
23	16	0	-2.627167	-0.607279	-0.255202
24	6	0	-2.305494	-2.430647	-0.208670
25	1	0	-2.268121	-2.768873	0.829408
26	1	0	-3.126879	-2.937927	-0.712854
27	6	0	-0.977824	-2.786425	-0.874932
28	1	0	-0.791339	-3.861719	-0.727542
29	7	0	0.102574	-1.978322	-0.274582
30	1	0	0.986402	-2.145963	-0.747985
31	6	0	-0.952502	-2.577991	-2.383925
32	8	0	-2.060879	-3.063736	-2.976374
33	8	0	-0.027122	-2.099040	-2.988383
34	1	0	-3.122839	4.646488	-0.535169
35	1	0	0.187972	-2.211983	0.714739
36	1	0	1.938492	-0.927119	1.504113
37	1	0	-1.973445	-2.912986	-3.929499
38	1	0	-2.219156	-0.449169	1.922399
39	6	0	-0.636194	-0.725632	4.738113
40	1	0	-1.524902	-0.833567	5.362494
41	6	0	-0.973900	-1.010698	3.297934
42	8	0	-2.052367	-0.347611	2.899623
43	8	0	-0.320449	-1.757331	2.587645
44	1	0	-0.302109	0.312025	4.822620
45	1	0	0.152884	-1.394432	5.075175

HF=-1651.0035693\ZeroPoint=0.3316914\Thermal=0.3584326

G = 28.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.261524	-0.475806	-0.165761
2	7	0	-0.134882	1.620202	-0.432073
3	7	0	-1.162138	2.211231	-0.866507
4	6	0	-2.298740	1.392480	-0.911150
5	6	0	-2.321934	0.142686	-0.232667
6	6	0	-3.465160	-0.654289	-0.351427
7	1	0	-3.497789	-1.600971	0.174763
8	6	0	-4.553661	-0.223171	-1.108425
9	6	0	-4.520627	1.020385	-1.745251
10	1	0	-5.375856	1.353411	-2.321964
11	6	0	-3.397224	1.838474	-1.645171
12	1	0	-3.351532	2.800466	-2.141087
13	6	0	1.057470	2.395559	-0.366308
14	6	0	1.881357	2.226923	0.750924
15	6	0	3.059400	2.963998	0.835236
16	1	0	3.692352	2.858412	1.708699
17	6	0	3.420426	3.837622	-0.191042
18	1	0	4.345498	4.398770	-0.125161
19	6	0	2.590958	3.991648	-1.303862
20	1	0	2.874114	4.666326	-2.103439
21	6	0	1.401078	3.278742	-1.394409
22	1	0	0.745818	3.381232	-2.249738
23	16	0	-0.610167	-2.749986	-0.149756
24	6	0	0.977607	-3.213979	0.658717
25	1	0	0.909718	-3.030582	1.733250
26	1	0	1.156764	-4.275739	0.488731
27	6	0	2.117313	-2.375384	0.088237
28	1	0	3.046491	-2.598217	0.633600
29	7	0	1.770035	-0.947039	0.235541
30	1	0	2.429843	-0.351616	-0.259168
31	6	0	2.421868	-2.646021	-1.379544
32	8	0	2.510687	-3.964959	-1.635284
33	8	0	2.629740	-1.788443	-2.199904
34	1	0	-5.435487	-0.847884	-1.192670
35	1	0	1.711622	-0.682701	1.228179
36	1	0	1.563008	1.564521	1.549902
37	1	0	2.718656	-4.068943	-2.575904
38	1	0	-1.800814	0.100147	0.883624
39	6	0	-0.739833	0.152596	4.639707
40	1	0	-1.023329	-0.855027	4.959920
41	6	0	-0.569234	0.139933	3.121379
42	8	0	-1.634076	0.308709	2.449749
43	8	0	0.587247	-0.052526	2.662720
44	1	0	-1.539484	0.833773	4.932764
45	1	0	0.196920	0.419235	5.130145

HF=-1650.9473183\ZeroPoint=0.3280615\Thermal=0.3541038

G = 22.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.566090	0.151006	0.043009
2	7	0	1.172762	1.359036	-0.194707
3	7	0	0.872935	2.575464	-0.294697
4	6	0	-0.507114	2.761640	0.017720
5	6	0	-1.074242	2.131947	1.158418
6	6	0	-2.450511	2.298152	1.398303
7	1	0	-2.889821	1.813379	2.260940
8	6	0	-3.226818	3.067257	0.543774
9	6	0	-2.635898	3.720801	-0.544950
10	1	0	-3.245279	4.334397	-1.198402
11	6	0	-1.279085	3.582700	-0.808080
12	1	0	-0.815025	4.066402	-1.658480
13	6	0	2.513591	0.979741	-0.465858
14	6	0	2.989442	-0.168568	0.174077

15	6	0	4.295413	-0.583048	-0.069786
16	1	0	4.676438	-1.462355	0.435646
17	6	0	5.104447	0.128861	-0.954617
18	1	0	6.116824	-0.205330	-1.151107
19	6	0	4.614015	1.271315	-1.594579
20	1	0	5.242672	1.816578	-2.288844
21	6	0	3.319167	1.708041	-1.350250
22	1	0	2.917875	2.585322	-1.840501
23	16	0	-2.620019	-0.876436	0.077305
24	6	0	-2.023294	-2.619227	0.004674
25	1	0	-1.706886	-2.943696	0.997078
26	1	0	-2.842411	-3.250261	-0.340429
27	6	0	-0.827406	-2.698572	-0.934689
28	1	0	-0.398817	-3.711620	-0.900071
29	7	0	0.181084	-1.724767	-0.475203
30	1	0	0.919032	-1.620141	-1.168675
31	6	0	-1.158580	-2.434885	-2.397840
32	8	0	-2.235488	-3.137793	-2.801852
33	8	0	-0.503886	-1.738274	-3.131860
34	1	0	-4.288710	3.177046	0.727313
35	1	0	0.582974	-2.030698	0.480485
36	1	0	2.356518	-0.687905	0.882750
37	1	0	-2.378043	-2.941841	-3.739911
38	1	0	-0.439589	1.679441	1.919120
39	6	0	0.771085	-1.981434	4.271163
40	1	0	-0.187680	-2.474994	4.458880
41	6	0	0.797977	-1.506606	2.821227
42	8	0	0.639379	-0.288881	2.576991
43	8	0	0.973255	-2.412778	1.937707
44	1	0	0.876797	-1.142269	4.958781
45	1	0	1.556891	-2.719767	4.442255

HF=-1650.9566718\ZeroPoint=0.3298889\Thermal=0.3568572

G = 1.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.063572	-0.167058	-0.401300
2	7	0	-2.044816	0.388124	-0.155058
3	7	0	-2.355180	1.590569	-0.408200
4	6	0	-1.272303	2.395191	-0.729351
5	6	0	0.030168	1.830167	-0.728922
6	6	0	1.089345	2.682756	-1.038173
7	1	0	2.111100	2.316887	-1.040282
8	6	0	0.863655	4.033169	-1.328313
9	6	0	-0.429128	4.566980	-1.322349
10	1	0	-0.586761	5.614467	-1.550054
11	6	0	-1.507764	3.746532	-1.020345
12	1	0	-2.523549	4.124276	-1.006430
13	6	0	-3.137069	-0.468217	0.181241
14	6	0	-2.955187	-1.437291	1.169470
15	6	0	-4.018687	-2.262858	1.521001
16	1	0	-3.878842	-3.011796	2.291477
17	6	0	-5.250374	-2.134984	0.881358
18	1	0	-6.071953	-2.789542	1.148843
19	6	0	-5.422034	-1.168578	-0.111996
20	1	0	-6.375168	-1.073807	-0.619505
21	6	0	-4.371978	-0.328851	-0.461808
22	1	0	-4.487275	0.422990	-1.231401
23	16	0	-0.226767	-2.538011	-0.247826
24	6	0	1.499711	-2.909439	-0.775534
25	1	0	1.797669	-3.878711	-0.374028
26	1	0	1.553845	-2.961219	-1.867742
27	6	0	2.456303	-1.826861	-0.267658
28	1	0	2.470848	-1.846153	0.823052
29	7	0	1.980550	-0.486678	-0.689230
30	1	0	2.221816	-0.339468	-1.669247
31	6	0	3.864046	-2.060866	-0.795008
32	8	0	4.480454	-3.061931	-0.135415
33	8	0	4.362449	-1.460612	-1.715593
34	1	0	1.706596	4.676963	-1.557745
35	1	0	2.471390	0.222476	-0.135178
36	1	0	-1.993833	-1.534604	1.655987
37	1	0	5.350004	-3.196302	-0.542797
38	1	0	0.604625	1.100953	1.489494
39	6	0	2.767093	2.050942	3.684211
40	1	0	2.363298	1.481961	4.524314
41	6	0	2.248771	1.485532	2.390593
42	8	0	0.916342	1.438094	2.362756
43	8	0	2.959887	1.116680	1.473256
44	1	0	3.854168	2.019990	3.691549
45	1	0	2.420246	3.081583	3.791574

HF=-1650.9913558\ZeroPoint=0.3317644\Thermal=0.3587381

G = 20.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.006393	-0.139981	-0.292178
2	7	0	-2.010647	0.348713	-0.109884
3	7	0	-2.343029	1.538938	-0.377543
4	6	0	-1.274453	2.392380	-0.647085
5	6	0	0.050659	2.049079	-0.264823
6	6	0	1.084685	2.912039	-0.644875
7	1	0	2.094425	2.684869	-0.318880
8	6	0	0.813872	4.077857	-1.359410
9	6	0	-0.502033	4.416584	-1.692639
10	1	0	-0.704779	5.333006	-2.234397
11	6	0	-1.552691	3.582302	-1.328241
12	1	0	-2.578050	3.816953	-1.587605
13	6	0	-3.079097	-0.544722	0.196555
14	6	0	-2.830119	-1.595811	1.082383
15	6	0	-3.862743	-2.467601	1.414104
16	1	0	-3.674187	-3.276784	2.109364
17	6	0	-5.126580	-2.305975	0.850444
18	1	0	-5.924503	-2.995593	1.100659
19	6	0	-5.364102	-1.259293	-0.044528
20	1	0	-6.343638	-1.139653	-0.492679
21	6	0	-4.347967	-0.371629	-0.370272
22	1	0	-4.514742	0.443040	-1.062031
23	16	0	-0.192823	-2.395279	-0.786611
24	6	0	1.583818	-2.723461	-1.171069

25	1	0	1.792795	-3.773730	-0.962881
26	1	0	1.773973	-2.534557	-2.231486
27	6	0	2.471458	-1.815686	-0.316834
28	1	0	2.368305	-2.085574	0.734867
29	7	0	2.033711	-0.411730	-0.475588
30	1	0	2.359085	-0.060737	-1.376545
31	6	0	3.928146	-1.955509	-0.737695
32	8	0	4.498227	-3.048698	-0.193069
33	8	0	4.493098	-1.213114	-1.501049
34	1	0	1.625948	4.740582	-1.637034
35	1	0	2.438398	0.200887	0.278529
36	1	0	-1.844584	-1.713546	1.512289
37	1	0	5.406954	-3.109380	-0.526146
38	1	0	0.298424	1.543505	0.862173
39	6	0	2.396317	1.609165	3.918599
40	1	0	1.664132	1.217577	4.625990
41	6	0	1.927537	1.386454	2.489302
42	8	0	0.676715	1.505847	2.282862
43	8	0	2.785382	1.128827	1.606462
44	1	0	3.373748	1.154490	4.078285
45	1	0	2.479659	2.686854	4.089438

HF=-1650.9597256\ZeroPoint=0.328074\Thermal=0.35412

G = -1.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.247858	-0.137808	0.100319
2	7	0	-1.809434	0.086231	-0.189407
3	7	0	-2.455916	1.152688	-0.266301
4	6	0	-1.815629	2.359325	0.076828
5	6	0	-0.992171	2.490296	1.205800
6	6	0	-0.441553	3.733662	1.497114
7	1	0	0.181119	3.846616	2.377151
8	6	0	-0.690388	4.830690	0.671203
9	6	0	-1.528156	4.696586	-0.437239
10	1	0	-1.732387	5.550466	-1.072397
11	6	0	-2.116715	3.469766	-0.719621
12	1	0	-2.782318	3.347020	-1.565254
13	6	0	-2.552608	-1.103059	-0.503228
14	6	0	-2.136074	-2.307073	0.068688
15	6	0	-2.836998	-3.475037	-0.214706
16	1	0	-2.524346	-4.408328	0.238330
17	6	0	-3.929192	-3.445716	-1.080392
18	1	0	-4.463432	-4.360217	-1.311126
19	6	0	-4.329491	-2.239201	-1.658900
20	1	0	-5.169297	-2.217288	-2.343649
21	6	0	-3.650645	-1.062628	-1.368376
22	1	0	-3.944908	-0.120967	-1.811466
23	16	0	0.609836	0.237573	-2.159130
24	6	0	2.451542	0.297892	-2.093534
25	1	0	2.840979	0.028604	-3.076289
26	1	0	2.788951	1.310211	-1.851124
27	6	0	2.963568	-0.677136	-1.027181
28	1	0	2.703982	-1.696573	-1.315015
29	7	0	2.299800	-0.369265	0.256894
30	1	0	2.713650	0.473981	0.654879
31	6	0	4.473545	-0.552520	-0.882824
32	8	0	5.121588	-1.234018	-1.849612
33	8	0	5.029855	0.108297	-0.041648
34	1	0	-0.247654	5.793024	0.901343
35	1	0	2.388262	-1.111516	0.973209
36	1	0	-1.289213	-2.312938	0.742504
37	1	0	6.072422	-1.080420	-1.737083
38	1	0	-0.828973	1.644289	1.861667
39	6	0	0.148896	-1.530395	4.278555
40	1	0	-0.892614	-1.858886	4.265414
41	6	0	0.645825	-1.329402	2.855530
42	8	0	-0.102851	-0.548652	2.146503
43	8	0	1.682918	-1.885361	2.467119
44	1	0	0.769399	-2.259564	4.797131
45	1	0	0.181789	-0.575528	4.809675

HF=-1650.9953787\ZeroPoint=0.3313774\Thermal=0.3584102

Structures from Table S4

Table S4. **PATH I**: B3LYP-D3/6-311+G**/SDD(Pd)/gas phase free energies for the pre- and postreaction complexes and the transition states for **the first D-transfer to D1-1**. Free energies relative to **B1-1** (in kcal mol^{-1}).

D-source→	**Cys^{4D}**·DCl	**Cys^{4D}**·DCl	DCl
Donor group→	COOD	ND_3^+	DCl
Prereaction complex	**-17.6**	-15.6	15.3
Transition state	**9.0**	10.8	24.0
Postreaction complex	**-3.5**	3.3	-8.2

G = -17.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	46	0	2.587172	-0.471695	-0.513895
2	7	0	1.011647	0.614954	-1.409004
3	7	0	-0.058289	-0.084293	-1.577785
4	6	0	0.176794	-1.460308	-1.646986
5	6	0	1.426636	-1.939052	-1.183716
6	6	0	1.662486	-3.308811	-1.258530
7	1	0	2.598988	-3.719723	-0.899575
8	6	0	0.699922	-4.166361	-1.798708
9	6	0	-0.515582	-3.672640	-2.278212
10	1	0	-1.253088	-4.346252	-2.696005
11	6	0	-0.782624	-2.315642	-2.203046
12	1	0	-1.705469	-1.911356	-2.594157
13	6	0	0.791573	1.993244	-1.311167
14	6	0	1.865309	2.874727	-1.497672
15	6	0	1.643751	4.240719	-1.399149
16	1	0	2.459107	4.936994	-1.556307
17	6	0	0.357368	4.710933	-1.116858
18	1	0	0.182475	5.778299	-1.032912
19	6	0	-0.714498	3.826108	-0.972265
20	1	0	-1.706282	4.224033	-0.791999
21	6	0	-0.528253	2.446752	-1.084237
22	16	0	3.749268	-1.856981	0.957098
23	6	0	4.621696	-0.560561	1.945683
24	1	0	3.974900	-0.231849	2.762188
25	1	0	5.524988	-1.000702	2.366410
26	6	0	4.974839	0.656534	1.096293
27	1	0	5.414153	1.423270	1.752967
28	7	0	3.761389	1.168043	0.426890
29	1	0	4.011618	1.920739	-0.206372
30	6	0	6.026145	0.395220	0.023682
31	8	0	7.060350	-0.323254	0.497782
32	8	0	5.971925	0.834371	-1.097083
33	1	0	0.901560	-5.231025	-1.845340
34	1	0	3.106451	1.527497	1.119423
35	1	0	2.836037	2.481092	-1.774013
36	1	0	7.696307	-0.438507	-0.224402
37	1	0	1.919526	-1.645391	2.047283
38	16	0	-2.975044	1.582528	3.432449
39	6	0	-1.172877	1.325354	3.190112
40	1	0	-0.745139	2.159521	2.637706
41	1	0	-0.725189	1.319093	4.186307
42	6	0	-0.842730	0.029839	2.436393
43	1	0	-1.193988	0.130407	1.399928
44	7	0	-1.547148	-1.157410	3.002951
45	1	0	-2.433823	-0.835230	3.411665
46	6	0	0.662632	-0.199855	2.350149
47	8	0	0.984113	-1.481187	2.387566
48	8	0	1.432987	0.729162	2.235291
49	1	0	-0.992555	-1.642703	3.706771
50	1	0	-3.250679	1.836774	2.108281
51	46	0	-1.851595	0.947003	-1.070894
52	16	0	-3.548247	2.243309	-0.192586
53	6	0	-4.949966	1.058449	-0.382416
54	1	0	-5.724850	1.320521	0.339755
55	1	0	-5.368374	1.155732	-1.387748
56	6	0	-4.469678	-0.375510	-0.150956
57	1	0	-4.144197	-0.494862	0.882349
58	7	0	-3.317423	-0.680091	-1.023835
59	6	0	-5.605172	-1.356325	-0.412552
60	1	0	-3.675271	-0.895496	-1.954554
61	1	0	-2.894196	-1.544988	-0.655560
62	8	0	-6.446793	-1.431942	0.637234
63	8	0	-5.767192	-1.954741	-1.446606
64	1	0	-7.153401	-2.054822	0.407796
65	1	0	-1.822738	-1.897083	2.212839
66	17	0	-2.475883	-2.994965	0.959010

HF=-3453.6776377\ZeroPoint=0.4598708\Thermal=0.5022469

G = 9.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	46	0	2.671516	-0.615885	-0.380015
2	7	0	1.023850	0.469003	-1.170126
3	7	0	-0.062755	-0.199883	-1.352139
4	6	0	0.114667	-1.593208	-1.325502
5	6	0	1.235916	-2.123723	-0.628779

6	6	0	1.410485	-3.514838	-0.643351
7	1	0	2.235427	-3.943101	-0.086421
8	6	0	0.512234	-4.341812	-1.315473
9	6	0	-0.580499	-3.791959	-1.984225
10	1	0	-1.287858	-4.437648	-2.490011
11	6	0	-0.786686	-2.414623	-1.992338
12	1	0	-1.620918	-1.983727	-2.528464
13	6	0	0.859628	1.851749	-1.215228
14	6	0	1.974234	2.676085	-1.442764
15	6	0	1.796906	4.048781	-1.484070
16	1	0	2.641094	4.699926	-1.676938
17	6	0	0.517237	4.585882	-1.295384
18	1	0	0.380557	5.661938	-1.315293
19	6	0	-0.592145	3.757541	-1.116339
20	1	0	-1.574744	4.202643	-1.015066
21	6	0	-0.454126	2.367959	-1.097436
22	16	0	4.311515	-1.966599	0.486311
23	6	0	4.980047	-0.780597	1.721048
24	1	0	4.315931	-0.743159	2.588056
25	1	0	5.958248	-1.137602	2.044336
26	6	0	5.087175	0.616336	1.117341
27	1	0	5.418669	1.322538	1.893452
28	7	0	3.772214	1.013756	0.579132
29	1	0	3.855255	1.880382	0.057639
30	6	0	6.106266	0.732984	-0.009997
31	8	0	7.278948	0.157645	0.311287
32	8	0	5.911110	1.328892	-1.039795
33	1	0	0.651578	-5.416351	-1.302153
34	1	0	3.082033	1.145623	1.327395
35	1	0	2.939827	2.230962	-1.650270
36	1	0	7.883005	0.278250	-0.436850
37	1	0	1.237360	-1.666281	0.629469
38	16	0	-3.053179	1.746437	3.541511
39	6	0	-1.264086	1.384905	3.282707
40	1	0	-0.769630	2.236197	2.820395
41	1	0	-0.830629	1.247916	4.276306
42	6	0	-1.031031	0.163683	2.402316
43	1	0	-1.490362	0.347307	1.422690
44	7	0	-1.693193	-1.064483	2.944133
45	1	0	-2.554573	-0.795911	3.431737
46	6	0	0.453994	-0.129880	2.102310
47	8	0	0.688271	-1.366780	1.866338
48	8	0	1.236057	0.822565	2.053065
49	1	0	-1.072883	-1.576047	3.571213
50	1	0	-3.320315	2.008610	2.229521
51	46	0	-1.837236	0.926259	-1.054413
52	16	0	-3.507634	2.318008	-0.292966
53	6	0	-4.953047	1.198025	-0.541732
54	1	0	-5.751213	1.510363	0.133403
55	1	0	-5.311455	1.297431	-1.569850
56	6	0	-4.557021	-0.252910	-0.262235
57	1	0	-4.301733	-0.372407	0.790772
58	7	0	-3.368408	-0.627263	-1.056971
59	6	0	-5.718930	-1.183421	-0.584793
60	1	0	-3.678978	-0.844131	-2.004364
61	1	0	-3.014982	-1.506796	-0.643745
62	8	0	-6.628088	-1.204805	0.408734
63	8	0	-5.842784	-1.787378	-1.621258
64	1	0	-7.346865	-1.798334	0.142314
65	1	0	-1.985655	-1.765149	2.159941
66	17	0	-2.740688	-2.953350	0.933832

HF=-3453.6328328\ZeroPoint=0.4562125\Thermal=0.4982375

G = -3.5 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-2.438325	0.780156	-0.290224
2	7	0	-0.664178	-0.089606	-1.286538
3	7	0	0.374765	0.669608	-1.217965
4	6	0	0.105882	2.024756	-0.922416
5	6	0	-0.804975	2.370071	0.095291
6	6	0	-1.137092	3.716957	0.295019
7	1	0	-1.819554	3.972000	1.095956
8	6	0	-0.553740	4.700436	-0.494156
9	6	0	0.384604	4.344487	-1.466811
10	1	0	0.853112	5.114386	-2.069047
11	6	0	0.721377	3.009365	-1.686843
12	1	0	1.420564	2.724869	-2.463521
13	6	0	-0.358484	-1.395107	-1.663194
14	6	0	-1.381168	-2.279548	-2.037338
15	6	0	-1.055701	-3.568051	-2.415390
16	1	0	-1.834583	-4.261484	-2.707382
17	6	0	0.284856	-3.973650	-2.407095
18	1	0	0.537529	-4.990110	-2.689862
19	6	0	1.304239	-3.087171	-2.054883
20	1	0	2.333344	-3.426258	-2.075064
21	6	0	1.013219	-1.771135	-1.696494
22	16	0	-4.012908	1.853164	0.977724
23	6	0	-4.767083	0.330600	1.683425
24	1	0	-4.066350	-0.134248	2.378834
25	1	0	-5.682394	0.611963	2.205113
26	6	0	-5.046433	-0.628968	0.537850
27	1	0	-5.385320	-1.595459	0.937351
28	7	0	-3.798757	-0.842058	-0.239001
29	1	0	-4.057740	-1.123376	-1.182724
30	6	0	-6.134470	-0.164300	-0.422654
31	8	0	-7.222752	0.283304	0.227178
32	8	0	-6.058712	-0.247455	-1.623801
33	1	0	-0.802205	5.742967	-0.337879
34	1	0	-3.203820	-1.578655	0.218764
35	1	0	-2.407264	-1.947381	-2.048581
36	1	0	-7.880149	0.540147	-0.436977
37	1	0	-0.939077	1.672556	0.936621
38	16	0	2.463664	-3.402297	2.197963
39	6	0	0.656554	-3.250329	1.880987
40	1	0	0.402191	-3.664643	0.907753
41	1	0	0.182159	-3.873557	2.643154
42	6	0	0.114087	-1.822172	1.938131
43	1	0	0.490989	-1.260811	1.082626
44	7	0	0.541952	-1.079739	3.164314
45	1	0	1.264523	-1.585882	3.680763
46	6	0	-1.444079	-1.809155	1.900726
47	8	0	-2.017394	-1.193663	2.823022

48	8	0	-1.949474	-2.413007	0.923489
49	1	0	-0.325980	-0.931562	3.708075
50	1	0	2.895343	-2.647054	1.154207
51	46	0	2.211201	-0.267128	-1.163416
52	16	0	4.082456	-1.560683	-0.882922
53	6	0	5.274471	-0.233987	-0.401170
54	1	0	6.059347	-0.681368	0.209592
55	1	0	5.732284	0.179059	-1.304684
56	6	0	4.562980	0.874179	0.381719
57	1	0	4.184752	0.477541	1.325735
58	7	0	3.397559	1.379612	-0.373991
59	6	0	5.534230	2.007926	0.679375
60	1	0	3.711261	2.073663	-1.051130
61	1	0	2.777503	1.844746	0.302138
62	8	0	6.400483	1.675122	1.656236
63	8	0	5.561947	3.062415	0.092911
64	1	0	7.006036	2.421068	1.785670
65	1	0	0.938880	-0.125708	2.897646
66	17	0	1.601123	1.567102	2.212681

HF=-3453.654051\ZeroPoint=0.4602939\Thermal=0.5029912

G = -15.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-2.248155	0.117242	0.829400
2	7	0	-0.592376	1.395869	0.655861
3	7	0	0.486777	0.978446	1.222725
4	6	0	0.268896	-0.041669	2.158925
5	6	0	-1.024315	-0.620136	2.233859
6	6	0	-1.219694	-1.623527	3.184736
7	1	0	-2.191080	-2.096791	3.275202
8	6	0	-0.186348	-2.019031	4.039435
9	6	0	1.069898	-1.410332	3.971042
10	1	0	1.857986	-1.701638	4.654997
11	6	0	1.299217	-0.413986	3.032377
12	1	0	2.246600	0.106225	2.999550
13	6	0	-0.413855	2.464470	-0.222366
14	6	0	-1.518587	3.255895	-0.578200
15	6	0	-1.319214	4.339166	-1.420078
16	1	0	-2.155110	4.971766	-1.693850
17	6	0	-0.034748	4.619272	-1.898879
18	1	0	0.117151	5.462148	-2.564591
19	6	0	1.062216	3.842653	-1.517198
20	1	0	2.048063	4.098363	-1.886272
21	6	0	0.901085	2.757691	-0.655966
22	16	0	-3.921053	-1.440303	1.176443
23	6	0	-4.950708	-1.144502	-0.335072
24	1	0	-4.632119	-1.815888	-1.133484
25	1	0	-5.988815	-1.354182	-0.079429
26	6	0	-4.806920	0.290892	-0.838584
27	1	0	-5.330115	0.368836	-1.802941
28	7	0	-3.372943	0.607792	-0.996953
29	1	0	-3.257424	1.564792	-1.318431
30	6	0	-5.429732	1.344514	0.065784
31	8	0	-6.679949	1.016552	0.438577
32	8	0	-4.893542	2.381875	0.372344
33	1	0	-0.368645	-2.794409	4.775893
34	1	0	-2.991753	-0.008671	-1.731853
35	1	0	-2.493389	3.052480	-0.149300
36	1	0	-7.019932	1.733605	0.994775
37	1	0	-1.411844	-1.847930	0.031095
38	16	0	0.652929	-3.817783	-3.203759
39	6	0	0.403622	-4.328056	-1.457630
40	1	0	-0.395823	-5.069570	-1.381984
41	1	0	1.336056	-4.814367	-1.170229
42	6	0	0.136924	-3.194249	-0.455965
43	1	0	0.253878	-3.583507	0.559502
44	7	0	-1.251323	-2.675742	-0.573862
45	1	0	-1.942117	-3.361925	-0.265223
46	6	0	1.165445	-2.074287	-0.591395
47	8	0	0.658432	-0.971305	-1.119534
48	8	0	2.307701	-2.231393	-0.226114
49	1	0	-1.571434	-2.355118	-1.562068
50	1	0	-0.554089	-3.223502	-3.394217
51	46	0	2.250843	1.520153	0.144155
52	16	0	3.823234	1.990555	-1.459420
53	6	0	5.259887	1.097028	-0.729934
54	1	0	5.970275	0.884959	-1.529714
55	1	0	5.755059	1.727410	0.014867
56	6	0	4.795008	-0.209600	-0.082680
57	1	0	4.364238	-0.858749	-0.845754
58	7	0	3.738874	0.070816	0.915742
59	6	0	5.965624	-0.928606	0.573587
60	1	0	4.187320	0.388995	1.774655
61	1	0	3.271382	-0.806781	1.134638
62	8	0	6.792646	-1.466118	-0.343525
63	8	0	6.156734	-0.989560	1.763995
64	1	0	7.533631	-1.879963	0.125303
65	17	0	-2.547720	-1.774304	-3.070682
66	1	0	1.326470	-0.245390	-1.130615

HF=-3453.6764417\ZeroPoint=0.4611937\Thermal=0.5036638

G = 10.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	2.340754	-0.334370	-0.536081
2	7	0	0.513818	0.833379	-0.692471
3	7	0	-0.493706	0.163274	-1.147075
4	6	0	-0.234358	-1.178674	-1.462406
5	6	0	0.857749	-1.836834	-0.847472
6	6	0	1.076136	-3.184912	-1.174647
7	1	0	1.900536	-3.709649	-0.704609
8	6	0	0.251113	-3.850446	-2.074587
9	6	0	-0.805568	-3.169401	-2.687201
10	1	0	-1.433477	-3.679004	-3.408733
11	6	0	-1.052831	-1.835442	-2.385139
12	1	0	-1.839215	-1.288052	-2.888304
13	6	0	0.193993	2.140223	-0.343347
14	6	0	1.166827	2.992216	0.207296
15	6	0	0.842589	4.310702	0.470984

16	1	0	1.582025	4.968829	0.910161
17	6	0	-0.447108	4.778298	0.196985
18	1	0	-0.695101	5.816074	0.392660
19	6	0	-1.435964	3.915744	-0.281447
20	1	0	-2.441029	4.291528	-0.431456
21	6	0	-1.148605	2.578221	-0.539585
22	16	0	4.048003	-1.868206	-0.371787
23	6	0	5.290295	-0.764545	0.418582
24	1	0	5.043431	-0.627480	1.472834
25	1	0	6.272020	-1.228344	0.322425
26	6	0	5.253757	0.590667	-0.273142
27	1	0	5.931400	1.284776	0.245023
28	7	0	3.868183	1.109630	-0.207072
29	1	0	3.772809	1.930761	-0.800247
30	6	0	5.700856	0.573395	-1.728479
31	8	0	6.850892	-0.107977	-1.889443
32	8	0	5.135374	1.154412	-2.619936
33	1	0	0.432899	-4.892334	-2.311040
34	1	0	3.647512	1.327515	0.786422
35	1	0	2.127092	2.605241	0.499643
36	1	0	7.090834	-0.063391	-2.827212
37	1	0	1.049859	-1.599266	0.418321
38	16	0	-0.105328	-0.404320	4.949223
39	6	0	-0.276908	-2.016180	4.087752
40	1	0	0.518480	-2.693668	4.409531
41	1	0	-1.223942	-2.429497	4.442148
42	6	0	-0.280873	-2.005342	2.541822
43	1	0	-0.492556	-3.028029	2.216689
44	7	0	0.997284	-1.602133	1.945264
45	1	0	1.747296	-2.235412	2.216402
46	6	0	-1.413198	-1.163861	1.959899
47	8	0	-1.087884	0.119307	1.859642
48	8	0	-2.481046	-1.631251	1.619315
49	1	0	1.316947	-0.660408	2.229055
50	1	0	1.035116	0.015604	4.344112
51	46	0	-2.371582	1.057151	-0.933431
52	16	0	-4.271444	2.202478	-0.337757
53	6	0	-5.514951	0.871034	-0.621147
54	1	0	-6.391223	1.085941	-0.008734
55	1	0	-5.821352	0.863580	-1.671705
56	6	0	-4.930864	-0.492622	-0.239569
57	1	0	-4.686150	-0.500867	0.823362
58	7	0	-3.676796	-0.727654	-0.989690
59	6	0	-5.934600	-1.600707	-0.527300
60	1	0	-3.918763	-1.049425	-1.926203
61	1	0	-3.172044	-1.490431	-0.540898
62	8	0	-6.946841	-1.594400	0.360442
63	8	0	-5.860233	-2.373067	-1.452358
64	1	0	-7.569969	-2.294557	0.112097
65	17	0	2.847944	0.920801	2.732226
66	1	0	-1.808637	0.618283	1.421977

HF=-3453.6302252\ZeroPoint=0.4569333\Thermal=0.4992883

G = 3.3 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	2.317191	-0.712086	0.067135
2	7	0	0.554524	0.190576	-0.846210
3	7	0	-0.402758	-0.667079	-0.836302
4	6	0	-0.072871	-1.881907	-0.176225
5	6	0	0.499147	-1.836659	1.115701
6	6	0	0.849580	-3.053704	1.729510
7	1	0	1.298775	-3.027947	2.714511
8	6	0	0.612525	-4.261483	1.090628
9	6	0	0.000652	-4.279609	-0.170056
10	1	0	-0.188973	-5.226522	-0.662277
11	6	0	-0.348016	-3.096181	-0.809116
12	1	0	-0.791527	-3.094115	-1.797438
13	6	0	0.200705	1.412013	-1.396811
14	6	0	1.156362	2.430760	-1.541652
15	6	0	0.774300	3.623676	-2.129584
16	1	0	1.493149	4.426727	-2.234217
17	6	0	-0.549589	3.800353	-2.547229
18	1	0	-0.844069	4.740558	-3.001319
19	6	0	-1.510983	2.803927	-2.355864
20	1	0	-2.536763	2.987231	-2.652236
21	6	0	-1.163568	1.590716	-1.771600
22	16	0	3.967068	-1.922525	1.100909
23	6	0	5.292320	-0.646677	0.993511
24	1	0	5.114498	0.136171	1.732413
25	1	0	6.249953	-1.129772	1.188409
26	6	0	5.252859	-0.027885	-0.394310
27	1	0	5.961601	0.811192	-0.449656
28	7	0	3.883739	0.486063	-0.630158
29	1	0	3.753043	0.690279	-1.619581
30	6	0	5.625933	-0.978530	-1.523640
31	8	0	6.753701	-1.660253	-1.249934
32	8	0	5.025786	-1.065735	-2.565250
33	1	0	0.887665	-5.193695	1.568899
34	1	0	3.736423	1.346678	-0.036511
35	1	0	2.148410	2.318529	-1.131416
36	1	0	6.949207	-2.225657	-2.012237
37	1	0	0.454818	-0.911653	1.706113
38	16	0	-0.275046	3.898885	1.256207
39	6	0	-0.700557	3.230280	2.917616
40	1	0	0.050630	3.569513	3.632483
41	1	0	-1.656603	3.679462	3.185476
42	6	0	-0.791432	1.694471	2.981890
43	1	0	-1.090531	1.429803	4.006297
44	7	0	0.462528	0.994653	2.699926
45	1	0	1.074494	1.039549	3.508173
46	6	0	-1.921261	1.105698	2.118349
47	8	0	-2.831280	2.011516	1.753606
48	8	0	-2.001098	-0.073441	1.837363
49	1	0	0.982821	1.475343	1.965037
50	1	0	1.064914	3.690181	1.331607
51	46	0	-2.287377	0.044523	-1.212595
52	16	0	-4.298251	1.188291	-1.148194
53	6	0	-5.389169	-0.252808	-0.770374
54	1	0	-6.317532	0.121470	-0.337445
55	1	0	-5.630146	-0.782434	-1.696484
56	6	0	-4.701562	-1.209551	0.212856
57	1	0	-4.514064	-0.685110	1.151054

58	7	0	-3.392395	-1.640341	-0.324249
59	6	0	-5.590317	-2.415063	0.486906
60	1	0	-3.532801	-2.438477	-0.943039
61	1	0	-2.810092	-1.960631	0.446570
62	8	0	-6.643999	-2.087010	1.259365
63	8	0	-5.402864	-3.522887	0.046080
64	1	0	-7.195265	-2.877124	1.369725
65	17	0	3.267013	2.625403	1.406958
66	1	0	-3.414793	1.656445	1.043291

HF=-3453.64377\ZeroPoint=0.4597871\Thermal=0.502759

G = 15.3 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	2.354196	0.056973	0.096837
2	46	0	-2.513985	0.031787	-0.248342
3	7	0	0.330662	-0.457101	-0.016215
4	7	0	-0.491001	0.530587	-0.193523
5	6	0	0.107143	1.796182	-0.208653
6	6	0	1.481169	1.868939	0.124642
7	6	0	2.051532	3.133970	0.229221
8	1	0	3.088661	3.256701	0.526082
9	6	0	1.307996	4.287241	-0.041441
10	6	0	-0.020996	4.187210	-0.452622
11	1	0	-0.588202	5.076799	-0.698140
12	6	0	-0.628442	2.942508	-0.541068
13	1	0	-1.656907	2.857777	-0.862615
14	6	0	-0.272026	-1.720961	-0.006297
15	6	0	-1.654143	-1.778856	-0.317525
16	6	0	-2.229643	-3.042732	-0.436665
17	1	0	-3.269502	-3.156472	-0.730309
18	6	0	-1.487632	-4.203949	-0.200004
19	1	0	-1.958994	-5.175003	-0.309897
20	6	0	-0.151582	-4.117109	0.192622
21	1	0	0.415633	-5.013254	0.413155
22	6	0	0.462863	-2.877012	0.293030
23	1	0	1.497125	-2.803934	0.598411
24	16	0	-3.661423	2.089874	0.270080
25	6	0	-5.360642	1.510028	-0.117677
26	1	0	-5.564101	1.596280	-1.190441
27	1	0	-6.083482	2.127524	0.416318
28	6	0	-5.519744	0.049955	0.314485
29	1	0	-5.389559	-0.010680	1.396448
30	6	0	-6.888460	-0.494714	-0.066087
31	8	0	-7.857958	0.019435	0.713250
32	8	0	-7.093265	-1.266203	-0.971959
33	7	0	-4.458254	-0.769128	-0.324744
34	1	0	-4.444394	-1.695733	0.093856
35	1	0	-4.704908	-0.914260	-1.304989
36	16	0	3.556940	-1.986792	-0.311991
37	6	0	5.150466	-1.412958	0.401858
38	1	0	5.110279	-1.441034	1.493732
39	1	0	5.952445	-2.071190	0.067889
40	6	0	5.432064	0.013764	-0.047608
41	1	0	6.343630	0.393662	0.436234
42	7	0	4.283543	0.894555	0.307578
43	1	0	4.310638	1.720445	-0.289667
44	6	0	5.666160	0.158892	-1.548104
45	8	0	5.201394	1.047099	-2.218730
46	8	0	6.517646	-0.767455	-2.014083
47	1	0	1.774773	5.261917	0.053518
48	1	0	6.626290	-0.618924	-2.965548
49	1	0	4.364399	1.192197	1.278131
50	1	0	-8.709506	-0.324512	0.401836
51	1	0	2.564820	-0.161214	2.242656
52	17	0	3.109953	-0.075715	3.450648

HF=-2731.5126104\ZeroPoint=0.3603878\Thermal=0.3940292

G = 24.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-2.358572	0.136175	0.144232
2	46	0	2.465379	0.060054	-0.293712
3	7	0	-0.358886	0.644215	-0.111852
4	7	0	0.440540	-0.351172	-0.325758
5	6	0	-0.179378	-1.610250	-0.365532
6	6	0	-1.422065	-1.772664	0.300262
7	6	0	-2.033805	-3.030557	0.217372
8	1	0	-2.948157	-3.210890	0.772990
9	6	0	-1.454780	-4.075086	-0.495729
10	6	0	-0.243181	-3.878043	-1.163163
11	1	0	0.203577	-4.684301	-1.732512
12	6	0	0.400322	-2.649436	-1.102371
13	1	0	1.329626	-2.485919	-1.629430
14	6	0	0.274544	1.885284	-0.005807
15	6	0	1.682742	1.905267	-0.179288
16	6	0	2.308878	3.150381	-0.146512
17	1	0	3.378895	3.239574	-0.311576
18	6	0	1.582189	4.322012	0.083099
19	1	0	2.095254	5.277983	0.096591
20	6	0	0.203949	4.269543	0.302756
21	1	0	-0.353605	5.176785	0.501350
22	6	0	-0.458834	3.052291	0.259838
23	1	0	-1.526465	3.000055	0.419534
24	16	0	3.450727	-2.125268	-0.178188
25	6	0	5.200849	-1.596176	-0.372472
26	1	0	5.456363	-1.489274	-1.432216
27	1	0	5.856166	-2.352540	0.060232
28	6	0	5.424752	-0.260590	0.342256
29	1	0	5.241566	-0.399660	1.409294
30	6	0	6.841899	0.251945	0.130636
31	8	0	7.737969	-0.476289	0.821119
32	8	0	7.136762	1.175813	-0.588617
33	7	0	4.449253	0.738892	-0.166412
34	1	0	4.474893	1.570605	0.418565
35	1	0	4.749718	1.045538	-1.092850
36	16	0	-3.552189	1.999957	-0.635935
37	6	0	-5.035337	1.723064	0.420190
38	1	0	-4.824842	2.010537	1.452618
39	1	0	-5.851610	2.341479	0.046410

40	6	0	-5.420171	0.250092	0.379319
41	1	0	-6.238561	0.050391	1.085320
42	7	0	-4.241538	-0.582274	0.733343
43	1	0	-4.365303	-1.513765	0.338129
44	6	0	-5.921427	-0.220697	-0.983074
45	8	0	-5.601373	-1.263958	-1.495105
46	8	0	-6.821286	0.627833	-1.505992
47	1	0	-1.941954	-5.043005	-0.529253
48	1	0	-7.107179	0.269070	-2.359722
49	1	0	-4.122809	-0.678644	1.746462
50	1	0	8.623589	-0.136108	0.620062
51	1	0	-1.671108	-1.318376	1.610239
52	17	0	-2.111578	-1.273187	3.172038

HF=-2731.5004488\ZeroPoint=0.3588819\Thermal=0.3915532

G = -8.2 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-2.470727	0.856310	0.227249
2	46	0	2.321657	-0.006040	-0.076401
3	7	0	-0.404280	0.865539	0.114495
4	7	0	0.298232	-0.202547	0.119476
5	6	0	-0.378510	-1.432269	0.373654
6	6	0	-1.160182	-1.576361	1.525434
7	6	0	-1.833029	-2.773736	1.735129
8	1	0	-2.447285	-2.890329	2.619300
9	6	0	-1.726952	-3.810731	0.808453
10	6	0	-0.928710	-3.660151	-0.324939
11	1	0	-0.839460	-4.467241	-1.042299
12	6	0	-0.237842	-2.473472	-0.543094
13	1	0	0.385159	-2.337842	-1.415941
14	6	0	0.328895	2.045785	-0.049437
15	6	0	1.731023	1.916073	-0.195502
16	6	0	2.451473	3.092614	-0.402703
17	1	0	3.528137	3.067036	-0.545973
18	6	0	1.811077	4.334163	-0.441045
19	1	0	2.396331	5.233709	-0.601793
20	6	0	0.426232	4.432497	-0.270892
21	1	0	-0.058486	5.400902	-0.288546
22	6	0	-0.326285	3.285210	-0.076427
23	1	0	-1.397186	3.332766	0.072758
24	16	0	2.996905	-2.290359	0.084756
25	6	0	4.776652	-2.022061	-0.305074
26	1	0	4.936144	-2.026165	-1.388903
27	1	0	5.367398	-2.830396	0.126773
28	6	0	5.252654	-0.684882	0.272440
29	1	0	5.164585	-0.722850	1.359860
30	6	0	6.697025	-0.396475	-0.110297
31	8	0	7.552275	-1.202559	0.545541
32	8	0	7.040129	0.429989	-0.920803
33	7	0	4.374054	0.408137	-0.222579
34	1	0	4.581607	1.271035	0.274683
35	1	0	4.601959	0.593798	-1.200244
36	16	0	-2.669035	-0.013346	-1.931649
37	6	0	-4.469429	0.339774	-2.108248
38	1	0	-4.635101	1.387716	-2.373802
39	1	0	-4.867806	-0.284670	-2.908492
40	6	0	-5.187791	0.038513	-0.798679
41	1	0	-6.253228	0.300993	-0.876452
42	7	0	-4.551934	0.820539	0.296257
43	1	0	-4.784223	0.429766	1.210295
44	6	0	-5.149725	-1.433781	-0.396162
45	8	0	-4.944127	-1.822693	0.724919
46	8	0	-5.454966	-2.238902	-1.427885
47	1	0	-2.259469	-4.740130	0.976229
48	1	0	-5.410353	-3.153232	-1.110316
49	1	0	-4.867278	1.787560	0.287028
50	1	0	8.449996	-1.005703	0.236108
51	1	0	-1.224385	-0.770057	2.244774
52	17	0	-2.516130	1.781034	2.427815

HF=-2731.5550071\ZeroPoint=0.3636041\Thermal=0.3967983

Structures from Table S5

Table S5. **PATH I**: B3LYP-D3/6-311+G**/SDD(Pd)/gas phase free energies for the pre- and postreaction complexes and the transition states for **the first D-transfer to the bridged complexes**. Free energies relative to **B1-1** (in kcal mol^{-1}).

D-source→	**Cys^{4D}**·DCl	**Cys^{4D}**·DCl	DCl	**Cys^{3D}** (bridge)[a]	**Cys^{4D}** (coord)	**Cys^{4D}** (coord)
Donor group→	COOD	ND_3^+	DCl	COOD	COOD	ND_3^+
B1-1[b]				**B1-3**[b]	**B1-Cl-1**[b]	
Prereaction complex	**-21.4**	-17.2	-6.1	24.9	15.9	4.9
Transition state	**-0.6**	2.7	20.6	37.0	30.6	15.3
Postreaction complex	**-7.6**	-16.0	-17.0	11.6	25.1	10.9
B1-2[b]				**B1-4**[b]	**B1-Cl-2**[b]	
Prereaction complex	**-15.8**	-8.7	-0.6	33.5	6.8	13.8
Transition state	**-1.9**	2.3	12.2	40.1	31.9	25.5
Postreaction complex	**-35.7**	-28.8	-25.8	14.6	28.0	21.8

[a]Intramolecular D-transfer from the bridging COOD group. [b]Mother complex.

G = -21.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.604145	0.451709	1.623038
2	46	0	-1.398846	1.255985	0.114329
3	7	0	2.019935	1.549545	-0.053962
4	7	0	3.066601	1.265039	-0.706132
5	6	0	3.749988	0.164136	-0.206964
6	6	0	3.262529	-0.470659	0.964586
7	6	0	3.943094	-1.600450	1.406212
8	1	0	3.616860	-2.144207	2.287634
9	6	0	5.056078	-2.085865	0.706658
10	6	0	5.513336	-1.448809	-0.449298
11	1	0	6.366886	-1.843811	-0.986722
12	6	0	4.859378	-0.314016	-0.913845
13	1	0	5.166821	0.191450	-1.820649
14	6	0	1.299901	2.708367	-0.475885
15	6	0	-0.107154	2.726697	-0.448136
16	6	0	-0.718957	3.914888	-0.886448
17	1	0	-1.799927	3.973138	-0.914421
18	6	0	0.017950	5.021650	-1.297125
19	1	0	-0.498198	5.923491	-1.608589
20	6	0	1.413680	4.972452	-1.311429
21	1	0	1.994067	5.830444	-1.629935
22	6	0	2.053171	3.813300	-0.910670
23	1	0	3.133191	3.742504	-0.912490
24	16	0	-2.239391	1.152713	-2.107443
25	6	0	-3.707647	0.052279	-1.815921
26	1	0	-3.473200	-0.994876	-2.017705
27	1	0	-4.494894	0.363426	-2.499646
28	6	0	-4.178811	0.188489	-0.369731
29	1	0	-4.501564	1.222163	-0.202703
30	6	0	-5.377831	-0.687673	-0.001512
31	8	0	-6.238589	-0.843862	-1.026189
32	8	0	-5.561430	-1.138668	1.100197
33	7	0	-3.051094	-0.094543	0.546202
34	1	0	-3.389339	-0.080293	1.505263
35	1	0	-2.773907	-1.067391	0.376952
36	16	0	-0.464860	1.519443	2.290417
37	6	0	-1.009827	0.219094	3.499193
38	1	0	-0.900317	0.678381	4.484571
39	1	0	-2.063173	-0.019722	3.366075
40	6	0	-0.186445	-1.075018	3.456387
41	1	0	-0.367370	-1.626830	4.389609
42	7	0	1.263564	-0.774225	3.313126
43	1	0	1.769353	-1.646215	3.175948
44	6	0	-0.559272	-2.044042	2.330670
45	8	0	0.277912	-2.557489	1.621194
46	8	0	-1.858553	-2.267640	2.281119
47	1	0	5.561919	-2.976981	1.063187
48	1	0	-2.081879	-2.810234	1.462652
49	1	0	1.619647	-0.324517	4.153285
50	1	0	-0.018240	0.782373	-2.773361
51	8	0	0.844619	0.612259	-3.203935
52	6	0	1.480245	-0.478203	-2.761894
53	6	0	0.738517	-1.352631	-1.726586
54	8	0	2.582193	-0.756282	-3.153873
55	6	0	1.487477	-2.637517	-1.385861
56	1	0	0.614711	-0.758520	-0.813312
57	7	0	-0.643078	-1.663457	-2.210278
58	16	0	1.551578	-3.862284	-2.759221
59	1	0	0.981798	-3.132633	-0.557605
60	1	0	2.497150	-2.386433	-1.070269
61	1	0	-0.595635	-2.229126	-3.062761
62	1	0	-1.201437	-2.232713	-1.502782
63	1	0	2.421978	-3.166404	-3.518043

64	17	0	-2.562400	-3.205279	-0.445620
65	1	0	-6.976912	-1.387721	-0.710609
66	1	0	-1.185705	-0.782743	-2.372164

HF=-3453.6882292\ZeroPoint=0.4614252\Thermal=0.5033511

G = -0.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.764491	0.285419	1.440156
2	46	0	-1.413931	1.095076	-0.071519
3	7	0	2.260852	1.607244	-0.015530
4	7	0	3.410452	1.538514	-0.533028
5	6	0	4.132216	0.433973	-0.105927
6	6	0	3.550481	-0.431096	0.859636
7	6	0	4.274492	-1.557186	1.226797
8	1	0	3.882623	-2.264290	1.952112
9	6	0	5.526409	-1.819830	0.650086
10	6	0	6.079777	-0.956911	-0.296860
11	1	0	7.043637	-1.179871	-0.737962
12	6	0	5.380224	0.180899	-0.682253
13	1	0	5.766500	0.862283	-1.430284
14	6	0	1.446861	2.716535	-0.409567
15	6	0	0.129150	2.478713	-0.874480
16	6	0	-0.556211	3.609196	-1.368225
17	1	0	-1.535225	3.476910	-1.809164
18	6	0	-0.011908	4.890233	-1.313741
19	1	0	-0.586719	5.734869	-1.676288
20	6	0	1.272356	5.081165	-0.811209
21	1	0	1.705406	6.074227	-0.771355
22	6	0	2.016568	3.985856	-0.382993
23	1	0	3.034250	4.102831	-0.032498
24	16	0	-2.614800	1.040287	-2.120982
25	6	0	-4.195156	0.281991	-1.534304
26	1	0	-4.200199	-0.787785	-1.748051
27	1	0	-5.021736	0.754526	-2.062246
28	6	0	-4.330808	0.503408	-0.031933
29	1	0	-4.439698	1.575268	0.164107
30	6	0	-5.531382	-0.176159	0.623468
31	8	0	-6.633680	-0.112945	-0.145603
32	8	0	-5.507233	-0.664342	1.725108
33	7	0	-3.084296	0.033878	0.621758
34	1	0	-3.205795	0.028615	1.631356
35	1	0	-2.957919	-0.952792	0.349818
36	16	0	-0.329972	1.300876	2.066457
37	6	0	-0.810550	0.042412	3.341243
38	1	0	-0.560103	0.506811	4.298000
39	1	0	-1.884734	-0.135578	3.340302
40	6	0	-0.077524	-1.298129	3.225616
41	1	0	-0.233076	-1.852862	4.161562
42	7	0	1.379118	-1.104639	2.986082
43	1	0	1.775240	-1.996575	2.693406
44	6	0	-0.597350	-2.215617	2.115160
45	8	0	0.155116	-2.805986	1.370882
46	8	0	-1.911465	-2.295484	2.116724
47	1	0	6.068591	-2.713595	0.940904
48	1	0	-2.242437	-2.782895	1.293994
49	1	0	1.848807	-0.806792	3.837525
50	1	0	0.194895	1.363551	-1.614182
51	8	0	0.681627	0.564510	-2.556123
52	6	0	1.328752	-0.511664	-2.251516
53	6	0	0.450690	-1.628998	-1.630527
54	8	0	2.525595	-0.716646	-2.393215
55	6	0	1.116545	-2.994966	-1.548759
56	1	0	0.202924	-1.302058	-0.615953
57	7	0	-0.851186	-1.716285	-2.364730
58	16	0	1.444432	-3.755539	-3.195312
59	1	0	0.478545	-3.692289	-1.006027
60	1	0	2.053927	-2.888225	-1.007797
61	1	0	-0.697724	-2.175015	-3.267905
62	1	0	-1.553655	-2.266585	-1.811390
63	1	0	2.357845	-2.835487	-3.569902
64	17	0	-2.978874	-3.020978	-0.522859
65	1	0	-7.358375	-0.539562	0.337500
66	1	0	-1.261284	-0.770570	-2.513212

HF=-3453.6525867\ZeroPoint=0.457378\Thermal=0.4987135

G = -7.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.849762	-0.699349	1.239202
2	46	0	1.474842	-1.078826	-0.391501
3	7	0	-2.286018	-1.707882	-0.449974
4	7	0	-3.388175	-1.544181	-1.029314
5	6	0	-4.175598	-0.594002	-0.389033
6	6	0	-3.673564	0.021015	0.791675
7	6	0	-4.467000	0.981904	1.399153
8	1	0	-4.138131	1.491909	2.299860
9	6	0	-5.709252	1.331482	0.847076
10	6	0	-6.180428	0.721164	-0.315231
11	1	0	-7.136295	1.012512	-0.733154
12	6	0	-5.409910	-0.251759	-0.942720
13	1	0	-5.731386	-0.730979	-1.859172
14	6	0	-1.345484	-2.667388	-0.954867
15	6	0	-0.284017	-2.219766	-1.769356
16	6	0	0.704147	-3.154102	-2.128491
17	1	0	1.484121	-2.860030	-2.817543
18	6	0	0.654185	-4.470476	-1.653466
19	1	0	1.431692	-5.172917	-1.928283
20	6	0	-0.404961	-4.874529	-0.854143
21	1	0	-0.456965	-5.895697	-0.494023
22	6	0	-1.413628	-3.969832	-0.497466
23	1	0	-2.229886	-4.270450	0.147625
24	16	0	2.676384	-0.462178	-2.324332
25	6	0	4.234568	0.163658	-1.549151
26	1	0	4.226117	1.253731	-1.528703
27	1	0	5.082165	-0.177396	-2.141302
28	6	0	4.331922	-0.375235	-0.127913
29	1	0	4.489745	-1.457890	-0.161409
30	6	0	5.460921	0.195903	0.728980
31	8	0	6.573636	0.433471	0.014483

32	8	0	5.374252	0.357541	1.920179
33	7	0	3.036748	-0.114569	0.554956
34	1	0	3.117382	-0.325983	1.547001
35	1	0	2.870835	0.905277	0.494890
36	16	0	0.308852	-1.737617	1.627872
37	6	0	0.711054	-0.812630	3.181544
38	1	0	0.433881	-1.497390	3.986307
39	1	0	1.780332	-0.626666	3.270372
40	6	0	-0.045846	0.508316	3.362792
41	1	0	0.064705	0.815428	4.412348
42	7	0	-1.492066	0.381389	3.026262
43	1	0	-1.860406	1.321894	2.881917
44	6	0	0.504586	1.679944	2.543398
45	8	0	-0.228871	2.466440	1.986299
46	8	0	1.820568	1.727570	2.572323
47	1	0	-6.308681	2.096021	1.330378
48	1	0	2.176581	2.410094	1.916080
49	1	0	-2.004755	-0.052144	3.789716
50	1	0	-0.365010	-1.243029	-2.261962
51	8	0	-0.670579	0.524174	-2.908539
52	6	0	-1.351266	1.223619	-2.113990
53	6	0	-0.490049	2.161658	-1.204710
54	8	0	-2.572654	1.245131	-1.909761
55	6	0	-1.176939	3.446860	-0.776589
56	1	0	-0.236032	1.586550	-0.310648
57	7	0	0.801909	2.433207	-1.912074
58	16	0	-1.594840	4.543950	-2.198928
59	1	0	-0.543113	4.029320	-0.107360
60	1	0	-2.091269	3.179622	-0.252679
61	1	0	0.645790	3.168686	-2.608569
62	1	0	1.559573	2.720113	-1.255274
63	1	0	-2.462288	3.674470	-2.760513
64	17	0	2.998289	3.067811	0.239324
65	1	0	7.249983	0.775617	0.619746
66	1	0	1.062147	1.560954	-2.406012

HF=-3453.6636542\ZeroPoint=0.4608244\Thermal=0.5032794

G = -15.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.609803	-2.122302	0.637053
2	46	0	2.175845	-0.060604	0.677702
3	7	0	0.332807	-2.122290	-1.191847
4	7	0	-0.380163	-2.139682	-2.235035
5	6	0	-1.747928	-2.125419	-1.968476
6	6	0	-2.184698	-2.215357	-0.620194
7	6	0	-3.562310	-2.224207	-0.402429
8	1	0	-3.961905	-2.268675	0.604527
9	6	0	-4.463529	-2.126888	-1.471650
10	6	0	-4.007410	-2.021740	-2.788259
11	1	0	-4.714280	-1.943550	-3.605583
12	6	0	-2.639540	-2.031134	-3.043684
13	1	0	-2.250101	-1.965947	-4.053133
14	6	0	1.738039	-2.312817	-1.372636
15	6	0	2.650408	-1.608673	-0.568682
16	6	0	4.010696	-1.881715	-0.787789
17	1	0	4.759116	-1.366890	-0.193149
18	6	0	4.436943	-2.808340	-1.737147
19	1	0	5.496570	-3.006662	-1.859792
20	6	0	3.503442	-3.488457	-2.524225
21	1	0	3.828458	-4.214519	-3.260214
22	6	0	2.152834	-3.237404	-2.347559
23	1	0	1.407339	-3.756500	-2.936802
24	16	0	1.753906	1.945541	1.939748
25	6	0	2.960061	2.975828	1.007774
26	1	0	3.970836	2.740905	1.352421
27	1	0	2.763452	4.029122	1.211174
28	6	0	2.847588	2.715166	-0.499964
29	1	0	1.867729	3.046767	-0.841852
30	6	0	3.919244	3.488714	-1.251877
31	8	0	3.658462	4.810762	-1.262796
32	8	0	4.904338	2.999504	-1.749806
33	7	0	2.960722	1.267288	-0.803476
34	1	0	2.413448	1.065690	-1.637911
35	1	0	3.930900	1.036639	-1.016921
36	16	0	1.240777	-1.639486	2.117349
37	6	0	0.227136	-0.826846	3.460770
38	1	0	0.560157	-1.289976	4.390626
39	1	0	0.465724	0.232613	3.514569
40	6	0	-1.295745	-1.020201	3.310837
41	1	0	-1.722300	-1.140388	4.316615
42	7	0	-1.619952	-2.223064	2.490190
43	1	0	-2.627613	-2.252672	2.352051
44	6	0	-2.107164	0.131732	2.694528
45	8	0	-3.072843	-0.127234	1.994051
46	8	0	-1.709478	1.323354	3.044243
47	1	0	-5.530168	-2.131400	-1.272071
48	1	0	-2.267045	2.032910	2.583400
49	1	0	-1.330857	-3.071968	2.970047
50	1	0	0.132315	1.658249	0.702066
51	8	0	-0.770656	1.450505	0.278274
52	6	0	-0.801000	1.531795	-1.030686
53	6	0	-2.232519	1.526291	-1.567025
54	8	0	0.142375	1.665784	-1.782744
55	6	0	-2.564849	2.963950	-2.019117
56	1	0	-2.292302	0.829174	-2.403103
57	7	0	-3.192773	1.089077	-0.517664
58	16	0	-4.342005	3.229529	-2.412428
59	1	0	-1.986129	3.186909	-2.913665
60	1	0	-2.294328	3.670260	-1.234133
61	1	0	-3.284483	1.846765	0.250218
62	1	0	-4.116450	0.951619	-0.929637
63	1	0	-4.689176	3.589037	-1.154959
64	17	0	-3.379417	3.314553	1.460673
65	1	0	4.391749	5.257120	-1.713524
66	1	0	-2.911631	0.225922	-0.046167

HF=-3453.679164\ZeroPoint=0.4610797\Thermal=0.5028416

G = -1.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	46	0	-2.454638	-0.310899	0.831046
2	46	0	0.969223	-1.649662	0.404715
3	7	0	-2.527328	-1.020078	-1.079964
4	7	0	-3.358525	-0.505290	-1.879008
5	6	0	-4.074601	0.553325	-1.328790
6	6	0	-3.811244	0.931382	0.013329
7	6	0	-4.517919	2.020570	0.513600
8	1	0	-4.364376	2.366611	1.531877
9	6	0	-5.447775	2.703492	-0.283171
10	6	0	-5.692762	2.309938	-1.600207
11	1	0	-6.415277	2.846195	-2.203596
12	6	0	-5.001615	1.226539	-2.132396
13	1	0	-5.162411	0.895043	-3.151613
14	6	0	-1.744902	-2.098647	-1.616294
15	6	0	-0.342327	-2.079913	-1.454803
16	6	0	0.346882	-3.070582	-2.180957
17	1	0	1.429327	-3.084384	-2.181820
18	6	0	-0.301541	-4.060747	-2.915852
19	1	0	0.279282	-4.819800	-3.428149
20	6	0	-1.693193	-4.074587	-2.990340
21	1	0	-2.208672	-4.846668	-3.549785
22	6	0	-2.417688	-3.070387	-2.362560
23	1	0	-3.496498	-3.025797	-2.444130
24	16	0	2.438368	-1.620042	2.210067
25	6	0	4.036662	-1.392273	1.319090
26	1	0	4.515629	-2.363583	1.159022
27	1	0	4.688014	-0.778531	1.941735
28	6	0	3.800354	-0.700068	-0.023967
29	1	0	3.463758	0.323109	0.156536
30	6	0	5.081684	-0.678838	-0.843839
31	8	0	5.948146	0.244851	-0.388104
32	8	0	5.316925	-1.419879	-1.767766
33	7	0	2.743715	-1.432636	-0.761537
34	1	0	2.534498	-0.940483	-1.637669
35	1	0	3.108098	-2.350025	-1.014845
36	16	0	-0.917028	-1.906893	1.775450
37	6	0	-0.678398	-1.061957	3.411744
38	1	0	-1.270213	-1.633692	4.130587
39	1	0	0.368419	-1.117326	3.706870
40	6	0	-1.139853	0.398186	3.422871
41	1	0	-1.196828	0.732734	4.467757
42	7	0	-2.472758	0.527630	2.770214
43	1	0	-2.701916	1.514008	2.673433
44	6	0	-0.188874	1.374046	2.720112
45	8	0	-0.590305	2.137558	1.857495
46	8	0	1.025493	1.304174	3.190673
47	1	0	-5.984952	3.550445	0.131060
48	1	0	1.669712	1.823670	2.612491
49	1	0	-3.191143	0.084957	3.338452
50	1	0	0.010689	-0.663690	-1.410161
51	8	0	-0.036161	0.542386	-1.540950
52	6	0	0.991826	1.106311	-2.081962
53	6	0	0.949874	2.644733	-1.944947
54	8	0	1.933428	0.560516	-2.641479
55	6	0	2.315750	3.286644	-2.189126
56	1	0	0.213663	3.020997	-2.660394
57	7	0	0.436167	2.962361	-0.575711
58	16	0	2.374824	5.081317	-1.774935
59	1	0	2.565063	3.181941	-3.243288
60	1	0	3.081970	2.778304	-1.607837
61	1	0	1.211095	2.816486	0.148166
62	1	0	0.153242	3.939948	-0.503640
63	1	0	2.745183	4.893282	-0.487116
64	17	0	2.834121	2.667779	1.225885
65	1	0	6.754423	0.186613	-0.923182
66	1	0	-0.340528	2.349316	-0.311219

HF=-3453.6538078\ZeroPoint=0.4578468\Thermal=0.4993109

G = -35.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-2.005699	-0.907451	0.970448
2	46	0	1.636553	-0.841728	0.304126
3	7	0	-2.436416	-1.433804	-0.985893
4	7	0	-3.380514	-0.838360	-1.574367
5	6	0	-3.920466	0.204043	-0.825167
6	6	0	-3.469970	0.391478	0.507441
7	6	0	-3.977354	1.492586	1.194654
8	1	0	-3.649809	1.721039	2.203912
9	6	0	-4.905680	2.353309	0.591974
10	6	0	-5.348912	2.134522	-0.714058
11	1	0	-6.067464	2.807347	-1.166184
12	6	0	-4.855088	1.050635	-1.432106
13	1	0	-5.164934	0.855393	-2.452102
14	6	0	-1.891256	-2.563214	-1.675420
15	6	0	-0.513293	-2.639940	-1.867010
16	6	0	0.018638	-3.748797	-2.515514
17	1	0	1.089468	-3.808429	-2.668407
18	6	0	-0.818105	-4.772747	-2.958950
19	1	0	-0.396975	-5.641516	-3.451763
20	6	0	-2.197987	-4.681364	-2.768603
21	1	0	-2.849387	-5.476744	-3.111895
22	6	0	-2.743540	-3.571868	-2.131515
23	1	0	-3.810313	-3.484373	-1.967512
24	16	0	3.372557	-2.261944	0.825944
25	6	0	4.652235	-1.443539	-0.228103
26	1	0	4.577949	-1.811326	-1.255819
27	1	0	5.636284	-1.706286	0.163088
28	6	0	4.460050	0.076168	-0.215192
29	1	0	4.613773	0.448080	0.799058
30	6	0	5.454365	0.749139	-1.150378
31	8	0	6.687323	0.803555	-0.602205
32	8	0	5.198970	1.150675	-2.257700
33	7	0	3.073983	0.398848	-0.613578
34	1	0	2.840825	1.361043	-0.336399
35	1	0	2.956828	0.341809	-1.626279
36	16	0	0.041190	-2.176973	1.454872
37	6	0	0.286512	-1.558608	3.188330
38	1	0	-0.048601	-2.353698	3.860019
39	1	0	1.351235	-1.399125	3.349586
40	6	0	-0.495750	-0.285167	3.500823
41	1	0	-0.484422	-0.127624	4.589677

42	7	0	-1.902752	-0.431758	3.030368
43	1	0	-2.399368	0.437706	3.207971
44	6	0	0.017619	1.031705	2.900294
45	8	0	-0.777994	1.907209	2.599126
46	8	0	1.317602	1.108970	2.815634
47	1	0	-5.284889	3.202502	1.151057
48	1	0	1.602708	1.912570	2.272138
49	1	0	-2.369573	-1.174715	3.545746
50	1	0	0.124326	-1.825655	-1.547504
51	8	0	0.159403	0.660761	-0.142455
52	6	0	0.091758	1.155829	-1.319291
53	6	0	-0.691384	2.492097	-1.361720
54	8	0	0.564857	0.719039	-2.363124
55	6	0	0.007189	3.497116	-2.276262
56	1	0	-1.708823	2.292000	-1.707818
57	7	0	-0.787427	3.032509	0.028165
58	16	0	-0.812945	5.154295	-2.316301
59	1	0	0.005034	3.097521	-3.287516
60	1	0	1.044056	3.630385	-1.967752
61	1	0	0.190708	3.222137	0.392259
62	1	0	-1.336370	3.893471	0.047547
63	1	0	0.019782	5.761497	-1.446544
64	17	0	2.156144	3.247863	0.862806
65	1	0	7.282175	1.208318	-1.251904
66	1	0	-1.177684	2.345177	0.680561

HF=-3453.7058453\ZeroPoint=0.4610044\Thermal=0.5036036

G = -17.2 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.528608	0.107917	-0.682407
2	46	0	2.004905	1.351591	-0.276692
3	7	0	-1.357700	1.954844	-0.142289
4	7	0	-2.591604	2.184394	-0.144253
5	6	0	-3.530700	1.251475	-0.600489
6	6	0	-3.340281	0.387891	-1.692569
7	6	0	-4.361481	-0.475753	-2.070659
8	1	0	-4.209800	-1.146987	-2.907361
9	6	0	-5.573335	-0.483711	-1.379285
10	6	0	-5.781535	0.410207	-0.327233
11	1	0	-6.726412	0.419334	0.202470
12	6	0	-4.777028	1.294571	0.043595
13	1	0	-4.920789	1.999249	0.852421
14	6	0	-0.524037	3.076637	0.205476
15	6	0	0.884680	2.974909	0.153769
16	6	0	1.607403	4.156436	0.420092
17	1	0	2.688088	4.121254	0.400865
18	6	0	0.984482	5.353649	0.737704
19	1	0	1.584244	6.234607	0.940108
20	6	0	-0.412161	5.420209	0.814688
21	1	0	-0.907524	6.347236	1.078614
22	6	0	-1.158431	4.293662	0.545534
23	1	0	-2.237423	4.329243	0.583911
24	16	0	2.866354	1.498984	1.891633
25	6	0	4.281580	0.332025	1.704006
26	1	0	4.551065	-0.032991	2.695377
27	1	0	5.148980	0.843973	1.276095
28	6	0	3.902098	-0.846432	0.814086
29	1	0	4.762492	-1.520513	0.698900
30	6	0	2.775496	-1.675399	1.425784
31	8	0	1.755548	-1.943584	0.804056
32	8	0	3.027294	-2.069246	2.641697
33	7	0	3.462446	-0.333647	-0.515097
34	1	0	4.273354	0.073265	-0.977480
35	1	0	3.172615	-1.123546	-1.091431
36	16	0	0.674170	1.166460	-2.385692
37	6	0	1.377760	-0.306223	-3.260284
38	1	0	1.282812	-0.132504	-4.333225
39	1	0	2.438467	-0.358372	-3.023409
40	6	0	0.667617	-1.612898	-2.890100
41	1	0	-0.231599	-1.728085	-3.494085
42	7	0	0.256353	-1.663100	-1.464706
43	1	0	1.039058	-1.883478	-0.834158
44	6	0	1.635101	-2.767574	-3.151662
45	8	0	2.651793	-2.918928	-2.516407
46	8	0	1.248418	-3.564359	-4.156829
47	1	0	-6.358524	-1.171056	-1.671292
48	1	0	1.908790	-4.268452	-4.262763
49	1	0	-0.450505	-2.394684	-1.344314
50	1	0	-0.237791	-3.803754	1.972612
51	1	0	-2.419477	0.426544	-2.259031
52	7	0	-0.934677	-0.755378	1.285087
53	6	0	-1.799571	-1.915651	1.648787
54	1	0	0.023264	-0.985700	1.562673
55	1	0	-1.223449	0.022357	1.880815
56	6	0	-3.278915	-1.554503	1.605966
57	1	0	-1.521209	-2.224759	2.659359
58	6	0	-1.500539	-3.067702	0.676173
59	16	0	-3.707429	-0.204110	2.781920
60	1	0	-3.878858	-2.435185	1.834297
61	1	0	-3.561987	-1.203778	0.615835
62	8	0	-1.996877	-3.079004	-0.439549
63	8	0	-0.662105	-3.993835	1.068464
64	1	0	-3.320368	-0.853928	3.900673
65	1	0	2.215145	-2.552210	3.028892
66	17	0	0.551333	-3.302876	3.684967

HF=-3453.6788411\ZeroPoint=0.4615827\Thermal=0.5034194

G = 2.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.875911	-0.832465	1.099563
2	46	0	1.743914	1.514640	-0.455621
3	7	0	2.065144	-1.811657	-0.249596
4	7	0	1.840599	-3.035836	-0.479255
5	6	0	0.778935	-3.563513	0.241640
6	6	0	-0.184811	-2.703576	0.850478
7	6	0	-1.152466	-3.308981	1.666491
8	1	0	-1.909551	-2.689369	2.125132
9	6	0	-1.197216	-4.693749	1.823804

10	6	0	-0.283424	-5.516950	1.159829
11	1	0	-0.340181	-6.593395	1.271364
12	6	0	0.705658	-4.954828	0.361583
13	1	0	1.443857	-5.566732	-0.142299
14	6	0	3.127181	-1.194079	-0.964980
15	6	0	3.096987	0.200264	-1.177659
16	6	0	4.143273	0.735880	-1.949182
17	1	0	4.137880	1.792969	-2.181467
18	6	0	5.180656	-0.054081	-2.429577
19	1	0	5.979637	0.401988	-3.004330
20	6	0	5.199168	-1.431906	-2.178779
21	1	0	6.012037	-2.047101	-2.546203
22	6	0	4.169419	-2.004502	-1.459660
23	1	0	4.151164	-3.067495	-1.260509
24	16	0	0.899678	1.803059	-2.611434
25	6	0	0.176687	3.479973	-2.341048
26	1	0	-0.547222	3.672470	-3.133359
27	1	0	0.960696	4.240455	-2.399789
28	6	0	-0.518076	3.579254	-0.982995
29	1	0	-0.901455	4.598442	-0.843043
30	6	0	-1.727328	2.652354	-0.904093
31	8	0	-1.820151	1.756770	-0.073171
32	8	0	-2.613275	2.961018	-1.808291
33	7	0	0.441905	3.234100	0.098497
34	1	0	1.100847	4.004442	0.194678
35	1	0	-0.066524	3.183154	0.981873
36	16	0	2.455239	0.795915	1.753783
37	6	0	1.452428	1.752141	2.985280
38	1	0	2.047343	1.823517	3.896678
39	1	0	1.317283	2.759448	2.599307
40	6	0	0.096444	1.108637	3.312854
41	1	0	0.202354	0.402913	4.135245
42	7	0	-0.466957	0.358568	2.159596
43	1	0	-0.793282	1.002473	1.424029
44	6	0	-0.915217	2.198921	3.679337
45	8	0	-1.100906	3.178296	2.996820
46	8	0	-1.593473	1.922997	4.800560
47	1	0	-1.964454	-5.135566	2.449693
48	1	0	-2.261748	2.614789	4.935459
49	1	0	-1.311937	-0.160132	2.413528
50	1	0	-4.810702	0.567493	-0.364341
51	1	0	-0.710714	-1.774421	0.087637
52	7	0	-1.482685	-1.053367	-1.006131
53	6	0	-2.950742	-0.944428	-0.922111
54	1	0	-1.068519	-0.121744	-1.068920
55	1	0	-1.252237	-1.527720	-1.880545
56	6	0	-3.617963	-2.296106	-1.220815
57	1	0	-3.317170	-0.218415	-1.650044
58	6	0	-3.413725	-0.497322	0.472554
59	16	0	-3.258683	-2.918683	-2.915390
60	1	0	-4.696432	-2.209089	-1.093914
61	1	0	-3.248095	-3.065624	-0.539989
62	8	0	-2.827312	-0.841006	1.487243
63	8	0	-4.530456	0.183663	0.531188
64	1	0	-3.871837	-1.905900	-3.564445
65	1	0	-3.455948	2.381901	-1.819568
66	17	0	-5.104320	1.410268	-2.091109

HF=-3453.6467932\ZeroPoint=0.457563\Thermal=0.498894

G = -16.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.528608	0.107917	-0.682407
2	46	0	2.004905	1.351591	-0.276692
3	7	0	-1.357700	1.954844	-0.142289
4	7	0	-2.591604	2.184394	-0.144253
5	6	0	-3.530700	1.251475	-0.600489
6	6	0	-3.340281	0.387891	-1.692569
7	6	0	-4.361481	-0.475753	-2.070659
8	1	0	-4.209800	-1.146987	-2.907361
9	6	0	-5.573335	-0.483711	-1.379285
10	6	0	-5.781535	0.410207	-0.327233
11	1	0	-6.726412	0.419334	0.202470
12	6	0	-4.777028	1.294571	0.043595
13	1	0	-4.920789	1.999249	0.852421
14	6	0	-0.524037	3.076637	0.205476
15	6	0	0.884680	2.974909	0.153769
16	6	0	1.607403	4.156436	0.420092
17	1	0	2.688088	4.121254	0.400865
18	6	0	0.984482	5.353649	0.737704
19	1	0	1.584244	6.234607	0.940108
20	6	0	-0.412161	5.420209	0.814688
21	1	0	-0.907524	6.347236	1.078614
22	6	0	-1.158431	4.293662	0.545534
23	1	0	-2.237423	4.329243	0.583911
24	16	0	2.866354	1.498984	1.891633
25	6	0	4.281580	0.332025	1.704006
26	1	0	4.551065	-0.032991	2.695377
27	1	0	5.148980	0.843973	1.276095
28	6	0	3.902098	-0.846432	0.814086
29	1	0	4.762492	-1.520513	0.698900
30	6	0	2.775496	-1.675399	1.425784
31	8	0	1.755548	-1.943584	0.804056
32	8	0	3.027294	-2.069246	2.641697
33	7	0	3.462446	-0.333647	-0.515097
34	1	0	4.273354	0.073265	-0.977480
35	1	0	3.172615	-1.123546	-1.091431
36	16	0	0.674170	1.166460	-2.385692
37	6	0	1.377760	-0.306223	-3.260284
38	1	0	1.282812	-0.132504	-4.333225
39	1	0	2.438467	-0.358372	-3.023409
40	6	0	0.667617	-1.612898	-2.890100
41	1	0	-0.231599	-1.728085	-3.494085
42	7	0	0.256353	-1.663100	-1.464706
43	1	0	1.039058	-1.883478	-0.834158
44	6	0	1.635101	-2.767574	-3.151662
45	8	0	2.651793	-2.918928	-2.516407
46	8	0	1.248418	-3.564359	-4.156829
47	1	0	-6.358524	-1.171056	-1.671292
48	1	0	1.908790	-4.268452	-4.262763
49	1	0	-0.450505	-2.394684	-1.344314
50	1	0	-0.237791	-3.803754	1.972612
51	1	0	-2.419477	0.426544	-2.259031

52	7	0	-0.934677	-0.755378	1.285087
53	6	0	-1.799571	-1.915651	1.648787
54	1	0	0.023264	-0.985700	1.562673
55	1	0	-1.223449	0.022357	1.880815
56	6	0	-3.278915	-1.554503	1.605966
57	1	0	-1.521209	-2.224759	2.659359
58	6	0	-1.500539	-3.067702	0.676173
59	16	0	-3.707429	-0.204110	2.781920
60	1	0	-3.878858	-2.435185	1.834297
61	1	0	-3.561987	-1.203778	0.615835
62	8	0	-1.996877	-3.079004	-0.439549
63	8	0	-0.662105	-3.993835	1.068464
64	1	0	-3.320368	-0.853928	3.900673
65	1	0	2.215145	-2.552210	3.028892
66	17	0	0.551333	-3.302876	3.684967

HF=-3453.6788411\ZeroPoint=0.4615827\Thermal=0.5034194

G = -8.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.633865	-1.349629	-0.938094
2	46	0	-1.820382	-0.840022	-0.246737
3	7	0	1.506362	-1.640284	1.099245
4	7	0	2.568383	-1.471274	1.769348
5	6	0	3.651563	-1.026972	1.022270
6	6	0	3.477439	-0.771789	-0.361436
7	6	0	4.573210	-0.269859	-1.058826
8	1	0	4.505460	-0.050290	-2.120878
9	6	0	5.792126	-0.029575	-0.410726
10	6	0	5.942988	-0.298175	0.951391
11	1	0	6.893385	-0.116045	1.439182
12	6	0	4.867847	-0.798743	1.677783
13	1	0	4.946911	-1.015281	2.736872
14	6	0	0.360012	-2.073706	1.838754
15	6	0	-0.944323	-1.695551	1.448734
16	6	0	-1.967610	-2.122450	2.326721
17	1	0	-2.999483	-1.872984	2.104116
18	6	0	-1.734012	-2.892816	3.459167
19	1	0	-2.568738	-3.208471	4.076086
20	6	0	-0.430222	-3.274623	3.788349
21	1	0	-0.234873	-3.891420	4.657783
22	6	0	0.611844	-2.856842	2.985453
23	1	0	1.632293	-3.126675	3.222097
24	16	0	-3.429025	-0.296841	-1.937073
25	6	0	-4.765080	-0.149015	-0.689827
26	1	0	-4.972044	-1.117472	-0.224116
27	1	0	-5.677774	0.195081	-1.179521
28	6	0	-4.340321	0.867742	0.381534
29	1	0	-4.319720	1.858570	-0.076903
30	6	0	-5.321792	0.876381	1.537018
31	8	0	-6.528717	1.342724	1.160529
32	8	0	-5.084910	0.483000	2.655647
33	7	0	-2.970718	0.570685	0.895146
34	1	0	-2.436280	1.436679	0.803908
35	1	0	-3.026504	0.324823	1.883217
36	16	0	-0.510225	-2.205313	-1.592973
37	6	0	-0.518645	-1.519497	-3.318795
38	1	0	-0.286905	-2.357703	-3.981320
39	1	0	-1.518311	-1.161369	-3.557411
40	6	0	0.515955	-0.412574	-3.532410
41	1	0	0.600444	-0.211970	-4.609657
42	7	0	1.835164	-0.848647	-2.986861
43	1	0	2.496085	-0.077925	-3.050261
44	6	0	0.180312	0.931992	-2.870820
45	8	0	-1.039723	1.328523	-3.118657
46	8	0	1.011035	1.536928	-2.216032
47	1	0	6.628067	0.370525	-0.974625
48	1	0	2.199323	-1.630451	-3.526680
49	1	0	-7.119141	1.288713	1.927366
50	1	0	0.605507	0.672244	0.216934
51	7	0	0.603506	1.624501	0.607961
52	6	0	1.933897	2.281636	0.447492
53	1	0	-0.172882	2.158413	0.110016
54	1	0	0.374977	1.545076	1.603336
55	6	0	1.800751	3.758133	0.053965
56	1	0	2.458350	1.755691	-0.349657
57	6	0	2.709417	2.074170	1.737794
58	16	0	0.967094	4.811990	1.309502
59	1	0	1.256368	3.819993	-0.887233
60	1	0	2.802280	4.161222	-0.089822
61	8	0	2.262535	1.545451	2.723304
62	8	0	3.956774	2.552670	1.627943
63	1	0	-0.285497	4.580999	0.848134
64	17	0	-1.679116	3.145864	-0.693195
65	1	0	-1.315042	2.044886	-2.477883
66	1	0	4.426009	2.365589	2.454940

HF=-3453.665964\ZeroPoint=0.4610344\Thermal=0.5033347

G = 2.3 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.875223	-1.451281	-0.302459
2	46	0	-1.739948	-0.922280	0.491435
3	7	0	2.031874	-0.575982	1.529955
4	7	0	3.165370	-0.132464	1.879875
5	6	0	4.129222	-0.226170	0.884705
6	6	0	3.749371	-0.723239	-0.389734
7	6	0	4.713545	-0.710754	-1.390980
8	1	0	4.484276	-1.069764	-2.390015
9	6	0	6.004582	-0.227479	-1.136830
10	6	0	6.361113	0.244507	0.128479
11	1	0	7.365013	0.609176	0.309764
12	6	0	5.418647	0.250058	1.150030
13	1	0	5.656815	0.616515	2.142057
14	6	0	0.974764	-0.398459	2.481379
15	6	0	-0.287055	0.069013	2.042080
16	6	0	-1.165645	0.433716	3.083312
17	1	0	-2.112768	0.901336	2.846733
18	6	0	-0.881834	0.232239	4.431002
19	1	0	-1.614271	0.501425	5.183806

20	6	0	0.343174	-0.316055	4.806296
21	1	0	0.572170	-0.494736	5.850390
22	6	0	1.286440	-0.601201	3.829669
23	1	0	2.267442	-0.972782	4.096394
24	16	0	-3.441168	-2.256659	-0.365576
25	6	0	-4.848813	-1.213256	0.182276
26	1	0	-5.033649	-1.354975	1.251041
27	1	0	-5.736886	-1.527725	-0.368793
28	6	0	-4.527291	0.249812	-0.109189
29	1	0	-4.412429	0.394547	-1.184427
30	6	0	-5.633749	1.161382	0.398373
31	8	0	-6.736872	1.075631	-0.367458
32	8	0	-5.558983	1.849753	1.388131
33	7	0	-3.238939	0.625770	0.529982
34	1	0	-2.859856	1.391298	-0.041896
35	1	0	-3.444531	0.998774	1.455694
36	16	0	-0.202300	-2.618760	0.026511
37	6	0	-0.468129	-3.076740	-1.756743
38	1	0	-0.139850	-4.114231	-1.858405
39	1	0	-1.529530	-3.023216	-1.991636
40	6	0	0.323591	-2.192348	-2.717180
41	1	0	0.239891	-2.608080	-3.730953
42	7	0	1.754907	-2.144673	-2.298147
43	1	0	2.244507	-1.457663	-2.868216
44	6	0	-0.163488	-0.735667	-2.802813
45	8	0	-1.462216	-0.643064	-2.932065
46	8	0	0.626788	0.187820	-2.770087
47	1	0	6.737789	-0.219655	-1.936489
48	1	0	2.197549	-3.051322	-2.427069
49	1	0	-7.412688	1.656366	0.014634
50	1	0	-0.224593	0.917744	0.919541
51	7	0	-0.068038	1.986616	0.101209
52	6	0	1.274859	2.216938	-0.450632
53	1	0	-0.745159	1.900019	-0.675097
54	1	0	-0.343561	2.804826	0.644742
55	6	0	1.260710	3.109406	-1.708073
56	1	0	1.690662	1.249806	-0.753633
57	6	0	2.160183	2.766549	0.651999
58	16	0	0.452637	4.745107	-1.469816
59	1	0	0.741305	2.576827	-2.501623
60	1	0	2.285616	3.297808	-2.025257
61	8	0	1.796263	3.022442	1.771145
62	8	0	3.429079	2.928431	0.222842
63	1	0	-0.800325	4.305086	-1.727035
64	17	0	-2.343661	2.112740	-2.146502
65	1	0	-1.766431	0.313140	-2.808656
66	1	0	3.952540	3.255165	0.969440

HF=-3453.6450197\ZeroPoint=0.4571834\Thermal=0.4992004

G = -28.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-2.139115	0.050758	-1.073532
2	46	0	1.774161	0.556516	-0.215451
3	7	0	-2.959542	1.368162	0.311057
4	7	0	-4.109714	1.098668	0.762050
5	6	0	-4.622298	-0.109013	0.312199
6	6	0	-3.879055	-0.863987	-0.630883
7	6	0	-4.427818	-2.069851	-1.052691
8	1	0	-3.912248	-2.700098	-1.771206
9	6	0	-5.661936	-2.511092	-0.554367
10	6	0	-6.377164	-1.751123	0.372899
11	1	0	-7.329570	-2.105044	0.748396
12	6	0	-5.858561	-0.538112	0.810478
13	1	0	-6.386561	0.080029	1.527087
14	6	0	-2.441793	2.649857	0.676221
15	6	0	-1.091676	2.776645	1.002160
16	6	0	-0.584585	4.023560	1.348974
17	1	0	0.464169	4.114819	1.603446
18	6	0	-1.416999	5.141460	1.358191
19	1	0	-1.014930	6.114970	1.613745
20	6	0	-2.767921	5.008811	1.029826
21	1	0	-3.415327	5.878051	1.027395
22	6	0	-3.287743	3.765092	0.692652
23	1	0	-4.329690	3.646324	0.425217
24	16	0	2.941728	2.132660	-1.445475
25	6	0	4.568535	1.973883	-0.586420
26	1	0	4.598952	2.643027	0.278668
27	1	0	5.352148	2.274992	-1.283490
28	6	0	4.788735	0.532765	-0.127833
29	1	0	4.842118	-0.127355	-0.994556
30	6	0	6.080077	0.424070	0.672069
31	8	0	7.159708	0.387312	-0.133164
32	8	0	6.140554	0.418868	1.876434
33	7	0	3.641513	0.094345	0.701216
34	1	0	3.676972	-0.936559	0.779044
35	1	0	3.739009	0.486289	1.638436
36	16	0	-0.060021	1.139470	-1.617097
37	6	0	0.296018	0.146207	-3.138354
38	1	0	-0.225280	0.642328	-3.960667
39	1	0	1.367154	0.180335	-3.330632
40	6	0	-0.184477	-1.295502	-3.022455
41	1	0	-0.093925	-1.782385	-4.002583
42	7	0	-1.608313	-1.339387	-2.572179
43	1	0	-1.773340	-2.264222	-2.173662
44	6	0	0.618382	-2.159544	-2.040737
45	8	0	1.910539	-2.070359	-2.225591
46	8	0	0.050268	-2.850697	-1.215995
47	1	0	-6.065308	-3.458809	-0.895101
48	1	0	-2.238630	-1.206902	-3.358843
49	1	0	7.949619	0.350108	0.427941
50	1	0	-0.446358	1.911089	1.018756
51	7	0	0.991723	-1.060374	1.084302
52	6	0	-0.383014	-1.414925	1.458554
53	1	0	1.454343	-1.882042	0.676860
54	1	0	1.489807	-0.893073	1.958163
55	6	0	-0.514243	-2.887943	1.904059
56	1	0	-1.034512	-1.284869	0.587445
57	6	0	-0.864546	-0.449759	2.522627
58	16	0	0.655641	-3.393247	3.232913
59	1	0	-0.352762	-3.523552	1.036231
60	1	0	-1.519738	-3.065060	2.285256
61	8	0	-0.181677	0.375257	3.075270

62	8	0	-2.179617	-0.617809	2.778898
63	1	0	1.730046	-3.557641	2.425611
64	17	0	3.344552	-3.037950	0.176264
65	1	0	2.422681	-2.528957	-1.471501
66	1	0	-2.431287	0.023172	3.460874

HF=-3453.7006807\ZeroPoint=0.4649438\Thermal=0.5070997

46	8	0	0.138459	3.288937	0.537597
47	1	0	-5.525510	-3.009510	-0.374978
48	1	0	1.540227	-4.692148	-1.347386
49	1	0	0.181105	4.441367	-2.566713
50	1	0	0.779764	2.729023	1.030525

HF=-2270.6473927\ZeroPoint=0.3521741\Thermal=0.3831045

G = 24.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.463896	0.230697	-0.277694
2	46	0	1.841875	0.235168	-0.198102
3	7	0	-0.690423	-0.349759	1.616976
4	7	0	-1.380559	-1.190121	2.265283
5	6	0	-2.463815	-1.676504	1.545819
6	6	0	-2.789366	-1.115553	0.282090
7	6	0	-3.900358	-1.605622	-0.393588
8	1	0	-4.181020	-1.196127	-1.356676
9	6	0	-4.664164	-2.634559	0.167794
10	6	0	-4.339350	-3.181894	1.412696
11	1	0	-4.945619	-3.975376	1.833372
12	6	0	-3.240387	-2.699147	2.109477
13	1	0	-2.964045	-3.091316	3.081273
14	6	0	0.314201	0.347321	2.358511
15	6	0	1.505961	0.745789	1.715004
16	6	0	2.435367	1.469894	2.478496
17	1	0	3.381198	1.750195	2.029761
18	6	0	2.181555	1.814396	3.808187
19	1	0	2.915082	2.386696	4.365763
20	6	0	0.993203	1.414589	4.418505
21	1	0	0.789801	1.678993	5.449798
22	6	0	0.062008	0.678393	3.697326
23	1	0	-0.870863	0.364245	4.148067
24	16	0	3.370364	-1.315892	0.511141
25	6	0	3.956648	-1.821005	-1.168808
26	1	0	4.406539	-2.810723	-1.081663
27	1	0	4.721453	-1.127213	-1.529767
28	6	0	2.811171	-1.859570	-2.178684
29	1	0	3.204937	-2.147880	-3.164700
30	6	0	1.734889	-2.889036	-1.845905
31	8	0	0.551799	-2.673729	-1.902535
32	8	0	2.269529	-4.088073	-1.553074
33	7	0	2.155750	-0.528102	-2.244684
34	1	0	2.714669	0.106614	-2.808094
35	1	0	1.236133	-0.615453	-2.676871
36	16	0	-2.733425	1.078085	-2.030470
37	6	0	-1.746613	2.542204	-2.568415
38	1	0	-0.902609	2.220954	-3.185153
39	1	0	-2.407271	3.149012	-3.188574
40	6	0	-1.231803	3.435672	-1.436158
41	1	0	-2.062088	3.728356	-0.790007
42	7	0	-0.617880	4.654337	-1.977673
43	1	0	-0.320225	5.288196	-1.243873
44	6	0	-0.221558	2.684982	-0.573614
45	8	0	0.299782	1.621692	-0.959481

G = 37.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.597582	0.305617	-0.150138
2	46	0	1.758293	0.506534	-0.100223
3	7	0	-0.689360	-1.081291	1.253559
4	7	0	-1.337514	-2.164848	1.402490
5	6	0	-2.475985	-2.260168	0.628792
6	6	0	-2.907867	-1.161551	-0.165216
7	6	0	-4.093392	-1.298628	-0.881000
8	1	0	-4.460827	-0.480826	-1.489658
9	6	0	-4.821001	-2.490413	-0.819999
10	6	0	-4.386552	-3.569161	-0.040226
11	1	0	-4.966040	-4.484010	-0.004825
12	6	0	-3.215559	-3.454860	0.690802
13	1	0	-2.851409	-4.262547	1.314981
14	6	0	0.383527	-0.887689	2.179988
15	6	0	1.331635	0.147256	1.949757
16	6	0	2.366314	0.303689	2.899637
17	1	0	3.096766	1.087550	2.737839
18	6	0	2.459947	-0.497807	4.027503
19	1	0	3.261300	-0.349745	4.742114
20	6	0	1.505555	-1.497438	4.232265
21	1	0	1.563535	-2.129735	5.111509
22	6	0	0.471372	-1.689209	3.325558
23	1	0	-0.270807	-2.457792	3.489693
24	16	0	3.492776	-0.998627	0.024379
25	6	0	4.155192	-0.700332	-1.674303
26	1	0	4.753721	-1.565272	-1.962334
27	1	0	4.800736	0.182497	-1.683474
28	6	0	3.018410	-0.494248	-2.669800
29	1	0	3.428626	-0.268710	-3.664974
30	6	0	2.129053	-1.721010	-2.853224
31	8	0	0.926338	-1.684279	-2.881687
32	8	0	2.856489	-2.833460	-3.053713
33	7	0	2.153045	0.622028	-2.203936
34	1	0	2.580228	1.516661	-2.428733
35	1	0	1.241956	0.577460	-2.661958
36	16	0	-2.968059	1.815579	-1.254226
37	6	0	-2.003418	3.387063	-1.127839
38	1	0	-1.229938	3.408794	-1.899718
39	1	0	-2.710251	4.193027	-1.330643
40	6	0	-1.364991	3.657535	0.237942
41	1	0	-2.129657	3.618327	1.016423
42	7	0	-0.758717	4.995058	0.261840
43	1	0	-0.365273	5.200970	1.174547
44	6	0	-0.318169	2.592342	0.589402
45	8	0	0.106433	1.840297	-0.361033

46	8	0	0.137419	2.511247	1.763414	46	8	0	-1.348526	3.185894	-0.774219
47	1	0	-5.741768	-2.576981	-1.387467	47	1	0	6.342426	-1.160166	2.011523
48	1	0	2.240136	-3.573135	-3.164657	48	1	0	-3.656437	-1.138269	4.381559
49	1	0	-0.015693	5.072496	-0.426395	49	1	0	-0.032330	5.283801	-1.161890
50	1	0	0.796482	1.401495	1.798162	50	1	0	-0.104312	-0.199842	-2.492680

HF=-2270.6257683\ZeroPoint=0.3482036\Thermal=0.3785085

HF=-2270.670053\ZeroPoint=0.3527484\Thermal=0.3834317

G = 11.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.827640	0.339020	-0.140572
2	46	0	-1.685331	0.070874	-0.441097
3	7	0	1.139149	-1.616273	-0.658233
4	7	0	1.873524	-2.587136	-0.273902
5	6	0	3.035411	-2.184933	0.340093
6	6	0	3.309826	-0.795546	0.518612
7	6	0	4.519811	-0.459752	1.125169
8	1	0	4.778100	0.581408	1.280098
9	6	0	5.409438	-1.451907	1.540340
10	6	0	5.123437	-2.813717	1.363908
11	1	0	5.829026	-3.566369	1.694923
12	6	0	3.935575	-3.183990	0.761896
13	1	0	3.675769	-4.223665	0.600292
14	6	0	-0.066553	-1.999784	-1.297426
15	6	0	-0.664494	-1.078474	-2.197441
16	6	0	-1.806136	-1.468957	-2.931669
17	1	0	-2.233897	-0.773481	-3.642905
18	6	0	-2.359366	-2.727018	-2.752578
19	1	0	-3.248699	-3.015245	-3.298299
20	6	0	-1.775389	-3.613535	-1.839823
21	1	0	-2.218548	-4.590910	-1.687020
22	6	0	-0.647510	-3.262446	-1.111368
23	1	0	-0.199867	-3.946476	-0.404366
24	16	0	-3.500845	-1.255085	0.056150
25	6	0	-4.475014	0.056324	0.911733
26	1	0	-5.283292	-0.421169	1.466504
27	1	0	-4.911746	0.739462	0.179779
28	6	0	-3.561965	0.837888	1.846803
29	1	0	-4.099644	1.690841	2.284317
30	6	0	-3.046929	0.017786	3.026686
31	8	0	-1.904038	0.021506	3.404613
32	8	0	-4.040565	-0.652094	3.636219
33	7	0	-2.383446	1.323826	1.084820
34	1	0	-2.540015	2.201568	0.582852
35	1	0	-1.593624	1.461024	1.717252
36	16	0	2.861973	2.261100	0.599292
37	6	0	1.815104	3.690043	0.094058
38	1	0	1.147179	3.969117	0.915676
39	1	0	2.507604	4.517552	-0.066703
40	6	0	1.002625	3.529674	-1.205756
41	1	0	1.622062	2.997541	-1.932199
42	7	0	0.674722	4.845673	-1.746611
43	1	0	0.251570	4.749137	-2.664676
44	6	0	-0.239803	2.674458	-0.905461
45	8	0	-0.023324	1.386383	-0.774552

G = 33.5 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.903617	0.242614	-0.262887
2	46	0	1.558425	0.393594	0.094423
3	7	0	-1.121630	-1.541593	0.586044
4	7	0	-1.781670	-2.599257	0.347564
5	6	0	-2.840522	-2.403581	-0.524036
6	6	0	-3.191536	-1.088847	-0.933639
7	6	0	-4.292124	-0.930547	-1.769272
8	1	0	-4.589234	0.057031	-2.100630
9	6	0	-5.017974	-2.048525	-2.192697
10	6	0	-4.665870	-3.340053	-1.786374
11	1	0	-5.243019	-4.192972	-2.123181
12	6	0	-3.579068	-3.521070	-0.944077
13	1	0	-3.284839	-4.504498	-0.596312
14	6	0	-0.181264	-1.629121	1.661993
15	6	0	0.964854	-0.806395	1.666385
16	6	0	1.812064	-0.916751	2.784445
17	1	0	2.711684	-0.308210	2.833671
18	6	0	1.539537	-1.776760	3.850059
19	1	0	2.211403	-1.817657	4.700680
20	6	0	0.395938	-2.573244	3.816989
21	1	0	0.166196	-3.239427	4.640580
22	6	0	-0.461785	-2.499652	2.727899
23	1	0	-1.361915	-3.099559	2.690658
24	16	0	2.402957	1.705295	-1.707038
25	6	0	4.047839	0.883564	-1.781141
26	1	0	4.740424	1.328973	-1.058557
27	1	0	4.470593	1.010505	-2.778404
28	6	0	3.901982	-0.613551	-1.483604
29	1	0	3.268708	-1.064339	-2.249318
30	6	0	5.256577	-1.306243	-1.460424
31	8	0	5.829538	-1.654596	-0.456228
32	8	0	5.759726	-1.449466	-2.699527
33	7	0	3.232018	-0.792648	-0.164650
34	1	0	2.975688	-1.767800	-0.023603
35	1	0	3.904648	-0.583344	0.574245
36	16	0	-3.201296	2.085982	-0.801988
37	6	0	-2.072158	3.485475	-0.401584
38	1	0	-1.253062	3.522502	-1.123652
39	1	0	-2.658732	4.399270	-0.504009
40	6	0	-1.499762	3.462939	1.017961
41	1	0	-2.306850	3.414749	1.751353
42	7	0	-0.706756	4.672292	1.268156
43	1	0	-0.353631	4.714300	2.217860
44	6	0	-0.602283	2.251064	1.222360
45	8	0	-0.130586	1.636202	0.241980

46	8	0	-0.253220	1.978497	2.456684
47	1	0	-5.870985	-1.906896	-2.847966
48	1	0	6.639122	-1.851518	-2.624744
49	1	0	0.073024	4.749785	0.621963
50	1	0	0.328978	1.184213	2.462606

HF=-2270.6342739\ZeroPoint=0.352536\Thermal=0.3835132

G = 40.1 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.898210	0.164607	-0.228408
2	46	0	1.462156	0.685642	0.058776
3	7	0	-0.907369	-1.559081	0.637914
4	7	0	-1.503613	-2.661500	0.420276
5	6	0	-2.639869	-2.555316	-0.352369
6	6	0	-3.128750	-1.280312	-0.749565
7	6	0	-4.307401	-1.234214	-1.488665
8	1	0	-4.716047	-0.282361	-1.806193
9	6	0	-4.974073	-2.414407	-1.828422
10	6	0	-4.484990	-3.666364	-1.435294
11	1	0	-5.018401	-4.569451	-1.706981
12	6	0	-3.319672	-3.739847	-0.691090
13	1	0	-2.914930	-4.688165	-0.357258
14	6	0	0.171701	-1.634982	1.580456
15	6	0	0.936236	-0.474511	1.849275
16	6	0	1.951565	-0.582113	2.823218
17	1	0	2.526755	0.305550	3.070810
18	6	0	2.228063	-1.773145	3.483007
19	1	0	3.013185	-1.821253	4.229348
20	6	0	1.471051	-2.908998	3.178393
21	1	0	1.673195	-3.847879	3.681913
22	6	0	0.445186	-2.842565	2.246198
23	1	0	-0.154383	-3.714224	2.024230
24	16	0	2.149698	1.712058	-1.921881
25	6	0	3.829548	0.962896	-1.997167
26	1	0	4.543018	1.548692	-1.408113
27	1	0	4.166247	0.955770	-3.034409
28	6	0	3.780419	-0.470103	-1.460834
29	1	0	3.128178	-1.066361	-2.101146
30	6	0	5.167278	-1.095965	-1.416270
31	8	0	5.804798	-1.272153	-0.406870
32	8	0	5.610846	-1.397887	-2.649410
33	7	0	3.194908	-0.449818	-0.092576
34	1	0	3.005119	-1.396835	0.231488
35	1	0	3.890811	-0.081333	0.557135
36	16	0	-3.390110	1.848838	-0.776641
37	6	0	-2.475774	3.369684	-0.273544
38	1	0	-1.701429	3.594704	-1.009987
39	1	0	-3.203926	4.182093	-0.279468
40	6	0	-1.851194	3.305252	1.122282
41	1	0	-2.616247	3.079680	1.867203
42	7	0	-1.234409	4.592329	1.463926
43	1	0	-0.849695	4.585393	2.402783
44	6	0	-0.796528	2.200068	1.203522
45	8	0	-0.284845	1.797416	0.097698

46	8	0	-0.397407	1.769705	2.326525
47	1	0	-5.890279	-2.355369	-2.406560
48	1	0	6.509706	-1.753599	-2.570687
49	1	0	-0.491482	4.829283	0.812997
50	1	0	0.275169	0.789342	2.073258

HF=-2270.6214646\ZeroPoint=0.3489617\Thermal=0.3792856

G = 14.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-2.012988	0.176180	-0.097581
2	46	0	1.468775	0.415004	0.220448
3	7	0	-1.144150	-1.615805	0.652404
4	7	0	-1.784935	-2.697383	0.422990
5	6	0	-2.985390	-2.487553	-0.217025
6	6	0	-3.393328	-1.161386	-0.559682
7	6	0	-4.634834	-1.016647	-1.178768
8	1	0	-4.989834	-0.030567	-1.455300
9	6	0	-5.430071	-2.130994	-1.450197
10	6	0	-5.014206	-3.427970	-1.112728
11	1	0	-5.648986	-4.277878	-1.333292
12	6	0	-3.791939	-3.609846	-0.493100
13	1	0	-3.436686	-4.593354	-0.207984
14	6	0	0.088946	-1.777344	1.331786
15	6	0	0.534011	-0.727191	2.165517
16	6	0	1.731251	-0.870514	2.889536
17	1	0	2.045261	-0.062288	3.538638
18	6	0	2.479278	-2.037883	2.787631
19	1	0	3.399424	-2.149679	3.348543
20	6	0	2.027366	-3.077489	1.961313
21	1	0	2.603117	-3.993960	1.890087
22	6	0	0.851093	-2.955055	1.232458
23	1	0	0.494248	-3.755515	0.598368
24	16	0	2.114912	1.666510	-1.594674
25	6	0	3.833833	1.020920	-1.733610
26	1	0	4.502335	1.550042	-1.047386
27	1	0	4.182945	1.186652	-2.753556
28	6	0	3.835652	-0.473628	-1.409780
29	1	0	3.220795	-0.996210	-2.144731
30	6	0	5.243574	-1.053813	-1.421893
31	8	0	5.851142	-1.390746	-0.435452
32	8	0	5.736403	-1.118214	-2.670708
33	7	0	3.223398	-0.668981	-0.067266
34	1	0	3.050936	-1.658791	0.106642
35	1	0	3.899907	-0.387869	0.643864
36	16	0	-3.205226	1.958142	-0.908846
37	6	0	-2.103497	3.393867	-0.568764
38	1	0	-1.285954	3.407306	-1.294299
39	1	0	-2.727555	4.273354	-0.737015
40	6	0	-1.545140	3.491204	0.861075
41	1	0	-2.313119	3.127499	1.553014
42	7	0	-1.265872	4.888200	1.197839
43	1	0	-0.794051	4.927596	2.097015
44	6	0	-0.307583	2.589427	1.081136
45	8	0	-0.280327	1.486939	0.341778

46	8	0	0.572749	2.876406	1.869508
47	1	0	-6.391075	-1.989174	-1.933887
48	1	0	6.643279	-1.459251	-2.624499
49	1	0	-0.608928	5.275997	0.524934
50	1	0	-0.120116	0.111238	2.363051

HF=-2270.6638096\ZeroPoint=0.3524457\Thermal=0.3834775

G = 15.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.067929	-0.139817	-1.016747
2	46	0	1.234642	1.503499	-0.229723
3	7	0	-2.024543	1.314182	0.151164
4	7	0	-3.145170	1.002890	0.653989
5	6	0	-3.583694	-0.258097	0.271408
6	6	0	-2.736705	-1.091591	-0.514890
7	6	0	-3.273570	-2.295408	-0.978661
8	1	0	-2.692947	-2.919989	-1.647641
9	6	0	-4.562801	-2.695004	-0.611057
10	6	0	-5.353269	-1.893190	0.215189
11	1	0	-6.346642	-2.217893	0.500955
12	6	0	-4.868566	-0.666254	0.651751
13	1	0	-5.468510	-0.004887	1.265507
14	6	0	-1.505913	2.597006	0.481448
15	6	0	-0.115148	2.822332	0.432529
16	6	0	0.340348	4.090273	0.824696
17	1	0	1.405235	4.291302	0.832516
18	6	0	-0.540230	5.100684	1.197898
19	1	0	-0.153031	6.075689	1.474785
20	6	0	-1.918930	4.865449	1.210115
21	1	0	-2.609217	5.654025	1.486703
22	6	0	-2.399450	3.616076	0.863163
23	1	0	-3.460761	3.406031	0.869841
24	16	0	2.335882	1.436536	1.814673
25	6	0	3.359236	-0.048006	1.459184
26	1	0	2.781279	-0.950127	1.669434
27	1	0	4.218724	-0.048876	2.135791
28	6	0	3.854673	-0.102150	0.003882
29	1	0	4.556523	0.714569	-0.160682
30	6	0	4.546216	-1.428477	-0.252489
31	8	0	5.807332	-1.314870	-0.667907
32	8	0	4.013643	-2.519399	-0.096897
33	7	0	2.729700	0.064429	-0.940634
34	1	0	3.048164	0.360560	-1.860099
35	1	0	2.177417	-0.790248	-1.088081
36	1	0	-4.951811	-3.639131	-0.977212
37	1	0	6.171623	-2.203646	-0.812673
38	1	0	-1.928545	-2.002329	1.267776
39	7	0	1.750155	-3.250593	1.300194
40	6	0	0.400203	-2.679988	0.951250
41	1	0	1.700907	-4.271535	1.310449
42	6	0	-0.061626	-3.203392	-0.427646
43	1	0	0.504633	-1.590843	0.925515
44	6	0	-0.535285	-3.060127	2.103832
45	16	0	0.154913	-2.005513	-1.800734
46	1	0	-1.106668	-3.502356	-0.358864
47	1	0	0.498847	-4.110280	-0.679664
48	8	0	-1.757486	-2.557874	2.058939
49	8	0	-0.156983	-3.780583	2.998009
50	1	0	2.010960	-2.977602	2.250846
51	17	0	0.289477	1.499272	-2.453768
52	1	0	2.505217	-2.941155	0.643671

HF=-2731.5214215\ZeroPoint=0.363346\Thermal=0.3962762

G = 30.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.105374	-0.376047	0.864967
2	46	0	-1.086031	1.495815	0.358088
3	7	0	2.143768	1.104312	-0.202600
4	7	0	3.278171	0.784013	-0.668779
5	6	0	3.659424	-0.517064	-0.374247
6	6	0	2.701597	-1.465940	0.094979
7	6	0	3.181375	-2.712207	0.524582
8	1	0	2.488381	-3.437298	0.932170
9	6	0	4.530895	-3.035160	0.418020
10	6	0	5.438488	-2.116801	-0.119775
11	1	0	6.484942	-2.382575	-0.214167
12	6	0	5.007325	-0.856981	-0.518099
13	1	0	5.697982	-0.117591	-0.904699
14	6	0	1.700511	2.432358	-0.430277
15	6	0	0.329811	2.747986	-0.297390
16	6	0	-0.047452	4.070811	-0.580397
17	1	0	-1.093543	4.346522	-0.520059
18	6	0	0.884354	5.039988	-0.933117
19	1	0	0.555448	6.055439	-1.127549
20	6	0	2.241599	4.712047	-1.034200
21	1	0	2.971907	5.467654	-1.299301
22	6	0	2.646603	3.414774	-0.791540
23	1	0	3.688173	3.134211	-0.868383
24	16	0	-2.328582	1.771113	-1.575997
25	6	0	-3.436878	0.328072	-1.328386
26	1	0	-2.945632	-0.585831	-1.668660
27	1	0	-4.323326	0.468878	-1.953556
28	6	0	-3.867813	0.174735	0.136236
29	1	0	-4.469324	1.038345	0.417963
30	6	0	-4.691685	-1.089564	0.313059
31	8	0	-5.853815	-0.885155	0.940480
32	8	0	-4.348834	-2.197719	-0.066292
33	7	0	-2.688606	0.144261	1.038920
34	1	0	-2.945718	0.398573	1.989515
35	1	0	-2.235302	-0.772940	1.107516
36	1	0	4.878382	-4.009017	0.743814
37	1	0	-6.317617	-1.734594	1.020978
38	1	0	1.690107	-1.589207	-0.748852
39	7	0	-2.158208	-3.214402	-1.526556
40	6	0	-0.928260	-2.525406	-0.989160
41	1	0	-2.124108	-4.219446	-1.359812
42	6	0	-0.335450	-3.234593	0.239239
43	1	0	-1.232445	-1.510845	-0.734345

44	6	0	0.018217	-2.383874	-2.221893
45	16	0	-0.155765	-2.156249	1.719175
46	1	0	0.621614	-3.683652	-0.030553
47	1	0	-0.990696	-4.049503	0.562539
48	8	0	1.189576	-1.971264	-1.996688
49	8	0	-0.490798	-2.669471	-3.315668
50	1	0	-2.044155	-3.063268	-2.562375
51	17	0	0.078941	1.170292	2.479724
52	1	0	-3.028197	-2.833503	-1.116209

HF=-2731.4958011\ZeroPoint=0.3587658\Thermal=0.3910296

G = 25.1 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.103718	-0.411566	-0.708962
2	46	0	0.950248	1.528217	-0.362222
3	7	0	-2.248544	1.043836	0.292787
4	7	0	-3.421969	0.719951	0.635963
5	6	0	-3.769068	-0.595829	0.329332
6	6	0	-2.799139	-1.625459	0.209766
7	6	0	-3.210071	-2.893351	-0.214952
8	1	0	-2.480794	-3.687259	-0.300268
9	6	0	-4.549134	-3.146870	-0.488597
10	6	0	-5.502771	-2.138840	-0.314817
11	1	0	-6.548338	-2.345276	-0.511901
12	6	0	-5.120567	-0.869511	0.104025
13	1	0	-5.843144	-0.071824	0.223029
14	6	0	-1.835960	2.374488	0.548651
15	6	0	-0.478011	2.724018	0.376249
16	6	0	-0.123795	4.052155	0.667763
17	1	0	0.911449	4.356652	0.572916
18	6	0	-1.064450	4.988424	1.078272
19	1	0	-0.752982	6.007073	1.284046
20	6	0	-2.408704	4.623821	1.228349
21	1	0	-3.144279	5.353811	1.545189
22	6	0	-2.792288	3.324514	0.969148
23	1	0	-3.822800	3.017061	1.080831
24	16	0	2.242101	1.848818	1.528228
25	6	0	3.473557	0.529440	1.184793
26	1	0	3.093029	-0.439732	1.515409
27	1	0	4.370616	0.745646	1.771343
28	6	0	3.833110	0.465632	-0.305544
29	1	0	4.299650	1.405714	-0.597902
30	6	0	4.804448	-0.677685	-0.549202
31	8	0	5.969302	-0.279440	-1.075142
32	8	0	4.573668	-1.843508	-0.286768
33	7	0	2.607092	0.299231	-1.123296
34	1	0	2.775936	0.540625	-2.096971
35	1	0	2.245169	-0.659345	-1.131684
36	1	0	-4.857397	-4.133628	-0.812858
37	1	0	6.541999	-1.056432	-1.181000
38	1	0	-1.850916	-1.575734	0.809812
39	7	0	2.555190	-3.264378	1.192257
40	6	0	1.214547	-2.640686	0.918230
41	1	0	2.610078	-4.219782	0.844802
42	6	0	0.461231	-3.235915	-0.275388
43	1	0	1.384753	-1.574139	0.773635
44	6	0	0.459555	-2.759908	2.296961
45	16	0	0.194468	-2.083713	-1.683621
46	1	0	-0.495080	-3.617000	0.078981
47	1	0	1.006863	-4.082562	-0.704803
48	8	0	-0.738877	-2.470472	2.290069
49	8	0	1.227859	-3.118764	3.233664
50	1	0	2.442961	-3.293797	2.288243
51	17	0	-0.318273	1.151084	-2.432830
52	1	0	3.345443	-2.729769	0.811212

HF=-2731.5027378\ZeroPoint=0.3604875\Thermal=0.3938215

G = 6.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.771005	0.470925	-0.776148
2	46	0	1.727967	0.458151	-0.866548
3	7	0	-0.937947	2.005557	0.434919
4	7	0	-1.539294	2.249221	1.519195
5	6	0	-2.670326	1.465876	1.722564
6	6	0	-3.073484	0.532608	0.730010
7	6	0	-4.276194	-0.140400	0.946385
8	1	0	-4.659846	-0.812989	0.188972
9	6	0	-5.013926	0.064713	2.118926
10	6	0	-4.580688	0.959685	3.099568
11	1	0	-5.163848	1.109907	4.000332
12	6	0	-3.407121	1.674412	2.896262
13	1	0	-3.052995	2.403676	3.615654
14	6	0	0.140864	2.889888	0.123829
15	6	0	1.316113	2.393870	-0.458092
16	6	0	2.334574	3.320019	-0.727338
17	1	0	3.262831	2.980936	-1.177279
18	6	0	2.181058	4.680044	-0.461031
19	1	0	2.980011	5.371467	-0.707013
20	6	0	0.995955	5.151223	0.106768
21	1	0	0.863839	6.208136	0.307114
22	6	0	-0.020253	4.256999	0.405834
23	1	0	-0.950324	4.597349	0.843421
24	16	0	2.591958	-1.781523	-1.326335
25	6	0	3.538559	-2.005497	0.241181
26	1	0	4.601048	-1.869283	0.017300
27	1	0	3.406494	-3.016026	0.627011
28	6	0	3.116766	-0.995927	1.323056
29	1	0	2.114981	-1.248445	1.676113
30	6	0	4.079415	-1.048561	2.502616
31	8	0	3.930517	-2.188475	3.204621
32	8	0	4.887827	-0.194021	2.765813
33	7	0	3.065580	0.373780	0.759821
34	1	0	2.792167	1.046061	1.473317
35	1	0	4.000254	0.654004	0.463776
36	1	0	-5.943921	-0.476512	2.259992
37	1	0	4.586332	-2.193297	3.919065
38	1	0	-1.487950	-3.033250	2.009173
39	7	0	-0.253758	-2.907099	-1.597605

40	6	0	-1.016277	-2.792424	-0.331792
41	1	0	-0.283959	-3.865185	-1.952133
42	6	0	-2.526756	-2.655821	-0.623621
43	1	0	-0.669897	-1.870856	0.148289
44	6	0	-0.709328	-4.002534	0.538505
45	16	0	-2.856389	-1.336700	-1.852674
46	1	0	-3.045183	-2.449898	0.315248
47	1	0	-2.913200	-3.598010	-1.024285
48	8	0	-1.083202	-3.892876	1.828655
49	8	0	-0.204520	-5.007455	0.116292
50	1	0	0.773420	-2.626026	-1.443129
51	17	0	0.038348	0.459713	-2.524706
52	1	0	-0.692281	-2.249447	-2.271951

HF=-2731.5330215\ZeroPoint=0.3624388\Thermal=0.3956756

G = 31.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.741552	-0.087769	-0.835303
2	46	0	1.469719	0.607945	-0.881569
3	7	0	-1.474821	1.665923	0.368833
4	7	0	-2.319006	1.845625	1.291861
5	6	0	-3.278444	0.841775	1.400037
6	6	0	-3.114093	-0.403354	0.728901
7	6	0	-4.177099	-1.315392	0.790008
8	1	0	-4.096861	-2.253438	0.255742
9	6	0	-5.322204	-1.032859	1.530947
10	6	0	-5.435985	0.174589	2.225447
11	1	0	-6.326655	0.383133	2.806806
12	6	0	-4.414168	1.116494	2.164622
13	1	0	-4.490666	2.070005	2.672812
14	6	0	-0.527172	2.711862	0.187554
15	6	0	0.748698	2.412169	-0.319573
16	6	0	1.648967	3.481905	-0.444596
17	1	0	2.646536	3.301077	-0.833518
18	6	0	1.290956	4.788104	-0.120843
19	1	0	2.005733	5.592684	-0.257081
20	6	0	0.007732	5.064063	0.360200
21	1	0	-0.282514	6.080189	0.600178
22	6	0	-0.896102	4.029331	0.521404
23	1	0	-1.894726	4.216602	0.893558
24	16	0	2.762443	-1.359681	-1.581472
25	6	0	4.049726	-1.174613	-0.271155
26	1	0	4.814716	-0.477236	-0.625863
27	1	0	4.534810	-2.134139	-0.088076
28	6	0	3.452543	-0.652474	1.043394
29	1	0	2.736387	-1.375329	1.440583
30	6	0	4.548283	-0.437147	2.078337
31	8	0	5.047092	-1.608186	2.516663
32	8	0	4.947907	0.641677	2.442594
33	7	0	2.730445	0.622876	0.804469
34	1	0	2.156777	0.850944	1.613944
35	1	0	3.405607	1.384502	0.730135
36	1	0	-6.127082	-1.757772	1.574514
37	1	0	5.751786	-1.415592	3.154269
38	1	0	-1.963079	-0.962632	1.007273
39	7	0	1.108845	-3.596068	-0.226671
40	6	0	-0.074588	-2.702165	-0.000466
41	1	0	1.482200	-3.779385	0.725018
42	6	0	-1.418278	-3.241275	-0.517364
43	1	0	0.172352	-1.791713	-0.545458
44	6	0	-0.048943	-2.292703	1.492910
45	16	0	-2.134030	-2.175028	-1.844399
46	1	0	-2.114084	-3.340448	0.317962
47	1	0	-1.304048	-4.236370	-0.957722
48	8	0	-0.988661	-1.537458	1.884017
49	8	0	0.916842	-2.694006	2.162742
50	1	0	1.825518	-3.002213	-0.771336
51	17	0	-0.195117	0.549074	-2.588965
52	1	0	0.891368	-4.454436	-0.727425

HF=-2731.4927577\ZeroPoint=0.3583819\Thermal=0.3906686

G = 28.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.798574	-0.225975	-0.662666
2	46	0	1.343204	0.595865	-0.875101
3	7	0	-1.677903	1.685315	0.332624
4	7	0	-2.656678	1.941793	1.082352
5	6	0	-3.536964	0.851778	1.240072
6	6	0	-3.049489	-0.469826	1.389724
7	6	0	-3.978887	-1.513978	1.516337
8	1	0	-3.620872	-2.527897	1.638702
9	6	0	-5.341360	-1.256550	1.501951
10	6	0	-5.802787	0.060697	1.386940
11	1	0	-6.868251	0.260057	1.386685
12	6	0	-4.908538	1.117001	1.271112
13	1	0	-5.250854	2.139847	1.175158
14	6	0	-0.723704	2.718202	0.149353
15	6	0	0.569648	2.378125	-0.285894
16	6	0	1.495390	3.433280	-0.377457
17	1	0	2.511970	3.226255	-0.697569
18	6	0	1.145195	4.750697	-0.102388
19	1	0	1.883903	5.537970	-0.209226
20	6	0	-0.159671	5.063883	0.296862
21	1	0	-0.441333	6.090620	0.498468
22	6	0	-1.088761	4.051253	0.430920
23	1	0	-2.101380	4.264487	0.746585
24	16	0	2.817694	-1.160718	-1.698860
25	6	0	4.146608	-0.753109	-0.483196
26	1	0	4.673274	0.137455	-0.837331
27	1	0	4.864261	-1.573058	-0.435801
28	6	0	3.577097	-0.498190	0.919600
29	1	0	3.173486	-1.428399	1.322906
30	6	0	4.675318	-0.009649	1.851202
31	8	0	5.565716	-0.982854	2.117884
32	8	0	4.770096	1.116927	2.276149
33	7	0	2.477341	0.509795	0.888599
34	1	0	1.774957	0.257985	1.588866
35	1	0	2.850045	1.422955	1.150880

36	1	0	-6.049272	-2.071029	1.596489
37	1	0	6.251889	-0.611192	2.693194
38	1	0	-1.994169	-0.650714	1.631372
39	7	0	1.302230	-3.627091	-0.490419
40	6	0	0.244591	-2.705559	0.039285
41	1	0	1.753037	-4.000303	0.371938
42	6	0	-1.189116	-3.233962	-0.085247
43	1	0	0.346231	-1.794653	-0.541105
44	6	0	0.681624	-2.319066	1.485189
45	16	0	-2.124727	-2.396162	-1.437938
46	1	0	-1.697985	-3.097099	0.868441
47	1	0	-1.208756	-4.306249	-0.305522
48	8	0	0.085556	-1.330783	1.959301
49	8	0	1.621590	-3.001755	1.957861
50	1	0	2.004576	-2.996678	-0.984623
51	17	0	-0.409067	0.352459	-2.509209
52	1	0	0.963203	-4.348165	-1.123722

HF=-2731.4999561\ZeroPoint=0.362073\Thermal=0.3952248

G = 4.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.287371	-0.381158	-0.762308
2	46	0	1.253662	1.024142	-0.333532
3	7	0	-2.067075	1.406830	-0.005923
4	7	0	-3.274605	1.383938	0.384834
5	6	0	-3.890322	0.153428	0.187833
6	6	0	-3.139609	-0.942449	-0.321787
7	6	0	-3.804706	-2.152019	-0.533863
8	1	0	-3.270652	-2.987671	-0.969921
9	6	0	-5.161839	-2.280991	-0.215637
10	6	0	-5.881211	-1.203864	0.310435
11	1	0	-6.932150	-1.315954	0.549365
12	6	0	-5.248369	0.017764	0.508229
13	1	0	-5.784281	0.877146	0.894000
14	6	0	-1.339512	2.612150	0.175277
15	6	0	0.074122	2.588065	0.142332
16	6	0	0.726283	3.809865	0.386534
17	1	0	1.808794	3.835416	0.402099
18	6	0	0.027037	4.991569	0.603534
19	1	0	0.571885	5.915389	0.767746
20	6	0	-1.372327	4.993883	0.603153
21	1	0	-1.922000	5.915215	0.757750
22	6	0	-2.051427	3.808797	0.398978
23	1	0	-3.132719	3.781169	0.397357
24	16	0	2.495022	1.163288	1.665797
25	6	0	3.882049	0.006824	1.227632
26	1	0	3.711534	-0.951462	1.719108
27	1	0	4.811288	0.436191	1.598977
28	6	0	3.986735	-0.209321	-0.289782
29	1	0	4.321501	0.723689	-0.752381
30	6	0	5.021706	-1.280651	-0.616111
31	8	0	6.255653	-0.912947	-0.198728
32	8	0	4.792804	-2.321244	-1.175359
33	7	0	2.667507	-0.544800	-0.847828
34	1	0	2.703452	-0.644401	-1.859907
35	1	0	2.337607	-1.442880	-0.491881
36	1	0	-5.662132	-3.227655	-0.391167
37	1	0	6.868884	-1.627850	-0.427527
38	1	0	-1.692428	-1.345415	1.174059
39	7	0	-1.618349	-2.027748	1.988546
40	6	0	-0.439614	-2.920253	1.711092
41	6	0	-0.568532	-3.552110	0.317189
42	1	0	-0.442892	-3.707450	2.471762
43	6	0	0.842819	-2.096806	1.897162
44	16	0	-0.315112	-2.464968	-1.150387
45	1	0	-1.531689	-4.071866	0.265726
46	1	0	0.213353	-4.309222	0.244682
47	8	0	0.605268	-0.963195	2.532868
48	8	0	1.908424	-2.506390	1.507112
49	1	0	-1.475923	-1.479280	2.837884
50	17	0	0.229462	0.805898	-2.490493
51	1	0	-2.500746	-2.539677	2.018219
52	1	0	1.341313	-0.244697	2.376777

HF=-2731.539569\ZeroPoint=0.3623087\Thermal=0.3948098

G = 15.3 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.260824	-0.429284	0.686050
2	46	0	-1.291285	1.009469	0.374243
3	7	0	2.010735	1.388662	-0.057106
4	7	0	3.218771	1.388098	-0.451707
5	6	0	3.870271	0.177915	-0.264432
6	6	0	3.139108	-1.004816	0.051538
7	6	0	3.867420	-2.158472	0.380658
8	1	0	3.332040	-3.055588	0.666191
9	6	0	5.258587	-2.161132	0.330368
10	6	0	5.957726	-1.009771	-0.051261
11	1	0	7.040320	-1.024140	-0.097651
12	6	0	5.268265	0.158445	-0.349424
13	1	0	5.788977	1.072472	-0.608406
14	6	0	1.285997	2.600021	-0.179749
15	6	0	-0.126342	2.586961	-0.084337
16	6	0	-0.774710	3.824213	-0.252845
17	1	0	-1.856323	3.859623	-0.218280
18	6	0	-0.073633	5.005558	-0.460838
19	1	0	-0.615324	5.939647	-0.567099
20	6	0	1.325069	4.995424	-0.528212
21	1	0	1.876124	5.916467	-0.679039
22	6	0	1.999983	3.799498	-0.395557
23	1	0	3.079583	3.763545	-0.444904
24	16	0	-2.585472	1.275456	-1.562943
25	6	0	-3.920450	0.040997	-1.190373
26	1	0	-3.709354	-0.883206	-1.728366
27	1	0	-4.866755	0.451619	-1.539533
28	6	0	-4.011771	-0.254418	0.313261
29	1	0	-4.363216	0.646782	0.824412
30	6	0	-5.018214	-1.363737	0.598840
31	8	0	-6.259655	-1.019147	0.184807

32	8	0	-4.763819	-2.412652	1.131471
33	7	0	-2.679385	-0.589960	0.843808
34	1	0	-2.710225	-0.757945	1.846688
35	1	0	-2.336057	-1.456746	0.426718
36	1	0	5.803291	-3.063262	0.585488
37	1	0	-6.853370	-1.757356	0.389772
38	1	0	2.158299	-1.340775	-0.839377
39	7	0	1.714897	-2.062688	-2.061729
40	6	0	0.483170	-2.828090	-1.782705
41	6	0	0.560492	-3.529359	-0.409015
42	1	0	0.353519	-3.613902	-2.538341
43	6	0	-0.756086	-1.942052	-1.904255
44	16	0	0.342788	-2.517272	1.119038
45	1	0	1.500161	-4.089386	-0.372331
46	1	0	-0.254391	-4.253073	-0.364355
47	8	0	-0.495201	-0.769117	-2.460680
48	8	0	-1.843082	-2.329642	-1.539573
49	1	0	1.557390	-1.359691	-2.779139
50	17	0	-0.107731	0.630600	2.450984
51	1	0	2.479093	-2.670601	-2.341223
52	1	0	-1.258506	-0.111560	-2.329988

HF=-2731.5201777\ZeroPoint=0.3584339\Thermal=0.3905803

G = 10.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.218735	-0.438682	-0.503482
2	46	0	1.224147	1.037657	-0.380652
3	7	0	-2.062727	1.379206	0.129654
4	7	0	-3.310375	1.392397	0.356570
5	6	0	-3.948043	0.171045	0.151539
6	6	0	-3.252846	-1.065836	0.186978
7	6	0	-3.926396	-2.240165	-0.163940
8	1	0	-3.389496	-3.179401	-0.143905
9	6	0	-5.271531	-2.199719	-0.513065
10	6	0	-5.965686	-0.984729	-0.489435
11	1	0	-7.018109	-0.959924	-0.747030
12	6	0	-5.314021	0.195078	-0.150223
13	1	0	-5.830140	1.147160	-0.155854
14	6	0	-1.352335	2.593420	0.284369
15	6	0	0.057697	2.593393	0.156564
16	6	0	0.699549	3.833046	0.336080
17	1	0	1.778968	3.881001	0.270369
18	6	0	-0.005677	5.000200	0.599374
19	1	0	0.530971	5.935465	0.719787
20	6	0	-1.402030	4.974843	0.711683
21	1	0	-1.954690	5.884484	0.915933
22	6	0	-2.070891	3.779106	0.558219
23	1	0	-3.147744	3.731381	0.641553
24	16	0	2.594991	1.319483	1.494620
25	6	0	3.958317	0.144533	1.044103
26	1	0	3.812973	-0.790366	1.584809
27	1	0	4.903075	0.593652	1.346786
28	6	0	3.980227	-0.136724	-0.463700
29	1	0	4.270611	0.780340	-0.985719
30	6	0	5.007290	-1.205055	-0.823719
31	8	0	6.249852	-0.847083	-0.425621
32	8	0	4.766118	-2.232165	-1.402852
33	7	0	2.632481	-0.516920	-0.921363
34	1	0	2.617296	-0.700873	-1.921833
35	1	0	2.337579	-1.386975	-0.473933
36	1	0	-5.787272	-3.112435	-0.787257
37	1	0	6.857055	-1.557014	-0.684049
38	1	0	-2.353970	-1.208893	0.867742
39	7	0	-1.475361	-2.480726	2.325492
40	6	0	-0.216208	-3.047019	1.832255
41	6	0	-0.387403	-3.606469	0.399129
42	1	0	0.127344	-3.890578	2.450243
43	6	0	0.931055	-2.044977	1.885949
44	16	0	-0.259529	-2.470052	-1.050844
45	1	0	-1.331700	-4.157642	0.369178
46	1	0	0.416883	-4.320661	0.209909
47	8	0	0.590270	-0.879917	2.420655
48	8	0	2.035944	-2.326482	1.471742
49	1	0	-1.318916	-1.885293	3.131386
50	17	0	-0.063840	0.635856	-2.406784
51	1	0	-2.114307	-3.220422	2.596892
52	1	0	1.310528	-0.192658	2.283285

HF=-2731.5276635\ZeroPoint=0.3610536\Thermal=0.3941322

G = 13.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.678828	-0.079855	-0.777829
2	46	0	1.473591	0.452469	-0.786515
3	7	0	-1.524678	1.776178	0.226049
4	7	0	-2.467440	2.062286	1.024708
5	6	0	-3.489024	1.118340	1.040855
6	6	0	-3.365101	-0.076177	0.279214
7	6	0	-4.449924	-0.958559	0.280287
8	1	0	-4.411685	-1.850467	-0.333237
9	6	0	-5.590154	-0.688341	1.044596
10	6	0	-5.679315	0.473980	1.816925
11	1	0	-6.569179	0.672726	2.402451
12	6	0	-4.629730	1.384456	1.811480
13	1	0	-4.677895	2.308642	2.375630
14	6	0	-0.462008	2.721739	0.141334
15	6	0	0.829301	2.300746	-0.236325
16	6	0	1.824736	3.293482	-0.266598
17	1	0	2.835153	3.027995	-0.563109
18	6	0	1.558328	4.627674	0.027144
19	1	0	2.353502	5.363156	-0.034987
20	6	0	0.264050	5.020014	0.378908
21	1	0	0.041667	6.059295	0.591450
22	6	0	-0.739443	4.070065	0.440882
23	1	0	-1.750272	4.349508	0.706873
24	16	0	2.635738	-1.585610	-1.471058
25	6	0	4.114189	-1.216191	-0.437387
26	1	0	4.699208	-0.437165	-0.933795
27	1	0	4.737077	-2.107542	-0.351445

28	6	0	3.700542	-0.747387	0.965806
29	1	0	3.192898	-1.568113	1.470224
30	6	0	4.923740	-0.348171	1.774532
31	8	0	5.664628	-1.422209	2.113976
32	8	0	5.227992	0.785607	2.057298
33	7	0	2.749357	0.392912	0.897972
34	1	0	2.114352	0.338494	1.690140
35	1	0	3.262322	1.269876	0.990639
36	1	0	-6.419641	-1.387740	1.028723
37	1	0	6.452263	-1.105574	2.582506
38	1	0	-1.896992	-1.158356	1.218222
39	7	0	-1.700131	-1.907947	1.939214
40	6	0	-1.083949	-3.073899	1.218651
41	6	0	-1.876779	-3.413860	-0.049164
42	1	0	-1.109202	-3.926299	1.906190
43	6	0	0.391109	-2.673397	1.023481
44	16	0	-1.716888	-2.291299	-1.499658
45	1	0	-2.924237	-3.565180	0.236548
46	1	0	-1.498029	-4.372864	-0.405758
47	8	0	1.015876	-3.372147	0.140720
48	8	0	0.844071	-1.765095	1.715795
49	1	0	-1.001102	-1.524040	2.585639
50	17	0	-0.042747	0.496501	-2.590959
51	1	0	-2.579517	-2.132264	2.402128
52	1	0	1.751640	-2.764670	-0.393071

HF=-2731.5238283\ZeroPoint=0.3609969\Thermal=0.3935033

G = 25.5 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.621707	-0.172429	-0.694748
2	46	0	1.493596	0.438846	-0.815640
3	7	0	-1.498816	1.724745	0.262655
4	7	0	-2.477389	2.041459	1.006884
5	6	0	-3.514764	1.118760	1.011248
6	6	0	-3.340468	-0.187612	0.470612
7	6	0	-4.479602	-1.000020	0.353982
8	1	0	-4.382078	-1.979630	-0.096252
9	6	0	-5.718860	-0.565762	0.815796
10	6	0	-5.854064	0.694373	1.409762
11	1	0	-6.820413	1.020602	1.776044
12	6	0	-4.755163	1.537750	1.508908
13	1	0	-4.841714	2.534226	1.925126
14	6	0	-0.454816	2.683942	0.157649
15	6	0	0.830933	2.281380	-0.260847
16	6	0	1.808590	3.291610	-0.324009
17	1	0	2.813076	3.041316	-0.652029
18	6	0	1.531446	4.620580	-0.022621
19	1	0	2.312401	5.368607	-0.110500
20	6	0	0.242341	4.994090	0.372384
21	1	0	0.012411	6.029907	0.593300
22	6	0	-0.743442	4.031059	0.465637
23	1	0	-1.748697	4.296879	0.763160
24	16	0	2.662608	-1.582982	-1.487887
25	6	0	4.158158	-1.182899	-0.490593
26	1	0	4.732669	-0.402766	-0.998192
27	1	0	4.788900	-2.068824	-0.404020
28	6	0	3.756185	-0.703801	0.911238
29	1	0	3.249745	-1.518132	1.428189
30	6	0	4.982335	-0.291956	1.708831
31	8	0	5.720584	-1.360460	2.069286
32	8	0	5.291612	0.847108	1.964989
33	7	0	2.804675	0.435489	0.832763
34	1	0	2.175591	0.393755	1.630996
35	1	0	3.319386	1.313448	0.901551
36	1	0	-6.584344	-1.211430	0.717407
37	1	0	6.510276	-1.036442	2.529193
38	1	0	-2.334903	-0.911069	1.014089
39	7	0	-1.787674	-1.861317	2.035152
40	6	0	-1.091087	-2.971749	1.360010
41	6	0	-1.837235	-3.421309	0.086444
42	1	0	-1.036570	-3.842451	2.027563
43	6	0	0.356121	-2.531868	1.118512
44	16	0	-1.711506	-2.371261	-1.423126
45	1	0	-2.882105	-3.602077	0.358859
46	1	0	-1.410220	-4.375411	-0.225305
47	8	0	0.996636	-3.311618	0.288875
48	8	0	0.814416	-1.555601	1.692536
49	1	0	-1.120566	-1.330215	2.593726
50	17	0	-0.139350	0.384577	-2.535479
51	1	0	-2.554131	-2.183174	2.617473
52	1	0	1.714486	-2.779719	-0.238476

HF=-2731.5031462\ZeroPoint=0.3577569\Thermal=0.3898125

G = 21.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.563289	-0.211875	0.567241
2	46	0	-1.425663	0.484115	0.798811
3	7	0	1.587229	1.734072	-0.301223
4	7	0	2.652778	2.078707	-0.895297
5	6	0	3.667566	1.125456	-0.876631
6	6	0	3.414525	-0.254172	-0.664891
7	6	0	4.494672	-1.132021	-0.526990
8	1	0	4.300513	-2.182106	-0.356565
9	6	0	5.799258	-0.661597	-0.624568
10	6	0	6.040273	0.691579	-0.887136
11	1	0	7.058691	1.051169	-0.976898
12	6	0	4.982386	1.582093	-1.022460
13	1	0	5.150763	2.637408	-1.198050
14	6	0	0.545445	2.697094	-0.250571
15	6	0	-0.746573	2.300477	0.158363
16	6	0	-1.727535	3.310899	0.174142
17	1	0	-2.735983	3.070221	0.496823
18	6	0	-1.451143	4.628558	-0.170138
19	1	0	-2.236712	5.375395	-0.122371
20	6	0	-0.157527	4.994001	-0.561776
21	1	0	0.069122	6.021205	-0.822484
22	6	0	0.833541	4.034684	-0.603023
23	1	0	1.840766	4.294093	-0.898579

24	16	0	-2.638294	-1.454408	1.594859
25	6	0	-4.163923	-1.003357	0.667608
26	1	0	-4.656592	-0.161387	1.162252
27	1	0	-4.853670	-1.848709	0.665638
28	6	0	-3.813227	-0.626030	-0.778129
29	1	0	-3.408058	-1.504099	-1.280417
30	6	0	-5.047984	-0.149727	-1.524096
31	8	0	-5.900260	-1.163873	-1.769663
32	8	0	-5.271534	0.996633	-1.832819
33	7	0	-2.769138	0.433394	-0.818102
34	1	0	-2.152958	0.250191	-1.607090
35	1	0	-3.210836	1.339297	-0.974656
36	1	0	6.630463	-1.347748	-0.512668
37	1	0	-6.686097	-0.795759	-2.202138
38	1	0	2.449265	-0.732384	-1.047944
39	7	0	1.586480	-2.229037	-2.255397
40	6	0	0.872802	-3.186694	-1.408721
41	6	0	1.668708	-3.513475	-0.122272
42	1	0	0.712590	-4.148547	-1.921152
43	6	0	-0.525149	-2.650047	-1.115624
44	16	0	1.551625	-2.388758	1.335201
45	1	0	2.711341	-3.674250	-0.411269
46	1	0	1.291814	-4.454137	0.285391
47	8	0	-1.169992	-3.374129	-0.227303
48	8	0	-0.966219	-1.660819	-1.677157
49	1	0	0.926024	-1.726394	-2.840805
50	17	0	0.256300	0.433016	2.479658
51	1	0	2.263363	-2.694515	-2.848770
52	1	0	-1.819075	-2.791323	0.305369

HF=-2731.5097221\ZeroPoint=0.3603521\Thermal=0.3932931

G = -6.1 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.878110	-0.470880	-0.796493
2	46	0	1.164794	0.803125	-0.331867
3	7	0	-2.148276	1.319464	0.152840
4	7	0	-3.077315	1.414987	1.004385
5	6	0	-3.781351	0.231367	1.183190
6	6	0	-3.407512	-0.908641	0.424158
7	6	0	-4.131112	-2.077347	0.632350
8	1	0	-3.898682	-2.986089	0.084680
9	6	0	-5.178976	-2.116847	1.562125
10	6	0	-5.527763	-0.984990	2.301393
11	1	0	-6.337992	-1.031871	3.018948
12	6	0	-4.826852	0.200641	2.113506
13	1	0	-5.069156	1.098324	2.670059
14	6	0	-1.413054	2.506853	-0.138692
15	6	0	-0.039092	2.429147	-0.415523
16	6	0	0.617300	3.633012	-0.712289
17	1	0	1.681772	3.625474	-0.919723
18	6	0	-0.060859	4.848452	-0.753672
19	1	0	0.476988	5.755832	-1.006603
20	6	0	-1.428460	4.898845	-0.473943
21	1	0	-1.963010	5.840936	-0.507950
22	6	0	-2.102541	3.730947	-0.159555
23	1	0	-3.163004	3.738472	0.057555
24	16	0	2.001942	1.455232	1.836551
25	6	0	3.716303	0.755373	1.730070
26	1	0	3.772548	-0.017513	2.496570
27	1	0	4.422857	1.548757	1.960992
28	6	0	3.992209	0.168335	0.339009
29	1	0	4.148365	0.996049	-0.362741
30	6	0	5.284793	-0.647020	0.291631
31	8	0	6.278894	-0.042734	0.979781
32	8	0	5.423133	-1.669946	-0.323504
33	7	0	2.839061	-0.617974	-0.128283
34	1	0	3.097002	-1.175590	-0.938932
35	1	0	2.583851	-1.301222	0.596902
36	16	0	-0.020501	0.129935	-2.265587
37	6	0	0.373013	-1.595813	-2.827878
38	1	0	-0.042484	-1.660171	-3.836721
39	1	0	1.449521	-1.742621	-2.898453
40	6	0	-0.224844	-2.704614	-1.952840
41	1	0	-0.165631	-3.649890	-2.507158
42	7	0	-1.647087	-2.404960	-1.616376
43	1	0	-1.973387	-3.068916	-0.918478
44	6	0	0.621514	-2.912007	-0.690938
45	8	0	-0.075731	-2.850655	0.424822
46	8	0	1.810948	-3.110370	-0.792851
47	1	0	-5.723726	-3.043127	1.711681
48	1	0	-2.231923	-2.506259	-2.443269
49	1	0	1.491974	0.273556	2.376101
50	1	0	7.077340	-0.584907	0.885858
51	1	0	0.514681	-2.685059	1.236778
52	17	0	1.576623	-1.846776	2.653323

HF=-2731.5534321\ZeroPoint=0.3610786\Thermal=0.3934441

G = 20.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.852048	-0.786322	-0.706520
2	46	0	1.532770	0.676702	-0.220678
3	7	0	-2.241696	1.176524	-0.356740
4	7	0	-3.366160	1.484489	0.130077
5	6	0	-4.186638	0.390718	0.366314
6	6	0	-3.682851	-0.907985	0.100126
7	6	0	-4.517349	-1.985419	0.373484
8	1	0	-4.194843	-3.005663	0.184493
9	6	0	-5.800116	-1.780958	0.901393
10	6	0	-6.274056	-0.494108	1.162984
11	1	0	-7.265804	-0.352843	1.575318
12	6	0	-5.463910	0.604185	0.896059
13	1	0	-5.795601	1.616848	1.092506
14	6	0	-1.346608	2.280189	-0.555283
15	6	0	-0.008157	2.230661	-0.085436
16	6	0	0.676778	3.466417	-0.129187
17	1	0	1.674908	3.535080	0.280145
18	6	0	0.135573	4.614305	-0.701575
19	1	0	0.726791	5.522637	-0.735698

20	6	0	-1.153119	4.592754	-1.226500
21	1	0	-1.581283	5.475526	-1.687323
22	6	0	-1.903656	3.430603	-1.121756
23	1	0	-2.929864	3.400222	-1.464277
24	16	0	2.922776	1.701867	1.391227
25	6	0	4.223131	0.408677	1.437462
26	1	0	3.900901	-0.439609	2.049297
27	1	0	5.125041	0.835159	1.876868
28	6	0	4.497424	-0.061157	0.010983
29	1	0	4.829990	0.797717	-0.577644
30	6	0	5.566627	-1.142642	-0.077859
31	8	0	6.750257	-0.705778	0.397469
32	8	0	5.393327	-2.251684	-0.520293
33	7	0	3.226360	-0.561443	-0.560665
34	1	0	3.341446	-0.754312	-1.552099
35	1	0	2.986723	-1.446927	-0.106169
36	16	0	0.264188	-0.562830	-1.869363
37	6	0	0.727199	-2.360437	-1.727646
38	1	0	0.421006	-2.831845	-2.665059
39	1	0	1.804188	-2.489721	-1.639538
40	6	0	0.033166	-3.071087	-0.560326
41	1	0	0.281521	-4.140343	-0.589943
42	7	0	-1.438977	-2.871718	-0.687631
43	1	0	-1.918350	-3.251125	0.124988
44	6	0	0.545435	-2.529926	0.786814
45	8	0	-0.435164	-2.210184	1.615800
46	8	0	1.728655	-2.427286	1.013079
47	1	0	-6.432173	-2.637209	1.112957
48	1	0	-1.787410	-3.351804	-1.514570
49	1	0	-0.031132	1.371107	1.112608
50	1	0	7.388459	-1.431702	0.322480
51	1	0	-0.227701	-1.415383	2.178337
52	17	0	-0.575762	0.698111	2.476447

HF=-2731.5090651\ZeroPoint=0.3582348\Thermal=0.3903952

G = -17.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-2.041388	-0.175404	-0.871065
2	46	0	1.444258	-0.518101	0.581209
3	7	0	-1.636449	1.790042	-0.422443
4	7	0	-2.522879	2.459358	0.175289
5	6	0	-3.737714	1.789888	0.273848
6	6	0	-3.829864	0.461448	-0.220562
7	6	0	-5.065211	-0.169611	-0.115780
8	1	0	-5.205559	-1.183561	-0.480292
9	6	0	-6.163342	0.489972	0.452598
10	6	0	-6.047092	1.793394	0.940222
11	1	0	-6.903065	2.287072	1.384255
12	6	0	-4.825792	2.451874	0.853727
13	1	0	-4.696143	3.460933	1.226984
14	6	0	-0.334541	2.374325	-0.491394
15	6	0	0.259135	2.897525	0.657744
16	6	0	1.551622	3.403520	0.581569
17	1	0	2.033844	3.769306	1.479337
18	6	0	2.236008	3.403815	-0.633804
19	1	0	3.241494	3.806792	-0.688078
20	6	0	1.633875	2.875190	-1.776859
21	1	0	2.162532	2.876316	-2.723606
22	6	0	0.349907	2.343165	-1.706864
23	1	0	-0.124663	1.908244	-2.576971
24	16	0	2.861811	0.105954	2.321935
25	6	0	4.454938	-0.130987	1.426433
26	1	0	4.781430	-1.175142	1.482114
27	1	0	5.217157	0.491257	1.898097
28	6	0	4.289074	0.270438	-0.041862
29	1	0	4.011155	1.324141	-0.090979
30	6	0	5.570131	0.046107	-0.828788
31	8	0	6.501040	0.976632	-0.532627
32	8	0	5.756450	-0.860705	-1.603277
33	7	0	3.179792	-0.521235	-0.625800
34	1	0	2.928473	-0.170063	-1.548057
35	1	0	3.492598	-1.482127	-0.765616
36	16	0	0.172962	-0.914293	-1.505064
37	6	0	-0.239131	-2.698533	-1.767490
38	1	0	-0.481328	-2.818079	-2.826404
39	1	0	0.629892	-3.312331	-1.535680
40	6	0	-1.416530	-3.159833	-0.914053
41	1	0	-1.724138	-4.165026	-1.235075
42	7	0	-2.571686	-2.219694	-1.061690
43	1	0	-3.260240	-2.415649	-0.338627
44	6	0	-0.995197	-3.300258	0.552316
45	8	0	-1.985215	-2.959912	1.393873
46	8	0	0.084444	-3.708126	0.878991
47	1	0	-7.118273	-0.021546	0.515741
48	1	0	-3.016621	-2.361131	-1.965932
49	1	0	-0.269970	2.841890	1.598903
50	1	0	7.308051	0.759039	-1.024075
51	1	0	-1.590809	-2.723369	2.251669
52	17	0	-0.390650	-0.344316	2.072151

HF=-2731.5691184\ZeroPoint=0.3627532\Thermal=0.396187

G = -0.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.440038	-0.128085	-0.208126
2	46	0	-1.325018	0.399242	-0.831501
3	7	0	0.920910	-2.055187	-0.622471
4	7	0	1.569593	-2.983346	-0.056028
5	6	0	2.526829	-2.515964	0.833228
6	6	0	2.619910	-1.116549	1.073765
7	6	0	3.536945	-0.683684	2.025092
8	1	0	3.639968	0.371074	2.259894
9	6	0	4.338400	-1.603560	2.712873
10	6	0	4.239735	-2.973809	2.459111
11	1	0	4.865858	-3.672875	3.000432
12	6	0	3.327710	-3.437652	1.518630
13	1	0	3.218467	-4.494852	1.307519
14	6	0	-0.166712	-2.410341	-1.475465
15	6	0	-1.204464	-1.474868	-1.674437

16	6	0	-2.275028	-1.898532	-2.478791
17	1	0	-3.100051	-1.218451	-2.667566
18	6	0	-2.304377	-3.158473	-3.071393
19	1	0	-3.141118	-3.439237	-3.702534
20	6	0	-1.250964	-4.055540	-2.867268
21	1	0	-1.263316	-5.032842	-3.335712
22	6	0	-0.185484	-3.686670	-2.064420
23	1	0	0.637898	-4.365240	-1.883202
24	16	0	-1.545561	2.514963	0.281576
25	6	0	-3.128444	2.139810	1.138652
26	1	0	-3.963142	2.344166	0.460996
27	1	0	-3.231050	2.786257	2.010856
28	6	0	-3.174439	0.673449	1.586957
29	1	0	-2.386190	0.507439	2.320328
30	6	0	-4.519753	0.353958	2.221595
31	8	0	-4.633908	0.906496	3.446042
32	8	0	-5.398297	-0.283491	1.693373
33	7	0	-2.924719	-0.233110	0.439307
34	1	0	-2.692268	-1.162487	0.783860
35	1	0	-3.784232	-0.337611	-0.099551
36	16	0	0.490156	0.956241	-2.224100
37	6	0	1.024851	2.684567	-1.833510
38	1	0	1.371537	3.134704	-2.762587
39	1	0	0.168911	3.257189	-1.474985
40	6	0	2.169176	2.703459	-0.809875
41	1	0	3.065115	2.287630	-1.281222
42	7	0	1.847181	1.853452	0.362528
43	1	0	0.963016	2.173639	0.780340
44	6	0	2.526346	4.113751	-0.349754
45	8	0	2.642675	4.446480	0.802249
46	8	0	2.730328	4.938998	-1.394734
47	1	0	5.041511	-1.245433	3.457442
48	1	0	2.964779	5.812606	-1.045243
49	1	0	2.562071	1.972207	1.076119
50	1	0	0.192691	-0.888088	1.649925
51	1	0	-5.520538	0.705307	3.782928
52	17	0	-0.543112	-1.504013	2.550380

HF=-2731.5414917\ZeroPoint=0.360366\Thermal=0.3939839

G = 12.2 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.864448	0.113146	0.094266
2	46	0	1.593156	0.230087	0.569267
3	7	0	-1.451861	-1.837370	0.498397
4	7	0	-2.199198	-2.727523	0.007865
5	6	0	-3.164749	-2.217496	-0.853125
6	6	0	-3.219581	-0.813975	-1.066299
7	6	0	-4.170718	-0.343647	-1.964350
8	1	0	-4.252728	0.716900	-2.185407
9	6	0	-5.034335	-1.230321	-2.624008
10	6	0	-4.967258	-2.605534	-2.394359
11	1	0	-5.640095	-3.277537	-2.913243
12	6	0	-4.024782	-3.108535	-1.503706
13	1	0	-3.935730	-4.170822	-1.309464
14	6	0	-0.420059	-2.287504	1.384648
15	6	0	0.894829	-1.810800	1.185705
16	6	0	1.879678	-2.391534	2.008740
17	1	0	2.919891	-2.117042	1.872281
18	6	0	1.572788	-3.313058	3.006031
19	1	0	2.359806	-3.710035	3.637571
20	6	0	0.253583	-3.728218	3.187688
21	1	0	0.005735	-4.446190	3.960970
22	6	0	-0.745261	-3.232470	2.357541
23	1	0	-1.770384	-3.567941	2.453130
24	16	0	2.466231	2.336926	0.032361
25	6	0	4.075910	1.790393	-0.674431
26	1	0	4.826877	1.714674	0.118183
27	1	0	4.410055	2.538485	-1.394616
28	6	0	3.915972	0.430109	-1.357477
29	1	0	3.224060	0.520234	-2.196002
30	6	0	5.263553	-0.069913	-1.859303
31	8	0	5.625187	0.544378	-3.003348
32	8	0	5.949530	-0.882128	-1.289467
33	7	0	3.339093	-0.532204	-0.393017
34	1	0	3.047224	-1.379878	-0.891193
35	1	0	4.061575	-0.800717	0.274534
36	16	0	-0.300327	1.099671	1.651578
37	6	0	-0.583934	2.852703	1.126127
38	1	0	-0.322845	3.515600	1.949165
39	1	0	0.053158	3.090915	0.271882
40	6	0	-2.056027	3.041856	0.744130
41	1	0	-2.687559	2.821340	1.608448
42	7	0	-2.422383	2.098880	-0.343250
43	1	0	-1.949287	2.384460	-1.201754
44	6	0	-2.322036	4.477398	0.304329
45	8	0	-2.611366	4.802060	-0.819762
46	8	0	-2.182578	5.338419	1.328115
47	1	0	-5.762541	-0.840248	-3.327552
48	1	0	-2.331548	6.236354	0.993218
49	1	0	-3.417387	2.168840	-0.542821
50	1	0	1.061432	-1.852958	-0.232869
51	1	0	6.502478	0.216364	-3.254314
52	17	0	1.143034	-2.388594	-1.724543

HF=-2731.5183004\ZeroPoint=0.3584111\Thermal=0.3914521

G = -25.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.758356	0.007401	-0.009496
2	46	0	1.840712	-0.695865	-0.119285
3	7	0	-1.908166	2.087870	0.090974
4	7	0	-2.833209	2.571087	0.806443
5	6	0	-3.540498	1.616263	1.522271
6	6	0	-3.223595	0.247025	1.336996
7	6	0	-3.925493	-0.678156	2.103392
8	1	0	-3.710596	-1.739971	2.036971
9	6	0	-4.913922	-0.258929	3.004092
10	6	0	-5.223410	1.094304	3.157678
11	1	0	-5.991990	1.401566	3.856609

12	6	0	-4.531821	2.043438	2.414837	34	1	0	3.582121	-1.765891	1.522242
13	1	0	-4.735957	3.103169	2.513816	35	1	0	3.168247	-0.309572	2.110704
14	6	0	-1.209092	3.030579	-0.720521	36	16	0	0.047652	-0.438452	-1.647691
15	6	0	0.159375	2.859670	-0.920705	37	6	0	-0.396528	-2.199379	-2.038194
16	6	0	0.856423	3.766938	-1.711017	38	1	0	-0.343107	-2.332305	-3.117069
17	1	0	1.917971	3.614905	-1.861844	39	1	0	0.331881	-2.853981	-1.563392
18	6	0	0.187090	4.834227	-2.307807	40	6	0	-1.807852	-2.529509	-1.541706
19	1	0	0.729074	5.532385	-2.935603	41	1	0	-2.536046	-2.003321	-2.167375
20	6	0	-1.186109	4.997328	-2.108125	42	7	0	-1.980588	-2.065447	-0.148337
21	1	0	-1.710828	5.819623	-2.581069	43	1	0	-1.221205	-2.448535	0.437617
22	6	0	-1.889971	4.101247	-1.313071	44	6	0	-2.140055	-4.014823	-1.646928
23	1	0	-2.955175	4.207692	-1.154800	45	8	0	-2.616651	-4.673579	-0.758426
24	16	0	3.143202	0.837402	-1.288677	46	8	0	-1.869460	-4.496812	-2.876638
25	6	0	4.379552	1.129625	0.046313	47	1	0	-5.443818	-0.999874	3.593457
26	1	0	3.992504	1.844687	0.779301	48	1	0	-2.116981	-5.434229	-2.890773
27	1	0	5.278722	1.552490	-0.404554	49	1	0	-2.861322	-2.413049	0.221204
28	6	0	4.714658	-0.189853	0.752656	50	1	0	0.684073	2.040100	-0.450552
29	1	0	5.156287	-0.874332	0.026764	51	1	0	7.517583	0.438681	2.193488
30	6	0	5.694908	0.045963	1.892872	52	17	0	0.846373	-2.495017	1.192883
31	8	0	6.946329	0.249572	1.433072	---					
32	8	0	5.396089	0.085787	3.060455	HF=-2731.5832121\ZeroPoint=0.3637664\Thermal=0.3970488					
33	7	0	3.459929	-0.789843	1.258882						

Structures from Table S7

Table S7. PATH II: B3LYP-D3/6-311+G**/SDD(Pd)/gas phase free energies for the pre- and postreaction complexes and the transition states for **the first D-transfer**. Free energies relative to **B1-1** (in kcal mol^{-1}).

Mother complex→	B1- 1			B1-2		
D-source→	**Cys^{4D}**·DCl	**Cys^{4D}**·DCl	DCl	**Cys^{4D}**·DCl	**Cys^{4D}**·DCl	DCl
Donor group→	COOD	ND_3^+	DCl	COOD	ND_3^+	DCl
Inside D-transfer						
Prereaction complex	-9.5	**-21.3**	-0.0	**-11.7**	-15.4	-0.6
Transition state	7.0	**1.4**	12.4	**6.2**	11.3	11.3
Postreaction complex	2.2	**-1.6**	1.4	**-6.3**	-12.4	-11.4
Outside D-transfer						
Prereaction complex	-13.8	-6.9	-0.8	-10.4	-3.7	3.3
Transition state	6.4	6.8	13.6	10.6	13.0	18.0
Postreaction complex	-3.0	-3.3	8.0	4.9	2.1	13.9

G = -9.5 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	2.278474	-0.196310	0.375944
2	46	0	-0.405503	1.826582	0.336744
3	7	0	2.372852	0.887183	-1.368432
4	7	0	2.867866	0.322705	-2.386430
5	6	0	3.222633	-1.006278	-2.175366
6	6	0	3.004642	-1.583806	-0.896164
7	6	0	3.334007	-2.927917	-0.735617
8	1	0	3.172269	-3.431012	0.213447
9	6	0	3.863877	-3.670038	-1.800470
10	6	0	4.077976	-3.078608	-3.045904
11	1	0	4.487264	-3.662652	-3.861386
12	6	0	3.755559	-1.738962	-3.240870
13	1	0	3.904910	-1.253201	-4.197877
14	6	0	2.045266	2.269085	-1.500449
15	6	0	0.913285	2.797985	-0.851050
16	6	0	0.658760	4.164746	-1.060944
17	1	0	-0.222560	4.610530	-0.617262
18	6	0	1.498159	4.963592	-1.830565
19	1	0	1.274273	6.018485	-1.948258
20	6	0	2.623485	4.413473	-2.451308
21	1	0	3.284005	5.032868	-3.046726
22	6	0	2.889591	3.065592	-2.296963
23	1	0	3.750992	2.609708	-2.767713
24	16	0	-2.087539	2.122014	-1.271375
25	6	0	-3.592085	1.673096	-0.287275
26	1	0	-4.018773	0.738140	-0.660277
27	1	0	-4.352386	2.433385	-0.464817
28	6	0	-3.343742	1.591191	1.233664
29	1	0	-3.394976	2.596912	1.652275
30	6	0	-4.442568	0.715507	1.823024
31	8	0	-5.619459	1.354980	1.880005
32	8	0	-4.279680	-0.439009	2.141168
33	7	0	-2.012742	1.032127	1.584749
34	1	0	-1.825215	1.247519	2.560585
35	1	0	-2.041019	0.013180	1.540242
36	16	0	1.415505	1.506044	1.864096
37	6	0	0.885252	0.302449	3.170410
38	1	0	0.746235	0.831568	4.112115
39	1	0	-0.048507	-0.183925	2.884827
40	6	0	1.964112	-0.772597	3.328202
41	1	0	2.909649	-0.289280	3.590053
42	7	0	2.142023	-1.477478	2.037517
43	1	0	1.296071	-2.017520	1.833098
44	6	0	1.630982	-1.774878	4.429740
45	8	0	1.517821	-2.961675	4.260087
46	8	0	1.488414	-1.165411	5.622493
47	1	0	4.104874	-4.717409	-1.654166
48	1	0	1.283497	-1.842789	6.285782
49	1	0	2.909478	-2.140776	2.103813
50	1	0	-6.305165	0.713408	2.124281
51	1	0	0.861241	-1.775548	-1.028517
52	7	0	-2.531812	-0.990951	-2.000299
53	6	0	-2.357614	-1.715712	-0.719934
54	1	0	-3.616443	-0.978817	-2.205655
55	1	0	-2.050914	-1.480833	-2.755888
56	6	0	-3.019662	-3.119341	-0.746498
57	1	0	-2.888052	-1.153690	0.047189
58	6	0	-0.904158	-1.793333	-0.301791
59	16	0	-2.826399	-4.047039	-2.318590
60	1	0	-4.085999	-2.989622	-0.574640
61	1	0	-2.598754	-3.722008	0.058191
62	8	0	-0.072771	-1.810081	-1.334076
63	8	0	-0.573980	-1.870612	0.866450
64	1	0	-3.926582	-3.500759	-2.889546
65	1	0	-2.185883	-0.003211	-1.931022
66	17	0	-5.435404	-1.171976	-2.140815

HF=-3453.6662317\ZeroPoint=0.461132\Thermal=0.5037065

G = 7.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-2.077512	0.195169	0.375129
2	46	0	0.431177	-1.825885	0.399000
3	7	0	-2.312527	-0.962511	-1.317923
4	7	0	-2.938733	-0.435572	-2.282783
5	6	0	-3.296706	0.898428	-2.090705
6	6	0	-2.704545	1.670854	-1.054575
7	6	0	-3.164409	2.980967	-0.872497
8	1	0	-2.699906	3.609708	-0.119091
9	6	0	-4.153226	3.515882	-1.696079
10	6	0	-4.696650	2.747207	-2.729691
11	1	0	-5.454688	3.172613	-3.376881
12	6	0	-4.266941	1.440039	-2.937825
13	1	0	-4.685352	0.826579	-3.726425
14	6	0	-1.986514	-2.339629	-1.440212
15	6	0	-0.854118	-2.851993	-0.774260
16	6	0	-0.584350	-4.218671	-0.966791
17	1	0	0.298127	-4.649680	-0.511393
18	6	0	-1.410481	-5.031634	-1.733647
19	1	0	-1.176861	-6.085669	-1.839216
20	6	0	-2.538927	-4.498967	-2.369152
21	1	0	-3.188004	-5.133068	-2.961463
22	6	0	-2.820965	-3.154709	-2.233573
23	1	0	-3.683156	-2.714262	-2.716126
24	16	0	2.090010	-2.137477	-1.219639
25	6	0	3.585984	-1.553694	-0.297265
26	1	0	3.929228	-0.595024	-0.694148
27	1	0	4.394742	-2.258313	-0.488739
28	6	0	3.357289	-1.478542	1.221074
29	1	0	3.398325	-2.490825	1.627826
30	6	0	4.465835	-0.635266	1.840581
31	8	0	5.650253	-1.267608	1.795968
32	8	0	4.306125	0.477051	2.280247
33	7	0	2.028137	-0.917249	1.573694
34	1	0	1.887568	-1.050275	2.571843
35	1	0	2.011697	0.096556	1.439289
36	16	0	-1.432637	-1.488571	1.891341
37	6	0	-0.902319	-0.340921	3.250729
38	1	0	-0.913851	-0.889809	4.190575
39	1	0	0.103812	0.031607	3.060511
40	6	0	-1.864707	0.842340	3.302405
41	1	0	-2.873696	0.467952	3.505053
42	7	0	-1.868149	1.507486	1.982442
43	1	0	-0.927676	1.887545	1.754252
44	6	0	-1.544239	1.856171	4.399343
45	8	0	-1.519053	3.047121	4.230998
46	8	0	-1.332610	1.254561	5.586105
47	1	0	-4.484133	4.538004	-1.552329
48	1	0	-1.164109	1.943457	6.248019
49	1	0	-2.526424	2.282384	1.979213
50	1	0	6.337372	-0.649533	2.090252
51	1	0	-1.407769	1.641557	-0.957176
52	7	0	2.353206	1.030197	-2.117398
53	6	0	2.266379	1.775419	-0.835714
54	1	0	3.405495	1.019159	-2.413667
55	1	0	1.782150	1.500033	-2.821788
56	6	0	2.925526	3.171268	-0.933011
57	1	0	2.847251	1.219431	-0.102200
58	6	0	0.820423	1.851635	-0.346963
59	16	0	2.638073	4.071787	-2.510001
60	1	0	4.001795	3.055584	-0.825198
61	1	0	2.548614	3.790353	-0.119084
62	8	0	-0.062954	1.869323	-1.262448
63	8	0	0.643145	1.903326	0.886657
64	1	0	3.709358	3.526094	-3.132920
65	1	0	2.029329	0.049392	-2.000802
66	17	0	5.258718	1.178577	-2.442638

HF=-3453.6375697\ZeroPoint=0.4575432\Thermal=0.4994312

G = 2.2 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	2.053594	-0.358354	0.167743
2	46	0	-0.323287	1.740584	0.687597
3	7	0	2.564732	1.235067	-1.058232
4	7	0	3.411726	0.930836	-1.943315
5	6	0	3.645623	-0.464456	-2.001223
6	6	0	2.566744	-1.375920	-1.926169
7	6	0	2.827434	-2.754000	-1.921699
8	1	0	1.981462	-3.428524	-1.865719
9	6	0	4.135393	-3.213043	-2.011650
10	6	0	5.191009	-2.299018	-2.135868
11	1	0	6.207980	-2.663591	-2.225090
12	6	0	4.956106	-0.928484	-2.141392
13	1	0	5.767815	-0.216015	-2.219868
14	6	0	2.230257	2.602129	-0.892064
15	6	0	1.044602	2.948337	-0.207590
16	6	0	0.773178	4.327534	-0.110017
17	1	0	-0.142737	4.649126	0.368274
18	6	0	1.634557	5.290026	-0.618938
19	1	0	1.390623	6.340859	-0.504949
20	6	0	2.812245	4.913807	-1.279407
21	1	0	3.487503	5.664501	-1.672464
22	6	0	3.105253	3.575147	-1.424868
23	1	0	4.004229	3.254122	-1.933364
24	16	0	-1.901324	2.417162	-0.891480
25	6	0	-3.462531	1.825555	-0.089784
26	1	0	-3.874272	0.978314	-0.642891
27	1	0	-4.202779	2.620705	-0.172681
28	6	0	-3.271511	1.492414	1.398304
29	1	0	-3.234605	2.430379	1.956421
30	6	0	-4.464322	0.672868	1.878052
31	8	0	-5.585586	1.414951	1.911699
32	8	0	-4.418277	-0.498769	2.158613
33	7	0	-2.001710	0.771443	1.668052
34	1	0	-1.867605	0.739087	2.675617
35	1	0	-2.043385	-0.213714	1.381351
36	16	0	1.464905	0.885292	2.033729
37	6	0	0.853455	-0.512507	3.090982

38	1	0	0.947329	-0.209941	4.132297
39	1	0	-0.185432	-0.733894	2.856269
40	6	0	1.707026	-1.740354	2.788649
41	1	0	2.749448	-1.527492	3.051005
42	7	0	1.616562	-2.008210	1.336857
43	1	0	0.597456	-2.168027	1.094780
44	6	0	1.320856	-2.995462	3.570974
45	8	0	1.364605	-4.106348	3.112334
46	8	0	0.980889	-2.714238	4.843730
47	1	0	4.340948	-4.276874	-2.013445
48	1	0	0.778641	-3.550329	5.292451
49	1	0	2.136876	-2.847664	1.091038
50	1	0	-6.331874	0.828931	2.112181
51	1	0	1.536658	-1.048690	-2.050516
52	7	0	-2.422681	-0.668481	-2.168664
53	6	0	-2.529692	-1.547559	-0.972495
54	1	0	-3.435569	-0.482600	-2.532972
55	1	0	-1.858508	-1.145010	-2.875076
56	6	0	-3.354124	-2.819318	-1.275423
57	1	0	-3.090348	-0.997922	-0.219946
58	6	0	-1.130814	-1.871562	-0.436349
59	16	0	-3.081707	-3.567631	-2.934729
60	1	0	-4.412583	-2.576922	-1.210081
61	1	0	-3.114053	-3.574570	-0.527261
62	8	0	-0.213614	-2.041520	-1.261672
63	8	0	-1.035285	-1.943882	0.827834
64	1	0	-4.040117	-2.825993	-3.538504
65	1	0	-1.989213	0.239565	-1.927974
66	17	0	-5.286749	-0.356502	-2.695307

HF=-3453.6468555\ZeroPoint=0.4609044\Thermal=0.5034792

G = -13.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.671400	-0.327700	0.235673
2	46	0	2.475100	0.556471	-0.598127
3	7	0	-0.311870	1.506766	1.071097
4	7	0	-0.834038	1.764292	2.193634
5	6	0	-1.579310	0.709498	2.709624
6	6	0	-1.690254	-0.488428	1.956018
7	6	0	-2.506248	-1.494339	2.463577
8	1	0	-2.681281	-2.405140	1.902184
9	6	0	-3.158924	-1.328925	3.692461
10	6	0	-3.017084	-0.153240	4.432630
11	1	0	-3.530329	-0.040889	5.380281
12	6	0	-2.227991	0.879369	3.938702
13	1	0	-2.112223	1.813647	4.475646
14	6	0	0.363018	2.577799	0.410007
15	6	0	1.521259	2.330199	-0.350003
16	6	0	2.093852	3.442619	-0.990956
17	1	0	3.009113	3.311157	-1.554159
18	6	0	1.532170	4.713531	-0.912122
19	1	0	1.998560	5.539847	-1.438311
20	6	0	0.379596	4.928314	-0.152188
21	1	0	-0.062350	5.915898	-0.085331
22	6	0	-0.198291	3.862656	0.515544
23	1	0	-1.092284	3.995698	1.111607
24	16	0	4.157669	1.362175	0.818059
25	6	0	5.531408	0.344434	0.136370
26	1	0	6.365094	0.371715	0.838730
27	1	0	5.880462	0.746181	-0.820086
28	6	0	5.074785	-1.097718	-0.081097
29	1	0	5.907355	-1.692403	-0.490173
30	6	0	4.708615	-1.787477	1.224098
31	8	0	5.666521	-1.638371	2.145435
32	8	0	3.728836	-2.475361	1.422553
33	7	0	3.919913	-1.113777	-1.004887
34	1	0	4.253869	-0.864689	-1.933260
35	1	0	3.526296	-2.052340	-1.090376
36	16	0	0.488069	-0.001096	-1.888046
37	6	0	0.140009	-1.697499	-2.554098
38	1	0	-0.769015	-1.590224	-3.146814
39	1	0	0.955084	-2.021586	-3.199140
40	6	0	-0.083812	-2.743867	-1.454697
41	1	0	-0.436982	-3.670588	-1.925442
42	7	0	-1.078821	-2.267694	-0.461368
43	1	0	-1.068812	-2.880140	0.350600
44	6	0	1.251774	-3.075489	-0.799541
45	8	0	2.218131	-3.395215	-1.463068
46	8	0	1.248580	-2.954586	0.518189
47	1	0	-3.790538	-2.126941	4.068692
48	1	0	2.174754	-2.929578	0.861123
49	1	0	-2.037691	-2.322740	-0.831238
50	1	0	5.380343	-2.094371	2.951403
51	1	0	-1.214446	1.425928	-2.300240
52	8	0	-2.133150	1.713126	-2.061125
53	6	0	-2.980942	0.765413	-2.418378
54	6	0	-4.323755	0.913875	-1.701619
55	8	0	-2.763019	-0.138326	-3.193099
56	6	0	-4.136198	0.941711	-0.173914
57	1	0	-4.810604	1.832861	-2.038139
58	7	0	-5.165184	-0.248204	-2.114620
59	16	0	-5.698389	0.752998	0.773217
60	1	0	-3.685215	1.893458	0.099221
61	1	0	-3.460109	0.149132	0.141500
62	1	0	-5.089142	-0.416942	-3.118133
63	1	0	-6.135696	-0.099586	-1.836585
64	1	0	-4.820253	-1.169569	-1.600631
65	1	0	-5.609214	-0.594072	0.870647
66	17	0	-4.280693	-2.588640	-0.606052

HF=-3453.674357\ZeroPoint=0.4605091\Thermal=0.5025925

G = 6.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.459221	0.431192	-0.331580
2	46	0	2.899039	0.089668	-0.661984
3	7	0	0.534222	1.908478	0.685862
4	7	0	0.204604	2.167441	1.873501
5	6	0	-0.792703	1.328309	2.376686

6	6	0	-1.525124	0.484028	1.500770
7	6	0	-2.375665	-0.465055	2.077040
8	1	0	-2.951880	-1.131896	1.444628
9	6	0	-2.525003	-0.539870	3.463258
10	6	0	-1.837312	0.340603	4.301510
11	1	0	-1.972771	0.285103	5.375442
12	6	0	-0.964956	1.281931	3.761207
13	1	0	-0.390238	1.951406	4.389801
14	6	0	1.566859	2.719263	0.115874
15	6	0	2.644869	2.096085	-0.532356
16	6	0	3.625819	2.948722	-1.060631
17	1	0	4.499870	2.519101	-1.533807
18	6	0	3.512944	4.334863	-0.978530
19	1	0	4.281966	4.961154	-1.418377
20	6	0	2.425838	4.922101	-0.326174
21	1	0	2.339687	6.000348	-0.258654
22	6	0	1.454726	4.111044	0.239219
23	1	0	0.600461	4.530514	0.756570
24	16	0	4.580146	0.291912	0.959269
25	6	0	5.430550	-1.305417	0.618221
26	1	0	6.055267	-1.556673	1.475749
27	1	0	6.077916	-1.223176	-0.260624
28	6	0	4.413237	-2.416801	0.367089
29	1	0	4.940796	-3.360607	0.155134
30	6	0	3.560828	-2.714052	1.592606
31	8	0	4.314511	-2.872329	2.687568
32	8	0	2.360674	-2.883140	1.605561
33	7	0	3.545762	-2.040641	-0.772333
34	1	0	4.109311	-2.069848	-1.619225
35	1	0	2.801337	-2.727708	-0.902300
36	16	0	1.021871	0.274673	-2.170971
37	6	0	0.322106	-1.261376	-2.951722
38	1	0	-0.263431	-0.917945	-3.807127
39	1	0	1.128032	-1.897778	-3.312491
40	6	0	-0.582777	-2.043048	-1.994559
41	1	0	-1.160267	-2.787076	-2.558095
42	7	0	-1.497618	-1.099133	-1.316267
43	1	0	-2.182966	-1.604218	-0.742433
44	6	0	0.284870	-2.826612	-1.016488
45	8	0	1.161658	-3.566858	-1.417398
46	8	0	0.021873	-2.591857	0.257455
47	1	0	-3.192889	-1.280666	3.888784
48	1	0	0.777889	-2.899788	0.806997
49	1	0	-2.063313	-0.591318	-2.000762
50	1	0	3.723764	-3.062491	3.431883
51	1	0	-2.226088	1.142354	0.489250
52	8	0	-3.352209	1.704209	0.091189
53	6	0	-3.893283	1.235173	-0.962646
54	6	0	-5.422118	0.990395	-0.837023
55	8	0	-3.360376	0.929436	-2.034103
56	6	0	-5.838782	0.615205	0.588739
57	1	0	-5.954433	1.884928	-1.170464
58	7	0	-5.736234	-0.108950	-1.806826
59	16	0	-7.519689	-0.132781	0.715439
60	1	0	-5.830555	1.515251	1.199462
61	1	0	-5.129166	-0.088885	1.014566
62	1	0	-5.268566	0.098180	-2.692488
63	1	0	-6.742449	-0.234449	-1.918540
64	1	0	-5.297648	-1.026107	-1.418614
65	1	0	-7.094759	-1.407240	0.563154
66	17	0	-4.388088	-2.381170	-0.467973

HF=-3453.6392914\ZeroPoint=0.4567643\Thermal=0.4982929

G = -3.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.519967	0.474553	-0.186848
2	46	0	2.833700	0.183677	-0.734708
3	7	0	0.563903	1.797158	0.964914
4	7	0	0.349782	1.882242	2.198458
5	6	0	-0.605791	0.972510	2.695174
6	6	0	-1.671444	0.473682	1.914387
7	6	0	-2.453561	-0.570413	2.408267
8	1	0	-3.244505	-0.988153	1.796306
9	6	0	-2.205208	-1.082061	3.681976
10	6	0	-1.194718	-0.536123	4.474446
11	1	0	-1.019544	-0.923300	5.471605
12	6	0	-0.393231	0.495232	3.987970
13	1	0	0.421981	0.904282	4.571823
14	6	0	1.551199	2.689987	0.431850
15	6	0	2.588788	2.162439	-0.351723
16	6	0	3.529442	3.084486	-0.832457
17	1	0	4.375205	2.726939	-1.406165
18	6	0	3.411624	4.449546	-0.577433
19	1	0	4.146983	5.134724	-0.985606
20	6	0	2.363685	4.939677	0.205207
21	1	0	2.273733	6.000911	0.404956
22	6	0	1.435640	4.053562	0.729637
23	1	0	0.611026	4.396642	1.342545
24	16	0	4.630785	0.213426	0.764103
25	6	0	5.428864	-1.353145	0.213778
26	1	0	6.098383	-1.696988	1.002492
27	1	0	6.024668	-1.188356	-0.689331
28	6	0	4.379074	-2.421064	-0.086340
29	1	0	4.876459	-3.342161	-0.429145
30	6	0	3.598181	-2.836038	1.152700
31	8	0	4.416137	-3.124548	2.172342
32	8	0	2.397380	-2.980823	1.225380
33	7	0	3.448987	-1.917854	-1.123338
34	1	0	3.958658	-1.864356	-2.002674
35	1	0	2.686597	-2.580746	-1.276393
36	16	0	0.861144	0.530384	-2.053089
37	6	0	0.119848	-0.892335	-3.001639
38	1	0	-0.502588	-0.435292	-3.772418
39	1	0	0.912341	-1.472358	-3.470903
40	6	0	-0.744278	-1.773063	-2.098347
41	1	0	-1.353757	-2.448770	-2.711848
42	7	0	-1.614312	-0.894658	-1.292871
43	1	0	-2.277861	-1.446202	-0.726232
44	6	0	0.164382	-2.658919	-1.253408
45	8	0	1.013015	-3.357484	-1.772714
46	8	0	-0.023233	-2.550513	0.051425
47	1	0	-2.812660	-1.896412	4.058606

48	1	0	0.753966	-2.926858	0.521206
49	1	0	-2.209789	-0.311182	-1.912629
50	1	0	3.870780	-3.390453	2.928024
51	1	0	-2.055480	1.049406	1.046675
52	8	0	-3.300094	1.866629	-0.472096
53	6	0	-3.928483	1.249616	-1.342261
54	6	0	-5.438406	0.958180	-1.049302
55	8	0	-3.517095	0.771391	-2.438598
56	6	0	-5.732042	0.825236	0.442683
57	1	0	-6.042740	1.754222	-1.491559
58	7	0	-5.758210	-0.304166	-1.797125
59	16	0	-7.374243	0.079490	0.837216
60	1	0	-5.704910	1.815859	0.891184
61	1	0	-4.970591	0.217850	0.922609
62	1	0	-5.261666	-0.226935	-2.694420
63	1	0	-6.760080	-0.458349	-1.900155
64	1	0	-5.315453	-1.130357	-1.275121
65	1	0	-6.931613	-1.197871	0.829041
66	17	0	-4.288445	-2.344082	-0.157043

HF=-3453.6555421\ZeroPoint=0.4602898\Thermal=0.5025223

G = -21.3 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.203218	0.964175	-1.079892
2	46	0	-1.589090	-0.632437	-1.182501
3	7	0	1.718040	-0.901024	-1.793613
4	7	0	2.866337	-1.349765	-1.495567
5	6	0	3.579978	-0.520386	-0.634653
6	6	0	2.969363	0.671943	-0.162582
7	6	0	3.674913	1.424912	0.774164
8	1	0	3.241577	2.322409	1.202366
9	6	0	4.943767	1.023041	1.208990
10	6	0	5.536540	-0.142348	0.713982
11	1	0	6.520397	-0.439449	1.056941
12	6	0	4.853126	-0.925034	-0.210591
13	1	0	5.278734	-1.840839	-0.604150
14	6	0	0.917832	-1.703899	-2.654545
15	6	0	-0.480648	-1.704142	-2.492531
16	6	0	-1.202532	-2.568522	-3.335350
17	1	0	-2.278171	-2.637269	-3.224127
18	6	0	-0.579030	-3.339504	-4.310370
19	1	0	-1.176486	-3.974052	-4.956534
20	6	0	0.811524	-3.297826	-4.463649
21	1	0	1.299274	-3.889201	-5.229835
22	6	0	1.561450	-2.492173	-3.627398
23	1	0	2.639192	-2.445077	-3.715258
24	16	0	-1.922814	-2.563138	0.156623
25	6	0	-3.036633	-1.794686	1.426506
26	1	0	-2.445759	-1.373136	2.242761
27	1	0	-3.672620	-2.576773	1.837400
28	6	0	-3.890473	-0.703158	0.786635
29	1	0	-4.497965	-1.161328	-0.002403
30	6	0	-4.879597	-0.033426	1.738976
31	8	0	-5.495631	-0.925143	2.545824
32	8	0	-5.130507	1.144786	1.742665
33	7	0	-3.013119	0.307024	0.162525
34	1	0	-3.585800	1.026782	-0.270931
35	1	0	-2.460393	0.780215	0.896993
36	16	0	-0.851712	1.335968	-2.328236
37	6	0	-1.376734	2.826887	-1.355434
38	1	0	-2.061304	3.415885	-1.962494
39	1	0	-1.874903	2.532383	-0.433592
40	6	0	-0.139076	3.649338	-1.001489
41	1	0	0.365602	3.944665	-1.928506
42	7	0	0.799316	2.816764	-0.211613
43	1	0	0.340684	2.555531	0.685570
44	6	0	-0.424607	4.948873	-0.248524
45	8	0	-1.541726	5.560856	-0.688194
46	8	0	0.295785	5.400781	0.603734
47	1	0	5.467553	1.619482	1.947913
48	1	0	1.623606	3.363354	0.024233
49	1	0	-6.127880	-0.434414	3.092920
50	1	0	1.079208	-0.580516	0.829035
51	7	0	0.514390	-1.038039	1.557748
52	6	0	1.308314	-1.993945	2.356423
53	1	0	0.081962	-0.234380	2.088654
54	1	0	-0.269618	-1.546957	1.060017
55	6	0	2.628800	-1.401710	2.877464
56	1	0	1.550895	-2.843072	1.709608
57	6	0	0.431167	-2.520435	3.483927
58	16	0	2.474101	0.177395	3.794307
59	1	0	3.274292	-1.168202	2.031678
60	1	0	3.129689	-2.155943	3.483378
61	8	0	1.038261	-3.547428	4.112399
62	8	0	-0.642088	-2.077264	3.789515
63	1	0	1.671397	-0.278482	4.779442
64	17	0	-0.882251	1.605902	2.189738
65	1	0	0.453988	-3.850799	4.824075
66	1	0	-1.644136	6.385058	-0.187370

HF=-3453.6856405\ZeroPoint=0.461322\Thermal=0.5039315

G = 1.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.697941	-1.438735	0.661676
2	46	0	-1.496088	0.640720	1.301561
3	7	0	1.695668	-0.053625	1.851506
4	7	0	2.950389	0.036599	1.686329
5	6	0	3.441659	-0.696944	0.604940
6	6	0	2.553596	-1.144414	-0.411680
7	6	0	3.087535	-1.853732	-1.496201
8	1	0	2.431390	-2.153205	-2.306593
9	6	0	4.455399	-2.103196	-1.573963
10	6	0	5.314561	-1.636842	-0.571458
11	1	0	6.379466	-1.823955	-0.647047
12	6	0	4.817407	-0.924169	0.516526
13	1	0	5.471510	-0.556402	1.297907
14	6	0	1.125836	0.694859	2.910632
15	6	0	-0.227388	1.077761	2.812360

16	6	0	-0.727081	1.869388	3.861942
17	1	0	-1.749199	2.225128	3.813156
18	6	0	0.053541	2.210881	4.959758
19	1	0	-0.376137	2.803451	5.760620
20	6	0	1.389522	1.793567	5.041062
21	1	0	1.994142	2.052109	5.902451
22	6	0	1.931297	1.048533	4.013247
23	1	0	2.961552	0.719420	4.043259
24	16	0	-1.245997	2.834935	0.506653
25	6	0	-2.289798	2.664737	-1.014292
26	1	0	-1.695560	2.273330	-1.842630
27	1	0	-2.643424	3.656651	-1.291255
28	6	0	-3.467589	1.741819	-0.729089
29	1	0	-4.054044	2.176217	0.089247
30	6	0	-4.451538	1.551783	-1.883095
31	8	0	-4.591480	2.662376	-2.636217
32	8	0	-5.083239	0.542038	-2.068665
33	7	0	-2.961531	0.425713	-0.279041
34	1	0	-3.754910	-0.172529	-0.061560
35	1	0	-2.466997	-0.025499	-1.072110
36	16	0	-1.271350	-1.679444	1.933244
37	6	0	-2.176986	-2.738100	0.705011
38	1	0	-2.959337	-3.277853	1.235211
39	1	0	-2.624552	-2.124064	-0.073660
40	6	0	-1.179417	-3.700524	0.073582
41	1	0	-0.739154	-4.323863	0.860316
42	7	0	-0.093360	-2.915962	-0.559488
43	1	0	-0.485665	-2.353638	-1.359780
44	6	0	-1.761604	-4.675324	-0.951516
45	8	0	-3.043425	-4.995199	-0.692003
46	8	0	-1.120345	-5.140668	-1.857150
47	1	0	4.861332	-2.636760	-2.425533
48	1	0	0.606355	-3.543965	-0.948657
49	1	0	-5.247504	2.467307	-3.322975
50	1	0	1.706725	-0.273355	-0.754807
51	7	0	1.079253	1.037388	-1.323191
52	6	0	1.967961	2.186589	-1.395226
53	1	0	0.697728	0.759957	-2.229484
54	1	0	0.282536	1.268664	-0.723516
55	6	0	3.313110	1.848868	-2.071266
56	1	0	2.187974	2.512705	-0.374309
57	6	0	1.312569	3.367989	-2.106699
58	16	0	3.183352	1.030473	-3.713365
59	1	0	3.852738	1.130488	-1.454519
60	1	0	3.921095	2.750081	-2.148448
61	8	0	1.931810	4.529102	-1.795450
62	8	0	0.398821	3.288487	-2.886106
63	1	0	2.483936	2.004361	-4.332610
64	17	0	-1.215253	-0.924541	-2.578495
65	1	0	1.485884	5.241052	-2.278921
66	1	0	-3.335486	-5.626438	-1.368256

HF=-3453.6435994\ZeroPoint=0.456923\Thermal=0.4995063

G = -1.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.278100	-1.316362	0.425922
2	46	0	0.266171	1.442522	1.295146
3	7	0	0.519611	-1.936170	1.249450
4	7	0	0.818777	-3.111777	0.898761
5	6	0	-0.062387	-3.618710	-0.092201
6	6	0	-0.453386	-2.810520	-1.188138
7	6	0	-1.358665	-3.335538	-2.125937
8	1	0	-1.645432	-2.718399	-2.970131
9	6	0	-1.848901	-4.626234	-1.981982
10	6	0	-1.413316	-5.426127	-0.915350
11	1	0	-1.782960	-6.440754	-0.820195
12	6	0	-0.514119	-4.936930	0.024203
13	1	0	-0.180783	-5.543859	0.856956
14	6	0	1.303125	-1.321030	2.261653
15	6	0	1.273559	0.084062	2.418890
16	6	0	2.079912	0.599256	3.454414
17	1	0	2.118070	1.671539	3.601742
18	6	0	2.838958	-0.215671	4.282527
19	1	0	3.433036	0.228549	5.074262
20	6	0	2.842833	-1.606001	4.102569
21	1	0	3.429646	-2.244695	4.752160
22	6	0	2.083039	-2.156628	3.093123
23	1	0	2.060893	-3.226358	2.934832
24	16	0	2.320016	2.338369	0.630333
25	6	0	1.686970	3.371911	-0.760601
26	1	0	1.538494	2.759847	-1.653319
27	1	0	2.440346	4.123823	-0.991732
28	6	0	0.382724	4.033848	-0.335551
29	1	0	0.587576	4.640776	0.554390
30	6	0	-0.243651	4.989169	-1.349653
31	8	0	0.679655	5.662609	-2.066542
32	8	0	-1.430346	5.170528	-1.460831
33	7	0	-0.595795	2.990845	0.044250
34	1	0	-1.430201	3.443306	0.408691
35	1	0	-0.897670	2.475024	-0.803840
36	16	0	-1.772234	0.371485	1.931296
37	6	0	-3.197639	1.094935	0.990003
38	1	0	-3.798194	1.678214	1.685768
39	1	0	-2.834919	1.728717	0.183499
40	6	0	-3.997458	-0.056234	0.392845
41	1	0	-4.365173	-0.698193	1.201477
42	7	0	-3.091066	-0.851921	-0.465826
43	1	0	-2.737731	-0.247294	-1.253252
44	6	0	-5.230577	0.357829	-0.410451
45	8	0	-5.839341	1.440052	0.109616
46	8	0	-5.634041	-0.251078	-1.366404
47	1	0	-2.545024	-5.029683	-2.707913
48	1	0	-3.586668	-1.642249	-0.872892
49	1	0	0.205747	6.264416	-2.660924
50	1	0	0.128508	-1.901850	-1.419984
51	7	0	1.508882	-0.456181	-1.684783
52	6	0	2.862527	-0.608220	-1.193473
53	1	0	1.497922	-0.320471	-2.691593
54	1	0	1.061551	0.362126	-1.283026
55	6	0	3.409839	-2.021759	-1.462081
56	1	0	2.852038	-0.472609	-0.108179
57	6	0	3.823524	0.455099	-1.726376

58	16	0	3.421129	-2.531707	-3.233355
59	1	0	2.757324	-2.744955	-0.972226
60	1	0	4.411801	-2.130237	-1.049192
61	8	0	5.042438	0.361688	-1.139333
62	8	0	3.569836	1.262085	-2.583938
63	1	0	4.380128	-1.674931	-3.641583
64	17	0	-1.520683	1.011876	-2.291609
65	1	0	5.589343	1.080510	-1.489328
66	1	0	-6.619857	1.634392	-0.432713

HF=-3453.6486707\ZeroPoint=0.4593555\Thermal=0.5029643

G = -6.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.409612	-1.452845	0.243728
2	46	0	1.429458	1.388993	-0.178304
3	7	0	-0.130714	-0.571091	2.068142
4	7	0	0.055231	-1.313140	3.075263
5	6	0	0.063678	-2.665820	2.760949
6	6	0	-0.174522	-3.059228	1.416450
7	6	0	-0.215861	-4.423154	1.148833
8	1	0	-0.425660	-4.788372	0.148952
9	6	0	-0.003688	-5.357805	2.170359
10	6	0	0.247841	-4.950476	3.483549
11	1	0	0.410045	-5.687950	4.260395
12	6	0	0.277011	-3.595460	3.787552
13	1	0	0.454896	-3.242051	4.796527
14	6	0	-0.294288	0.828274	2.319087
15	6	0	0.270879	1.776561	1.444412
16	6	0	0.007265	3.126473	1.748021
17	1	0	0.466059	3.897007	1.140216
18	6	0	-0.802200	3.507597	2.817382
19	1	0	-0.985199	4.560043	3.007511
20	6	0	-1.362254	2.539449	3.656285
21	1	0	-1.983226	2.827955	4.496513
22	6	0	-1.091850	1.199190	3.415762
23	1	0	-1.492996	0.424691	4.058441
24	16	0	3.254555	2.158529	1.061680
25	6	0	4.346125	2.563853	-0.365889
26	1	0	5.370845	2.647239	-0.003057
27	1	0	4.064278	3.522634	-0.811589
28	6	0	4.252869	1.482872	-1.440649
29	1	0	4.893718	1.754773	-2.294312
30	6	0	4.782855	0.135521	-0.970519
31	8	0	5.975332	0.255539	-0.376519
32	8	0	4.263280	-0.941244	-1.169008
33	7	0	2.844201	1.343891	-1.875216
34	1	0	2.592962	2.174842	-2.406456
35	1	0	2.732109	0.556029	-2.517107
36	16	0	-0.646594	0.552472	-1.118403
37	6	0	-0.830181	-0.320714	-2.746413
38	1	0	-1.901807	-0.433215	-2.915752
39	1	0	-0.399243	0.288564	-3.538139
40	6	0	-0.170730	-1.703444	-2.731482
41	1	0	-0.456218	-2.218729	-3.657944
42	7	0	-0.640188	-2.485129	-1.561365
43	1	0	-0.136576	-3.366709	-1.517475
44	6	0	1.343692	-1.544919	-2.751163
45	8	0	1.897886	-0.802382	-3.537508
46	8	0	1.973101	-2.257092	-1.826224
47	1	0	-0.039573	-6.416792	1.936971
48	1	0	2.891454	-1.920926	-1.720502
49	1	0	-1.650503	-2.705209	-1.715052
50	1	0	6.267222	-0.628414	-0.106324
51	1	0	-2.170916	1.092879	0.331522
52	7	0	-3.093144	1.312821	0.769421
53	6	0	-4.013219	1.772300	-0.328465
54	1	0	-3.431509	0.433924	1.167634
55	1	0	-2.960935	2.012955	1.507196
56	6	0	-3.495824	3.054811	-0.968236
57	1	0	-4.993418	1.936533	0.125398
58	6	0	-4.133535	0.617619	-1.352285
59	16	0	-3.428126	4.482551	0.192455
60	1	0	-4.176672	3.324810	-1.773154
61	1	0	-2.513930	2.890785	-1.411155
62	8	0	-4.215193	0.835661	-2.535168
63	8	0	-4.137348	-0.541590	-0.732212
64	1	0	-2.180908	4.250892	0.651260
65	1	0	-4.041121	-1.368474	-1.375004
66	17	0	-3.607175	-2.840173	-2.355799

HF=-3453.6685749\ZeroPoint=0.4605407\Thermal=0.5025752

G = 6.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.906150	-0.127325	-0.092924
2	46	0	2.401816	0.524421	-0.715579
3	7	0	-0.157925	1.350880	1.144896
4	7	0	-0.384018	1.283884	2.384257
5	6	0	-1.142301	0.172200	2.759879
6	6	0	-1.852191	-0.564931	1.771242
7	6	0	-2.516037	-1.728268	2.178132
8	1	0	-3.066323	-2.325831	1.458114
9	6	0	-2.491797	-2.122856	3.518600
10	6	0	-1.823368	-1.358346	4.477628
11	1	0	-1.824092	-1.669962	5.515768
12	6	0	-1.146786	-0.198301	4.104711
13	1	0	-0.600320	0.398819	4.824866
14	6	0	0.566888	2.498152	0.691124
15	6	0	1.644773	2.328977	-0.192075
16	6	0	2.278955	3.503961	-0.625503
17	1	0	3.137721	3.428191	-1.280508
18	6	0	1.848822	4.764780	-0.218930
19	1	0	2.352509	5.649296	-0.593700
20	6	0	0.790451	4.896993	0.684138
21	1	0	0.467271	5.876306	1.017158
22	6	0	0.157002	3.758029	1.156501
23	1	0	-0.656834	3.822726	1.868726
24	16	0	4.175208	0.974771	0.749890
25	6	0	5.354315	-0.274115	0.085236

26	1	0	6.127239	-0.453918	0.832787
27	1	0	5.839540	0.093535	-0.824165
28	6	0	4.628117	-1.576821	-0.243774
29	1	0	5.344149	-2.309186	-0.648283
30	6	0	4.042459	-2.239840	0.995312
31	8	0	4.959097	-2.355305	1.964203
32	8	0	2.923716	-2.691217	1.105538
33	7	0	3.554452	-1.304474	-1.227485
34	1	0	3.994512	-1.076950	-2.116598
35	1	0	2.997521	-2.145410	-1.392344
36	16	0	0.379882	0.373377	-2.012062
37	6	0	0.049893	-1.178845	-2.983770
38	1	0	-0.681562	-0.904857	-3.746244
39	1	0	0.963572	-1.510820	-3.473000
40	6	0	-0.523812	-2.288160	-2.097871
41	1	0	-0.932386	-3.090434	-2.724664
42	7	0	-1.603594	-1.714610	-1.263233
43	1	0	-2.103887	-2.463252	-0.749308
44	6	0	0.605798	-2.908332	-1.286901
45	8	0	1.595251	-3.348773	-1.839007
46	8	0	0.432468	-2.868816	0.023550
47	1	0	-3.008922	-3.029097	3.813153
48	1	0	1.295416	-3.033464	0.465614
49	1	0	-2.326813	-1.353602	-1.892259
50	1	0	4.539375	-2.785915	2.724248
51	1	0	-2.666048	0.277276	1.059364
52	7	0	-3.791376	1.155451	0.889449
53	6	0	-4.283279	1.307987	-0.501859
54	1	0	-4.496753	0.700022	1.463664
55	1	0	-3.580985	2.075721	1.278725
56	6	0	-3.365947	2.205954	-1.334104
57	1	0	-5.294074	1.734140	-0.485343
58	6	0	-4.381273	-0.097060	-1.119524
59	16	0	-3.162507	3.891154	-0.602621
60	1	0	-3.789238	2.308166	-2.330965
61	1	0	-2.380297	1.754594	-1.440900
62	8	0	-3.986451	-0.337483	-2.243322
63	8	0	-4.883883	-0.957261	-0.264659
64	1	0	-1.836554	3.810033	-0.370186
65	1	0	-4.683358	-1.947701	-0.505276
66	17	0	-3.911811	-3.662217	-0.535020

HF=-3453.6394624\ZeroPoint=0.4564283\Thermal=0.4979191

G = -3.3 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.896883	-0.478841	-0.052074
2	46	0	2.154412	0.955683	-0.625889
3	7	0	-0.339459	0.820437	1.466814
4	7	0	-0.406528	0.468497	2.666769
5	6	0	-0.843103	-0.854881	2.882304
6	6	0	-1.767427	-1.507638	2.038558
7	6	0	-2.054284	-2.858049	2.236297
8	1	0	-2.752011	-3.353270	1.568382
9	6	0	-1.440109	-3.544853	3.284413
10	6	0	-0.566447	-2.881499	4.147436
11	1	0	-0.107863	-3.417389	4.970608
12	6	0	-0.271147	-1.532484	3.958690
13	1	0	0.421774	-1.006817	4.603907
14	6	0	0.075573	2.172544	1.230427
15	6	0	1.108957	2.420657	0.315429
16	6	0	1.458310	3.765587	0.124726
17	1	0	2.273832	4.010627	-0.543974
18	6	0	0.794150	4.795110	0.788495
19	1	0	1.078307	5.824556	0.599534
20	6	0	-0.222544	4.511141	1.703863
21	1	0	-0.731651	5.311081	2.228678
22	6	0	-0.576345	3.190539	1.938335
23	1	0	-1.359572	2.930206	2.639266
24	16	0	3.916404	1.418791	0.836729
25	6	0	5.245481	0.549837	-0.098453
26	1	0	6.071862	0.347385	0.583080
27	1	0	5.621311	1.179633	-0.910511
28	6	0	4.725451	-0.755438	-0.696699
29	1	0	5.529305	-1.245737	-1.267821
30	6	0	4.324688	-1.768728	0.366771
31	8	0	5.286791	-1.919831	1.284164
32	8	0	3.310655	-2.431771	0.373231
33	7	0	3.568441	-0.465672	-1.575825
34	1	0	3.913492	0.027785	-2.396479
35	1	0	3.151687	-1.333516	-1.918366
36	16	0	0.092230	0.684970	-1.802117
37	6	0	-0.049286	-0.605222	-3.141569
38	1	0	-0.879058	-0.283077	-3.772351
39	1	0	0.868128	-0.623049	-3.726640
40	6	0	-0.355220	-1.981065	-2.546077
41	1	0	-0.673348	-2.667266	-3.340870
42	7	0	-1.437537	-1.812933	-1.555616
43	1	0	-1.810194	-2.706966	-1.180543
44	6	0	0.925351	-2.558681	-1.954105
45	8	0	1.939057	-2.636170	-2.618972
46	8	0	0.836260	-2.900954	-0.678193
47	1	0	-1.660798	-4.594686	3.436896
48	1	0	1.742314	-2.993974	-0.309171
49	1	0	-2.258677	-1.401858	-2.019839
50	1	0	4.988806	-2.580372	1.927771
51	1	0	-2.424495	-0.916530	1.381496
52	7	0	-3.699575	1.355750	1.021144
53	6	0	-4.218480	1.392421	-0.354797
54	1	0	-4.276298	0.737990	1.583982
55	1	0	-3.777924	2.287032	1.421053
56	6	0	-3.426710	2.375981	-1.220327
57	1	0	-5.283746	1.673018	-0.394040
58	6	0	-4.126037	-0.012700	-0.959116
59	16	0	-3.487976	4.119604	-0.624197
60	1	0	-3.836920	2.380708	-2.228664
61	1	0	-2.384129	2.072090	-1.290717
62	8	0	-3.747846	-0.218842	-2.100249
63	8	0	-4.472524	-0.951114	-0.098138
64	1	0	-2.379721	4.066002	0.142064
65	1	0	-4.308925	-1.900138	-0.440996
66	17	0	-3.670223	-3.723566	-0.732435

HF=-3453.6565132\ZeroPoint=0.4598658\Thermal=0.5022117

G = -0.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.575974	0.387536	-0.385450
2	46	0	-1.379721	-0.985288	-0.505442
3	7	0	1.832299	-1.618709	-0.004355
4	7	0	2.731550	-1.950982	0.818359
5	6	0	3.371062	-0.869517	1.413541
6	6	0	2.982461	0.444420	1.048859
7	6	0	3.604168	1.505491	1.697201
8	1	0	3.325852	2.533082	1.481550
9	6	0	4.590240	1.271664	2.665473
10	6	0	4.969810	-0.028895	3.001346
11	1	0	5.732982	-0.195650	3.752060
12	6	0	4.356965	-1.110308	2.376726
13	1	0	4.620717	-2.132237	2.622303
14	6	0	1.165142	-2.670145	-0.698549
15	6	0	-0.203853	-2.547602	-0.996011
16	6	0	-0.798950	-3.633876	-1.658669
17	1	0	-1.860336	-3.603210	-1.873626
18	6	0	-0.065723	-4.754502	-2.037189
19	1	0	-0.558003	-5.564294	-2.565474
20	6	0	1.297889	-4.842312	-1.739374
21	1	0	1.872391	-5.711675	-2.037473
22	6	0	1.911942	-3.805795	-1.058920
23	1	0	2.964367	-3.846699	-0.808489
24	16	0	-2.391659	-2.336154	1.115052
25	6	0	-3.367676	-1.002410	1.926819
26	1	0	-2.738249	-0.432584	2.617639
27	1	0	-4.175698	-1.463222	2.496461
28	6	0	-3.955536	-0.049399	0.878214
29	1	0	-4.594544	-0.629492	0.208781
30	6	0	-4.790060	1.045807	1.527814
31	8	0	-5.920133	0.550079	2.073765
32	8	0	-4.488226	2.213935	1.574094
33	7	0	-2.855212	0.541561	0.082775
34	1	0	-3.240011	1.034833	-0.718538
35	1	0	-2.396049	1.248254	0.657823
36	16	0	-0.122816	0.288880	-2.127500
37	6	0	-0.553849	2.084169	-1.997544
38	1	0	-1.093879	2.389985	-2.893202
39	1	0	-1.186374	2.269671	-1.126727
40	6	0	0.733128	2.907414	-1.864913
41	1	0	1.361901	2.714840	-2.737419
42	7	0	1.478801	2.483934	-0.653323
43	1	0	1.026734	2.884026	0.171650
44	6	0	0.434544	4.401178	-1.799031
45	8	0	0.611753	5.091083	-0.827134
46	8	0	-0.069842	4.851919	-2.962933
47	1	0	5.058766	2.113623	3.163977
48	1	0	-0.263797	5.797050	-2.863647
49	1	0	2.417454	2.875892	-0.668016
50	1	0	-6.391499	1.283001	2.498428
51	1	0	0.272347	0.791892	1.445062
52	17	0	-0.377756	1.645696	2.216224

HF=-2731.5388628\ZeroPoint=0.3599254\Thermal=0.3938556

G = 12.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.217053	0.671908	-0.368033
2	46	0	-1.111009	-1.325812	-0.569732
3	7	0	2.002100	-1.191679	0.058143
4	7	0	2.921262	-1.248106	0.921632
5	6	0	3.239292	-0.029707	1.516008
6	6	0	2.422469	1.119229	1.322058
7	6	0	2.873948	2.329923	1.861182
8	1	0	2.249539	3.213696	1.778223
9	6	0	4.061832	2.399463	2.587521
10	6	0	4.826160	1.249142	2.799885
11	1	0	5.739896	1.304887	3.379757
12	6	0	4.415710	0.030698	2.269692
13	1	0	5.000371	-0.871111	2.405261
14	6	0	1.686489	-2.395656	-0.633004
15	6	0	0.353416	-2.622924	-1.023460
16	6	0	0.086831	-3.834896	-1.676671
17	1	0	-0.932242	-4.068939	-1.960702
18	6	0	1.099187	-4.747273	-1.958792
19	1	0	0.862124	-5.666739	-2.483782
20	6	0	2.419488	-4.489111	-1.570079
21	1	0	3.206870	-5.198794	-1.795593
22	6	0	2.714902	-3.318876	-0.894517
23	1	0	3.724665	-3.095155	-0.575138
24	16	0	-1.783092	-2.798180	1.110356
25	6	0	-2.783323	-1.585565	2.072710
26	1	0	-2.131053	-0.959652	2.687952
27	1	0	-3.456821	-2.139287	2.726615
28	6	0	-3.590547	-0.700365	1.122584
29	1	0	-4.228556	-1.349761	0.514076
30	6	0	-4.507743	0.295442	1.824408
31	8	0	-5.283495	-0.301466	2.753552
32	8	0	-4.570965	1.472762	1.567504
33	7	0	-2.662522	0.012379	0.216480
34	1	0	-3.203835	0.556588	-0.449708
35	1	0	-2.127565	0.684663	0.776205
36	16	0	-0.092531	0.092672	-2.261176
37	6	0	-0.991516	1.709147	-2.375041
38	1	0	-1.381823	1.816058	-3.386105
39	1	0	-1.828397	1.729867	-1.675371
40	6	0	-0.028788	2.853342	-2.056375
41	1	0	0.787405	2.834682	-2.783853
42	7	0	0.552780	2.643814	-0.710354
43	1	0	-0.147775	2.809308	0.020341
44	6	0	-0.698171	4.222067	-2.137777
45	8	0	-0.770733	5.000600	-1.222898
46	8	0	-1.192945	4.451814	-3.369534
47	1	0	4.380141	3.345664	3.010253
48	1	0	-1.607040	5.328903	-3.370712
49	1	0	1.291564	3.321425	-0.536902

50	1	0	-5.849391	0.380653	3.146090
51	1	0	1.044358	1.119267	1.609413
52	17	0	-0.412266	1.580147	2.293043

HF=-2731.5195218\ZeroPoint=0.3582909\Thermal=0.39122

G = 1.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.505843	-0.198471	-0.225631
2	46	0	1.379378	1.059635	-0.562364
3	7	0	-1.665906	1.821491	0.246313
4	7	0	-2.594752	2.031020	1.068624
5	6	0	-3.102483	0.798577	1.579616
6	6	0	-2.216982	-0.201786	2.053438
7	6	0	-2.745901	-1.420488	2.513516
8	1	0	-2.050463	-2.177303	2.857433
9	6	0	-4.118165	-1.626372	2.515430
10	6	0	-4.984266	-0.608378	2.089507
11	1	0	-6.055996	-0.769366	2.113736
12	6	0	-4.487342	0.604302	1.630749
13	1	0	-5.145654	1.392481	1.287050
14	6	0	-1.026694	2.921680	-0.374791
15	6	0	0.293649	2.746137	-0.834477
16	6	0	0.893033	3.867596	-1.432400
17	1	0	1.919970	3.799218	-1.770766
18	6	0	0.207685	5.067214	-1.589363
19	1	0	0.698168	5.905440	-2.073132
20	6	0	-1.108410	5.205956	-1.126554
21	1	0	-1.639627	6.141681	-1.254479
22	6	0	-1.725410	4.137521	-0.506209
23	1	0	-2.739592	4.212200	-0.135097
24	16	0	2.456573	2.153108	1.186918
25	6	0	3.257179	0.654263	1.912309
26	1	0	2.538430	0.093445	2.514604
27	1	0	4.071864	0.984380	2.556062
28	6	0	3.787368	-0.231105	0.792181
29	1	0	4.489839	0.360833	0.193451
30	6	0	4.561247	-1.475899	1.224346
31	8	0	5.227665	-1.303256	2.384328
32	8	0	4.621955	-2.487655	0.570956
33	7	0	2.660696	-0.624637	-0.084102
34	1	0	3.026092	-1.158098	-0.869052
35	1	0	2.045953	-1.266958	0.449639
36	16	0	-0.112325	-0.042459	-2.077342
37	6	0	0.280996	-1.852334	-2.185444
38	1	0	0.666772	-2.051067	-3.183871
39	1	0	1.028318	-2.123756	-1.442011
40	6	0	-1.002436	-2.629356	-1.919481
41	1	0	-1.751495	-2.347268	-2.668265
42	7	0	-1.509091	-2.247203	-0.582435
43	1	0	-0.823218	-2.542515	0.159700
44	6	0	-0.874434	-4.150370	-2.005215
45	8	0	-1.519245	-4.909402	-1.330561
46	8	0	-0.004867	-4.536858	-2.957998
47	1	0	-4.524680	-2.566189	2.870043
48	1	0	0.009165	-5.506707	-2.975166
49	1	0	-2.391089	-2.716255	-0.386356
50	1	0	5.709440	-2.124486	2.567631
51	1	0	-1.163058	0.008555	2.214574
52	17	0	0.601045	-2.396617	1.621957

HF=-2731.5403748\ZeroPoint=0.3627599\Thermal=0.3958884

G = -0.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.481865	-0.333324	-0.293946
2	46	0	1.716114	0.594253	-0.500574
3	7	0	-1.317419	1.485755	0.627624
4	7	0	-2.010753	1.697090	1.661304
5	6	0	-2.785700	0.606935	2.042239
6	6	0	-2.733706	-0.577149	1.262932
7	6	0	-3.530244	-1.643246	1.664090
8	1	0	-3.549176	-2.571485	1.100060
9	6	0	-4.337495	-1.545538	2.805549
10	6	0	-4.368158	-0.373857	3.563692
11	1	0	-4.998065	-0.311062	4.442953
12	6	0	-3.590430	0.714143	3.181801
13	1	0	-3.595534	1.641163	3.742963
14	6	0	-0.559186	2.578970	0.113019
15	6	0	0.720618	2.357144	-0.425443
16	6	0	1.389053	3.486966	-0.925301
17	1	0	2.393015	3.376131	-1.314822
18	6	0	0.805274	4.750096	-0.922505
19	1	0	1.348575	5.592266	-1.337980
20	6	0	-0.469982	4.938787	-0.382637
21	1	0	-0.928824	5.920689	-0.379805
22	6	0	-1.148668	3.854893	0.145440
23	1	0	-2.139624	3.965869	0.567068
24	16	0	3.084196	1.409021	1.225722
25	6	0	4.578758	0.415659	0.820809
26	1	0	5.261052	0.449816	1.670711
27	1	0	5.100781	0.825473	-0.049643
28	6	0	4.190910	-1.031172	0.517880
29	1	0	5.093970	-1.617601	0.284398
30	6	0	3.579803	-1.718702	1.729166
31	8	0	4.351357	-1.580227	2.811821
32	8	0	2.572163	-2.396357	1.743812
33	7	0	3.243311	-1.058441	-0.617719
34	1	0	3.751768	-0.791376	-1.457814
35	1	0	2.900280	-2.004942	-0.784577
36	16	0	0.015619	0.054115	-2.162354
37	6	0	-0.070274	-1.659463	-2.868052
38	1	0	-0.799594	-1.607172	-3.680042
39	1	0	0.891534	-1.948453	-3.289744
40	6	0	-0.515850	-2.728447	-1.861649
41	1	0	-0.731217	-3.658590	-2.402840
42	7	0	-1.727279	-2.268919	-1.127495
43	1	0	-1.948613	-2.916353	-0.375346
44	6	0	0.632970	-3.042632	-0.913105
45	8	0	1.711757	-3.398352	-1.341518

46	8	0	0.341267	-2.865337	0.363783
47	1	0	-4.948020	-2.392203	3.101497
48	1	0	1.172981	-2.819954	0.900843
49	1	0	-2.526555	-2.243469	-1.760332
50	1	0	3.915059	-2.029749	3.551409
51	1	0	-3.282666	0.037520	-1.457055
52	17	0	-4.271008	-0.216232	-2.309096

HF=-2731.5427253\ZeroPoint=0.3600072\Thermal=0.3929988

G = 13.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.511917	-0.081877	-0.553121
2	46	0	1.822656	0.493960	-0.479612
3	7	0	-1.145505	1.619967	0.507453
4	7	0	-1.768394	1.810381	1.585091
5	6	0	-2.598120	0.755504	1.969417
6	6	0	-2.919945	-0.297041	1.070062
7	6	0	-3.587575	-1.407535	1.597850
8	1	0	-3.896084	-2.204873	0.930467
9	6	0	-3.952963	-1.461879	2.942113
10	6	0	-3.676176	-0.388722	3.791995
11	1	0	-3.983151	-0.424980	4.830600
12	6	0	-3.000322	0.726541	3.307270
13	1	0	-2.744515	1.558814	3.951678
14	6	0	-0.273568	2.668666	0.077796
15	6	0	1.015711	2.353659	-0.383302
16	6	0	1.815332	3.439068	-0.773507
17	1	0	2.832465	3.256567	-1.096264
18	6	0	1.341678	4.748279	-0.744184
19	1	0	1.984306	5.557023	-1.075636
20	6	0	0.051624	5.026512	-0.285181
21	1	0	-0.319078	6.044551	-0.263085
22	6	0	-0.754750	3.985384	0.142499
23	1	0	-1.759858	4.163836	0.503836
24	16	0	3.152460	1.070561	1.361335
25	6	0	4.495172	-0.156394	1.077780
26	1	0	5.070338	-0.260258	1.998196
27	1	0	5.175097	0.182631	0.289885
28	6	0	3.913861	-1.507953	0.666733
29	1	0	4.731859	-2.225456	0.492855
30	6	0	3.072854	-2.137595	1.767220
31	8	0	3.712060	-2.129404	2.940640
32	8	0	1.993876	-2.675702	1.626028
33	7	0	3.100809	-1.340229	-0.558535
34	1	0	3.732279	-1.128675	-1.328142
35	1	0	2.632704	-2.212117	-0.808415
36	16	0	0.142986	0.233381	-2.201200
37	6	0	-0.074184	-1.381665	-3.097710
38	1	0	-0.704458	-1.156903	-3.960586
39	1	0	0.889787	-1.742443	-3.452831
40	6	0	-0.746741	-2.455485	-2.239604
41	1	0	-1.031229	-3.302874	-2.876604
42	7	0	-1.939204	-1.877674	-1.572757
43	1	0	-2.345123	-2.537122	-0.913880
44	6	0	0.262368	-2.989901	-1.228194
45	8	0	1.345619	-3.403239	-1.586802
46	8	0	-0.146740	-2.924195	0.028201
47	1	0	-4.479686	-2.330037	3.321865
48	1	0	0.627493	-3.004877	0.637195
49	1	0	-2.681271	-1.627742	-2.231275
50	1	0	3.136167	-2.543888	3.600935
51	1	0	-3.497481	-0.082035	-0.120066
52	17	0	-4.686451	-0.196556	-1.366752

HF=-2731.5211187\ZeroPoint=0.3588198\Thermal=0.3908277

G = 8.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.547588	-0.014946	-0.233944
2	46	0	1.811514	0.375255	-0.581970
3	7	0	-1.030779	1.815349	0.560597
4	7	0	-1.635339	2.134535	1.612951
5	6	0	-2.605356	1.156414	1.995890
6	6	0	-3.553603	0.650077	1.077605
7	6	0	-4.424016	-0.372271	1.485311
8	1	0	-5.125331	-0.757044	0.752988
9	6	0	-4.365601	-0.854822	2.787600
10	6	0	-3.457118	-0.307083	3.701600
11	1	0	-3.428851	-0.675373	4.720737
12	6	0	-2.580898	0.701428	3.316713
13	1	0	-1.859057	1.119119	4.007533
14	6	0	-0.096125	2.747948	0.021384
15	6	0	1.113075	2.290807	-0.536268
16	6	0	1.950955	3.282718	-1.072002
17	1	0	2.911700	2.996719	-1.479727
18	6	0	1.594027	4.628237	-1.079587
19	1	0	2.264233	5.355775	-1.524718
20	6	0	0.386788	5.047310	-0.514399
21	1	0	0.106213	6.093771	-0.521495
22	6	0	-0.455833	4.106711	0.049358
23	1	0	-1.405200	4.393349	0.484123
24	16	0	3.419904	1.033141	0.987794
25	6	0	4.677088	-0.251214	0.588558
26	1	0	5.393202	-0.301083	1.409073
27	1	0	5.223058	0.009216	-0.323178
28	6	0	4.010332	-1.610104	0.386315
29	1	0	4.772618	-2.363367	0.132443
30	6	0	3.358190	-2.127511	1.659826
31	8	0	4.200080	-2.072247	2.696736
32	8	0	2.251772	-2.615995	1.752598
33	7	0	3.004869	-1.506098	-0.695785
34	1	0	3.503218	-1.391555	-1.575941
35	1	0	2.473520	-2.374369	-0.785861
36	16	0	-0.087528	0.019917	-2.021276
37	6	0	-0.513952	-1.650359	-2.730277
38	1	0	-1.283031	-1.451939	-3.477744
39	1	0	0.367259	-2.077462	-3.206720
40	6	0	-1.071325	-2.592069	-1.666009
41	1	0	-1.488084	-3.481051	-2.157207

42	7	0	-2.123816	-1.884689	-0.910663
43	1	0	-2.439955	-2.444963	-0.121531
44	6	0	0.068256	-3.069881	-0.774227
45	8	0	1.072417	-3.568531	-1.242044
46	8	0	-0.129552	-2.850707	0.517890
47	1	0	-5.039660	-1.642414	3.103363
48	1	0	0.724517	-2.940263	1.003765
49	1	0	-2.999748	-1.652590	-1.486790
50	1	0	3.741965	-2.419427	3.477196
51	1	0	-3.716723	1.111229	0.106127
52	17	0	-4.648591	-0.837724	-2.024950

HF=-2731.5322235\ZeroPoint=0.3627373\Thermal=0.3950531

G = -11.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.991789	0.701990	-0.547266
2	46	0	1.319511	0.321232	-1.295808
3	7	0	-0.962450	2.351287	0.131694
4	7	0	-1.331608	2.874380	1.217773
5	6	0	-2.387193	2.199389	1.828942
6	6	0	-2.975567	1.095486	1.161318
7	6	0	-4.029373	0.447690	1.808336
8	1	0	-4.516814	-0.407695	1.350056
9	6	0	-4.473709	0.875869	3.070576
10	6	0	-3.867227	1.959120	3.710962
11	1	0	-4.212205	2.276705	4.687623
12	6	0	-2.819327	2.630273	3.086650
13	1	0	-2.322988	3.470416	3.557419
14	6	0	0.042159	3.052184	-0.605150
15	6	0	1.009862	2.338858	-1.332366
16	6	0	1.941750	3.105938	-2.050014
17	1	0	2.707533	2.604670	-2.633917
18	6	0	1.909729	4.498554	-2.053673
19	1	0	2.637093	5.053244	-2.637196
20	6	0	0.938805	5.179261	-1.315093
21	1	0	0.905018	6.262524	-1.315312
22	6	0	0.009051	4.457037	-0.586087
23	1	0	-0.756110	4.958327	-0.007226
24	16	0	2.039959	-2.002674	-1.274240
25	6	0	3.778228	-1.584931	-0.817857
26	1	0	4.307617	-1.223341	-1.703266
27	1	0	4.291876	-2.480513	-0.461349
28	6	0	3.805940	-0.504370	0.272626
29	1	0	3.312485	-0.886216	1.166665
30	6	0	5.244116	-0.157001	0.625447
31	8	0	5.788065	-1.077396	1.451243
32	8	0	5.851906	0.790686	0.193818
33	7	0	3.075655	0.701626	-0.161097
34	1	0	2.747193	1.203346	0.674749
35	1	0	3.706292	1.321536	-0.668205
36	16	0	-0.670420	0.170965	-2.497153
37	6	0	-1.238625	-1.590568	-2.551758
38	1	0	-0.955041	-2.030545	-3.506312
39	1	0	-0.771663	-2.161568	-1.748123
40	6	0	-2.762592	-1.594036	-2.388623
41	1	0	-3.199151	-0.983452	-3.184062
42	7	0	-3.131250	-0.992007	-1.083676
43	1	0	-2.953304	-1.665820	-0.334134
44	6	0	-3.341164	-2.999519	-2.505188
45	8	0	-3.911599	-3.584945	-1.619960
46	8	0	-3.132502	-3.512791	-3.733604
47	1	0	-5.296466	0.357179	3.552019
48	1	0	-3.501017	-4.409415	-3.752164
49	1	0	-4.127979	-0.793156	-1.059720
50	1	0	6.711910	-0.827099	1.605847
51	1	0	-2.407750	-0.645133	3.008546
52	7	0	1.066496	-1.520065	3.123613
53	6	0	0.284097	-2.118729	2.009086
54	1	0	1.263055	-0.416401	2.950007
55	1	0	1.974761	-1.996618	3.163127
56	6	0	0.471016	-3.642563	1.924919
57	1	0	0.664668	-1.672607	1.079936
58	6	0	-1.186330	-1.765590	2.082437
59	16	0	2.236287	-4.108260	1.736021
60	1	0	-0.104747	-4.011516	1.078110
61	1	0	0.102226	-4.133613	2.828859
62	8	0	-1.492438	-0.974104	3.109864
63	8	0	-1.978533	-2.192188	1.275132
64	1	0	2.324587	-3.470795	0.521078
65	1	0	0.597005	-1.614883	4.023401
66	17	0	1.644972	1.264645	2.638112

HF=-3453.6679498\ZeroPoint=0.459872\Thermal=0.502472

G = 6.2 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-2.151684	0.235135	-0.349200
2	46	0	1.081609	0.413382	-1.251545
3	7	0	-1.545158	2.152472	0.165313
4	7	0	-2.212754	2.719115	1.080176
5	6	0	-3.222263	1.946709	1.652219
6	6	0	-3.278956	0.541659	1.449294
7	6	0	-4.379878	-0.146000	1.975344
8	1	0	-4.432878	-1.225787	1.872155
9	6	0	-5.370654	0.520457	2.695293
10	6	0	-5.272033	1.897688	2.912994
11	1	0	-6.036608	2.410289	3.485084
12	6	0	-4.196272	2.615822	2.399739
13	1	0	-4.111916	3.686267	2.543011
14	6	0	-0.599675	2.968919	-0.522454
15	6	0	0.503318	2.386550	-1.183944
16	6	0	1.355274	3.285559	-1.855236
17	1	0	2.210576	2.900711	-2.401519
18	6	0	1.134797	4.656738	-1.878793
19	1	0	1.812039	5.303004	-2.427131
20	6	0	0.032380	5.201845	-1.209746
21	1	0	-0.152985	6.269304	-1.230587
22	6	0	-0.829461	4.363225	-0.533687
23	1	0	-1.693423	4.759353	-0.017857

24	16	0	2.013717	-1.790627	-1.361762
25	6	0	3.748734	-1.189921	-1.443563
26	1	0	3.946017	-0.754127	-2.426821
27	1	0	4.427702	-2.031832	-1.298597
28	6	0	3.982558	-0.146001	-0.347159
29	1	0	3.909938	-0.626455	0.626375
30	6	0	5.368562	0.463246	-0.472281
31	8	0	6.323106	-0.385687	-0.045734
32	8	0	5.604761	1.550831	-0.941291
33	7	0	2.960367	0.931763	-0.392835
34	1	0	2.839731	1.265136	0.572957
35	1	0	3.347704	1.719121	-0.913196
36	16	0	-0.937442	0.000325	-2.339350
37	6	0	-1.190900	-1.830027	-2.516187
38	1	0	-0.993366	-2.100891	-3.551260
39	1	0	-0.492167	-2.361707	-1.872002
40	6	0	-2.629829	-2.147848	-2.124677
41	1	0	-3.312251	-1.598114	-2.781481
42	7	0	-2.853816	-1.693603	-0.733163
43	1	0	-2.273602	-2.244448	-0.075537
44	6	0	-2.982212	-3.626923	-2.254556
45	8	0	-3.486478	-4.283913	-1.380622
46	8	0	-2.689701	-4.097217	-3.481483
47	1	0	-6.207183	-0.032753	3.106992
48	1	0	-2.940190	-5.033528	-3.513874
49	1	0	-3.825434	-1.832392	-0.467864
50	1	0	7.181820	0.046488	-0.169761
51	1	0	-2.169796	-0.147518	1.741968
52	7	0	1.182836	-0.841305	3.549646
53	6	0	1.010138	-1.591771	2.262558
54	1	0	1.994790	-0.127582	3.420170
55	1	0	1.412895	-1.459798	4.327438
56	6	0	1.676387	-2.963502	2.250362
57	1	0	1.481864	-0.974502	1.490174
58	6	0	-0.478915	-1.624815	1.886037
59	16	0	3.336260	-2.996559	3.057605
60	1	0	1.751807	-3.271037	1.208904
61	1	0	1.075478	-3.699679	2.788304
62	8	0	-1.167994	-0.684438	2.440967
63	8	0	-0.877321	-2.461928	1.078817
64	1	0	3.765457	-1.787992	2.624183
65	1	0	0.309673	-0.332412	3.726535
66	17	0	3.361135	0.974759	2.802650

HF=-3453.6375377\ZeroPoint=0.4567582\Thermal=0.4988926

G = -6.3 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.951611	0.561164	-0.318916
2	46	0	1.327742	0.665777	-1.138843
3	7	0	-1.222975	2.387897	0.399441
4	7	0	-1.961001	2.872890	1.291807
5	6	0	-2.967299	1.962205	1.717436
6	6	0	-2.649372	0.623684	2.052865
7	6	0	-3.687657	-0.252691	2.413138
8	1	0	-3.422033	-1.273360	2.664237
9	6	0	-4.999754	0.202052	2.450234
10	6	0	-5.290937	1.543744	2.168198
11	1	0	-6.314482	1.896659	2.224622
12	6	0	-4.282383	2.430261	1.813139
13	1	0	-4.494607	3.466850	1.582284
14	6	0	-0.213601	3.222840	-0.158196
15	6	0	0.832791	2.646779	-0.899066
16	6	0	1.755958	3.545136	-1.465665
17	1	0	2.577072	3.158028	-2.060903
18	6	0	1.651040	4.921723	-1.303064
19	1	0	2.379219	5.577318	-1.768952
20	6	0	0.604890	5.462250	-0.546262
21	1	0	0.516412	6.534233	-0.415325
22	6	0	-0.324690	4.616554	0.025332
23	1	0	-1.147575	5.008887	0.607667
24	16	0	2.344350	-1.484944	-1.525382
25	6	0	4.018863	-0.919605	-0.996910
26	1	0	4.469722	-0.303451	-1.779815
27	1	0	4.663695	-1.786911	-0.840547
28	6	0	3.911529	-0.103920	0.298702
29	1	0	3.501944	-0.738514	1.086123
30	6	0	5.285617	0.386916	0.726485
31	8	0	6.012551	-0.603144	1.284247
32	8	0	5.705182	1.504966	0.553234
33	7	0	2.995843	1.041510	0.112487
34	1	0	2.533899	1.259612	1.008214
35	1	0	3.526802	1.861964	-0.177706
36	16	0	-0.679637	0.385714	-2.240874
37	6	0	-1.020019	-1.417004	-2.518049
38	1	0	-0.692229	-1.663343	-3.526153
39	1	0	-0.473296	-2.014676	-1.790324
40	6	0	-2.521127	-1.602483	-2.338820
41	1	0	-3.050417	-0.950299	-3.043628
42	7	0	-2.884434	-1.195750	-0.956899
43	1	0	-2.493706	-1.927094	-0.306935
44	6	0	-3.045585	-3.012758	-2.605711
45	8	0	-4.005371	-3.478534	-2.049483
46	8	0	-2.352949	-3.642357	-3.572895
47	1	0	-5.798894	-0.475432	2.727610
48	1	0	-2.755328	-4.514434	-3.708099
49	1	0	-3.896076	-1.185999	-0.845587
50	1	0	6.889168	-0.246895	1.495601
51	1	0	-1.608943	0.338928	2.200613
52	7	0	0.958656	-2.085298	2.969855
53	6	0	0.612610	-2.613787	1.615172
54	1	0	1.006929	-1.014174	2.925638
55	1	0	1.854913	-2.446420	3.301696
56	6	0	1.224244	-3.987962	1.362779
57	1	0	0.983869	-1.904445	0.874590
58	6	0	-0.931707	-2.679657	1.516220
59	16	0	3.066155	-3.987136	1.428470
60	1	0	0.895027	-4.329640	0.383660
61	1	0	0.889155	-4.712762	2.109224
62	8	0	-1.569728	-2.513185	2.573618
63	8	0	-1.360278	-2.900626	0.354827
64	1	0	3.184697	-3.181580	0.346629
65	1	0	0.169736	-2.331062	3.585672

66	17	0	0.981829	0.877013	2.574615

HF=-3453.6606035\ZeroPoint=0.4606073\Thermal=0.5032452

G = -10.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.320426	-0.058014	0.226641
2	46	0	-2.321292	0.369151	-0.908722
3	7	0	-0.295641	-1.992296	-0.068108
4	7	0	0.052178	-2.868533	0.776896
5	6	0	0.796725	-2.346358	1.826390
6	6	0	1.035310	-0.944603	1.874251
7	6	0	1.758443	-0.454213	2.957241
8	1	0	1.998068	0.598740	3.035763
9	6	0	2.228794	-1.321440	3.950989
10	6	0	1.987922	-2.696137	3.886107
11	1	0	2.365860	-3.352637	4.660712
12	6	0	1.265532	-3.216497	2.820048
13	1	0	1.057977	-4.277055	2.737455
14	6	0	-1.105954	-2.418050	-1.166756
15	6	0	-2.036723	-1.505785	-1.702573
16	6	0	-2.827780	-1.971392	-2.763518
17	1	0	-3.560399	-1.307228	-3.210960
18	6	0	-2.688156	-3.260541	-3.276504
19	1	0	-3.305416	-3.580059	-4.109831
20	6	0	-1.746955	-4.137594	-2.729332
21	1	0	-1.628531	-5.136749	-3.132693
22	6	0	-0.957835	-3.720804	-1.668239
23	1	0	-0.224435	-4.381291	-1.222911
24	16	0	-2.650915	2.447663	0.249861
25	6	0	-4.177940	1.965751	1.156041
26	1	0	-5.062272	2.238401	0.569745
27	1	0	-4.221752	2.503292	2.103557
28	6	0	-4.205556	0.454663	1.431058
29	1	0	-3.363938	0.199748	2.078104
30	6	0	-5.505576	0.055567	2.114265
31	8	0	-5.538012	0.468922	3.397041
32	8	0	-6.413100	-0.532547	1.578271
33	7	0	-4.046047	-0.284980	0.156420
34	1	0	-3.982926	-1.285638	0.328690
35	1	0	-4.883618	-0.156412	-0.410721
36	16	0	-0.307905	0.902918	-1.993335
37	6	0	0.203935	2.639100	-1.614990
38	1	0	0.611571	3.065716	-2.530402
39	1	0	-0.686658	3.201557	-1.333775
40	6	0	1.273730	2.698550	-0.515935
41	1	0	2.208328	2.293396	-0.900481
42	7	0	0.902826	1.900181	0.674403
43	1	0	0.106569	2.336186	1.146334
44	6	0	1.530401	4.143837	-0.107511
45	8	0	1.233762	4.624845	0.954499
46	8	0	2.119452	4.835153	-1.107726
47	1	0	2.797292	-0.914782	4.780710
48	1	0	2.248311	5.744716	-0.798561
49	1	0	1.707123	1.914377	1.305343
50	1	0	-6.399506	0.224668	3.768856
51	1	0	1.381011	-0.568915	-2.702145
52	8	0	2.183053	-1.074388	-2.431716
53	6	0	3.165567	-0.214777	-2.212024
54	6	0	4.304445	-0.841028	-1.404780
55	8	0	3.193138	0.937869	-2.576999
56	6	0	3.788371	-1.558152	-0.147003
57	1	0	4.842216	-1.544451	-2.046732
58	7	0	5.231094	0.271563	-1.040674
59	16	0	5.116180	-2.049103	1.023168
60	1	0	3.255628	-2.456151	-0.452633
61	1	0	3.090869	-0.920277	0.391589
62	1	0	5.353712	0.912729	-1.825801
63	1	0	6.126060	-0.099858	-0.722122
64	1	0	4.807983	0.860734	-0.191476
65	1	0	5.053455	-0.906627	1.747168
66	17	0	4.127769	1.664527	1.270291

HF=-3453.6657718\ZeroPoint=0.460406\Thermal=0.5034248

G = 10.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.500651	0.208290	-0.018301
2	46	0	-2.776422	-0.438061	0.674504
3	7	0	-0.539074	1.983632	0.129796
4	7	0	-0.337265	2.866439	-0.749294
5	6	0	0.605564	2.509491	-1.719167
6	6	0	1.461581	1.396668	-1.510801
7	6	0	2.313721	1.019890	-2.555019
8	1	0	3.003018	0.192777	-2.412813
9	6	0	2.323944	1.734366	-3.754730
10	6	0	1.497372	2.847827	-3.923883
11	1	0	1.523785	3.404666	-4.853397
12	6	0	0.636708	3.246986	-2.903510
13	1	0	-0.024224	4.097565	-3.019930
14	6	0	-1.470744	2.329338	1.164552
15	6	0	-2.441965	1.394258	1.562681
16	6	0	-3.320642	1.821004	2.572458
17	1	0	-4.092580	1.143829	2.925835
18	6	0	-3.225168	3.081859	3.159920
19	1	0	-3.910447	3.360467	3.953781
20	6	0	-2.243307	3.981804	2.738719
21	1	0	-2.158018	4.959782	3.197860
22	6	0	-1.368626	3.609915	1.729495
23	1	0	-0.595544	4.284530	1.382571
24	16	0	-3.321593	-2.486675	-0.433406
25	6	0	-5.043581	-2.031990	-0.891613
26	1	0	-5.729739	-2.255261	-0.067249
27	1	0	-5.351472	-2.619734	-1.757263
28	6	0	-5.140646	-0.537876	-1.232582
29	1	0	-4.503078	-0.335162	-2.094844
30	6	0	-6.576080	-0.153372	-1.558786
31	8	0	-6.944265	-0.598179	-2.777202
32	8	0	-7.315363	0.445089	-0.815364
33	7	0	-4.642306	0.262151	-0.088429

34	1	0	-4.558652	1.243278	-0.343703
35	1	0	-5.334529	0.235311	0.660374
36	16	0	-0.722836	-1.025854	1.555685
37	6	0	-0.174875	-2.701158	0.988308
38	1	0	-0.341854	-3.403508	1.805118
39	1	0	-0.761974	-3.015199	0.124485
40	6	0	1.308593	-2.612093	0.623069
41	1	0	1.901997	-2.304637	1.483547
42	7	0	1.488769	-1.586472	-0.431352
43	1	0	1.104566	-1.953906	-1.304237
44	6	0	1.780119	-3.967221	0.108224
45	8	0	1.667644	-4.330666	-1.033011
46	8	0	2.284987	-4.730362	1.099323
47	1	0	2.992097	1.432461	-4.553471
48	1	0	2.530531	-5.586390	0.715038
49	1	0	2.500888	-1.467772	-0.602408
50	1	0	-7.876949	-0.368843	-2.909984
51	1	0	2.153467	1.417178	-0.358338
52	8	0	3.238596	1.735984	0.382823
53	6	0	3.672024	0.804266	1.136920
54	6	0	5.220851	0.754523	1.262933
55	8	0	3.033173	-0.057540	1.744560
56	6	0	5.937498	1.282811	0.020187
57	1	0	5.520544	1.319408	2.149515
58	7	0	5.548618	-0.686469	1.516217
59	16	0	7.744863	0.903753	-0.020372
60	1	0	5.828163	2.364663	-0.006350
61	1	0	5.484059	0.871134	-0.878095
62	1	0	4.910866	-1.034451	2.237167
63	1	0	6.529246	-0.814144	1.766390
64	1	0	5.315859	-1.228219	0.605672
65	1	0	7.625485	-0.235588	-0.735033
66	17	0	4.642916	-1.755981	-1.086937

HF=-3453.6273033\ZeroPoint=0.4564381\Thermal=0.4990288

G = 4.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.626265	-0.116045	0.274301
2	46	0	-2.675643	0.307476	-0.668256
3	7	0	-0.345315	-1.944750	0.219405
4	7	0	-0.145682	-2.732383	1.175293
5	6	0	0.752377	-2.221113	2.150975
6	6	0	1.940227	-1.546450	1.789566
7	6	0	2.722514	-0.960489	2.793260
8	1	0	3.619209	-0.416881	2.516521
9	6	0	2.341378	-1.071274	4.128133
10	6	0	1.196295	-1.793881	4.473495
11	1	0	0.915753	-1.895097	5.515670
12	6	0	0.401241	-2.379292	3.490938
13	1	0	-0.501133	-2.922320	3.743535
14	6	0	-1.193461	-2.423298	-0.832616
15	6	0	-2.189352	-1.581848	-1.356165
16	6	0	-2.980570	-2.139449	-2.373688
17	1	0	-3.766283	-1.541719	-2.826135
18	6	0	-2.776500	-3.433506	-2.851201
19	1	0	-3.395509	-3.813887	-3.657026
20	6	0	-1.768381	-4.234086	-2.309708
21	1	0	-1.594392	-5.234037	-2.688990
22	6	0	-0.977904	-3.732267	-1.288097
23	1	0	-0.177280	-4.320592	-0.857687
24	16	0	-3.408735	2.421450	0.169947
25	6	0	-5.165044	1.947366	0.439550
26	1	0	-5.738545	2.065961	-0.486108
27	1	0	-5.599955	2.603882	1.194083
28	6	0	-5.269828	0.490436	0.912130
29	1	0	-4.749914	0.395241	1.866945
30	6	0	-6.726291	0.083293	1.082051
31	8	0	-7.267257	0.629304	2.189106
32	8	0	-7.340294	-0.613032	0.310757
33	7	0	-4.601742	-0.395332	-0.071372
34	1	0	-4.523137	-1.342913	0.290315
35	1	0	-5.191807	-0.471882	-0.900205
36	16	0	-0.585647	0.906490	-1.395820
37	6	0	-0.161110	2.649314	-0.940365
38	1	0	-0.391404	3.276226	-1.801969
39	1	0	-0.761952	2.971965	-0.089363
40	6	0	1.330309	2.671883	-0.601814
41	1	0	1.920590	2.342863	-1.457048
42	7	0	1.584985	1.718425	0.506653
43	1	0	1.254786	2.141066	1.377221
44	6	0	1.726869	4.077702	-0.172319
45	8	0	1.703497	4.469879	0.965811
46	8	0	2.054147	4.845741	-1.229825
47	1	0	2.946037	-0.611709	4.900829
48	1	0	2.253231	5.735872	-0.900007
49	1	0	2.609716	1.597429	0.630244
50	1	0	-8.203368	0.378311	2.220973
51	1	0	2.325472	-1.633992	0.767691
52	8	0	2.681114	-1.617111	-1.276555
53	6	0	3.305250	-0.640381	-1.729967
54	6	0	4.870557	-0.744762	-1.670956
55	8	0	2.877617	0.435354	-2.213806
56	6	0	5.368389	-1.498805	-0.442415
57	1	0	5.220139	-1.230223	-2.585416
58	7	0	5.365417	0.671585	-1.706662
59	16	0	7.180752	-1.336824	-0.127014
60	1	0	5.151057	-2.556132	-0.576178
61	1	0	4.850878	-1.154154	0.448959
62	1	0	4.692922	1.161377	-2.318489
63	1	0	6.334323	0.752715	-2.008561
64	1	0	5.248870	1.098237	-0.736048
65	1	0	7.072409	-0.218914	0.625283
66	17	0	4.724279	1.567126	1.093366

HF=-3453.6387202\ZeroPoint=0.4602382\Thermal=0.5035014

G = -15.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.846935	0.982912	-0.148136

2	46	0	1.377052	0.713892	-1.219178
3	7	0	-0.689743	2.202326	1.050738
4	7	0	-1.046562	2.325966	2.261427
5	6	0	-2.130390	1.533158	2.615393
6	6	0	-2.720727	0.694229	1.635838
7	6	0	-3.721524	-0.179068	2.047143
8	1	0	-4.160567	-0.886827	1.351862
9	6	0	-4.144891	-0.190344	3.383631
10	6	0	-3.578433	0.669572	4.328315
11	1	0	-3.923108	0.651602	5.355358
12	6	0	-2.558846	1.534916	3.948963
13	1	0	-2.084383	2.199709	4.661694
14	6	0	0.387097	3.038440	0.613864
15	6	0	1.293189	2.579230	-0.363045
16	6	0	2.311003	3.477043	-0.730687
17	1	0	3.029801	3.185341	-1.490700
18	6	0	2.419867	4.751904	-0.180824
19	1	0	3.208782	5.418117	-0.513625
20	6	0	1.502703	5.177838	0.783025
21	1	0	1.570154	6.173003	1.206855
22	6	0	0.490268	4.321814	1.182052
23	1	0	-0.239687	4.631754	1.918823
24	16	0	1.686577	-1.497971	-2.128721
25	6	0	3.503298	-1.546623	-1.846458
26	1	0	3.998878	-0.972332	-2.634266
27	1	0	3.851232	-2.578560	-1.908883
28	6	0	3.866674	-0.967535	-0.473838
29	1	0	3.447935	-1.603367	0.303148
30	6	0	5.377151	-0.921538	-0.300205
31	8	0	5.886282	-2.151946	-0.092463
32	8	0	6.050229	0.077554	-0.372682
33	7	0	3.294255	0.390881	-0.303054
34	1	0	3.226317	0.598599	0.690730
35	1	0	3.945682	1.075585	-0.687640
36	16	0	-0.660145	1.232846	-2.232125
37	6	0	-1.426298	-0.280641	-2.987148
38	1	0	-1.246275	-0.274659	-4.059949
39	1	0	-0.985442	-1.188477	-2.576915
40	6	0	-2.920386	-0.244480	-2.690048
41	1	0	-3.342453	0.688659	-3.079675
42	7	0	-3.149975	-0.255820	-1.216392
43	1	0	-3.033407	-1.231239	-0.866707
44	6	0	-3.670286	-1.380087	-3.391123
45	8	0	-3.266525	-1.987662	-4.344634
46	8	0	-4.883535	-1.573689	-2.827605
47	1	0	-4.921085	-0.884364	3.688197
48	1	0	-5.299403	-2.334513	-3.260576
49	1	0	-4.117967	-0.014262	-1.017984
50	1	0	6.851127	-2.073205	-0.035639
51	1	0	-0.621107	-0.881687	0.518546
52	7	0	-0.233436	-1.840892	0.488103
53	6	0	0.311614	-2.262799	1.809616
54	1	0	-1.075605	-2.461367	0.200079
55	1	0	0.490854	-1.853372	-0.271824
56	6	0	1.099468	-3.557380	1.642981
57	1	0	-0.539908	-2.411807	2.475210
58	6	0	1.150656	-1.102527	2.350928
59	16	0	1.714691	-4.230070	3.234329
60	1	0	1.929024	-3.420917	0.948791
61	1	0	0.435282	-4.318193	1.229578
62	8	0	2.350249	-0.999493	2.249585
63	8	0	0.360047	-0.183818	2.909824
64	1	0	2.708736	-3.332670	3.389988
65	17	0	-2.733275	-3.218113	-0.245811
66	1	0	0.875940	0.601965	3.152854

HF=-3453.6752668\ZeroPoint=0.4608453\Thermal=0.5035233

G = 11.3 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.524211	0.452036	0.619961
2	46	0	0.974210	1.801311	-0.140160
3	7	0	-0.492554	0.323432	2.402288
4	7	0	-0.755725	-0.651583	3.164359
5	6	0	-1.710752	-1.531356	2.666545
6	6	0	-2.064350	-1.518236	1.286155
7	6	0	-3.083156	-2.381287	0.865920
8	1	0	-3.341586	-2.424064	-0.188494
9	6	0	-3.702500	-3.243707	1.773356
10	6	0	-3.313686	-3.267689	3.114376
11	1	0	-3.792942	-3.949870	3.806933
12	6	0	-2.309369	-2.417011	3.565891
13	1	0	-2.000891	-2.406444	4.604310
14	6	0	0.499657	1.248664	2.848125
15	6	0	1.220972	1.987145	1.887350
16	6	0	2.216205	2.845210	2.383673
17	1	0	2.802050	3.438383	1.688451
18	6	0	2.460907	2.984958	3.746740
19	1	0	3.224654	3.674525	4.090624
20	6	0	1.711945	2.253316	4.675713
21	1	0	1.886922	2.373595	5.738392
22	6	0	0.735493	1.380841	4.229819
23	1	0	0.142196	0.805466	4.928386
24	16	0	0.776948	1.355495	-2.477609
25	6	0	2.557454	1.009792	-2.780100
26	1	0	3.093596	1.952988	-2.919363
27	1	0	2.659242	0.420270	-3.692122
28	6	0	3.158094	0.238397	-1.601213
29	1	0	2.669365	-0.728853	-1.521402
30	6	0	4.646887	0.004687	-1.804029
31	8	0	4.869313	-0.982582	-2.693925
32	8	0	5.523754	0.635500	-1.266717
33	7	0	2.923129	0.956641	-0.325415
34	1	0	3.072559	0.308693	0.445980
35	1	0	3.621291	1.693424	-0.224201
36	16	0	-1.158427	2.757438	0.227844
37	6	0	-2.072505	2.925623	-1.381813
38	1	0	-2.583253	3.887881	-1.355569
39	1	0	-1.360006	2.936842	-2.205284
40	6	0	-3.075611	1.791672	-1.542424
41	1	0	-3.882717	1.886999	-0.812486
42	7	0	-2.398636	0.492146	-1.274174
43	1	0	-1.600915	0.393031	-1.912740

44	6	0	-3.715006	1.771688	-2.935673
45	8	0	-3.408405	2.481353	-3.855680
46	8	0	-4.672779	0.827659	-2.978138
47	1	0	-4.479703	-3.913541	1.423181
48	1	0	-4.977531	0.723485	-3.892413
49	1	0	-2.982392	-0.327156	-1.511974
50	1	0	5.826789	-1.065590	-2.823115
51	1	0	-1.106776	-1.515445	0.360305
52	7	0	-0.203237	-1.996047	-0.739914
53	6	0	0.713320	-3.080508	-0.362520
54	1	0	-0.927046	-2.295253	-1.434489
55	1	0	0.290076	-1.198434	-1.150133
56	6	0	1.557558	-3.571096	-1.541714
57	1	0	0.112526	-3.902449	0.029635
58	6	0	1.569938	-2.527288	0.774778
59	16	0	2.706520	-4.940956	-1.109664
60	1	0	2.124655	-2.753561	-1.986658
61	1	0	0.886526	-3.965717	-2.305951
62	8	0	2.566307	-1.855440	0.619018
63	8	0	1.052064	-2.804788	1.977347
64	1	0	3.605312	-4.172503	-0.461436
65	17	0	-2.671400	-2.332197	-2.583210
66	1	0	1.569325	-2.343604	2.657264

HF=-3453.628271\ZeroPoint=0.4567867\Thermal=0.4995323

G = -12.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.561142	0.738931	-0.397188
2	46	0	-2.120495	0.029912	-0.934469
3	7	0	1.149212	-0.868969	-1.607416
4	7	0	2.335756	-1.180328	-1.873385
5	6	0	3.436570	-0.480175	-1.365701
6	6	0	3.488353	0.891021	-1.069460
7	6	0	4.635458	1.429690	-0.501205
8	1	0	4.645788	2.474873	-0.223303
9	6	0	5.741363	0.618217	-0.247805
10	6	0	5.713576	-0.736415	-0.588447
11	1	0	6.577035	-1.364122	-0.402567
12	6	0	4.575634	-1.282348	-1.165185
13	1	0	4.524682	-2.331087	-1.431019
14	6	0	0.150514	-1.727528	-2.211203
15	6	0	-1.220248	-1.447787	-2.040566
16	6	0	-2.119082	-2.337808	-2.662753
17	1	0	-3.185600	-2.150558	-2.584010
18	6	0	-1.699216	-3.443794	-3.390124
19	1	0	-2.429468	-4.099661	-3.852409
20	6	0	-0.330967	-3.705167	-3.526657
21	1	0	0.012566	-4.565938	-4.088689
22	6	0	0.586562	-2.850223	-2.946497
23	1	0	1.646766	-3.033704	-3.046525
24	16	0	-3.255914	1.572874	0.505170
25	6	0	-4.170037	0.328105	1.504707
26	1	0	-5.126014	0.096850	1.024003
27	1	0	-4.376378	0.742510	2.491867
28	6	0	-3.347300	-0.957542	1.647650
29	1	0	-2.422947	-0.737287	2.182471
30	6	0	-4.124572	-2.014888	2.418460
31	8	0	-4.178890	-1.727142	3.733820
32	8	0	-4.656540	-2.977539	1.921365
33	7	0	-2.977480	-1.472054	0.309638
34	1	0	-2.273230	-2.199604	0.415882
35	1	0	-3.791547	-1.910298	-0.119769
36	16	0	-0.776129	1.598257	-2.133799
37	6	0	-1.089480	3.287954	-1.425823
38	1	0	-0.949191	4.007517	-2.231455
39	1	0	-2.127118	3.331438	-1.094771
40	6	0	-0.120113	3.594240	-0.276798
41	1	0	0.875042	3.792812	-0.680494
42	7	0	-0.001650	2.446934	0.645148
43	1	0	-0.903360	2.284236	1.109966
44	6	0	-0.572169	4.839587	0.482357
45	8	0	-1.004456	4.847248	1.601830
46	8	0	-0.442342	5.941252	-0.290919
47	1	0	6.625556	1.043889	0.211886
48	1	0	-0.749932	6.702816	0.224168
49	1	0	0.743650	2.651676	1.343093
50	1	0	-4.718884	-2.405396	4.168075
51	1	0	2.643002	1.530779	-1.288009
52	7	0	1.365296	-0.022916	1.438324
53	6	0	1.931559	-1.377028	1.552263
54	1	0	2.045889	0.718937	1.736993
55	1	0	0.575460	0.049319	2.078951
56	6	0	2.401247	-1.642774	2.996671
57	1	0	2.780557	-1.462823	0.878746
58	6	0	0.851733	-2.368709	1.136566
59	16	0	3.381931	-3.177731	3.221497
60	1	0	1.550279	-1.635551	3.680883
61	1	0	3.071765	-0.831427	3.285939
62	8	0	-0.308430	-2.273799	1.470523
63	8	0	1.324513	-3.354316	0.364796
64	1	0	2.377997	-4.049969	2.997322
65	17	0	2.742404	2.608247	2.128127
66	1	0	0.583715	-3.915661	0.084801

HF=-3453.6687956\ZeroPoint=0.4607809\Thermal=0.5039793

G = -3.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.221440	-1.058696	0.340945
2	46	0	1.818110	0.343566	-0.413013
3	7	0	-0.446606	-0.361942	2.111455
4	7	0	-0.685608	-1.024410	3.165229
5	6	0	-1.462835	-2.151266	2.944848
6	6	0	-1.914207	-2.429466	1.626549
7	6	0	-2.733622	-3.539311	1.453232
8	1	0	-3.134489	-3.788042	0.476436
9	6	0	-3.071248	-4.353077	2.541940
10	6	0	-2.602006	-4.073952	3.829280
11	1	0	-2.872914	-4.716676	4.658178

12	6	0	-1.795342	-2.963726	4.038823
13	1	0	-1.422897	-2.708506	5.024134
14	6	0	0.257651	0.875216	2.285575
15	6	0	1.177726	1.305890	1.310061
16	6	0	1.800782	2.544117	1.567775
17	1	0	2.528159	2.926754	0.857135
18	6	0	1.512876	3.317653	2.692074
19	1	0	2.010255	4.271181	2.836307
20	6	0	0.572984	2.869597	3.623348
21	1	0	0.333260	3.465087	4.496528
22	6	0	-0.046433	1.643539	3.424824
23	1	0	-0.762484	1.260942	4.142264
24	16	0	2.883062	-0.492355	-2.391233
25	6	0	4.599422	-0.449833	-1.730918
26	1	0	5.027354	0.552236	-1.843106
27	1	0	5.216327	-1.147098	-2.298726
28	6	0	4.616356	-0.842054	-0.249839
29	1	0	4.233956	-1.859432	-0.151669
30	6	0	6.027706	-0.767601	0.315236
31	8	0	6.786708	-1.794525	-0.111791
32	8	0	6.435403	0.116067	1.029791
33	7	0	3.718754	0.067134	0.504293
34	1	0	3.576442	-0.278772	1.450348
35	1	0	4.181842	0.969527	0.614490
36	16	0	-0.371977	0.653510	-1.150585
37	6	0	-0.966530	-0.107402	-2.731461
38	1	0	-1.896134	0.414353	-2.965897
39	1	0	-0.235894	0.082956	-3.514943
40	6	0	-1.250126	-1.610614	-2.609198
41	1	0	-1.845218	-1.893111	-3.487439
42	7	0	-2.021946	-1.917684	-1.381069
43	1	0	-2.030889	-2.926939	-1.252792
44	6	0	0.016418	-2.455068	-2.626038
45	8	0	0.332044	-3.227497	-1.756612
46	8	0	0.716678	-2.230557	-3.746248
47	1	0	-3.710901	-5.214639	2.381973
48	1	0	1.631412	-2.528668	-3.601992
49	1	0	-3.003564	-1.603759	-1.540826
50	1	0	7.682729	-1.673689	0.238867
51	1	0	-1.461191	1.830127	0.365844
52	7	0	-2.172735	2.458155	0.792953
53	6	0	-2.710592	3.348348	-0.296119
54	1	0	-2.915123	1.844690	1.140097
55	1	0	-1.741523	2.988388	1.556626
56	6	0	-1.599137	4.204784	-0.890536
57	1	0	-3.477974	3.976198	0.163102
58	6	0	-3.388810	2.439297	-1.349201
59	16	0	-0.788423	5.297998	0.352333
60	1	0	-2.037920	4.843145	-1.654820
61	1	0	-0.850076	3.579426	-1.375007
62	8	0	-3.332673	2.694005	-2.525614
63	8	0	-3.989054	1.433623	-0.753289
64	1	0	0.199202	4.443405	0.691930
65	1	0	-4.336461	0.679260	-1.408481
66	17	0	-4.733928	-0.796877	-2.359597

HF=-3453.6518863\ZeroPoint=0.4595455\Thermal=0.5025672

G = 13.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.096190	-0.152208	0.001271
2	46	0	2.283485	0.080534	-0.750409
3	7	0	-0.228709	1.424879	1.026269
4	7	0	-0.487950	1.560264	2.255512
5	6	0	-1.385660	0.614769	2.753828
6	6	0	-2.158309	-0.169595	1.852532
7	6	0	-2.970857	-1.171647	2.394457
8	1	0	-3.571518	-1.801439	1.745623
9	6	0	-3.028209	-1.363398	3.777553
10	6	0	-2.293655	-0.551048	4.644399
11	1	0	-2.357385	-0.704530	5.715409
12	6	0	-1.469293	0.451143	4.137266
13	1	0	-0.870973	1.078421	4.787248
14	6	0	0.634127	2.416251	0.453207
15	6	0	1.666650	2.019848	-0.412299
16	6	0	2.435834	3.060756	-0.960681
17	1	0	3.242672	2.819650	-1.646235
18	6	0	2.191292	4.402511	-0.672105
19	1	0	2.794978	5.173790	-1.138474
20	6	0	1.170411	4.756265	0.213428
21	1	0	0.977495	5.796711	0.446917
22	6	0	0.395784	3.759716	0.788383
23	1	0	-0.400600	4.002886	1.481471
24	16	0	3.263204	-2.080728	-1.106712
25	6	0	4.939623	-1.640614	-0.493384
26	1	0	5.517448	-1.144454	-1.280432
27	1	0	5.466831	-2.552033	-0.209247
28	6	0	4.839663	-0.709253	0.721417
29	1	0	4.302515	-1.229132	1.516498
30	6	0	6.224057	-0.313164	1.214124
31	8	0	6.827578	-1.327897	1.863177
32	8	0	6.740770	0.760904	1.022944
33	7	0	4.065138	0.499123	0.349319
34	1	0	3.829075	1.041593	1.176868
35	1	0	4.658075	1.110970	-0.212134
36	16	0	0.292780	-0.147165	-1.908425
37	6	0	-0.037980	-1.877580	-2.507509
38	1	0	-0.612736	-1.758323	-3.427863
39	1	0	0.908152	-2.362419	-2.740073
40	6	0	-0.857745	-2.688138	-1.494179
41	1	0	-1.312506	-3.546611	-2.002511
42	7	0	-1.920039	-1.827676	-0.930208
43	1	0	-2.567488	-2.391419	-0.347540
44	6	0	0.023233	-3.245173	-0.381718
45	8	0	0.009361	-2.886108	0.766474
46	8	0	0.837721	-4.186851	-0.882480
47	1	0	-3.659348	-2.149127	4.177061
48	1	0	1.557073	-4.337154	-0.248497
49	1	0	-2.520976	-1.506653	-1.694050
50	1	0	7.719221	-1.038384	2.111210
51	1	0	-2.841561	0.639850	0.980944
52	7	0	-3.845183	1.593410	0.610779
53	6	0	-4.242099	1.582632	-0.819089

54	1	0	-4.628254	1.306723	1.193412
55	1	0	-3.552112	2.534728	0.876207
56	6	0	-3.181084	2.231225	-1.709517
57	1	0	-5.192831	2.117470	-0.935284
58	6	0	-4.480791	0.117925	-1.225958
59	16	0	-2.802480	3.972747	-1.217373
60	1	0	-3.539747	2.231274	-2.736509
61	1	0	-2.256401	1.656185	-1.685537
62	8	0	-4.058299	-0.340740	-2.268084
63	8	0	-5.137121	-0.528695	-0.290678
64	1	0	-1.513793	3.770663	-0.877326
65	1	0	-5.049174	-1.562612	-0.357726
66	17	0	-4.501800	-3.328986	-0.059200

HF=-3453.6265554\ZeroPoint=0.4558908\Thermal=0.4980881

G = 2.1 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.158939	-0.416123	0.059365
2	46	0	2.130879	0.293389	-0.689811
3	7	0	-0.350742	0.897681	1.440119
4	7	0	-0.513252	0.683715	2.666004
5	6	0	-1.260677	-0.469946	2.969321
6	6	0	-2.279340	-0.960258	2.121634
7	6	0	-2.894649	-2.178060	2.410608
8	1	0	-3.668038	-2.551402	1.746246
9	6	0	-2.507326	-2.891509	3.545447
10	6	0	-1.535850	-2.378347	4.405545
11	1	0	-1.253403	-2.931150	5.294078
12	6	0	-0.915467	-1.160947	4.129551
13	1	0	-0.143467	-0.759482	4.774277
14	6	0	0.365018	2.094231	1.102221
15	6	0	1.390986	2.032063	0.147556
16	6	0	2.034128	3.247296	-0.138724
17	1	0	2.829715	3.268289	-0.877271
18	6	0	1.672017	4.442885	0.480839
19	1	0	2.178068	5.364000	0.212677
20	6	0	0.654441	4.460318	1.437853
21	1	0	0.367806	5.387066	1.920901
22	6	0	0.000926	3.278745	1.757884
23	1	0	-0.799018	3.258106	2.487465
24	16	0	3.205151	-1.649996	-1.590334
25	6	0	4.888479	-1.255242	-0.963490
26	1	0	5.394594	-0.560353	-1.641816
27	1	0	5.476410	-2.172528	-0.917440
28	6	0	4.810359	-0.629252	0.434894
29	1	0	4.352060	-1.349178	1.115087
30	6	0	6.198089	-0.260699	0.940582
31	8	0	6.895768	-1.352134	1.309387
32	8	0	6.638859	0.862124	0.978222
33	7	0	3.949269	0.577538	0.385269
34	1	0	3.739340	0.907562	1.324432
35	1	0	4.470768	1.336630	-0.054383
36	16	0	0.106705	0.216750	-1.780630
37	6	0	-0.140091	-1.291071	-2.851439
38	1	0	-0.736379	-0.939540	-3.694892
39	1	0	0.828736	-1.633753	-3.209201
40	6	0	-0.902611	-2.390258	-2.101338
41	1	0	-1.342292	-3.083880	-2.828053
42	7	0	-1.964655	-1.757775	-1.296863
43	1	0	-2.612071	-2.440954	-0.854232
44	6	0	0.027510	-3.204892	-1.207828
45	8	0	0.008448	-3.209725	-0.004426
46	8	0	0.886071	-3.903747	-1.965086
47	1	0	-2.980367	-3.840931	3.766011
48	1	0	1.610083	-4.217391	-1.400235
49	1	0	-2.589396	-1.213709	-1.905388
50	1	0	7.783277	-1.066855	1.576746
51	1	0	-2.761823	-0.282604	1.396131
52	7	0	-3.447589	2.189521	0.777387
53	6	0	-3.862166	2.189936	-0.634323
54	1	0	-4.185022	1.783001	1.344944
55	1	0	-3.332452	3.152656	1.081237
56	6	0	-2.800129	2.839277	-1.524575
57	1	0	-4.816565	2.719040	-0.789938
58	6	0	-4.102205	0.745737	-1.088642
59	16	0	-2.453750	4.603544	-1.117861
60	1	0	-3.137230	2.824484	-2.559561
61	1	0	-1.865825	2.283847	-1.476736
62	8	0	-3.742704	0.325261	-2.174445
63	8	0	-4.715078	0.028369	-0.164462
64	1	0	-1.474908	4.371755	-0.220458
65	1	0	-4.799383	-0.961443	-0.405587
66	17	0	-4.676642	-2.907429	-0.485983

HF=-3453.6435725\ZeroPoint=0.4586604\Thermal=0.5020024

G = -0.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.440043	-0.128091	-0.208132
2	46	0	-1.325018	0.399246	-0.831498
3	7	0	0.920901	-2.055192	-0.622470
4	7	0	1.569570	-2.983355	-0.056021
5	6	0	2.526810	-2.515977	0.833236
6	6	0	2.619900	-1.116563	1.073768
7	6	0	3.536940	-0.683700	2.025091
8	1	0	3.639970	0.371058	2.259889
9	6	0	4.338392	-1.603577	2.712873
10	6	0	4.239716	-2.973826	2.459117
11	1	0	4.865837	-3.672894	3.000437
12	6	0	3.327685	-3.437669	1.518639
13	1	0	3.218437	-4.494869	1.307533
14	6	0	-0.166722	-2.410339	-1.475469
15	6	0	-1.204469	-1.474861	-1.674441
16	6	0	-2.275032	-1.898519	-2.478800
17	1	0	-3.100052	-1.218434	-2.667575
18	6	0	-2.304383	-3.158458	-3.071406
19	1	0	-3.141122	-3.439216	-3.702552
20	6	0	-1.250975	-4.055530	-2.867281
21	1	0	-1.263326	-5.032830	-3.335728

22	6	0	-0.185497	-3.686667	-2.064427
23	1	0	0.637883	-4.365240	-1.883208
24	16	0	-1.545552	2.514965	0.281584
25	6	0	-3.128440	2.139817	1.138651
26	1	0	-3.963135	2.344172	0.460991
27	1	0	-3.231050	2.786265	2.010854
28	6	0	-3.174438	0.673457	1.586958
29	1	0	-2.386189	0.507445	2.320329
30	6	0	-4.519752	0.353967	2.221596
31	8	0	-4.633902	0.906499	3.446048
32	8	0	-5.398301	-0.283473	1.693372
33	7	0	-2.924720	-0.233104	0.439308
34	1	0	-2.692269	-1.162481	0.783862
35	1	0	-3.784236	-0.337605	-0.099547
36	16	0	0.490161	0.956243	-2.224091
37	6	0	1.024859	2.684570	-1.833507
38	1	0	1.371540	3.134704	-2.762585
39	1	0	0.168920	3.257193	-1.474977
40	6	0	2.169188	2.703457	-0.809876
41	1	0	3.065125	2.287628	-1.281228
42	7	0	1.847194	1.853447	0.362524
43	1	0	0.963030	2.173635	0.780340
44	6	0	2.526358	4.113747	-0.349752
45	8	0	2.642683	4.446476	0.802251
46	8	0	2.730349	4.938994	-1.394731
47	1	0	5.041507	-1.245452	3.457439
48	1	0	2.964802	5.812602	-1.045239
49	1	0	2.562085	1.972197	1.076114
50	1	0	-5.520534	0.705314	3.782933
51	1	0	0.192710	-0.888080	1.649935
52	17	0	-0.543112	-1.504006	2.550374

HF=-2731.5414917\ZeroPoint=0.360366\Thermal=0.3939839

G = 11.3 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.320514	0.017974	-0.179465
2	46	0	-1.412701	0.141071	-0.913284
3	7	0	1.123291	-1.988078	-0.518663
4	7	0	1.956501	-2.767078	0.029882
5	6	0	2.835511	-2.120988	0.891820
6	6	0	2.514804	-0.812100	1.360581
7	6	0	3.420348	-0.189938	2.229045
8	1	0	3.185046	0.786864	2.638458
9	6	0	4.585956	-0.839738	2.627912
10	6	0	4.865300	-2.134875	2.176838
11	1	0	5.767309	-2.637131	2.506196
12	6	0	3.986415	-2.787068	1.318111
13	1	0	4.184322	-3.790516	0.961156
14	6	0	0.090956	-2.551828	-1.318356
15	6	0	-1.063938	-1.778358	-1.563923
16	6	0	-2.084745	-2.404953	-2.297966
17	1	0	-2.998157	-1.858701	-2.510999
18	6	0	-1.955274	-3.701886	-2.785299
19	1	0	-2.759648	-4.143579	-3.364225
20	6	0	-0.787154	-4.434894	-2.541352
21	1	0	-0.680935	-5.441948	-2.927323
22	6	0	0.232766	-3.866817	-1.801759
23	1	0	1.139138	-4.416753	-1.585792
24	16	0	-1.943042	2.332284	-0.096381
25	6	0	-3.348495	1.812833	0.971190
26	1	0	-4.253256	1.742795	0.360124
27	1	0	-3.512458	2.566218	1.742221
28	6	0	-3.054143	0.462857	1.631754
29	1	0	-2.190538	0.565925	2.289931
30	6	0	-4.248090	-0.001798	2.450843
31	8	0	-4.400849	0.736475	3.567647
32	8	0	-4.997432	-0.894850	2.135632
33	7	0	-2.707984	-0.567474	0.618671
34	1	0	-2.165089	-1.296092	1.085299
35	1	0	-3.559567	-1.004505	0.267667
36	16	0	0.417627	0.758778	-2.280950
37	6	0	0.702680	2.580178	-2.079357
38	1	0	1.091005	2.955072	-3.024858
39	1	0	-0.250423	3.068815	-1.878115
40	6	0	1.716955	2.857455	-0.963533
41	1	0	2.707286	2.542948	-1.307986
42	7	0	1.394594	2.064916	0.247636
43	1	0	0.428495	2.278227	0.549196
44	6	0	1.833841	4.337052	-0.604555
45	8	0	1.878337	4.758311	0.522304
46	8	0	1.926865	5.109302	-1.703629
47	1	0	5.270655	-0.349523	3.310805
48	1	0	2.019389	6.031087	-1.416595
49	1	0	2.009729	2.337304	1.011225
50	1	0	-5.186596	0.411848	4.033460
51	1	0	1.262106	-0.739495	1.798475
52	17	0	-0.114289	-1.047215	2.749126

HF=-2731.5233189\ZeroPoint=0.3590765\Thermal=0.3915962

G = -11.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.952979	0.185099	0.478227
2	46	0	-1.424850	-0.258575	-1.046411
3	7	0	1.470026	-1.773495	0.067125
4	7	0	2.632882	-2.222952	-0.026043
5	6	0	3.738387	-1.426508	0.343058
6	6	0	3.834864	-0.727860	1.552926
7	6	0	4.994640	-0.008475	1.828146
8	1	0	5.076264	0.521588	2.770111
9	6	0	6.042843	0.028278	0.908941
10	6	0	5.948527	-0.689043	-0.285432
11	1	0	6.767113	-0.676120	-0.995638
12	6	0	4.811381	-1.440110	-0.557931
13	1	0	4.726185	-2.021458	-1.468052
14	6	0	0.436124	-2.690057	-0.344401
15	6	0	-0.736166	-2.198481	-0.952951
16	6	0	-1.616701	-3.177880	-1.450760
17	1	0	-2.515635	-2.865450	-1.973669

18	6	0	-1.384557	-4.542699	-1.305197
19	1	0	-2.100642	-5.256776	-1.698358
20	6	0	-0.240275	-4.990792	-0.640363
21	1	0	-0.066054	-6.049988	-0.492288
22	6	0	0.674461	-4.064327	-0.171682
23	1	0	1.575540	-4.383187	0.335884
24	16	0	-2.461483	1.918637	-0.892218
25	6	0	-3.942480	1.423835	0.081775
26	1	0	-4.778227	1.225308	-0.597474
27	1	0	-4.230253	2.241461	0.742389
28	6	0	-3.658258	0.167803	0.915830
29	1	0	-2.883141	0.389311	1.652898
30	6	0	-4.916380	-0.295413	1.637830
31	8	0	-5.243870	0.539672	2.642297
32	8	0	-5.560413	-1.270826	1.338066
33	7	0	-3.151448	-0.904395	0.029292
34	1	0	-2.905243	-1.729028	0.572642
35	1	0	-3.897786	-1.200652	-0.598844
36	16	0	0.702229	0.493597	-1.855335
37	6	0	0.671670	2.350854	-1.866989
38	1	0	1.365014	2.680021	-2.639108
39	1	0	-0.329217	2.682201	-2.140093
40	6	0	1.102974	2.932147	-0.510291
41	1	0	2.185845	2.807998	-0.411733
42	7	0	0.465303	2.198492	0.604402
43	1	0	-0.561448	2.258357	0.506238
44	6	0	0.822028	4.428204	-0.393187
45	8	0	0.303264	4.953692	0.555976
46	8	0	1.266167	5.098034	-1.477342
47	1	0	6.938738	0.597357	1.129791
48	1	0	1.078695	6.039935	-1.343445
49	1	0	0.715611	2.596220	1.508016
50	1	0	-6.062131	0.215527	3.049127
51	1	0	3.031687	-0.772267	2.275179
52	17	0	0.658013	-0.037718	2.822495

HF=-2731.5607209\ZeroPoint=0.3634804\Thermal=0.3966906

G = 3.3 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.674540	-0.291517	-0.093295
2	46	0	1.613781	-0.035992	-0.786756
3	7	0	-1.225710	1.701874	0.095707
4	7	0	-1.824628	2.362043	0.991983
5	6	0	-2.723720	1.607964	1.735010
6	6	0	-2.873750	0.229487	1.437106
7	6	0	-3.790095	-0.491967	2.192814
8	1	0	-3.964198	-1.547004	2.003966
9	6	0	-4.520178	0.127259	3.215917
10	6	0	-4.351631	1.484128	3.499612
11	1	0	-4.924059	1.949294	4.293088
12	6	0	-3.449238	2.235063	2.755334
13	1	0	-3.298039	3.291578	2.943247
14	6	0	-0.333342	2.428629	-0.751936
15	6	0	0.835957	1.812522	-1.228965
16	6	0	1.655225	2.596681	-2.059366
17	1	0	2.568087	2.169046	-2.462942
18	6	0	1.324204	3.903041	-2.411931
19	1	0	1.973492	4.463565	-3.076177
20	6	0	0.150595	4.483711	-1.924929
21	1	0	-0.120593	5.495375	-2.203311
22	6	0	-0.675479	3.749714	-1.090544
23	1	0	-1.593230	4.173052	-0.702844
24	16	0	3.043517	-1.981685	-0.471509
25	6	0	4.350376	-1.154271	0.526127
26	1	0	5.135629	-0.780839	-0.139768
27	1	0	4.800302	-1.877257	1.206276
28	6	0	3.776381	0.015540	1.334620
29	1	0	3.046626	-0.373318	2.047510
30	6	0	4.882111	0.741231	2.088958
31	8	0	5.333453	0.010215	3.127708
32	8	0	5.326243	1.821881	1.787756
33	7	0	3.077919	0.947387	0.421669
34	1	0	2.619913	1.688241	0.947133
35	1	0	3.762208	1.419680	-0.168859
36	16	0	-0.243208	-0.835214	-1.972774
37	6	0	-0.482964	-2.672664	-1.907333
38	1	0	-1.188100	-2.893016	-2.712505
39	1	0	0.456800	-3.177191	-2.124112
40	6	0	-1.052439	-3.191771	-0.577715
41	1	0	-1.387818	-4.226368	-0.726267
42	7	0	-2.184297	-2.342752	-0.118442
43	1	0	-2.427763	-2.599331	0.835710
44	6	0	0.009173	-3.216693	0.518820
45	8	0	-0.072174	-2.575845	1.537666
46	8	0	1.015908	-4.017912	0.174661
47	1	0	-5.227718	-0.457262	3.794466
48	1	0	1.871012	-3.576876	0.434676
49	1	0	-3.003768	-2.483616	-0.707517
50	1	0	6.058026	0.499720	3.546710
51	1	0	-3.512748	-0.154249	-1.260808
52	17	0	-4.574800	-0.563507	-1.943832

HF=-2731.53297\ZeroPoint=0.3593072\Thermal=0.3928397

G = 18.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.743439	-0.149634	-0.372387
2	46	0	1.651208	-0.062935	-0.713573
3	7	0	-1.111553	1.751557	0.040222
4	7	0	-1.631480	2.360749	1.014007
5	6	0	-2.560626	1.616770	1.740588
6	6	0	-3.077991	0.389830	1.243800
7	6	0	-3.846831	-0.382156	2.120599
8	1	0	-4.298185	-1.299564	1.759740
9	6	0	-4.123382	0.052771	3.415732
10	6	0	-3.653056	1.290416	3.860548
11	1	0	-3.891021	1.634706	4.860031
12	6	0	-2.872515	2.079541	3.022405
13	1	0	-2.469622	3.029587	3.351998

14	6	0	-0.149654	2.488436	-0.724741
15	6	0	1.031032	1.855133	-1.147669
16	6	0	1.926800	2.652797	-1.878536
17	1	0	2.854102	2.218743	-2.240439
18	6	0	1.655905	3.985147	-2.185980
19	1	0	2.365268	4.557333	-2.774531
20	6	0	0.468401	4.579034	-1.752577
21	1	0	0.245918	5.610606	-1.998633
22	6	0	-0.433951	3.832750	-1.011705
23	1	0	-1.365326	4.263701	-0.666174
24	16	0	2.709434	-2.178718	-0.247095
25	6	0	4.210548	-1.482578	0.555864
26	1	0	4.954802	-1.215622	-0.202004
27	1	0	4.649302	-2.236171	1.210507
28	6	0	3.860271	-0.235639	1.377582
29	1	0	3.157218	-0.519511	2.162563
30	6	0	5.110793	0.363868	2.004942
31	8	0	5.544227	-0.373645	3.046409
32	8	0	5.672084	1.355441	1.607302
33	7	0	3.200347	0.759334	0.500100
34	1	0	2.815993	1.524391	1.049426
35	1	0	3.902257	1.188572	-0.103170
36	16	0	-0.163422	-0.655866	-2.032663
37	6	0	-0.492862	-2.478355	-2.192144
38	1	0	-1.018680	-2.584130	-3.143226
39	1	0	0.455332	-3.009295	-2.254009
40	6	0	-1.358091	-3.049594	-1.061966
41	1	0	-1.777945	-4.007196	-1.396914
42	7	0	-2.441825	-2.103189	-0.706348
43	1	0	-2.909608	-2.411426	0.143069
44	6	0	-0.549274	-3.344504	0.198899
45	8	0	-0.777377	-2.860485	1.277333
46	8	0	0.423025	-4.221240	-0.072739
47	1	0	-4.729340	-0.562098	4.071340
48	1	0	1.129464	-4.125703	0.591540
49	1	0	-3.158970	-2.013811	-1.428846
50	1	0	6.363942	0.025634	3.376541
51	1	0	-3.677281	0.284085	0.064632
52	17	0	-4.939316	-0.063709	-1.077606

HF=-2731.510252\ZeroPoint=0.3583723\Thermal=0.3911795

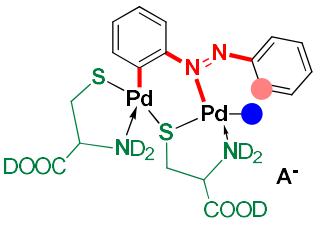
G = 13.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.742666	0.011040	-0.155029
2	46	0	1.645865	-0.078816	-0.655752
3	7	0	-1.040974	1.928205	0.184035
4	7	0	-1.601984	2.538144	1.128015
5	6	0	-2.675824	1.789951	1.698470
6	6	0	-3.665509	1.177276	0.895546
7	6	0	-4.646918	0.382081	1.506229
8	1	0	-5.379064	-0.093307	0.862623
9	6	0	-4.653258	0.226248	2.887357
10	6	0	-3.698548	0.881335	3.674889
11	1	0	-3.718728	0.768140	4.752668
12	6	0	-2.714950	1.670464	3.090385
13	1	0	-1.959124	2.165979	3.686956
14	6	0	-0.004408	2.615320	-0.519886
15	6	0	1.114940	1.901163	-0.986711
16	6	0	2.061026	2.661488	-1.696441
17	1	0	2.940306	2.171965	-2.104407
18	6	0	1.904358	4.025924	-1.930641
19	1	0	2.651674	4.562626	-2.505359
20	6	0	0.781489	4.699738	-1.444013
21	1	0	0.646979	5.757933	-1.633399
22	6	0	-0.173395	3.994864	-0.732126
23	1	0	-1.064232	4.484320	-0.358760
24	16	0	2.617768	-2.251898	-0.364003
25	6	0	4.248906	-1.662987	0.248065
26	1	0	4.896138	-1.391986	-0.592695
27	1	0	4.732417	-2.468029	0.802372
28	6	0	4.072218	-0.445462	1.162537
29	1	0	3.464991	-0.737076	2.021109
30	6	0	5.421366	0.071447	1.642447
31	8	0	5.953413	-0.733998	2.581705
32	8	0	5.969093	1.058740	1.216283
33	7	0	3.352896	0.618330	0.421539
34	1	0	3.064398	1.362780	1.051993
35	1	0	4.000493	1.059650	-0.231922
36	16	0	-0.276578	-0.594514	-1.823137
37	6	0	-0.717958	-2.400447	-1.955625
38	1	0	-1.339238	-2.456594	-2.850400
39	1	0	0.195113	-2.974861	-2.103456
40	6	0	-1.513649	-2.904007	-0.750226
41	1	0	-2.019962	-3.834807	-1.037640
42	7	0	-2.507976	-1.893243	-0.344184
43	1	0	-2.919400	-2.152255	0.551436
44	6	0	-0.618276	-3.233546	0.439953
45	8	0	-0.681161	-2.687674	1.512173
46	8	0	0.231298	-4.219549	0.124637
47	1	0	-5.411395	-0.387771	3.358975
48	1	0	0.958146	-4.221633	0.769380
49	1	0	-3.322824	-1.744365	-1.020783
50	1	0	6.827850	-0.386715	2.816844
51	1	0	-3.770251	1.402584	-0.163635
52	17	0	-4.870883	-0.859505	-1.786306

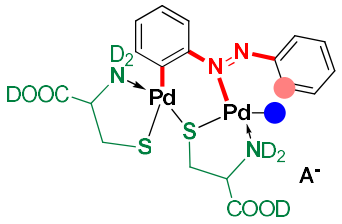
HF=-2731.519573\ZeroPoint=0.3622664\Thermal=0.395348

Structures from Table S8

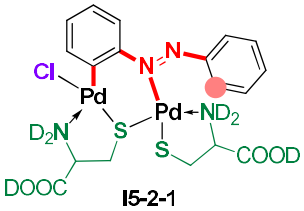
Table S8. B3LYP-D3/6-311+G**/SDD(Pd)/gas phase relative stabilities for the main isomers of the bridged intermediates that could be formed by deuteration of the bridged dipalladated complex by D-transfer to the 5-ring. Free energies relative to **B1-1** (in kcal mol^{-1}).



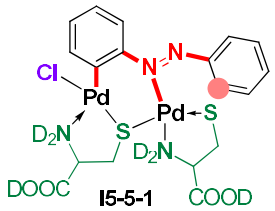
● = none, A = Cl (**I4-1**)
= Cys^{4D}, A = Cl (**I5-1**)
= Cl$^-$, A = none (**I5-2**)



● = none, A = Cl (**I4-2**)
= Cys^{4D}, A = Cl (**I5-4**)
= Cl$^-$, A = none (**I5-5**)



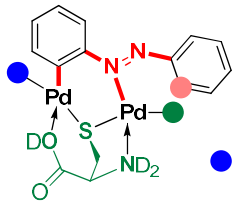
I5-2-1



I5-5-1

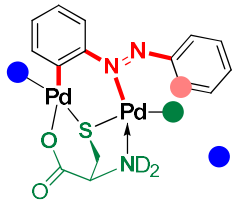
Functional/donor groups in group ●				*G*$_{rel}$ (kcal mol^{-1})			
S/SD	ND_2/ND_3	COO/COOD	Cl$^-$	Complex	**B1-1***	Complex	**B1-2***
-	-	-	anion	**I4-1**	2.5	**I4-2**	-**
S-coord	ND_3	COOD	anion	**I5-1-1**	**-30.3**	**I5-4-1**	**-18.8**
SD-coord	ND_2	COOD	anion	**I5-1-2**	-14.9	**I5-4-2**	-5.4
SD-coord	ND_3	COO	anion	**I5-1-3**	-16.5	**I5-4-3**	-12.7
SD	ND_2-coord	COOD	anion	**I5-1-4**	-18.6	**I5-4-4**	-6.7
SD	ND_3	COO-coord	anion	**I5-1-5**	-14.2	**I5-4-5**	-12.5
-	-	-	coord	**I5-2**	-4.8	**I5-5**	-11.7
-	-	-	coord	**I5-2-1**	-17.0	**I5-5-1**	-5.4

* Mother complex. **Optimization ends in the coordinated Cl$^-$ unless Cl$^-$ is far from the empty coordination site.



● = Cl$^-$, = *S*-coord Cys^{3D}; ● = *S*-coord Cys^{3D} (**I7-1**) = Cl$^-$ (**I8-1**)

Complex	*G*$_{rel}$ (kcal mol^{-1})
I7-1	-2.9
I8-1	2.7



● = Cl$^-$, = *S*-coord Cys^{4D}; ● = *S*-coord Cys^{4D} (**I7-2**) = Cl$^-$ (**I8-2**)

Complex	*G*$_{rel}$ (kcal mol^{-1})
I7-2	-10.7
I8-2	-11.4

G = 2.5 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.505831	-0.198492	-0.225629
2	46	0	1.379370	1.059647	-0.562367
3	7	0	-1.665920	1.821472	0.246309
4	7	0	-2.594770	2.030997	1.068616
5	6	0	-3.102491	0.798555	1.579617
6	6	0	-2.216984	-0.201804	2.053436
7	6	0	-2.745896	-1.420506	2.513521
8	1	0	-2.050451	-2.177317	2.857434
9	6	0	-4.118159	-1.626395	2.515446
10	6	0	-4.984266	-0.608404	2.089527
11	1	0	-6.055995	-0.769394	2.113766
12	6	0	-4.487349	0.604275	1.630761
13	1	0	-5.145666	1.392452	1.287064
14	6	0	-1.026718	2.921666	-0.374799
15	6	0	0.293624	2.746138	-0.834487
16	6	0	0.892996	3.867602	-1.432414
17	1	0	1.919932	3.799233	-1.770783
18	6	0	0.207636	5.067212	-1.589377
19	1	0	0.698110	5.905442	-2.073149
20	6	0	-1.108460	5.205941	-1.126565
21	1	0	-1.639687	6.141660	-1.254489
22	6	0	-1.725448	4.137500	-0.506218
23	1	0	-2.739629	4.212169	-0.135105
24	16	0	2.456549	2.153134	1.186914
25	6	0	3.257164	0.654297	1.912314
26	1	0	2.538416	0.093477	2.514608
27	1	0	4.071844	0.984423	2.556069
28	6	0	3.787363	-0.231071	0.792191
29	1	0	4.489832	0.360868	0.193462
30	6	0	4.561247	-1.475859	1.224363
31	8	0	5.227649	-1.303215	2.384355
32	8	0	4.621974	-2.487612	0.570971
33	7	0	2.660697	-0.624614	-0.084096
34	1	0	3.026100	-1.158077	-0.869042
35	1	0	2.045956	-1.266937	0.449647
36	16	0	-0.112319	-0.042462	-2.077344
37	6	0	0.281018	-1.852332	-2.185453
38	1	0	0.666793	-2.051059	-3.183881
39	1	0	1.028344	-2.123752	-1.442021
40	6	0	-1.002408	-2.629365	-1.919488
41	1	0	-1.751473	-2.347278	-2.668267
42	7	0	-1.509058	-2.247224	-0.582437
43	1	0	-0.823178	-2.542536	0.159690
44	6	0	-0.874396	-4.150379	-2.005233
45	8	0	-0.004839	-4.536853	-2.958032
46	8	0	-1.519191	-4.909420	-1.330574
47	1	0	-4.524668	-2.566211	2.870064
48	1	0	-2.391049	-2.716288	-0.386354
49	1	0	5.709428	-2.124441	2.567662
50	1	0	-1.163060	0.008541	2.214565
51	17	0	0.601071	-2.396597	1.621978
52	1	0	0.009199	-5.506702	-2.975207

HF=-2731.5403748\ZeroPoint=0.3627599\Thermal=0.3958884

G = -30.3 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.017269	0.828893	-0.088649
2	46	0	-1.210290	-0.262373	-1.664873
3	7	0	2.150742	-0.743499	-0.805280
4	7	0	3.373113	-0.886966	-0.573964
5	6	0	4.090617	0.110505	0.104692
6	6	0	4.995622	-0.324210	1.081051
7	6	0	5.748514	0.608119	1.782402
8	1	0	6.420057	0.276052	2.565180
9	6	0	5.648547	1.966782	1.474228
10	6	0	4.794063	2.389929	0.456858
11	1	0	4.745197	3.439618	0.190415
12	6	0	4.006037	1.470419	-0.228590
13	1	0	3.369778	1.786628	-1.045000
14	6	0	1.548918	-1.767063	-1.628283
15	6	0	0.218205	-1.648179	-2.096219
16	6	0	-0.205699	-2.641201	-3.004686
17	1	0	-1.208103	-2.588995	-3.406211
18	6	0	0.598792	-3.707275	-3.380381
19	1	0	0.216645	-4.448609	-4.073911
20	6	0	1.884501	-3.837106	-2.846833
21	1	0	2.510141	-4.682977	-3.105960
22	6	0	2.356357	-2.868981	-1.986589
23	1	0	3.353576	-2.938068	-1.577339
24	16	0	-2.655476	-2.003925	-0.971166
25	6	0	-4.233401	-1.047252	-0.947882
26	1	0	-4.937077	-1.551070	-0.286294
27	1	0	-4.657103	-1.029582	-1.955651
28	6	0	-4.007700	0.381772	-0.465308
29	1	0	-4.956767	0.934733	-0.500857
30	6	0	-3.536060	0.421498	0.988183
31	8	0	-2.542376	1.041661	1.338114
32	8	0	-4.317354	-0.265007	1.774805
33	7	0	-2.989449	1.040739	-1.324218
34	1	0	-3.388897	1.171485	-2.251741
35	1	0	-2.815476	1.975642	-0.955374
36	16	0	0.383201	1.469448	-2.294850
37	6	0	-0.422334	3.085656	-1.884215
38	1	0	0.040771	3.841880	-2.520014
39	1	0	-1.470086	3.026113	-2.168030
40	6	0	-0.275316	3.525286	-0.415581
41	1	0	0.650174	4.086152	-0.292404
42	7	0	-0.218771	2.384669	0.541054
43	1	0	-1.142170	1.946845	0.688839
44	6	0	-1.469465	4.400579	-0.027333
45	8	0	-1.104025	5.543314	0.572506
46	8	0	-2.617680	4.073056	-0.211889
47	1	0	6.249904	2.689903	2.012747
48	1	0	0.097897	2.703856	1.455867
49	1	0	5.063603	-1.383059	1.299452
50	7	0	-1.555572	-2.503622	2.056204
51	6	0	-0.201986	-1.904909	1.840694

52	6	0	-0.011097	-0.630692	2.677788
53	1	0	-0.150732	-1.634189	0.782589
54	6	0	0.838025	-3.017239	2.067456
55	16	0	1.497215	0.307966	2.180703
56	1	0	0.089114	-0.870793	3.738267
57	1	0	-0.892581	-0.002947	2.571991
58	8	0	0.498489	-4.166169	2.228216
59	8	0	2.112072	-2.648751	2.032109
60	1	0	2.182451	-1.653244	2.004336
61	1	0	-1.906264	6.026066	0.830630
62	1	0	-2.120877	-2.369618	1.188357
63	1	0	-2.074925	-2.066917	2.882017
64	1	0	-1.433227	-3.510270	2.223474
65	1	0	-3.920599	-0.402551	2.716470
66	17	0	-3.081107	-1.098268	4.265827

HF=-3453.7050788\ZeroPoint=0.4635458\Thermal=0.5046889

G = -14.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.220120	0.581136	-0.082203
2	46	0	-1.370690	-0.826825	-1.111962
3	7	0	2.089733	-1.235090	-0.666030
4	7	0	3.339026	-1.353323	-0.638892
5	6	0	4.136683	-0.222559	-0.371629
6	6	0	5.124786	-0.343108	0.611191
7	6	0	5.947255	0.742214	0.895245
8	1	0	6.689233	0.660400	1.680680
9	6	0	5.827666	1.925486	0.165091
10	6	0	4.885105	2.018389	-0.859223
11	1	0	4.818126	2.921676	-1.455007
12	6	0	4.032700	0.952703	-1.131423
13	1	0	3.323756	1.003589	-1.947696
14	6	0	1.363993	-2.392484	-1.102182
15	6	0	-0.013824	-2.316123	-1.406650
16	6	0	-0.570751	-3.473582	-1.995330
17	1	0	-1.615601	-3.466764	-2.277505
18	6	0	0.152482	-4.638938	-2.194126
19	1	0	-0.333602	-5.503526	-2.633465
20	6	0	1.494809	-4.708998	-1.801887
21	1	0	2.057894	-5.627968	-1.912947
22	6	0	2.096599	-3.590542	-1.272739
23	1	0	3.136090	-3.614381	-0.980058
24	16	0	-2.698715	-2.356862	0.101789
25	6	0	-3.910260	-1.141966	0.778191
26	1	0	-3.485804	-0.601057	1.624130
27	1	0	-4.793783	-1.687168	1.107223
28	6	0	-4.266747	-0.154197	-0.325440
29	1	0	-4.676742	-0.714619	-1.173655
30	6	0	-5.323633	0.890081	0.034496
31	8	0	-6.235717	0.428330	0.912442
32	8	0	-5.370592	1.989402	-0.457915
33	7	0	-3.032967	0.528188	-0.777142
34	1	0	-3.267226	1.139490	-1.555161
35	1	0	-2.721052	1.131237	0.006187
36	16	0	0.113088	0.784003	-2.140086
37	6	0	-0.592639	2.483198	-1.864630
38	1	0	-0.659052	2.973927	-2.833847
39	1	0	-1.590003	2.419717	-1.438410
40	6	0	0.311144	3.268407	-0.924036
41	1	0	1.289951	3.400820	-1.398839
42	7	0	0.512382	2.497566	0.326015
43	1	0	-0.399642	2.377192	0.837094
44	6	0	-0.169768	4.680372	-0.576439
45	8	0	-0.938254	5.217775	-1.541572
46	8	0	0.153014	5.253247	0.430503
47	1	0	6.480434	2.763388	0.379541
48	1	0	1.113892	3.031734	0.951653
49	1	0	-6.878052	1.137820	1.068565
50	1	0	5.215465	-1.274639	1.157372
51	7	0	-1.421061	-1.173235	3.521452
52	6	0	-0.282941	-1.031609	2.607312
53	6	0	0.643593	0.017190	3.218042
54	1	0	-0.593530	-0.685131	1.609583
55	6	0	0.421318	-2.380945	2.411797
56	16	0	2.101131	0.463963	2.175960
57	1	0	1.042529	-0.322171	4.173322
58	1	0	0.088406	0.945717	3.350952
59	8	0	1.578563	-2.576628	2.720500
60	8	0	-0.310136	-3.346771	1.865200
61	1	0	2.645700	-0.772360	2.198043
62	17	0	-2.067553	1.913020	1.890292
63	1	0	-1.145506	-3.002081	1.449505
64	1	0	-1.190884	6.111633	-1.260961
65	1	0	-1.990653	-0.332495	3.444634
66	1	0	-2.004052	-1.960812	3.258205

HF=-3453.6757545\ZeroPoint=0.4607747\Thermal=0.503268

G = -16.5 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.069216	-0.889400	0.428686
2	46	0	2.188789	1.021117	0.340748
3	7	0	1.417316	-2.227951	-0.458801
4	7	0	1.107500	-3.399306	-0.786550
5	6	0	-0.154461	-3.926198	-0.470758
6	6	0	-0.741705	-4.738057	-1.451285
7	6	0	-2.012843	-5.258264	-1.244064
8	1	0	-2.480549	-5.857151	-2.016762
9	6	0	-2.686318	-5.009419	-0.046169
10	6	0	-2.071785	-4.263017	0.958827
11	1	0	-2.586801	-4.084028	1.894173
12	6	0	-0.803362	-3.729516	0.759749
13	1	0	-0.305392	-3.187150	1.552793
14	6	0	2.778054	-1.843036	-0.718502
15	6	0	3.217662	-0.525315	-0.457767
16	6	0	4.576490	-0.256901	-0.723101
17	1	0	4.950150	0.745436	-0.564050
18	6	0	5.446588	-1.225656	-1.200336
19	1	0	6.484680	-0.971088	-1.385875

20	6	0	4.986075	-2.524532	-1.448089
21	1	0	5.659005	-3.287698	-1.821204
22	6	0	3.663633	-2.829826	-1.208037
23	1	0	3.290045	-3.828213	-1.384800
24	16	0	2.500795	2.192545	-1.653258
25	6	0	2.164723	3.883014	-0.998401
26	1	0	1.910723	4.526764	-1.840791
27	1	0	3.056024	4.288472	-0.510147
28	6	0	1.008628	3.867092	-0.006033
29	1	0	0.843217	4.880651	0.387469
30	6	0	-0.308711	3.445054	-0.650825
31	8	0	-1.053172	2.624668	-0.123954
32	8	0	-0.562433	4.065960	-1.763091
33	7	0	1.315917	2.927011	1.108051
34	1	0	2.045065	3.340608	1.685596
35	1	0	0.487034	2.847167	1.697397
36	16	0	1.592806	-0.515788	2.178131
37	6	0	0.505759	0.442308	3.328883
38	1	0	0.654878	0.040716	4.332302
39	1	0	0.843899	1.476708	3.330292
40	6	0	-0.978830	0.352866	2.956228
41	1	0	-1.409275	-0.571720	3.338773
42	7	0	-1.202427	0.367898	1.488499
43	1	0	-1.079007	1.307827	1.086413
44	6	0	-1.686088	1.560060	3.573116
45	8	0	-2.516323	1.229035	4.570795
46	8	0	-1.478890	2.692130	3.205786
47	1	0	-3.681672	-5.407599	0.110870
48	1	0	-2.178222	0.071556	1.316584
49	1	0	-0.205513	-4.910653	-2.376449
50	7	0	-4.379896	0.261741	-1.792959
51	6	0	-3.158109	1.137064	-1.760273
52	6	0	-1.902675	0.444497	-2.258257
53	1	0	-3.028189	1.461328	-0.729468
54	6	0	-3.553105	2.405967	-2.620783
55	16	0	-1.479285	-1.173375	-1.422549
56	1	0	-1.049906	1.104846	-2.127231
57	1	0	-1.985131	0.199427	-3.319475
58	8	0	-4.759230	2.448480	-2.925677
59	8	0	-2.641541	3.213841	-2.895417
60	1	0	-2.923603	2.041032	4.913114
61	1	0	-4.563829	-0.159120	-0.850251
62	1	0	-4.306017	-0.488400	-2.478891
63	1	0	-5.101933	0.949745	-2.139772
64	1	0	-1.427538	3.705098	-2.195680
65	17	0	-4.028275	-1.011513	0.959658
66	1	0	-2.582681	-1.299715	-0.590235

HF=-3453.6804352\ZeroPoint=0.4611221\Thermal=0.5025944

G = -18.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.584829	-0.200217	0.841333
2	46	0	-1.999701	0.997868	0.528068
3	7	0	1.339301	1.739578	0.908460
4	7	0	2.566619	2.007623	0.882626
5	6	0	3.511059	0.969408	0.939780
6	6	0	4.638093	1.123335	0.120184
7	6	0	5.580062	0.103789	0.050700
8	1	0	6.429897	0.202888	-0.614260
9	6	0	5.426668	-1.047380	0.825233
10	6	0	4.343890	-1.166210	1.696069
11	1	0	4.230930	-2.055026	2.303470
12	6	0	3.389416	-0.159330	1.767406
13	1	0	2.568052	-0.230327	2.468915
14	6	0	0.451379	2.870443	0.966366
15	6	0	-0.941836	2.704796	0.788834
16	6	0	-1.723325	3.875112	0.863609
17	1	0	-2.790510	3.800781	0.703708
18	6	0	-1.171730	5.122848	1.119084
19	1	0	-1.816400	5.993600	1.174445
20	6	0	0.208650	5.257429	1.303677
21	1	0	0.646963	6.226710	1.510541
22	6	0	1.012698	4.139195	1.227058
23	1	0	2.080700	4.217920	1.373319
24	16	0	-2.670737	1.772457	-1.579137
25	6	0	-4.096886	0.634115	-1.838074
26	1	0	-4.305228	0.589365	-2.907364
27	1	0	-4.987634	1.018083	-1.331935
28	6	0	-3.791961	-0.764400	-1.316312
29	1	0	-4.669020	-1.414515	-1.455707
30	6	0	-2.640330	-1.442511	-2.050976
31	8	0	-2.635610	-1.237029	-3.358266
32	8	0	-1.813928	-2.124132	-1.477707
33	7	0	-3.427741	-0.692670	0.127852
34	1	0	-4.264867	-0.454678	0.655883
35	1	0	-3.142303	-1.621807	0.441885
36	16	0	-0.898575	0.219271	2.604007
37	6	0	-1.518656	-1.501078	2.901705
38	1	0	-1.488204	-1.678753	3.977822
39	1	0	-2.559971	-1.538949	2.587570
40	6	0	-0.689058	-2.570863	2.177910
41	1	0	0.183324	-2.839789	2.772225
42	7	0	-0.197034	-2.119393	0.855067
43	1	0	-0.941198	-2.152253	0.151632
44	6	0	-1.579434	-3.795700	1.963772
45	8	0	-1.136462	-4.889857	2.593748
46	8	0	-2.589431	-3.757230	1.298793
47	1	0	6.150973	-1.849803	0.755094
48	1	0	0.560001	-2.765193	0.513269
49	1	0	-1.770471	-1.545484	-3.718938
50	1	0	4.724713	2.015314	-0.486552
51	7	0	1.593172	-0.611010	-1.001587
52	6	0	0.719517	-0.305180	-2.150857
53	6	0	0.784958	1.175572	-2.565329
54	1	0	-0.309698	-0.473310	-1.851275
55	6	0	0.941493	-1.226853	-3.341141
56	16	0	2.465928	1.853924	-2.868277
57	1	0	0.378789	1.774261	-1.750233
58	1	0	0.142869	1.341355	-3.428892
59	8	0	2.225800	-1.541111	-3.531772
60	8	0	0.048609	-1.615863	-4.066594
61	1	0	2.797242	1.040721	-3.891827

62	1	0	-1.734311	-5.626059	2.386836
63	1	0	1.838134	-1.626836	-0.945664
64	1	0	2.478818	-0.116109	-1.110274
65	1	0	2.285469	-2.207776	-4.233937
66	17	0	2.175365	-3.598416	-0.371318

HF=-3453.6836939\ZeroPoint=0.4619005\Thermal=0.5040161

G = -14.2 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.298900	-0.461430	0.084389
2	46	0	0.182339	1.405658	-1.496276
3	7	0	-2.471289	1.121613	0.679053
4	7	0	-3.646482	1.011760	1.099070
5	6	0	-4.193268	-0.259424	1.361157
6	6	0	-3.534677	-1.267816	2.079360
7	6	0	-4.185970	-2.477141	2.305318
8	1	0	-3.681085	-3.252750	2.869546
9	6	0	-5.475268	-2.689996	1.818131
10	6	0	-6.136292	-1.672797	1.126307
11	1	0	-7.144678	-1.828451	0.760958
12	6	0	-5.510057	-0.449533	0.920300
13	1	0	-6.011585	0.359171	0.402717
14	6	0	-2.006202	2.461124	0.462473
15	6	0	-0.983862	2.731047	-0.479976
16	6	0	-0.746288	4.097076	-0.738462
17	1	0	0.010639	4.367580	-1.460839
18	6	0	-1.416486	5.114286	-0.071235
19	1	0	-1.179968	6.148132	-0.299452
20	6	0	-2.361389	4.811895	0.914462
21	1	0	-2.854205	5.600185	1.471237
22	6	0	-2.660122	3.490093	1.171671
23	1	0	-3.398853	3.224655	1.915663
24	16	0	2.066276	2.523462	-0.668011
25	6	0	3.254112	1.951021	-1.952309
26	1	0	4.265057	2.147596	-1.594865
27	1	0	3.107444	2.496699	-2.889278
28	6	0	3.079985	0.456188	-2.208724
29	1	0	3.787194	0.124104	-2.981021
30	6	0	3.417718	-0.351756	-0.958052
31	8	0	4.640332	-0.128696	-0.582670
32	8	0	2.623739	-1.126471	-0.420794
33	7	0	1.682279	0.197641	-2.645545
34	1	0	1.583402	0.562784	-3.591218
35	1	0	1.549965	-0.811105	-2.720968
36	16	0	-1.844960	0.079253	-2.102019
37	6	0	-1.221492	-1.442578	-2.960254
38	1	0	-2.030567	-1.819455	-3.587056
39	1	0	-0.405709	-1.145486	-3.616801
40	6	0	-0.777251	-2.551413	-1.988697
41	1	0	-1.639752	-3.152219	-1.704328
42	7	0	-0.186558	-2.013166	-0.739781
43	1	0	0.766190	-1.652579	-0.874393
44	6	0	0.261381	-3.417376	-2.698661
45	8	0	-0.172435	-4.658726	-2.956602
46	8	0	1.355368	-3.005065	-3.006125
47	1	0	-5.972260	-3.637124	1.994146
48	1	0	-0.113505	-2.726948	-0.005639
49	1	0	-2.548857	-1.091523	2.485267
50	7	0	2.840676	-1.931246	2.298708
51	6	0	1.760440	-1.083285	2.901984
52	1	0	2.644709	-2.918292	2.464480
53	6	0	2.059674	0.402927	2.720461
54	1	0	1.708488	-1.328526	3.965353
55	6	0	0.454424	-1.547737	2.207066
56	16	0	3.414285	1.039278	3.785549
57	1	0	1.168865	0.955862	3.012156
58	1	0	2.246022	0.649739	1.673252
59	8	0	-0.416224	-0.639073	2.013008
60	8	0	0.392247	-2.736384	1.856786
61	1	0	4.449005	0.492554	3.101895
62	1	0	2.837708	-1.789005	1.269648
63	1	0	0.532547	-5.141411	-3.418358
64	1	0	3.828412	-1.701193	2.574104
65	1	0	4.956211	-0.612068	0.269085
66	17	0	5.726003	-1.318061	1.855878

HF=-3453.6768457\ZeroPoint=0.4617086\Thermal=0.5033985

G = -4.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.280158	-0.680552	-0.073761
2	46	0	1.538272	0.701901	-0.438708
3	7	0	-1.916698	1.280926	0.158897
4	7	0	-3.086601	1.548705	0.520047
5	6	0	-4.087141	0.565365	0.506071
6	6	0	-4.296277	-0.257380	-0.610348
7	6	0	-5.361903	-1.151379	-0.610382
8	1	0	-5.537402	-1.775545	-1.479629
9	6	0	-6.207581	-1.238311	0.494656
10	6	0	-6.010250	-0.395716	1.591007
11	1	0	-6.670954	-0.456383	2.447799
12	6	0	-4.972855	0.526055	1.587781
13	1	0	-4.803401	1.186217	2.428956
14	6	0	-1.086704	2.428082	-0.110962
15	6	0	0.292094	2.304299	-0.374608
16	6	0	0.964580	3.493577	-0.733062
17	1	0	2.027449	3.455955	-0.928243
18	6	0	0.326493	4.720571	-0.825341
19	1	0	0.892424	5.600845	-1.111330
20	6	0	-1.039535	4.818750	-0.543890
21	1	0	-1.553630	5.770566	-0.610309
22	6	0	-1.736434	3.681450	-0.198170
23	1	0	-2.798323	3.729376	-0.004557
24	16	0	2.746502	1.659553	1.332713
25	6	0	4.408190	1.381647	0.601734
26	1	0	5.165296	1.644878	1.341276
27	1	0	4.565338	2.010005	-0.280682
28	6	0	4.555192	-0.085857	0.196168
29	1	0	5.554118	-0.256986	-0.234725

30	6	0	4.488726	-0.997878	1.410404
31	8	0	5.365588	-0.627357	2.348564
32	8	0	3.810850	-1.998406	1.528889
33	7	0	3.499575	-0.440215	-0.777964
34	1	0	3.745103	-0.021762	-1.672270
35	1	0	3.471342	-1.447564	-0.941399
36	16	0	-0.088589	-0.226009	-2.041435
37	6	0	0.123170	-1.995970	-2.569689
38	1	0	-0.741177	-2.220375	-3.198270
39	1	0	1.023782	-2.089326	-3.176215
40	6	0	0.180780	-2.993314	-1.408641
41	1	0	0.068074	-4.007860	-1.812823
42	7	0	-0.893770	-2.710413	-0.425012
43	1	0	-0.691015	-3.108267	0.492327
44	6	0	1.552403	-2.968333	-0.750369
45	8	0	2.565728	-3.063462	-1.414019
46	8	0	1.502439	-2.837416	0.559593
47	1	0	-7.029195	-1.945304	0.495114
48	1	0	2.398400	-2.625781	0.930153
49	1	0	-1.783384	-3.094970	-0.733750
50	1	0	5.273010	-1.230983	3.101503
51	1	0	-3.654509	-0.159187	-1.476918
52	17	0	-2.061957	-1.378244	2.053351

HF=-2731.5539789\ZeroPoint=0.3631068\Thermal=0.3956673

G = -17.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.788932	-0.705894	-0.070322
2	46	0	1.638865	1.120441	-0.263262
3	7	0	-1.794985	1.151289	-0.598215
4	7	0	-3.050430	1.158654	-0.681972
5	6	0	-3.715869	-0.082205	-0.750019
6	6	0	-3.339840	-1.091188	-1.649005
7	6	0	-4.052873	-2.285632	-1.673749
8	1	0	-3.763517	-3.064764	-2.368994
9	6	0	-5.127621	-2.485124	-0.807032
10	6	0	-5.518247	-1.466335	0.064747
11	1	0	-6.366826	-1.609457	0.723824
12	6	0	-4.832199	-0.255369	0.076514
13	1	0	-5.133430	0.555162	0.730231
14	6	0	-1.157713	2.427978	-0.659155
15	6	0	0.239792	2.542635	-0.489345
16	6	0	0.779480	3.842434	-0.562352
17	1	0	1.841647	3.979769	-0.408175
18	6	0	-0.007012	4.957605	-0.805949
19	1	0	0.453644	5.938549	-0.856102
20	6	0	-1.390530	4.820145	-0.981758
21	1	0	-2.011403	5.687747	-1.172604
22	6	0	-1.958473	3.567732	-0.908122
23	1	0	-3.023466	3.438385	-1.039590
24	16	0	0.673082	-0.308441	-1.857215
25	6	0	2.035670	-1.557267	-1.958176
26	1	0	2.632996	-1.248118	-2.820853
27	1	0	1.600804	-2.533135	-2.170820
28	6	0	2.904934	-1.641476	-0.693385
29	1	0	2.300657	-2.122202	0.081141
30	6	0	4.130575	-2.498825	-0.965918
31	8	0	3.790936	-3.777221	-1.233272
32	8	0	5.268328	-2.098535	-0.962188
33	7	0	3.283564	-0.305499	-0.209073
34	1	0	3.611324	-0.346240	0.753621
35	1	0	4.065052	0.063463	-0.749898
36	16	0	0.021554	-2.752810	0.687508
37	6	0	-0.260693	-2.491231	2.505791
38	1	0	-0.853857	-3.334929	2.866269
39	1	0	0.695098	-2.494936	3.027268
40	6	0	-0.994713	-1.185922	2.807420
41	1	0	-1.522479	-1.272724	3.767333
42	7	0	-1.964537	-0.883181	1.717591
43	1	0	-2.440789	-0.008133	1.929085
44	6	0	-0.144282	0.094892	2.911595
45	8	0	1.160603	-0.110657	3.005905
46	8	0	-0.689280	1.174117	2.900230
47	1	0	-5.671675	-3.422219	-0.824603
48	1	0	-2.659210	-1.618738	1.614948
49	1	0	4.606143	-4.271625	-1.409170
50	1	0	-2.518582	-0.923058	-2.333398
51	1	0	1.639184	0.744654	2.837259
52	17	0	2.659135	2.185052	1.636885

HF=-2731.5732211\ZeroPoint=0.3631944\Thermal=0.3961037

G = -18.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.042904	0.701152	0.157748
2	46	0	-1.563885	0.590958	-1.154898
3	7	0	1.667664	-0.811231	-1.091530
4	7	0	2.855691	-1.123273	-1.331528
5	6	0	3.914965	-0.357351	-0.806046
6	6	0	5.015197	-1.068052	-0.310897
7	6	0	6.105696	-0.376354	0.202509
8	1	0	6.939616	-0.927456	0.620861
9	6	0	6.134450	1.018745	0.166185
10	6	0	5.067829	1.721222	-0.394512
11	1	0	5.107915	2.802278	-0.467320
12	6	0	3.953209	1.043060	-0.876574
13	1	0	3.145696	1.580089	-1.353305
14	6	0	0.662949	-1.613358	-1.752808
15	6	0	-0.654040	-1.120199	-1.915861
16	6	0	-1.508283	-1.960447	-2.661586
17	1	0	-2.517680	-1.630941	-2.880361
18	6	0	-1.128361	-3.208140	-3.138353
19	1	0	-1.840350	-3.814411	-3.688173
20	6	0	0.162887	-3.687659	-2.894784
21	1	0	0.463190	-4.671737	-3.234898
22	6	0	1.060095	-2.883953	-2.219868
23	1	0	2.071520	-3.220623	-2.035750
24	16	0	-2.736229	2.401904	-0.117319
25	6	0	-4.307528	1.522427	0.245064

26	1	0	-4.970258	1.605566	-0.621064
27	1	0	-4.796083	1.995878	1.097526
28	6	0	-4.035721	0.049463	0.551359
29	1	0	-3.470866	-0.045307	1.477176
30	6	0	-5.354460	-0.699528	0.693325
31	8	0	-5.891008	-0.535218	1.916347
32	8	0	-5.890529	-1.308402	-0.199817
33	7	0	-3.230995	-0.563537	-0.532493
34	1	0	-2.927541	-1.484280	-0.192568
35	1	0	-3.849102	-0.739539	-1.324685
36	16	0	0.315953	1.914787	-1.766212
37	6	0	0.144414	3.578129	-0.960823
38	1	0	0.703315	4.287769	-1.568816
39	1	0	-0.906342	3.865142	-0.980538
40	6	0	0.702158	3.588959	0.473352
41	1	0	1.795184	3.613326	0.420043
42	7	0	0.325967	2.360197	1.210117
43	1	0	-0.702736	2.280221	1.233437
44	6	0	0.281870	4.827985	1.261015
45	8	0	0.471999	5.953935	0.543934
46	8	0	-0.130708	4.809263	2.390589
47	1	0	6.994394	1.554165	0.551575
48	1	0	0.648108	2.407314	2.175453
49	1	0	-6.728269	-1.023056	1.940170
50	1	0	4.979331	-2.149145	-0.294328
51	7	0	-0.219422	-3.978919	1.904670
52	6	0	0.775348	-2.919427	1.552883
53	6	0	0.630934	-1.732938	2.517044
54	1	0	0.509957	-2.586347	0.546807
55	6	0	2.150062	-3.618262	1.457834
56	16	0	1.789508	-0.338750	2.165884
57	1	0	0.846321	-2.053058	3.541895
58	1	0	-0.403148	-1.387796	2.478145
59	8	0	3.223634	-2.850313	1.446881
60	8	0	2.209403	-4.823106	1.357023
61	17	0	-2.892397	-2.897365	1.608396
62	1	0	0.203087	6.707331	1.092136
63	1	0	-1.253910	-3.609962	1.759497
64	1	0	-0.120757	-4.262669	2.879973
65	1	0	-0.044562	-4.811065	1.337034
66	1	0	2.975433	-1.888470	1.613544

HF=-3453.6824633\ZeroPoint=0.4627154\Thermal=0.5049534

G = -5.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.355115	0.387599	0.090358
2	46	0	-1.497284	0.181276	-1.281931
3	7	0	1.712834	-1.427010	-0.877642
4	7	0	2.870539	-1.880818	-1.026324
5	6	0	3.970796	-1.083478	-0.641608
6	6	0	4.923499	-1.669488	0.198103
7	6	0	6.032591	-0.931099	0.598793
8	1	0	6.754779	-1.373252	1.274998
9	6	0	6.223468	0.365821	0.119927
10	6	0	5.302214	0.922190	-0.767591
11	1	0	5.468596	1.914315	-1.171753
12	6	0	4.170003	0.208135	-1.148981
13	1	0	3.467824	0.620297	-1.861396
14	6	0	0.639964	-2.259117	-1.337679
15	6	0	-0.652871	-1.717921	-1.515348
16	6	0	-1.591867	-2.619788	-2.066386
17	1	0	-2.588463	-2.267903	-2.309074
18	6	0	-1.305344	-3.947746	-2.348684
19	1	0	-2.077681	-4.590356	-2.758369
20	6	0	-0.028542	-4.458926	-2.091287
21	1	0	0.196747	-5.503975	-2.266024
22	6	0	0.941595	-3.614052	-1.601247
23	1	0	1.934708	-3.981599	-1.387507
24	16	0	-2.855177	2.134184	-1.437234
25	6	0	-4.406510	1.427990	-0.746567
26	1	0	-5.008749	0.984441	-1.547285
27	1	0	-4.984381	2.230182	-0.287704
28	6	0	-4.075589	0.373099	0.308704
29	1	0	-3.523875	0.853587	1.122845
30	6	0	-5.325670	-0.285024	0.863576
31	8	0	-6.085933	0.588437	1.552105
32	8	0	-5.627256	-1.445282	0.704093
33	7	0	-3.187862	-0.660651	-0.283728
34	1	0	-2.855341	-1.278126	0.456744
35	1	0	-3.741243	-1.253961	-0.900132
36	16	0	0.496921	1.270839	-1.898763
37	6	0	0.323422	3.044536	-1.353486
38	1	0	0.596124	3.675510	-2.196985
39	1	0	-0.718084	3.224953	-1.087271
40	6	0	1.234042	3.315566	-0.161411
41	1	0	2.279360	3.250645	-0.486187
42	7	0	1.024051	2.287290	0.881466
43	1	0	0.038711	2.243439	1.231756
44	6	0	1.080370	4.713240	0.439596
45	8	0	0.906111	5.652844	-0.509853
46	8	0	1.162426	4.949136	1.616034
47	1	0	7.097091	0.931911	0.420952
48	1	0	1.581040	2.515624	1.703347
49	1	0	-6.871017	0.114675	1.866158
50	1	0	4.769269	-2.685225	0.543195
51	7	0	-1.778888	-1.803050	2.618440
52	6	0	-0.394469	-1.774839	2.140086
53	6	0	0.600301	-1.089122	3.083663
54	1	0	-0.421796	-1.190397	1.212761
55	6	0	0.059425	-3.178336	1.730383
56	16	0	2.129190	-0.483944	2.236155
57	1	0	0.931147	-1.742882	3.892583
58	1	0	0.136204	-0.186153	3.478972
59	8	0	1.219982	-3.515195	1.672774
60	8	0	-0.935750	-4.006910	1.403579
61	17	0	-1.522389	1.440016	2.409193
62	1	0	-1.767610	-3.518385	1.573042
63	1	0	0.840398	6.514499	-0.069393
64	1	0	-2.092935	-0.828286	2.680941
65	1	0	-1.843510	-2.197842	3.554125
66	1	0	2.561813	-1.705950	1.859539

HF=-3453.6592879\ZeroPoint=0.4609749\Thermal=0.5037983

G = -12.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.945533	0.648138	0.083389
2	46	0	-1.653123	0.063203	-1.280282
3	7	0	1.811833	-0.803722	-1.076411
4	7	0	3.018392	-0.930299	-1.362838
5	6	0	3.947135	0.053441	-0.955341
6	6	0	5.130353	-0.409061	-0.368232
7	6	0	6.087909	0.510386	0.045472
8	1	0	6.986456	0.157222	0.537279
9	6	0	5.900237	1.874890	-0.179553
10	6	0	4.746146	2.322937	-0.822723
11	1	0	4.616313	3.378092	-1.035272
12	6	0	3.759497	1.420072	-1.205867
13	1	0	2.879892	1.756025	-1.736391
14	6	0	0.930281	-1.854980	-1.530130
15	6	0	-0.452266	-1.602998	-1.726930
16	6	0	-1.161708	-2.698667	-2.265250
17	1	0	-2.211177	-2.581252	-2.508808
18	6	0	-0.589807	-3.941712	-2.508008
19	1	0	-1.200362	-4.744375	-2.908205
20	6	0	0.759861	-4.165815	-2.217382
21	1	0	1.206237	-5.142409	-2.362516
22	6	0	1.524917	-3.117406	-1.745158
23	1	0	2.571588	-3.252350	-1.505761
24	16	0	-3.153126	1.817624	-0.671817
25	6	0	-4.580555	0.787375	-0.147782
26	1	0	-5.214229	0.574579	-1.014045
27	1	0	-5.169382	1.341377	0.583968
28	6	0	-4.066344	-0.513088	0.466351
29	1	0	-3.495202	-0.290913	1.369262
30	6	0	-5.222972	-1.434366	0.816742
31	8	0	-5.871111	-1.019524	1.924816
32	8	0	-5.561404	-2.397919	0.172310
33	7	0	-3.147120	-1.200946	-0.469758
34	1	0	-2.646693	-1.903007	0.095591
35	1	0	-3.693680	-1.682319	-1.181640
36	16	0	0.055487	1.573597	-1.893772
37	6	0	-0.382408	3.247092	-1.218444
38	1	0	0.175862	3.977025	-1.802728
39	1	0	-1.443366	3.414148	-1.392862
40	6	0	-0.022307	3.404815	0.271857
41	1	0	1.034731	3.682646	0.339408
42	7	0	-0.179200	2.139976	1.026333
43	1	0	-1.154044	1.809779	0.979829
44	6	0	-0.792127	4.528110	0.965136
45	8	0	-0.923226	5.606337	0.167969
46	8	0	-1.184599	4.474863	2.100587
47	1	0	6.659001	2.584885	0.128748
48	1	0	0.011024	2.289492	2.015302
49	1	0	-6.613156	-1.624566	2.076087
50	1	0	5.252846	-1.469911	-0.194387
51	7	0	0.769307	-2.933430	1.650467
52	6	0	0.239375	-2.033372	2.735293
53	6	0	1.255747	-1.028108	3.252155
54	1	0	-0.009946	-2.688811	3.574631
55	6	0	-1.107461	-1.449899	2.201507
56	16	0	2.174695	0.008685	2.036558
57	1	0	2.046546	-1.521982	3.819623
58	1	0	0.717874	-0.335561	3.896970
59	8	0	-1.340212	-0.248063	2.398706
60	8	0	-1.789147	-2.329138	1.612850
61	1	0	-1.399233	6.290153	0.664285
62	1	0	1.805031	-3.169670	1.744074
63	1	0	0.665812	-2.479738	0.737000
64	1	0	3.001454	-1.049764	1.634952
65	1	0	0.177467	-3.762140	1.594514
66	17	0	3.751922	-2.980481	1.576349

HF=-3453.6704613\ZeroPoint=0.4585294\Thermal=0.5006846

G = -6.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.848447	0.729092	-0.100149
2	46	0	-1.719514	0.107816	-1.236935
3	7	0	1.722783	-0.616852	-1.416704
4	7	0	2.945581	-0.724007	-1.661456
5	6	0	3.864748	0.180058	-1.097224
6	6	0	5.050973	-0.378757	-0.602620
7	6	0	6.014775	0.446594	-0.034285
8	1	0	6.918652	0.011796	0.375957
9	6	0	5.827313	1.830204	-0.008832
10	6	0	4.672640	2.387061	-0.559480
11	1	0	4.546233	3.463620	-0.579470
12	6	0	3.683337	1.570457	-1.099695
13	1	0	2.804944	1.998185	-1.563174
14	6	0	0.861370	-1.570864	-2.065961
15	6	0	-0.537825	-1.381727	-2.048380
16	6	0	-1.289132	-2.373267	-2.713727
17	1	0	-2.368451	-2.270962	-2.767556
18	6	0	-0.710544	-3.483934	-3.314801
19	1	0	-1.337667	-4.222128	-3.803552
20	6	0	0.678732	-3.655602	-3.278630
21	1	0	1.139587	-4.529493	-3.723722
22	6	0	1.462148	-2.698772	-2.664236
23	1	0	2.535882	-2.814254	-2.614783
24	16	0	-3.344407	1.635734	-0.400272
25	6	0	-4.594023	0.346472	-0.004911
26	1	0	-5.062341	0.006078	-0.932772
27	1	0	-5.366049	0.779964	0.631841
28	6	0	-3.928518	-0.827112	0.719309
29	1	0	-3.585546	-0.488281	1.699227
30	6	0	-4.906865	-1.971706	0.908710
31	8	0	-5.902894	-1.640387	1.752082
32	8	0	-4.836752	-3.044094	0.354608
33	7	0	-2.729222	-1.318413	-0.016588
34	1	0	-2.013484	-1.526301	0.686692
35	1	0	-2.958175	-2.189809	-0.494010

36	16	0	-0.170232	1.774531	-1.954035
37	6	0	-0.692084	3.355926	-1.130410
38	1	0	-0.279259	4.177459	-1.713695
39	1	0	-1.777970	3.417183	-1.177455
40	6	0	-0.183127	3.448766	0.316572
41	1	0	0.870394	3.747221	0.290359
42	7	0	-0.243412	2.138187	1.006629
43	1	0	-1.210327	1.777337	1.012905
44	6	0	-0.891584	4.516777	1.150098
45	8	0	-1.169221	5.616425	0.422149
46	8	0	-1.121159	4.407960	2.325001
47	1	0	6.589152	2.472898	0.416799
48	1	0	-0.011632	2.238342	1.994853
49	1	0	-6.501790	-2.399762	1.817135
50	1	0	5.176830	-1.454343	-0.639259
51	7	0	1.531630	-0.202019	1.704801
52	6	0	2.562764	-1.253464	1.812974
53	1	0	1.817621	0.559936	2.316510
54	1	0	0.608055	-0.511020	2.090258
55	6	0	2.829885	-1.663527	3.278394
56	1	0	3.496669	-0.851872	1.416287
57	6	0	2.256193	-2.485630	0.975500
58	16	0	1.522044	-2.645957	4.113561
59	1	0	3.053934	-0.762047	3.855642
60	1	0	3.717271	-2.298300	3.298485
61	8	0	0.950943	-2.636228	0.721464
62	8	0	3.116961	-3.241678	0.597651
63	1	0	0.481205	-1.796574	3.897373
64	17	0	-1.273751	-0.397501	2.850352
65	1	0	0.834479	-3.428303	0.173422
66	1	0	-1.595488	6.262253	1.006910

HF=-3453.661093\ZeroPoint=0.4609569\Thermal=0.5037741

G = -12.5 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.348361	0.068022	0.341160
2	46	0	0.151670	-0.924889	-1.896335
3	7	0	-1.536717	1.850225	-0.704165
4	7	0	-2.462966	2.680431	-0.561016
5	6	0	-3.399229	2.517668	0.480026
6	6	0	-3.052630	2.239509	1.809886
7	6	0	-4.059877	2.136911	2.765829
8	1	0	-3.794564	1.938665	3.798107
9	6	0	-5.398135	2.295442	2.406977
10	6	0	-5.734568	2.594669	1.085252
11	1	0	-6.772145	2.734440	0.805415
12	6	0	-4.737651	2.734441	0.127161
13	1	0	-4.975376	2.986216	-0.899233
14	6	0	-0.619745	2.126097	-1.775166
15	6	0	0.030077	1.062764	-2.436657
16	6	0	0.812179	1.430365	-3.548104
17	1	0	1.310737	0.656060	-4.122689
18	6	0	0.983729	2.752917	-3.943227
19	1	0	1.609810	2.983105	-4.798782
20	6	0	0.369701	3.784887	-3.226990
21	1	0	0.527824	4.820066	-3.504940
22	6	0	-0.439473	3.470398	-2.151923
23	1	0	-0.933099	4.248436	-1.584295
24	16	0	0.662107	-3.172778	-1.144852
25	6	0	2.451524	-2.907111	-0.750954
26	1	0	3.070785	-3.302741	-1.561337
27	1	0	2.698203	-3.445823	0.164026
28	6	0	2.718422	-1.415658	-0.560994
29	1	0	2.128467	-1.067007	0.282416
30	6	0	4.173842	-1.057688	-0.279475
31	8	0	4.474789	-1.215356	1.018454
32	8	0	4.933057	-0.636874	-1.117622
33	7	0	2.247253	-0.686142	-1.762771
34	1	0	2.461320	0.304037	-1.659186
35	1	0	2.758739	-1.009049	-2.582899
36	16	0	-2.217300	-1.006691	-1.542966
37	6	0	-2.618014	-2.653964	-0.783505
38	1	0	-3.635233	-2.906797	-1.076968
39	1	0	-1.939731	-3.398614	-1.196059
40	6	0	-2.514471	-2.593322	0.746182
41	1	0	-3.386337	-2.053706	1.130637
42	7	0	-1.304936	-1.847075	1.152891
43	1	0	-0.470931	-2.295537	0.734151
44	6	0	-2.537698	-3.967194	1.413468
45	8	0	-3.465219	-4.773320	0.858847
46	8	0	-1.847639	-4.277443	2.348542
47	1	0	-6.175375	2.207049	3.157308
48	1	0	-1.164515	-1.873496	2.160171
49	1	0	5.288313	-0.699500	1.244648
50	1	0	-2.013619	2.152605	2.094534
51	7	0	3.141774	0.451393	3.196102
52	6	0	1.956575	1.317194	2.880878
53	1	0	3.208771	0.249213	4.191112
54	6	0	2.318249	2.509354	1.990596
55	1	0	1.567374	1.712039	3.823714
56	6	0	0.863292	0.404805	2.268550
57	16	0	2.905741	2.107249	0.294919
58	1	0	3.078414	3.125160	2.472701
59	1	0	1.414634	3.103213	1.863594
60	8	0	-0.158275	1.033676	1.837994
61	8	0	1.071283	-0.811795	2.243023
62	1	0	4.197084	1.875091	0.650506
63	17	0	5.862402	1.198264	2.319930
64	1	0	3.003659	-0.448578	2.712505
65	1	0	-3.451176	-5.618084	1.335038
66	1	0	4.114746	0.836627	2.883393

HF=-3453.6729466\ZeroPoint=0.4611033\Thermal=0.503311

G = -11.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.029312	0.204691	0.191843
2	46	0	-1.555922	-0.173153	-0.946393
3	7	0	1.390459	-1.802397	-0.189077

4	7	0	2.465608	-2.368763	0.105304
5	6	0	3.566878	-1.586184	0.502774
6	6	0	4.000071	-0.485712	-0.249609
7	6	0	5.134649	0.211232	0.153230
8	1	0	5.484065	1.051423	-0.436260
9	6	0	5.823808	-0.171079	1.303500
10	6	0	5.398102	-1.281491	2.034909
11	1	0	5.934965	-1.582852	2.926624
12	6	0	4.289065	-2.008594	1.621932
13	1	0	3.943905	-2.871715	2.176976
14	6	0	0.367164	-2.646350	-0.762518
15	6	0	-0.850739	-2.083713	-1.196924
16	6	0	-1.763756	-2.969016	-1.802629
17	1	0	-2.706081	-2.580880	-2.177092
18	6	0	-1.504168	-4.325789	-1.953263
19	1	0	-2.237385	-4.968724	-2.428964
20	6	0	-0.295211	-4.857962	-1.492963
21	1	0	-0.083052	-5.915544	-1.597863
22	6	0	0.636899	-4.022222	-0.908464
23	1	0	1.582544	-4.412511	-0.558807
24	16	0	-2.547622	1.967076	-0.429284
25	6	0	-3.848695	1.363071	0.724062
26	1	0	-4.785744	1.219962	0.175601
27	1	0	-4.021011	2.110024	1.498698
28	6	0	-3.437629	0.036779	1.378307
29	1	0	-2.552073	0.199455	1.996782
30	6	0	-4.562555	-0.506188	2.249067
31	8	0	-4.724526	0.232825	3.363134
32	8	0	-5.245279	-1.461907	1.971955
33	7	0	-3.085078	-0.943701	0.325349
34	1	0	-2.761471	-1.813406	0.742918
35	1	0	-3.923170	-1.186437	-0.201911
36	16	0	0.393304	0.625749	-2.059058
37	6	0	0.365088	2.481979	-1.973182
38	1	0	0.891986	2.855569	-2.849678
39	1	0	-0.669734	2.818266	-2.025449
40	6	0	1.054591	2.998187	-0.700223
41	1	0	2.134847	2.863369	-0.811857
42	7	0	0.625555	2.218401	0.479210
43	1	0	-0.399199	2.290947	0.585495
44	6	0	0.820367	4.489254	-0.470972
45	8	0	0.458939	4.973906	0.568183
46	8	0	1.105387	5.205615	-1.579458
47	1	0	6.699158	0.383700	1.620896
48	1	0	0.953290	6.141560	-1.376729
49	1	0	1.053481	2.562559	1.337218
50	1	0	-5.466476	-0.137733	3.865443
51	1	0	3.477135	-0.215454	-1.157989
52	17	0	1.320448	-0.052532	2.520028

HF=-2731.5623657\ZeroPoint=0.3632776\Thermal=0.3965724

G = -2.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.755315	-0.578824	-0.363210
2	46	0	1.866717	0.662764	-0.852557
3	7	0	-1.439278	1.348467	-0.088750
4	7	0	-2.641003	1.692676	-0.027985
5	6	0	-3.664142	0.767260	-0.288044
6	6	0	-3.643967	-0.100737	-1.388836
7	6	0	-4.727629	-0.943432	-1.612100
8	1	0	-4.722260	-1.604858	-2.471062
9	6	0	-5.819433	-0.934647	-0.744557
10	6	0	-5.848587	-0.043416	0.330167
11	1	0	-6.702105	-0.024434	0.997504
12	6	0	-4.789397	0.828351	0.542147
13	1	0	-4.797163	1.531923	1.365399
14	6	0	-0.488657	2.431521	0.058014
15	6	0	0.866435	2.301779	-0.324695
16	6	0	1.664242	3.457931	-0.273395
17	1	0	2.700950	3.397114	-0.573954
18	6	0	1.173017	4.670144	0.190743
19	1	0	1.828256	5.533436	0.227444
20	6	0	-0.148997	4.765862	0.633009
21	1	0	-0.533596	5.698336	1.029056
22	6	0	-0.970623	3.659803	0.556269
23	1	0	-2.002532	3.719319	0.871352
24	16	0	0.244240	0.060785	-2.447568
25	6	0	0.745379	-1.656516	-2.938734
26	1	0	1.594748	-1.592725	-3.621460
27	1	0	-0.104832	-2.051935	-3.498364
28	6	0	1.066216	-2.614916	-1.786822
29	1	0	1.015879	-3.638831	-2.167263
30	6	0	2.494486	-2.515015	-1.241218
31	8	0	3.013197	-1.253897	-1.290123
32	8	0	3.117556	-3.454306	-0.843059
33	7	0	0.088382	-2.484761	-0.654312
34	1	0	-0.664276	-3.161315	-0.753545
35	1	0	0.547096	-2.669447	0.246877
36	16	0	-1.867851	-1.431166	1.534094
37	6	0	-1.004374	-0.853770	3.047583
38	1	0	-0.802790	0.218521	2.982956
39	1	0	-1.716902	-1.009543	3.861001
40	6	0	0.281686	-1.611614	3.438000
41	1	0	0.105891	-2.680984	3.311213
42	7	0	0.577583	-1.350155	4.848903
43	1	0	0.844538	-0.378327	4.976089
44	6	0	1.404850	-1.225877	2.479911
45	8	0	1.952450	-0.061746	2.797294
46	8	0	1.742490	-1.894663	1.515987
47	1	0	-6.654540	-1.603679	-0.916844
48	1	0	1.362161	-1.913908	5.160917
49	1	0	3.837590	-1.210001	-0.767880
50	1	0	-2.810266	-0.079131	-2.077670
51	1	0	2.611078	0.226281	2.113348
52	17	0	3.745179	1.055063	0.599725

HF=-2731.5510574\ZeroPoint=0.3622515\Thermal=0.3952735

G = 2.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	46	0	1.182288	-0.714384	0.335819
2	46	0	-1.077827	1.151948	0.723035
3	7	0	2.102800	1.004172	-0.422700
4	7	0	3.212560	0.944805	-1.000447
5	6	0	3.993305	-0.218375	-0.907407
6	6	0	4.250857	-0.838860	0.323581
7	6	0	5.094209	-1.944466	0.366835
8	1	0	5.312472	-2.414531	1.319218
9	6	0	5.666103	-2.439031	-0.804493
10	6	0	5.424863	-1.800120	-2.022824
11	1	0	5.873975	-2.179566	-2.933027
12	6	0	4.614888	-0.674148	-2.074151
13	1	0	4.414844	-0.165886	-3.008890
14	6	0	1.522430	2.322991	-0.345706
15	6	0	0.202900	2.536838	0.105030
16	6	0	-0.247976	3.866738	0.183097
17	1	0	-1.264387	4.060681	0.502830
18	6	0	0.565614	4.938706	-0.150884
19	1	0	0.181853	5.949968	-0.069963
20	6	0	1.874712	4.713356	-0.590165
21	1	0	2.521239	5.543752	-0.848426
22	6	0	2.346003	3.420503	-0.682608
23	1	0	3.358940	3.228917	-1.007013
24	16	0	0.573398	0.360505	2.341043
25	6	0	-0.237925	-1.097598	3.150784
26	1	0	-1.073610	-0.731989	3.748783
27	1	0	0.498265	-1.540865	3.825253
28	6	0	-0.721814	-2.159779	2.171516
29	1	0	-0.967429	-3.079468	2.717422
30	6	0	-1.994764	-1.775271	1.412939
31	8	0	-2.492496	-0.660770	1.432515
32	8	0	-2.476833	-2.797903	0.747829
33	7	0	0.337931	-2.449194	1.160713
34	1	0	1.103080	-2.969092	1.586068
35	1	0	-0.014963	-3.017391	0.388657
36	16	0	-2.458072	1.814425	-1.061775
37	6	0	-3.081143	0.192025	-1.659263
38	1	0	-2.938473	0.146268	-2.742215
39	1	0	-2.476020	-0.603686	-1.224597
40	6	0	-4.589505	-0.036928	-1.330385
41	1	0	-5.188501	0.554921	-2.024004
42	7	0	-5.038594	0.268445	0.025705
43	1	0	-4.944089	1.272108	0.157281
44	6	0	-4.895380	-1.497471	-1.578675
45	8	0	-5.675921	-1.724980	-2.636716
46	8	0	-4.459091	-2.423553	-0.908415
47	1	0	6.313170	-3.307779	-0.767207
48	1	0	-4.395519	-0.147580	0.693181
49	1	0	3.832420	-0.425711	1.232853
50	1	0	-5.791009	-2.684677	-2.728686
51	1	0	-3.267396	-2.554593	0.171803
52	17	0	1.298134	-1.907954	-1.705459

HF=-2731.5407663\ZeroPoint=0.3624755\Thermal=0.3955295

G = -11.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.693986	-0.194735	0.933359
2	46	0	2.076503	-0.678554	0.226933
3	7	0	-1.054437	-1.569623	-0.617940
4	7	0	-2.202901	-1.770045	-1.085178
5	6	0	-3.328259	-1.241704	-0.435963
6	6	0	-3.510043	-1.330463	0.952207
7	6	0	-4.681538	-0.841551	1.521331
8	1	0	-4.831694	-0.924131	2.591906
9	6	0	-5.664100	-0.259471	0.720905
10	6	0	-5.492524	-0.204034	-0.664159
11	1	0	-6.261224	0.234942	-1.289246
12	6	0	-4.342414	-0.719131	-1.246505
13	1	0	-4.193788	-0.691102	-2.318874
14	6	0	-0.008438	-2.355986	-1.221307
15	6	0	1.350100	-2.108594	-0.936537
16	6	0	2.304503	-2.941354	-1.545286
17	1	0	3.355492	-2.754576	-1.364988
18	6	0	1.936479	-3.979683	-2.387319
19	1	0	2.700730	-4.604874	-2.836346
20	6	0	0.582881	-4.220252	-2.655004
21	1	0	0.286711	-5.035727	-3.304452
22	6	0	-0.378602	-3.417972	-2.076809
23	1	0	-1.428217	-3.597079	-2.262266
24	16	0	0.868624	-1.644349	2.031817
25	6	0	1.316243	-0.489340	3.409061
26	1	0	2.387040	-0.583625	3.589759
27	1	0	0.779091	-0.835460	4.296313
28	6	0	0.976371	0.961168	3.107702
29	1	0	1.073563	1.559332	4.022398
30	6	0	1.850043	1.657048	2.029438
31	8	0	1.484709	2.824904	1.768155
32	8	0	2.782695	1.018230	1.473586
33	7	0	-0.418556	1.075780	2.584221
34	1	0	-1.107296	0.850881	3.299120
35	1	0	-0.564296	2.041625	2.282847
36	16	0	-1.543868	1.637274	-0.325689
37	6	0	-0.426827	1.609222	-1.794819
38	1	0	0.198600	0.716650	-1.788017
39	1	0	-1.049111	1.573407	-2.689944
40	6	0	0.494925	2.827451	-1.940353
41	1	0	0.990531	2.743153	-2.915327
42	7	0	1.581248	2.872266	-0.923916
43	1	0	1.278222	2.865312	0.084956
44	6	0	-0.218970	4.172129	-1.929324
45	8	0	-1.301406	4.160038	-2.723547
46	8	0	0.172352	5.140086	-1.328523
47	1	0	-6.570380	0.128856	1.171048
48	1	0	2.122478	3.732737	-1.017556
49	1	0	-2.761977	-1.820977	1.562509
50	1	0	-1.711108	5.037509	-2.683237
51	17	0	3.134558	0.322577	-1.687941
52	1	0	2.224001	2.054239	-1.068311

HF=-2731.5657244\ZeroPoint=0.3631234\Thermal=0.395571

G = -10.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.051097	-0.527865	-0.600086
2	46	0	1.242117	1.269622	-0.772886
3	7	0	-1.813237	0.980224	0.642499
4	7	0	-2.862713	0.799653	1.305133
5	6	0	-3.692669	-0.294303	1.004909
6	6	0	-4.087199	-0.586094	-0.309246
7	6	0	-4.964808	-1.640698	-0.540135
8	1	0	-5.286631	-1.857077	-1.552563
9	6	0	-5.438944	-2.407511	0.523582
10	6	0	-5.063259	-2.094041	1.831557
11	1	0	-5.437705	-2.683624	2.660022
12	6	0	-4.214984	-1.022766	2.078149
13	1	0	-3.913783	-0.763828	3.085394
14	6	0	-1.170545	2.255390	0.832457
15	6	0	0.105840	2.522727	0.288583
16	6	0	0.618940	3.819835	0.485687
17	1	0	1.598864	4.061627	0.092425
18	6	0	-0.083806	4.797766	1.173339
19	1	0	0.347646	5.785743	1.293893
20	6	0	-1.347475	4.511950	1.704045
21	1	0	-1.907802	5.271994	2.235779
22	6	0	-1.886037	3.254225	1.530584
23	1	0	-2.868083	3.020062	1.916697
24	16	0	-0.598770	1.002342	-2.310285
25	6	0	0.117369	-0.183573	-3.538238
26	1	0	0.926874	0.332637	-4.054877
27	1	0	-0.671003	-0.418484	-4.258215
28	6	0	0.649294	-1.444578	-2.882675
29	1	0	0.860543	-2.199096	-3.649604
30	6	0	1.959643	-1.298605	-2.051197
31	8	0	2.469820	-0.143228	-1.910062
32	8	0	2.368500	-2.363067	-1.569412
33	7	0	-0.364669	-1.991176	-1.925758
34	1	0	-1.170673	-2.378403	-2.412937
35	1	0	0.070123	-2.747282	-1.392783
36	16	0	2.870101	1.505724	0.938136
37	6	0	3.823395	-0.055147	0.867370
38	1	0	4.191593	-0.236183	-0.139623
39	1	0	4.670470	0.077374	1.544440
40	6	0	2.981631	-1.313530	1.278058
41	1	0	2.613621	-1.787850	0.365999
42	7	0	1.821885	-0.943503	2.143094
43	1	0	2.012519	-1.210417	3.113872
44	6	0	3.828195	-2.302076	2.045207
45	8	0	4.802532	-2.811629	1.284784
46	8	0	3.668496	-2.572595	3.215231
47	1	0	-6.114100	-3.234607	0.337179
48	1	0	0.932273	-1.389810	1.834787
49	1	0	-3.746236	0.038369	-1.125443
50	1	0	5.331006	-3.412378	1.832000
51	17	0	-0.944230	-2.148812	1.181120
52	1	0	1.733094	0.105093	2.054313

HF=-2731.5640542\ZeroPoint=0.3631844\Thermal=0.3956817

Structures from Table S9

Table S9. PATH II: B3LYP-D3/6-311+G**/SDD(Pd)/gas phase free energies for the pre- (R) and postreaction (P) complexes and the transition states (TS) for **the second D-transfer**. Free energies relative to **B1-1** (in kcal mol^{-1}). Donor group that is involved in the D-transfer is grey-shaded. Chloride that bonds to the Pd center is marked with "coord".

Mother complex→				**B1-1**			**B1-2**		
Functional/donor groups									
S/SD	ND_2/ND_3	COO/COOD	Cl^-	R	TS	P	R	TS	P
D-source: coordinated **Cys^{4D}**					**I5-1**			**I5-4**	
S-coord	**ND_3**	COOD	anion	-19.0	5.0	-7.8	-5.8	5.2	-41.5
S-coord	ND_3	**COOD**	anion	**-29.4 (-16.6)**	**-2.0 (5.5)**	**-6.6 (-7.2)**	-14.4 (-6.3)	4.9 (11.9)	-14.6 (-10.7)
SD-coord	**ND_3**	COO	anion	-13.5	14.2	-0.6	-12.7	7.8	-22.2
SD-coord	ND_2	**COOD**	anion	-14.9	16.9	-13.4*	-5.4	14.8	-37.3*
SD	**ND_3**	COO-coord	anion	-9.7	11.4	1.1	-3.0	13.2	-23.8
SD	ND_2-coord	**COOD**	anion	-14.2	14.9	2.5	-6.7	11.7	3.5
D-source: non-coordinated **Cys^{4D}**					**I5-2**			**I5-5**	
SD	**ND_3**	COO	coord	-18.4	4.2	-9.3	-6.1	5.8	-34.1
SD	ND_2	**COOD**	coord	-17.5 (-5.1)	3.5 (14.3)	-14.3 (-6.4)	**-12.4 (-0.6)**	**-2.1 (12.4)**	**-38.6 (-15.3)**
D-source: non-coordinated **Cys^{5D+}** formed by an intermolecular D-transfer					**I5-3**			**I5-6**	
SD	**ND_3**	COOD	coord	**-25.2 (-10.2)**	**-3.0 (8.5)**	**-11.8 (-2.6)**	-12.2 (1.0)	2.8 (13.9)	-34.8 (-14.1)
D-source: coordinated **Cys^{4D}**					**I7-2**			**I8-2**	
S-coord	**ND_3**	COOD	coord	-1.9	25.6	12.7	-10.7	16.3	3.2
S-coord	ND_3	**COOD**	coord	6.4	33.1	9.2	-13.0	20.2	13.2

* Postreaction complex optimization leads to the D-transfer from SD to COO^- group ending with three *S*-coordinated cysteines with the ND_2 and COOD groups.

G = -19.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.343479	-0.358432	-0.101040
2	46	0	1.066370	1.136704	-1.131157
3	7	0	-2.322742	1.466012	-0.306250
4	7	0	-3.563869	1.555534	-0.157062
5	6	0	-4.312711	0.367440	-0.009913
6	6	0	-5.199055	0.281979	1.066502
7	6	0	-5.969889	-0.863763	1.229956
8	1	0	-6.628805	-0.948275	2.086100
9	6	0	-5.901577	-1.897255	0.294805
10	6	0	-5.059108	-1.780757	-0.810538
11	1	0	-5.029376	-2.566738	-1.556779
12	6	0	-4.255299	-0.655853	-0.966733
13	1	0	-3.618570	-0.544391	-1.834796
14	6	0	-1.633890	2.692882	-0.598656
15	6	0	-0.276149	2.669099	-0.987858
16	6	0	0.265520	3.919798	-1.368626
17	1	0	1.298627	3.965528	-1.687184
18	6	0	-0.461842	5.099822	-1.331133
19	1	0	0.008627	6.030176	-1.631693
20	6	0	-1.791208	5.093139	-0.891595
21	1	0	-2.361839	6.012997	-0.836876
22	6	0	-2.373868	3.895343	-0.537038
23	1	0	-3.405736	3.858080	-0.217197
24	16	0	2.476216	2.304349	0.359948
25	6	0	3.863030	1.086095	0.443809
26	1	0	3.655245	0.331826	1.201592
27	1	0	4.767570	1.625512	0.719693
28	6	0	4.025521	0.429766	-0.921480
29	1	0	4.257620	1.207525	-1.658600
30	6	0	5.158601	-0.590559	-1.027314
31	8	0	6.219842	-0.272822	-0.258002

32	8	0	5.136507	-1.543877	-1.764850
33	7	0	2.747470	-0.207274	-1.312656
34	1	0	2.860565	-0.629001	-2.231148
35	1	0	2.582174	-0.977780	-0.638183
36	16	0	-0.519470	-0.265637	-2.341505
37	6	0	0.169697	-1.993500	-2.384126
38	1	0	0.052902	-2.372027	-3.397973
39	1	0	1.229397	-1.993399	-2.141989
40	6	0	-0.577863	-2.885068	-1.396754
41	1	0	-1.626066	-2.956341	-1.707979
42	7	0	-0.551078	-2.276026	-0.046051
43	1	0	0.433246	-2.250298	0.304410
44	6	0	-0.079456	-4.330998	-1.310329
45	8	0	0.557304	-4.731593	-2.428119
46	8	0	-0.283338	-5.041012	-0.361071
47	1	0	-6.514454	-2.782403	0.419094
48	1	0	-1.067069	-2.864457	0.606309
49	1	0	6.896921	-0.951462	-0.402985
50	1	0	-5.243694	1.094812	1.780660
51	7	0	0.435925	1.463312	2.601976
52	6	0	0.450849	0.320841	3.566127
53	6	0	-0.309416	-0.898945	3.003048
54	1	0	-0.056115	0.662675	4.472498
55	6	0	1.899517	0.003163	3.916908
56	16	0	-1.912905	-0.451185	2.220836
57	1	0	-0.503965	-1.570366	3.838788
58	1	0	0.343736	-1.424010	2.308748
59	8	0	2.839406	0.674498	3.579812
60	8	0	1.971820	-1.099979	4.672281
61	1	0	1.202805	1.469329	1.859398
62	1	0	0.831997	-5.652838	-2.298103
63	1	0	-0.483594	1.427602	2.123478
64	1	0	0.540473	2.361422	3.071516
65	1	0	2.906802	-1.334960	4.775914
66	17	0	2.363261	-2.182255	1.098318

HF=-3453.6831581\ZeroPoint=0.463263\Thermal=0.5058469

G = 5.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.331733	0.682917	-0.104065
2	46	0	-1.233763	-0.794326	-0.930126
3	7	0	2.405950	-0.922442	-0.849596
4	7	0	3.652180	-1.088430	-0.782695
5	6	0	4.454374	-0.084400	-0.224994
6	6	0	5.550928	-0.524827	0.530690
7	6	0	6.389142	0.402188	1.132835
8	1	0	7.213673	0.063285	1.748585
9	6	0	6.176449	1.769474	0.936879
10	6	0	5.127450	2.206302	0.129181
11	1	0	4.985504	3.265299	-0.051736
12	6	0	4.260366	1.287807	-0.452325
13	1	0	3.472538	1.617060	-1.117963
14	6	0	1.710767	-1.960591	-1.560563
15	6	0	0.381977	-2.265395	-1.176337
16	6	0	-0.195734	-3.391091	-1.804125
17	1	0	-1.183603	-3.712172	-1.498096
18	6	0	0.457453	-4.091959	-2.814960
19	1	0	-0.035861	-4.928784	-3.296641
20	6	0	1.738680	-3.711233	-3.212885
21	1	0	2.244225	-4.238595	-4.013686
22	6	0	2.378116	-2.657971	-2.570046
23	1	0	3.382932	-2.366358	-2.845356
24	16	0	-2.515890	-2.270240	0.354041
25	6	0	-3.927734	-1.138493	0.697413
26	1	0	-3.676976	-0.454659	1.509985
27	1	0	-4.789432	-1.742272	0.980544
28	6	0	-4.212952	-0.352900	-0.572045
29	1	0	-4.467785	-1.056135	-1.372559
30	6	0	-5.362340	0.652574	-0.509579
31	8	0	-6.320990	0.295299	0.365997
32	8	0	-5.429351	1.628123	-1.214139
33	7	0	-2.973341	0.366161	-0.961520
34	1	0	-3.123153	0.845295	-1.846292
35	1	0	-2.809105	1.092683	-0.224562
36	16	0	0.074681	0.946776	-2.128427
37	6	0	-0.691398	2.590142	-1.703171
38	1	0	-0.706806	3.187401	-2.613414
39	1	0	-1.715104	2.465773	-1.362326
40	6	0	0.111857	3.305368	-0.619362
41	1	0	1.085421	3.595036	-1.028872
42	7	0	0.358641	2.393503	0.524799
43	1	0	-0.567049	2.172722	0.960116
44	6	0	-0.513659	4.602988	-0.093782
45	8	0	-1.457832	5.100324	-0.911779
46	8	0	-0.143634	5.137462	0.918735
47	1	0	6.840799	2.491455	1.397260
48	1	0	0.897208	2.871550	1.246024
49	1	0	-7.012450	0.974535	0.336067
50	1	0	5.702809	-1.589386	0.660464
51	7	0	0.791896	-2.570616	1.456118
52	6	0	0.365749	-1.967631	2.743604
53	6	0	0.308296	-0.442380	2.688095
54	1	0	1.111789	-2.242279	3.503799
55	6	0	-0.895415	-2.692719	3.205823
56	16	0	1.936924	0.268489	2.148685
57	1	0	0.095893	-0.064096	3.687910
58	1	0	-0.501354	-0.104155	2.041167
59	8	0	-1.058687	-3.878527	3.048545
60	8	0	-1.727687	-1.903060	3.898484
61	1	0	0.295718	-2.185908	0.194798
62	1	0	-1.822345	5.895888	-0.493742
63	1	0	1.787787	-2.389155	1.341934
64	1	0	0.636778	-3.578214	1.493159
65	1	0	-2.481127	-2.443331	4.181273
66	17	0	-2.559710	2.180367	1.471036

HF=-3453.6424971\ZeroPoint=0.4592814\Thermal=0.5012975

G = -7.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	46	0	1.304589	0.728164	-0.092010
2	46	0	-1.397749	-0.821384	-1.065955
3	7	0	2.413568	-0.739884	-1.044385
4	7	0	3.646601	-0.921830	-1.166419
5	6	0	4.541255	-0.050242	-0.523254
6	6	0	5.718874	-0.640876	-0.043387
7	6	0	6.652921	0.136134	0.627088
8	1	0	7.546252	-0.324018	1.032153
9	6	0	6.446622	1.510621	0.767912
10	6	0	5.307589	2.108261	0.228594
11	1	0	5.164736	3.179173	0.311127
12	6	0	4.350400	1.335459	-0.417111
13	1	0	3.476609	1.794660	-0.862593
14	6	0	1.604239	-1.591749	-1.872059
15	6	0	0.546918	-2.306864	-1.266487
16	6	0	-0.297356	-3.057811	-2.101568
17	1	0	-1.049229	-3.699711	-1.662547
18	6	0	-0.119366	-3.048780	-3.494954
19	1	0	-0.794430	-3.614951	-4.124940
20	6	0	0.929296	-2.336276	-4.053334
21	1	0	1.074055	-2.331731	-5.127450
22	6	0	1.807268	-1.606624	-3.239888
23	1	0	2.616711	-1.029318	-3.667784
24	16	0	-2.496206	-2.426611	0.230114
25	6	0	-3.914824	-1.385065	0.781892
26	1	0	-3.623432	-0.763442	1.629552
27	1	0	-4.730142	-2.045831	1.074552
28	6	0	-4.323975	-0.509147	-0.388294
29	1	0	-4.627194	-1.148165	-1.224397
30	6	0	-5.479796	0.464100	-0.154644
31	8	0	-6.336016	0.040405	0.791204
32	8	0	-5.631601	1.471442	-0.799001
33	7	0	-3.133418	0.278249	-0.811936
34	1	0	-3.365878	0.833292	-1.632988
35	1	0	-2.923943	0.940946	-0.021501
36	16	0	-0.128472	1.081803	-2.026765
37	6	0	-0.933098	2.646686	-1.421694
38	1	0	-1.011158	3.323453	-2.270931
39	1	0	-1.934598	2.451000	-1.050330
40	6	0	-0.108530	3.293770	-0.309867
41	1	0	0.829761	3.668395	-0.732705
42	7	0	0.236015	2.293593	0.730099
43	1	0	-0.657113	1.974736	1.168420
44	6	0	-0.766076	4.505585	0.361560
45	8	0	-1.748052	5.046224	-0.381277
46	8	0	-0.385978	4.951262	1.412195
47	1	0	7.183370	2.117963	1.280730
48	1	0	0.771184	2.732557	1.478816
49	1	0	-7.035954	0.706472	0.874939
50	1	0	5.862036	-1.706342	-0.176406
51	7	0	1.601728	-2.770589	1.718891
52	6	0	1.046789	-2.152721	2.922123
53	6	0	0.716000	-0.668450	2.698717
54	1	0	1.737943	-2.210694	3.781499
55	6	0	-0.165403	-2.968529	3.357817
56	16	0	2.178751	0.282196	2.058280
57	1	0	0.402350	-0.215419	3.638160
58	1	0	-0.116201	-0.577521	1.998934
59	8	0	-0.355274	-4.121234	3.057855
60	8	0	-0.983518	-2.277010	4.178537
61	1	0	0.561256	-2.434664	-0.181823
62	1	0	-2.130364	5.780559	0.123753
63	1	0	2.522429	-2.380493	1.545065
64	1	0	1.678588	-3.774757	1.845382
65	1	0	-1.715365	-2.864129	4.420209
66	17	0	-2.675207	1.939855	1.694037

HF=-3453.6620708\ZeroPoint=0.4620679\Thermal=0.505109

G = -29.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.298311	0.553945	-0.024240
2	46	0	-1.403341	-0.681144	-1.039034
3	7	0	2.120956	-1.150625	-0.853761
4	7	0	3.359297	-1.255628	-1.011921
5	6	0	4.170551	-0.128248	-0.755075
6	6	0	5.259109	-0.288519	0.106147
7	6	0	6.094506	0.793300	0.362344
8	1	0	6.916554	0.680977	1.059348
9	6	0	5.882490	2.014406	-0.279303
10	6	0	4.829559	2.151210	-1.183403
11	1	0	4.683880	3.087152	-1.711058
12	6	0	3.963800	1.087770	-1.421469
13	1	0	3.161711	1.175873	-2.142727
14	6	0	1.337699	-2.290112	-1.247605
15	6	0	-0.063826	-2.189879	-1.414510
16	6	0	-0.682001	-3.334276	-1.969705
17	1	0	-1.746815	-3.315996	-2.157241
18	6	0	0.006384	-4.503027	-2.260526
19	1	0	-0.530765	-5.352207	-2.669440
20	6	0	1.377146	-4.594338	-2.000635
21	1	0	1.918384	-5.515095	-2.183308
22	6	0	2.036963	-3.489005	-1.510468
23	1	0	3.100353	-3.523405	-1.321908
24	16	0	-2.804554	-2.216712	0.135986
25	6	0	-4.223848	-1.087446	0.496364
26	1	0	-4.070979	-0.561154	1.442133
27	1	0	-5.128377	-1.688770	0.570902
28	6	0	-4.359465	-0.062227	-0.624862
29	1	0	-4.558097	-0.596439	-1.560775
30	6	0	-5.510550	0.925400	-0.443975
31	8	0	-6.644089	0.314922	-0.041001
32	8	0	-5.437028	2.105240	-0.677778
33	7	0	-3.082760	0.664836	-0.767019
34	1	0	-3.182875	1.368778	-1.493371
35	1	0	-2.893815	1.159601	0.118878
36	16	0	0.051039	1.010740	-1.999892
37	6	0	-0.584747	2.675938	-1.459892
38	1	0	-0.642830	3.312190	-2.340780
39	1	0	-1.581136	2.590009	-1.033285
40	6	0	0.349066	3.295975	-0.420207
41	1	0	1.325662	3.472695	-0.884385

42	7	0	0.545976	2.351868	0.701907
43	1	0	-0.357468	2.170259	1.179243
44	6	0	-0.109262	4.655362	0.111756
45	8	0	-0.669588	5.413616	-0.852866
46	8	0	0.057866	5.022123	1.244179
47	1	0	6.545703	2.849839	-0.087758
48	1	0	1.162501	2.759220	1.403203
49	1	0	-7.337221	0.990114	0.021284
50	1	0	5.414533	-1.244267	0.590987
51	7	0	-1.442877	-1.334170	2.827166
52	6	0	-0.005547	-1.359627	2.433374
53	6	0	0.806975	-0.216239	3.063529
54	1	0	-0.016890	-1.221066	1.348480
55	6	0	0.561343	-2.746373	2.741107
56	16	0	2.339011	0.106364	2.083857
57	1	0	1.112660	-0.460886	4.084502
58	1	0	0.192351	0.682542	3.096563
59	8	0	-0.099164	-3.596695	3.285843
60	8	0	1.826283	-2.937552	2.373574
61	17	0	-2.209977	1.591056	2.174946
62	1	0	2.231149	-2.080269	2.078369
63	1	0	-0.909522	6.266866	-0.458734
64	1	0	-1.791832	-0.341873	2.802480
65	1	0	-1.980799	-1.845030	2.070985
66	1	0	-1.599412	-1.790176	3.726594

HF=-3453.7023056\ZeroPoint=0.4638943\Thermal=0.505815

G = -2.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.373451	0.625560	-0.229490
2	46	0	-1.437733	-0.961761	-0.591503
3	7	0	2.279495	-1.152883	-0.789807
4	7	0	3.501371	-1.426722	-0.814954
5	6	0	4.446716	-0.440578	-0.494554
6	6	0	5.548083	-0.862154	0.262852
7	6	0	6.527733	0.055024	0.613503
8	1	0	7.358724	-0.256875	1.234762
9	6	0	6.447777	1.374946	0.160825
10	6	0	5.384727	1.775743	-0.646531
11	1	0	5.340129	2.791159	-1.022581
12	6	0	4.376359	0.875818	-0.974064
13	1	0	3.563394	1.168281	-1.626963
14	6	0	1.442769	-2.205778	-1.309360
15	6	0	0.201670	-2.473052	-0.678716
16	6	0	-0.495087	-3.606277	-1.156124
17	1	0	-1.397738	-3.916151	-0.645834
18	6	0	-0.053577	-4.343448	-2.253322
19	1	0	-0.634223	-5.186878	-2.609190
20	6	0	1.137987	-3.997548	-2.883933
21	1	0	1.485715	-4.557685	-3.744545
22	6	0	1.905789	-2.942186	-2.394681
23	1	0	2.854576	-2.689625	-2.849730
24	16	0	-2.705678	-2.180236	1.005849
25	6	0	-4.235071	-1.142577	0.993771
26	1	0	-4.158977	-0.340852	1.732735
27	1	0	-5.085273	-1.775635	1.242227
28	6	0	-4.410102	-0.531082	-0.390012
29	1	0	-4.540142	-1.338540	-1.118356
30	6	0	-5.619131	0.389539	-0.541097
31	8	0	-6.724761	-0.135574	0.021833
32	8	0	-5.600540	1.439066	-1.132135
33	7	0	-3.175634	0.210935	-0.729140
34	1	0	-3.286532	0.664282	-1.632620
35	1	0	-3.026223	0.951789	-0.018395
36	16	0	-0.182685	0.533586	-2.075491
37	6	0	-0.885839	2.241950	-1.836570
38	1	0	-1.070570	2.666573	-2.821338
39	1	0	-1.828581	2.201985	-1.296810
40	6	0	0.084814	3.127388	-1.054175
41	1	0	0.988022	3.281581	-1.654546
42	7	0	0.481749	2.450361	0.200303
43	1	0	-0.367172	2.310486	0.779615
44	6	0	-0.445393	4.528965	-0.738463
45	8	0	-1.274391	4.990208	-1.695676
46	8	0	-0.113715	5.161798	0.228355
47	1	0	7.223175	2.084692	0.424812
48	1	0	1.112365	3.039456	0.742286
49	1	0	-7.459412	0.477791	-0.135147
50	1	0	5.589430	-1.890837	0.598504
51	7	0	-1.288032	-0.340246	3.300284
52	6	0	0.013451	-0.474386	2.554441
53	6	0	0.987621	0.623796	2.966651
54	1	0	-0.260890	-0.350746	1.507443
55	6	0	0.517064	-1.907871	2.849568
56	16	0	2.468018	0.694714	1.868759
57	1	0	1.362178	0.428186	3.974938
58	1	0	0.469704	1.587074	2.967460
59	8	0	0.594570	-2.204618	4.040997
60	8	0	0.769262	-2.655496	1.845695
61	17	0	-2.329601	2.086016	1.680880
62	1	0	0.316617	-2.354504	0.591321
63	1	0	-1.554824	5.883138	-1.440697
64	1	0	-1.703668	0.596895	3.113937
65	1	0	-1.931084	-1.043454	2.881799
66	1	0	-1.139194	-0.548218	4.290310

HF=-3453.6562362\ZeroPoint=0.4602284\Thermal=0.5018406

G = -6.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.374980	0.679109	-0.275273
2	46	0	-1.524074	-1.054529	-0.683115
3	7	0	2.326186	-1.062274	-0.896791
4	7	0	3.523207	-1.402188	-0.968648
5	6	0	4.524426	-0.504752	-0.555944
6	6	0	5.593073	-1.061367	0.157600
7	6	0	6.616918	-0.236394	0.600445
8	1	0	7.423838	-0.651771	1.192054
9	6	0	6.610886	1.123461	0.279515

10	6	0	5.577526	1.659695	-0.487699
11	1	0	5.588323	2.709031	-0.757812
12	6	0	4.526039	0.852333	-0.905319
13	1	0	3.727012	1.253465	-1.516368
14	6	0	1.414299	-1.997810	-1.509100
15	6	0	0.401616	-2.578764	-0.712927
16	6	0	-0.523418	-3.422024	-1.356146
17	1	0	-1.234222	-3.980691	-0.762004
18	6	0	-0.466853	-3.629587	-2.745257
19	1	0	-1.199086	-4.268898	-3.223079
20	6	0	0.544139	-3.043778	-3.487658
21	1	0	0.603279	-3.212107	-4.556733
22	6	0	1.502570	-2.227325	-2.867784
23	1	0	2.290685	-1.757790	-3.442675
24	16	0	-2.664400	-2.345618	0.933435
25	6	0	-4.163100	-1.282777	1.137483
26	1	0	-3.995086	-0.530686	1.911322
27	1	0	-4.999158	-1.916871	1.427494
28	6	0	-4.449238	-0.589521	-0.185851
29	1	0	-4.675312	-1.347929	-0.942670
30	6	0	-5.627678	0.382983	-0.181092
31	8	0	-6.671708	-0.091978	0.521926
32	8	0	-5.635642	1.428766	-0.778862
33	7	0	-3.224811	0.137354	-0.601484
34	1	0	-3.400144	0.635704	-1.470912
35	1	0	-2.994941	0.840587	0.133870
36	16	0	-0.295395	0.569631	-2.068010
37	6	0	-1.038367	2.245506	-1.748204
38	1	0	-1.284004	2.690930	-2.710138
39	1	0	-1.951892	2.163679	-1.164721
40	6	0	-0.058473	3.140614	-0.987407
41	1	0	0.809683	3.340966	-1.624793
42	7	0	0.417628	2.446674	0.228560
43	1	0	-0.399442	2.247777	0.836936
44	6	0	-0.620323	4.514657	-0.610109
45	8	0	-1.501267	4.973828	-1.521152
46	8	0	-0.271519	5.130846	0.360963
47	1	0	7.419999	1.761303	0.615893
48	1	0	1.043522	3.046243	0.765096
49	1	0	-7.392764	0.554063	0.461647
50	1	0	5.573334	-2.117930	0.393561
51	7	0	-1.045574	-0.580622	3.321541
52	6	0	0.255878	-0.641179	2.564139
53	6	0	1.115781	0.576079	2.906324
54	1	0	-0.016532	-0.622764	1.510147
55	6	0	0.902039	-2.009205	2.976087
56	16	0	2.549306	0.792397	1.767714
57	1	0	1.542210	0.456840	3.906550
58	1	0	0.500354	1.480311	2.903958
59	8	0	0.758528	-2.264372	4.191168
60	8	0	1.444071	-2.655512	2.059171
61	17	0	-2.299212	1.894602	1.799363
62	1	0	0.548866	-2.574285	0.375463
63	1	0	-1.799892	5.849747	-1.230261
64	1	0	-1.492938	0.348354	3.249168
65	1	0	-1.680854	-1.263426	2.876068
66	1	0	-0.824686	-0.905632	4.274827

HF=-3453.6651348\ZeroPoint=0.4634755\Thermal=0.5057656

G = -13.5 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.204313	0.557254	-0.149047
2	46	0	-1.635330	-0.829713	-0.874968
3	7	0	1.858412	-1.353105	-0.746855
4	7	0	3.084407	-1.528359	-0.919659
5	6	0	3.975208	-0.443696	-0.773178
6	6	0	5.034881	-0.590095	0.126662
7	6	0	5.949489	0.447168	0.275366
8	1	0	6.750409	0.352362	0.999029
9	6	0	5.842627	1.600334	-0.503517
10	6	0	4.815993	1.714512	-1.440896
11	1	0	4.752242	2.592901	-2.073381
12	6	0	3.874540	0.698323	-1.580241
13	1	0	3.094798	0.760709	-2.329011
14	6	0	1.038284	-2.498559	-1.028859
15	6	0	-0.350031	-2.372349	-1.245553
16	6	0	-0.988702	-3.524268	-1.758274
17	1	0	-2.045680	-3.481287	-1.982627
18	6	0	-0.329018	-4.730198	-1.941954
19	1	0	-0.876074	-5.586733	-2.321487
20	6	0	1.020936	-4.853079	-1.594179
21	1	0	1.529465	-5.806985	-1.667815
22	6	0	1.700420	-3.741398	-1.150227
23	1	0	2.743694	-3.803043	-0.879189
24	16	0	-2.903710	-2.330983	0.451445
25	6	0	-4.312182	-1.225662	0.900531
26	1	0	-4.102694	-0.721837	1.843866
27	1	0	-5.203883	-1.841867	1.007058
28	6	0	-4.525215	-0.187197	-0.199623
29	1	0	-4.796750	-0.710396	-1.123225
30	6	0	-5.656942	0.794246	0.090640
31	8	0	-6.785157	0.162754	0.477236
32	8	0	-5.580145	1.990092	-0.045525
33	7	0	-3.261492	0.543923	-0.429156
34	1	0	-3.430898	1.299195	-1.087528
35	1	0	-2.972063	0.960201	0.470965
36	16	0	-0.201735	0.735382	-2.021557
37	6	0	-0.812240	2.447452	-1.627471
38	1	0	-1.180492	2.897458	-2.547470
39	1	0	-1.622015	2.404709	-0.900901
40	6	0	0.336253	3.259449	-1.041867
41	1	0	1.155859	3.283992	-1.769293
42	7	0	0.825458	2.588763	0.182565
43	1	0	0.141433	2.648385	0.967877
44	6	0	0.002155	4.721472	-0.742002
45	8	0	-0.770519	5.268727	-1.702302
46	8	0	0.420912	5.322222	0.210998
47	1	0	6.566932	2.398752	-0.392573
48	1	0	1.664983	3.053090	0.523351
49	1	0	-7.467234	0.837196	0.617767
50	1	0	5.097438	-1.491617	0.724176
51	7	0	-0.364563	-1.232687	2.289816

52	6	0	-0.239523	0.000029	3.137032
53	6	0	1.212704	0.396413	3.383145
54	1	0	-0.680979	-0.248322	4.106292
55	6	0	-1.135010	1.118654	2.504662
56	16	0	2.390101	0.422487	1.951802
57	1	0	1.687499	-0.297049	4.080018
58	1	0	1.208041	1.399014	3.804423
59	8	0	-0.642178	2.264095	2.422598
60	8	0	-2.260951	0.721296	2.144480
61	1	0	2.565673	-1.046442	2.034046
62	1	0	-0.919028	6.199368	-1.472324
63	1	0	-1.333940	-1.590638	2.240989
64	1	0	-0.165022	-1.000095	1.305876
65	1	0	0.322163	-1.976367	2.543822
66	17	0	2.353494	-2.784366	2.402168

HF=-3453.6741188\ZeroPoint=0.4607782\Thermal=0.5027546

G = 14.2 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.345596	0.600707	-0.071877
2	46	0	-1.718517	-0.890146	-0.752568
3	7	0	2.027477	-1.184292	-0.884382
4	7	0	3.231932	-1.299448	-1.208545
5	6	0	4.050679	-0.151586	-1.130657
6	6	0	5.226587	-0.254323	-0.382518
7	6	0	6.062167	0.851666	-0.273577
8	1	0	6.953243	0.790436	0.339747
9	6	0	5.760629	2.032006	-0.955073
10	6	0	4.615899	2.107720	-1.748399
11	1	0	4.398327	3.012289	-2.304961
12	6	0	3.748293	1.022773	-1.834259
13	1	0	2.870659	1.061006	-2.467008
14	6	0	1.234784	-2.368716	-1.032737
15	6	0	-0.027365	-2.438288	-0.395310
16	6	0	-0.598836	-3.729169	-0.365682
17	1	0	-1.509673	-3.886326	0.195762
18	6	0	-0.045517	-4.824948	-1.016798
19	1	0	-0.544031	-5.786690	-0.972810
20	6	0	1.140535	-4.675956	-1.732801
21	1	0	1.572567	-5.512959	-2.269052
22	6	0	1.792185	-3.453939	-1.721110
23	1	0	2.748148	-3.336218	-2.210865
24	16	0	-3.332219	-2.390945	0.101182
25	6	0	-4.654381	-1.182276	0.499138
26	1	0	-4.442658	-0.700202	1.455544
27	1	0	-5.602646	-1.715500	0.556811
28	6	0	-4.690810	-0.138210	-0.611190
29	1	0	-4.912661	-0.638591	-1.559159
30	6	0	-5.738309	0.953186	-0.420877
31	8	0	-6.960093	0.434766	-0.183283
32	8	0	-5.519311	2.135932	-0.503767
33	7	0	-3.346026	0.468825	-0.697333
34	1	0	-3.339294	1.214403	-1.387245
35	1	0	-3.108696	0.867514	0.227582
36	16	0	-0.301422	0.862194	-1.743690
37	6	0	-0.933772	2.472319	-1.046262
38	1	0	-1.478585	3.002524	-1.824948
39	1	0	-1.591742	2.283151	-0.198173
40	6	0	0.250216	3.298844	-0.552656
41	1	0	0.950857	3.450823	-1.382178
42	7	0	0.941356	2.548902	0.517547
43	1	0	0.328158	2.485241	1.364003
44	6	0	-0.112486	4.699218	-0.054913
45	8	0	-1.087963	5.266454	-0.794385
46	8	0	0.445948	5.250279	0.856028
47	1	0	6.424702	2.885167	-0.879739
48	1	0	1.797435	3.021258	0.798008
49	1	0	-7.583228	1.172052	-0.092646
50	1	0	5.442767	-1.179817	0.136760
51	7	0	-0.406403	-1.551986	2.176461
52	6	0	-0.265302	-0.288929	2.951906
53	6	0	1.180878	0.112948	3.264219
54	1	0	-0.713930	-0.462434	3.942170
55	6	0	-1.178297	0.829273	2.354074
56	16	0	2.493798	0.178289	1.951050
57	1	0	1.597445	-0.590633	3.990781
58	1	0	1.135261	1.096348	3.728736
59	8	0	-0.787671	2.015160	2.464406
60	8	0	-2.260843	0.431729	1.866317
61	1	0	2.658183	-1.681803	1.931593
62	1	0	-1.249500	6.154979	-0.440663
63	1	0	-1.395070	-1.813159	2.174928
64	1	0	-0.203131	-1.733151	0.794785
65	1	0	0.140757	-2.302296	2.598171
66	17	0	2.668392	-3.095652	2.059175

HF=-3453.6251473\ZeroPoint=0.4561745\Thermal=0.4978902

G = -0.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.326682	0.616692	-0.265813
2	46	0	-1.875998	-1.217130	-0.560899
3	7	0	2.146494	-1.248679	-0.712093
4	7	0	3.337568	-1.593128	-0.867726
5	6	0	4.366774	-0.660116	-0.634086
6	6	0	5.469093	-1.119285	0.097262
7	6	0	6.520816	-0.251290	0.355451
8	1	0	7.355599	-0.585942	0.959543
9	6	0	6.506733	1.045727	-0.163954
10	6	0	5.434592	1.477180	-0.943002
11	1	0	5.435882	2.474656	-1.366595
12	6	0	4.355291	0.631852	-1.175913
13	1	0	3.525288	0.947966	-1.795427
14	6	0	1.200257	-2.234767	-1.146010
15	6	0	0.171231	-2.609288	-0.258189
16	6	0	-0.757988	-3.560036	-0.706494
17	1	0	-1.437774	-4.014628	-0.000562
18	6	0	-0.707412	-4.050429	-2.027962
19	1	0	-1.451959	-4.764702	-2.356810

20	6	0	0.300383	-3.639161	-2.879160
21	1	0	0.347382	-4.014764	-3.894479
22	6	0	1.277860	-2.738106	-2.430786
23	1	0	2.078415	-2.413347	-3.083061
24	16	0	-3.337254	-2.593511	0.659464
25	6	0	-4.565857	-1.326089	1.171272
26	1	0	-4.216377	-0.806716	2.064080
27	1	0	-5.509590	-1.828644	1.379210
28	6	0	-4.716893	-0.345377	0.018386
29	1	0	-5.088780	-0.885744	-0.858990
30	6	0	-5.682319	0.813273	0.253736
31	8	0	-6.807522	0.415767	0.879000
32	8	0	-5.487588	1.942448	-0.120192
33	7	0	-3.374137	0.200488	-0.290497
34	1	0	-3.445919	0.893815	-1.029309
35	1	0	-3.005296	0.655415	0.586749
36	16	0	-0.474024	0.350171	-1.855188
37	6	0	-1.145249	2.063120	-1.586173
38	1	0	-1.731588	2.350749	-2.456521
39	1	0	-1.766238	2.095640	-0.691447
40	6	0	0.017815	3.027636	-1.369334
41	1	0	0.688015	2.984784	-2.236082
42	7	0	0.763230	2.608459	-0.164816
43	1	0	0.141107	2.693867	0.680929
44	6	0	-0.394048	4.495299	-1.235772
45	8	0	-1.411457	4.817482	-2.060629
46	8	0	0.162307	5.282752	-0.517202
47	1	0	7.337604	1.714341	0.029131
48	1	0	1.574331	3.202988	-0.013139
49	1	0	-7.385862	1.189118	0.967911
50	1	0	5.451979	-2.124888	0.496567
51	7	0	-0.049854	-0.805896	2.596551
52	6	0	-0.093992	0.598828	3.014186
53	6	0	1.281946	1.290257	3.010890
54	1	0	-0.441962	0.702782	4.058237
55	6	0	-1.212285	1.317118	2.208624
56	16	0	2.561525	0.904229	1.715897
57	1	0	1.812170	1.028691	3.931269
58	1	0	1.120888	2.367835	3.016665
59	8	0	-1.017937	2.474051	1.757695
60	8	0	-2.280987	0.663571	2.093951
61	1	0	2.851216	-0.967310	2.170336
62	1	0	-1.603457	5.760483	-1.939853
63	1	0	-0.998189	-1.171879	2.623888
64	1	0	0.218824	-2.269997	0.773167
65	1	0	0.530138	-1.357997	3.221504
66	17	0	3.064742	-2.297999	2.520021

HF=-3453.6497995\ZeroPoint=0.4589639\Thermal=0.5014496

G = -14.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.220120	0.581136	-0.082203
2	46	0	-1.370690	-0.826825	-1.111962
3	7	0	2.089733	-1.235090	-0.666030
4	7	0	3.339026	-1.353323	-0.638892
5	6	0	4.136683	-0.222559	-0.371629
6	6	0	5.124786	-0.343108	0.611191
7	6	0	5.947255	0.742214	0.895245
8	1	0	6.689233	0.660400	1.680680
9	6	0	5.827666	1.925486	0.165091
10	6	0	4.885105	2.018389	-0.859223
11	1	0	4.818126	2.921676	-1.455007
12	6	0	4.032700	0.952703	-1.131423
13	1	0	3.323756	1.003589	-1.947696
14	6	0	1.363993	-2.392484	-1.102182
15	6	0	-0.013824	-2.316123	-1.406650
16	6	0	-0.570751	-3.473582	-1.995330
17	1	0	-1.615601	-3.466764	-2.277505
18	6	0	0.152482	-4.638938	-2.194126
19	1	0	-0.333602	-5.503526	-2.633465
20	6	0	1.494809	-4.708998	-1.801887
21	1	0	2.057894	-5.627968	-1.912947
22	6	0	2.096599	-3.590542	-1.272739
23	1	0	3.136090	-3.614381	-0.980058
24	16	0	-2.698715	-2.356862	0.101789
25	6	0	-3.910260	-1.141966	0.778191
26	1	0	-3.485804	-0.601057	1.624130
27	1	0	-4.793783	-1.687168	1.107223
28	6	0	-4.266747	-0.154197	-0.325440
29	1	0	-4.676742	-0.714619	-1.173655
30	6	0	-5.323633	0.890081	0.034496
31	8	0	-6.235717	0.428330	0.912442
32	8	0	-5.370592	1.989402	-0.457915
33	7	0	-3.032967	0.528188	-0.777142
34	1	0	-3.267226	1.139490	-1.555161
35	1	0	-2.721052	1.131237	0.006187
36	16	0	0.113088	0.784003	-2.140086
37	6	0	-0.592639	2.483198	-1.864630
38	1	0	-0.659052	2.973927	-2.833847
39	1	0	-1.590003	2.419717	-1.438410
40	6	0	0.311144	3.268407	-0.924036
41	1	0	1.289951	3.400820	-1.398839
42	7	0	0.512382	2.497566	0.326015
43	1	0	-0.399642	2.377192	0.837094
44	6	0	-0.169768	4.680372	-0.576439
45	8	0	-0.938254	5.217775	-1.541572
46	8	0	0.153014	5.253247	0.430503
47	1	0	6.480434	2.763388	0.379541
48	1	0	1.113892	3.031734	0.951653
49	1	0	-6.878052	1.137820	1.068565
50	1	0	5.215465	-1.274639	1.157372
51	7	0	-1.421061	-1.173235	3.521452
52	6	0	-0.282941	-1.031609	2.607312
53	6	0	0.643593	0.017190	3.218042
54	1	0	-0.593530	-0.685131	1.609583
55	6	0	0.421318	-2.380945	2.411797
56	16	0	2.101131	0.463963	2.175960
57	1	0	1.042529	-0.322171	4.173322
58	1	0	0.088406	0.945717	3.350952
59	8	0	1.578563	-2.576628	2.720500
60	8	0	-0.310136	-3.346771	1.865200
61	1	0	2.645700	-0.772360	2.198043

62	17	0	-2.067553	1.913020	1.890292
63	1	0	-1.145506	-3.002081	1.449505
64	1	0	-1.190884	6.111633	-1.260961
65	1	0	-1.990653	-0.332495	3.444634
66	1	0	-2.004052	-1.960812	3.258205

HF=-3453.6757545\ZeroPoint=0.4607747\Thermal=0.503268

G = 16.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.368017	0.526124	-0.115880
2	46	0	-1.333435	-1.028654	-0.729035
3	7	0	2.330903	-1.220607	-0.713218
4	7	0	3.575929	-1.373395	-0.736453
5	6	0	4.400286	-0.268399	-0.451526
6	6	0	5.479029	-0.492925	0.411799
7	6	0	6.322203	0.561303	0.740692
8	1	0	7.135179	0.400861	1.438567
9	6	0	6.130721	1.819147	0.165110
10	6	0	5.094421	2.021677	-0.746363
11	1	0	4.970478	2.987559	-1.222187
12	6	0	4.219887	0.985192	-1.055784
13	1	0	3.437740	1.120228	-1.791966
14	6	0	1.572779	-2.350140	-1.165002
15	6	0	0.284190	-2.562756	-0.616376
16	6	0	-0.336609	-3.776315	-0.981089
17	1	0	-1.282069	-4.040511	-0.526666
18	6	0	0.226094	-4.649762	-1.908847
19	1	0	-0.301540	-5.555705	-2.184759
20	6	0	1.462695	-4.358516	-2.482223
21	1	0	1.897206	-5.024021	-3.219202
22	6	0	2.153730	-3.217714	-2.091861
23	1	0	3.130875	-2.994006	-2.498686
24	16	0	-2.719968	-2.264286	0.682701
25	6	0	-4.108445	-1.064962	0.803163
26	1	0	-3.876648	-0.284117	1.529648
27	1	0	-4.996843	-1.605581	1.127751
28	6	0	-4.315434	-0.452225	-0.571959
29	1	0	-4.554161	-1.252867	-1.280492
30	6	0	-5.434531	0.579688	-0.698157
31	8	0	-6.488304	0.294234	0.088917
32	8	0	-5.399576	1.513541	-1.459804
33	7	0	-3.035248	0.173198	-0.989171
34	1	0	-3.132093	0.549806	-1.929122
35	1	0	-2.860121	0.972931	-0.342632
36	16	0	0.085637	0.514064	-2.085921
37	6	0	-0.639855	2.221852	-1.931714
38	1	0	-0.670004	2.656227	-2.929384
39	1	0	-1.651072	2.179128	-1.538543
40	6	0	0.217231	3.078092	-1.006354
41	1	0	1.186076	3.265259	-1.481198
42	7	0	0.468190	2.351125	0.266594
43	1	0	-0.466029	2.213854	0.728964
44	6	0	-0.354696	4.461128	-0.674166
45	8	0	-1.251017	4.885897	-1.577966
46	8	0	0.021719	5.104444	0.270718
47	1	0	6.800901	2.634258	0.411645
48	1	0	1.005029	2.958010	0.885109
49	1	0	-7.163170	0.974260	-0.061479
50	1	0	5.616767	-1.479379	0.837518
51	7	0	-1.524364	0.033336	3.751418
52	6	0	-0.485291	-0.330535	2.809824
53	6	0	0.733764	0.558036	3.165618
54	1	0	-0.774541	-0.122011	1.773296
55	6	0	-0.116014	-1.826204	2.884830
56	16	0	2.257021	0.343645	2.116883
57	1	0	1.044870	0.364899	4.193056
58	1	0	0.448574	1.607311	3.084594
59	8	0	-0.501647	-2.520251	3.803658
60	8	0	0.694021	-2.228555	1.921270
61	1	0	2.102223	-1.023955	2.070256
62	17	0	-2.439132	2.291817	1.208076
63	1	0	0.263095	-2.212311	0.645584
64	1	0	-1.580662	5.751936	-1.290689
65	1	0	-2.197520	0.661356	3.326765
66	1	0	-1.967480	-0.796763	4.128188

HF=-3453.6205235\ZeroPoint=0.455663\Thermal=0.4978756

G = -13.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.344157	0.589322	-0.232634
2	46	0	-1.478008	-1.239456	-0.765169
3	7	0	2.387575	-1.156631	-0.683852
4	7	0	3.610278	-1.419859	-0.727369
5	6	0	4.547365	-0.429079	-0.389610
6	6	0	5.673507	-0.869048	0.320119
7	6	0	6.642771	0.048449	0.698716
8	1	0	7.494176	-0.278189	1.283515
9	6	0	6.526652	1.387468	0.316328
10	6	0	5.439706	1.808199	-0.448984
11	1	0	5.367112	2.840730	-0.769125
12	6	0	4.442668	0.907244	-0.802175
13	1	0	3.606353	1.218136	-1.415623
14	6	0	1.549891	-2.186310	-1.236736
15	6	0	0.485448	-2.695693	-0.459930
16	6	0	-0.379936	-3.625794	-1.060175
17	1	0	-1.119586	-4.135400	-0.458191
18	6	0	-0.215067	-3.990824	-2.409037
19	1	0	-0.904761	-4.694022	-2.858929
20	6	0	0.839643	-3.474084	-3.139594
21	1	0	0.977775	-3.759473	-4.175810
22	6	0	1.737131	-2.570994	-2.550779
23	1	0	2.553235	-2.145098	-3.120062
24	16	0	-2.686018	-2.456185	0.815997
25	6	0	-3.991717	-1.201476	1.154904
26	1	0	-3.618893	-0.436666	1.837141
27	1	0	-4.841307	-1.709309	1.609875
28	6	0	-4.376254	-0.577981	-0.173541
29	1	0	-4.755654	-1.361170	-0.838046

30	6	0	-5.444020	0.516148	-0.147622
31	8	0	-6.300582	0.382239	0.878297
32	8	0	-5.531942	1.367530	-0.996390
33	7	0	-3.143790	-0.007505	-0.785652
34	1	0	-3.358438	0.347191	-1.715119
35	1	0	-2.866731	0.807550	-0.186884
36	16	0	-0.124794	0.320373	-2.146801
37	6	0	-0.905351	2.006073	-2.060211
38	1	0	-1.035886	2.363023	-3.080137
39	1	0	-1.880937	1.962237	-1.585154
40	6	0	-0.019734	2.971310	-1.274556
41	1	0	0.902790	3.150807	-1.837008
42	7	0	0.353657	2.377715	0.032903
43	1	0	-0.526817	2.238626	0.579683
44	6	0	-0.630875	4.356442	-1.032421
45	8	0	-1.582422	4.668729	-1.929684
46	8	0	-0.248498	5.094328	-0.163156
47	1	0	7.293299	2.098571	0.601101
48	1	0	0.922266	3.039047	0.560344
49	1	0	-6.947132	1.103118	0.822327
50	1	0	5.745944	-1.914087	0.595084
51	7	0	-1.221231	0.187446	3.794453
52	6	0	-0.122100	-0.157460	2.911752
53	6	0	0.933679	0.968065	3.005448
54	1	0	-0.435655	-0.228372	1.853627
55	6	0	0.380338	-1.569889	3.244739
56	16	0	2.395174	0.866571	1.868270
57	1	0	1.347761	0.996700	4.016239
58	1	0	0.411776	1.911989	2.843764
59	8	0	-0.252754	-2.352782	3.902816
60	8	0	1.546345	-1.945051	2.671490
61	1	0	2.022659	-1.154398	2.313199
62	17	0	-2.479804	2.201634	1.235457
63	1	0	0.483383	-2.532294	0.611366
64	1	0	-1.926075	5.547840	-1.705790
65	1	0	-1.844472	0.843962	3.333328
66	1	0	-1.731258	-0.647503	4.061796

HF=-3453.6730401\ZeroPoint=0.4621728\Thermal=0.5047415

G = -9.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.326625	-0.414780	0.105204
2	46	0	1.139662	1.161875	-1.089658
3	7	0	-2.316786	1.310902	-0.420626
4	7	0	-3.498441	1.347256	-0.833032
5	6	0	-4.284218	0.176658	-0.806534
6	6	0	-4.388218	-0.664956	0.311316
7	6	0	-5.222981	-1.776966	0.240836
8	1	0	-5.320481	-2.420535	1.107502
9	6	0	-5.935030	-2.058307	-0.925144
10	6	0	-5.844979	-1.200942	-2.023856
11	1	0	-6.410457	-1.408047	-2.924806
12	6	0	-5.045210	-0.066557	-1.957268
13	1	0	-4.976128	0.622943	-2.789850
14	6	0	-1.636232	2.575202	-0.434011
15	6	0	-0.261661	2.649161	-0.766111
16	6	0	0.224102	3.969973	-0.914723
17	1	0	1.252123	4.119259	-1.217387
18	6	0	-0.549117	5.101525	-0.676038
19	1	0	-0.105103	6.084182	-0.794993
20	6	0	-1.877242	4.976484	-0.263337
21	1	0	-2.475595	5.850261	-0.034248
22	6	0	-2.422943	3.711246	-0.160874
23	1	0	-3.455206	3.573024	0.133050
24	16	0	2.737179	2.424382	0.141664
25	6	0	4.099718	1.180662	0.157638
26	1	0	3.932171	0.434211	0.934906
27	1	0	5.034576	1.704276	0.351305
28	6	0	4.136157	0.501476	-1.206041
29	1	0	4.302791	1.266305	-1.973314
30	6	0	5.246714	-0.531995	-1.394282
31	8	0	6.383875	-0.189755	-0.756856
32	8	0	5.137675	-1.514589	-2.082938
33	7	0	2.822929	-0.132205	-1.456841
34	1	0	2.831977	-0.565613	-2.376898
35	1	0	2.724350	-0.890586	-0.756867
36	16	0	-0.457279	-0.465165	-2.042813
37	6	0	0.313660	-2.162037	-1.938278
38	1	0	0.217294	-2.623713	-2.919065
39	1	0	1.367513	-2.095943	-1.686044
40	6	0	-0.400566	-3.000705	-0.879638
41	1	0	-1.433585	-3.177201	-1.197712
42	7	0	-0.439523	-2.255107	0.402975
43	1	0	0.543259	-2.139732	0.735592
44	6	0	0.204899	-4.386882	-0.638795
45	8	0	0.864406	-4.857862	-1.713398
46	8	0	0.053136	-4.998557	0.385045
47	1	0	-6.575939	-2.931328	-0.971284
48	1	0	-0.925436	-2.796067	1.117456
49	1	0	7.042768	-0.876822	-0.941678
50	1	0	-3.864727	-0.426765	1.228759
51	7	0	0.539970	2.055463	2.342298
52	6	0	0.314194	0.590659	2.656978
53	1	0	1.489566	2.215241	1.908379
54	1	0	0.382196	2.620673	3.178868
55	6	0	1.172788	0.191088	3.849700
56	1	0	0.631211	0.049788	1.767174
57	6	0	-1.207252	0.461670	2.943567
58	16	0	0.953927	-1.578453	4.282089
59	1	0	0.863169	0.756795	4.730970
60	1	0	2.227367	0.384316	3.642067
61	8	0	-1.911885	-0.235664	2.119443
62	8	0	-1.631001	1.076246	3.913773
63	1	0	1.663939	-2.046091	3.223053
64	17	0	2.591024	-2.018715	1.021931
65	1	0	-0.113550	2.368718	1.614612
66	1	0	1.215400	-5.733448	-1.487141

HF=-3453.6674434\ZeroPoint=0.4618021\Thermal=0.5042702

G = 11.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.390067	-0.348230	0.090794
2	46	0	1.300458	1.206052	-0.727922
3	7	0	-2.353302	1.440569	-0.373063
4	7	0	-3.489734	1.478192	-0.899838
5	6	0	-4.298109	0.330077	-0.939020
6	6	0	-4.476612	-0.542906	0.146774
7	6	0	-5.337624	-1.625688	0.002582
8	1	0	-5.492508	-2.291886	0.843257
9	6	0	-6.003203	-1.851102	-1.203441
10	6	0	-5.840392	-0.964345	-2.269828
11	1	0	-6.370184	-1.127375	-3.200943
12	6	0	-5.014890	0.144166	-2.130111
13	1	0	-4.889889	0.857238	-2.935914
14	6	0	-1.647671	2.697770	-0.356285
15	6	0	-0.288653	2.733641	0.048697
16	6	0	0.312620	4.013662	0.053842
17	1	0	1.335178	4.111351	0.394804
18	6	0	-0.355271	5.165399	-0.341738
19	1	0	0.157209	6.120632	-0.331163
20	6	0	-1.691547	5.084617	-0.731648
21	1	0	-2.233763	5.975771	-1.026470
22	6	0	-2.340003	3.858966	-0.723228
23	1	0	-3.382594	3.787605	-0.998297
24	16	0	2.999711	2.276236	0.499793
25	6	0	4.335123	1.037204	0.235501
26	1	0	4.208811	0.188976	0.909961
27	1	0	5.292320	1.520134	0.427261
28	6	0	4.243543	0.572171	-1.210606
29	1	0	4.380040	1.436894	-1.868983
30	6	0	5.272772	-0.469174	-1.645889
31	8	0	6.482773	-0.249668	-1.098568
32	8	0	5.040597	-1.352906	-2.431387
33	7	0	2.882441	0.024173	-1.431692
34	1	0	2.781866	-0.270574	-2.400012
35	1	0	2.787000	-0.818276	-0.822513
36	16	0	-0.345844	-0.203833	-1.980149
37	6	0	0.319674	-1.945803	-2.043442
38	1	0	0.204809	-2.300161	-3.065965
39	1	0	1.373679	-1.965092	-1.781990
40	6	0	-0.450428	-2.847568	-1.077682
41	1	0	-1.475371	-2.972630	-1.442206
42	7	0	-0.517346	-2.208337	0.259120
43	1	0	0.460676	-2.128765	0.612389
44	6	0	0.118712	-4.262251	-0.933717
45	8	0	0.783291	-4.663974	-2.033126
46	8	0	-0.066218	-4.947765	0.036050
47	1	0	-6.664952	-2.703622	-1.305317
48	1	0	-1.020469	-2.799434	0.920599
49	1	0	7.087988	-0.929380	-1.433702
50	1	0	-3.984351	-0.355599	1.093164
51	7	0	0.384940	1.693049	2.500777
52	6	0	0.146509	0.253359	2.762482
53	1	0	1.385843	1.902141	2.484212
54	1	0	-0.075138	2.262428	3.209756
55	6	0	0.946570	-0.269710	3.954847
56	1	0	0.476589	-0.275347	1.869028
57	6	0	-1.381229	0.109388	2.992261
58	16	0	0.780177	-2.091752	4.148462
59	1	0	0.569904	0.174469	4.877125
60	1	0	2.003133	-0.021229	3.836019
61	8	0	-2.095752	-0.407473	2.035916
62	8	0	-1.842359	0.527771	4.042367
63	1	0	1.557162	-2.403644	3.083673
64	17	0	2.550253	-2.129064	0.768085
65	1	0	0.049043	2.057648	1.143182
66	1	0	1.113975	-5.561051	-1.869465

HF=-3453.6301553\ZeroPoint=0.4574173\Thermal=0.4995795

G = 1.1 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.376302	-0.335013	-0.128136
2	46	0	1.376859	1.487956	-0.148299
3	7	0	-2.501118	1.433492	0.003216
4	7	0	-3.683460	1.707526	-0.304359
5	6	0	-4.661651	0.724673	-0.502652
6	6	0	-4.724277	-0.518668	0.149740
7	6	0	-5.785040	-1.370001	-0.134444
8	1	0	-5.847436	-2.321649	0.380225
9	6	0	-6.767683	-1.006763	-1.058231
10	6	0	-6.715632	0.239711	-1.685222
11	1	0	-7.488002	0.531781	-2.386730
12	6	0	-5.682329	1.117057	-1.387061
13	1	0	-5.632933	2.100850	-1.837832
14	6	0	-1.646351	2.586360	0.087625
15	6	0	-0.584443	2.561831	1.020793
16	6	0	0.279962	3.667847	1.056496
17	1	0	1.023587	3.734387	1.838328
18	6	0	0.131830	4.731950	0.153629
19	1	0	0.824935	5.563462	0.186596
20	6	0	-0.907519	4.714492	-0.763189
21	1	0	-1.026549	5.529166	-1.468070
22	6	0	-1.807364	3.644019	-0.795296
23	1	0	-2.613339	3.615196	-1.515646
24	16	0	2.855580	1.918867	1.612149
25	6	0	4.258562	0.870089	1.038251
26	1	0	4.090716	-0.173537	1.306436
27	1	0	5.170011	1.230032	1.513844
28	6	0	4.342599	1.014537	-0.470902
29	1	0	4.529394	2.064424	-0.719953
30	6	0	5.427335	0.204147	-1.180591
31	8	0	6.520632	0.028092	-0.419644
32	8	0	5.325760	-0.179316	-2.318524
33	7	0	3.024486	0.625680	-1.042422
34	1	0	3.035973	0.754796	-2.052049
35	1	0	2.905488	-0.399196	-0.845637
36	16	0	-0.158167	0.613890	-1.910032
37	6	0	0.568787	-0.966700	-2.583867
38	1	0	0.457444	-0.937660	-3.666076
39	1	0	1.626665	-1.033027	-2.347595

40	6	0	-0.153949	-2.186530	-2.007937
41	1	0	-1.158811	-2.245737	-2.438029
42	7	0	-0.299880	-2.038205	-0.539390
43	1	0	0.659093	-2.011053	-0.140644
44	6	0	0.510477	-3.532673	-2.317507
45	8	0	1.269938	-3.486873	-3.427138
46	8	0	0.307801	-4.523953	-1.669932
47	1	0	-7.585719	-1.685303	-1.272102
48	1	0	-0.748378	-2.856481	-0.122768
49	1	0	7.165215	-0.479592	-0.937006
50	1	0	-3.985791	-0.796561	0.892819
51	7	0	0.056363	0.418498	3.425565
52	6	0	-0.071707	-0.889607	2.765959
53	1	0	1.036331	0.681180	3.499079
54	1	0	-0.343345	0.370046	4.358919
55	6	0	0.677972	-2.025192	3.474366
56	1	0	0.338914	-0.776668	1.761209
57	6	0	-1.581815	-1.209512	2.707087
58	16	0	0.551801	-3.649875	2.605316
59	1	0	0.245072	-2.177552	4.464179
60	1	0	1.732733	-1.766361	3.581974
61	8	0	-2.187419	-1.197594	1.544118
62	8	0	-2.171208	-1.451349	3.746362
63	1	0	1.524698	-3.405832	1.696762
64	17	0	2.799215	-2.264141	-0.120314
65	1	0	-0.549667	1.814899	1.819497
66	1	0	1.668637	-4.362463	-3.549760

HF=-3453.6482789\ZeroPoint=0.4605067\Thermal=0.5034431

G = -14.2 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.113964	-0.092211	-0.321724
2	46	0	1.449906	1.432405	-0.628662
3	7	0	-1.949149	1.858299	-0.212090
4	7	0	-3.177755	2.003912	0.025210
5	6	0	-4.020317	0.875196	0.017580
6	6	0	-4.932545	0.746435	1.072336
7	6	0	-5.779094	-0.356767	1.123215
8	1	0	-6.462208	-0.471222	1.956637
9	6	0	-5.759609	-1.304627	0.098097
10	6	0	-4.900875	-1.135575	-0.988611
11	1	0	-4.913620	-1.847929	-1.805499
12	6	0	-4.027983	-0.052462	-1.036260
13	1	0	-3.384503	0.103577	-1.892324
14	6	0	-1.206381	3.064041	-0.393362
15	6	0	0.192576	3.016398	-0.576459
16	6	0	0.831760	4.256756	-0.793716
17	1	0	1.906795	4.275510	-0.920857
18	6	0	0.138139	5.455924	-0.833417
19	1	0	0.674880	6.382511	-1.007652
20	6	0	-1.251476	5.473460	-0.646962
21	1	0	-1.800816	6.407057	-0.678385
22	6	0	-1.917327	4.287862	-0.431356
23	1	0	-2.989816	4.277225	-0.298463
24	16	0	2.488638	2.289190	1.301406
25	6	0	3.602529	0.840349	1.599102
26	1	0	3.056237	0.035442	2.090362
27	1	0	4.402392	1.165602	2.263898
28	6	0	4.168806	0.378713	0.266287
29	1	0	4.685153	1.220322	-0.207153
30	6	0	5.195198	-0.756391	0.312061
31	8	0	5.623152	-1.049257	1.553392
32	8	0	5.601157	-1.304489	-0.682253
33	7	0	3.054027	-0.021280	-0.634676
34	1	0	3.441509	-0.196009	-1.559882
35	1	0	2.700824	-0.940768	-0.310499
36	16	0	0.006611	0.407681	-2.305566
37	6	0	0.612963	-1.308877	-2.695781
38	1	0	0.690835	-1.392405	-3.778412
39	1	0	1.590894	-1.481344	-2.253046
40	6	0	-0.381316	-2.317079	-2.138695
41	1	0	-1.346291	-2.192662	-2.641791
42	7	0	-0.573969	-2.049345	-0.691276
43	1	0	0.341997	-2.283658	-0.232926
44	6	0	-0.010567	-3.794484	-2.307234
45	8	0	0.854370	-4.006451	-3.310627
46	8	0	-0.506602	-4.665041	-1.638349
47	1	0	-6.426951	-2.157398	0.134622
48	1	0	-1.258337	-2.702570	-0.308799
49	1	0	6.243032	-1.791532	1.480830
50	1	0	-4.947147	1.501565	1.849940
51	7	0	-1.910680	-0.575043	1.655323
52	6	0	-1.029972	-1.006658	2.780092
53	6	0	-0.427822	-2.404527	2.603035
54	1	0	-1.631953	-0.994569	3.699093
55	6	0	0.120164	-0.011469	2.994223
56	16	0	-1.698861	-3.672674	2.157091
57	1	0	0.046506	-2.684740	3.540523
58	1	0	0.352472	-2.409886	1.842784
59	8	0	1.140786	-0.328798	3.551676
60	8	0	-0.152572	1.192916	2.500873
61	1	0	-0.889934	-4.403762	1.362383
62	17	0	2.181736	-2.947843	0.206263
63	1	0	0.706642	1.696034	2.355368
64	1	0	1.058655	-4.954462	-3.334299
65	1	0	-2.645416	-1.271876	1.534923
66	1	0	-2.367619	0.285007	1.942857

HF=-3453.6746323\ZeroPoint=0.4612679\Thermal=0.5036985

G = 14.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.213128	-0.386913	-0.281472
2	46	0	1.265441	1.361563	-0.415149
3	7	0	-2.325698	1.375372	-0.570233
4	7	0	-3.574759	1.443601	-0.578181
5	6	0	-4.310534	0.248078	-0.421876
6	6	0	-5.348274	0.267968	0.517138
7	6	0	-6.091562	-0.886548	0.740932

8	1	0	-6.874413	-0.883885	1.490045
9	6	0	-5.840477	-2.039064	-0.006638
10	6	0	-4.847699	-2.033606	-0.986668
11	1	0	-4.677668	-2.916400	-1.592075
12	6	0	-4.073638	-0.895742	-1.197230
13	1	0	-3.323788	-0.870118	-1.977417
14	6	0	-1.647098	2.613760	-0.830591
15	6	0	-0.382454	2.808601	-0.225871
16	6	0	0.182305	4.090819	-0.372947
17	1	0	1.111715	4.316307	0.134129
18	6	0	-0.421855	5.071869	-1.156852
19	1	0	0.055200	6.038459	-1.273788
20	6	0	-1.637268	4.813492	-1.790782
21	1	0	-2.100922	5.569535	-2.413932
22	6	0	-2.270472	3.588748	-1.608598
23	1	0	-3.231089	3.384738	-2.063035
24	16	0	2.391474	2.232411	1.419849
25	6	0	3.843696	1.098611	1.386022
26	1	0	3.598104	0.145207	1.857757
27	1	0	4.654002	1.571595	1.940057
28	6	0	4.233886	0.875894	-0.063984
29	1	0	4.479451	1.843642	-0.514624
30	6	0	5.434278	-0.032087	-0.329508
31	8	0	6.329781	-0.019502	0.674041
32	8	0	5.585233	-0.645236	-1.356651
33	7	0	3.051754	0.322557	-0.776939
34	1	0	3.267698	0.237783	-1.767845
35	1	0	2.907460	-0.642601	-0.411596
36	16	0	0.015123	0.120349	-2.205534
37	6	0	0.836242	-1.532114	-2.450517
38	1	0	0.875765	-1.723080	-3.521388
39	1	0	1.850999	-1.523900	-2.061413
40	6	0	0.032626	-2.614922	-1.740262
41	1	0	-0.936311	-2.731874	-2.236528
42	7	0	-0.217252	-2.198546	-0.336127
43	1	0	0.721546	-2.136168	0.120115
44	6	0	0.664874	-4.011719	-1.733555
45	8	0	1.578603	-4.174669	-2.703418
46	8	0	0.315142	-4.874628	-0.971342
47	1	0	-6.431687	-2.931814	0.159742
48	1	0	-0.698598	-2.944184	0.168706
49	1	0	7.061550	-0.604632	0.423719
50	1	0	-5.536525	1.177683	1.074874
51	7	0	-2.020863	-0.743599	1.685266
52	6	0	-1.165189	-0.425827	2.876820
53	6	0	0.124782	-1.240018	2.905035
54	1	0	-1.750728	-0.652432	3.775691
55	6	0	-0.798322	1.085516	2.955963
56	16	0	-0.204573	-3.062760	2.919605
57	1	0	0.669237	-0.961804	3.804405
58	1	0	0.756380	-1.010316	2.046230
59	8	0	-0.177831	1.456604	3.931374
60	8	0	-1.229865	1.791729	1.956055
61	1	0	0.919292	-3.398743	2.243193
62	17	0	2.705490	-2.463729	0.566730
63	1	0	-0.483967	2.228186	0.973084
64	1	0	1.951680	-5.065855	-2.616436
65	1	0	-2.316827	-1.716653	1.756036
66	1	0	-2.857555	-0.169493	1.746583

HF=-3453.6251473\ZeroPoint=0.4570099\Thermal=0.4990321

G = 2.5 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.281836	0.464432	-0.268838
2	46	0	-1.631000	-1.431658	-0.307763
3	7	0	2.253475	-1.364688	-0.541626
4	7	0	3.456990	-1.618799	-0.722358
5	6	0	4.378563	-0.548969	-0.724276
6	6	0	5.510190	-0.681150	0.086965
7	6	0	6.442105	0.349336	0.110957
8	1	0	7.301148	0.275568	0.766982
9	6	0	6.275921	1.474435	-0.701507
10	6	0	5.167458	1.575403	-1.541522
11	1	0	5.052075	2.434672	-2.191921
12	6	0	4.206358	0.567595	-1.552006
13	1	0	3.352901	0.619408	-2.216942
14	6	0	1.368676	-2.482080	-0.737468
15	6	0	0.376976	-2.749516	0.236506
16	6	0	-0.516154	-3.800455	-0.029209
17	1	0	-1.184768	-4.137760	0.750440
18	6	0	-0.460849	-4.512542	-1.243256
19	1	0	-1.175167	-5.304975	-1.429630
20	6	0	0.520829	-4.217559	-2.170595
21	1	0	0.577158	-4.767676	-3.102538
22	6	0	1.453228	-3.200553	-1.914619
23	1	0	2.218628	-2.952416	-2.638596
24	16	0	-2.888955	-2.319099	1.437094
25	6	0	-4.210058	-1.035525	1.480643
26	1	0	-3.862539	-0.144273	2.005427
27	1	0	-5.070809	-1.452693	2.002298
28	6	0	-4.554737	-0.698152	0.042630
29	1	0	-4.906824	-1.604583	-0.460989
30	6	0	-5.628596	0.365034	-0.187016
31	8	0	-6.545889	0.394404	0.794029
32	8	0	-5.671044	1.056266	-1.173754
33	7	0	-3.304268	-0.249152	-0.629073
34	1	0	-3.488629	-0.087102	-1.616695
35	1	0	-3.046204	0.669218	-0.196308
36	16	0	-0.264421	-0.146883	-1.954762
37	6	0	-1.048484	1.520215	-2.218358
38	1	0	-1.168454	1.661294	-3.290881
39	1	0	-2.026400	1.567870	-1.749418
40	6	0	-0.166791	2.618728	-1.629388
41	1	0	0.741835	2.719622	-2.231969
42	7	0	0.235361	2.246682	-0.249596
43	1	0	-0.645733	2.138126	0.302160
44	6	0	-0.802706	4.013361	-1.601658
45	8	0	-1.778679	4.155206	-2.513472
46	8	0	-0.412095	4.889563	-0.876492
47	1	0	7.016581	2.265594	-0.687331
48	1	0	0.720590	3.026476	0.195761
49	1	0	-7.196612	1.078948	0.573192

50	1	0	5.590839	-1.543892	0.733986
51	7	0	2.491507	1.075784	1.373879
52	6	0	2.043411	0.530833	2.696220
53	6	0	0.606278	0.896493	3.016925
54	1	0	2.712320	0.944375	3.461226
55	6	0	2.329153	-1.014040	2.626417
56	16	0	0.409607	2.740989	3.134870
57	1	0	0.334738	0.436143	3.964070
58	1	0	-0.080806	0.515881	2.259931
59	8	0	1.390260	-1.773748	2.926674
60	8	0	3.481664	-1.274341	2.208151
61	1	0	-0.841390	2.801802	2.619975
62	17	0	-2.627176	2.316504	0.913876
63	1	0	0.478430	-2.328686	1.240081
64	1	0	-2.143064	5.050029	-2.426269
65	1	0	2.539381	2.092063	1.414232
66	1	0	3.434791	0.705786	1.244275

HF=-3453.6469824\ZeroPoint=0.4610271\Thermal=0.5035013

G = -5.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.451348	0.291802	0.218200
2	46	0	-1.398880	-0.437425	-1.407291
3	7	0	2.030181	-1.413261	-0.772470
4	7	0	3.168242	-1.695339	-1.196568
5	6	0	4.182400	-0.705905	-1.147351
6	6	0	5.388774	-1.080604	-0.548852
7	6	0	6.432478	-0.164462	-0.476362
8	1	0	7.356220	-0.442069	0.017595
9	6	0	6.296345	1.100202	-1.049678
10	6	0	5.109855	1.446722	-1.695546
11	1	0	5.012211	2.416346	-2.170405
12	6	0	4.043958	0.553343	-1.741992
13	1	0	3.129058	0.810597	-2.256772
14	6	0	1.067050	-2.483656	-0.757566
15	6	0	-0.317774	-2.202161	-0.866292
16	6	0	-1.117914	-3.367004	-0.746764
17	1	0	-2.191622	-3.295442	-0.849881
18	6	0	-0.623602	-4.644767	-0.501019
19	1	0	-1.313934	-5.476823	-0.405836
20	6	0	0.752514	-4.855054	-0.381079
21	1	0	1.154826	-5.842404	-0.185630
22	6	0	1.596249	-3.769256	-0.528025
23	1	0	2.669321	-3.884640	-0.444792
24	16	0	-2.831112	1.170708	-2.412296
25	6	0	-4.440462	0.611477	-1.711755
26	1	0	-4.939912	-0.068543	-2.411026
27	1	0	-5.080735	1.480385	-1.560547
28	6	0	-4.207527	-0.090421	-0.375262
29	1	0	-3.794769	0.630895	0.335722
30	6	0	-5.495847	-0.663826	0.190733
31	8	0	-6.368936	0.305898	0.524567
32	8	0	-5.734514	-1.843007	0.315488
33	7	0	-3.213804	-1.175859	-0.556253
34	1	0	-2.949858	-1.539236	0.358212
35	1	0	-3.651220	-1.933092	-1.077506
36	16	0	0.445122	1.007196	-1.776881
37	6	0	-0.118771	2.681233	-1.170796
38	1	0	-0.048322	3.373431	-2.007119
39	1	0	-1.157131	2.607185	-0.856826
40	6	0	0.771490	3.131353	-0.017426
41	1	0	1.800743	3.262157	-0.370009
42	7	0	0.786048	2.083339	1.039045
43	1	0	-0.190986	1.986932	1.367058
44	6	0	0.380100	4.469460	0.614962
45	8	0	-0.197039	5.307893	-0.261849
46	8	0	0.627549	4.752173	1.759220
47	1	0	7.117613	1.806135	-1.007329
48	1	0	1.330612	2.409649	1.835416
49	1	0	-7.170137	-0.120810	0.864021
50	1	0	5.484059	-2.071938	-0.123075
51	7	0	0.508506	-2.635814	2.434714
52	6	0	0.218875	-1.503968	3.376497
53	6	0	1.479906	-0.633386	3.590438
54	1	0	-0.111101	-1.922747	4.330459
55	6	0	-0.995563	-0.755990	2.789906
56	16	0	2.611466	-0.566186	2.142704
57	1	0	2.075842	-1.048922	4.406251
58	1	0	1.145634	0.356358	3.893521
59	8	0	-1.137229	0.423313	3.300119
60	8	0	-1.704840	-1.317041	1.971322
61	1	0	-0.415730	6.126466	0.210029
62	1	0	1.385272	-2.347310	1.921579
63	1	0	-0.273691	-2.709433	1.760016
64	1	0	0.659522	-3.532964	2.889293
65	1	0	-1.772284	1.062828	2.736264
66	17	0	-2.384116	2.306054	1.626604

HF=-3453.6611848\ZeroPoint=0.4618817\Thermal=0.5042377

G = 5.2 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.514346	0.287235	0.106991
2	46	0	-1.440204	-0.620713	-0.935713
3	7	0	2.112395	-1.630714	-0.453054
4	7	0	3.289236	-2.006155	-0.666915
5	6	0	4.317107	-1.045859	-0.659257
6	6	0	5.497075	-1.395220	0.009033
7	6	0	6.549648	-0.491225	0.061008
8	1	0	7.448686	-0.743883	0.610534
9	6	0	6.454936	0.734841	-0.601760
10	6	0	5.303523	1.053053	-1.320048
11	1	0	5.244415	1.987485	-1.866168
12	6	0	4.226352	0.172701	-1.348281
13	1	0	3.347590	0.393640	-1.938639
14	6	0	1.099260	-2.644926	-0.564647
15	6	0	-0.158801	-2.379468	0.025167
16	6	0	-1.042577	-3.483383	0.045266
17	1	0	-1.989046	-3.389315	0.567928

18	6	0	-0.753961	-4.699890	-0.562004
19	1	0	-1.477461	-5.508004	-0.537672
20	6	0	0.468963	-4.874582	-1.218717
21	1	0	0.691395	-5.806866	-1.724818
22	6	0	1.406585	-3.854464	-1.206400
23	1	0	2.370251	-3.981382	-1.681445
24	16	0	-2.861832	0.398775	-2.467917
25	6	0	-4.484195	0.052803	-1.658917
26	1	0	-4.942399	-0.831086	-2.114814
27	1	0	-5.137545	0.909479	-1.824564
28	6	0	-4.285412	-0.167550	-0.160976
29	1	0	-3.938649	0.763985	0.296098
30	6	0	-5.574756	-0.612637	0.508381
31	8	0	-6.494078	0.371324	0.519558
32	8	0	-5.773880	-1.716495	0.957971
33	7	0	-3.233232	-1.191765	0.042566
34	1	0	-3.009172	-1.245768	1.037272
35	1	0	-3.584115	-2.099240	-0.256218
36	16	0	0.379939	0.508763	-1.957550
37	6	0	-0.069746	2.313844	-1.813214
38	1	0	0.073187	2.766663	-2.792300
39	1	0	-1.118092	2.385911	-1.533361
40	6	0	0.817163	2.997221	-0.774359
41	1	0	1.848439	3.042025	-1.141300
42	7	0	0.825324	2.210336	0.486519
43	1	0	-0.151443	2.185403	0.820578
44	6	0	0.430331	4.444330	-0.455395
45	8	0	-0.158564	5.061948	-1.493191
46	8	0	0.693336	4.978180	0.591054
47	1	0	7.284993	1.431108	-0.572769
48	1	0	1.364410	2.703345	1.196519
49	1	0	-7.293952	0.026697	0.944893
50	1	0	5.553828	-2.354692	0.508122
51	7	0	0.357934	-1.836899	2.597397
52	6	0	0.167041	-0.611044	3.426331
53	6	0	1.446009	0.257069	3.504936
54	1	0	-0.090429	-0.925894	4.443707
55	6	0	-1.098191	0.084936	2.904906
56	16	0	2.681648	0.042808	2.158976
57	1	0	1.992902	-0.001326	4.414755
58	1	0	1.139944	1.296757	3.592988
59	8	0	-1.057957	1.384825	2.981711
60	8	0	-2.030129	-0.593626	2.509945
61	1	0	-0.383963	5.962551	-1.212912
62	1	0	1.363761	-2.026824	2.523333
63	1	0	-0.007499	-1.798494	1.403192
64	1	0	-0.131084	-2.638807	2.985623
65	1	0	-1.750665	1.847085	2.360002
66	17	0	-2.383203	2.704573	0.849894

HF=-3453.6422434\ZeroPoint=0.4590659\Thermal=0.5009419

G = -41.5 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.165034	0.373087	0.608570
2	46	0	0.926251	-1.154790	-1.501659
3	7	0	-0.392954	2.302785	0.234439
4	7	0	-1.049779	3.163213	-0.389827
5	6	0	-2.408450	2.893247	-0.676040
6	6	0	-3.328876	2.545464	0.320546
7	6	0	-4.652955	2.300560	-0.033587
8	1	0	-5.370285	2.044689	0.737889
9	6	0	-5.055190	2.389071	-1.366588
10	6	0	-4.136287	2.764891	-2.348063
11	1	0	-4.447367	2.845133	-3.383042
12	6	0	-2.818674	3.044796	-2.002863
13	1	0	-2.090689	3.331130	-2.751512
14	6	0	0.973160	2.667288	0.499329
15	6	0	1.635780	2.061983	1.563942
16	6	0	2.949076	2.432328	1.846479
17	1	0	3.451243	1.966246	2.685160
18	6	0	3.601059	3.377287	1.060749
19	1	0	4.626976	3.653767	1.277491
20	6	0	2.935769	3.958631	-0.024458
21	1	0	3.447865	4.674096	-0.657415
22	6	0	1.624260	3.611075	-0.307802
23	1	0	1.105981	4.034113	-1.156057
24	16	0	1.839683	0.771042	-2.401463
25	6	0	3.440457	0.650729	-1.504260
26	1	0	3.316768	0.969314	-0.467605
27	1	0	4.158251	1.313581	-1.988086
28	6	0	3.939985	-0.797723	-1.543314
29	1	0	4.084264	-1.085308	-2.587524
30	6	0	5.267592	-0.956932	-0.814354
31	8	0	6.253567	-0.276708	-1.443028
32	8	0	5.439683	-1.591971	0.194553
33	7	0	2.906953	-1.674519	-0.953859
34	1	0	3.095521	-2.656583	-1.139445
35	1	0	2.880059	-1.568888	0.066924
36	16	0	-1.178398	-0.157601	-1.764062
37	6	0	-2.467655	-1.487805	-1.712568
38	1	0	-3.200419	-1.268316	-2.487089
39	1	0	-1.990465	-2.441706	-1.928443
40	6	0	-3.158677	-1.519914	-0.343266
41	1	0	-3.801669	-0.638487	-0.252238
42	7	0	-2.151948	-1.457302	0.739842
43	1	0	-1.486178	-2.226310	0.629849
44	6	0	-4.051559	-2.742195	-0.163601
45	8	0	-4.921592	-2.870640	-1.186579
46	8	0	-4.011841	-3.486401	0.781758
47	1	0	-6.085008	2.186039	-1.637273
48	1	0	-2.601412	-1.574456	1.644881
49	1	0	7.068355	-0.401392	-0.933058
50	1	0	-3.020795	2.496836	1.356074
51	7	0	1.499362	0.108309	4.196148
52	6	0	0.658754	-1.025960	3.850217
53	6	0	-0.845801	-0.674703	3.874054
54	1	0	0.760447	-1.877032	4.547952
55	6	0	1.098794	-1.601153	2.508840
56	16	0	-1.416071	0.795400	2.924029
57	1	0	-1.119685	-0.439924	4.907408
58	1	0	-1.403430	-1.570546	3.598706
59	8	0	0.338209	-2.640199	2.163863

60	8	0	2.045309	-1.199996	1.865587
61	1	0	-5.467481	-3.653844	-1.016863
62	1	0	1.252661	0.480841	5.105626
63	1	0	1.141634	1.346546	2.202579
64	1	0	2.478994	-0.152415	4.200406
65	1	0	0.562643	-2.964279	1.254171
66	17	0	0.216608	-3.371872	-0.751780

HF=-3453.7183273\ZeroPoint=0.4625088\Thermal=0.5055282

G = -14.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.363390	0.136217	0.057632
2	46	0	-1.313442	-0.221567	-1.544236
3	7	0	1.717770	-1.833112	-0.495210
4	7	0	2.854897	-2.349250	-0.412794
5	6	0	3.947123	-1.514229	-0.080690
6	6	0	4.763020	-1.899504	0.985637
7	6	0	5.858949	-1.114297	1.327610
8	1	0	6.471309	-1.391258	2.177664
9	6	0	6.174578	0.018815	0.577004
10	6	0	5.389516	0.365695	-0.522363
11	1	0	5.652022	1.225428	-1.128569
12	6	0	4.269556	-0.390758	-0.854008
13	1	0	3.669635	-0.144482	-1.720209
14	6	0	0.657402	-2.702086	-0.922400
15	6	0	-0.554212	-2.155449	-1.391428
16	6	0	-1.477755	-3.103167	-1.886059
17	1	0	-2.408404	-2.758286	-2.325593
18	6	0	-1.254435	-4.473345	-1.860004
19	1	0	-2.008237	-5.151327	-2.246747
20	6	0	-0.063651	-4.976289	-1.325969
21	1	0	0.110995	-6.044161	-1.268910
22	6	0	0.892382	-4.091677	-0.872594
23	1	0	1.827612	-4.451824	-0.466697
24	16	0	-2.584737	1.768333	-1.963897
25	6	0	-4.072303	1.386405	-0.942883
26	1	0	-4.894096	1.030069	-1.570010
27	1	0	-4.389086	2.298141	-0.433036
28	6	0	-3.710583	0.332546	0.099138
29	1	0	-2.947747	0.770995	0.737090
30	6	0	-4.865341	-0.078335	0.997993
31	8	0	-5.901356	-0.596305	0.315054
32	8	0	-4.861873	0.022808	2.206063
33	7	0	-3.124661	-0.852730	-0.583445
34	1	0	-2.930183	-1.601260	0.082155
35	1	0	-3.787003	-1.214354	-1.267224
36	16	0	0.769404	0.689940	-2.169065
37	6	0	0.673379	2.534962	-1.924331
38	1	0	1.030700	3.008334	-2.836630
39	1	0	-0.367374	2.813391	-1.756303
40	6	0	1.536429	2.945024	-0.735355
41	1	0	2.584490	2.708232	-0.953300
42	7	0	1.150620	2.167851	0.469017
43	1	0	0.178569	2.396102	0.753092
44	6	0	1.523105	4.440622	-0.412059
45	8	0	1.383205	5.202385	-1.514409
46	8	0	1.680460	4.882144	0.695669
47	1	0	7.038099	0.619235	0.838427
48	1	0	1.730240	2.453752	1.256559
49	1	0	-6.583856	-0.861623	0.951138
50	1	0	4.508815	-2.785568	1.554019
51	7	0	-2.145365	0.362177	3.224505
52	6	0	-0.982513	-0.281388	2.533887
53	6	0	0.312007	0.139458	3.230717
54	1	0	-0.970694	0.152675	1.527451
55	6	0	-1.273681	-1.775765	2.323429
56	16	0	1.831179	-0.421363	2.347843
57	1	0	0.362312	-0.281618	4.240465
58	1	0	0.304091	1.228193	3.309853
59	8	0	-2.421502	-2.143543	2.173662
60	8	0	-0.250300	-2.601399	2.253445
61	17	0	-1.657495	2.904385	1.873169
62	1	0	0.616871	-2.094987	2.285265
63	1	0	1.408807	6.131575	-1.237419
64	1	0	-2.098165	1.408327	2.924182
65	1	0	-2.084686	0.271463	4.237714
66	1	0	-3.058488	-0.010873	2.915405

HF=-3453.6784924\ZeroPoint=0.4634052\Thermal=0.5053036

G = 4.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.413861	0.291872	-0.053070
2	46	0	-1.380622	-0.655349	-1.271220
3	7	0	2.102316	-1.639630	-0.388189
4	7	0	3.282239	-2.023970	-0.213116
5	6	0	4.262008	-1.072886	0.123315
6	6	0	5.158320	-1.419470	1.141029
7	6	0	6.146984	-0.519962	1.516567
8	1	0	6.815922	-0.767110	2.332268
9	6	0	6.284800	0.695352	0.841512
10	6	0	5.430106	1.010059	-0.213554
11	1	0	5.558640	1.937575	-0.759513
12	6	0	4.409816	0.135470	-0.573731
13	1	0	3.765591	0.352140	-1.416289
14	6	0	1.202995	-2.646157	-0.878419
15	6	0	-0.178638	-2.498249	-0.636868
16	6	0	-0.978361	-3.583015	-1.057503
17	1	0	-2.038440	-3.580524	-0.830330
18	6	0	-0.469647	-4.681798	-1.739801
19	1	0	-1.131130	-5.478980	-2.060472
20	6	0	0.897003	-4.749193	-2.016123
21	1	0	1.305527	-5.588060	-2.567656
22	6	0	1.737613	-3.740037	-1.572002
23	1	0	2.802189	-3.785122	-1.758034
24	16	0	-2.938910	0.756140	-2.304883
25	6	0	-4.352247	0.558371	-1.123899
26	1	0	-5.125075	-0.079213	-1.559463
27	1	0	-4.776413	1.545094	-0.931932

28	6	0	-3.835056	-0.030311	0.176714
29	1	0	-3.140163	0.689265	0.613722
30	6	0	-4.864322	-0.335647	1.256298
31	8	0	-6.073678	-0.676281	0.794928
32	8	0	-4.594704	-0.321170	2.440742
33	7	0	-3.073366	-1.276829	-0.132676
34	1	0	-2.729084	-1.748280	0.708947
35	1	0	-3.661264	-1.925565	-0.652995
36	16	0	0.472283	0.452572	-2.252283
37	6	0	0.076462	2.275888	-2.178188
38	1	0	0.236138	2.689432	-3.171901
39	1	0	-0.972977	2.392105	-1.911402
40	6	0	0.975298	2.967245	-1.158590
41	1	0	2.019150	2.894567	-1.484758
42	7	0	0.869242	2.286227	0.155143
43	1	0	-0.102251	2.402357	0.507972
44	6	0	0.718025	4.466132	-0.973425
45	8	0	0.174358	5.040442	-2.062324
46	8	0	1.026623	5.066483	0.022531
47	1	0	7.068223	1.387272	1.128064
48	1	0	1.471933	2.751523	0.832158
49	1	0	-6.644056	-0.881703	1.553345
50	1	0	5.036131	-2.368401	1.648195
51	7	0	-1.998231	0.732845	3.223255
52	6	0	-0.836945	0.056858	2.528515
53	6	0	0.447295	0.699077	3.048194
54	1	0	-0.965066	0.274441	1.469154
55	6	0	-0.965474	-1.451256	2.815278
56	16	0	1.982508	0.113657	2.231390
57	1	0	0.562670	0.450876	4.107935
58	1	0	0.350906	1.784803	2.956613
59	8	0	-1.091899	-1.790300	3.978867
60	8	0	-1.047668	-2.249775	1.788638
61	17	0	-2.067594	2.921225	1.197143
62	1	0	-0.587692	-2.054469	0.653078
63	1	0	0.053360	5.983398	-1.869699
64	1	0	-2.074766	1.704838	2.804366
65	1	0	-1.849815	0.732873	4.232540
66	1	0	-2.897995	0.261587	3.034507

HF=-3453.644023\ZeroPoint=0.4599046\Thermal=0.5017076

G = -14.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.376860	0.111395	0.149719
2	46	0	-0.991106	-0.410708	-1.420750
3	7	0	2.006662	-1.855018	-0.145214
4	7	0	3.174500	-2.293102	-0.118450
5	6	0	4.226817	-1.387792	0.153477
6	6	0	5.166085	-1.798083	1.104958
7	6	0	6.216819	-0.950641	1.435407
8	1	0	6.925170	-1.247429	2.199566
9	6	0	6.367627	0.270856	0.776276
10	6	0	5.464063	0.645032	-0.217436
11	1	0	5.602885	1.575353	-0.756114
12	6	0	4.383876	-0.174911	-0.529791
13	1	0	3.703304	0.088660	-1.328308
14	6	0	1.008915	-2.828816	-0.506668
15	6	0	-0.104571	-2.968821	0.320799
16	6	0	-1.074707	-3.911773	-0.010139
17	1	0	-1.921487	-4.029468	0.655601
18	6	0	-0.944174	-4.671207	-1.171503
19	1	0	-1.708780	-5.392414	-1.436984
20	6	0	0.171348	-4.508857	-1.997970
21	1	0	0.265600	-5.092903	-2.905796
22	6	0	1.165780	-3.597369	-1.662027
23	1	0	2.038037	-3.456514	-2.287746
24	16	0	-2.519359	0.552388	-2.846640
25	6	0	-4.046849	0.384477	-1.797997
26	1	0	-4.682100	-0.410436	-2.194216
27	1	0	-4.585755	1.332076	-1.840931
28	6	0	-3.626638	0.076238	-0.365733
29	1	0	-3.100315	0.946164	0.028998
30	6	0	-4.765119	-0.209743	0.603406
31	8	0	-5.571536	-1.200405	0.190865
32	8	0	-4.915277	0.364393	1.659844
33	7	0	-2.682280	-1.072801	-0.387848
34	1	0	-2.454961	-1.395776	0.592779
35	1	0	-3.103800	-1.861440	-0.876219
36	16	0	0.977959	0.544423	-2.240248
37	6	0	0.659766	2.373162	-2.064357
38	1	0	1.042464	2.862684	-2.957723
39	1	0	-0.415641	2.533991	-1.998257
40	6	0	1.365092	2.899803	-0.821936
41	1	0	2.447680	2.775186	-0.936061
42	7	0	0.944682	2.117862	0.369143
43	1	0	-0.073738	2.307768	0.508539
44	6	0	1.160473	4.389609	-0.520889
45	8	0	0.766218	5.091170	-1.594966
46	8	0	1.396853	4.868965	0.557569
47	1	0	7.198745	0.920444	1.024628
48	1	0	1.420492	2.488766	1.190432
49	1	0	-6.214672	-1.382451	0.894244
50	1	0	5.039373	-2.755949	1.594278
51	7	0	-2.474549	1.414889	2.911751
52	6	0	-1.446728	0.377883	2.509519
53	6	0	-0.089368	0.773461	3.087600
54	1	0	-1.412337	0.416873	1.423501
55	6	0	-1.998918	-0.983346	3.044971
56	16	0	1.322075	-0.240852	2.475022
57	1	0	-0.104791	0.600425	4.167613
58	1	0	0.097268	1.837789	2.918308
59	8	0	-2.166861	-1.017768	4.267356
60	8	0	-2.262057	-1.853887	2.164700
61	17	0	-1.930576	3.203365	0.538459
62	1	0	-0.201880	-2.382861	1.223380
63	1	0	0.641384	6.012758	-1.319209
64	1	0	-2.272923	2.311447	2.404996
65	1	0	-2.491856	1.498099	3.929596
66	1	0	-3.412408	1.117495	2.596134

HF=-3453.677894\ZeroPoint=0.4641482\Thermal=0.5064818

G = -12.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.945533	0.648138	0.083389
2	46	0	-1.653123	0.063203	-1.280282
3	7	0	1.811833	-0.803722	-1.076411
4	7	0	3.018392	-0.930299	-1.362838
5	6	0	3.947135	0.053441	-0.955341
6	6	0	5.130353	-0.409061	-0.368232
7	6	0	6.087909	0.510386	0.045472
8	1	0	6.986456	0.157222	0.537279
9	6	0	5.900237	1.874890	-0.179553
10	6	0	4.746146	2.322937	-0.822723
11	1	0	4.616313	3.378092	-1.035272
12	6	0	3.759497	1.420072	-1.205867
13	1	0	2.879892	1.756025	-1.736391
14	6	0	0.930281	-1.854980	-1.530130
15	6	0	-0.452266	-1.602998	-1.726930
16	6	0	-1.161708	-2.698667	-2.265250
17	1	0	-2.211177	-2.581252	-2.508808
18	6	0	-0.589807	-3.941712	-2.508008
19	1	0	-1.200362	-4.744375	-2.908205
20	6	0	0.759861	-4.165815	-2.217382
21	1	0	1.206237	-5.142409	-2.362516
22	6	0	1.524917	-3.117406	-1.745158
23	1	0	2.571588	-3.252350	-1.505761
24	16	0	-3.153126	1.817624	-0.671817
25	6	0	-4.580555	0.787375	-0.147782
26	1	0	-5.214229	0.574579	-1.014045
27	1	0	-5.169382	1.341377	0.583968
28	6	0	-4.066344	-0.513088	0.466351
29	1	0	-3.495202	-0.290913	1.369262
30	6	0	-5.222972	-1.434366	0.816742
31	8	0	-5.871111	-1.019524	1.924816
32	8	0	-5.561404	-2.397919	0.172310
33	7	0	-3.147120	-1.200946	-0.469758
34	1	0	-2.646693	-1.903007	0.095591
35	1	0	-3.693680	-1.682319	-1.181640
36	16	0	0.055487	1.573597	-1.893772
37	6	0	-0.382408	3.247092	-1.218444
38	1	0	0.175862	3.977025	-1.802728
39	1	0	-1.443366	3.414148	-1.392862
40	6	0	-0.022307	3.404815	0.271857
41	1	0	1.034731	3.682646	0.339408
42	7	0	-0.179200	2.139976	1.026333
43	1	0	-1.154044	1.809779	0.979829
44	6	0	-0.792127	4.528110	0.965136
45	8	0	-0.923226	5.606337	0.167969
46	8	0	-1.184599	4.474863	2.100587
47	1	0	6.659001	2.584885	0.128748
48	1	0	0.011024	2.289492	2.015302
49	1	0	-6.613156	-1.624566	2.076087
50	1	0	5.252846	-1.469911	-0.194387
51	7	0	0.769307	-2.933430	1.650467
52	6	0	0.239375	-2.033372	2.735293
53	6	0	1.255747	-1.028108	3.252155
54	1	0	-0.009946	-2.688811	3.574631
55	6	0	-1.107461	-1.449899	2.201507
56	16	0	2.174695	0.008685	2.036558
57	1	0	2.046546	-1.521982	3.819623
58	1	0	0.717874	-0.335561	3.896970
59	8	0	-1.340212	-0.248063	2.398706
60	8	0	-1.789147	-2.329138	1.612850
61	1	0	-1.399233	6.290153	0.664285
62	1	0	1.805031	-3.169670	1.744074
63	1	0	0.665812	-2.479738	0.737000
64	1	0	3.001454	-1.049764	1.634952
65	1	0	0.177467	-3.762140	1.594514
66	17	0	3.751922	-2.980481	1.576349

HF=-3453.6704613\ZeroPoint=0.4585294\Thermal=0.5006846

G = 7.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.366698	0.530745	-0.006062
2	46	0	-1.770998	-0.169615	-0.923044
3	7	0	1.812822	-1.275846	-0.934723
4	7	0	2.963147	-1.636764	-1.267650
5	6	0	4.026087	-0.728936	-1.088295
6	6	0	5.162661	-1.212351	-0.430829
7	6	0	6.237625	-0.358319	-0.216611
8	1	0	7.103647	-0.714686	0.328412
9	6	0	6.207074	0.949359	-0.706166
10	6	0	5.094038	1.406649	-1.410504
11	1	0	5.083586	2.410537	-1.819425
12	6	0	3.992441	0.576728	-1.597702
13	1	0	3.137198	0.909784	-2.171425
14	6	0	0.765951	-2.226248	-1.185321
15	6	0	-0.434968	-2.087760	-0.455348
16	6	0	-1.334597	-3.168861	-0.593169
17	1	0	-2.226794	-3.194461	0.023172
18	6	0	-1.120984	-4.229675	-1.464890
19	1	0	-1.854873	-5.023919	-1.548149
20	6	0	0.043220	-4.266378	-2.237094
21	1	0	0.211697	-5.075597	-2.938020
22	6	0	1.000789	-3.276790	-2.081878
23	1	0	1.930265	-3.313180	-2.633705
24	16	0	-3.306081	1.295658	-1.882573
25	6	0	-4.853436	0.555145	-1.214552
26	1	0	-5.211767	-0.233496	-1.882973
27	1	0	-5.610178	1.339364	-1.164093
28	6	0	-4.576641	-0.020494	0.170911
29	1	0	-4.286734	0.774880	0.859253
30	6	0	-5.806928	-0.731708	0.716100
31	8	0	-6.742282	0.144522	1.131249
32	8	0	-5.955571	-1.929347	0.740937
33	7	0	-3.443681	-0.968400	0.091819
34	1	0	-3.084465	-1.088654	1.053465
35	1	0	-3.777445	-1.856423	-0.275965
36	16	0	-0.014059	1.166871	-1.808731
37	6	0	-0.441891	2.870084	-1.168881

38	1	0	-0.565052	3.529711	-2.024852
39	1	0	-1.387227	2.808622	-0.632843
40	6	0	0.667167	3.375911	-0.250466
41	1	0	1.586341	3.501276	-0.834042
42	7	0	0.929202	2.385672	0.811969
43	1	0	0.096641	2.201370	1.413638
44	6	0	0.364918	4.743350	0.360670
45	8	0	-0.050326	5.623268	-0.573975
46	8	0	0.518060	5.017544	1.521482
47	1	0	7.056113	1.604953	-0.551080
48	1	0	1.666745	2.716298	1.430103
49	1	0	-7.509398	-0.361629	1.440018
50	1	0	5.159591	-2.228037	-0.055369
51	7	0	-0.105819	-1.903433	2.205996
52	6	0	-0.102775	-0.703877	3.090185
53	6	0	1.270859	-0.047929	3.289335
54	1	0	-0.419752	-1.028542	4.088335
55	6	0	-1.282594	0.195911	2.596535
56	16	0	2.544729	-0.050595	1.948318
57	1	0	1.785866	-0.535753	4.120576
58	1	0	1.087852	0.988161	3.574668
59	8	0	-1.087480	1.406914	2.373004
60	8	0	-2.357156	-0.450521	2.501472
61	1	0	-0.204707	6.474013	-0.134878
62	1	0	0.717541	-2.497953	2.324583
63	1	0	-0.275325	-1.716096	0.904335
64	1	0	2.814352	-1.829279	1.837943
65	1	0	-0.936555	-2.447512	2.428796
66	17	0	2.938675	-3.276893	1.813457

HF=-3453.6334399\ZeroPoint=0.4556058\Thermal=0.49765

G = -22.2 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.524800	0.347285	0.030744
2	46	0	-1.861267	0.880404	-0.278798
3	7	0	1.358609	-1.443210	-0.986107
4	7	0	2.225730	-2.045396	-1.644757
5	6	0	3.521833	-1.475140	-1.700727
6	6	0	4.591076	-2.306521	-1.357629
7	6	0	5.883614	-1.795869	-1.395641
8	1	0	6.714888	-2.422242	-1.094353
9	6	0	6.112167	-0.487881	-1.827799
10	6	0	5.042419	0.317405	-2.216166
11	1	0	5.221553	1.323275	-2.578645
12	6	0	3.738584	-0.165691	-2.144083
13	1	0	2.901691	0.440803	-2.466147
14	6	0	0.040117	-2.029825	-1.038666
15	6	0	-0.577720	-2.386275	0.156281
16	6	0	-1.859372	-2.925728	0.105317
17	1	0	-2.343694	-3.219044	1.029129
18	6	0	-2.519717	-3.066308	-1.116159
19	1	0	-3.526888	-3.467247	-1.140270
20	6	0	-1.890000	-2.683558	-2.300782
21	1	0	-2.406188	-2.771382	-3.249244
22	6	0	-0.594680	-2.176757	-2.269691
23	1	0	-0.092835	-1.863489	-3.176306
24	16	0	-3.046334	1.066006	-2.242892
25	6	0	-4.520854	0.085662	-1.741542
26	1	0	-4.326880	-0.978798	-1.898398
27	1	0	-5.361448	0.386124	-2.369173
28	6	0	-4.840237	0.325794	-0.262003
29	1	0	-5.129679	1.367331	-0.118171
30	6	0	-5.976654	-0.592577	0.165885
31	8	0	-7.182188	-0.063543	-0.135112
32	8	0	-5.830510	-1.680043	0.664823
33	7	0	-3.624288	0.053918	0.528447
34	1	0	-3.704131	0.306039	1.511776
35	1	0	-3.437187	-0.949362	0.553559
36	16	0	0.080113	1.569092	-1.470559
37	6	0	0.368804	3.281965	-0.806332
38	1	0	0.461498	3.966897	-1.647332
39	1	0	-0.503359	3.570263	-0.218992
40	6	0	1.633193	3.327541	0.056129
41	1	0	2.510530	3.230528	-0.589371
42	7	0	1.628580	2.196849	0.997795
43	1	0	0.762009	2.161386	1.547586
44	6	0	1.750462	4.652134	0.802999
45	8	0	1.850259	5.687226	-0.055719
46	8	0	1.756286	4.766711	2.001181
47	1	0	7.124197	-0.102412	-1.873412
48	1	0	2.416126	2.251590	1.639077
49	1	0	-7.860843	-0.712713	0.106605
50	1	0	4.387627	-3.315555	-1.021719
51	7	0	0.119451	-2.056291	3.388330
52	6	0	0.120820	-0.592516	3.452027
53	6	0	1.541785	-0.041018	3.278417
54	1	0	-0.197301	-0.217540	4.442716
55	6	0	-1.013028	-0.103957	2.507337
56	16	0	2.615819	-0.610381	1.878108
57	1	0	2.118315	-0.331032	4.163148
58	1	0	1.501653	1.048833	3.297330
59	8	0	-0.765656	0.835659	1.659292
60	8	0	-2.100859	-0.670130	2.652548
61	1	0	1.915041	6.504360	0.462500
62	1	0	0.785524	-2.458714	4.039065
63	1	0	-0.064958	-2.279027	1.105195
64	1	0	2.427096	-2.701626	1.635561
65	1	0	-0.807137	-2.402812	3.612902
66	17	0	2.500458	-4.008646	1.335661

HF=-3453.6784948\ZeroPoint=0.4557868\Thermal=0.4992706

G = -5.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.355115	0.387599	0.090358
2	46	0	-1.497284	0.181276	-1.281931
3	7	0	1.712834	-1.427010	-0.877642
4	7	0	2.870539	-1.880818	-1.026324
5	6	0	3.970796	-1.083478	-0.641608

6	6	0	4.923499	-1.669488	0.198103
7	6	0	6.032591	-0.931099	0.598793
8	1	0	6.754779	-1.373252	1.274998
9	6	0	6.223468	0.365821	0.119927
10	6	0	5.302214	0.922190	-0.767591
11	1	0	5.468596	1.914315	-1.171753
12	6	0	4.170003	0.208135	-1.148981
13	1	0	3.467824	0.620297	-1.861396
14	6	0	0.639964	-2.259117	-1.337679
15	6	0	-0.652871	-1.717921	-1.515348
16	6	0	-1.591867	-2.619788	-2.066386
17	1	0	-2.588463	-2.267903	-2.309074
18	6	0	-1.305344	-3.947746	-2.348684
19	1	0	-2.077681	-4.590356	-2.758369
20	6	0	-0.028542	-4.458926	-2.091287
21	1	0	0.196747	-5.503975	-2.266024
22	6	0	0.941595	-3.614052	-1.601247
23	1	0	1.934708	-3.981599	-1.387507
24	16	0	-2.855177	2.134184	-1.437234
25	6	0	-4.406510	1.427990	-0.746567
26	1	0	-5.008749	0.984441	-1.547285
27	1	0	-4.984381	2.230182	-0.287704
28	6	0	-4.075589	0.373099	0.308704
29	1	0	-3.523875	0.853587	1.122845
30	6	0	-5.325670	-0.285024	0.863576
31	8	0	-6.085933	0.588437	1.552105
32	8	0	-5.627256	-1.445282	0.704093
33	7	0	-3.187862	-0.660651	-0.283728
34	1	0	-2.855341	-1.278126	0.456744
35	1	0	-3.741243	-1.253961	-0.900132
36	16	0	0.496921	1.270839	-1.898763
37	6	0	0.323422	3.044536	-1.353486
38	1	0	0.596124	3.675510	-2.196985
39	1	0	-0.718084	3.224953	-1.087271
40	6	0	1.234042	3.315566	-0.161411
41	1	0	2.279360	3.250645	-0.486187
42	7	0	1.024051	2.287290	0.881466
43	1	0	0.038711	2.243439	1.231756
44	6	0	1.080370	4.713240	0.439596
45	8	0	0.906111	5.652844	-0.509853
46	8	0	1.162426	4.949136	1.616034
47	1	0	7.097091	0.931911	0.420952
48	1	0	1.581040	2.515624	1.703347
49	1	0	-6.871017	0.114675	1.866158
50	1	0	4.769269	-2.685225	0.543195
51	7	0	-1.778888	-1.803050	2.618440
52	6	0	-0.394469	-1.774839	2.140086
53	6	0	0.600301	-1.089122	3.083663
54	1	0	-0.421796	-1.190397	1.212761
55	6	0	0.059425	-3.178336	1.730383
56	16	0	2.129190	-0.483944	2.236155
57	1	0	0.931147	-1.742882	3.892583
58	1	0	0.136204	-0.186153	3.478972
59	8	0	1.219982	-3.515195	1.672774
60	8	0	-0.935750	-4.006910	1.403579
61	17	0	-1.522389	1.440016	2.409193
62	1	0	-1.767610	-3.518385	1.573042
63	1	0	0.840398	6.514499	-0.069393
64	1	0	-2.092935	-0.828286	2.680941
65	1	0	-1.843510	-2.197842	3.554125
66	1	0	2.561813	-1.705950	1.859539

HF=-3453.6592879\ZeroPoint=0.4609749\Thermal=0.5037983

G = 14.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.410644	0.462255	-0.161513
2	46	0	-1.579671	-0.535844	-1.014912
3	7	0	1.985898	-1.502351	-0.642187
4	7	0	3.141571	-1.966839	-0.489721
5	6	0	4.172207	-1.128297	-0.027918
6	6	0	5.003165	-1.645406	0.974287
7	6	0	6.038576	-0.864998	1.473329
8	1	0	6.659406	-1.246799	2.274949
9	6	0	6.287112	0.400487	0.936357
10	6	0	5.497923	0.885336	-0.105887
11	1	0	5.711971	1.852476	-0.545553
12	6	0	4.434641	0.129806	-0.590656
13	1	0	3.838552	0.481419	-1.423682
14	6	0	1.076065	-2.402680	-1.297678
15	6	0	-0.287579	-2.389929	-0.940895
16	6	0	-1.084690	-3.383700	-1.543096
17	1	0	-2.121251	-3.480239	-1.240828
18	6	0	-0.590504	-4.255719	-2.506192
19	1	0	-1.247089	-4.984933	-2.967318
20	6	0	0.752999	-4.186484	-2.882223
21	1	0	1.143352	-4.846357	-3.648100
22	6	0	1.594992	-3.274661	-2.262846
23	1	0	2.643345	-3.221376	-2.526119
24	16	0	-3.247437	0.878735	-1.810973
25	6	0	-4.613297	0.370071	-0.681940
26	1	0	-5.220355	-0.406846	-1.156891
27	1	0	-5.240492	1.242583	-0.496310
28	6	0	-4.030264	-0.139417	0.633441
29	1	0	-3.505330	0.680201	1.127503
30	6	0	-5.126890	-0.679041	1.536165
31	8	0	-5.820354	0.314399	2.124324
32	8	0	-5.379820	-1.850263	1.683319
33	7	0	-3.043230	-1.213573	0.351595
34	1	0	-2.575343	-1.464693	1.231235
35	1	0	-3.539323	-2.049432	0.043551
36	16	0	0.160233	0.634234	-2.151107
37	6	0	-0.296776	2.437100	-2.010670
38	1	0	-0.365040	2.838171	-3.019812
39	1	0	-1.265492	2.512442	-1.517985
40	6	0	0.769311	3.155180	-1.201225
41	1	0	1.727320	3.120226	-1.733131
42	7	0	0.931234	2.460884	0.099929
43	1	0	0.001779	2.501756	0.620823
44	6	0	0.505575	4.640887	-0.937836
45	8	0	-0.275123	5.204557	-1.873656
46	8	0	1.001814	5.236264	-0.016839
47	1	0	7.105998	0.998720	1.318076

48	1	0	1.600656	2.978066	0.668989
49	1	0	-6.524358	-0.088483	2.655287
50	1	0	4.800167	-2.634135	1.367929
51	7	0	-1.750018	-0.342476	3.079908
52	6	0	-0.429541	-0.437327	2.461240
53	6	0	0.619215	0.477617	3.094972
54	1	0	-0.564729	-0.107746	1.424611
55	6	0	0.014781	-1.915040	2.440647
56	16	0	2.222575	0.459036	2.152458
57	1	0	0.869563	0.168795	4.109880
58	1	0	0.273432	1.511722	3.072572
59	8	0	0.889571	-2.300541	3.211578
60	8	0	-0.606759	-2.660298	1.580724
61	17	0	-1.736066	2.594885	1.493955
62	1	0	-0.543619	-2.257513	0.374061
63	1	0	-0.394859	6.138804	-1.641125
64	1	0	-2.060497	0.628512	3.044512
65	1	0	-1.735622	-0.659631	4.044423
66	1	0	2.475369	-0.850966	2.370201

HF=-3453.6224261\ZeroPoint=0.4560889\Thermal=0.4984812

G = -37.3 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.294761	0.462462	0.393166
2	46	0	0.980336	-1.700381	-0.865243
3	7	0	-1.083348	2.248351	-0.673859
4	7	0	-2.033723	2.739846	-1.318898
5	6	0	-3.264972	2.028428	-1.283156
6	6	0	-3.966552	1.863477	-0.083460
7	6	0	-5.183528	1.185084	-0.096343
8	1	0	-5.738619	1.068576	0.827535
9	6	0	-5.683833	0.660922	-1.288161
10	6	0	-4.982246	0.847054	-2.480674
11	1	0	-5.371937	0.446304	-3.408972
12	6	0	-3.784571	1.555335	-2.488396
13	1	0	-3.228872	1.709088	-3.404933
14	6	0	0.092989	3.070581	-0.621287
15	6	0	1.334550	2.472840	-0.820728
16	6	0	2.475942	3.265829	-0.779647
17	1	0	3.448270	2.819297	-0.946990
18	6	0	2.375816	4.628402	-0.504064
19	1	0	3.272686	5.232560	-0.437920
20	6	0	1.126549	5.211385	-0.291651
21	1	0	1.050325	6.267042	-0.059997
22	6	0	-0.025914	4.437399	-0.361914
23	1	0	-1.004707	4.868187	-0.194182
24	16	0	1.800269	-0.551603	-2.703512
25	6	0	3.502207	-0.306482	-2.040244
26	1	0	3.525700	0.514722	-1.318270
27	1	0	4.163060	-0.044982	-2.866069
28	6	0	3.975465	-1.584800	-1.360337
29	1	0	3.990162	-2.387131	-2.105636
30	6	0	5.404649	-1.459589	-0.833994
31	8	0	5.615983	-2.239820	0.252258
32	8	0	6.260727	-0.780877	-1.337366
33	7	0	2.998161	-1.966551	-0.313710
34	1	0	3.141360	-2.924959	-0.004441
35	1	0	3.087067	-1.380856	0.540343
36	16	0	-1.231182	-1.056658	-1.478683
37	6	0	-2.337204	-2.372234	-0.774617
38	1	0	-3.114178	-2.581512	-1.507559
39	1	0	-1.739250	-3.267834	-0.618591
40	6	0	-2.976904	-1.903897	0.538517
41	1	0	-3.757372	-1.173009	0.302862
42	7	0	-1.969864	-1.234812	1.390037
43	1	0	-1.180673	-1.882663	1.546632
44	6	0	-3.658501	-3.026821	1.313341
45	8	0	-4.448744	-3.770291	0.511836
46	8	0	-3.542590	-3.206850	2.497492
47	1	0	-6.624830	0.123224	-1.291347
48	1	0	-2.366824	-0.996957	2.297238
49	1	0	6.539009	-2.122773	0.524986
50	1	0	-3.576785	2.283351	0.835195
51	7	0	2.607854	-0.628429	2.291457
52	6	0	1.709455	0.521184	2.174578
53	6	0	0.441166	0.433798	3.063850
54	1	0	1.358727	0.566604	1.137033
55	6	0	2.502216	1.810619	2.431130
56	16	0	-0.948235	1.527180	2.491406
57	1	0	0.663003	0.714485	4.097209
58	1	0	0.100617	-0.602316	3.069911
59	8	0	1.803749	2.951407	2.392740
60	8	0	3.687130	1.812500	2.658545
61	17	0	0.470255	-3.123394	1.064271
62	1	0	1.383909	1.420038	-1.065370
63	1	0	-4.867258	-4.454302	1.057206
64	1	0	2.093336	-1.467379	2.543999
65	1	0	3.341199	-0.447889	2.969697
66	1	0	0.844201	2.771894	2.250321

HF=-3453.711004\ZeroPoint=0.4627975\Thermal=0.505474

G = -3.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.459651	-0.290389	0.341131
2	46	0	1.581705	-0.812302	-1.142679
3	7	0	-1.792656	0.063494	-1.651415
4	7	0	-2.692900	-0.351048	-2.407558
5	6	0	-3.723951	-1.144826	-1.863283
6	6	0	-4.380846	-0.825685	-0.665182
7	6	0	-5.414293	-1.648610	-0.225950
8	1	0	-5.941677	-1.396202	0.686716
9	6	0	-5.780022	-2.778682	-0.956890
10	6	0	-5.135117	-3.074719	-2.160104
11	1	0	-5.428922	-3.944299	-2.736014
12	6	0	-4.126967	-2.243626	-2.631898
13	1	0	-3.625172	-2.442778	-3.570970
14	6	0	-0.855521	1.002924	-2.199941
15	6	0	0.528292	0.870020	-1.921818

16	6	0	1.291592	1.942374	-2.437232
17	1	0	2.365609	1.960095	-2.309533
18	6	0	0.752511	3.026113	-3.129823
19	1	0	1.408638	3.818356	-3.475163
20	6	0	-0.617738	3.095371	-3.378778
21	1	0	-1.048809	3.935967	-3.908953
22	6	0	-1.423302	2.068031	-2.918024
23	1	0	-2.495829	2.088410	-3.067739
24	16	0	2.970528	-2.717569	-0.757015
25	6	0	4.599824	-1.865699	-0.835047
26	1	0	4.955555	-1.818157	-1.869729
27	1	0	5.323167	-2.434119	-0.249706
28	6	0	4.467135	-0.454210	-0.268497
29	1	0	4.148605	-0.504179	0.774427
30	6	0	5.783342	0.304861	-0.351728
31	8	0	6.691517	-0.182365	0.515427
32	8	0	6.010321	1.213534	-1.114699
33	7	0	3.417083	0.280242	-1.015348
34	1	0	3.164908	1.107259	-0.475873
35	1	0	3.803749	0.592405	-1.904531
36	16	0	-0.261859	-2.113628	-0.368180
37	6	0	0.363153	-2.661655	1.307010
38	1	0	0.476297	-3.742722	1.278814
39	1	0	1.337280	-2.208219	1.477176
40	6	0	-0.630376	-2.233087	2.381584
41	1	0	-1.592068	-2.729937	2.214998
42	7	0	-0.838563	-0.769071	2.278281
43	1	0	0.072430	-0.288162	2.394575
44	6	0	-0.191393	-2.601908	3.797173
45	8	0	0.195729	-3.888395	3.877987
46	8	0	-0.229174	-1.845867	4.732736
47	1	0	-6.581323	-3.416832	-0.602328
48	1	0	-1.449167	-0.445596	3.026048
49	1	0	7.512785	0.320037	0.401530
50	1	0	-4.127854	0.078617	-0.125283
51	7	0	0.016656	2.650410	0.688411
52	6	0	-0.903466	2.810994	1.860927
53	1	0	0.907065	2.169732	1.027954
54	1	0	0.189985	3.563806	0.253587
55	6	0	-0.672966	4.167433	2.522118
56	1	0	-0.599604	2.034269	2.568245
57	6	0	-2.381257	2.531852	1.463841
58	16	0	-0.831872	5.596731	1.371604
59	1	0	0.341057	4.220100	2.923702
60	1	0	-1.382235	4.284774	3.338349
61	8	0	-2.596266	1.431681	0.827221
62	8	0	-3.238874	3.339316	1.790137
63	1	0	-2.141592	5.390494	1.117542
64	17	0	1.998077	0.878836	2.021355
65	1	0	-0.370810	2.028636	-0.027953
66	1	0	0.442202	-4.071753	4.797886

HF=-3453.6536033\ZeroPoint=0.4606946\Thermal=0.5038111

G = 13.2 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.529485	0.121138	0.318402
2	46	0	-1.407666	0.643578	-1.059711
3	7	0	1.883309	-0.664254	-1.575472
4	7	0	2.861788	-0.414604	-2.313215
5	6	0	3.970552	0.266000	-1.777928
6	6	0	4.526530	-0.038273	-0.524745
7	6	0	5.652432	0.661512	-0.102789
8	1	0	6.100424	0.416443	0.853275
9	6	0	6.210538	1.659761	-0.902697
10	6	0	5.664086	1.940022	-2.156817
11	1	0	6.106061	2.703778	-2.785767
12	6	0	4.562744	1.224546	-2.610391
13	1	0	4.133595	1.411168	-3.587329
14	6	0	0.829831	-1.452184	-2.146256
15	6	0	-0.401732	-1.501278	-1.457542
16	6	0	-1.370953	-2.359219	-2.020791
17	1	0	-2.311152	-2.509513	-1.499279
18	6	0	-1.163503	-3.065497	-3.198436
19	1	0	-1.940029	-3.712505	-3.591565
20	6	0	0.062705	-2.957845	-3.862257
21	1	0	0.240891	-3.512505	-4.776085
22	6	0	1.066964	-2.165835	-3.329744
23	1	0	2.035369	-2.100706	-3.807340
24	16	0	-2.541076	2.634917	-1.459556
25	6	0	-4.259049	1.970006	-1.419400
26	1	0	-4.552981	1.626214	-2.416066
27	1	0	-4.926711	2.779017	-1.120824
28	6	0	-4.344698	0.820301	-0.420652
29	1	0	-4.090163	1.176250	0.580393
30	6	0	-5.735682	0.203988	-0.397871
31	8	0	-6.638937	1.043171	0.141024
32	8	0	-6.009808	-0.889882	-0.829529
33	7	0	-3.342133	-0.214044	-0.781809
34	1	0	-3.239032	-0.838608	0.017304
35	1	0	-3.691950	-0.765110	-1.563998
36	16	0	0.562095	1.927293	-0.751275
37	6	0	0.096700	2.918460	0.764883
38	1	0	0.186447	3.972124	0.511635
39	1	0	-0.936402	2.691209	1.020131
40	6	0	1.031124	2.544436	1.911788
41	1	0	2.054993	2.843472	1.661597
42	7	0	1.009306	1.073548	2.092568
43	1	0	0.029091	0.786566	2.299089
44	6	0	0.703096	3.234700	3.235770
45	8	0	0.358924	4.524557	3.060407
46	8	0	0.795408	2.699473	4.309033
47	1	0	7.083301	2.203587	-0.559685
48	1	0	1.581261	0.808234	2.892350
49	1	0	-7.505311	0.608413	0.117745
50	1	0	4.114617	-0.839010	0.077672
51	7	0	-0.657344	-2.189861	1.132303
52	6	0	0.324871	-2.368386	2.231454
53	1	0	-1.401994	-1.569728	1.496009
54	1	0	-1.040542	-3.110206	0.902811
55	6	0	-0.139075	-3.455410	3.212050
56	1	0	0.327155	-1.427055	2.785776
57	6	0	1.771928	-2.594998	1.717746

58	16	0	-0.553642	-5.074332	2.435765
59	1	0	-1.057526	-3.126908	3.702726
60	1	0	0.625535	-3.614547	3.971069
61	8	0	2.361892	-1.576518	1.171467
62	8	0	2.322468	-3.673210	1.893551
63	1	0	0.701374	-5.311030	1.999651
64	17	0	-2.096512	0.298464	2.302206
65	1	0	-0.417142	-1.621086	-0.072131
66	1	0	0.189292	4.910127	3.934091

HF=-3453.6259494\ZeroPoint=0.4572065\Thermal=0.499656

G = -23.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.298056	-0.032820	-0.322305
2	46	0	1.441929	-0.969423	1.335421
3	7	0	-0.196198	-0.538142	-2.044291
4	7	0	-0.531216	-1.448246	-2.831324
5	6	0	-1.802400	-2.035053	-2.675131
6	6	0	-2.968511	-1.267810	-2.525534
7	6	0	-4.191228	-1.922287	-2.407030
8	1	0	-5.098746	-1.336575	-2.314871
9	6	0	-4.253680	-3.316359	-2.418709
10	6	0	-3.089391	-4.068302	-2.589617
11	1	0	-3.138145	-5.150662	-2.611218
12	6	0	-1.864735	-3.430354	-2.748932
13	1	0	-0.950181	-3.993039	-2.890586
14	6	0	1.074474	0.076577	-2.302928
15	6	0	1.424787	1.183296	-1.530730
16	6	0	2.646071	1.815054	-1.754879
17	1	0	2.916351	2.683289	-1.164620
18	6	0	3.512266	1.342161	-2.737932
19	1	0	4.463348	1.834131	-2.906139
20	6	0	3.155363	0.225305	-3.500815
21	1	0	3.831043	-0.151874	-4.259683
22	6	0	1.940577	-0.412305	-3.289394
23	1	0	1.658726	-1.281761	-3.866135
24	16	0	2.559092	-2.504386	0.004945
25	6	0	4.069652	-1.488550	-0.263726
26	1	0	3.899353	-0.765224	-1.062740
27	1	0	4.879961	-2.153928	-0.565849
28	6	0	4.452048	-0.748475	1.024394
29	1	0	4.699157	-1.479019	1.796124
30	6	0	5.648035	0.159666	0.773824
31	8	0	6.795677	-0.543650	0.703183
32	8	0	5.583365	1.353924	0.616854
33	7	0	3.289946	0.046320	1.485054
34	1	0	3.414873	0.387280	2.436197
35	1	0	3.196414	0.874889	0.896177
36	16	0	-0.579768	-1.997871	0.748856
37	6	0	-1.673383	-1.934443	2.248852
38	1	0	-2.019706	-2.946471	2.449668
39	1	0	-1.085344	-1.574181	3.091144
40	6	0	-2.860554	-1.007356	1.982594
41	1	0	-3.515050	-1.466672	1.235403
42	7	0	-2.366411	0.274091	1.432749
43	1	0	-1.687485	0.685338	2.087368
44	6	0	-3.704118	-0.755444	3.228661
45	8	0	-4.101003	-1.911545	3.795171
46	8	0	-3.999623	0.336098	3.640331
47	1	0	-5.210086	-3.816621	-2.317278
48	1	0	-3.135436	0.929688	1.316477
49	1	0	7.514939	0.074245	0.499931
50	1	0	-2.918290	-0.185497	-2.546442
51	7	0	-0.263851	2.978742	0.481054
52	6	0	-1.663292	3.372567	0.318283
53	1	0	-0.022390	2.791515	1.448592
54	1	0	0.331500	3.726693	0.133046
55	6	0	-1.923360	4.877849	0.501899
56	1	0	-2.240164	2.874904	1.107132
57	6	0	-2.258257	2.848160	-1.023471
58	16	0	-0.910039	5.963645	-0.589898
59	1	0	-1.650910	5.168140	1.519043
60	1	0	-2.975010	5.108047	0.337610
61	8	0	-2.112865	1.588105	-1.312816
62	8	0	-2.878436	3.613297	-1.751590
63	1	0	-1.499760	5.558189	-1.733306
64	17	0	0.509956	0.628986	2.930375
65	1	0	0.741362	1.567838	-0.778501
66	1	0	-4.641305	-1.696974	4.571490

HF=-3453.6842346\ZeroPoint=0.4602209\Thermal=0.5037553

G = -6.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.848447	0.729092	-0.100149
2	46	0	-1.719514	0.107816	-1.236935
3	7	0	1.722783	-0.616852	-1.416704
4	7	0	2.945581	-0.724007	-1.661456
5	6	0	3.864748	0.180058	-1.097224
6	6	0	5.050973	-0.378757	-0.602620
7	6	0	6.014775	0.446594	-0.034285
8	1	0	6.918652	0.011796	0.375957
9	6	0	5.827313	1.830204	-0.008832
10	6	0	4.672640	2.387061	-0.559480
11	1	0	4.546233	3.463620	-0.579470
12	6	0	3.683337	1.570457	-1.099695
13	1	0	2.804944	1.998185	-1.563174
14	6	0	0.861370	-1.570864	-2.065961
15	6	0	-0.537825	-1.381727	-2.048380
16	6	0	-1.289132	-2.373267	-2.713727
17	1	0	-2.368451	-2.270962	-2.767556
18	6	0	-0.710544	-3.483934	-3.314801
19	1	0	-1.337667	-4.222128	-3.803552
20	6	0	0.678732	-3.655602	-3.278630
21	1	0	1.139587	-4.529493	-3.723722
22	6	0	1.462148	-2.698772	-2.664236
23	1	0	2.535882	-2.814254	-2.614783
24	16	0	-3.344407	1.635734	-0.400272
25	6	0	-4.594023	0.346472	-0.004911

26	1	0	-5.062341	0.006078	-0.932772
27	1	0	-5.366049	0.779964	0.631841
28	6	0	-3.928518	-0.827112	0.719309
29	1	0	-3.585546	-0.488281	1.699227
30	6	0	-4.906865	-1.971706	0.908710
31	8	0	-5.902894	-1.640387	1.752082
32	8	0	-4.836752	-3.044094	0.354608
33	7	0	-2.729222	-1.318413	-0.016588
34	1	0	-2.013484	-1.526301	0.686692
35	1	0	-2.958175	-2.189809	-0.494010
36	16	0	-0.170232	1.774531	-1.954035
37	6	0	-0.692084	3.355926	-1.130410
38	1	0	-0.279259	4.177459	-1.713695
39	1	0	-1.777970	3.417183	-1.177455
40	6	0	-0.183127	3.448766	0.316572
41	1	0	0.870394	3.747221	0.290359
42	7	0	-0.243412	2.138187	1.006629
43	1	0	-1.210327	1.777337	1.012905
44	6	0	-0.891584	4.516777	1.150098
45	8	0	-1.169221	5.616425	0.422149
46	8	0	-1.121159	4.407960	2.325001
47	1	0	6.589152	2.472898	0.416799
48	1	0	-0.011632	2.238342	1.994853
49	1	0	-6.501790	-2.399762	1.817135
50	1	0	5.176830	-1.454343	-0.639259
51	7	0	1.531630	-0.202019	1.704801
52	6	0	2.562764	-1.253464	1.812974
53	1	0	1.817621	0.559936	2.316510
54	1	0	0.608055	-0.511020	2.090258
55	6	0	2.829885	-1.663527	3.278394
56	1	0	3.496669	-0.851872	1.416287
57	6	0	2.256193	-2.485630	0.975500
58	16	0	1.522044	-2.645957	4.113561
59	1	0	3.053934	-0.762047	3.855642
60	1	0	3.717271	-2.298300	3.298485
61	8	0	0.950943	-2.636228	0.721464
62	8	0	3.116961	-3.241678	0.597651
63	1	0	0.481205	-1.796574	3.897373
64	17	0	-1.273751	-0.397501	2.850352
65	1	0	0.834479	-3.428303	0.173422
66	1	0	-1.595488	6.262253	1.006910

HF=-3453.661093\ZeroPoint=0.4609569\Thermal=0.5037741

G = 11.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.946301	0.732992	-0.070606
2	46	0	-1.496006	-0.084228	-1.440990
3	7	0	2.087428	-0.619650	-1.201131
4	7	0	3.317413	-0.834434	-1.110991
5	6	0	4.080575	-0.135384	-0.162001
6	6	0	5.057313	-0.889106	0.504582
7	6	0	5.837418	-0.288278	1.484473
8	1	0	6.568213	-0.877319	2.025542
9	6	0	5.689205	1.072975	1.761667
10	6	0	4.762906	1.835653	1.049713
11	1	0	4.679076	2.900148	1.235893
12	6	0	3.951926	1.238821	0.089278
13	1	0	3.260550	1.830352	-0.497395
14	6	0	1.422996	-1.333347	-2.263449
15	6	0	0.050991	-1.627704	-2.101972
16	6	0	-0.539787	-2.413746	-3.105577
17	1	0	-1.574741	-2.720060	-2.998640
18	6	0	0.165593	-2.817090	-4.236050
19	1	0	-0.326223	-3.402723	-5.004620
20	6	0	1.509721	-2.466450	-4.378865
21	1	0	2.061115	-2.768819	-5.261561
22	6	0	2.150982	-1.739540	-3.383887
23	1	0	3.198544	-1.483016	-3.469753
24	16	0	-3.146878	1.447296	-0.866777
25	6	0	-4.312113	0.317683	0.009015
26	1	0	-5.077768	-0.023391	-0.694040
27	1	0	-4.792898	0.880581	0.808831
28	6	0	-3.552416	-0.868851	0.597199
29	1	0	-2.887583	-0.513982	1.394199
30	6	0	-4.511558	-1.900865	1.168760
31	8	0	-5.154512	-1.433444	2.250934
32	8	0	-4.697515	-2.996738	0.694925
33	7	0	-2.715851	-1.502322	-0.458280
34	1	0	-2.075795	-2.163437	-0.009640
35	1	0	-3.314291	-2.040691	-1.084018
36	16	0	0.092147	1.603981	-2.098453
37	6	0	-0.493537	3.251537	-1.488119
38	1	0	-0.053600	4.009971	-2.133031
39	1	0	-1.576086	3.298949	-1.593123
40	6	0	-0.064198	3.488233	-0.033154
41	1	0	0.998328	3.753435	-0.027557
42	7	0	-0.221466	2.257733	0.773601
43	1	0	-1.195145	1.925078	0.733649
44	6	0	-0.785623	4.665273	0.623572
45	8	0	-0.887965	5.710742	-0.226898
46	8	0	-1.168237	4.680499	1.760586
47	1	0	6.311242	1.542738	2.514589
48	1	0	-0.080173	2.429822	1.771652
49	1	0	-5.746649	-2.130020	2.573273
50	1	0	5.155213	-1.941565	0.267242
51	7	0	1.208041	-0.225657	1.821169
52	6	0	1.697625	-1.627144	1.910959
53	1	0	1.784280	0.352770	2.430334
54	1	0	0.240497	-0.139892	2.204240
55	6	0	1.560891	-2.212821	3.328652
56	1	0	2.763913	-1.610519	1.679260
57	6	0	1.048262	-2.536941	0.849193
58	16	0	-0.121817	-2.706245	3.875491
59	1	0	1.997074	-1.519684	4.053541
60	1	0	2.144152	-3.134814	3.358424
61	8	0	-0.126955	-2.140733	0.442621
62	8	0	1.676133	-3.493885	0.433750
63	1	0	-0.700376	-1.476062	3.797363
64	17	0	-1.492584	0.640769	3.087143
65	1	0	-0.170167	-1.889401	-0.794239
66	1	0	-1.325157	6.436189	0.245507

HF=-3453.6283117\ZeroPoint=0.4565721\Thermal=0.4988432

G = 3.5 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.846296	-0.641995	0.436732
2	46	0	1.678770	-0.926200	-1.170125
3	7	0	-1.998663	-0.604263	-1.345160
4	7	0	-3.218797	-0.462621	-1.557248
5	6	0	-4.082557	-0.143802	-0.493085
6	6	0	-5.110282	0.756204	-0.806048
7	6	0	-5.986174	1.165136	0.191090
8	1	0	-6.756954	1.891732	-0.035554
9	6	0	-5.877808	0.635699	1.478999
10	6	0	-4.894278	-0.311337	1.769105
11	1	0	-4.837568	-0.749444	2.758851
12	6	0	-3.989905	-0.703878	0.788468
13	1	0	-3.238824	-1.456667	0.994691
14	6	0	-1.253001	-1.063623	-2.495176
15	6	0	-0.117751	-0.339881	-2.897442
16	6	0	0.706009	-0.890057	-3.885449
17	1	0	1.554823	-0.321503	-4.246400
18	6	0	0.398526	-2.130380	-4.459485
19	1	0	1.050527	-2.554768	-5.213187
20	6	0	-0.754830	-2.801518	-4.074978
21	1	0	-1.004470	-3.755120	-4.524999
22	6	0	-1.591147	-2.270359	-3.086963
23	1	0	-2.467843	-2.808112	-2.749104
24	16	0	3.218752	-1.112813	0.520585
25	6	0	4.046360	0.536423	0.414568
26	1	0	4.989858	0.419509	-0.124449
27	1	0	4.239351	0.871540	1.433804
28	6	0	3.125403	1.531284	-0.281475
29	1	0	2.288960	1.771038	0.380792
30	6	0	3.871324	2.811859	-0.625566
31	8	0	4.172280	3.521364	0.470491
32	8	0	4.184500	3.133412	-1.747970
33	7	0	2.562018	0.946867	-1.530628
34	1	0	1.746038	1.539019	-1.764412
35	1	0	3.251755	1.000312	-2.278907
36	16	0	0.231835	-2.655834	-0.318491
37	6	0	0.865317	-3.275316	1.305515
38	1	0	0.578550	-4.321835	1.387846
39	1	0	1.952429	-3.215000	1.310624
40	6	0	0.260895	-2.468072	2.459422
41	1	0	-0.786588	-2.765583	2.577273
42	7	0	0.289570	-1.022329	2.148052
43	1	0	1.248617	-0.724301	1.912554
44	6	0	0.918152	-2.748064	3.811676
45	8	0	1.199612	-4.062600	3.955829
46	8	0	1.111846	-1.920125	4.657447
47	1	0	-6.572127	0.945910	2.251150
48	1	0	0.069352	-0.441812	2.962560
49	1	0	4.640422	4.323239	0.191867
50	1	0	-5.165587	1.156359	-1.810811
51	7	0	-1.293743	1.302170	1.147784
52	6	0	-1.843399	2.319914	0.214237
53	1	0	-1.891055	1.250416	1.971821
54	1	0	-0.357019	1.593490	1.502526
55	6	0	-1.944097	3.710197	0.867076
56	1	0	-2.862894	2.020404	-0.027665
57	6	0	-1.045913	2.350081	-1.114041
58	16	0	-0.387729	4.655886	1.114385
59	1	0	-2.480989	3.633059	1.817834
60	1	0	-2.540784	4.333633	0.198978
61	8	0	0.159578	1.964627	-1.027479
62	8	0	-1.672344	2.697112	-2.121166
63	1	0	0.257796	3.748898	1.894687
64	17	0	1.316087	1.780024	2.798093
65	1	0	0.010828	0.673549	-2.526557
66	1	0	1.578815	-4.189358	4.839509

HF=-3453.6441904\ZeroPoint=0.4606952\Thermal=0.5035095

G = -18.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.473137	-0.128819	-0.205803
2	46	0	1.148124	1.537785	-0.457329
3	7	0	-2.286587	1.714992	0.308700
4	7	0	-3.522232	1.796449	0.494590
5	6	0	-4.340782	0.704409	0.131449
6	6	0	-4.330907	0.194051	-1.174312
7	6	0	-5.200380	-0.839968	-1.509462
8	1	0	-5.207112	-1.225663	-2.522814
9	6	0	-6.064808	-1.370791	-0.552570
10	6	0	-6.084878	-0.838967	0.737912
11	1	0	-6.758985	-1.245958	1.482365
12	6	0	-5.244974	0.215421	1.076466
13	1	0	-5.244614	0.634772	2.074427
14	6	0	-1.534747	2.920265	0.505372
15	6	0	-0.159528	2.963031	0.194927
16	6	0	0.448182	4.235933	0.300277
17	1	0	1.500412	4.334192	0.071851
18	6	0	-0.239870	5.367297	0.711596
19	1	0	0.279890	6.317472	0.775547
20	6	0	-1.592904	5.279387	1.058593
21	1	0	-2.135468	6.152310	1.402434
22	6	0	-2.235095	4.065600	0.947588
23	1	0	-3.285282	3.974764	1.186063
24	16	0	2.532238	1.992907	1.411844
25	6	0	4.120944	1.254019	0.809664
26	1	0	4.254986	0.268786	1.253092
27	1	0	4.936098	1.907711	1.115394
28	6	0	4.101760	1.130699	-0.714610
29	1	0	4.081877	2.138891	-1.144093
30	6	0	5.340809	0.451633	-1.293717
31	8	0	6.479374	0.906226	-0.728430
32	8	0	5.321500	-0.358399	-2.185872
33	7	0	2.879526	0.418514	-1.147199
34	1	0	2.927297	0.264633	-2.151172
35	1	0	2.891150	-0.509136	-0.688347

36	16	0	-0.419739	0.713888	-2.114516
37	6	0	0.252456	-0.922810	-2.701400
38	1	0	0.403607	-0.860795	-3.777347
39	1	0	1.204466	-1.135005	-2.218930
40	6	0	-0.740894	-2.024437	-2.349481
41	1	0	-1.696472	-1.810687	-2.842080
42	7	0	-0.966584	-2.020512	-0.886768
43	1	0	-0.115030	-2.356061	-0.386846
44	6	0	-0.346684	-3.429595	-2.809950
45	8	0	-0.689692	-4.433460	-2.244797
46	8	0	0.375982	-3.413987	-3.948733
47	1	0	-6.731467	-2.184068	-0.814694
48	1	0	0.565857	-4.333633	-4.192001
49	1	0	-1.706724	-2.673392	-0.635592
50	1	0	7.221613	0.458586	-1.162749
51	1	0	-3.677832	0.632021	-1.918391
52	17	0	-2.062751	-1.051361	1.927717
53	1	0	1.570454	0.172875	2.225624
54	7	0	1.023667	-0.586723	2.719238
55	6	0	1.703763	-1.941044	2.651118
56	6	0	0.803362	-2.988711	3.291142
57	1	0	2.649620	-1.843575	3.183886
58	6	0	2.013665	-2.184175	1.138146
59	16	0	1.607740	-4.637276	3.348901
60	1	0	-0.137652	-3.060095	2.747825
61	1	0	0.585944	-2.732453	4.332012
62	8	0	1.189246	-2.879908	0.500976
63	8	0	3.033037	-1.606736	0.715834
64	1	0	1.562967	-4.832704	2.014745
65	1	0	0.067132	-0.639551	2.312447
66	1	0	0.905728	-0.282225	3.686317

HF=-3453.6792311\ZeroPoint=0.4613645\Thermal=0.5040777

G = 4.2 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.882485	-0.328956	0.343691
2	46	0	1.234238	0.885739	-0.971491
3	7	0	-2.360465	1.564162	-0.341973
4	7	0	-3.512019	1.850178	-0.732164
5	6	0	-4.456829	0.811404	-0.885340
6	6	0	-4.223120	-0.292660	-1.715227
7	6	0	-5.220472	-1.251302	-1.865641
8	1	0	-5.052339	-2.097187	-2.522441
9	6	0	-6.429300	-1.124249	-1.182333
10	6	0	-6.658658	-0.011584	-0.371356
11	1	0	-7.598048	0.090991	0.158717
12	6	0	-5.688114	0.974735	-0.244881
13	1	0	-5.849303	1.844378	0.379364
14	6	0	-1.442543	2.673902	-0.228971
15	6	0	-0.092807	2.449605	0.147078
16	6	0	0.655509	3.617861	0.418540
17	1	0	1.666024	3.502080	0.789455
18	6	0	0.162537	4.901865	0.236542
19	1	0	0.791660	5.759825	0.444966
20	6	0	-1.146623	5.074710	-0.211966
21	1	0	-1.550892	6.068500	-0.366992
22	6	0	-1.950500	3.966325	-0.424503
23	1	0	-2.983031	4.087212	-0.719083
24	16	0	3.139686	2.256650	-0.778845
25	6	0	4.414147	0.955544	-1.024420
26	1	0	4.565850	0.394941	-0.098523
27	1	0	5.347044	1.440161	-1.309960
28	6	0	3.930622	0.019748	-2.123935
29	1	0	3.789193	0.599777	-3.041797
30	6	0	4.878947	-1.125623	-2.463571
31	8	0	6.144028	-0.692566	-2.634356
32	8	0	4.540345	-2.273828	-2.604006
33	7	0	2.622492	-0.527003	-1.703191
34	1	0	2.262634	-1.162044	-2.410482
35	1	0	2.754387	-1.063961	-0.826098
36	16	0	-0.523704	-0.708148	-1.496805
37	6	0	0.075207	-2.399003	-0.988766
38	1	0	0.322543	-2.959055	-1.888667
39	1	0	0.958868	-2.310120	-0.357004
40	6	0	-1.042765	-3.098275	-0.214283
41	1	0	-1.913071	-3.220568	-0.868922
42	7	0	-1.435160	-2.255391	0.935342
43	1	0	-0.613418	-2.158417	1.566372
44	6	0	-0.673424	-4.502217	0.266251
45	8	0	-0.994980	-4.955236	1.331818
46	8	0	0.006244	-5.190924	-0.673978
47	1	0	-7.196564	-1.881750	-1.292239
48	1	0	0.195985	-6.072605	-0.317421
49	1	0	-2.195104	-2.673444	1.468010
50	1	0	6.690216	-1.457466	-2.872751
51	1	0	-3.292692	-0.373626	-2.260336
52	17	0	-3.033522	0.053704	2.364650
53	1	0	0.242296	1.522532	1.074780
54	7	0	0.592695	0.982393	2.352853
55	6	0	1.956506	0.398014	2.335345
56	6	0	2.566180	0.339929	3.742173
57	1	0	2.582187	1.012740	1.687184
58	6	0	1.852526	-1.037535	1.750583
59	16	0	4.355878	-0.096052	3.744984
60	1	0	2.006100	-0.362185	4.362539
61	1	0	2.527001	1.327404	4.210529
62	8	0	0.890226	-1.715778	2.184207
63	8	0	2.733466	-1.400337	0.935087
64	1	0	4.243710	-1.184283	2.954694
65	1	0	-0.090071	0.275951	2.636492
66	1	0	0.518723	1.767805	2.995842

HF=-3453.6396421\ZeroPoint=0.457249\Thermal=0.4997837

G = 9.3 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	2.098464	0.547583	0.329704
2	46	0	-1.188657	-1.183160	-0.642235
3	7	0	2.717451	-1.422110	0.072388

4	7	0	3.858113	-1.874893	-0.180231
5	6	0	4.887848	-0.993998	-0.536673
6	6	0	4.703415	0.125930	-1.362144
7	6	0	5.797119	0.916191	-1.689066
8	1	0	5.663632	1.773686	-2.338154
9	6	0	7.062592	0.610433	-1.186353
10	6	0	7.246356	-0.518201	-0.385036
11	1	0	8.231045	-0.760130	-0.003486
12	6	0	6.168681	-1.339563	-0.085217
13	1	0	6.286724	-2.225042	0.526945
14	6	0	1.700501	-2.409426	0.280051
15	6	0	0.559175	-2.035024	1.028574
16	6	0	-0.425171	-2.992003	1.292453
17	1	0	-1.227192	-2.715409	1.964274
18	6	0	-0.305090	-4.290387	0.767741
19	1	0	-1.084529	-5.017469	0.957975
20	6	0	0.806715	-4.630192	0.010987
21	1	0	0.898318	-5.628661	-0.400383
22	6	0	1.816177	-3.694730	-0.236105
23	1	0	2.684385	-3.955043	-0.826409
24	16	0	-2.996462	-2.659824	-0.324962
25	6	0	-4.350618	-1.538523	-0.863228
26	1	0	-4.666385	-0.890382	-0.040327
27	1	0	-5.198796	-2.150787	-1.168241
28	6	0	-3.844804	-0.700975	-2.027946
29	1	0	-3.592311	-1.368746	-2.857854
30	6	0	-4.843810	0.321879	-2.560081
31	8	0	-6.046559	-0.237820	-2.795111
32	8	0	-4.586351	1.478415	-2.778079
33	7	0	-2.613751	-0.003837	-1.593669
34	1	0	-2.233421	0.544292	-2.360771
35	1	0	-2.813895	0.660447	-0.809718
36	16	0	0.544942	0.361751	-1.418233
37	6	0	-0.151984	2.085998	-1.316725
38	1	0	-0.368300	2.428836	-2.326992
39	1	0	-1.065121	2.066436	-0.718585
40	6	0	0.862646	3.016176	-0.646481
41	1	0	1.737447	3.138421	-1.294358
42	7	0	1.296607	2.416702	0.629572
43	1	0	0.460641	2.228812	1.235000
44	6	0	0.300285	4.418201	-0.413225
45	8	0	0.405337	5.031503	0.614502
46	8	0	-0.290660	4.903040	-1.526299
47	1	0	7.908535	1.241549	-1.433039
48	1	0	-0.621759	5.791619	-1.323683
49	1	0	1.933897	3.025027	1.140203
50	1	0	-6.633611	0.450966	-3.143410
51	1	0	3.724724	0.342933	-1.769599
52	17	0	3.637127	0.903033	2.061549
53	1	0	0.525573	-1.084575	1.551982
54	7	0	-1.777497	-0.664506	3.311317
55	6	0	-2.720115	0.045931	2.442425
56	6	0	-3.894184	0.690060	3.215410
57	1	0	-3.142335	-0.665594	1.729497
58	6	0	-1.966652	1.127637	1.633422
59	16	0	-5.347219	1.168295	2.182666
60	1	0	-3.548690	1.552346	3.790501
61	1	0	-4.299246	-0.042299	3.918344
62	8	0	-0.842263	1.483175	2.051289
63	8	0	-2.556626	1.587662	0.609446
64	1	0	-4.633152	1.884066	1.287395
65	1	0	-1.069889	-0.011275	3.637752
66	1	0	-2.242712	-1.072377	4.115381

HF=-3453.6621868\ZeroPoint=0.4600714\Thermal=0.5033447

G = -17.5 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.834268	0.239517	0.456945
2	46	0	-1.123975	-0.473468	-1.583622
3	7	0	1.965426	-1.630365	-0.359380
4	7	0	3.006000	-2.173323	-0.772107
5	6	0	4.173942	-1.373039	-0.903149
6	6	0	4.223628	-0.275221	-1.767636
7	6	0	5.416667	0.428818	-1.903554
8	1	0	5.463009	1.271996	-2.583435
9	6	0	6.545459	0.052221	-1.176299
10	6	0	6.488470	-1.053192	-0.326943
11	1	0	7.364385	-1.352858	0.236426
12	6	0	5.311390	-1.784837	-0.206223
13	1	0	5.253717	-2.650526	0.441763
14	6	0	0.838216	-2.484673	-0.118736
15	6	0	-0.484391	-2.099940	-0.446734
16	6	0	-1.459526	-3.005305	0.017372
17	1	0	-2.505353	-2.803810	-0.165068
18	6	0	-1.166471	-4.172942	0.716496
19	1	0	-1.983974	-4.802223	1.051601
20	6	0	0.152780	-4.521598	0.991260
21	1	0	0.395067	-5.421512	1.544125
22	6	0	1.155306	-3.669354	0.569133
23	1	0	2.191848	-3.869323	0.805776
24	16	0	-3.106672	-1.619339	-2.142307
25	6	0	-4.037047	-0.285932	-3.016482
26	1	0	-5.094834	-0.408495	-2.781844
27	1	0	-3.907359	-0.374440	-4.099808
28	6	0	-3.581614	1.094586	-2.568197
29	1	0	-4.078500	1.866743	-3.175026
30	6	0	-3.983168	1.381981	-1.115792
31	8	0	-3.031255	2.011148	-0.428673
32	8	0	-5.072283	1.095254	-0.676613
33	7	0	-2.105603	1.173135	-2.735283
34	1	0	-1.867740	1.053938	-3.717445
35	1	0	-1.771464	2.086456	-2.444681
36	16	0	0.826883	1.004166	-1.460664
37	6	0	0.252122	2.612284	-0.723010
38	1	0	0.051036	3.316412	-1.530144
39	1	0	-0.659648	2.442052	-0.152378
40	6	0	1.361118	3.161313	0.177881
41	1	0	2.259924	3.319148	-0.426104
42	7	0	1.671970	2.168558	1.227903
43	1	0	0.890809	2.107190	1.892871
44	6	0	0.990236	4.505774	0.797964
45	8	0	0.977476	4.740798	1.976866

46	8	0	0.694223	5.416959	-0.155265
47	1	0	7.469464	0.609039	-1.280675
48	1	0	0.481398	6.253008	0.287405
49	1	0	2.500791	2.425147	1.758832
50	1	0	-3.256328	2.008738	0.570469
51	1	0	3.347400	0.006704	-2.335156
52	17	0	2.417032	-0.550536	2.629822
53	1	0	0.181135	-0.495936	2.820857
54	7	0	-3.459847	1.806154	2.197429
55	6	0	-2.920992	0.510455	2.662067
56	1	0	-4.455118	1.855365	2.395918
57	1	0	-2.996370	2.571882	2.679876
58	6	0	-3.502936	-0.636306	1.807184
59	1	0	-3.173488	0.320886	3.713331
60	6	0	-1.397960	0.588400	2.606414
61	16	0	-3.682261	-2.229186	2.692661
62	1	0	-2.929597	-0.779695	0.891126
63	1	0	-4.514528	-0.367510	1.499408
64	8	0	-0.819276	1.637066	2.382867
65	8	0	-0.805991	-0.564643	2.858227
66	1	0	-2.366085	-2.500483	2.779785

HF=-3453.6795841\ZeroPoint=0.4609432\Thermal=0.5034082

G = 3.5 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.927235	0.387985	0.563316
2	46	0	-1.068386	-0.697831	-1.308922
3	7	0	2.199838	-1.563018	-0.017466
4	7	0	3.253362	-2.079910	-0.438424
5	6	0	4.372236	-1.262039	-0.709478
6	6	0	4.314171	-0.131279	-1.532786
7	6	0	5.480700	0.581727	-1.789970
8	1	0	5.443202	1.447132	-2.441746
9	6	0	6.690314	0.187688	-1.219111
10	6	0	6.742641	-0.951111	-0.414088
11	1	0	7.681695	-1.263918	0.026778
12	6	0	5.593176	-1.696640	-0.183777
13	1	0	5.616702	-2.587751	0.430819
14	6	0	1.133651	-2.487800	0.291631
15	6	0	-0.227137	-2.082019	0.285042
16	6	0	-1.148413	-3.059090	0.722470
17	1	0	-2.191657	-2.781882	0.794232
18	6	0	-0.779241	-4.340436	1.108287
19	1	0	-1.534473	-5.042155	1.443040
20	6	0	0.565156	-4.702083	1.081504
21	1	0	0.878189	-5.691493	1.394909
22	6	0	1.517909	-3.774794	0.684901
23	1	0	2.569321	-4.024535	0.704435
24	16	0	-2.956665	-2.079816	-1.544674
25	6	0	-3.834422	-1.161951	-2.885512
26	1	0	-4.906084	-1.299179	-2.737728
27	1	0	-3.559754	-1.565016	-3.864778
28	6	0	-3.504749	0.319970	-2.828789
29	1	0	-3.932430	0.840269	-3.697640
30	6	0	-4.112284	0.988314	-1.585748
31	8	0	-3.266371	1.796582	-0.964351
32	8	0	-5.259870	0.787850	-1.263155
33	7	0	-2.018396	0.464211	-2.841290
34	1	0	-1.648757	0.156010	-3.738383
35	1	0	-1.765612	1.441102	-2.717354
36	16	0	0.780080	0.858346	-1.399587
37	6	0	0.159161	2.544831	-0.929025
38	1	0	0.057863	3.141284	-1.834698
39	1	0	-0.806601	2.444037	-0.439871
40	6	0	1.178284	3.200060	0.012483
41	1	0	2.114940	3.355125	-0.532994
42	7	0	1.446975	2.307650	1.158594
43	1	0	0.561402	2.161651	1.671927
44	6	0	0.720328	4.573797	0.496411
45	8	0	0.704221	4.928980	1.644098
46	8	0	0.364479	5.365730	-0.541056
47	1	0	7.592348	0.756549	-1.412572
48	1	0	0.111573	6.229421	-0.180209
49	1	0	2.137139	2.696730	1.797374
50	1	0	-3.609408	2.034946	-0.005315
51	1	0	3.380631	0.160081	-1.992346
52	17	0	3.166443	0.046040	2.526865
53	1	0	-0.698595	-0.939062	0.922321
54	7	0	-3.845137	2.192949	1.551702
55	6	0	-3.370936	0.956016	2.228315
56	1	0	-4.804090	2.398271	1.817613
57	1	0	-3.254423	2.967528	1.846290
58	6	0	-4.210368	-0.248483	1.782768
59	1	0	-3.443918	1.058205	3.318484
60	6	0	-1.865815	0.809436	1.901200
61	16	0	-4.211568	-1.637647	2.986556
62	1	0	-3.889702	-0.617026	0.808920
63	1	0	-5.259191	0.040978	1.693260
64	8	0	-1.214844	1.849109	1.736679
65	8	0	-1.431559	-0.392583	1.841523
66	1	0	-2.877548	-1.824425	2.967645

HF=-3453.6421267\ZeroPoint=0.4560732\Thermal=0.4979856

G = -14.3 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.959518	0.501745	0.328550
2	46	0	-1.309494	-1.163501	-0.940085
3	7	0	2.481144	-1.511572	0.202846
4	7	0	3.612989	-2.028326	0.054916
5	6	0	4.711635	-1.218013	-0.261406
6	6	0	4.649205	-0.135056	-1.151664
7	6	0	5.805041	0.581299	-1.432369
8	1	0	5.765495	1.410136	-2.129514
9	6	0	7.012074	0.239238	-0.821286
10	6	0	7.075181	-0.853947	0.045087
11	1	0	8.014645	-1.124832	0.511805
12	6	0	5.935579	-1.603239	0.301654
13	1	0	5.960604	-2.460194	0.963291

14	6	0	1.402059	-2.439874	0.368159
15	6	0	0.215177	-1.960336	0.969015
16	6	0	-0.846600	-2.846896	1.172587
17	1	0	-1.715938	-2.510200	1.723723
18	6	0	-0.744392	-4.184461	0.749645
19	1	0	-1.580589	-4.855772	0.895791
20	6	0	0.422811	-4.629489	0.147266
21	1	0	0.502693	-5.657728	-0.185655
22	6	0	1.502021	-3.762154	-0.048615
23	1	0	2.411709	-4.104601	-0.523343
24	16	0	-3.230320	-2.479416	-0.669436
25	6	0	-4.239070	-1.850643	-2.081374
26	1	0	-5.284398	-1.864958	-1.770102
27	1	0	-4.112196	-2.508032	-2.945878
28	6	0	-3.846138	-0.431173	-2.425514
29	1	0	-4.294115	-0.130763	-3.383410
30	6	0	-4.304048	0.624067	-1.384483
31	8	0	-3.448229	1.558560	-1.179567
32	8	0	-5.411945	0.506939	-0.867578
33	7	0	-2.355485	-0.352928	-2.556242
34	1	0	-2.031453	-0.819309	-3.400791
35	1	0	-2.116471	0.636802	-2.602020
36	16	0	0.540521	0.325149	-1.529468
37	6	0	-0.160309	2.048109	-1.459216
38	1	0	-0.388752	2.368368	-2.474659
39	1	0	-1.074335	2.041602	-0.871661
40	6	0	0.873446	2.984576	-0.836370
41	1	0	1.752657	3.035401	-1.489046
42	7	0	1.300989	2.449965	0.475089
43	1	0	0.463556	2.466252	1.094341
44	6	0	0.395008	4.428383	-0.677447
45	8	0	0.765667	5.165134	0.196451
46	8	0	-0.436745	4.803278	-1.673520
47	1	0	7.906556	0.813653	-1.032866
48	1	0	-0.662698	5.735219	-1.529990
49	1	0	2.011297	3.041277	0.903709
50	1	0	-3.765380	2.162149	0.123789
51	1	0	3.715539	0.111259	-1.639915
52	17	0	3.411445	0.858396	2.134781
53	1	0	0.172414	-0.969775	1.409441
54	7	0	-3.890406	2.527428	1.162008
55	6	0	-3.256480	1.561937	2.128878
56	1	0	-4.881369	2.673519	1.344689
57	1	0	-3.362770	3.401852	1.227358
58	6	0	-3.893249	0.179116	2.019354
59	1	0	-3.402937	1.964291	3.135299
60	6	0	-1.727889	1.602360	1.821683
61	16	0	-3.547184	-0.866436	3.490776
62	1	0	-3.556763	-0.339589	1.125114
63	1	0	-4.980935	0.251524	1.962161
64	8	0	-1.299595	2.732177	1.455023
65	8	0	-1.080805	0.551232	1.955025
66	1	0	-2.207766	-0.721578	3.409223

HF=-3453.6730648\ZeroPoint=0.4606143\Thermal=0.5030662

G = -6.1 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.817255	0.296192	0.310634
2	46	0	1.312980	-1.463365	-0.055856
3	7	0	-1.972294	-0.900438	-1.347248
4	7	0	-2.933587	-1.559989	-1.781441
5	6	0	-4.070938	-1.758333	-0.964684
6	6	0	-4.002629	-2.172020	0.371297
7	6	0	-5.182449	-2.392219	1.074003
8	1	0	-5.133561	-2.731348	2.102304
9	6	0	-6.419463	-2.186768	0.462608
10	6	0	-6.479659	-1.793145	-0.874663
11	1	0	-7.438769	-1.644215	-1.356414
12	6	0	-5.308278	-1.607797	-1.599576
13	1	0	-5.334083	-1.321304	-2.643713
14	6	0	-0.892219	-0.669559	-2.283131
15	6	0	0.466566	-0.722425	-1.873720
16	6	0	1.358141	-0.370513	-2.916948
17	1	0	2.424089	-0.370656	-2.739699
18	6	0	0.967162	0.012770	-4.198276
19	1	0	1.722681	0.280870	-4.930055
20	6	0	-0.385041	0.056256	-4.535825
21	1	0	-0.708899	0.360630	-5.524210
22	6	0	-1.313978	-0.298345	-3.572257
23	1	0	-2.374742	-0.259749	-3.782812
24	16	0	2.355445	-2.594530	1.768216
25	6	0	4.046459	-2.698127	1.051990
26	1	0	4.122737	-3.558295	0.379136
27	1	0	4.764210	-2.830008	1.862802
28	6	0	4.348601	-1.413384	0.284610
29	1	0	4.312082	-0.563666	0.968425
30	6	0	5.724474	-1.472420	-0.362127
31	8	0	6.708637	-1.363539	0.553317
32	8	0	5.930953	-1.633247	-1.541432
33	7	0	3.315764	-1.184318	-0.752639
34	1	0	3.332639	-0.181938	-0.968756
35	1	0	3.557992	-1.714121	-1.588048
36	16	0	-0.575818	-1.344044	1.341232
37	6	0	0.094910	-0.274274	2.713295
38	1	0	0.383189	-0.925853	3.534065
39	1	0	0.968286	0.256321	2.338175
40	6	0	-0.988602	0.720901	3.124822
41	1	0	-1.870231	0.179257	3.483047
42	7	0	-1.373048	1.514772	1.936669
43	1	0	-0.547673	2.030403	1.599776
44	6	0	-0.540862	1.641654	4.256406
45	8	0	-0.595745	2.842951	4.220677
46	8	0	-0.106355	0.936632	5.320334
47	1	0	-7.333837	-2.350392	1.021085
48	1	0	0.158937	1.566331	6.008184
49	1	0	-2.102214	2.191973	2.148637
50	1	0	7.555578	-1.442762	0.088477
51	1	0	-3.045686	-2.356513	0.837982
52	17	0	-2.982075	2.086340	-0.775246
53	1	0	-0.180420	1.524902	-1.824396
54	7	0	0.010557	2.532828	-1.752817
55	6	0	1.482694	2.764527	-1.578380

56	6	0	1.808287	4.255542	-1.583733
57	1	0	1.981618	2.282841	-2.417768
58	6	0	1.931693	2.060236	-0.254381
59	16	0	0.875698	5.192011	-0.277575
60	1	0	1.569478	4.696643	-2.553896
61	1	0	2.880205	4.356561	-1.413471
62	8	0	1.075592	2.070105	0.659554
63	8	0	3.086454	1.603060	-0.275345
64	1	0	0.648907	6.281036	-1.038723
65	1	0	-0.512029	2.859991	-0.929758
66	1	0	-0.390996	2.987213	-2.573436

HF=-3453.6571312\ZeroPoint=0.4610922\Thermal=0.5047559

G = 5.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.750081	0.166366	-0.034406
2	46	0	-1.572015	-0.709483	-0.790570
3	7	0	1.839877	-1.912406	0.096841
4	7	0	2.894042	-2.574809	-0.032105
5	6	0	4.044954	-1.933385	-0.524368
6	6	0	4.030657	-1.130251	-1.673952
7	6	0	5.219445	-0.563824	-2.121919
8	1	0	5.217084	0.040739	-3.021593
9	6	0	6.408293	-0.777768	-1.425324
10	6	0	6.418772	-1.597391	-0.294812
11	1	0	7.343458	-1.770273	0.242841
12	6	0	5.246735	-2.201763	0.139942
13	1	0	5.234305	-2.843643	1.011822
14	6	0	0.676962	-2.658599	0.522379
15	6	0	-0.491560	-1.959276	0.913687
16	6	0	-1.495160	-2.761571	1.502467
17	1	0	-2.367124	-2.275084	1.927777
18	6	0	-1.416497	-4.145240	1.588370
19	1	0	-2.226090	-4.713709	2.033361
20	6	0	-0.286330	-4.799820	1.090289
21	1	0	-0.218303	-5.881066	1.122820
22	6	0	0.765350	-4.059275	0.576216
23	1	0	1.662700	-4.550482	0.226198
24	16	0	-2.719822	-0.148493	-2.737623
25	6	0	-4.425797	-0.526517	-2.158941
26	1	0	-4.649835	-1.586050	-2.315718
27	1	0	-5.122491	0.067725	-2.752046
28	6	0	-4.548958	-0.176923	-0.680014
29	1	0	-4.380601	0.890158	-0.526016
30	6	0	-5.924653	-0.546857	-0.145498
31	8	0	-6.873491	0.297622	-0.594207
32	8	0	-6.157687	-1.496626	0.562758
33	7	0	-3.503155	-0.891762	0.090317
34	1	0	-3.434497	-0.403450	0.992050
35	1	0	-3.800478	-1.852253	0.251260
36	16	0	0.375585	0.021348	-1.891271
37	6	0	0.010196	1.842923	-2.083054
38	1	0	-0.133174	2.043789	-3.141796
39	1	0	-0.902621	2.062086	-1.533477
40	6	0	1.179282	2.646032	-1.514983
41	1	0	2.079246	2.455139	-2.110001
42	7	0	1.433177	2.208595	-0.126295
43	1	0	0.566485	2.329881	0.436025
44	6	0	0.946929	4.154841	-1.562179
45	8	0	1.164585	4.904892	-0.648377
46	8	0	0.512393	4.550589	-2.776984
47	1	0	7.328555	-0.322009	-1.771881
48	1	0	0.400957	5.513523	-2.753279
49	1	0	2.173658	2.750740	0.313524
50	1	0	-7.726832	0.001588	-0.242066
51	1	0	3.113809	-0.998581	-2.232290
52	17	0	3.128229	0.428316	1.896582
53	1	0	-0.352792	-0.753444	1.661001
54	7	0	-0.095907	0.090206	2.627774
55	6	0	-1.213111	0.981946	3.008660
56	6	0	-0.763329	2.107644	3.956705
57	1	0	-1.949424	0.376951	3.542414
58	6	0	-1.903445	1.503263	1.714923
59	16	0	0.633257	3.165721	3.378273
60	1	0	-0.495913	1.696115	4.932803
61	1	0	-1.602041	2.789572	4.108066
62	8	0	-1.148353	1.966510	0.826271
63	8	0	-3.145504	1.366546	1.681049
64	1	0	1.630060	2.294039	3.641213
65	1	0	0.701325	0.630479	2.285128
66	1	0	0.251130	-0.451864	3.417466

HF=-3453.6371721\ZeroPoint=0.4568772\Thermal=0.4996478

G = -34.1 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.798737	-0.226143	0.320921
2	46	0	-1.566711	0.094756	-0.954799
3	7	0	1.006994	-2.067675	0.855486
4	7	0	1.553413	-3.186422	0.794423
5	6	0	2.821377	-3.295313	0.179129
6	6	0	3.086082	-2.802367	-1.103974
7	6	0	4.347790	-2.997473	-1.657936
8	1	0	4.551316	-2.636923	-2.659734
9	6	0	5.340838	-3.657788	-0.935560
10	6	0	5.061957	-4.161210	0.336445
11	1	0	5.829816	-4.681967	0.896152
12	6	0	3.794378	-4.009838	0.884885
13	1	0	3.553900	-4.403275	1.864664
14	6	0	-0.321756	-2.073966	1.410514
15	6	0	-0.682847	-1.064465	2.301366
16	6	0	-1.971890	-1.059179	2.825103
17	1	0	-2.252693	-0.275739	3.518548
18	6	0	-2.892959	-2.035770	2.444765
19	1	0	-3.905213	-2.009993	2.831222
20	6	0	-2.519477	-3.033512	1.540240
21	1	0	-3.238710	-3.782885	1.231196
22	6	0	-1.230297	-3.062228	1.022476
23	1	0	-0.932092	-3.809983	0.299812

24	16	0	-2.337426	-1.435483	-2.502754
25	6	0	-3.990335	-1.733623	-1.739716
26	1	0	-3.906514	-2.487272	-0.951775
27	1	0	-4.662362	-2.109101	-2.512980
28	6	0	-4.535831	-0.433537	-1.134381
29	1	0	-4.708487	0.291001	-1.930907
30	6	0	-5.840841	-0.717999	-0.404062
31	8	0	-6.889272	-0.749141	-1.253072
32	8	0	-5.933803	-0.940250	0.778086
33	7	0	-3.531245	0.113701	-0.204049
34	1	0	-3.690898	1.090098	0.077775
35	1	0	-3.524928	-0.438152	0.654556
36	16	0	0.638326	-0.078595	-1.738500
37	6	0	1.085012	1.683429	-2.111350
38	1	0	1.013635	1.835225	-3.186225
39	1	0	0.380927	2.336390	-1.596216
40	6	0	2.501850	1.939674	-1.604138
41	1	0	3.194610	1.250783	-2.099349
42	7	0	2.526024	1.658230	-0.153218
43	1	0	1.906965	2.333206	0.312303
44	6	0	3.024990	3.347157	-1.880916
45	8	0	3.592981	4.031308	-1.069030
46	8	0	2.816251	3.712497	-3.159619
47	1	0	6.324887	-3.795794	-1.368468
48	1	0	3.190023	4.598987	-3.283090
49	1	0	3.454307	1.786050	0.246734
50	1	0	-7.679590	-0.983416	-0.742383
51	1	0	2.305207	-2.318562	-1.673745
52	17	0	3.038072	-0.129290	2.323717
53	1	0	0.021140	-0.297689	2.590735
54	7	0	0.072896	2.206150	2.975653
55	6	0	-0.959063	3.023541	2.356900
56	6	0	-0.549916	4.450857	1.924012
57	1	0	-1.763115	3.166484	3.086137
58	6	0	-1.620642	2.297441	1.167951
59	16	0	0.837893	4.566670	0.709821
60	1	0	-0.268873	5.043875	2.796252
61	1	0	-1.400617	4.941291	1.446709
62	8	0	-0.847183	1.519195	0.504753
63	8	0	-2.813227	2.537810	0.935077
64	1	0	1.855970	4.594987	1.591392
65	1	0	0.758367	1.882896	2.302489
66	1	0	0.558868	2.697510	3.718175

HF=-3453.7021716\ZeroPoint=0.4603064\Thermal=0.5038509

G = -12.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	2.312372	0.773937	-0.457848
2	46	0	-0.659760	-1.399849	-0.167791
3	7	0	2.497325	-0.318862	1.248925
4	7	0	3.521605	-0.829037	1.734867
5	6	0	4.703842	-0.873677	0.955400
6	6	0	4.738833	-1.426513	-0.329344
7	6	0	5.953203	-1.493706	-1.005183
8	1	0	5.988842	-1.938275	-1.993235
9	6	0	7.117145	-0.999156	-0.417394
10	6	0	7.074169	-0.463386	0.870333
11	1	0	7.977396	-0.082738	1.332417
12	6	0	5.874865	-0.426214	1.571899
13	1	0	5.824275	-0.023301	2.575632
14	6	0	1.351888	-0.248965	2.132014
15	6	0	0.043383	-0.582773	1.702044
16	6	0	-0.912698	-0.428780	2.736605
17	1	0	-1.949189	-0.680277	2.563949
18	6	0	-0.630434	0.037232	4.023615
19	1	0	-1.436710	0.136413	4.743307
20	6	0	0.670986	0.380521	4.370255
21	1	0	0.910491	0.766481	5.353690
22	6	0	1.662166	0.222402	3.416979
23	1	0	2.686662	0.492501	3.636902
24	16	0	-1.558982	-2.465831	-2.116115
25	6	0	-2.836624	-3.451084	-1.243832
26	1	0	-2.384181	-4.305719	-0.731435
27	1	0	-3.555092	-3.827496	-1.973708
28	6	0	-3.539412	-2.552971	-0.224085
29	1	0	-4.019175	-1.732126	-0.759476
30	6	0	-4.595397	-3.324772	0.552514
31	8	0	-4.484888	-3.693508	1.696692
32	8	0	-5.675621	-3.590416	-0.211351
33	7	0	-2.547878	-1.968550	0.707900
34	1	0	-2.929685	-1.096722	1.069974
35	1	0	-2.403898	-2.605473	1.490330
36	16	0	1.252609	-1.013909	-1.433752
37	6	0	0.814854	-0.193802	-3.043563
38	1	0	1.606620	-0.486822	-3.736329
39	1	0	-0.132149	-0.593750	-3.402519
40	6	0	0.753299	1.328591	-2.948109
41	1	0	0.752827	1.732473	-3.970798
42	7	0	1.917567	1.870043	-2.194097
43	1	0	1.713744	2.817409	-1.870243
44	6	0	-0.520506	1.889154	-2.307031
45	8	0	-0.482358	2.841789	-1.554007
46	8	0	-1.608909	1.281599	-2.723779
47	1	0	8.057473	-1.044146	-0.954630
48	1	0	-2.433014	1.691183	-2.287341
49	1	0	2.755872	1.902951	-2.768345
50	1	0	3.837743	-1.825987	-0.773750
51	17	0	3.467138	2.616227	0.470192
52	1	0	-1.435192	1.480180	1.930960
53	7	0	-3.747017	2.415680	-1.494512
54	6	0	-3.272669	3.011627	-0.238137
55	1	0	-4.475362	1.733745	-1.290204
56	1	0	-4.168258	3.133174	-2.079014
57	6	0	-4.305193	3.880441	0.516578
58	1	0	-2.406080	3.634342	-0.462915
59	6	0	-2.793254	1.884592	0.663279
60	16	0	-5.935530	3.092382	0.844998
61	1	0	-4.544361	4.753187	-0.095433
62	1	0	-3.868922	4.243439	1.448680
63	8	0	-3.341403	0.799385	0.697673
64	8	0	-1.769706	2.247468	1.419953
65	1	0	-5.474246	2.072721	1.597694

66	1	0	-6.290303	-4.121575	0.317836

HF=-3453.6672327\ZeroPoint=0.4603905\Thermal=0.5035007

G = -2.1 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	2.179410	0.660638	-0.218363
2	46	0	-0.846419	-1.331800	-0.474219
3	7	0	2.353681	-0.765695	1.262349
4	7	0	3.442649	-1.293533	1.561143
5	6	0	4.582179	-1.017494	0.767633
6	6	0	4.632192	-1.359330	-0.588034
7	6	0	5.805469	-1.131594	-1.302118
8	1	0	5.854844	-1.411539	-2.348321
9	6	0	6.910048	-0.554577	-0.677661
10	6	0	6.852995	-0.231615	0.679073
11	1	0	7.709174	0.217892	1.167978
12	6	0	5.701454	-0.487926	1.413275
13	1	0	5.640210	-0.239879	2.465103
14	6	0	1.233290	-1.107903	2.112896
15	6	0	-0.094559	-0.816603	1.720207
16	6	0	-1.075886	-1.089540	2.697798
17	1	0	-2.093448	-0.774404	2.508296
18	6	0	-0.796039	-1.666888	3.928539
19	1	0	-1.595904	-1.846891	4.638562
20	6	0	0.523277	-1.981646	4.255655
21	1	0	0.766516	-2.421955	5.215718
22	6	0	1.533524	-1.685300	3.357988
23	1	0	2.566191	-1.877042	3.612696
24	16	0	-1.639609	-2.248723	-2.460775
25	6	0	-3.205663	-2.959165	-1.806945
26	1	0	-3.016641	-3.933216	-1.346405
27	1	0	-3.893230	-3.096742	-2.642954
28	6	0	-3.795836	-2.002871	-0.771699
29	1	0	-4.038623	-1.057342	-1.259307
30	6	0	-5.059311	-2.585779	-0.153896
31	8	0	-5.122222	-3.093403	0.938279
32	8	0	-6.105544	-2.504240	-1.001238
33	7	0	-2.791808	-1.730558	0.278119
34	1	0	-3.028693	-0.851110	0.757669
35	1	0	-2.794943	-2.487044	0.960488
36	16	0	1.148901	-0.879827	-1.592316
37	6	0	0.793041	0.236132	-3.038075
38	1	0	1.537967	-0.037358	-3.788162
39	1	0	-0.196792	-0.003946	-3.423359
40	6	0	0.901755	1.725934	-2.725599
41	1	0	1.081827	2.253156	-3.673385
42	7	0	2.025854	2.021942	-1.788805
43	1	0	1.885033	2.950842	-1.383647
44	6	0	-0.340202	2.425835	-2.151350
45	8	0	-0.214476	3.516257	-1.628800
46	8	0	-1.469651	1.789972	-2.345608
47	1	0	7.816928	-0.368824	-1.241413
48	1	0	-2.233067	2.299419	-1.869920
49	1	0	2.922677	2.027299	-2.268517
50	1	0	3.778031	-1.823840	-1.061535
51	17	0	3.288157	2.283758	1.077594
52	1	0	-0.507497	0.350449	1.077954
53	7	0	-3.262704	3.074650	-0.861323
54	6	0	-2.543627	3.182449	0.427798
55	1	0	-4.153681	2.606458	-0.702389
56	1	0	-3.476301	4.005097	-1.213125
57	6	0	-3.314300	3.911563	1.544195
58	1	0	-1.625100	3.736397	0.237423
59	6	0	-2.139742	1.755334	0.830033
60	16	0	-5.052884	3.374931	1.838494
61	1	0	-3.399102	4.969677	1.284155
62	1	0	-2.748995	3.849385	2.476257
63	8	0	-3.039494	0.926068	1.057816
64	8	0	-0.879109	1.542958	0.860499
65	1	0	-4.761455	2.074044	2.042440
66	1	0	-6.868812	-2.924099	-0.575304

HF=-3453.6513078\ZeroPoint=0.4571872\Thermal=0.4991368

G = -38.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-2.107176	-1.139907	0.155207
2	46	0	0.817043	0.759562	-1.140250
3	7	0	-1.985360	0.628027	1.241274
4	7	0	-2.901395	1.434625	1.488959
5	6	0	-4.127872	1.286824	0.802114
6	6	0	-4.191224	1.277217	-0.595494
7	6	0	-5.434711	1.187351	-1.214199
8	1	0	-5.492162	1.199856	-2.296486
9	6	0	-6.596622	1.089287	-0.449952
10	6	0	-6.521625	1.115321	0.944317
11	1	0	-7.424390	1.043729	1.539346
12	6	0	-5.290887	1.244072	1.576041
13	1	0	-5.211421	1.271654	2.655467
14	6	0	-0.731198	0.907287	1.887594
15	6	0	0.100866	-0.159366	2.228003
16	6	0	1.324623	0.105057	2.834006
17	1	0	1.971345	-0.719881	3.106673
18	6	0	1.723886	1.418237	3.075482
19	1	0	2.690622	1.621587	3.520920
20	6	0	0.886356	2.480253	2.720569
21	1	0	1.211135	3.500691	2.883979
22	6	0	-0.345337	2.229544	2.129224
23	1	0	-0.997715	3.035905	1.822070
24	16	0	-0.144483	2.737868	-1.863025
25	6	0	0.999376	3.897852	-0.999479
26	1	0	0.671679	4.053137	0.032247
27	1	0	0.973412	4.855863	-1.520957
28	6	0	2.422576	3.324582	-0.993475
29	1	0	2.788093	3.256450	-2.018617
30	6	0	3.334533	4.232541	-0.179630
31	8	0	3.596508	4.076060	0.987682
32	8	0	3.775997	5.277439	-0.909773
33	7	0	2.384767	1.971200	-0.410163

34	1	0	3.241491	1.418833	-0.538952
35	1	0	2.250991	2.042203	0.599066
36	16	0	-1.165999	-0.302558	-1.817224
37	6	0	-0.882411	-1.908131	-2.706507
38	1	0	-1.643577	-1.932461	-3.489056
39	1	0	0.099097	-1.885667	-3.174361
40	6	0	-1.007551	-3.142830	-1.812993
41	1	0	-1.228677	-4.006741	-2.454480
42	7	0	-2.094131	-2.983324	-0.808603
43	1	0	-1.958890	-3.652666	-0.047695
44	6	0	0.283615	-3.515884	-1.075483
45	8	0	0.286653	-3.789734	0.108094
46	8	0	1.307760	-3.565969	-1.892585
47	1	0	-7.561081	1.008640	-0.938071
48	1	0	2.190418	-3.618190	-1.347394
49	1	0	-3.011009	-3.147502	-1.216837
50	1	0	-3.288449	1.387408	-1.180475
51	17	0	-3.164373	-2.156644	1.999098
52	1	0	-0.208109	-1.175823	2.020918
53	7	0	3.469732	-3.549531	-0.407285
54	6	0	3.247345	-2.516308	0.630612
55	1	0	4.360793	-3.371077	-0.869518
56	1	0	3.560441	-4.459467	0.040503
57	6	0	4.377188	-2.421926	1.668507
58	1	0	2.328446	-2.802862	1.147277
59	6	0	2.944575	-1.165620	-0.068781
60	16	0	6.089243	-2.297603	0.998507
61	1	0	4.382955	-3.329558	2.277795
62	1	0	4.196158	-1.575928	2.333345
63	8	0	3.859452	-0.338476	-0.222037
64	8	0	1.725159	-1.042337	-0.420432
65	1	0	5.862247	-1.143093	0.337985
66	1	0	4.305902	5.845459	-0.329272

HF=-3453.7096639\ZeroPoint=0.4607027\Thermal=0.5032782

G = -25.2 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.785898	-0.131402	0.846497
2	46	0	0.941600	-0.925878	-1.116384
3	7	0	-2.360890	0.354642	-1.044324
4	7	0	-3.441461	0.072312	-1.601503
5	6	0	-4.461007	-0.565429	-0.861175
6	6	0	-5.108334	-1.626268	-1.505618
7	6	0	-6.125507	-2.308444	-0.849279
8	1	0	-6.607767	-3.149664	-1.333043
9	6	0	-6.538619	-1.897073	0.419713
10	6	0	-5.930408	-0.801070	1.031176
11	1	0	-6.275273	-0.456436	1.999254
12	6	0	-4.884167	-0.131653	0.402433
13	1	0	-4.435684	0.740995	0.858277
14	6	0	-1.433573	1.096904	-1.855045
15	6	0	-0.075549	0.709879	-1.969905
16	6	0	0.644159	1.495655	-2.899796
17	1	0	1.671855	1.242930	-3.124277
18	6	0	0.111587	2.596071	-3.567387
19	1	0	0.742948	3.161896	-4.244225
20	6	0	-1.212837	2.973321	-3.362242
21	1	0	-1.631130	3.845089	-3.850593
22	6	0	-1.991093	2.200273	-2.520166
23	1	0	-3.029999	2.446058	-2.341296
24	16	0	3.036118	0.058914	-1.589976
25	6	0	4.106129	-1.190301	-0.761429
26	1	0	4.125550	-1.025384	0.318810
27	1	0	5.115340	-1.092605	-1.159613
28	6	0	3.543709	-2.577904	-1.052998
29	1	0	3.517568	-2.720714	-2.138101
30	6	0	4.366874	-3.723081	-0.470834
31	8	0	5.670673	-3.619805	-0.802370
32	8	0	3.914505	-4.632516	0.178127
33	7	0	2.162413	-2.629076	-0.532507
34	1	0	1.735201	-3.520690	-0.769180
35	1	0	2.214300	-2.573380	0.493707
36	16	0	-0.973251	-2.089300	-0.085553
37	6	0	-0.378302	-2.835357	1.519478
38	1	0	-1.199949	-3.476177	1.846872
39	1	0	0.485665	-3.473399	1.341994
40	6	0	-0.055086	-1.810419	2.602781
41	1	0	0.049076	-2.346854	3.555670
42	7	0	-1.160672	-0.817624	2.712496
43	1	0	-0.825879	-0.008710	3.238397
44	6	0	1.297365	-1.063589	2.428142
45	8	0	2.283355	-1.729143	2.108173
46	8	0	1.251090	0.182112	2.697789
47	1	0	-7.347529	-2.416876	0.920162
48	1	0	2.303019	1.434584	2.946657
49	1	0	-1.966849	-1.206933	3.196344
50	1	0	6.134451	-4.382114	-0.423203
51	1	0	-4.786745	-1.913995	-2.499119
52	17	0	-2.251650	2.017961	1.761934
53	1	0	0.685743	1.561719	-0.088287
54	6	0	2.282204	2.622279	0.729425
55	7	0	0.900320	2.051235	0.795055
56	6	0	2.371914	3.656995	-0.388479
57	1	0	2.925301	1.776936	0.458089
58	6	0	2.753693	3.161764	2.098018
59	1	0	0.823201	1.327865	1.543686
60	1	0	0.178630	2.768066	0.939242
61	16	0	1.107995	4.990789	-0.304147
62	1	0	2.214055	3.159080	-1.345556
63	1	0	3.366627	4.096906	-0.385443
64	8	0	2.686943	2.335351	3.133517
65	8	0	3.215895	4.272158	2.195274
66	1	0	1.623662	5.583889	0.792017

HF=-3453.6933052\ZeroPoint=0.4622593\Thermal=0.5043439

G = -3.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.809926	-0.077327	0.842992

2	46	0	1.069628	-0.804633	-1.001631
3	7	0	-2.340391	0.457695	-1.070791
4	7	0	-3.369041	0.054967	-1.660651
5	6	0	-4.378964	-0.612474	-0.941588
6	6	0	-4.938409	-1.726541	-1.580816
7	6	0	-5.942934	-2.447782	-0.947723
8	1	0	-6.355675	-3.328574	-1.425211
9	6	0	-6.433613	-2.024125	0.289122
10	6	0	-5.915842	-0.877071	0.891775
11	1	0	-6.322079	-0.525161	1.832936
12	6	0	-4.881839	-0.167363	0.289694
13	1	0	-4.500554	0.738571	0.741656
14	6	0	-1.430096	1.194815	-1.905154
15	6	0	-0.024157	1.131514	-1.706346
16	6	0	0.738807	1.841717	-2.657201
17	1	0	1.815072	1.837427	-2.568560
18	6	0	0.182298	2.578917	-3.693953
19	1	0	0.827631	3.111572	-4.382578
20	6	0	-1.202042	2.657832	-3.816578
21	1	0	-1.656274	3.260719	-4.594073
22	6	0	-2.004183	1.964281	-2.923016
23	1	0	-3.081764	2.016568	-2.996911
24	16	0	3.162479	0.061374	-1.620118
25	6	0	4.194224	-1.220481	-0.796589
26	1	0	4.235403	-1.049253	0.281873
27	1	0	5.201105	-1.170019	-1.209199
28	6	0	3.557866	-2.573544	-1.081370
29	1	0	3.521078	-2.719850	-2.165690
30	6	0	4.288672	-3.777344	-0.494020
31	8	0	5.612958	-3.724096	-0.734587
32	8	0	3.746598	-4.687714	0.080218
33	7	0	2.170693	-2.541450	-0.560801
34	1	0	1.681329	-3.394568	-0.818659
35	1	0	2.208548	-2.496204	0.475856
36	16	0	-0.909528	-1.976826	-0.143953
37	6	0	-0.446292	-2.833292	1.442753
38	1	0	-1.309274	-3.458016	1.683354
39	1	0	0.407607	-3.489696	1.280448
40	6	0	-0.147352	-1.867357	2.579621
41	1	0	-0.097670	-2.439157	3.515704
42	7	0	-1.224634	-0.839784	2.687683
43	1	0	-0.853511	-0.054521	3.228547
44	6	0	1.230639	-1.144510	2.474204
45	8	0	2.197534	-1.817777	2.083775
46	8	0	1.207864	0.059017	2.845398
47	1	0	-7.233377	-2.574797	0.770923
48	1	0	2.093000	1.425874	3.132483
49	1	0	-2.049041	-1.200412	3.162565
50	1	0	6.016637	-4.523259	-0.362000
51	1	0	-4.557170	-2.023241	-2.550248
52	17	0	-2.447608	1.957056	1.859342
53	1	0	0.450865	1.305029	-0.506483
54	6	0	2.179639	2.549807	0.922690
55	7	0	0.798528	2.045696	0.780323
56	6	0	2.547909	3.535506	-0.187557
57	1	0	2.835730	1.678716	0.817593
58	6	0	2.444965	3.171311	2.318755
59	1	0	0.596604	1.374043	1.520952
60	1	0	0.119604	2.803650	0.848767
61	16	0	1.314696	4.862773	-0.511595
62	1	0	2.655555	2.997243	-1.124661
63	1	0	3.504568	3.998703	0.045416
64	8	0	2.366212	2.351800	3.362026
65	8	0	2.734057	4.337392	2.455172
66	1	0	1.543096	5.529978	0.637822

HF=-3453.6550454\ZeroPoint=0.4581764\Thermal=0.499756

G = -11.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-2.109117	-0.716923	-0.756853
2	46	0	0.612325	1.180771	0.684069
3	7	0	-2.659923	-0.358764	1.233693
4	7	0	-3.729859	0.119560	1.670584
5	6	0	-4.858317	0.240276	0.848360
6	6	0	-5.655731	1.366070	1.108168
7	6	0	-6.794661	1.593808	0.347413
8	1	0	-7.395014	2.477828	0.526195
9	6	0	-7.175423	0.670571	-0.628542
10	6	0	-6.414129	-0.480475	-0.840670
11	1	0	-6.732860	-1.217012	-1.568918
12	6	0	-5.250021	-0.703075	-0.115020
13	1	0	-4.683999	-1.614206	-0.253523
14	6	0	-1.589001	-0.430213	2.193253
15	6	0	-0.339905	-0.920130	1.749865
16	6	0	0.703485	-1.074635	2.671406
17	1	0	1.621334	-1.516238	2.310996
18	6	0	0.527559	-0.696338	4.001753
19	1	0	1.342834	-0.805433	4.706060
20	6	0	-0.702053	-0.188934	4.417444
21	1	0	-0.843221	0.103842	5.451551
22	6	0	-1.764789	-0.057389	3.526125
23	1	0	-2.722448	0.320687	3.854189
24	16	0	2.482025	1.362777	2.079015
25	6	0	3.584355	2.153502	0.838535
26	1	0	3.954063	1.408983	0.128191
27	1	0	4.436894	2.587498	1.360277
28	6	0	2.789367	3.226762	0.110801
29	1	0	2.457956	3.965356	0.847803
30	6	0	3.545664	3.989544	-0.973491
31	8	0	4.769739	4.363627	-0.556558
32	8	0	3.089931	4.258486	-2.055631
33	7	0	1.585128	2.600918	-0.485383
34	1	0	0.949341	3.322788	-0.813982
35	1	0	1.824472	2.006761	-1.305393
36	16	0	-1.350563	1.480734	-0.743108
37	6	0	-0.857418	1.555019	-2.530688
38	1	0	-1.741565	1.927477	-3.052608
39	1	0	-0.053036	2.276855	-2.666695
40	6	0	-0.430105	0.205665	-3.075800
41	1	0	-0.373526	0.271962	-4.170481
42	7	0	-1.416293	-0.856695	-2.707898
43	1	0	-0.927504	-1.754669	-2.790213

44	6	0	0.987981	-0.270434	-2.635785
45	8	0	1.839357	0.594007	-2.354917
46	8	0	1.127130	-1.519546	-2.666788
47	1	0	-8.077342	0.836366	-1.206519
48	1	0	2.608973	-2.302328	-2.645815
49	1	0	-2.216411	-0.871476	-3.336103
50	1	0	5.192664	4.861321	-1.273676
51	1	0	-5.352299	2.054753	1.887243
52	17	0	-2.623938	-3.012291	-0.789723
53	1	0	-0.229045	-1.375879	0.771202
54	6	0	3.373986	-1.879646	-0.374809
55	7	0	2.068855	-2.427805	0.024853
56	6	0	4.277371	-1.657085	0.839734
57	1	0	3.175361	-0.897864	-0.822436
58	6	0	4.093988	-2.712655	-1.462798
59	1	0	1.455309	-2.487542	-0.781630
60	1	0	2.190966	-3.363291	0.403142
61	16	0	4.522856	-3.120850	1.933955
62	1	0	3.827336	-0.900627	1.482104
63	1	0	5.256652	-1.305541	0.516438
64	8	0	3.447907	-2.833305	-2.622773
65	8	0	5.172872	-3.235530	-1.290802
66	1	0	5.220320	-3.844675	1.035448

HF=-3453.6673497\ZeroPoint=0.4605521\Thermal=0.5034241

G = -12.2 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.841675	0.119010	0.890531
2	46	0	0.557925	-1.409663	-1.135452
3	7	0	-2.301840	0.712484	-1.008380
4	7	0	-3.410368	0.682250	-1.579631
5	6	0	-4.555708	0.281654	-0.857271
6	6	0	-5.422726	-0.587640	-1.530213
7	6	0	-6.574135	-1.035061	-0.894119
8	1	0	-7.230919	-1.733065	-1.399646
9	6	0	-6.892718	-0.570424	0.383632
10	6	0	-6.055460	0.342656	1.024378
11	1	0	-6.320723	0.733209	2.000048
12	6	0	-4.878557	0.769843	0.416120
13	1	0	-4.246917	1.506189	0.894907
14	6	0	-1.217959	1.217816	-1.811994
15	6	0	0.003557	0.508445	-1.894111
16	6	0	0.909743	1.089751	-2.812047
17	1	0	1.848537	0.596461	-3.030814
18	6	0	0.674926	2.278786	-3.501838
19	1	0	1.433054	2.667945	-4.173506
20	6	0	-0.522118	2.967243	-3.323030
21	1	0	-0.707858	3.907397	-3.827815
22	6	0	-1.482150	2.415314	-2.490925
23	1	0	-2.435150	2.906259	-2.338803
24	16	0	1.295555	-3.683650	-0.933245
25	6	0	3.114246	-3.412795	-0.722825
26	1	0	3.646127	-3.813617	-1.591439
27	1	0	3.460416	-3.935224	0.167310
28	6	0	3.394470	-1.921927	-0.561982
29	1	0	3.010053	-1.636263	0.424892
30	6	0	4.850940	-1.489151	-0.569109
31	8	0	5.652910	-2.349017	0.074102
32	8	0	5.234203	-0.444087	-1.048130
33	7	0	2.640098	-1.161265	-1.593414
34	1	0	2.996453	-0.209414	-1.635521
35	1	0	2.816959	-1.571611	-2.509750
36	16	0	-1.435735	-1.972173	-0.007235
37	6	0	-0.896021	-2.797303	1.579651
38	1	0	-1.781782	-3.333433	1.928593
39	1	0	-0.109105	-3.507405	1.327617
40	6	0	-0.411340	-1.822428	2.645023
41	1	0	-0.380017	-2.357175	3.603691
42	7	0	-1.350685	-0.666820	2.756706
43	1	0	-0.902084	0.081255	3.286641
44	6	0	1.035773	-1.302764	2.439527
45	8	0	1.916614	-2.109318	2.181700
46	8	0	1.172755	-0.033412	2.626303
47	1	0	-7.802672	-0.904063	0.869051
48	1	0	2.469584	0.827199	2.852712
49	1	0	-2.209871	-0.932877	3.232992
50	1	0	6.544214	-1.967281	0.103082
51	1	0	-5.166312	-0.918343	-2.529288
52	17	0	-1.858950	2.340856	1.778176
53	1	0	0.767657	1.470720	-0.098560
54	6	0	2.677855	1.952867	0.609966
55	7	0	1.193885	1.831919	0.768794
56	6	0	3.027820	2.914943	-0.524026
57	1	0	3.031065	0.949229	0.353123
58	6	0	3.384673	2.329281	1.944382
59	1	0	0.955893	1.132008	1.519424
60	1	0	0.742589	2.728273	0.980494
61	16	0	2.253462	4.576349	-0.377370
62	1	0	2.661121	2.515693	-1.469131
63	1	0	4.109129	3.016438	-0.581091
64	8	0	3.139671	1.571156	2.993863
65	8	0	4.164520	3.250750	1.971426
66	1	0	3.009031	4.975362	0.665947

HF=-3453.6696738\ZeroPoint=0.4613832\Thermal=0.5036628

G = 2.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.918283	0.325585	0.797886
2	46	0	0.711695	-1.392617	-0.707025
3	7	0	-2.252129	0.540616	-1.228077
4	7	0	-3.317798	0.221793	-1.802070
5	6	0	-4.462233	-0.080218	-1.037178
6	6	0	-5.194493	-1.198227	-1.455876
7	6	0	-6.339331	-1.567148	-0.760239
8	1	0	-6.890079	-2.450466	-1.061197
9	6	0	-6.788492	-0.789697	0.309140
10	6	0	-6.088015	0.357759	0.682612
11	1	0	-6.454959	0.982362	1.488778

12	6	0	-4.917955	0.718110	0.021715
13	1	0	-4.388530	1.621989	0.292222
14	6	0	-1.177078	0.896473	-2.114420
15	6	0	0.168687	0.641737	-1.750813
16	6	0	1.110406	0.946589	-2.757723
17	1	0	2.162391	0.792916	-2.563097
18	6	0	0.776165	1.478996	-3.995393
19	1	0	1.553867	1.703573	-4.716405
20	6	0	-0.558550	1.759058	-4.285824
21	1	0	-0.836400	2.209288	-5.231386
22	6	0	-1.532162	1.465549	-3.345385
23	1	0	-2.573998	1.673409	-3.548296
24	16	0	1.234116	-3.658821	-0.451421
25	6	0	3.080487	-3.557530	-0.451554
26	1	0	3.466177	-3.904036	-1.415989
27	1	0	3.469050	-4.209361	0.329598
28	6	0	3.524547	-2.121902	-0.189059
29	1	0	3.227207	-1.839763	0.826254
30	6	0	5.024235	-1.904460	-0.317630
31	8	0	5.722087	-2.750940	0.458641
32	8	0	5.530685	-1.056537	-1.013445
33	7	0	2.804447	-1.221542	-1.127309
34	1	0	3.172410	-0.280191	-1.022969
35	1	0	3.007446	-1.493270	-2.088464
36	16	0	-1.351891	-1.874310	0.319571
37	6	0	-0.861063	-2.377257	2.047100
38	1	0	-1.715855	-2.940242	2.429564
39	1	0	0.001992	-3.035311	1.962971
40	6	0	-0.544216	-1.195200	2.946679
41	1	0	-0.535598	-1.544200	3.988484
42	7	0	-1.579958	-0.128009	2.798173
43	1	0	-1.218429	0.720165	3.242017
44	6	0	0.849009	-0.529224	2.729465
45	8	0	1.789866	-1.210823	2.319535
46	8	0	0.843558	0.704942	3.039301
47	1	0	-7.694098	-1.066905	0.836415
48	1	0	1.914377	1.825659	3.099984
49	1	0	-2.460666	-0.386355	3.237481
50	1	0	6.663984	-2.539708	0.365508
51	1	0	-4.838437	-1.775044	-2.300686
52	17	0	-2.153254	2.627941	1.296640
53	1	0	0.650990	1.050470	-0.529825
54	6	0	2.556677	2.036454	0.730512
55	7	0	1.100633	1.958648	0.459593
56	6	0	3.357431	2.425596	-0.516630
57	1	0	2.856735	1.033748	1.058449
58	6	0	2.897633	3.012044	1.898860
59	1	0	0.600868	1.706626	1.314793
60	1	0	0.744189	2.862939	0.149299
61	16	0	2.717967	3.881396	-1.445363
62	1	0	3.363048	1.618180	-1.245530
63	1	0	4.390415	2.616316	-0.234186
64	8	0	2.453356	2.679153	3.093134
65	8	0	3.558889	4.008459	1.707487
66	1	0	3.103199	4.783825	-0.520424

HF=-3453.6434115\ZeroPoint=0.4573775\Thermal=0.49937

G = -34.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-2.332734	-0.981368	0.657029
2	46	0	0.514540	0.223600	-0.703952
3	7	0	-2.777075	1.054591	0.680858
4	7	0	-3.667927	1.632433	0.025777
5	6	0	-4.634703	0.860934	-0.647161
6	6	0	-4.974144	1.286912	-1.936444
7	6	0	-5.916865	0.572738	-2.666040
8	1	0	-6.158494	0.878727	-3.677004
9	6	0	-6.562088	-0.523760	-2.091089
10	6	0	-6.261411	-0.906865	-0.783196
11	1	0	-6.789290	-1.734204	-0.323205
12	6	0	-5.291892	-0.226807	-0.053866
13	1	0	-5.077489	-0.501442	0.970877
14	6	0	-1.828964	1.916707	1.335608
15	6	0	-1.034854	1.389943	2.356931
16	6	0	-0.072647	2.194847	2.961074
17	1	0	0.538931	1.787384	3.757246
18	6	0	0.104517	3.513060	2.544764
19	1	0	0.872574	4.127141	2.999305
20	6	0	-0.696798	4.031861	1.524262
21	1	0	-0.556682	5.053675	1.191188
22	6	0	-1.659395	3.240698	0.912554
23	1	0	-2.257142	3.619722	0.096526
24	16	0	0.261281	2.074346	-2.045699
25	6	0	1.499820	3.175446	-1.230643
26	1	0	1.021601	3.730134	-0.420703
27	1	0	1.864086	3.884193	-1.975845
28	6	0	2.655978	2.346541	-0.663057
29	1	0	3.210001	1.893092	-1.485467
30	6	0	3.593049	3.236340	0.143870
31	8	0	4.464804	3.884660	-0.651353
32	8	0	3.538099	3.379008	1.340475
33	7	0	2.110765	1.271710	0.187950
34	1	0	2.844778	0.582974	0.466073
35	1	0	1.748747	1.683584	1.049404
36	16	0	-1.429710	-0.783787	-1.514101
37	6	0	-0.925607	-2.558345	-1.703174
38	1	0	-1.775688	-3.069650	-2.163362
39	1	0	-0.086648	-2.602197	-2.398625
40	6	0	-0.574451	-3.223445	-0.377946
41	1	0	-0.488116	-4.303159	-0.526652
42	7	0	-1.688837	-2.957288	0.590760
43	1	0	-1.431686	-3.221838	1.541790
44	6	0	0.783011	-2.782065	0.234699
45	8	0	1.009266	-1.553186	0.461129
46	8	0	1.573629	-3.705911	0.488167
47	1	0	-7.312961	-1.065606	-2.654591
48	1	0	3.260365	-3.744124	0.699405
49	1	0	-2.501874	-3.523377	0.351152
50	1	0	5.025469	4.444879	-0.092599
51	1	0	-4.470171	2.148437	-2.357016
52	17	0	-3.220093	-1.418759	2.804580
53	1	0	-1.180691	0.370816	2.686783

54	6	0	4.200727	-1.688505	-0.263514
55	7	0	3.846120	-0.893434	0.922990
56	6	0	4.969323	-0.850962	-1.290426
57	1	0	3.254344	-1.982075	-0.727556
58	6	0	4.960581	-2.975204	0.123449
59	1	0	3.141356	-1.379618	1.469839
60	1	0	4.667669	-0.715990	1.493523
61	16	0	6.401217	0.111558	-0.644635
62	1	0	4.294924	-0.102572	-1.709639
63	1	0	5.313957	-1.487261	-2.105266
64	8	0	4.236672	-3.916576	0.728627
65	8	0	6.149081	-3.112875	-0.055885
66	1	0	7.149151	-0.966754	-0.335560

HF=-3453.7034169\ZeroPoint=0.4611425\Thermal=0.5040031

G = -1.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.015343	-0.209803	0.713643
2	46	0	-1.583524	1.059736	0.876356
3	7	0	1.367865	1.135661	-0.849327
4	7	0	2.429518	1.112705	-1.520481
5	6	0	3.497034	0.313945	-1.071426
6	6	0	3.958683	0.364599	0.252630
7	6	0	5.062196	-0.399008	0.620770
8	1	0	5.433540	-0.345926	1.637845
9	6	0	5.693661	-1.220211	-0.312575
10	6	0	5.243279	-1.249440	-1.634021
11	1	0	5.738630	-1.879930	-2.362909
12	6	0	4.165865	-0.463298	-2.022948
13	1	0	3.808410	-0.466778	-3.045139
14	6	0	0.385390	2.103212	-1.264829
15	6	0	-0.867479	2.182884	-0.614796
16	6	0	-1.755340	3.176904	-1.075202
17	1	0	-2.734018	3.252381	-0.618943
18	6	0	-1.426548	4.042819	-2.105805
19	1	0	-2.139968	4.795371	-2.424135
20	6	0	-0.178861	3.943942	-2.737670
21	1	0	0.085726	4.618612	-3.543530
22	6	0	0.719063	2.985387	-2.319243
23	1	0	1.691588	2.901534	-2.783499
24	16	0	0.345198	1.555835	2.166949
25	6	0	0.048567	0.510648	3.664293
26	1	0	-0.790814	0.943591	4.207970
27	1	0	0.949550	0.583099	4.279960
28	6	0	-0.269884	-0.932334	3.314221
29	1	0	-0.266300	-1.540130	4.227214
30	6	0	-1.658968	-1.171614	2.631728
31	8	0	-1.870770	-2.340814	2.304343
32	8	0	-2.406475	-0.151950	2.472256
33	7	0	0.740927	-1.479793	2.357069
34	1	0	1.648191	-1.618018	2.798095
35	1	0	0.406124	-2.393708	2.046244
36	16	0	1.130987	-2.096181	-0.745653
37	6	0	-0.642586	-2.638620	-0.809887
38	1	0	-0.676354	-3.721093	-0.694009
39	1	0	-1.232897	-2.209663	0.001720
40	6	0	-1.252799	-2.290371	-2.167572
41	1	0	-0.637305	-2.736068	-2.956110
42	7	0	-1.232786	-0.809136	-2.380011
43	1	0	-1.943526	-0.338758	-1.727823
44	6	0	-2.686510	-2.748911	-2.433097
45	8	0	-2.999497	-3.859211	-1.759113
46	8	0	-3.409478	-2.187902	-3.216892
47	1	0	6.545626	-1.821492	-0.017287
48	1	0	-1.498056	-0.559225	-3.332252
49	1	0	3.487481	1.033401	0.961518
50	1	0	-3.917495	-4.093465	-1.967804
51	17	0	-3.353560	0.303348	-0.561769
52	1	0	-0.287746	-0.472258	-2.160698

HF=-2731.5491882\ZeroPoint=0.3628617\Thermal=0.3955335

G = 25.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.968410	-0.876388	-0.228624
2	46	0	1.828865	-0.160510	-0.939230
3	7	0	-1.527366	1.062876	-0.710164
4	7	0	-2.643688	1.609368	-0.516610
5	6	0	-3.702771	0.858956	0.007862
6	6	0	-3.975034	-0.470217	-0.354091
7	6	0	-5.069502	-1.119499	0.206019
8	1	0	-5.291186	-2.140734	-0.081092
9	6	0	-5.884229	-0.460154	1.125578
10	6	0	-5.631311	0.873412	1.458379
11	1	0	-6.274424	1.389609	2.161017
12	6	0	-4.563168	1.542831	0.879726
13	1	0	-4.355013	2.579867	1.112950
14	6	0	-0.568055	1.902304	-1.383197
15	6	0	0.808391	1.746195	-1.073576
16	6	0	1.693362	2.675827	-1.656699
17	1	0	2.739567	2.628631	-1.381626
18	6	0	1.252744	3.635037	-2.566031
19	1	0	1.964717	4.311416	-3.025224
20	6	0	-0.100939	3.720020	-2.888693
21	1	0	-0.447288	4.454655	-3.606621
22	6	0	-1.019691	2.869515	-2.279761
23	1	0	-2.076452	2.945250	-2.499344
24	16	0	0.132927	-1.119965	-2.332560
25	6	0	0.510724	-2.918863	-2.179210
26	1	0	1.416658	-3.119974	-2.750701
27	1	0	-0.325528	-3.457641	-2.633054
28	6	0	0.724387	-3.332395	-0.734867
29	1	0	0.797919	-4.424356	-0.671080
30	6	0	2.030285	-2.780054	-0.080099
31	8	0	2.231533	-3.138884	1.072389
32	8	0	2.774304	-2.023590	-0.815658
33	7	0	-0.409820	-2.872017	0.128126
34	1	0	-1.238860	-3.446403	-0.011536
35	1	0	-0.134058	-2.986073	1.105851

36	16	0	-1.328811	-0.585196	2.095618
37	6	0	0.443015	-0.363487	2.604208
38	1	0	0.572733	-0.884922	3.552558
39	1	0	1.123024	-0.829174	1.891391
40	6	0	0.805635	1.106357	2.806797
41	1	0	0.171543	1.498250	3.615216
42	7	0	0.573107	1.935039	1.598965
43	1	0	0.905851	1.534655	0.247160
44	6	0	2.229189	1.385546	3.291773
45	8	0	2.797137	0.322996	3.873637
46	8	0	2.731007	2.480983	3.231402
47	1	0	-6.729110	-0.976277	1.566497
48	1	0	1.083351	2.812677	1.702921
49	1	0	-3.365513	-0.960600	-1.102914
50	1	0	3.701955	0.566091	4.122321
51	17	0	3.507025	0.755529	0.421727
52	1	0	-0.421753	2.134036	1.527276

HF=-2731.5040178\ZeroPoint=0.3590675\Thermal=0.3912034

G = 12.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.816663	-0.618021	-0.796291
2	46	0	-2.171233	-0.691923	0.302428
3	7	0	1.477696	-0.555771	1.176710
4	7	0	2.608538	-0.455387	1.699226
5	6	0	3.737415	-0.288442	0.878839
6	6	0	3.924275	-0.956505	-0.339649
7	6	0	5.087549	-0.735070	-1.066187
8	1	0	5.240301	-1.253554	-2.005380
9	6	0	6.056553	0.148256	-0.590011
10	6	0	5.883246	0.784587	0.641216
11	1	0	6.644490	1.457280	1.017709
12	6	0	4.740935	0.544392	1.392158
13	1	0	4.590607	1.013218	2.357101
14	6	0	0.417235	-0.911378	2.083848
15	6	0	-0.766481	-0.126949	2.086802
16	6	0	-1.874199	-0.612392	2.805072
17	1	0	-2.738986	0.025459	2.928957
18	6	0	-1.802211	-1.852188	3.479751
19	1	0	-2.671951	-2.220034	4.010001
20	6	0	-0.620892	-2.564053	3.491393
21	1	0	-0.553999	-3.505080	4.024624
22	6	0	0.505037	-2.091445	2.789526
23	1	0	1.418522	-2.671625	2.751809
24	16	0	-0.690323	-2.462535	-0.313244
25	6	0	-1.182711	-2.784932	-2.058980
26	1	0	-2.183698	-3.215623	-2.056229
27	1	0	-0.478714	-3.523879	-2.451580
28	6	0	-1.178731	-1.516858	-2.893113
29	1	0	-1.345141	-1.770352	-3.946737
30	6	0	-2.291659	-0.489374	-2.531065
31	8	0	-2.354023	0.501722	-3.239317
32	8	0	-3.078407	-0.798859	-1.547883
33	7	0	0.125530	-0.796637	-2.769661
34	1	0	0.859428	-1.263368	-3.299246
35	1	0	0.024509	0.137424	-3.173190
36	16	0	1.713692	1.488453	-1.387825
37	6	0	0.168748	2.476385	-1.087023
38	1	0	-0.017545	3.083294	-1.972220
39	1	0	-0.683527	1.804722	-0.973442
40	6	0	0.280459	3.384301	0.148154
41	1	0	0.977514	4.202761	-0.102573
42	7	0	0.697972	2.639060	1.334611
43	1	0	-0.696315	0.901863	1.741543
44	6	0	-1.038600	4.082364	0.474063
45	8	0	-1.729868	4.412501	-0.632495
46	8	0	-1.400561	4.352772	1.591920
47	1	0	6.956382	0.325067	-1.167625
48	1	0	0.595626	3.218671	2.161688
49	1	0	3.177858	-1.659458	-0.688729
50	1	0	-2.574324	4.794922	-0.349967
51	17	0	-3.436160	1.240486	0.717789
52	1	0	1.668908	2.364662	1.233110

HF=-2731.5234602\ZeroPoint=0.3616845\Thermal=0.3949818

G = 6.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.655882	-0.797268	-0.655716
2	46	0	2.240459	0.072659	-0.388504
3	7	0	-0.954040	1.306445	-0.545398
4	7	0	-2.087973	1.829703	-0.358623
5	6	0	-3.266973	1.101456	-0.532566
6	6	0	-3.463012	0.169357	-1.564448
7	6	0	-4.693381	-0.466125	-1.689575
8	1	0	-4.845293	-1.182544	-2.488746
9	6	0	-5.732244	-0.180197	-0.803879
10	6	0	-5.553929	0.786071	0.189201
11	1	0	-6.370647	1.035113	0.856887
12	6	0	-4.337976	1.444743	0.307224
13	1	0	-4.190314	2.224479	1.046244
14	6	0	0.115358	2.263041	-0.653686
15	6	0	1.482207	1.893656	-0.608625
16	6	0	2.429792	2.924592	-0.757021
17	1	0	3.480905	2.676075	-0.701907
18	6	0	2.062276	4.245639	-0.948654
19	1	0	2.827912	5.005540	-1.063223
20	6	0	0.706531	4.595584	-1.004760
21	1	0	0.407811	5.623552	-1.174407
22	6	0	-0.250557	3.616500	-0.862870
23	1	0	-1.298689	3.870008	-0.924766
24	16	0	1.011974	-0.519593	-2.304725
25	6	0	1.495585	-2.296717	-2.483724
26	1	0	2.572952	-2.327213	-2.643747
27	1	0	0.987675	-2.680940	-3.372921
28	6	0	1.139000	-3.096235	-1.247096
29	1	0	1.284321	-4.166864	-1.438785
30	6	0	1.958427	-2.760569	0.049153
31	8	0	1.521318	-3.300380	1.071340

32	8	0	2.952348	-1.983262	-0.083940
33	7	0	-0.286378	-2.849584	-0.879432
34	1	0	-0.935713	-3.235039	-1.562265
35	1	0	-0.451670	-3.314811	0.015030
36	16	0	-2.167958	-1.445965	1.101622
37	6	0	-1.107793	-1.662620	2.591523
38	1	0	-1.635198	-2.357149	3.248251
39	1	0	-0.138809	-2.099432	2.342471
40	6	0	-0.879139	-0.318742	3.338720
41	1	0	-0.784218	-0.494254	4.411331
42	7	0	-2.018903	0.626038	3.087681
43	1	0	-2.515228	0.207890	2.234221
44	6	0	0.372026	0.444421	2.874817
45	8	0	1.442974	-0.269258	3.029382
46	8	0	0.268062	1.581442	2.449901
47	1	0	-6.685582	-0.685423	-0.904626
48	1	0	-1.574604	1.524353	2.812091
49	1	0	-2.666358	-0.024076	-2.271585
50	1	0	2.258151	0.151402	2.579558
51	17	0	3.625282	0.791235	1.434564
52	1	0	-2.655752	0.739587	3.871637

HF=-2731.5369156\ZeroPoint=0.3617884\Thermal=0.393823

G = 33.1 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.488735	-0.924914	-0.520503
2	46	0	2.408284	0.137238	-0.106585
3	7	0	-1.014038	1.095852	-0.795442
4	7	0	-2.169100	1.560980	-0.931812
5	6	0	-3.281570	0.710803	-0.972969
6	6	0	-3.334211	-0.467772	-1.729061
7	6	0	-4.496224	-1.232163	-1.718460
8	1	0	-4.542919	-2.143209	-2.303569
9	6	0	-5.597294	-0.831860	-0.962572
10	6	0	-5.557001	0.369051	-0.248613
11	1	0	-6.425701	0.696996	0.310819
12	6	0	-4.413878	1.156776	-0.277152
13	1	0	-4.361750	2.106021	0.243297
14	6	0	0.023210	2.100163	-0.931773
15	6	0	1.252498	1.969723	-0.230701
16	6	0	2.141986	3.058977	-0.320274
17	1	0	3.054838	3.016680	0.259776
18	6	0	1.879247	4.164050	-1.125760
19	1	0	2.603283	4.968284	-1.193141
20	6	0	0.691422	4.227006	-1.850931
21	1	0	0.485830	5.072997	-2.496974
22	6	0	-0.246787	3.207219	-1.738228
23	1	0	-1.185401	3.264164	-2.272334
24	16	0	1.262500	-0.586675	-2.062294
25	6	0	1.815275	-2.340340	-2.197697
26	1	0	2.877284	-2.331639	-2.442378
27	1	0	1.257625	-2.794551	-3.021212
28	6	0	1.599380	-3.077257	-0.893438
29	1	0	1.809378	-4.145484	-1.026427
30	6	0	2.508490	-2.605801	0.291011
31	8	0	2.282619	-3.155498	1.363553
32	8	0	3.403836	-1.726300	0.012159
33	7	0	0.186429	-2.914475	-0.426790
34	1	0	-0.459015	-3.490680	-0.963273
35	1	0	0.147545	-3.241251	0.541269
36	16	0	-2.057283	-1.542291	1.202472
37	6	0	-1.162674	-1.168767	2.773401
38	1	0	-1.512826	-1.880549	3.525338
39	1	0	-0.085842	-1.289216	2.660095
40	6	0	-1.437156	0.270182	3.227998
41	1	0	-1.149693	0.421992	4.270875
42	7	0	-2.898705	0.601009	3.073093
43	1	0	-3.222386	-0.001011	2.273813
44	6	0	-0.724327	1.343028	2.355902
45	8	0	0.486070	1.067043	2.122019
46	8	0	-1.404382	2.307624	1.982293
47	1	0	-6.495320	-1.438402	-0.951685
48	1	0	-2.881809	1.593166	2.741717
49	1	0	-2.482558	-0.758625	-2.331011
50	1	0	1.003848	1.471221	1.019583
51	17	0	3.682904	0.898658	1.698601
52	1	0	-3.466082	0.457880	3.904772

HF=-2731.4916323\ZeroPoint=0.3582337\Thermal=0.3899803

G = 9.2 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.265012	-0.394445	-1.068724
2	46	0	2.548232	0.194998	0.387525
3	7	0	-0.926769	1.428438	-0.285871
4	7	0	-2.031295	2.001554	-0.266168
5	6	0	-3.149096	1.358323	-0.830044
6	6	0	-3.119836	0.762463	-2.096827
7	6	0	-4.275909	0.173847	-2.595698
8	1	0	-4.266059	-0.280627	-3.579501
9	6	0	-5.443210	0.165601	-1.832244
10	6	0	-5.468242	0.782476	-0.579234
11	1	0	-6.377946	0.780526	0.009518
12	6	0	-4.332466	1.410392	-0.085949
13	1	0	-4.322868	1.881562	0.888620
14	6	0	0.181914	2.241338	0.151394
15	6	0	1.021892	1.762232	1.190765
16	6	0	2.222295	2.454141	1.438150
17	1	0	2.810904	2.187874	2.305526
18	6	0	2.573834	3.580092	0.659837
19	1	0	3.510306	4.088331	0.853313
20	6	0	1.708342	4.045957	-0.306557
21	1	0	1.959756	4.923638	-0.890304
22	6	0	0.497956	3.372849	-0.565770
23	1	0	-0.160514	3.704068	-1.358991
24	16	0	1.801975	0.609678	-1.840061
25	6	0	2.435888	-0.868701	-2.737895
26	1	0	3.524718	-0.826812	-2.733936
27	1	0	2.079757	-0.788742	-3.768696

28	6	0	1.972054	-2.158220	-2.087970
29	1	0	2.257186	-3.011384	-2.715145
30	6	0	2.585210	-2.447070	-0.684992
31	8	0	2.255036	-3.501609	-0.167100
32	8	0	3.424000	-1.575320	-0.221231
33	7	0	0.488340	-2.159564	-1.913386
34	1	0	0.007068	-2.300913	-2.799750
35	1	0	0.228530	-2.941454	-1.307845
36	16	0	-1.935264	-1.722680	-0.045945
37	6	0	-1.147349	-2.000298	1.614564
38	1	0	-0.881631	-3.054598	1.710747
39	1	0	-0.228252	-1.421089	1.696567
40	6	0	-2.106120	-1.605608	2.742085
41	1	0	-1.607232	-1.799941	3.699449
42	7	0	-3.394582	-2.319957	2.752131
43	1	0	-3.688530	-2.529355	1.800523
44	6	0	-2.381609	-0.088137	2.740593
45	8	0	-1.529956	0.742194	2.541351
46	8	0	-3.648219	0.237232	3.019244
47	1	0	-6.338382	-0.306589	-2.220305
48	1	0	-4.111884	-0.628023	3.118666
49	1	0	-2.210224	0.788701	-2.684280
50	1	0	0.623049	1.047309	1.898904
51	17	0	3.060238	-0.403627	2.596057
52	1	0	-3.337333	-3.191570	3.264867

HF=-2731.5300539\ZeroPoint=0.3621131\Thermal=0.3950847

G = -10.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.051100	-0.527873	0.600071
2	46	0	-1.242105	1.269617	0.772900
3	7	0	1.813241	0.980226	-0.642501
4	7	0	2.862720	0.799659	-1.305131
5	6	0	3.692673	-0.294302	-1.004911
6	6	0	4.087201	-0.586098	0.309243
7	6	0	4.964807	-1.640706	0.540129
8	1	0	5.286628	-1.857090	1.552556
9	6	0	5.438941	-2.407518	-0.523590
10	6	0	5.063257	-2.094041	-1.831565
11	1	0	5.437701	-2.683623	-2.660032
12	6	0	4.214986	-1.022763	-2.078154
13	1	0	3.913786	-0.763821	-3.085397
14	6	0	1.170549	2.255393	-0.832451
15	6	0	-0.105830	2.522730	-0.288564
16	6	0	-0.618929	3.819841	-0.485653
17	1	0	-1.598847	4.061634	-0.092378
18	6	0	0.083811	4.797773	-1.173310
19	1	0	-0.347639	5.785752	-1.293854
20	6	0	1.347471	4.511956	-1.704035
21	1	0	1.907792	5.272000	-2.235775
22	6	0	1.886033	3.254229	-1.530586
23	1	0	2.868073	3.020064	-1.916713
24	16	0	0.598786	1.002322	2.310287
25	6	0	-0.117348	-0.183604	3.538232
26	1	0	-0.926849	0.332603	4.054883
27	1	0	0.671028	-0.418525	4.258202
28	6	0	-0.649282	-1.444601	2.882661
29	1	0	-0.860529	-2.199125	3.649583
30	6	0	-1.959635	-1.298616	2.051192
31	8	0	-2.469811	-0.143237	1.910068
32	8	0	-2.368498	-2.363074	1.569401
33	7	0	0.364674	-1.991193	1.925732
34	1	0	1.170678	-2.378428	2.412904
35	1	0	-0.070124	-2.747293	1.392752
36	1	0	6.114093	-3.234617	-0.337191
37	1	0	3.746239	0.038362	1.125442
38	16	0	-2.870091	1.505737	-0.938119
39	6	0	-3.823405	-0.055123	-0.867357
40	1	0	-4.191602	-0.236156	0.139637
41	1	0	-4.670480	0.077412	-1.544423
42	6	0	-2.981657	-1.313514	-1.278050
43	1	0	-2.613648	-1.787842	-0.365994
44	7	0	-1.821911	-0.943497	-2.143089
45	6	0	-3.828235	-2.302047	-2.045200
46	1	0	-1.733110	0.105098	-2.054310
47	1	0	-2.012550	-1.210409	-3.113868
48	1	0	-0.932300	-1.389810	-1.834787
49	8	0	-4.802574	-2.811595	-1.284774
50	8	0	-3.668545	-2.572562	-3.215226
51	1	0	-5.331059	-3.412332	-1.831992
52	17	0	0.944219	-2.148799	-1.181152

HF=-2731.5640542\ZeroPoint=0.3631844\Thermal=0.3956817

G = 16.3 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.284842	-0.742246	0.136304
2	46	0	1.612007	-0.804998	-0.894190
3	7	0	-1.408097	1.158176	-0.697882
4	7	0	-2.385615	1.937211	-0.582238
5	6	0	-3.589711	1.467788	-0.039787
6	6	0	-4.147561	0.226248	-0.381573
7	6	0	-5.371877	-0.142286	0.162911
8	1	0	-5.815952	-1.092268	-0.110988
9	6	0	-6.030373	0.706790	1.052111
10	6	0	-5.484332	1.953337	1.366889
11	1	0	-6.002519	2.616979	2.048687
12	6	0	-4.282629	2.350438	0.798213
13	1	0	-3.845162	3.315780	1.020448
14	6	0	-0.313922	1.690414	-1.473705
15	6	0	1.018122	1.272206	-1.212510
16	6	0	2.030181	1.931711	-1.937300
17	1	0	3.059990	1.704086	-1.695200
18	6	0	1.743431	2.865014	-2.930173
19	1	0	2.550514	3.324920	-3.489108
20	6	0	0.420123	3.203070	-3.203192
21	1	0	0.184599	3.917289	-3.983848
22	6	0	-0.608900	2.632432	-2.461966
23	1	0	-1.638698	2.906388	-2.647444

24	16	0	-0.493117	-1.584667	-1.890234
25	6	0	-0.466597	-3.369012	-1.404056
26	1	0	0.312782	-3.855804	-1.989706
27	1	0	-1.437844	-3.794952	-1.667659
28	6	0	-0.167383	-3.527093	0.074780
29	1	0	-0.284446	-4.576322	0.372119
30	6	0	1.281258	-3.112653	0.489189
31	8	0	2.087842	-2.834869	-0.474164
32	8	0	1.506028	-3.103060	1.696874
33	7	0	-1.097773	-2.681326	0.887572
34	1	0	-2.026569	-3.092824	0.953512
35	1	0	-0.720651	-2.617603	1.836599
36	1	0	-6.978102	0.407217	1.484233
37	1	0	-3.647514	-0.410627	-1.100201
38	16	0	3.647955	-0.209099	0.108165
39	6	0	3.139910	-0.107864	1.864106
40	1	0	2.489900	-0.953412	2.105856
41	1	0	4.046093	-0.216555	2.461710
42	6	0	2.467970	1.222989	2.240947
43	1	0	2.290886	1.217579	3.327380
44	7	0	1.197960	1.431816	1.526300
45	6	0	3.360328	2.426890	1.968056
46	1	0	1.222319	1.117128	0.103127
47	1	0	0.933682	2.414325	1.561989
48	1	0	0.439661	0.883301	1.940083
49	8	0	4.593055	2.260117	2.480098
50	8	0	3.001083	3.434550	1.409744
51	1	0	5.108400	3.053802	2.272816
52	17	0	-1.729765	0.028675	2.346890

HF=-2731.517747\ZeroPoint=0.3586302\Thermal=0.3907581

G = 3.2 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.233670	0.815773	0.038212
2	46	0	-1.938016	0.181565	-0.990901
3	7	0	1.724996	-1.123192	-0.533834
4	7	0	2.786439	-1.777901	-0.470093
5	6	0	3.955784	-1.179197	0.029133
6	6	0	4.350011	0.124883	-0.298516
7	6	0	5.552817	0.614613	0.192405
8	1	0	5.868137	1.618970	-0.064597
9	6	0	6.349723	-0.178664	1.017877
10	6	0	5.964160	-1.486050	1.321822
11	1	0	6.589728	-2.104539	1.954189
12	6	0	4.785425	-2.001715	0.801344
13	1	0	4.472257	-3.017324	1.009641
14	6	0	0.674672	-1.751431	-1.294633
15	6	0	-0.618268	-1.872335	-0.735652
16	6	0	-1.658868	-2.306742	-1.574666
17	1	0	-2.615769	-2.549479	-1.133840
18	6	0	-1.415523	-2.576111	-2.938972
19	1	0	-2.236013	-2.889710	-3.572824
20	6	0	-0.135449	-2.474125	-3.446991
21	1	0	0.061355	-2.692940	-4.489738
22	6	0	0.922285	-2.067247	-2.617635
23	1	0	1.922644	-1.948037	-3.014533
24	16	0	0.080631	1.145581	-1.996752
25	6	0	-0.241600	2.950083	-1.794273
26	1	0	-1.137004	3.194920	-2.365113
27	1	0	0.611539	3.487147	-2.216298
28	6	0	-0.450063	3.300337	-0.334589
29	1	0	-0.509511	4.389286	-0.215505
30	6	0	-1.757594	2.738647	0.294966
31	8	0	-2.588639	2.145276	-0.483639
32	8	0	-1.893795	2.947401	1.500230
33	7	0	0.689032	2.783864	0.488837
34	1	0	1.521588	3.358787	0.375835
35	1	0	0.427740	2.829829	1.476006
36	1	0	7.279735	0.215330	1.411027
37	1	0	3.730105	0.727610	-0.950267
38	16	0	-3.893245	-0.617418	0.009093
39	6	0	-3.793176	0.074443	1.701966
40	1	0	-3.692992	1.158999	1.643714
41	1	0	-4.752491	-0.165729	2.166135
42	6	0	-2.645989	-0.488478	2.565626
43	1	0	-2.862067	-0.190343	3.605834
44	7	0	-1.356691	-0.007294	2.089747
45	6	0	-2.654728	-2.006766	2.564433
46	1	0	-0.761992	-1.785977	0.334846
47	1	0	-0.574836	-0.441730	2.569111
48	1	0	-1.299034	0.994178	2.236660
49	8	0	-3.813790	-2.495005	3.059112
50	8	0	-1.748450	-2.718417	2.202985
51	1	0	-3.766739	-3.460822	3.006082
52	17	0	2.086741	0.605658	2.228581

HF=-2731.541891\ZeroPoint=0.3625544\Thermal=0.395332

G = -13.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.202635	-0.643811	-0.411379
2	46	0	1.494499	0.314306	-1.190321
3	7	0	-1.456506	1.379354	0.088815
4	7	0	-2.450206	1.764104	0.748540
5	6	0	-3.554051	0.915054	0.919956
6	6	0	-4.124539	0.211206	-0.151094
7	6	0	-5.260227	-0.561199	0.068268
8	1	0	-5.716119	-1.090862	-0.760526
9	6	0	-5.818206	-0.644591	1.343402
10	6	0	-5.261267	0.081104	2.398842
11	1	0	-5.699717	0.023801	3.388012
12	6	0	-4.149715	0.884367	2.185311
13	1	0	-3.703885	1.455215	2.990042
14	6	0	-0.518722	2.418304	-0.264871
15	6	0	0.746426	2.125508	-0.818276
16	6	0	1.554588	3.216465	-1.185341
17	1	0	2.533824	3.029820	-1.609015
18	6	0	1.142353	4.530402	-1.015162
19	1	0	1.795721	5.341798	-1.316865

20	6	0	-0.112952	4.803513	-0.462786
21	1	0	-0.448378	5.825470	-0.331797
22	6	0	-0.935497	3.757500	-0.098352
23	1	0	-1.916712	3.950203	0.311602
24	16	0	-0.437756	-0.121790	-2.564802
25	6	0	-0.087569	-1.850930	-3.138729
26	1	0	0.813450	-1.817695	-3.750915
27	1	0	-0.929639	-2.161204	-3.762251
28	6	0	0.108972	-2.811806	-1.978660
29	1	0	0.124069	-3.845560	-2.346346
30	6	0	1.414018	-2.607981	-1.163669
31	8	0	2.256700	-1.756159	-1.552019
32	8	0	1.485039	-3.303784	-0.123653
33	7	0	-1.003827	-2.646393	-0.994369
34	1	0	-1.892453	-2.964923	-1.375490
35	1	0	-0.799935	-3.199758	-0.160073
36	16	0	3.340873	0.890652	0.185300
37	6	0	3.956921	-0.688138	0.912318
38	1	0	3.927931	-1.467152	0.149941
39	1	0	4.996475	-0.522236	1.202592
40	6	0	3.185263	-1.163850	2.152697
41	1	0	3.598552	-2.111006	2.501030
42	7	0	1.759495	-1.438922	1.775643
43	6	0	3.189057	-0.226908	3.383972
44	8	0	2.936109	1.060887	3.166595
45	8	0	3.364289	-0.679988	4.486479
46	1	0	-6.696509	-1.256941	1.511447
47	1	0	1.348500	-0.629436	1.288683
48	1	0	-3.709680	0.314241	-1.146162
49	1	0	2.924035	1.261785	2.186058
50	17	0	-1.435691	-1.393239	1.849764
51	1	0	1.143830	-1.647635	2.565190
52	1	0	1.708893	-2.250199	1.092471

HF=-2731.5686096\ZeroPoint=0.3635062\Thermal=0.3956442

G = 20.2 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.103266	0.855712	-0.327175
2	46	0	-1.908306	0.055961	-0.781688
3	7	0	1.422265	-1.208255	-0.427024
4	7	0	2.468375	-1.817826	-0.110460
5	6	0	3.636018	-1.108434	0.202198
6	6	0	4.096110	-0.034125	-0.572893
7	6	0	5.296610	0.579528	-0.238397
8	1	0	5.666520	1.400432	-0.841540
9	6	0	6.023567	0.141380	0.868148
10	6	0	5.572683	-0.946113	1.620216
11	1	0	6.144595	-1.291043	2.473215
12	6	0	4.398258	-1.596502	1.270321
13	1	0	4.031830	-2.446525	1.832166
14	6	0	0.405265	-2.074453	-0.985837
15	6	0	-0.965313	-1.896996	-0.654782
16	6	0	-1.865379	-2.843783	-1.186198
17	1	0	-2.900679	-2.796210	-0.873652
18	6	0	-1.454218	-3.845005	-2.063854
19	1	0	-2.179138	-4.537232	-2.476041
20	6	0	-0.109100	-3.955796	-2.399050
21	1	0	0.223541	-4.727588	-3.083760
22	6	0	0.828270	-3.085630	-1.840824
23	1	0	1.880032	-3.187294	-2.074298
24	16	0	-0.135934	0.767569	-2.309821
25	6	0	-0.518823	2.572217	-2.458823
26	1	0	-1.498163	2.661603	-2.928351
27	1	0	0.234620	3.016705	-3.113551
28	6	0	-0.533941	3.246326	-1.099788
29	1	0	-0.610713	4.334336	-1.219120
30	6	0	-1.708862	2.820324	-0.173199
31	8	0	-2.627540	2.092937	-0.667503
32	8	0	-1.626671	3.229665	0.997090
33	7	0	0.724073	2.916742	-0.360500
34	1	0	1.531467	3.383281	-0.769475
35	1	0	0.637721	3.239412	0.605311
36	16	0	-3.745274	-0.646848	0.481176
37	6	0	-3.610909	0.149411	2.129222
38	1	0	-3.833668	1.216881	2.049173
39	1	0	-4.397778	-0.324807	2.720221
40	6	0	-2.292905	-0.066219	2.882542
41	1	0	-2.424199	0.211183	3.929677
42	7	0	-1.233018	0.832030	2.315916
43	6	0	-1.796737	-1.541043	2.812910
44	8	0	-0.861220	-1.756219	1.944599
45	8	0	-2.308923	-2.331480	3.583905
46	1	0	6.951476	0.634180	1.134128
47	1	0	-0.975160	0.470458	1.385248
48	1	0	3.537056	0.279756	-1.445984
49	1	0	-1.078624	-1.652812	0.599291
50	17	0	1.964660	1.152608	1.876519
51	1	0	-0.351886	0.812774	2.838614
52	1	0	-1.537527	1.811081	2.162249

HF=-2731.5129244\ZeroPoint=0.3588269\Thermal=0.3907405

G = 13.2 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.157000	0.852091	-0.309785
2	46	0	-1.980156	-0.080935	-0.875749
3	7	0	1.605810	-1.181172	-0.456833
4	7	0	2.645088	-1.824830	-0.216285
5	6	0	3.809404	-1.157073	0.200881
6	6	0	4.266340	0.021997	-0.402173
7	6	0	5.458980	0.586462	0.029996
8	1	0	5.825958	1.491769	-0.438934
9	6	0	6.179710	-0.006001	1.066925
10	6	0	5.729865	-1.193355	1.648579
11	1	0	6.296452	-1.656460	2.447370
12	6	0	4.563388	-1.792699	1.194302
13	1	0	4.199715	-2.719662	1.619910
14	6	0	0.564186	-1.946382	-1.106690
15	6	0	-0.704115	-2.070716	-0.489548

16	6	0	-1.740797	-2.647460	-1.248122	36	16	0	-3.718268	-0.803669	0.487708
17	1	0	-2.674846	-2.879261	-0.753761	37	6	0	-3.677707	0.190620	2.030754
18	6	0	-1.518641	-3.065179	-2.577415	38	1	0	-3.766819	1.249606	1.779171
19	1	0	-2.335068	-3.492234	-3.146752	39	1	0	-4.599061	-0.118225	2.530365
20	6	0	-0.256370	-2.966551	-3.126541	40	6	0	-2.526116	-0.055757	3.015470
21	1	0	-0.069922	-3.306335	-4.138447	41	1	0	-2.844033	0.250004	4.012879
22	6	0	0.800528	-2.407602	-2.384366	42	7	0	-1.304277	0.742892	2.642957
23	1	0	1.783685	-2.292437	-2.823675	43	6	0	-2.053566	-1.558781	3.048810
24	16	0	-0.129553	0.762157	-2.296569	44	8	0	-0.939819	-1.733166	2.461485
25	6	0	-0.572376	2.553686	-2.391073	45	8	0	-2.807917	-2.349077	3.604269
26	1	0	-1.555684	2.628603	-2.854805	46	1	0	7.101768	0.447889	1.411033
27	1	0	0.162600	3.046483	-3.032096	47	1	0	-0.709251	0.020065	2.168276
28	6	0	-0.602218	3.181289	-1.010753	48	1	0	3.706384	0.463634	-1.217356
29	1	0	-0.732314	4.268092	-1.090351	49	1	0	-0.804020	-1.942360	0.593154
30	6	0	-1.737501	2.672225	-0.085395	50	17	0	1.989624	1.119025	1.885773
31	8	0	-2.645028	1.927900	-0.584407	51	1	0	-0.764281	1.023737	3.459696
32	8	0	-1.660043	3.044459	1.094928	52	1	0	-1.493068	1.588889	2.076778
33	7	0	0.676003	2.887009	-0.293133	---					
34	1	0	1.457522	3.399984	-0.696736	HF=-2731.5269685\ZeroPoint=0.362854\Thermal=0.3951275					
35	1	0	0.587129	3.175235	0.683522						

Structures from Table S10

Table S10. Free energies for the pre- and postreaction complexes and the transition states for **the D transfer from Ala^{3D}·DCl to the palladated complexes** with L-alanine. Free energies relative to **M1-Ala^{2D}-1** for the monopalladated and **D1-Ala^{2D}-1** for the dipalladated complexes (in kcal mol^{-1}).

D-source→	**Ala^{3D}·DCl**	**Ala^{3D}·DCl**
Donor group→	COOD	ND_3^+
M1-Ala^{2D}-1		
Prereaction complex	**-0.8**	-7.0
Transition state	**17.7**	22.0
Postreaction complex	**13.6**	16.0
D1-Ala^{2D}-1		
Prereaction complex	-12.4	**-13.9**
Transition state	17.8	**14.8**
Postreaction complex	15.4	**14.1**

G = -0.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.328977	-0.060993	-1.034162
2	7	0	1.938718	0.897969	-0.078133
3	7	0	1.868566	2.158699	0.020494
4	6	0	0.726735	2.704511	-0.550192
5	6	0	-0.234575	1.835203	-1.130251
6	6	0	-1.361980	2.430814	-1.702651
7	1	0	-2.126819	1.821067	-2.173692
8	6	0	-1.529150	3.824821	-1.691107
9	6	0	-0.574286	4.654690	-1.102215
10	1	0	-0.715604	5.728701	-1.094660
11	6	0	0.563065	4.093925	-0.528519
12	1	0	1.326305	4.709877	-0.067409
13	6	0	3.089955	0.291221	0.506152
14	6	0	3.121208	-1.101655	0.627715
15	6	0	4.227027	-1.711044	1.216776
16	1	0	4.245848	-2.790438	1.309182
17	6	0	5.296234	-0.946629	1.673548
18	1	0	6.156031	-1.427134	2.126747
19	6	0	5.264354	0.446002	1.538249
20	1	0	6.099927	1.044359	1.883285
21	6	0	4.170129	1.069110	0.959843
22	1	0	4.136306	2.143771	0.849621
23	6	0	-2.299716	-3.121529	-2.558585
24	1	0	-3.331610	-2.758873	-2.526690
25	1	0	-2.281522	-4.182557	-2.308805
26	6	0	-1.417093	-2.364317	-1.577304
27	1	0	-1.821097	-2.438575	-0.564724
28	7	0	-1.370439	-0.896960	-1.879917
29	1	0	-2.197106	-0.439754	-1.495527
30	6	0	0.020724	-2.936889	-1.471952
31	8	0	0.198013	-4.132345	-1.632725
32	8	0	0.933256	-2.068141	-1.162293
33	1	0	-2.413911	4.259275	-2.144321
34	1	0	-1.352622	-0.747734	-2.886768
35	1	0	2.305391	-1.703025	0.248095
36	1	0	-2.009860	2.022744	0.360798
37	6	0	-2.705398	0.664286	3.741386
38	1	0	-3.144728	0.295077	4.672019
39	1	0	-2.680684	1.752749	3.780770
40	6	0	-3.541590	0.191865	2.552350
41	1	0	-4.547707	0.633546	2.624383
42	7	0	-3.604608	-1.281631	2.514879
43	1	0	-2.023530	-1.761386	2.296428
44	6	0	-3.018961	0.652259	1.192437
45	8	0	-2.357622	1.801140	1.249286
46	8	0	-3.242601	0.036276	0.169251
47	1	0	-4.127544	-1.600503	1.703659
48	1	0	-4.043854	-1.648480	3.353196
49	17	0	-0.696198	-1.922379	2.019833
50	1	0	-1.682774	0.292926	3.666084
51	1	0	-1.920524	-3.021400	-3.580874

HF=-1808.3106097\ZeroPoint=0.37864\Thermal=0.4090932

G = 17.7 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.159054	-0.291441	-0.798906
2	7	0	-1.952473	-0.412481	0.205598
3	7	0	-2.394433	-1.563267	0.488456
4	6	0	-1.519574	-2.594169	0.143150
5	6	0	-0.154355	-2.310143	-0.144209
6	6	0	0.662351	-3.371019	-0.551633
7	1	0	1.716365	-3.182578	-0.728097
8	6	0	0.153098	-4.664228	-0.658545
9	6	0	-1.183684	-4.925532	-0.341677
10	1	0	-1.568413	-5.936085	-0.414106

11	6	0	-2.023272	-3.895079	0.069943
12	1	0	-3.065014	-4.074777	0.306710
13	6	0	-2.754863	0.707995	0.537845
14	6	0	-2.121938	1.951127	0.652832
15	6	0	-2.878286	3.064089	1.005352
16	1	0	-2.386894	4.024100	1.104821
17	6	0	-4.249909	2.944510	1.214624
18	1	0	-4.837053	3.818683	1.472544
19	6	0	-4.876984	1.699708	1.083553
20	1	0	-5.946474	1.611688	1.235638
21	6	0	-4.136292	0.576679	0.751424
22	1	0	-4.603599	-0.392709	0.643226
23	6	0	2.804259	1.313641	-3.433866
24	1	0	3.798097	0.952570	-3.154334
25	1	0	2.879953	2.349428	-3.766585
26	6	0	1.843568	1.240129	-2.257848
27	1	0	2.224940	1.802411	-1.400897
28	7	0	1.651385	-0.162568	-1.768873
29	1	0	2.360376	-0.435551	-1.075123
30	6	0	0.471703	1.880975	-2.549394
31	8	0	0.365606	2.812163	-3.319683
32	8	0	-0.534873	1.381798	-1.866938
33	1	0	0.801657	-5.476741	-0.966330
34	1	0	1.679905	-0.818764	-2.546258
35	1	0	-1.056076	2.046261	0.491678
36	1	0	0.501492	-1.573441	0.703972
37	6	0	2.044461	0.459756	3.909859
38	1	0	2.580024	0.953215	4.726937
39	1	0	1.494047	-0.388455	4.314979
40	6	0	3.011777	-0.040477	2.848905
41	1	0	3.749372	-0.725046	3.279935
42	7	0	3.761939	1.106000	2.232154
43	1	0	3.000566	1.788002	1.776320
44	6	0	2.355493	-0.781788	1.657041
45	8	0	1.201460	-1.248100	1.870173
46	8	0	3.032063	-0.858324	0.611270
47	1	0	4.329328	0.748061	1.460637
48	1	0	4.337635	1.609786	2.903498
49	17	0	1.581946	2.577240	1.006224
50	1	0	1.331225	1.158549	3.471054
51	1	0	2.437650	0.723489	-4.280375

HF=-1808.2863439\ZeroPoint=0.3773757\Thermal=0.4063323

G = 13.6 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.241469	0.179769	0.644857
2	7	0	-1.982702	0.667456	-0.370224
3	7	0	-2.247042	1.886116	-0.560707
4	6	0	-1.255581	2.772724	-0.127351
5	6	0	0.101271	2.393372	0.020283
6	6	0	1.018110	3.297811	0.555387
7	1	0	2.055608	2.995332	0.609586
8	6	0	0.593449	4.571183	0.933678
9	6	0	-0.736269	4.956250	0.749449
10	1	0	-1.054716	5.954096	1.027897
11	6	0	-1.660280	4.066542	0.209301
12	1	0	-2.699345	4.341002	0.076272
13	6	0	-2.973021	-0.277307	-0.747871
14	6	0	-2.575258	-1.601004	-0.963082
15	6	0	-3.528075	-2.538164	-1.348660
16	1	0	-3.219225	-3.560471	-1.528648
17	6	0	-4.862399	-2.167390	-1.491769
18	1	0	-5.602908	-2.906239	-1.776583
19	6	0	-5.254674	-0.843590	-1.259658
20	1	0	-6.295895	-0.559951	-1.359016
21	6	0	-4.316581	0.107043	-0.892704
22	1	0	-4.603172	1.132389	-0.703146
23	6	0	2.197525	-2.251786	3.173421
24	1	0	3.245819	-2.043259	2.947509
25	1	0	2.068387	-3.321229	3.346634
26	6	0	1.307889	-1.822184	2.017739
27	1	0	1.609069	-2.316171	1.088874
28	7	0	1.413890	-0.359282	1.732149
29	1	0	2.313539	-0.182710	1.228334
30	6	0	-0.167170	-2.196106	2.207254
31	8	0	-0.518493	-3.176681	2.825156
32	8	0	-1.027632	-1.391017	1.607300
33	1	0	1.307751	5.274891	1.344674
34	1	0	1.423306	0.168252	2.603678
35	1	0	-1.536446	-1.884246	-0.865081
36	1	0	0.539941	1.540551	-0.558874
37	6	0	3.190136	0.219601	-3.335289
38	1	0	3.607382	-0.209516	-4.251845
39	1	0	3.253289	1.305579	-3.394564
40	6	0	3.955856	-0.241489	-2.106671
41	1	0	5.022893	-0.015942	-2.199943
42	7	0	3.833372	-1.730631	-1.917740
43	1	0	2.775856	-1.975684	-1.874932
44	6	0	3.472167	0.379548	-0.761246
45	8	0	2.914983	1.482897	-0.802610
46	8	0	3.711479	-0.340670	0.254016
47	1	0	4.199014	-1.935067	-0.980255
48	1	0	4.300787	-2.276765	-2.638234
49	17	0	0.913445	-2.046528	-1.582181
50	1	0	2.139153	-0.062510	-3.254105
51	1	0	1.921035	-1.732921	4.096929

HF=-1808.2936292\ZeroPoint=0.3806969\Thermal=0.4104586

G = -7.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.153343	0.396066	-0.804588
2	7	0	2.126093	0.396967	-0.094039
3	7	0	2.615549	1.527426	0.208470
4	6	0	1.723547	2.576860	0.088210
5	6	0	0.396078	2.307197	-0.335960
6	6	0	-0.503145	3.366903	-0.363956
7	1	0	-1.546776	3.201672	-0.600339
8	6	0	-0.083391	4.656325	-0.012763

9	6	0	1.235418	4.912364	0.375486
10	1	0	1.538556	5.917919	0.641470
11	6	0	2.148053	3.868147	0.436982
12	1	0	3.173323	4.023529	0.751754
13	6	0	3.004535	-0.720132	0.034387
14	6	0	4.395221	-0.541965	0.117262
15	6	0	5.217712	-1.647993	0.272341
16	1	0	6.291587	-1.511252	0.328181
17	6	0	4.670438	-2.932702	0.348416
18	1	0	5.319754	-3.792623	0.466620
19	6	0	3.291778	-3.103559	0.256209
20	1	0	2.859212	-4.096176	0.299393
21	6	0	2.452452	-2.003921	0.091506
22	1	0	1.386966	-2.147889	-0.024165
23	6	0	-1.345140	-1.913794	-1.760858
24	6	0	-2.123177	-0.711699	-2.341421
25	1	0	-1.681741	-0.530543	-3.327800
26	7	0	-1.803540	0.499082	-1.512460
27	1	0	-2.426553	0.571036	-0.692800
28	6	0	-3.620862	-0.946396	-2.466681
29	1	0	-0.803331	5.467362	-0.030329
30	1	0	-1.967387	1.346114	-2.049931
31	1	0	4.808519	0.455137	0.055444
32	1	0	-0.453788	0.182550	1.467121
33	6	0	-2.308939	-1.589537	3.681636
34	1	0	-1.911543	-1.134114	4.592778
35	1	0	-2.475733	-2.650134	3.877001
36	6	0	-1.329672	-1.424424	2.520400
37	1	0	-0.361628	-1.874793	2.745640
38	7	0	-1.125213	0.032037	2.238422
39	1	0	-0.778820	0.525041	3.060633
40	6	0	-1.901311	-2.045767	1.242313
41	8	0	-1.367510	-3.222269	0.948575
42	8	0	-2.749465	-1.471617	0.604705
43	1	0	-2.040972	0.595311	1.888756
44	1	0	-1.606899	-3.450054	0.007934
45	1	0	-3.262728	-1.119454	3.433979
46	8	0	-0.182042	-1.630616	-1.281993
47	8	0	-1.829898	-3.046902	-1.757403
48	1	0	-4.108585	-0.094729	-2.949086
49	1	0	-3.797035	-1.842487	-3.063122
50	1	0	-4.060310	-1.101115	-1.481202
51	17	0	-3.219079	1.763993	1.206955

HF=-1808.3287159\ZeroPoint=0.3816565\Thermal=0.4109377

G = 22.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.080988	0.180997	-0.777922
2	7	0	1.727549	1.000100	-0.107663
3	7	0	1.739691	2.243513	0.125442
4	6	0	0.499274	2.865484	0.011474
5	6	0	-0.697860	2.097255	-0.073865
6	6	0	-1.904593	2.779786	-0.274110
7	1	0	-2.831222	2.209522	-0.287317
8	6	0	-1.919966	4.174376	-0.359639
9	6	0	-0.739376	4.909950	-0.239126
10	1	0	-0.766454	5.992012	-0.296562
11	6	0	0.478040	4.259830	-0.046139
12	1	0	1.408690	4.809003	0.029696
13	6	0	2.987246	0.341755	-0.042494
14	6	0	4.180649	1.052623	-0.250207
15	6	0	5.392014	0.384501	-0.164168
16	1	0	6.315546	0.924463	-0.337272
17	6	0	5.424070	-0.981656	0.136054
18	1	0	6.374908	-1.498164	0.200216
19	6	0	4.236187	-1.679546	0.339217
20	1	0	4.255382	-2.738565	0.566285
21	6	0	3.011061	-1.027131	0.240023
22	1	0	2.089678	-1.569536	0.379186
23	6	0	-0.374722	-2.518036	-1.535131
24	6	0	-1.695063	-1.927540	-2.063534
25	1	0	-1.517828	-1.780486	-3.134973
26	7	0	-1.877056	-0.564166	-1.465632
27	1	0	-2.568939	-0.556905	-0.678108
28	6	0	-2.909785	-2.816529	-1.847439
29	1	0	-2.864070	4.687525	-0.502771
30	1	0	-2.284592	0.070132	-2.148306
31	1	0	4.139522	2.107403	-0.485056
32	1	0	-0.852466	1.161276	0.792073
33	6	0	-0.856239	-1.177981	4.026562
34	1	0	-0.697369	-0.351554	4.724288
35	1	0	-0.229939	-2.015930	4.341427
36	6	0	-0.496164	-0.736211	2.597350
37	1	0	0.558617	-0.449618	2.560981
38	7	0	-1.313261	0.393358	2.119373
39	1	0	-1.432575	1.087185	2.852448
40	6	0	-0.697104	-1.919558	1.655625
41	8	0	0.388616	-2.707501	1.568862
42	8	0	-1.727543	-2.135581	1.071834
43	1	0	-2.261731	0.109102	1.808107
44	1	0	0.217676	-3.382282	0.881072
45	1	0	-1.904882	-1.479784	4.073504
46	8	0	0.587050	-1.636779	-1.381754
47	8	0	-0.222609	-3.705306	-1.306728
48	1	0	-3.794705	-2.380429	-2.316726
49	1	0	-2.716160	-3.798034	-2.283155
50	1	0	-3.103180	-2.938355	-0.782607
51	17	0	-4.085708	0.290568	0.520405

HF=-1808.2813309\ZeroPoint=0.3780841\Thermal=0.4071046

G = 16.0 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.502801	-0.316980	-0.415833
2	7	0	-1.356677	1.475306	0.160162
3	7	0	-2.597957	1.504966	0.379091
4	6	0	-3.229321	0.256948	0.333619
5	6	0	-2.520834	-0.959274	0.487781
6	6	0	-3.191484	-2.173621	0.352485

7	1	0	-2.632445	-3.083378	0.540782
8	6	0	-4.556849	-2.183440	0.068288
9	6	0	-5.258996	-0.981376	-0.052432
10	1	0	-6.323719	-0.995945	-0.254073
11	6	0	-4.604813	0.239464	0.090582
12	1	0	-5.133136	1.179344	-0.011005
13	6	0	-0.664882	2.715213	0.147962
14	6	0	-1.334058	3.911448	-0.153428
15	6	0	-0.617152	5.097659	-0.168965
16	1	0	-1.119857	6.025448	-0.415506
17	6	0	0.752338	5.096937	0.119836
18	1	0	1.306663	6.028367	0.099832
19	6	0	1.405606	3.903934	0.421919
20	1	0	2.465864	3.897462	0.643599
21	6	0	0.704914	2.703148	0.428788
22	1	0	1.193030	1.775013	0.690941
23	6	0	1.682916	-0.343989	-2.237032
24	6	0	1.110656	-1.765189	-2.362662
25	1	0	0.357995	-1.708306	-3.157546
26	7	0	0.372407	-2.050423	-1.097645
27	1	0	1.003238	-2.314761	-0.330101
28	6	0	2.154451	-2.818919	-2.696410
29	1	0	-5.080978	-3.127064	-0.027073
30	1	0	-0.289282	-2.817066	-1.186801
31	1	0	-2.390614	3.890976	-0.384353
32	1	0	-1.551087	-1.048936	1.062993
33	6	0	3.523506	-1.440260	2.915835
34	1	0	3.362661	-1.304637	3.988318
35	1	0	4.594928	-1.579240	2.740194
36	6	0	2.984399	-0.223785	2.158631
37	1	0	3.506481	0.686234	2.464685
38	7	0	1.536185	0.004391	2.320420
39	1	0	1.351886	0.391753	3.240373
40	6	0	3.184374	-0.383963	0.656579
41	8	0	3.592348	0.739503	0.050355
42	8	0	2.939800	-1.409098	0.056115
43	1	0	1.037876	-0.891149	2.269906
44	1	0	3.556444	0.612270	-0.919989
45	1	0	2.992074	-2.338750	2.596401
46	8	0	0.945953	0.491379	-1.539435
47	8	0	2.729577	0.001846	-2.754024
48	1	0	1.685115	-3.794071	-2.851958
49	1	0	2.677019	-2.527458	-3.609132
50	1	0	2.885079	-2.890762	-1.891264
51	17	0	-0.165539	-2.854034	1.877797

HF=-1808.2902738\ZeroPoint=0.3806926\Thermal=0.4108547

G = -12.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	2.100408	0.727757	-0.601849
2	7	0	0.111784	1.290972	-0.436085
3	7	0	-0.745041	0.369326	-0.712700
4	6	0	-0.214631	-0.783451	-1.293406
5	6	0	1.198894	-0.874966	-1.348681
6	6	0	1.739303	-2.017942	-1.933088
7	1	0	2.811606	-2.166856	-1.960245
8	6	0	0.906293	-3.002321	-2.476348
9	6	0	-0.484308	-2.874664	-2.433672
10	1	0	-1.117691	-3.652242	-2.841256
11	6	0	-1.059222	-1.767520	-1.829331
12	1	0	-2.133266	-1.676700	-1.745489
13	6	0	-0.460338	2.481185	0.022052
14	6	0	0.331893	3.601160	0.304606
15	6	0	-0.302311	4.779388	0.686498
16	1	0	0.293720	5.656492	0.907143
17	6	0	-1.692113	4.832847	0.785619
18	1	0	-2.177312	5.758611	1.075971
19	6	0	-2.474236	3.699524	0.518989
20	1	0	-3.552629	3.776203	0.616362
21	6	0	-1.874647	2.508688	0.134380
22	6	0	6.359914	0.723619	-0.059234
23	1	0	6.710415	-0.311274	-0.042835
24	1	0	6.937769	1.315146	0.651176
25	6	0	4.884919	0.799501	0.308661
26	1	0	4.727037	0.331204	1.285403
27	7	0	4.033738	0.017313	-0.643004
28	1	0	4.068633	-0.980755	-0.379621
29	6	0	4.356732	2.249895	0.445741
30	8	0	5.097232	3.128797	0.849459
31	8	0	3.095920	2.403950	0.154241
32	1	0	1.350778	-3.880856	-2.932195
33	1	0	4.400264	0.106609	-1.589087
34	1	0	1.413022	3.536119	0.238838
35	1	0	-2.367237	-2.044711	1.011205
36	6	0	1.149643	-1.610565	2.326100
37	1	0	2.054685	-1.652427	2.933734
38	1	0	0.416966	-0.965336	2.809109
39	6	0	0.552355	-3.004911	2.157123
40	1	0	0.284634	-3.416395	3.134274
41	7	0	1.523677	-3.951288	1.506480
42	1	0	2.441986	-3.470439	1.138636
43	6	0	-0.726387	-3.049465	1.302767
44	8	0	-1.577645	-2.109388	1.637115
45	8	0	-0.876627	-3.891562	0.442742
46	1	0	1.031917	-4.394094	0.716602
47	1	0	1.836259	-4.682578	2.141409
48	17	0	4.124873	-2.882630	0.650517
49	46	0	-2.666818	0.716312	-0.097361
50	6	0	-6.038244	0.125755	-1.187391
51	1	0	-6.630580	1.039397	-1.298461
52	1	0	-6.675373	-0.724984	-1.432236
53	6	0	-5.518834	-0.023169	0.242031
54	1	0	-6.356234	-0.048338	0.942459
55	7	0	-4.614169	1.127125	0.580132
56	6	0	-4.744790	-1.354977	0.385698
57	1	0	-4.562077	1.251353	1.589280
58	1	0	-4.981324	1.994742	0.195875
59	8	0	-5.335150	-2.362299	0.716099
60	8	0	-3.471256	-1.274591	0.089792
61	1	0	1.413488	-1.181477	1.358909
62	1	0	-5.209458	0.156254	-1.899426
63	1	0	6.533006	1.145833	-1.054722

HF=-2258.9835395\ZeroPoint=0.4639239\Thermal=0.5018701

G = 17.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.402239	0.230225	-0.694642
2	7	0	-0.531075	0.636095	-0.067170
3	7	0	-1.383335	-0.323581	-0.141118
4	6	0	-0.859706	-1.563399	-0.549744
5	6	0	0.514991	-1.834023	-0.329596
6	6	0	1.060708	-3.024340	-0.812505
7	1	0	2.099356	-3.228541	-0.583042
8	6	0	0.252554	-3.932308	-1.494919
9	6	0	-1.108560	-3.669863	-1.667092
10	1	0	-1.739669	-4.390890	-2.173196
11	6	0	-1.680391	-2.492116	-1.191508
12	1	0	-2.739802	-2.301264	-1.300129
13	6	0	-1.034416	1.831826	0.433813
14	6	0	-0.202865	2.952205	0.591149
15	6	0	-0.745333	4.106500	1.135607
16	1	0	-0.123671	4.983844	1.262819
17	6	0	-2.089476	4.135127	1.514956
18	1	0	-2.505563	5.040108	1.944731
19	6	0	-2.910590	3.013295	1.347055
20	1	0	-3.947245	3.080170	1.661310
21	6	0	-2.406370	1.839807	0.798466
22	6	0	4.695986	0.662167	-3.241029
23	1	0	5.532206	0.010338	-2.979891
24	1	0	5.083371	1.565517	-3.713709
25	6	0	3.926643	1.050126	-1.987683
26	1	0	4.622591	1.475069	-1.259333
27	7	0	3.321185	-0.145563	-1.311730
28	1	0	3.915468	-0.421352	-0.515839
29	6	0	2.871884	2.128669	-2.233907
30	8	0	3.076747	3.080715	-2.950275
31	8	0	1.740228	1.997154	-1.552509
32	1	0	0.674525	-4.859833	-1.864233
33	1	0	3.306912	-0.943484	-1.943256
34	1	0	0.829239	2.915727	0.272874
35	1	0	1.062467	-1.346781	0.536090
36	6	0	4.278817	0.049793	3.619669
37	1	0	4.995213	0.090590	4.445839
38	1	0	3.297587	0.348109	3.986957
39	6	0	4.168048	-1.355851	3.046472
40	1	0	3.911873	-2.074839	3.830993
41	7	0	5.469364	-1.798118	2.437271
42	1	0	5.817949	-1.032586	1.743790
43	6	0	3.096089	-1.506046	1.928202
44	8	0	2.011488	-0.918611	2.117923
45	8	0	3.431625	-2.219647	0.946757
46	1	0	5.256769	-2.600989	1.833668
47	1	0	6.191570	-2.011909	3.121387
48	17	0	6.117140	0.230262	0.403007
49	46	0	-3.314485	0.122611	0.412494
50	6	0	-6.630115	0.466341	-1.051540
51	1	0	-7.126829	1.423867	-0.864295
52	1	0	-7.317384	-0.175995	-1.602567
53	6	0	-6.240332	-0.223917	0.253806
54	1	0	-7.127352	-0.376894	0.872713
55	7	0	-5.251954	0.627528	1.003522
56	6	0	-5.621667	-1.613237	-0.054205
57	1	0	-5.305507	0.432445	2.001385
58	1	0	-5.463785	1.614890	0.881406
59	8	0	-6.374334	-2.527703	-0.334144
60	8	0	-4.323919	-1.663448	-0.034764
61	1	0	4.593606	0.752255	2.845632
62	1	0	-5.747599	0.643920	-1.672689
63	1	0	4.046309	0.156862	-3.963896

HF=-2258.9323835\ZeroPoint=0.4622209\Thermal=0.4998677

G = 15.4 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.420550	0.240180	-0.617012
2	7	0	-0.530362	0.657914	-0.056528
3	7	0	-1.369080	-0.316982	-0.074205
4	6	0	-0.829626	-1.568111	-0.420299
5	6	0	0.555512	-1.806253	-0.226226
6	6	0	1.109918	-3.008493	-0.668495
7	1	0	2.159408	-3.186792	-0.461079
8	6	0	0.301047	-3.961671	-1.284662
9	6	0	-1.068777	-3.731782	-1.430318
10	1	0	-1.700415	-4.486583	-1.883716
11	6	0	-1.648123	-2.542477	-0.995534
12	1	0	-2.713142	-2.374179	-1.086701
13	6	0	-1.050841	1.876261	0.366299
14	6	0	-0.234379	3.016701	0.442690
15	6	0	-0.792441	4.196879	0.911239
16	1	0	-0.183051	5.089508	0.976089
17	6	0	-2.135501	4.231356	1.293799
18	1	0	-2.563279	5.156963	1.664065
19	6	0	-2.941490	3.089487	1.203655
20	1	0	-3.978328	3.163314	1.515821
21	6	0	-2.422213	1.889231	0.732661
22	6	0	3.422702	-0.204882	-3.599251
23	1	0	4.051649	-1.099435	-3.602071
24	1	0	3.644391	0.378782	-4.493451
25	6	0	3.698181	0.641533	-2.358175
26	1	0	4.750964	0.929433	-2.313277
27	7	0	3.364762	-0.093917	-1.107958
28	1	0	3.956521	0.303673	-0.348239
29	6	0	2.864311	1.932565	-2.390298
30	8	0	3.111683	2.840553	-3.146752
31	8	0	1.831615	1.962877	-1.554276
32	1	0	0.731161	-4.897831	-1.621290
33	1	0	3.594577	-1.088083	-1.126750
34	1	0	0.797317	2.976598	0.120935
35	1	0	1.142510	-1.312034	0.617101
36	6	0	4.412022	-0.263647	3.712382
37	1	0	5.195309	-0.203236	4.474385

38	1	0	3.444422	-0.344236	4.206031
39	6	0	4.599331	-1.480326	2.820487
40	1	0	4.636113	-2.398440	3.415612
41	7	0	5.890762	-1.401032	2.051226
42	1	0	5.934623	-0.443095	1.540917
43	6	0	3.486064	-1.687237	1.749259
44	8	0	2.345788	-1.287489	2.047470
45	8	0	3.868629	-2.257552	0.689525
46	1	0	5.825312	-2.106173	1.306398
47	1	0	6.719718	-1.530611	2.627163
48	17	0	5.676254	1.159841	0.571469
49	46	0	-3.307336	0.138916	0.456809
50	6	0	-6.629956	0.356066	-1.014082
51	1	0	-7.135216	1.318575	-0.883966
52	1	0	-7.312763	-0.325282	-1.522115
53	6	0	-6.229387	-0.249252	0.329559
54	1	0	-7.113098	-0.373768	0.959493
55	7	0	-5.248439	0.656605	1.023000
56	6	0	-5.596397	-1.648006	0.104716
57	1	0	-5.297169	0.521704	2.031004
58	1	0	-5.471383	1.632421	0.842083
59	8	0	-6.339610	-2.585628	-0.117921
60	8	0	-4.298160	-1.683091	0.124754
61	1	0	4.423906	0.651099	3.117733
62	1	0	-5.751148	0.503474	-1.648241
63	1	0	2.374160	-0.514621	-3.637134

HF=-2258.935991\ZeroPoint=0.4626361\Thermal=0.5007715

G = -13.9 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	2.156796	-0.733546	0.551333
2	7	0	0.185378	-1.369600	0.402123
3	7	0	-0.702656	-0.483552	0.700246
4	6	0	-0.206493	0.676856	1.301513
5	6	0	1.202834	0.820314	1.341843
6	6	0	1.708452	1.977456	1.933654
7	1	0	2.775520	2.163637	1.948428
8	6	0	0.847339	2.931313	2.486525
9	6	0	-0.539845	2.758582	2.444945
10	1	0	-1.197328	3.515388	2.853251
11	6	0	-1.080399	1.630909	1.844543
12	1	0	-2.151563	1.504018	1.765416
13	6	0	-0.344564	-2.569682	-0.076788
14	6	0	0.486703	-3.659303	-0.370884
15	6	0	-0.106139	-4.851637	-0.771956
16	1	0	0.518982	-5.705913	-1.001088
17	6	0	-1.493406	-4.948133	-0.880082
18	1	0	-1.946369	-5.885303	-1.185451
19	6	0	-2.314130	-3.845146	-0.603334
20	1	0	-3.388560	-3.956964	-0.708648
21	6	0	-1.757386	-2.640443	-0.197790
22	6	0	6.414362	-0.607559	0.032956
23	1	0	6.740337	0.435195	0.016211
24	1	0	7.016249	-1.187263	-0.667182
25	6	0	4.947653	-0.720093	-0.356944
26	1	0	4.793218	-0.255230	-1.335873
27	7	0	4.063935	0.044087	0.581172
28	1	0	4.066417	1.039010	0.296595
29	6	0	4.457079	-2.181315	-0.498395
30	8	0	5.219016	-3.044832	-0.891409
31	8	0	3.194322	-2.365141	-0.222331
32	1	0	1.263267	3.824223	2.940544
33	1	0	4.430626	-0.017364	1.529522
34	1	0	1.564711	-3.559562	-0.299372
35	1	0	0.904081	1.620575	-0.892004
36	6	0	0.778286	4.750930	-2.146951
37	1	0	0.312501	5.679964	-1.819043
38	1	0	0.361200	4.485263	-3.123264
39	6	0	0.495769	3.662897	-1.114904
40	1	0	0.946577	3.935972	-0.159262
41	7	0	1.166214	2.386266	-1.517568
42	1	0	2.247265	2.513288	-1.406417
43	6	0	-0.999735	3.477959	-0.852150
44	8	0	-1.655986	4.352381	-0.350264
45	8	0	-1.436151	2.273071	-1.218226
46	1	0	0.921605	2.114202	-2.468725
47	17	0	3.993619	2.849722	-0.879110
48	46	0	-2.607701	-0.876786	0.053467
49	6	0	-6.028169	-0.435694	1.083362
50	1	0	-6.593720	-1.370077	1.154601
51	1	0	-6.698577	0.388096	1.331132
52	6	0	-5.474794	-0.232385	-0.326307
53	1	0	-6.292737	-0.218028	-1.049558
54	7	0	-4.522713	-1.343162	-0.667523
55	6	0	-4.744151	1.128683	-0.414231
56	1	0	-4.447463	-1.446494	-1.677575
57	1	0	-4.865224	-2.230550	-0.306241
58	8	0	-5.366731	2.124739	-0.714017
59	8	0	-3.471121	1.081559	-0.105808
60	1	0	-2.343912	2.061669	-0.844258
61	1	0	-5.218962	-0.458207	1.818008
62	1	0	6.583440	-1.022035	1.032380
63	1	0	1.855037	4.902930	-2.242510

HF=-2258.9860376\ZeroPoint=0.4643378\Thermal=0.5023368

G = 14.8 kcal mol^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	2.174986	0.529143	-0.485259
2	7	0	0.203581	1.203236	-0.266185
3	7	0	-0.713487	0.372870	-0.620687
4	6	0	-0.265182	-0.817249	-1.208212
5	6	0	1.047187	-1.258239	-0.891657
6	6	0	1.531422	-2.418865	-1.510350
7	1	0	2.500691	-2.801700	-1.208114
8	6	0	0.726826	-3.113528	-2.410969
9	6	0	-0.573312	-2.679614	-2.677062
10	1	0	-1.206824	-3.252492	-3.343020
11	6	0	-1.087197	-1.533400	-2.073666

12	1	0	-2.103679	-1.213994	-2.255529
13	6	0	-0.282293	2.388902	0.282884
14	6	0	0.592300	3.426311	0.642824
15	6	0	0.050443	4.597925	1.153916
16	1	0	0.706352	5.413876	1.430879
17	6	0	-1.332037	4.724731	1.304951
18	1	0	-1.746259	5.645642	1.701349
19	6	0	-2.195316	3.680118	0.948196
20	1	0	-3.263061	3.818857	1.083779
21	6	0	-1.692918	2.495931	0.424856
22	6	0	6.439271	0.563531	-0.559230
23	1	0	6.804301	-0.441383	-0.337580
24	1	0	7.098828	1.299885	-0.098068
25	6	0	5.028731	0.748610	-0.018765
26	1	0	5.016710	0.535034	1.055443
27	7	0	4.064394	-0.212209	-0.624391
28	1	0	4.106536	-1.140272	-0.111254
29	6	0	4.498205	2.183371	-0.176963
30	8	0	5.217672	3.152022	-0.075840
31	8	0	3.195653	2.274646	-0.383686
32	1	0	1.093781	-4.024630	-2.867790
33	1	0	4.289846	-0.369575	-1.605607
34	1	0	1.660235	3.313912	0.500029
35	1	0	1.299674	-1.177135	0.271159
36	6	0	0.382968	-3.847786	3.129672
37	1	0	0.003243	-4.861214	2.980034
38	1	0	-0.306343	-3.309721	3.787013
39	6	0	0.531767	-3.121043	1.783173
40	1	0	1.236756	-3.675037	1.161561
41	7	0	1.068897	-1.757926	1.903414
42	1	0	2.049645	-1.811960	2.184707
43	6	0	-0.798775	-3.133226	1.038618
44	8	0	-1.136807	-4.016213	0.289396
45	8	0	-1.565191	-2.063926	1.326061
46	1	0	0.530402	-1.193911	2.553980
47	17	0	4.016425	-2.714617	1.039519
48	46	0	-2.619883	0.812956	-0.039841
49	6	0	-5.987370	0.799167	-1.333075
50	1	0	-6.519390	1.750515	-1.232835
51	1	0	-6.667034	0.072731	-1.779596
52	6	0	-5.518706	0.280635	0.025288
53	1	0	-6.375329	0.154553	0.690753
54	7	0	-4.549951	1.255243	0.637703
55	6	0	-4.844308	-1.104739	-0.145836
56	1	0	-4.538178	1.150189	1.650448
57	1	0	-4.835064	2.212485	0.443901
58	8	0	-5.541860	-2.095906	-0.187905
59	8	0	-3.543067	-1.073028	-0.277701
60	1	0	-2.371803	-2.058405	0.758293
61	1	0	-5.138501	0.941467	-2.007564
62	1	0	6.465648	0.726262	-1.641467
63	1	0	1.359372	-3.910538	3.614723

HF=-2258.9388037\ZeroPoint=0.4612798\Thermal=0.4987619

G = 14.1 kcal mol^{-1}

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	46	0	2.193000	0.507239	-0.489993
2	7	0	0.223221	1.186604	-0.254506
3	7	0	-0.699009	0.363387	-0.609223
4	6	0	-0.260779	-0.829839	-1.200353
5	6	0	1.037057	-1.300696	-0.872978
6	6	0	1.514652	-2.460206	-1.494793
7	1	0	2.472209	-2.859801	-1.177777
8	6	0	0.713360	-3.128742	-2.417889
9	6	0	-0.574672	-2.669089	-2.697545
10	1	0	-1.207317	-3.222185	-3.380893
11	6	0	-1.079321	-1.521623	-2.087989
12	1	0	-2.086964	-1.182491	-2.282498
13	6	0	-0.253256	2.371014	0.304955
14	6	0	0.629293	3.399337	0.671578
15	6	0	0.097318	4.568729	1.197475
16	1	0	0.759394	5.377694	1.480139
17	6	0	-1.283758	4.702101	1.356201
18	1	0	-1.690489	5.620947	1.764952
19	6	0	-2.154960	3.667038	0.991474
20	1	0	-3.221144	3.811077	1.133535
21	6	0	-1.662548	2.485197	0.453164
22	6	0	6.454695	0.532312	-0.587144
23	1	0	6.818673	-0.470684	-0.355437
24	1	0	7.117301	1.272272	-0.136122
25	6	0	5.046431	0.726096	-0.043997
26	1	0	5.037055	0.525766	1.032857
27	7	0	4.077449	-0.238324	-0.634606
28	1	0	4.107456	-1.160510	-0.104759
29	6	0	4.517488	2.158699	-0.218856
30	8	0	5.234954	3.129768	-0.136150
31	8	0	3.212350	2.248859	-0.420183
32	1	0	1.071499	-4.040498	-2.880150
33	1	0	4.298555	-0.410669	-1.614310
34	1	0	1.695542	3.282479	0.522050
35	1	0	1.325415	-1.171021	0.244595
36	6	0	0.265138	-3.838337	3.188706
37	1	0	-0.100828	-4.853191	3.014614
38	1	0	-0.454831	-3.311204	3.821771
39	6	0	0.466841	-3.094797	1.857501
40	1	0	1.198262	-3.639720	1.258694
41	7	0	0.986931	-1.728899	2.006748
42	1	0	1.957989	-1.776403	2.314187
43	6	0	-0.832428	-3.110706	1.060127
44	8	0	-1.128864	-3.980289	0.277361
45	8	0	-1.628496	-2.060206	1.339423
46	1	0	0.430443	-1.184437	2.658362
47	17	0	3.958965	-2.701192	1.063960
48	46	0	-2.605034	0.817925	-0.037251
49	6	0	-5.958130	0.892735	-1.369513
50	1	0	-6.478291	1.848361	-1.249616
51	1	0	-6.642371	0.187864	-1.842766
52	6	0	-5.512117	0.331460	-0.020580
53	1	0	-6.377855	0.201337	0.632238
54	7	0	-4.535581	1.274644	0.627712
55	6	0	-4.857100	-1.059392	-0.220961
56	1	0	-4.536973	1.142944	1.637439

57	1	0	-4.803654	2.240916	0.455791	62	1	0	6.477942	0.682921	-1.671147
58	8	0	-5.570743	-2.036354	-0.306691	63	1	0	1.220136	-3.899324	3.715107
59	8	0	-3.553453	-1.046848	-0.326448						
60	1	0	-2.412498	-2.060043	0.742729						
61	1	0	-5.099791	1.041259	-2.030573						

HF=-2258.9388497\ZeroPoint=0.4618464\Thermal=0.5002