

Electronic Supplementary Information for:

“Mapping the Potential Energy Surfaces for Ring-closing Metathesis Reactions of Prototypical Dienes by Electronic Structure Calculations”

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The coordinates of the structures A, B, BC, C, CD and D (Table 1 and Scheme 1, with BC and CD being transition structures linking B and C, and C and D, respectively) that lead to the cycloalkenes (Z-cyclopentene to Z-cyclodecene). Each set of structures is designated by the number of carbons in the product alkene (i.e. five, six, seven, eight, nine and ten) and the point on the potential energy surface (i.e. A, B, BC, C, CD and D). The free energy (which includes solvation, rotational, translational and vibrational effects) is also given. The units used are Ångstroms, for coordinates, and unless otherwise stated, Hartrees for the free energies.

Molecule	Electronic Energy (B2)	Solvation Energy (B2)	Entropic Energy^a
A for 5 membered ring	-2175.63850	-0.01834	-0.10900
A for 6 membered ring	-2214.95585	-0.01866	-0.11234
A for 7 membered ring	-2254.27328	-0.01898	-0.11540
A for 8 membered ring	-2293.59063	-0.01897	-0.11852
A for 9 membered ring	-2332.90788	-0.01921	-0.12258
A for 10 membered ring	-2372.22526	-0.01930	-0.12559
B for 5 membered ring	-2175.66211	-0.01876	-0.10351
B for 6 membered ring	-2214.97224	-0.019006	-0.10617
B for 7 membered ring	-2254.29288	-0.01884	-0.10837
B for 8 membered ring	2293.60804	-0.01928	-0.10901
B for 9 membered ring	-2332.91868	-0.01891	-0.11426
B for 10 membered ring	-2372.24342	-0.01896	-0.11482
BC for 5 membered ring	-2175.65850	-0.01964	-0.10014
BC for 6 membered ring	-2214.97038	-0.01883	-0.10366
BC for 7 membered ring	-2254.28595	-0.01920	-0.10548
BC for 8 membered ring	-2293.60122	-0.01922	-0.10731
BC for 9 membered ring	-2332.91253	-0.01914	-0.10973
BC for 10 membered ring	-2372.23271	-0.01977	-0.11146
C for 5 membered ring	-2175.66386	-0.01915	-0.10074
C for 6 membered ring	-2214.98055	-0.01923	-0.10529
C for 7 membered ring	-2254.29842	-0.01979	-0.10536
C for 8 membered ring	-2293.61178	-0.01914	-0.10707
C for 9 membered ring	-2332.92259	-0.01938	-0.11184
C for 10 membered ring	-2372.24093	-0.01995	-0.11179
CD for 5 membered ring	-2175.64005	-0.01887	-0.10041
CD for 6 membered ring	-2214.96359	-0.01855	-0.10289
CD for 7 membered ring	-2254.27947	-0.01932	-0.10698
CD for 8 membered ring	-2293.59484	-0.01964	-0.10922
CD for 9 membered ring	-2332.90596	-0.01965	-0.11037
CD for 10 membered ring	-2372.22862	-0.01997	-0.11225
D for 5 membered ring	-2175.64562	-0.01853	-0.10606
D for 6 membered ring	-2214.96996	-0.01840	-0.10581
D for 7 membered ring	-2254.28279	-0.01862	-0.10823
D for 8 membered ring	-2293.59895	-0.01909	-0.11136
D for 9 membered ring	-2332.91133	-0.01905	-0.11377
D for 10 membered ring	-2372.23617	-0.01926	-0.11490

Z-Cyclopentene formation

Five A Free Energy = -2175.155185

1	44	0	-0.508283	-0.337861	-0.934876
2	17	0	0.137242	-0.561593	-3.160840
3	17	0	-0.997090	-1.378879	1.103750
4	6	0	-3.260865	-0.035170	-1.337601
5	1	0	-3.700474	0.276651	-2.297403
6	6	0	-5.562271	-0.467498	-0.334774
7	1	0	-6.048709	-0.179464	-1.274949
8	6	0	-4.230060	0.266034	-0.188921
9	1	0	-4.405176	1.348569	-0.137078
10	1	0	-3.751311	-0.013282	0.758067
11	1	0	-3.104024	-1.121749	-1.411229
12	6	0	0.869997	0.854128	-0.312187
13	7	0	0.896582	2.204164	-0.147484
14	7	0	2.101778	0.383970	0.038241
15	6	0	2.154058	2.672578	0.444231
16	1	0	2.534404	3.542409	-0.099355
17	1	0	1.991345	2.979166	1.486152
18	6	0	3.056086	1.450603	0.331327
19	1	0	3.787083	1.542583	-0.483270
20	1	0	3.607299	1.235008	1.251928
21	6	0	2.515943	-0.973926	-0.130870
22	6	0	3.232976	-3.647777	-0.473086
23	6	0	2.432469	-1.849457	0.963409
24	6	0	3.041431	-1.389002	-1.366133
25	6	0	3.376357	-2.732659	-1.514495
26	6	0	2.782449	-3.182619	0.760310
27	1	0	3.761967	-3.071501	-2.473284
28	1	0	2.698914	-3.876708	1.593560
29	6	0	-0.235847	3.069433	-0.176047
30	6	0	-2.484842	4.709334	-0.280347
31	6	0	-0.494087	3.791991	-1.344641
32	6	0	-1.077971	3.137519	0.941577
33	6	0	-2.195265	3.965642	0.865129
34	6	0	-1.624470	4.609586	-1.372697
35	1	0	-2.868034	4.017303	1.718494
36	1	0	-1.846518	5.169278	-2.278395
37	6	0	0.371941	3.608596	-2.551690
38	1	0	1.426463	3.806999	-2.336424
39	1	0	0.065033	4.269504	-3.363734
40	1	0	0.318384	2.575448	-2.914780
41	6	0	-0.840251	2.274049	2.140209
42	1	0	-1.000649	1.216811	1.896768
43	1	0	-1.516696	2.537408	2.954978
44	1	0	0.183603	2.353320	2.518530
45	6	0	3.319059	-0.421156	-2.475792
46	1	0	4.361324	-0.081957	-2.427789
47	1	0	2.673327	0.457342	-2.443440
48	1	0	3.172819	-0.888442	-3.450477
49	6	0	2.045727	-1.377771	2.331434
50	1	0	1.483981	-0.444120	2.307668
51	1	0	2.942895	-1.220248	2.942753
52	1	0	1.427618	-2.117587	2.842861
53	6	0	-3.692155	5.595668	-0.325924
54	1	0	-3.919629	5.916735	-1.344003

55	1	0	-3.543815	6.497888	0.276607
56	1	0	-4.575560	5.091327	0.074932
57	6	0	3.545350	-5.098080	-0.678312
58	1	0	2.665180	-5.638872	-1.042060
59	1	0	3.855795	-5.580531	0.251061
60	1	0	4.335886	-5.241453	-1.418125
61	6	0	-1.976788	0.691421	-1.124494
62	1	0	-2.043501	1.783282	-1.097600
63	6	0	-6.481752	-0.213319	0.812189
64	1	0	-6.108459	-0.514500	1.792171
65	6	0	-7.679200	0.356423	0.724400
66	1	0	-8.087720	0.673453	-0.231989
67	1	0	-8.301358	0.522947	1.597083
68	1	0	-5.357795	-1.544817	-0.409451

Five B Free Energy = -2175.173473

1	44	0	-0.408964	-0.741531	0.206990
2	17	0	-0.627399	-1.180287	-2.177652
3	17	0	-0.132200	-0.674073	2.612525
4	6	0	-3.125543	0.252607	-0.535740
5	1	0	-3.668682	1.202650	-0.448819
6	6	0	-3.346511	-2.251860	-0.195688
7	1	0	-4.069315	-3.037986	0.065839
8	1	0	-3.031379	-2.440121	-1.227817
9	6	0	-4.043640	-0.900867	-0.085362
10	1	0	-4.951875	-0.891507	-0.696016
11	1	0	-4.363247	-0.733477	0.951572
12	1	0	-2.851146	0.096852	-1.583587
13	6	0	0.951564	0.714575	0.030324
14	7	0	0.872074	2.056086	-0.081398
15	7	0	2.262698	0.377804	0.078577
16	6	0	2.194065	2.696024	-0.000637
17	1	0	2.300098	3.457389	-0.777964
18	1	0	2.316262	3.187871	0.972299
19	6	0	3.146282	1.517026	-0.173822
20	1	0	3.562717	1.461409	-1.188888
21	1	0	3.979587	1.528998	0.534470
22	6	0	2.667476	-0.993659	0.003129
23	6	0	3.243646	-3.719360	-0.130648
24	6	0	2.999286	-1.678679	1.183148
25	6	0	2.721793	-1.621918	-1.254714
26	6	0	2.993876	-2.986705	-1.291008
27	6	0	3.268722	-3.044409	1.087499
28	1	0	3.011808	-3.488849	-2.255684
29	1	0	3.506628	-3.593046	1.996107
30	6	0	-0.329188	2.824515	-0.131897
31	6	0	-2.673738	4.326593	-0.259300
32	6	0	-0.935065	3.037082	-1.378712
33	6	0	-0.860993	3.355914	1.049998
34	6	0	-2.034670	4.103565	0.959309
35	6	0	-2.106450	3.789950	-1.415299
36	1	0	-2.465665	4.512799	1.870265
37	1	0	-2.589893	3.958445	-2.375200
38	6	0	-0.354431	2.445209	-2.622961
39	1	0	0.711002	2.676992	-2.725467
40	1	0	-0.866736	2.818884	-3.511251
41	1	0	-0.438585	1.351487	-2.617871

42	6	0	-0.219236	3.079769	2.373340
43	1	0	-0.040608	2.007185	2.516589
44	1	0	-0.848794	3.428280	3.193630
45	1	0	0.748141	3.584344	2.472062
46	6	0	2.582789	-0.848814	-2.529661
47	1	0	3.563861	-0.474442	-2.848682
48	1	0	1.906198	0.001170	-2.436305
49	1	0	2.192145	-1.478185	-3.329707
50	6	0	3.143819	-0.974292	2.495715
51	1	0	2.607581	-0.026366	2.517418
52	1	0	4.204457	-0.780358	2.697810
53	1	0	2.758427	-1.581625	3.316324
54	6	0	-3.956911	5.097300	-0.327287
55	1	0	-4.816037	4.424434	-0.425549
56	1	0	-3.981155	5.765945	-1.191298
57	1	0	-4.116994	5.697419	0.570432
58	6	0	3.469931	-5.198582	-0.194384
59	1	0	2.516775	-5.738156	-0.213822
60	1	0	4.027167	-5.560791	0.671944
61	1	0	4.015332	-5.486795	-1.095992
62	6	0	-0.986396	-2.970382	0.388626
63	1	0	-0.269449	-3.229540	1.165560
64	1	0	-0.827023	-3.372267	-0.608430
65	6	0	-2.180326	-2.396249	0.724465
66	1	0	-2.344370	-2.135051	1.770888
67	6	0	-1.913021	0.295528	0.323504
68	1	0	-1.993979	0.942194	1.213862

Five BC Free Energy= -2175.168000

1	44	0	-0.134174	0.783508	0.412360
2	17	0	0.444707	0.160456	2.684896
3	17	0	-0.924615	1.501762	-1.774245
4	6	0	-1.186899	2.430460	1.220498
5	1	0	-1.925446	2.755873	0.489422
6	1	0	-1.549863	2.107640	2.193462
7	6	0	1.534679	1.599735	0.329453
8	1	0	2.187602	1.437458	1.202348
9	6	0	0.120483	2.978162	1.138616
10	1	0	0.687556	2.969132	2.071590
11	6	0	2.116568	2.459481	-0.743618
12	1	0	1.610205	2.307138	-1.699035
13	1	0	3.179511	2.216807	-0.859533
14	6	0	0.474517	4.048170	0.141102
15	1	0	-0.187362	3.961431	-0.726624
16	1	0	0.284907	5.024702	0.602576
17	6	0	1.928229	3.912527	-0.283274
18	1	0	2.199114	4.617789	-1.074338
19	1	0	2.586607	4.117546	0.570641
20	6	0	-0.169226	-1.176239	-0.145435
21	7	0	-1.313964	-1.843083	-0.386501
22	7	0	0.856674	-2.042522	-0.253831
23	6	0	-1.092899	-3.289200	-0.500047
24	1	0	-1.379927	-3.784172	0.438199
25	1	0	-1.691586	-3.717166	-1.307142
26	6	0	0.405139	-3.350635	-0.755906
27	1	0	0.904711	-4.164302	-0.226017
28	1	0	0.643042	-3.442634	-1.824633

29	6	0	2.240545	-1.693404	-0.190686
30	6	0	4.933642	-0.998703	-0.032087
31	6	0	2.827880	-1.008908	-1.261884
32	6	0	2.973241	-2.068202	0.943688
33	6	0	4.316391	-1.706822	1.000207
34	6	0	4.176469	-0.666690	-1.153371
35	1	0	4.894734	-1.981337	1.879398
36	1	0	4.646919	-0.130659	-1.975042
37	6	0	-2.606073	-1.236102	-0.304712
38	6	0	-5.056163	0.088984	-0.230572
39	6	0	-3.165879	-0.920454	0.938561
40	6	0	-3.270875	-0.957068	-1.512010
41	6	0	-4.491128	-0.301306	-1.449189
42	6	0	-4.387586	-0.236119	0.942183
43	1	0	-5.004105	-0.058426	-2.376964
44	1	0	-4.829839	0.031522	1.899780
45	6	0	-2.556126	-1.344158	2.240644
46	1	0	-3.233861	-2.028081	2.762667
47	1	0	-2.380173	-0.494259	2.904975
48	1	0	-1.591961	-1.838791	2.124274
49	6	0	-2.650674	-1.321688	-2.823641
50	1	0	-3.261818	-0.969625	-3.656027
51	1	0	-2.533675	-2.405443	-2.936071
52	1	0	-1.659760	-0.866579	-2.917390
53	6	0	2.321572	-2.819914	2.060890
54	1	0	1.962047	-3.802091	1.734411
55	1	0	1.462202	-2.264355	2.448092
56	1	0	3.019761	-2.983563	2.883059
57	6	0	2.037385	-0.654687	-2.483697
58	1	0	1.209771	0.029811	-2.263522
59	1	0	1.588192	-1.541271	-2.944782
60	1	0	2.672301	-0.180606	-3.234702
61	6	0	-6.350600	0.842238	-0.203378
62	1	0	-6.729925	0.958951	0.813328
63	1	0	-7.120884	0.339508	-0.795047
64	1	0	-6.231903	1.843663	-0.628984
65	6	0	6.376174	-0.606181	0.071113
66	1	0	6.526763	0.152760	0.845535
67	1	0	6.751722	-0.196372	-0.868167
68	1	0	7.006086	-1.458183	0.341341

Five C Free Energy = -2175.171237

1	44	0	-0.057572	0.782994	0.141920
2	17	0	-0.886641	0.494102	2.400702
3	17	0	0.613455	1.141175	-2.166701
4	6	0	-1.141214	2.438952	0.087749
5	1	0	-1.361913	2.782863	-0.924787
6	1	0	-1.973980	2.464203	0.789550
7	6	0	1.379806	1.828665	0.909777
8	1	0	1.471694	1.655268	1.987216
9	6	0	0.193557	2.948979	0.636143
10	1	0	-0.000460	3.280261	1.661283
11	6	0	2.628367	2.336824	0.220679
12	1	0	2.745084	1.876269	-0.763435
13	1	0	3.514435	2.093000	0.813987
14	6	0	0.915953	3.960704	-0.253627
15	1	0	0.744320	3.690316	-1.299464

16	1	0	0.509660	4.963837	-0.095964
17	6	0	2.397472	3.844863	0.081482
18	1	0	3.042591	4.305668	-0.671517
19	1	0	2.607203	4.342845	1.036627
20	6	0	-0.277674	-1.190186	-0.272772
21	7	0	-1.438226	-1.831011	-0.462122
22	7	0	0.738686	-2.051839	-0.419098
23	6	0	-1.240969	-3.248576	-0.800534
24	1	0	-1.799568	-3.882793	-0.106181
25	1	0	-1.613838	-3.448801	-1.811365
26	6	0	0.275632	-3.421539	-0.678272
27	1	0	0.565893	-4.081793	0.147426
28	1	0	0.734465	-3.808967	-1.592860
29	6	0	2.116318	-1.672650	-0.343347
30	6	0	4.752008	-0.789828	-0.185001
31	6	0	2.836695	-1.473571	-1.528467
32	6	0	2.698721	-1.496568	0.920580
33	6	0	4.016300	-1.047071	0.971235
34	6	0	4.152530	-1.027340	-1.420081
35	1	0	4.479721	-0.896317	1.943855
36	1	0	4.718066	-0.843622	-2.330868
37	6	0	-2.721425	-1.242305	-0.223253
38	6	0	-5.159344	-0.004105	0.298660
39	6	0	-3.339327	-1.454220	1.018444
40	6	0	-3.311632	-0.461308	-1.224326
41	6	0	-4.530411	0.153328	-0.933517
42	6	0	-4.554894	-0.821616	1.254385
43	1	0	-5.000216	0.769022	-1.697246
44	1	0	-5.033309	-0.954465	2.222028
45	6	0	-2.719918	-2.331735	2.061846
46	1	0	-3.065125	-2.051002	3.057897
47	1	0	-1.630377	-2.252224	2.065808
48	1	0	-2.988386	-3.384492	1.907958
49	6	0	-2.667676	-0.284093	-2.564105
50	1	0	-3.385171	0.104707	-3.288758
51	1	0	-2.271170	-1.226218	-2.954255
52	1	0	-1.818170	0.406736	-2.530185
53	6	0	1.935171	-1.784186	2.175640
54	1	0	1.448562	-2.764160	2.135817
55	1	0	1.140858	-1.051459	2.357742
56	1	0	2.598448	-1.777368	3.042171
57	6	0	2.233103	-1.742618	-2.871677
58	1	0	1.155667	-1.568365	-2.876368
59	1	0	2.419589	-2.777472	-3.184913
60	1	0	2.667309	-1.090069	-3.630595
61	6	0	-6.452631	0.688740	0.601854
62	1	0	-7.209070	-0.012475	0.965449
63	1	0	-6.857201	1.193242	-0.277452
64	1	0	-6.321660	1.442854	1.384219
65	6	0	6.141209	-0.236842	-0.099919
66	1	0	6.657548	-0.572838	0.802120
67	1	0	6.121418	0.858660	-0.068499
68	1	0	6.745455	-0.519889	-0.964261

Five CD Free Energy = -2175.149707

1	44	0	0.148615	0.711667	0.255523
2	17	0	-0.449634	0.290168	2.573759

3	17	0	0.731699	1.153416	-2.065504
4	6	0	-1.247738	1.887007	0.145282
5	1	0	-1.399093	2.498713	-0.754714
6	1	0	-1.987145	1.990610	0.950598
7	6	0	1.659144	2.091891	0.987264
8	1	0	1.994687	1.458359	1.808977
9	6	0	0.506551	2.893014	1.143923
10	1	0	-0.073124	2.853518	2.060503
11	6	0	2.641409	2.758600	0.056351
12	1	0	3.073348	2.074296	-0.679199
13	1	0	3.473055	3.139567	0.667312
14	6	0	0.666724	4.164962	0.347466
15	1	0	-0.236327	4.500437	-0.167748
16	1	0	0.907306	4.948942	1.079558
17	6	0	1.847741	3.900858	-0.594355
18	1	0	1.479138	3.571781	-1.566112
19	1	0	2.454725	4.795100	-0.754125
20	6	0	-0.321122	-1.184994	-0.277898
21	7	0	-1.501117	-1.816088	-0.386354
22	7	0	0.663970	-2.058945	-0.563463
23	6	0	-1.333960	-3.180356	-0.915756
24	1	0	-1.963066	-3.886982	-0.369456
25	1	0	-1.632240	-3.208811	-1.971858
26	6	0	0.159447	-3.425307	-0.727155
27	1	0	0.377213	-4.017905	0.172156
28	1	0	0.628415	-3.917408	-1.582817
29	6	0	2.037779	-1.690949	-0.408789
30	6	0	4.638124	-0.722144	-0.128038
31	6	0	2.797197	-1.427742	-1.561771
32	6	0	2.581403	-1.562615	0.879251
33	6	0	3.879219	-1.053121	0.988827
34	6	0	4.088933	-0.942912	-1.393554
35	1	0	4.307370	-0.930625	1.981480
36	1	0	4.678085	-0.709562	-2.277430
37	6	0	-2.785376	-1.208821	-0.219312
38	6	0	-5.272413	-0.012261	0.147964
39	6	0	-3.472490	-1.427604	0.981641
40	6	0	-3.324354	-0.436751	-1.255380
41	6	0	-4.569452	0.156596	-1.042707
42	6	0	-4.713313	-0.816082	1.141885
43	1	0	-5.002418	0.761033	-1.836851
44	1	0	-5.255465	-0.969285	2.072345
45	6	0	-2.881438	-2.275502	2.063001
46	1	0	-3.579900	-2.393374	2.893041
47	1	0	-1.965943	-1.817985	2.451703
48	1	0	-2.621417	-3.277186	1.704083
49	6	0	-2.590533	-0.247738	-2.545339
50	1	0	-3.222677	0.247522	-3.284505
51	1	0	-2.265852	-1.201936	-2.973510
52	1	0	-1.682400	0.352344	-2.420032
53	6	0	1.875329	-2.049334	2.108808
54	1	0	2.291310	-3.018563	2.408853
55	1	0	0.800367	-2.166031	1.975261
56	1	0	2.009447	-1.363395	2.947496
57	6	0	2.249788	-1.681166	-2.930757
58	1	0	1.171206	-1.524296	-2.970719
59	1	0	2.460577	-2.710523	-3.246896
60	1	0	2.706034	-1.013743	-3.663013

61	6	0	-6.594322	0.659902	0.363860
62	1	0	-6.488518	1.539799	1.007222
63	1	0	-7.310130	-0.004723	0.854212
64	1	0	-7.034716	0.996931	-0.576568
65	6	0	6.005684	-0.128352	0.016978
66	1	0	6.420933	-0.306705	1.010685
67	1	0	5.979182	0.956405	-0.134564
68	1	0	6.702929	-0.532690	-0.720754

Five D Free Energy = -2175.160640

1	6	0	0.251339	-1.161104	-0.004634
2	7	0	-0.834482	-1.971868	0.014380
3	7	0	1.346804	-1.922396	0.204760
4	6	0	-0.503529	-3.332828	0.437224
5	1	0	-0.792728	-3.488704	1.485840
6	1	0	-1.027024	-4.073119	-0.173286
7	6	0	1.007616	-3.353931	0.244397
8	1	0	1.540598	-3.854092	1.056553
9	1	0	1.301264	-3.835584	-0.698029
10	6	0	2.700794	-1.495976	0.057973
11	6	0	5.356179	-0.700740	-0.216157
12	6	0	3.236835	-1.348769	-1.228917
13	6	0	3.463746	-1.267671	1.211586
14	6	0	4.788100	-0.869209	1.047412
15	6	0	4.567087	-0.945331	-1.338397
16	1	0	5.390378	-0.676759	1.932423
17	1	0	4.994745	-0.816425	-2.329932
18	6	0	-2.156663	-1.435563	-0.098451
19	6	0	-4.634850	-0.201662	-0.424863
20	6	0	-2.811789	-0.918588	1.029999
21	6	0	-2.759570	-1.436006	-1.369676
22	6	0	-3.989016	-0.803300	-1.508659
23	6	0	-4.048292	-0.296399	0.832590
24	1	0	-4.451951	-0.769959	-2.492087
25	1	0	-4.560288	0.129162	1.693354
26	6	0	-2.270691	-1.087413	2.415693
27	1	0	-2.782062	-1.918522	2.915928
28	1	0	-2.431855	-0.191843	3.019684
29	1	0	-1.198401	-1.280529	2.431381
30	6	0	-2.096903	-2.110896	-2.527922
31	1	0	-1.101447	-1.699184	-2.708236
32	1	0	-2.679982	-1.979652	-3.440578
33	1	0	-1.990072	-3.186994	-2.350614
34	6	0	2.853583	-1.408100	2.569498
35	1	0	2.421292	-2.402409	2.723265
36	1	0	2.040646	-0.686045	2.706564
37	1	0	3.595808	-1.243757	3.352148
38	6	0	2.393888	-1.576063	-2.443353
39	1	0	1.587391	-0.836269	-2.516372
40	1	0	1.912757	-2.559922	-2.432086
41	1	0	2.991481	-1.510285	-3.353847
42	6	0	-5.917409	0.546343	-0.619924
43	1	0	-5.721443	1.568775	-0.962837
44	1	0	-6.489175	0.621585	0.307286
45	1	0	-6.551282	0.076179	-1.375336
46	6	0	6.790771	-0.292915	-0.359676
47	1	0	7.078736	0.441226	0.396592

48	1	0	6.992150	0.136439	-1.342994
49	1	0	7.459402	-1.152078	-0.238532
50	44	0	-0.059774	0.775872	-0.163136
51	17	0	0.190013	1.111150	2.218188
52	17	0	-0.393176	0.824515	-2.557925
53	6	0	1.672287	1.249598	-0.361379
54	1	0	2.128540	1.350602	-1.357559
55	1	0	2.314213	1.497384	0.496861
56	6	0	-0.757378	3.301382	-0.384839
57	1	0	-0.234315	3.325779	-1.335667
58	6	0	-1.861158	2.553379	-0.150393
59	1	0	-2.338289	1.925154	-0.902384
60	6	0	-0.425061	4.184152	0.779027
61	1	0	-0.345605	5.227684	0.452230
62	6	0	-2.470545	2.850913	1.186089
63	1	0	-3.513914	3.166740	1.054604
64	6	0	-1.576917	3.957221	1.783245
65	1	0	-2.146985	4.878215	1.932175
66	1	0	-1.187984	3.655545	2.756296
67	1	0	0.548258	3.920967	1.207985
68	1	0	-2.500170	1.960292	1.822463

Z-Cyclohexene formation

Six A Free Energy = -2214.446270

1	44	0	1.447375	1.978688	-0.238018
2	17	0	0.932421	0.574984	1.560570
3	17	0	2.261567	2.204467	-2.409467
4	6	0	-1.260388	2.094739	-0.854193
5	1	0	-1.657438	2.549660	-1.774717
6	1	0	-0.955410	1.073249	-1.130093
7	6	0	-4.638496	1.127001	0.860150
8	1	0	-4.196192	0.740105	1.789181
9	1	0	-4.994354	2.139244	1.089171
10	6	0	-2.352213	2.028559	0.219296
11	1	0	-1.915557	1.620387	1.139756
12	1	0	-2.677927	3.049641	0.461166
13	6	0	-3.545887	1.188335	-0.205562
14	1	0	-3.969815	1.583789	-1.137887
15	1	0	-3.207864	0.170218	-0.439989
16	6	0	2.666503	3.143804	0.691082
17	7	0	2.570179	4.451845	1.047500
18	7	0	3.892341	2.705488	1.102608
19	6	0	3.725614	4.907335	1.827155
20	1	0	4.078211	5.876196	1.461562
21	1	0	3.446564	5.033265	2.881888
22	6	0	4.731687	3.783112	1.622677
23	1	0	5.508449	4.046249	0.892229
24	1	0	5.229979	3.475391	2.546871
25	6	0	4.435975	1.430587	0.750680
26	6	0	5.403116	-1.084992	0.034524
27	6	0	4.361829	0.380999	1.679306
28	6	0	5.073772	1.270849	-0.491229
29	6	0	5.529945	-0.000258	-0.831428
30	6	0	4.840577	-0.868199	1.290596
31	1	0	6.002333	-0.142917	-1.800567
32	1	0	4.765897	-1.696462	1.991413
33	6	0	1.384615	5.241069	1.019028
34	6	0	-0.935852	6.778698	0.933062
35	6	0	1.178554	6.097085	-0.067948
36	6	0	0.449327	5.114812	2.053509
37	6	0	-0.702044	5.898188	1.989606
38	6	0	0.011220	6.858747	-0.088933
39	1	0	-1.444051	5.805132	2.779604
40	1	0	-0.169353	7.520344	-0.933280
41	6	0	2.148663	6.113182	-1.207631
42	1	0	3.171876	6.314798	-0.875153
43	1	0	1.879516	6.868650	-1.947355
44	1	0	2.172397	5.137912	-1.708726
45	6	0	0.633458	4.099005	3.137529
46	1	0	0.561556	3.080731	2.735589
47	1	0	-0.126081	4.208310	3.913127
48	1	0	1.613739	4.170982	3.618585
49	6	0	5.347560	2.430421	-1.400007
50	1	0	6.349153	2.832771	-1.203184
51	1	0	4.626492	3.240992	-1.286288
52	1	0	5.318403	2.124349	-2.446453
53	6	0	3.844556	0.588283	3.069619
54	1	0	3.164975	1.437833	3.137322

55	1	0	4.678154	0.760162	3.761764
56	1	0	3.303677	-0.291477	3.422374
57	6	0	-2.167621	7.631308	0.902437
58	1	0	-2.494371	7.832654	-0.120148
59	1	0	-1.985733	8.602140	1.376006
60	1	0	-2.996357	7.164415	1.438682
61	6	0	5.851343	-2.452721	-0.379611
62	1	0	5.064569	-2.967215	-0.941299
63	1	0	6.091411	-3.077880	0.482804
64	1	0	6.729962	-2.412431	-1.027418
65	6	0	-7.048832	0.676633	0.336864
66	1	0	-7.844692	0.005914	0.031880
67	1	0	-7.332057	1.705991	0.542292
68	6	0	-5.790590	0.266967	0.459666
69	1	0	-5.550124	-0.774156	0.238777
70	6	0	-0.099001	2.894920	-0.370013
71	1	0	-0.295997	3.943212	-0.126119

Six B Free Energy = -2214.456777

1	44	0	-0.238614	-0.791504	-0.114933
2	17	0	0.054953	-1.451097	2.203568
3	17	0	-0.508643	-0.472410	-2.509704
4	6	0	-3.079571	0.252244	-0.459654
5	1	0	-3.357011	1.292785	-0.236058
6	1	0	-2.932478	0.172501	-1.539589
7	6	0	-2.945786	-2.607167	-1.193269
8	1	0	-3.146842	-3.605700	-1.604397
9	1	0	-2.555294	-2.028677	-2.039533
10	6	0	-4.193876	-0.687802	0.042457
11	1	0	-4.043654	-0.857178	1.116791
12	1	0	-5.161774	-0.183890	-0.037665
13	6	0	-4.269319	-2.026650	-0.696760
14	1	0	-4.773757	-2.756539	-0.052272
15	1	0	-4.915892	-1.913023	-1.573929
16	6	0	0.940549	0.815623	-0.039360
17	7	0	0.686770	2.143036	-0.061018
18	7	0	2.280486	0.649957	-0.119017
19	6	0	1.923763	2.936121	0.000742
20	1	0	1.880454	3.775638	-0.697730
21	1	0	2.058413	3.345769	1.011480
22	6	0	2.990441	1.908523	-0.354499
23	1	0	3.305140	1.975968	-1.404894
24	1	0	3.883991	1.977367	0.271330
25	6	0	2.899136	-0.639949	-0.111972
26	6	0	3.983242	-3.205477	0.001542
27	6	0	3.346986	-1.141388	1.124398
28	6	0	3.062843	-1.359859	-1.303288
29	6	0	3.591282	-2.652073	-1.211705
30	6	0	3.875658	-2.424069	1.156345
31	1	0	3.709671	-3.231130	-2.125191
32	1	0	4.205369	-2.831257	2.109231
33	6	0	-0.580385	2.752360	0.182905
34	6	0	-3.035311	3.985008	0.659238
35	6	0	-1.283401	3.305124	-0.894458
36	6	0	-1.069010	2.812741	1.496840
37	6	0	-2.304327	3.422123	1.706780
38	6	0	-2.507124	3.919869	-0.629409

39	1	0	-2.701007	3.465688	2.718846
40	1	0	-3.067448	4.348796	-1.457246
41	6	0	-0.754420	3.197588	-2.288780
42	1	0	0.255470	3.611257	-2.377890
43	1	0	-1.394865	3.729921	-2.994077
44	1	0	-0.690617	2.148471	-2.599218
45	6	0	-0.297094	2.214521	2.630676
46	1	0	-0.208660	1.125298	2.535360
47	1	0	-0.776433	2.428000	3.587453
48	1	0	0.725079	2.605100	2.677195
49	6	0	2.785738	-0.765880	-2.649774
50	1	0	3.732179	-0.542177	-3.156021
51	1	0	2.196263	0.148409	-2.599177
52	1	0	2.229617	-1.457257	-3.286120
53	6	0	3.264731	-0.302897	2.360635
54	1	0	2.231765	-0.018272	2.574064
55	1	0	3.852829	0.616745	2.260524
56	1	0	3.643905	-0.847186	3.226862
57	6	0	-4.344080	4.665487	0.922811
58	1	0	-4.932217	4.779677	0.010149
59	1	0	-4.191218	5.667571	1.337438
60	1	0	-4.947155	4.113675	1.648276
61	6	0	4.511978	-4.604699	0.079583
62	1	0	3.787890	-5.272024	0.558329
63	1	0	5.427360	-4.656844	0.675136
64	1	0	4.728303	-5.011600	-0.909880
65	6	0	-0.556385	-3.030571	-0.542353
66	1	0	0.152865	-3.377491	0.205426
67	1	0	-0.292463	-3.137889	-1.592430
68	6	0	-1.847717	-2.756561	-0.186233
69	1	0	-2.106052	-2.797794	0.872720
70	6	0	-1.841620	-0.026188	0.316721
71	1	0	-1.983144	0.174962	1.396508

Six BC Free Energy = -2214.452847

1	44	0	0.280895	0.753633	-0.167607
2	17	0	0.731713	0.585086	-2.551172
3	17	0	0.059209	1.103075	2.227699
4	6	0	-2.584719	1.712649	0.258880
5	1	0	-3.321570	0.903496	0.147157
6	1	0	-2.319882	1.756613	1.317707
7	6	0	-0.831531	3.907662	0.380166
8	1	0	-0.276468	4.849449	0.475470
9	1	0	-0.779937	3.441896	1.370546
10	6	0	-3.183736	3.025430	-0.251574
11	1	0	-3.383278	2.914043	-1.324406
12	1	0	-4.159788	3.185752	0.216131
13	6	0	-2.272391	4.239927	-0.004866
14	1	0	-2.267788	4.882628	-0.892679
15	1	0	-2.688826	4.856634	0.798028
16	6	0	0.386178	-1.258392	0.103283
17	7	0	-0.585506	-2.171608	0.283212
18	7	0	1.575788	-1.887187	0.143156
19	6	0	-0.046304	-3.540879	0.319056
20	1	0	-0.495911	-4.110699	1.136380
21	1	0	-0.279063	-4.060727	-0.619557
22	6	0	1.451103	-3.304779	0.496543

23	1	0	1.784311	-3.467753	1.530345
24	1	0	2.066947	-3.925123	-0.160286
25	6	0	2.801705	-1.148340	0.123759
26	6	0	5.067836	0.470978	0.027389
27	6	0	3.485754	-1.005047	-1.095236
28	6	0	3.276007	-0.569141	1.311935
29	6	0	4.403480	0.249408	1.230779
30	6	0	4.608463	-0.182828	-1.116636
31	1	0	4.771781	0.720368	2.139487
32	1	0	5.134084	-0.042488	-2.058624
33	6	0	-1.989861	-1.919476	0.198406
34	6	0	-4.733065	-1.451194	0.050182
35	6	0	-2.719940	-1.780153	1.385491
36	6	0	-2.599812	-1.849562	-1.061768
37	6	0	-3.971877	-1.607612	-1.108603
38	6	0	-4.091976	-1.549551	1.284496
39	1	0	-4.458370	-1.546532	-2.079731
40	1	0	-4.672271	-1.436694	2.197629
41	6	0	-2.038615	-1.843219	2.715335
42	1	0	-1.416065	-2.738320	2.815797
43	1	0	-2.765044	-1.847428	3.529708
44	1	0	-1.374999	-0.980927	2.849534
45	6	0	-1.802663	-2.014378	-2.316489
46	1	0	-1.077238	-1.203216	-2.449161
47	1	0	-2.452478	-2.029472	-3.192911
48	1	0	-1.228595	-2.946871	-2.315007
49	6	0	2.672097	-0.879201	2.647225
50	1	0	3.251759	-1.668969	3.140871
51	1	0	1.634165	-1.206536	2.581353
52	1	0	2.682673	-0.005270	3.299923
53	6	0	3.068422	-1.746539	-2.326738
54	1	0	2.015762	-2.027736	-2.302171
55	1	0	3.666453	-2.659688	-2.437654
56	1	0	3.220490	-1.139748	-3.220403
57	6	0	-6.197939	-1.147492	-0.032440
58	1	0	-6.660938	-1.617679	-0.902948
59	1	0	-6.369945	-0.068938	-0.124575
60	1	0	-6.732402	-1.481257	0.859378
61	6	0	6.245933	1.393635	-0.044997
62	1	0	5.965610	2.353437	-0.491769
63	1	0	7.045288	0.979793	-0.665077
64	1	0	6.657398	1.603506	0.944054
65	6	0	1.258152	2.634239	-0.287097
66	1	0	1.967958	2.528986	-1.103534
67	1	0	1.652584	2.870130	0.700452
68	6	0	-0.061977	3.047206	-0.588642
69	1	0	-0.286207	3.154887	-1.651335
70	6	0	-1.430286	1.318823	-0.592714
71	1	0	-1.668515	1.317953	-1.672437

Six C Free Energy = -2214.462541

1	44	0	0.045934	0.672910	-0.092661
2	17	0	0.810124	0.446981	-2.388788
3	17	0	-0.612906	0.997309	2.210462
4	6	0	1.104751	2.316188	-0.028251
5	1	0	1.929370	2.372360	-0.738749
6	1	0	1.321651	2.679006	0.979204

7	6	0	-1.420502	1.743474	-0.820207
8	1	0	-1.532570	1.574831	-1.897809
9	6	0	-0.250427	2.839794	-0.591279
10	1	0	-0.019589	3.135520	-1.620169
11	6	0	-2.719449	2.079573	-0.140028
12	1	0	-3.462666	1.324775	-0.415890
13	1	0	-2.619805	2.047650	0.946592
14	6	0	-0.818823	3.968250	0.268652
15	1	0	-0.979590	3.579841	1.280150
16	1	0	-0.064605	4.756219	0.357838
17	6	0	-3.171274	3.467374	-0.608093
18	1	0	-3.376752	3.427771	-1.684176
19	6	0	-2.108089	4.543170	-0.313112
20	1	0	-1.868494	5.093619	-1.230183
21	6	0	0.403582	-1.300527	0.152384
22	7	0	1.611404	-1.885456	0.150018
23	7	0	-0.545384	-2.249004	0.202240
24	6	0	1.506611	-3.340696	0.337740
25	1	0	2.175414	-3.866346	-0.347397
26	1	0	1.791817	-3.605564	1.365041
27	6	0	0.030908	-3.593787	0.053570
28	1	0	-0.140734	-3.962448	-0.966154
29	1	0	-0.434198	-4.293492	0.751674
30	6	0	-1.949651	-1.980630	0.277712
31	6	0	-4.660277	-1.384087	0.492212
32	6	0	-2.546808	-1.975955	1.545734
33	6	0	-2.683672	-1.740564	-0.892012
34	6	0	-4.038745	-1.440815	-0.754203
35	6	0	-3.902273	-1.669158	1.626880
36	1	0	-4.621408	-1.239068	-1.650657
37	1	0	-4.374685	-1.641162	2.605997
38	6	0	2.849108	-1.170016	0.128916
39	6	0	5.195392	0.332056	0.027184
40	6	0	3.606456	-1.166188	-1.054361
41	6	0	3.272333	-0.491466	1.279457
42	6	0	4.445542	0.261162	1.196410
43	6	0	4.767460	-0.402209	-1.080840
44	1	0	4.782122	0.799915	2.079487
45	1	0	5.350472	-0.370751	-1.998569
46	6	0	3.199223	-1.970699	-2.249530
47	1	0	2.114638	-2.058678	-2.331637
48	1	0	3.626705	-2.980469	-2.206883
49	1	0	3.557532	-1.507210	-3.169994
50	6	0	2.521468	-0.557494	2.573066
51	1	0	1.907095	-1.457150	2.654592
52	1	0	1.835482	0.287147	2.693452
53	1	0	3.215069	-0.541513	3.417000
54	6	0	-2.049044	-1.821930	-2.245924
55	1	0	-2.701123	-1.389627	-3.007194
56	1	0	-1.865991	-2.863644	-2.534131
57	1	0	-1.090045	-1.297106	-2.295971
58	6	0	-1.744148	-2.274088	2.772160
59	1	0	-2.374648	-2.271087	3.662341
60	1	0	-0.963685	-1.520477	2.912277
61	1	0	-1.255475	-3.252851	2.713179
62	6	0	6.434656	1.170428	-0.048910
63	1	0	6.293596	2.023036	-0.720884
64	1	0	7.282912	0.600923	-0.439141

65	1	0	6.715784	1.565408	0.929011
66	6	0	-6.099003	-0.985029	0.610284
67	1	0	-6.557528	-1.381099	1.518702
68	1	0	-6.687016	-1.324856	-0.245303
69	1	0	-6.196519	0.105871	0.651935
70	1	0	-4.123340	3.717568	-0.130188
71	1	0	-2.500424	5.289903	0.383716

Six CD Free Energy = -2214.445284

1	6	0	0.414892	-1.328147	0.340542
2	7	0	-0.564124	-2.204849	0.644999
3	7	0	1.599251	-1.950156	0.469200
4	6	0	-0.047550	-3.563553	0.836529
5	1	0	-0.520098	-4.047541	1.694666
6	1	0	-0.249237	-4.172974	-0.055430
7	6	0	1.439983	-3.299083	1.036349
8	1	0	1.724477	-3.294154	2.096803
9	1	0	2.082936	-4.014852	0.518602
10	6	0	2.880628	-1.340654	0.293946
11	6	0	5.363797	-0.142525	-0.089745
12	6	0	3.572921	-1.582821	-0.899305
13	6	0	3.410896	-0.541831	1.313893
14	6	0	4.654178	0.052127	1.093364
15	6	0	4.812663	-0.971191	-1.067575
16	1	0	5.080648	0.677510	1.874703
17	1	0	5.359955	-1.143353	-1.991719
18	6	0	-1.942542	-1.865543	0.471410
19	6	0	-4.582415	-1.022546	0.158841
20	6	0	-2.709241	-1.579396	1.614741
21	6	0	-2.490910	-1.810064	-0.819663
22	6	0	-3.811263	-1.365988	-0.945586
23	6	0	-4.021028	-1.158239	1.431392
24	1	0	-4.244544	-1.298758	-1.941343
25	1	0	-4.616704	-0.908018	2.306089
26	6	0	-2.135774	-1.738973	2.987316
27	1	0	-2.163641	-2.789028	3.303043
28	1	0	-2.705091	-1.162652	3.717898
29	1	0	-1.099550	-1.397688	3.029814
30	6	0	-1.760238	-2.299694	-2.033054
31	1	0	-1.905438	-1.631764	-2.884383
32	1	0	-2.145187	-3.285467	-2.320097
33	1	0	-0.683614	-2.381596	-1.888229
34	6	0	2.667606	-0.325634	2.594366
35	1	0	2.349391	-1.271375	3.045587
36	1	0	1.755414	0.263624	2.447662
37	1	0	3.290306	0.195036	3.324029
38	6	0	2.983324	-2.448398	-1.967303
39	1	0	2.101388	-1.966907	-2.403556
40	1	0	2.663659	-3.421151	-1.578988
41	1	0	3.703172	-2.629380	-2.767129
42	6	0	-5.968596	-0.480982	-0.006575
43	1	0	-5.969799	0.611061	0.086906
44	1	0	-6.648888	-0.864331	0.757718
45	1	0	-6.384893	-0.723111	-0.986312
46	6	0	6.684130	0.529649	-0.315031
47	1	0	7.123997	0.880448	0.620581
48	1	0	6.576101	1.400684	-0.970029

49	1	0	7.401205	-0.139887	-0.796637
50	44	0	-0.048694	0.554483	-0.227559
51	17	0	-0.627310	1.162470	2.050202
52	17	0	0.521874	0.091115	-2.545673
53	6	0	1.377869	1.702221	-0.191082
54	1	0	2.081369	1.781406	-1.030131
55	1	0	1.593674	2.313365	0.695433
56	6	0	-1.533464	1.923001	-1.042112
57	1	0	-1.663012	1.416781	-1.999125
58	6	0	-0.414155	2.783989	-0.966918
59	1	0	0.175624	2.861621	-1.878186
60	6	0	-0.449275	3.969389	-0.028251
61	1	0	0.243774	4.736808	-0.385081
62	1	0	-0.116025	3.675818	0.973277
63	6	0	-2.799280	2.167434	-0.256061
64	1	0	-3.062025	1.281386	0.334042
65	1	0	-3.596749	2.258256	-1.008616
66	6	0	-2.781994	3.409010	0.638756
67	1	0	-3.805716	3.778545	0.759895
68	1	0	-2.425088	3.129874	1.634298
69	6	0	-1.877845	4.500313	0.087074
70	1	0	-2.232378	4.836302	-0.897337
71	1	0	-1.895445	5.378040	0.740372

Six D Free Energy = -2214.453816

1	6	0	-2.077736	4.598386	0.077216
2	6	0	-0.679543	4.131234	-0.322089
3	6	0	-0.758844	2.904971	-1.180482
4	6	0	-1.804512	2.044272	-1.090962
5	6	0	-2.964864	2.238578	-0.165343
6	6	0	-2.848349	3.465320	0.740067
7	44	0	0.044071	0.573501	-0.253442
8	6	0	1.690169	1.308185	-0.144164
9	6	0	0.529639	-1.253906	0.305006
10	7	0	-0.470120	-2.118108	0.610348
11	6	0	0.017097	-3.486504	0.787478
12	6	0	1.505567	-3.254931	1.005895
13	7	0	1.700783	-1.910375	0.445212
14	6	0	-1.848634	-1.775696	0.450365
15	6	0	-2.598049	-1.472486	1.602530
16	6	0	-3.925392	-1.095806	1.437760
17	6	0	-4.520225	-1.018619	0.174883
18	6	0	-3.764086	-1.373055	-0.936147
19	6	0	-2.429934	-1.781215	-0.827148
20	6	0	3.002450	-1.341871	0.317968
21	6	0	3.703869	-1.548865	-0.877119
22	6	0	4.973403	-0.988922	-0.991126
23	6	0	5.544611	-0.242031	0.040717
24	6	0	4.821589	-0.073243	1.219580
25	6	0	3.548166	-0.618712	1.387178
26	6	0	6.899405	0.375988	-0.127383
27	6	0	3.084313	-2.314566	-2.002453
28	6	0	2.778943	-0.429365	2.657154
29	6	0	-5.931698	-0.540318	0.030042
30	6	0	-1.993777	-1.585741	2.966533
31	6	0	-1.718599	-2.303881	-2.037648
32	17	0	-0.468007	1.296021	1.988483

33	17	0	0.448571	0.129291	-2.604746
34	1	0	-0.474251	-3.972073	1.634172
35	1	0	-0.186035	-4.081688	-0.114374
36	1	0	1.776432	-3.260933	2.070152
37	1	0	2.138572	-3.983368	0.493150
38	1	0	5.258414	0.496928	2.036404
39	1	0	5.529622	-1.135302	-1.914423
40	1	0	-4.222783	-1.353727	-1.922723
41	1	0	-4.509767	-0.839710	2.318473
42	1	0	-1.992016	-2.628864	3.305741
43	1	0	-2.562009	-1.006106	3.695423
44	1	0	-0.965027	-1.221675	2.981199
45	1	0	-1.877054	-1.660152	-2.905029
46	1	0	-2.108423	-3.297283	-2.289795
47	1	0	-0.639869	-2.381315	-1.905651
48	1	0	2.569560	-1.385887	3.148981
49	1	0	1.810830	0.053382	2.481122
50	1	0	3.336496	0.185774	3.365288
51	1	0	2.239674	-1.757803	-2.423977
52	1	0	2.694031	-3.283558	-1.674268
53	1	0	3.806714	-2.496059	-2.799806
54	1	0	-5.994508	0.542310	0.186493
55	1	0	-6.592889	-1.002907	0.767380
56	1	0	-6.331337	-0.750549	-0.963655
57	1	0	7.320507	0.693879	0.828221
58	1	0	6.851722	1.259252	-0.772749
59	1	0	7.603718	-0.317321	-0.594150
60	1	0	2.416307	1.241907	-0.966836
61	1	0	1.995185	1.899612	0.733245
62	1	0	-1.890431	1.260697	-1.846802
63	1	0	-0.032438	2.756364	-1.975857
64	1	0	-0.134060	4.916045	-0.855723
65	1	0	-0.096460	3.911088	0.582101
66	1	0	-3.107821	1.334522	0.440537
67	1	0	-3.862135	2.301427	-0.800142
68	1	0	-3.848033	3.800538	1.034999
69	1	0	-2.327936	3.175707	1.657104
70	1	0	-2.609310	4.944615	-0.819526
71	1	0	-2.010693	5.458467	0.750229

Z-Cycloheptene formation

Seven A Free Energy = -2253.737044

1	6	0	0.427999	-1.440609	2.282565
2	1	0	-0.162367	-1.602206	3.197509
3	6	0	4.705866	-3.041263	4.529961
4	1	0	4.722323	-3.943163	3.906254
5	1	0	4.108146	-3.295515	5.417484
6	6	0	1.882278	-1.114862	2.645209
7	1	0	1.901784	-0.189903	3.238244
8	1	0	2.434030	-0.896635	1.721823
9	6	0	4.006108	-1.907105	3.783192
10	1	0	4.579330	-1.660123	2.880467
11	1	0	4.022704	-0.999111	4.401776
12	6	0	2.571150	-2.237730	3.404127
13	1	0	1.997939	-2.478195	4.310656
14	1	0	2.554911	-3.149935	2.792724
15	6	0	-0.950522	1.015954	-1.019023
16	7	0	-1.248896	1.106712	-2.349306
17	7	0	-0.859835	2.287244	-0.546202
18	6	0	-1.541603	2.476952	-2.765752
19	1	0	-1.064206	2.702004	-3.723882
20	1	0	-2.625061	2.614554	-2.886306
21	6	0	-0.983026	3.290297	-1.608356
22	1	0	-0.000310	3.723984	-1.837833
23	1	0	-1.640252	4.105612	-1.292393
24	6	0	-0.439010	2.674637	0.757567
25	6	0	0.350041	3.389485	3.331419
26	6	0	-1.418151	2.883715	1.733902
27	6	0	0.928316	2.796108	1.038050
28	6	0	1.296953	3.156598	2.332101
29	6	0	-0.999957	3.244465	3.014731
30	1	0	2.355249	3.240709	2.570505
31	1	0	-1.748668	3.400621	3.787748
32	6	0	-1.624254	-0.013490	-3.155514
33	6	0	-2.331478	-2.243293	-4.673755
34	6	0	-0.665434	-0.597433	-3.997823
35	6	0	-2.953827	-0.467204	-3.127491
36	6	0	-3.276588	-1.590649	-3.883534
37	6	0	-1.042306	-1.719095	-4.734769
38	1	0	-4.296706	-1.966431	-3.850817
39	1	0	-0.303647	-2.194892	-5.375975
40	6	0	0.701659	-0.010299	-4.170946
41	1	0	1.461135	-0.790979	-4.240881
42	1	0	0.981018	0.641194	-3.342929
43	1	0	0.745421	0.573644	-5.098358
44	6	0	-4.025188	0.261534	-2.374553
45	1	0	-3.642342	0.795967	-1.503813
46	1	0	-4.788897	-0.428880	-2.014439
47	1	0	-4.521394	0.988425	-3.029784
48	6	0	1.955099	2.465785	0.000320
49	1	0	1.884247	3.120018	-0.874890
50	1	0	1.834326	1.438505	-0.362831
51	1	0	2.964894	2.563629	0.401950
52	6	0	-2.861329	2.634371	1.424133
53	1	0	-3.033985	1.572658	1.210274
54	1	0	-3.195948	3.187040	0.540683

55	1	0	-3.500942	2.917460	2.261406
56	6	0	-2.691973	-3.485059	-5.429831
57	1	0	-2.557436	-4.374228	-4.804659
58	1	0	-2.064922	-3.616747	-6.314164
59	1	0	-3.736328	-3.475837	-5.749542
60	6	0	0.780627	3.793876	4.708224
61	1	0	1.656669	3.229738	5.038048
62	1	0	-0.014352	3.643876	5.440914
63	1	0	1.057068	4.852960	4.740158
64	44	0	-0.696307	-0.696427	-0.178991
65	6	0	6.094747	-2.693409	4.950701
66	1	0	6.188673	-1.822441	5.601836
67	6	0	7.195058	-3.340307	4.581078
68	1	0	7.149014	-4.209262	3.929690
69	1	0	8.181039	-3.034032	4.913207
70	1	0	0.391538	-2.386757	1.722585
71	6	0	-0.166414	-0.317589	1.503310
72	1	0	-0.228061	0.644765	2.020724
73	17	0	1.372366	-1.167488	-1.162300
74	17	0	-2.891113	-1.370512	0.208495

Seven B Free Energy = -2253.749257

1	6	0	-0.588456	-1.571158	2.422340
2	1	0	-0.956806	-0.770499	3.085097
3	6	0	-0.439025	-3.975617	0.292310
4	1	0	-1.345842	-3.411421	0.537308
5	1	0	-0.804546	-4.817487	-0.311225
6	6	0	0.190724	-2.594790	3.256063
7	1	0	-0.510157	-3.138348	3.902208
8	1	0	0.869704	-2.053967	3.928307
9	6	0	0.250463	-4.547433	1.534111
10	1	0	0.957706	-5.317072	1.200094
11	1	0	-0.498484	-5.081119	2.132781
12	6	0	1.018753	-3.579173	2.432328
13	1	0	1.745662	-3.013955	1.831981
14	1	0	1.624095	-4.176175	3.123688
15	6	0	0.083635	1.398720	-0.280549
16	7	0	0.193836	2.059806	-1.460966
17	7	0	0.025487	2.318028	0.704364
18	6	0	0.020265	3.504627	-1.306416
19	1	0	0.744417	4.053871	-1.914066
20	1	0	-0.989362	3.807324	-1.618798
21	6	0	0.238358	3.679720	0.193230
22	1	0	1.257755	4.014453	0.426710
23	1	0	-0.461409	4.380086	0.656209
24	6	0	-0.085108	2.037308	2.098019
25	6	0	-0.338837	1.454223	4.811061
26	6	0	-1.364766	1.990691	2.666413
27	6	0	1.072883	1.827482	2.859053
28	6	0	0.918622	1.526839	4.211544
29	6	0	-1.465319	1.705292	4.027111
30	1	0	1.807154	1.340393	4.810833
31	1	0	-2.452723	1.659312	4.481274
32	6	0	0.054356	1.338310	-2.691023
33	6	0	-0.199752	-0.317919	-4.921028
34	6	0	1.202304	1.008938	-3.430143
35	6	0	-1.231073	0.949927	-3.114004

36	6	0	-1.327349	0.108829	-4.220847
37	6	0	1.047444	0.167340	-4.530729
38	1	0	-2.313187	-0.222497	-4.539156
39	1	0	1.932082	-0.121274	-5.093736
40	6	0	2.544813	1.580526	-3.100843
41	1	0	3.336697	0.846760	-3.257201
42	1	0	2.607130	1.911090	-2.064953
43	1	0	2.753328	2.438363	-3.752261
44	6	0	-2.472229	1.489422	-2.471777
45	1	0	-2.338180	1.715015	-1.413489
46	1	0	-3.293169	0.775213	-2.538688
47	1	0	-2.782489	2.409517	-2.983052
48	6	0	2.427044	1.891735	2.225409
49	1	0	2.687723	2.916614	1.938915
50	1	0	2.483489	1.280950	1.316691
51	1	0	3.199209	1.543057	2.913247
52	6	0	-2.584446	2.184569	1.823219
53	1	0	-2.727455	1.328300	1.152189
54	1	0	-2.511341	3.074893	1.190301
55	1	0	-3.478788	2.281986	2.440892
56	6	0	-0.325686	-1.291671	-6.051745
57	1	0	-0.340300	-2.321213	-5.676484
58	1	0	0.511687	-1.216131	-6.748446
59	1	0	-1.251703	-1.145489	-6.612495
60	6	0	-0.478823	1.072313	6.252714
61	1	0	-0.563047	-0.015093	6.361345
62	1	0	-1.374003	1.507144	6.702616
63	1	0	0.385684	1.385405	6.841829
64	44	0	0.091771	-0.585662	-0.357332
65	6	0	0.429577	-3.129931	-0.587714
66	1	0	1.500493	-3.109299	-0.386354
67	6	0	-0.012982	-2.490050	-1.704759
68	1	0	-1.051041	-2.560588	-2.019693
69	1	0	0.702869	-2.062984	-2.407682
70	1	0	-1.479987	-1.993179	1.957431
71	6	0	0.294830	-0.906038	1.431178
72	1	0	1.278123	-0.627283	1.853967
73	17	0	2.507526	-0.577175	-0.623556
74	17	0	-2.325637	-0.874489	-0.277383

Seven BC Free Energy = -2253.740504

1	44	0	0.394029	-0.625379	-0.109796
2	17	0	0.353520	-0.599615	-2.537687
3	17	0	0.496663	-0.913409	2.305827
4	6	0	1.401794	-2.469107	-0.277086
5	1	0	0.985598	-2.913327	-1.178794
6	1	0	1.298245	-3.028733	0.652071
7	6	0	1.862116	0.511138	-0.163813
8	1	0	2.182315	0.821018	-1.174917
9	6	0	2.511022	-1.595897	-0.403979
10	1	0	2.793781	-1.358006	-1.429896
11	6	0	2.542530	1.234693	0.944070
12	1	0	1.928671	2.138030	1.064896
13	1	0	2.439983	0.705691	1.895441
14	6	0	3.624565	-1.604416	0.615160
15	1	0	3.222670	-1.363435	1.607108
16	1	0	3.940731	-2.651813	0.692856

17	6	0	3.986335	1.647690	0.668337
18	1	0	4.212776	2.548776	1.250084
19	1	0	4.089675	1.937901	-0.387138
20	6	0	4.851173	-0.748394	0.262722
21	1	0	4.859604	-0.554559	-0.819051
22	1	0	5.750623	-1.342798	0.452740
23	6	0	5.003916	0.570423	1.015409
24	1	0	6.011321	0.962664	0.833305
25	1	0	4.952906	0.368899	2.094176
26	6	0	-1.409457	0.289297	0.133307
27	7	0	-2.548149	-0.407429	-0.035083
28	7	0	-1.724232	1.519232	0.580915
29	6	0	-3.726295	0.322019	0.444587
30	1	0	-4.553945	0.241883	-0.264499
31	1	0	-4.060794	-0.093348	1.404744
32	6	0	-3.181288	1.739083	0.578466
33	1	0	-3.460714	2.379236	-0.269552
34	1	0	-3.499733	2.239549	1.495863
35	6	0	-0.801409	2.595672	0.753832
36	6	0	0.988166	4.704262	1.113783
37	6	0	-0.473262	2.994292	2.055332
38	6	0	-0.275208	3.241984	-0.375142
39	6	0	0.624564	4.285876	-0.167153
40	6	0	0.422271	4.053588	2.208779
41	1	0	1.044694	4.793076	-1.033282
42	1	0	0.691743	4.368452	3.214317
43	6	0	-2.555432	-1.734028	-0.572454
44	6	0	-2.385988	-4.266336	-1.722850
45	6	0	-2.755307	-1.872228	-1.958194
46	6	0	-2.342056	-2.841067	0.258282
47	6	0	-2.245483	-4.097481	-0.350788
48	6	0	-2.663387	-3.143025	-2.507732
49	1	0	-2.061970	-4.966596	0.277504
50	1	0	-2.788980	-3.259505	-3.581554
51	6	0	-3.048062	-0.677701	-2.810078
52	1	0	-4.013825	-0.226129	-2.554115
53	1	0	-3.080439	-0.951111	-3.865452
54	1	0	-2.276273	0.086870	-2.692159
55	6	0	-2.282486	-2.731965	1.750640
56	1	0	-2.188501	-1.703766	2.098033
57	1	0	-1.425860	-3.274112	2.158016
58	1	0	-3.185161	-3.168142	2.193489
59	6	0	-0.652725	2.819075	-1.759831
60	1	0	-1.735787	2.704597	-1.870853
61	1	0	-0.212071	1.851319	-2.027592
62	1	0	-0.318454	3.552262	-2.495794
63	6	0	-1.043527	2.281872	3.240114
64	1	0	-0.830192	1.209127	3.185166
65	1	0	-2.131554	2.395577	3.299933
66	1	0	-0.623883	2.668743	4.169941
67	6	0	-2.235785	-5.615655	-2.356064
68	1	0	-1.297650	-5.682896	-2.916678
69	1	0	-3.041069	-5.819911	-3.066748
70	1	0	-2.230849	-6.413958	-1.611580
71	6	0	1.978827	5.812915	1.300200
72	1	0	2.994319	5.480742	1.058747
73	1	0	1.990340	6.175680	2.329530
74	1	0	1.762614	6.661016	0.645158

Seven C Free Energy = -2253.750752

1	44	0	0.449802	-0.216842	-0.297516
2	17	0	0.521273	1.136943	-2.312315
3	17	0	0.392823	-1.689539	1.625114
4	6	0	1.328374	-1.640653	-1.285216
5	1	0	1.216530	-1.622802	-2.370566
6	1	0	1.277434	-2.629759	-0.824311
7	6	0	2.239775	0.521837	0.056133
8	1	0	2.442918	1.401838	-0.563339
9	6	0	2.563757	-0.795801	-0.785183
10	1	0	2.965618	-0.376374	-1.713608
11	6	0	2.770546	0.674983	1.458519
12	1	0	2.232993	1.524432	1.894866
13	1	0	2.529673	-0.192776	2.078310
14	6	0	3.560526	-1.721865	-0.078882
15	1	0	3.124666	-2.066609	0.866340
16	1	0	3.662999	-2.614422	-0.704112
17	6	0	4.274839	0.964014	1.499630
18	1	0	4.510199	1.483352	2.435570
19	1	0	4.538275	1.663706	0.693816
20	6	0	4.947040	-1.109171	0.131271
21	1	0	5.207175	-0.495839	-0.743371
22	1	0	5.680013	-1.923285	0.142824
23	6	0	5.129704	-0.290245	1.404579
24	1	0	6.186806	-0.015093	1.498966
25	1	0	4.907995	-0.931856	2.268260
26	6	0	-1.476474	0.344116	-0.042689
27	7	0	-2.544849	-0.445812	-0.224128
28	7	0	-1.889050	1.578421	0.284220
29	6	0	-3.806994	0.297619	-0.102616
30	1	0	-4.290824	0.376805	-1.084053
31	1	0	-4.492963	-0.225795	0.568677
32	6	0	-3.348341	1.649317	0.443059
33	1	0	-3.752581	2.497213	-0.116013
34	1	0	-3.604565	1.789245	1.500866
35	6	0	-1.006632	2.673904	0.537535
36	6	0	0.812384	4.738019	0.970472
37	6	0	-0.292207	2.706540	1.742182
38	6	0	-0.874367	3.677648	-0.432922
39	6	0	0.045063	4.694147	-0.193840
40	6	0	0.617567	3.747644	1.930260
41	1	0	0.178543	5.464914	-0.949321
42	1	0	1.185408	3.783875	2.857750
43	6	0	-2.482777	-1.843911	-0.522124
44	6	0	-2.269021	-4.566954	-1.058998
45	6	0	-2.241653	-2.256860	-1.837966
46	6	0	-2.665011	-2.759574	0.524400
47	6	0	-2.549448	-4.113406	0.230651
48	6	0	-2.130737	-3.627451	-2.076900
49	1	0	-2.662531	-4.834715	1.036730
50	1	0	-1.935981	-3.965975	-3.092181
51	6	0	-2.102680	-1.272789	-2.957275
52	1	0	-2.849683	-0.475523	-2.898579
53	1	0	-2.216072	-1.767771	-3.923490
54	1	0	-1.129572	-0.770415	-2.949934
55	6	0	-2.972532	-2.298996	1.915140

56	1	0	-2.415149	-1.395506	2.173249
57	1	0	-2.707564	-3.064807	2.645501
58	1	0	-4.041987	-2.087111	2.038443
59	6	0	-1.691793	3.661006	-1.686673
60	1	0	-2.674915	4.120769	-1.526562
61	1	0	-1.842495	2.642962	-2.053595
62	1	0	-1.197745	4.223033	-2.480417
63	6	0	-0.492668	1.662415	2.798162
64	1	0	-0.080656	0.687943	2.510204
65	1	0	-1.554109	1.494859	3.007229
66	1	0	-0.012014	1.959604	3.732311
67	6	0	-2.115850	-6.032070	-1.331950
68	1	0	-2.025727	-6.237026	-2.400189
69	1	0	-2.965912	-6.604315	-0.949629
70	1	0	-1.222335	-6.432110	-0.842052
71	6	0	1.831171	5.817798	1.172372
72	1	0	2.725011	5.631262	0.567633
73	1	0	2.150628	5.882569	2.214194
74	1	0	1.447836	6.796893	0.873745

Seven CD Free Energy = -2253.735613

1	44	0	0.573301	0.077403	-0.193590
2	17	0	0.601482	1.208941	-2.343545
3	17	0	0.668145	-1.108034	1.927516
4	6	0	0.936317	-1.512907	-1.017236
5	1	0	0.983804	-1.598589	-2.112018
6	1	0	1.091565	-2.435031	-0.441139
7	6	0	2.628728	0.848987	0.005929
8	1	0	2.525864	1.719771	-0.644695
9	6	0	2.875304	-0.364739	-0.662223
10	1	0	2.910207	-0.301098	-1.748810
11	6	0	3.147740	1.114680	1.396304
12	1	0	2.732693	2.064963	1.746243
13	1	0	2.800268	0.346913	2.094405
14	6	0	3.643215	-1.483462	-0.008296
15	1	0	3.172528	-1.751199	0.945910
16	1	0	3.599646	-2.375354	-0.640022
17	6	0	4.680882	1.171051	1.422544
18	1	0	4.995482	1.719699	2.317489
19	1	0	5.048152	1.755754	0.567710
20	6	0	5.107137	-1.086487	0.221628
21	1	0	5.500011	-0.595245	-0.679478
22	1	0	5.696190	-2.002585	0.339722
23	6	0	5.345700	-0.202266	1.442452
24	1	0	6.426336	-0.072007	1.573195
25	1	0	4.998850	-0.741869	2.334611
26	6	0	-1.421485	0.340300	0.000070
27	7	0	-2.443837	-0.531157	-0.075921
28	7	0	-1.920810	1.562375	0.271936
29	6	0	-3.743147	0.156150	0.002916
30	1	0	-4.192142	0.220756	-0.997167
31	1	0	-4.433473	-0.393563	0.646780
32	6	0	-3.358511	1.524422	0.554977
33	1	0	-3.878051	2.350422	0.063279
34	1	0	-3.532993	1.605421	1.636964
35	6	0	-1.054445	2.668107	0.536895
36	6	0	0.795479	4.717767	0.925583

37	6	0	-0.362776	2.736995	1.756227
38	6	0	-0.898543	3.647693	-0.459715
39	6	0	0.035133	4.654055	-0.244666
40	6	0	0.566296	3.769252	1.916105
41	1	0	0.188381	5.399566	-1.021180
42	1	0	1.118691	3.829862	2.851814
43	6	0	-2.338357	-1.905328	-0.456502
44	6	0	-2.097925	-4.586571	-1.173357
45	6	0	-2.181683	-2.234423	-1.808193
46	6	0	-2.416722	-2.885209	0.542581
47	6	0	-2.288829	-4.217141	0.158748
48	6	0	-2.057328	-3.584009	-2.139899
49	1	0	-2.335425	-4.987882	0.924904
50	1	0	-1.930671	-3.855324	-3.185714
51	6	0	-2.141290	-1.174170	-2.863523
52	1	0	-3.020543	-0.522604	-2.818448
53	1	0	-2.112145	-1.617015	-3.860639
54	1	0	-1.268183	-0.520147	-2.760447
55	6	0	-2.619065	-2.506198	1.975163
56	1	0	-1.803004	-1.865726	2.322997
57	1	0	-2.651795	-3.390652	2.613068
58	1	0	-3.556345	-1.958268	2.122751
59	6	0	-1.719516	3.610051	-1.709758
60	1	0	-2.723411	4.015205	-1.532358
61	1	0	-1.826386	2.590668	-2.086140
62	1	0	-1.260105	4.207528	-2.498236
63	6	0	-0.647394	1.820682	2.907549
64	1	0	0.275092	1.467569	3.373904
65	1	0	-1.207900	0.930177	2.624672
66	1	0	-1.218284	2.358325	3.673565
67	6	0	-1.936407	-6.028199	-1.548434
68	1	0	-1.993433	-6.173071	-2.628822
69	1	0	-2.702811	-6.654071	-1.083126
70	1	0	-0.968502	-6.417451	-1.216208
71	6	0	1.849940	5.767406	1.097772
72	1	0	2.794247	5.448080	0.642572
73	1	0	2.052839	5.968501	2.151679
74	1	0	1.569468	6.708105	0.618391

Seven D Free Energy = -2253.738732

1	44	0	0.503604	0.058122	-0.241542
2	17	0	0.538248	1.065225	-2.441725
3	17	0	0.748089	-0.970275	1.943569
4	6	0	0.501535	-1.607496	-0.943528
5	1	0	0.480963	-1.768636	-2.032623
6	1	0	0.575945	-2.508234	-0.316955
7	6	0	2.790379	1.020784	-0.006145
8	1	0	2.417005	1.862340	-0.594528
9	6	0	3.038154	-0.136910	-0.677347
10	1	0	2.829462	-0.151912	-1.745097
11	6	0	3.277670	1.296705	1.387762
12	1	0	2.919191	2.282113	1.699542
13	1	0	2.838669	0.574943	2.087487
14	6	0	3.742639	-1.311134	-0.065506
15	1	0	3.213095	-1.610930	0.849221
16	1	0	3.688212	-2.163131	-0.749585
17	6	0	4.806538	1.242583	1.500176

18	1	0	5.100535	1.760637	2.420081
19	1	0	5.259273	1.811480	0.676781
20	6	0	5.205538	-1.007252	0.279197
21	1	0	5.692062	-0.515241	-0.573685
22	1	0	5.731812	-1.958293	0.416616
23	6	0	5.389426	-0.167735	1.539606
24	1	0	6.460485	-0.099667	1.763255
25	1	0	4.940238	-0.706323	2.385711
26	6	0	-1.452746	0.278775	-0.037883
27	7	0	-2.496472	-0.573246	-0.095279
28	7	0	-1.931322	1.510150	0.255879
29	6	0	-3.779745	0.132833	0.032680
30	1	0	-4.263386	0.212262	-0.949996
31	1	0	-4.455872	-0.411881	0.696361
32	6	0	-3.357561	1.491436	0.581571
33	1	0	-3.878868	2.328121	0.109606
34	1	0	-3.501722	1.567366	1.668563
35	6	0	-1.041995	2.601458	0.504032
36	6	0	0.855568	4.610870	0.869736
37	6	0	-0.379761	2.695315	1.739508
38	6	0	-0.840517	3.545891	-0.517784
39	6	0	0.119809	4.531340	-0.314236
40	6	0	0.572404	3.706317	1.888791
41	1	0	0.310425	5.247879	-1.109627
42	1	0	1.104314	3.783038	2.835042
43	6	0	-2.442867	-1.941874	-0.493359
44	6	0	-2.388233	-4.621064	-1.251722
45	6	0	-2.412486	-2.260781	-1.858454
46	6	0	-2.470436	-2.929350	0.500669
47	6	0	-2.440403	-4.261651	0.095293
48	6	0	-2.381142	-3.608970	-2.211125
49	1	0	-2.457139	-5.040031	0.854846
50	1	0	-2.353420	-3.873559	-3.265714
51	6	0	-2.392611	-1.182658	-2.896163
52	1	0	-3.275125	-0.536914	-2.829966
53	1	0	-2.372301	-1.606054	-3.901704
54	1	0	-1.519399	-0.528425	-2.787529
55	6	0	-2.500417	-2.557059	1.948669
56	1	0	-1.554993	-2.087159	2.243383
57	1	0	-2.657604	-3.435026	2.577452
58	1	0	-3.294779	-1.836957	2.171121
59	6	0	-1.649202	3.508782	-1.776019
60	1	0	-2.617235	4.003381	-1.627945
61	1	0	-1.835754	2.485446	-2.106358
62	1	0	-1.135602	4.026676	-2.586788
63	6	0	-0.723787	1.824003	2.908725
64	1	0	-1.246448	0.910231	2.625840
65	1	0	-1.356353	2.381188	3.610188
66	1	0	0.172447	1.511567	3.448273
67	6	0	-2.318724	-6.061746	-1.656921
68	1	0	-2.735276	-6.222553	-2.653471
69	1	0	-2.854823	-6.705633	-0.956072
70	1	0	-1.281362	-6.412455	-1.682475
71	6	0	1.945832	5.625167	1.030012
72	1	0	2.906278	5.217517	0.693714
73	1	0	2.073245	5.922688	2.073288
74	1	0	1.756892	6.523297	0.438374

Z-Cyclooctene formation

Eight A Free Energy = -2293.027433

1	6	0	1.961359	-0.087208	4.413224
2	6	0	1.671392	-1.043052	3.435479
3	6	0	0.867686	-2.159431	3.702311
4	6	0	0.367896	-2.308389	4.993770
5	6	0	0.643859	-1.382440	6.002014
6	6	0	1.437910	-0.278794	5.691998
7	7	0	2.172548	-0.841118	2.118219
8	6	0	1.490464	-0.281849	1.084678
9	7	0	2.264690	-0.423676	-0.027783
10	6	0	3.579534	-0.992267	0.259590
11	6	0	3.414194	-1.491790	1.689900
12	6	0	1.919606	0.085340	-1.316830
13	6	0	2.293603	1.392742	-1.669969
14	6	0	1.882081	1.876355	-2.909626
15	6	0	1.147622	1.094324	-3.799485
16	6	0	0.865737	-0.224187	-3.446755
17	6	0	1.254141	-0.758223	-2.220870
18	6	0	3.176104	2.227559	-0.793147
19	6	0	1.022032	-2.209510	-1.930967
20	6	0	0.662443	1.660844	-5.098207
21	44	0	-0.217139	0.607744	1.015270
22	17	0	-1.437094	-1.063772	-0.074927
23	6	0	0.482242	-3.104065	2.607511
24	6	0	0.098579	-1.577285	7.383871
25	6	0	2.732261	1.145535	4.057320
26	17	0	0.544049	2.810353	1.044574
27	6	0	-0.912151	0.482593	2.672324
28	6	0	-2.315813	0.973182	2.777660
29	6	0	-3.259720	-0.155348	3.206936
30	6	0	-4.714640	0.284142	3.252242
31	6	0	-5.665690	-0.813399	3.702859
32	6	0	-7.120505	-0.371119	3.727666
33	6	0	-8.077801	-1.464572	4.198364
34	6	0	-9.506890	-1.035335	4.173377
35	6	0	-10.310539	-0.975378	5.229924
36	1	0	-2.663008	1.396212	1.821527
37	1	0	-2.356731	1.801552	3.501699
38	1	0	-7.947648	-2.344636	3.552047
39	1	0	-7.805833	-1.787603	5.210900
40	1	0	-3.143389	-0.995322	2.510096
41	1	0	-2.945302	-0.528417	4.191505
42	1	0	-7.230375	0.506855	4.377637
43	1	0	-5.013318	0.639711	2.256705
44	1	0	-4.816150	1.152510	3.918297
45	1	0	4.243006	-1.206956	2.344823
46	1	0	3.310275	-2.583766	1.744646
47	1	0	4.356126	-0.220449	0.172069
48	1	0	3.819848	-1.790105	-0.449818
49	1	0	2.145214	2.894839	-3.185953
50	1	0	0.325876	-0.859721	-4.145082
51	1	0	-0.268471	-3.162875	5.213994
52	1	0	1.643828	0.462432	6.460786
53	1	0	3.702976	0.909720	3.609565
54	1	0	2.910203	1.768809	4.934901

55	1	0	2.186129	1.744682	3.318806
56	1	0	-0.135709	-2.599465	1.854534
57	1	0	-0.087756	-3.948343	2.998468
58	1	0	1.351931	-3.506695	2.078542
59	1	0	4.221982	2.129256	-1.109669
60	1	0	3.110254	1.946830	0.258798
61	1	0	2.912151	3.284025	-0.859433
62	1	0	1.021857	-2.430618	-0.863570
63	1	0	1.805297	-2.815965	-2.402571
64	1	0	0.064544	-2.543271	-2.333764
65	1	0	-0.953961	-1.871544	7.362584
66	1	0	0.636583	-2.370084	7.913855
67	1	0	0.183435	-0.669242	7.983387
68	1	0	1.342845	2.420813	-5.488703
69	1	0	-0.314038	2.140510	-4.973001
70	1	0	0.543186	0.886079	-5.858411
71	1	0	-11.339899	-0.642859	5.151649
72	1	0	-9.966350	-1.262810	6.220369
73	1	0	-9.893839	-0.732236	3.198915
74	1	0	-0.457315	0.089509	3.586286
75	1	0	-7.417343	-0.033743	2.725246
76	1	0	-5.558371	-1.684459	3.041886
77	1	0	-5.372966	-1.164697	4.702376

Eight B Free Energy = -2293.035634

1	44	0	-0.122330	0.180763	-0.600977
2	17	0	-0.190722	-2.021912	-1.631608
3	17	0	-0.193294	2.494177	0.160863
4	6	0	-2.456219	0.504688	1.318630
5	1	0	-1.950685	0.547844	2.296635
6	1	0	-2.497563	1.550150	0.999376
7	6	0	-3.093398	1.473694	-2.063976
8	1	0	-2.942108	1.936745	-1.078315
9	1	0	-3.152084	2.320834	-2.757817
10	6	0	-3.855399	-0.083044	1.512232
11	1	0	-4.257848	0.284296	2.463843
12	1	0	-3.786093	-1.175226	1.617800
13	6	0	-4.388423	0.666836	-2.106897
14	1	0	-5.247289	1.347736	-2.070337
15	6	0	-4.818617	0.282514	0.389140
16	1	0	-5.838516	0.019325	0.690052
17	1	0	-4.822326	1.377116	0.291971
18	6	0	1.376414	-0.337810	0.595452
19	7	0	1.501737	-0.683163	1.893442
20	7	0	2.616757	-0.353671	0.044980
21	6	0	2.873970	-1.097382	2.219438
22	1	0	3.183143	-0.689213	3.184904
23	1	0	2.931219	-2.192553	2.279813
24	6	0	3.668900	-0.543808	1.043777
25	1	0	4.151458	0.415569	1.280058
26	1	0	4.436543	-1.231237	0.679426
27	6	0	2.826080	0.092877	-1.298280
28	6	0	2.978866	0.941048	-3.950130
29	6	0	2.940262	-0.868648	-2.317169
30	6	0	2.894592	1.470575	-1.571800
31	6	0	2.953534	1.865913	-2.909035
32	6	0	3.000970	-0.418333	-3.632525

33	1	0	2.981739	2.929139	-3.137046
34	1	0	3.058146	-1.152369	-4.432954
35	6	0	0.434198	-0.826462	2.825809
36	6	0	-1.673861	-1.059074	4.631999
37	6	0	0.167337	0.236333	3.696910
38	6	0	-0.311546	-2.012999	2.849207
39	6	0	-1.371102	-2.097435	3.751019
40	6	0	-0.886690	0.092365	4.599313
41	1	0	-1.977328	-3.000607	3.762449
42	1	0	-1.115489	0.914630	5.273677
43	6	0	0.935660	1.515779	3.597741
44	1	0	2.017925	1.351264	3.603731
45	1	0	0.692826	2.187029	4.423058
46	1	0	0.698764	2.029581	2.657149
47	6	0	0.014829	-3.142592	1.923136
48	1	0	0.081503	-2.817681	0.878841
49	1	0	-0.740310	-3.928217	1.981220
50	1	0	0.978551	-3.598182	2.177712
51	6	0	3.010642	2.490096	-0.480815
52	1	0	4.069140	2.715367	-0.300006
53	1	0	2.564844	2.160908	0.458062
54	1	0	2.515256	3.422594	-0.753676
55	6	0	3.046221	-2.329039	-2.009042
56	1	0	2.496212	-2.599748	-1.107657
57	1	0	4.097915	-2.610616	-1.871148
58	1	0	2.647419	-2.931066	-2.826595
59	6	0	-2.812248	-1.186018	5.597549
60	1	0	-3.174547	-0.209540	5.925434
61	1	0	-2.511784	-1.737143	6.495139
62	1	0	-3.652316	-1.729793	5.158237
63	6	0	2.962648	1.393126	-5.377880
64	1	0	3.400490	2.386756	-5.493449
65	1	0	1.935664	1.448921	-5.756171
66	1	0	3.504023	0.702885	-6.028656
67	6	0	-0.654002	1.146569	-2.666432
68	1	0	0.109852	0.512073	-3.120244
69	1	0	-0.446210	2.210931	-2.592053
70	6	0	-1.893421	0.647179	-2.420981
71	1	0	-2.051954	-0.415790	-2.604081
72	6	0	-1.528684	-0.295015	0.476313
73	1	0	-1.733550	-1.382514	0.515261
74	1	0	-4.450651	0.157899	-3.076776
75	6	0	-4.506305	-0.352516	-0.977216
76	1	0	-3.578959	-0.939744	-0.924809
77	1	0	-5.281581	-1.083112	-1.229184

Eight BC Free Energy = -2293.027062

1	44	0	-0.270202	-0.088564	-0.643047
2	17	0	0.015844	-2.491899	-0.923963
3	17	0	-0.646725	2.306947	-0.609465
4	6	0	-1.233357	-0.166915	-2.487913
5	1	0	-0.790380	-1.009675	-3.014005
6	1	0	-1.176635	0.807594	-2.972111
7	6	0	-1.737005	-0.469060	0.444092
8	1	0	-1.947630	-1.540655	0.598274
9	6	0	-2.349015	-0.409728	-1.627252
10	1	0	-2.601290	-1.466749	-1.530437

11	6	0	-2.441642	0.454207	1.379558
12	1	0	-1.691791	0.649068	2.158767
13	1	0	-2.594335	1.440193	0.931035
14	6	0	-3.514884	0.557913	-1.590705
15	1	0	-3.358608	1.346334	-0.848511
16	1	0	-3.546309	1.091698	-2.546165
17	6	0	-3.708648	-0.079528	2.044209
18	1	0	-3.863274	0.485811	2.971444
19	1	0	-3.544900	-1.121372	2.355763
20	6	0	-4.847152	-0.153181	-1.375452
21	1	0	-5.003170	-0.863863	-2.197297
22	1	0	-5.655115	0.583946	-1.462394
23	6	0	-4.974607	0.005281	1.198270
24	1	0	-5.826811	-0.246694	1.838216
25	1	0	-5.135786	1.050977	0.901622
26	6	0	-4.992874	-0.892392	-0.049477
27	1	0	-4.212223	-1.660434	0.035890
28	1	0	-5.932559	-1.453579	-0.081022
29	6	0	1.553157	0.077840	0.261512
30	7	0	1.893387	0.220059	1.553882
31	7	0	2.680060	0.032831	-0.472508
32	6	0	3.351415	0.132181	1.746554
33	1	0	3.697960	0.909434	2.432451
34	1	0	3.613877	-0.841873	2.179688
35	6	0	3.880787	0.296194	0.325423
36	1	0	4.251156	1.311480	0.127752
37	1	0	4.676059	-0.411494	0.076979
38	6	0	2.627742	-0.016597	-1.901385
39	6	0	2.265124	-0.183682	-4.658030
40	6	0	2.802577	-1.257185	-2.537341
41	6	0	2.362984	1.157436	-2.624217
42	6	0	2.171344	1.040668	-4.002289
43	6	0	2.606632	-1.313937	-3.913203
44	1	0	1.944276	1.937361	-4.574588
45	1	0	2.708083	-2.273134	-4.415752
46	6	0	0.978036	0.263157	2.649876
47	6	0	-0.827494	0.380710	4.769032
48	6	0	0.623031	1.513508	3.170259
49	6	0	0.468601	-0.933438	3.174159
50	6	0	-0.440770	-0.845708	4.226409
51	6	0	-0.280320	1.545887	4.233943
52	1	0	-0.857294	-1.764325	4.634191
53	1	0	-0.574860	2.510255	4.641634
54	6	0	1.151624	2.774379	2.563323
55	1	0	2.241077	2.757199	2.456483
56	1	0	0.888563	3.642785	3.169150
57	1	0	0.734166	2.918376	1.559705
58	6	0	0.874520	-2.258125	2.610741
59	1	0	0.592330	-2.360223	1.557051
60	1	0	0.410698	-3.076541	3.163597
61	1	0	1.959232	-2.402500	2.659046
62	6	0	2.368938	2.509973	-1.980098
63	1	0	3.351663	2.979255	-2.110969
64	1	0	2.145625	2.476361	-0.913313
65	1	0	1.625279	3.167515	-2.432589
66	6	0	3.220837	-2.474546	-1.773434
67	1	0	2.833163	-2.470662	-0.753758
68	1	0	4.315127	-2.540688	-1.726525

69	1	0	2.855911	-3.382835	-2.254692
70	6	0	-1.795598	0.436340	5.911242
71	1	0	-2.229901	1.431436	6.024818
72	1	0	-1.306573	0.184876	6.858482
73	1	0	-2.613030	-0.277311	5.779548
74	6	0	1.986970	-0.293821	-6.125670
75	1	0	2.079094	0.670475	-6.629310
76	1	0	0.968339	-0.655719	-6.303472
77	1	0	2.662589	-0.999878	-6.614429

Eight C Free Energy = -2293.034858

1	44	0	-0.145037	0.497910	0.023415
2	17	0	-0.705370	0.633025	2.382421
3	17	0	0.346462	0.539422	-2.342961
4	6	0	-0.943471	2.259192	-0.139453
5	1	0	-1.668080	2.539929	0.625804
6	1	0	-1.192280	2.562483	-1.158299
7	6	0	1.539687	1.390202	0.512241
8	1	0	1.727997	1.300567	1.588864
9	6	0	0.547304	2.620260	0.261215
10	1	0	0.422834	3.023901	1.271871
11	6	0	2.781654	1.153946	-0.314728
12	1	0	2.916168	0.066547	-0.347705
13	1	0	2.639358	1.441993	-1.357873
14	6	0	1.132915	3.649287	-0.715723
15	1	0	1.667276	3.142441	-1.523326
16	1	0	0.319784	4.190730	-1.206458
17	6	0	4.061129	1.766638	0.254363
18	1	0	4.913219	1.280436	-0.236251
19	1	0	4.144428	1.508714	1.320418
20	6	0	2.017190	4.666887	0.001749
21	1	0	1.379276	5.287551	0.644383
22	1	0	2.431459	5.349573	-0.751184
23	6	0	4.197073	3.276469	0.087737
24	1	0	5.202245	3.563420	0.415429
25	1	0	4.158797	3.526335	-0.981861
26	6	0	3.158642	4.112349	0.848947
27	1	0	2.752577	3.520764	1.680759
28	1	0	3.654387	4.964072	1.326579
29	6	0	-0.818834	-1.400728	-0.048090
30	7	0	-0.040533	-2.490253	0.059891
31	7	0	-2.098622	-1.776973	-0.182172
32	6	0	-0.811271	-3.732476	-0.099801
33	1	0	-0.545583	-4.217548	-1.046299
34	1	0	-0.584731	-4.430858	0.711050
35	6	0	-2.257294	-3.235817	-0.082861
36	1	0	-2.853553	-3.613592	-0.918489
37	1	0	-2.778892	-3.491171	0.847002
38	6	0	-3.196276	-0.857072	-0.127996
39	6	0	-5.237989	1.033783	-0.028388
40	6	0	-3.804153	-0.579409	1.104753
41	6	0	-3.627888	-0.261233	-1.321274
42	6	0	-4.645612	0.688598	-1.241305
43	6	0	-4.816209	0.377171	1.127211
44	1	0	-4.986461	1.166607	-2.156933
45	1	0	-5.282600	0.619412	2.079675
46	6	0	1.389188	-2.448201	-0.027109

47	6	0	4.171058	-2.347719	-0.185644
48	6	0	2.003042	-2.546016	-1.285120
49	6	0	2.134532	-2.328158	1.155830
50	6	0	3.523549	-2.271464	1.046895
51	6	0	3.394856	-2.486327	-1.335501
52	1	0	4.114450	-2.165784	1.954108
53	1	0	3.883276	-2.539498	-2.306031
54	6	0	1.211514	-2.738916	-2.541752
55	1	0	1.086444	-3.806159	-2.763405
56	1	0	1.723221	-2.288210	-3.393332
57	1	0	0.223244	-2.278313	-2.487719
58	6	0	1.464136	-2.260534	2.491276
59	1	0	0.927546	-1.315540	2.632521
60	1	0	2.193129	-2.360345	3.297170
61	1	0	0.719828	-3.054222	2.609330
62	6	0	-3.026170	-0.632135	-2.639860
63	1	0	-2.926626	-1.716817	-2.747233
64	1	0	-2.021338	-0.213081	-2.763621
65	1	0	-3.644340	-0.268237	-3.462571
66	6	0	-3.422534	-1.304227	2.358501
67	1	0	-2.380948	-1.628674	2.349878
68	1	0	-4.060893	-2.184623	2.505083
69	1	0	-3.545052	-0.661801	3.231676
70	6	0	5.666060	-2.299605	-0.271339
71	1	0	6.001441	-1.795122	-1.180556
72	1	0	6.093818	-3.307886	-0.290369
73	1	0	6.102837	-1.781510	0.585179
74	6	0	-6.297709	2.090756	0.038710
75	1	0	-5.887488	3.034306	0.413690
76	1	0	-7.108461	1.808454	0.715173
77	1	0	-6.730039	2.292907	-0.943195

Eight CD Free Energy = -2293.023542

1	6	0	-0.390323	0.175532	1.681809
2	7	0	0.689302	0.235217	2.487345
3	7	0	-1.485815	0.426839	2.419178
4	6	0	0.354111	0.726620	3.828517
5	1	0	0.858761	0.137593	4.598737
6	1	0	0.672327	1.772604	3.936916
7	6	0	-1.162724	0.573556	3.847359
8	1	0	-1.489597	-0.317795	4.398905
9	1	0	-1.678012	1.439460	4.270391
10	6	0	-2.829416	0.391419	1.936781
11	6	0	-5.420581	0.325918	0.914673
12	6	0	-3.506888	1.598075	1.728847
13	6	0	-3.430882	-0.851538	1.685554
14	6	0	-4.723505	-0.856482	1.169407
15	6	0	-4.801114	1.536900	1.211675
16	1	0	-5.201095	-1.812660	0.965601
17	1	0	-5.334644	2.467082	1.029675
18	6	0	2.025120	0.103026	1.989837
19	6	0	4.589442	-0.248311	0.953466
20	6	0	2.647619	-1.153003	2.112492
21	6	0	2.683232	1.201977	1.420447
22	6	0	3.963875	0.991655	0.897070
23	6	0	3.922069	-1.304431	1.581852
24	1	0	4.481623	1.829905	0.435485

25	1	0	4.405640	-2.276135	1.650225
26	6	0	1.951059	-2.283253	2.800262
27	1	0	1.703043	-2.029953	3.836792
28	1	0	2.577898	-3.175899	2.815814
29	1	0	1.019334	-2.535637	2.286375
30	6	0	2.099163	2.581192	1.417107
31	1	0	1.039279	2.597157	1.667324
32	1	0	2.188065	3.050941	0.434971
33	1	0	2.635002	3.216351	2.131811
34	6	0	-2.700987	-2.129433	1.955028
35	1	0	-2.247136	-2.135124	2.951671
36	1	0	-1.882994	-2.292905	1.244109
37	1	0	-3.375299	-2.985121	1.890953
38	6	0	-2.878029	2.914051	2.064289
39	1	0	-1.811193	2.918224	1.832062
40	1	0	-3.000969	3.151858	3.128245
41	1	0	-3.340996	3.723836	1.498305
42	6	0	5.935469	-0.464188	0.332742
43	1	0	6.610038	-1.000832	1.005329
44	1	0	6.411117	0.478883	0.057024
45	1	0	5.852560	-1.069129	-0.576781
46	6	0	-6.799632	0.285168	0.330202
47	1	0	-7.439797	-0.427481	0.857636
48	1	0	-6.776272	-0.029444	-0.718168
49	1	0	-7.282914	1.263195	0.366923
50	44	0	-0.175264	-0.051006	-0.316738
51	17	0	0.220636	-2.445185	-0.196282
52	17	0	-0.616219	2.322641	-0.590032
53	6	0	-1.753715	-0.374208	-1.180998
54	1	0	-2.435337	0.434374	-1.475856
55	1	0	-2.071576	-1.403023	-1.394241
56	6	0	1.135955	0.175762	-2.051214
57	1	0	1.373610	1.236503	-1.938328
58	6	0	-0.088206	-0.092110	-2.699530
59	1	0	-0.657076	0.790558	-2.992498
60	6	0	-0.269097	-1.324835	-3.538059
61	1	0	-1.310609	-1.655098	-3.551958
62	1	0	0.304403	-2.150906	-3.108319
63	6	0	2.319922	-0.755667	-2.041728
64	1	0	2.884951	-0.574660	-1.120561
65	1	0	2.000600	-1.797991	-1.985654
66	6	0	0.163778	-1.037426	-4.983879
67	1	0	0.149414	-1.987171	-5.532338
68	1	0	-0.596699	-0.406101	-5.460536
69	6	0	3.251792	-0.559028	-3.241723
70	1	0	4.203183	-1.052318	-3.009757
71	1	0	3.490034	0.507754	-3.360076
72	6	0	1.524641	-0.368470	-5.168486
73	1	0	1.493177	0.653656	-4.768305
74	1	0	1.676509	-0.244618	-6.246016
75	6	0	2.729142	-1.109372	-4.567892
76	1	0	3.555366	-1.082310	-5.286617
77	1	0	2.487997	-2.174642	-4.445223

Eight D Free Energy = -2293.028660

1	6	0	-0.459742	0.239305	1.581207
2	7	0	0.611741	0.247075	2.408524

3	7	0	-1.563735	0.457758	2.328652
4	6	0	0.262569	0.670015	3.766159
5	1	0	0.774569	0.056998	4.512461
6	1	0	0.555713	1.717284	3.924688
7	6	0	-1.247974	0.484366	3.765376
8	1	0	-1.552762	-0.461441	4.233717
9	1	0	-1.785054	1.294516	4.264385
10	6	0	-2.912972	0.357117	1.876011
11	6	0	-5.545885	0.179241	0.983628
12	6	0	-3.643443	1.536901	1.675801
13	6	0	-3.475136	-0.909686	1.666569
14	6	0	-4.792453	-0.970277	1.211585
15	6	0	-4.956655	1.420984	1.228123
16	1	0	-5.239527	-1.945529	1.033029
17	1	0	-5.533040	2.327381	1.056207
18	6	0	1.951900	0.116339	1.926422
19	6	0	4.532184	-0.229308	0.926527
20	6	0	2.553524	-1.152684	2.005126
21	6	0	2.641650	1.231343	1.425935
22	6	0	3.926119	1.023021	0.914172
23	6	0	3.837549	-1.300497	1.494166
24	1	0	4.468884	1.874851	0.509203
25	1	0	4.307587	-2.280354	1.533985
26	6	0	1.833688	-2.299054	2.640197
27	1	0	1.606024	-2.094509	3.692365
28	1	0	2.436139	-3.207685	2.600935
29	1	0	0.889606	-2.501123	2.128207
30	6	0	2.090175	2.621264	1.507646
31	1	0	1.017044	2.644867	1.693991
32	1	0	2.252579	3.171273	0.578115
33	1	0	2.594989	3.174212	2.308340
34	6	0	-2.677809	-2.154375	1.897167
35	1	0	-2.222247	-2.168428	2.893047
36	1	0	-1.855236	-2.248301	1.178506
37	1	0	-3.304259	-3.043233	1.806897
38	6	0	-3.010476	2.873805	1.897231
39	1	0	-2.182218	3.029626	1.197062
40	1	0	-2.595510	2.968207	2.906327
41	1	0	-3.734195	3.678540	1.758742
42	6	0	5.886706	-0.432172	0.319967
43	1	0	6.441740	-1.226420	0.823646
44	1	0	6.487205	0.479151	0.354268
45	1	0	5.802489	-0.721276	-0.733967
46	6	0	-6.966411	0.089387	0.515211
47	1	0	-7.191227	-0.891848	0.092937
48	1	0	-7.188625	0.843638	-0.243737
49	1	0	-7.666670	0.256408	1.340619
50	44	0	-0.158266	0.077559	-0.370429
51	17	0	0.181288	-2.317544	-0.391162
52	17	0	-0.433621	2.469639	-0.654929
53	6	0	-1.876304	-0.163997	-0.876011
54	1	0	-2.580443	0.672911	-0.988833
55	1	0	-2.255831	-1.163861	-1.137532
56	6	0	1.426612	0.266596	-2.246062
57	1	0	1.686593	1.260052	-1.871637
58	6	0	0.243531	0.152810	-2.911120
59	1	0	-0.370054	1.047996	-3.005393
60	6	0	-0.124209	-1.044261	-3.722801

61	1	0	-1.201839	-1.227587	-3.680833
62	1	0	0.351589	-1.935071	-3.301062
63	6	0	2.509987	-0.771954	-2.221841
64	1	0	3.110955	-0.625520	-1.318817
65	1	0	2.080912	-1.773415	-2.132050
66	6	0	0.295637	-0.853406	-5.189174
67	1	0	0.130860	-1.803554	-5.711695
68	1	0	-0.375463	-0.128551	-5.666108
69	6	0	3.426258	-0.719253	-3.451513
70	1	0	4.322514	-1.306360	-3.218912
71	1	0	3.777909	0.309218	-3.614059
72	6	0	1.736658	-0.395475	-5.408022
73	1	0	1.849894	0.643401	-5.072154
74	1	0	1.904514	-0.363542	-6.489875
75	6	0	2.826041	-1.258238	-4.751354
76	1	0	3.650561	-1.381710	-5.461895
77	1	0	2.442939	-2.273203	-4.576840

Z-Cyclononene formation

Nine A Free Energy = -2332.319111

1	6	0	-0.929380	-2.120698	0.071709
2	7	0	-2.085963	-2.721880	0.470220
3	7	0	0.089191	-2.954486	0.412685
4	6	0	-1.878963	-4.067032	1.000588
5	1	0	-2.427010	-4.201569	1.938276
6	1	0	-2.244314	-4.818423	0.287574
7	6	0	-0.366815	-4.119400	1.176974
8	1	0	-0.062429	-4.026707	2.228266
9	1	0	0.082289	-5.036581	0.784380
10	6	0	1.479025	-2.659363	0.324533
11	6	0	4.183799	-2.034713	0.094786
12	6	0	2.182250	-3.095248	-0.802371
13	6	0	2.089339	-1.905589	1.335776
14	6	0	3.443418	-1.608783	1.199093
15	6	0	3.536090	-2.773132	-0.895263
16	1	0	3.929392	-1.012897	1.968855
17	1	0	4.093847	-3.093133	-1.772299
18	6	0	-3.392303	-2.189671	0.243610
19	6	0	-5.906514	-1.072796	-0.213426
20	6	0	-3.987082	-1.409181	1.248430
21	6	0	-4.073064	-2.502100	-0.944464
22	6	0	-5.321674	-1.919909	-1.153009
23	6	0	-5.235758	-0.850390	0.987705
24	1	0	-5.849582	-2.134963	-2.079438
25	1	0	-5.696006	-0.222501	1.747298
26	6	0	-3.352923	-1.227365	2.593744
27	1	0	-3.781692	-1.938703	3.310358
28	1	0	-3.534570	-0.223723	2.981367
29	1	0	-2.273176	-1.376997	2.573086
30	6	0	-3.532074	-3.491756	-1.930666
31	1	0	-2.445321	-3.573463	-1.892365
32	1	0	-3.796941	-3.215883	-2.952317
33	1	0	-3.956997	-4.484840	-1.738657
34	6	0	1.288160	-1.358870	2.475364
35	1	0	0.721594	-2.136226	2.997482
36	1	0	0.555105	-0.622887	2.123207
37	1	0	1.930208	-0.867796	3.208367
38	6	0	1.466235	-3.801776	-1.911506
39	1	0	0.701619	-3.152913	-2.355004
40	1	0	0.946777	-4.699365	-1.561045
41	1	0	2.156838	-4.101134	-2.701319
42	6	0	-7.218769	-0.407351	-0.493022
43	1	0	-7.783123	-0.222303	0.423645
44	1	0	-7.841492	-1.004106	-1.162921
45	1	0	-7.067077	0.563314	-0.976980
46	6	0	5.642076	-1.709396	-0.015461
47	1	0	5.850060	-0.683383	0.298747
48	1	0	6.007223	-1.831489	-1.036868
49	1	0	6.242561	-2.363812	0.625104
50	44	0	-0.948011	-0.411757	-0.817662
51	17	0	-1.452778	0.932291	1.029765
52	17	0	-1.524282	-1.120985	-2.960033
53	6	0	0.786857	0.018076	-1.058299
54	1	0	1.664593	-0.618557	-0.912518

55	6	0	6.343338	9.218529	1.602544
56	1	0	6.814068	9.734225	2.432313
57	1	0	6.910369	9.168291	0.676372
58	6	0	5.133931	8.677415	1.703590
59	1	0	4.602279	8.748205	2.654182
60	6	0	4.422469	7.941931	0.617399
61	6	0	1.060729	1.417282	-1.492736
62	1	0	1.612332	1.401193	-2.445343
63	1	0	0.129912	1.970934	-1.688108
64	6	0	4.087874	6.499397	0.992798
65	1	0	3.511176	6.491124	1.927884
66	1	0	5.017802	5.959965	1.216483
67	6	0	1.878067	2.148853	-0.421364
68	1	0	2.810820	1.594568	-0.245729
69	1	0	1.322290	2.116687	0.524564
70	6	0	3.311919	5.762368	-0.087215
71	1	0	3.883289	5.781466	-1.025944
72	1	0	2.380332	6.304833	-0.301256
73	6	0	2.190316	3.590254	-0.791360
74	1	0	2.740768	3.615592	-1.742443
75	1	0	1.250761	4.127568	-0.979218
76	6	0	2.985925	4.322375	0.277886
77	1	0	2.426343	4.302304	1.223176
78	1	0	3.919037	3.776814	0.478076
79	1	0	5.025424	7.959172	-0.298846
80	1	0	3.485722	8.464596	0.374619

Nine B Free Energy = -2332.320302

1	6	0	-0.175125	-1.703242	0.354309
2	7	0	-1.305786	-2.424915	0.571368
3	7	0	0.868578	-2.560036	0.383020
4	6	0	-1.064671	-3.865117	0.580007
5	1	0	-1.601110	-4.346769	1.402465
6	1	0	-1.405421	-4.319849	-0.360646
7	6	0	0.452353	-3.924579	0.737236
8	1	0	0.753793	-4.157556	1.766685
9	1	0	0.928340	-4.653825	0.076107
10	6	0	2.247746	-2.221764	0.256166
11	6	0	4.954438	-1.614705	-0.004813
12	6	0	2.824493	-2.225798	-1.020160
13	6	0	2.989635	-1.914897	1.405254
14	6	0	4.339688	-1.610149	1.248462
15	6	0	4.181343	-1.921106	-1.123992
16	1	0	4.924905	-1.354892	2.128913
17	1	0	4.643010	-1.915224	-2.109080
18	6	0	-2.590804	-1.804526	0.460795
19	6	0	-4.957494	-0.348075	0.228919
20	6	0	-3.238405	-1.363861	1.628413
21	6	0	-3.166813	-1.632249	-0.811014
22	6	0	-4.340577	-0.885239	-0.899170
23	6	0	-4.411045	-0.626044	1.481667
24	1	0	-4.778812	-0.717661	-1.880370
25	1	0	-4.905679	-0.250773	2.374943
26	6	0	-2.736042	-1.717315	2.992999
27	1	0	-3.300762	-2.571828	3.386309
28	1	0	-2.863731	-0.886966	3.688895
29	1	0	-1.677979	-1.977006	2.990157

30	6	0	-2.603561	-2.297588	-2.028573
31	1	0	-1.523169	-2.434951	-1.972683
32	1	0	-2.800426	-1.710037	-2.925543
33	1	0	-3.069872	-3.281957	-2.161488
34	6	0	2.327349	-1.854476	2.745946
35	1	0	1.951930	-2.833699	3.062097
36	1	0	1.466495	-1.173828	2.739072
37	1	0	3.023171	-1.510311	3.512701
38	6	0	1.992604	-2.502544	-2.231023
39	1	0	1.270926	-1.694254	-2.404002
40	1	0	1.406851	-3.421527	-2.122633
41	1	0	2.613639	-2.600921	-3.122880
42	6	0	-6.164224	0.529016	0.099515
43	1	0	-6.823114	0.444429	0.966532
44	1	0	-6.744246	0.294304	-0.795431
45	1	0	-5.870138	1.582232	0.024101
46	6	0	6.417021	-1.318738	-0.139739
47	1	0	6.751444	-0.586959	0.599212
48	1	0	6.662553	-0.936066	-1.132652
49	1	0	7.017455	-2.222109	0.013611
50	44	0	-0.407029	0.226473	0.075762
51	17	0	-0.519907	0.637126	2.466611
52	17	0	-0.553175	0.175235	-2.341894
53	6	0	1.375271	0.637114	0.124953
54	1	0	1.883401	0.461842	1.089741
55	6	0	-2.085698	1.986697	-0.111054
56	1	0	-2.493882	1.630731	0.833661
57	1	0	-2.627001	1.743291	-1.022805
58	6	0	-1.036064	2.839429	-0.140361
59	1	0	-0.565161	3.097139	0.809788
60	6	0	-0.534486	3.496642	-1.387683
61	1	0	-1.275150	3.349643	-2.180120
62	1	0	0.344685	2.951817	-1.741076
63	6	0	2.225726	1.365982	-0.853210
64	1	0	3.161409	0.806792	-1.000847
65	1	0	1.738184	1.443000	-1.828412
66	6	0	-0.220704	4.993225	-1.250188
67	1	0	-1.139997	5.505275	-0.941024
68	1	0	0.007836	5.382254	-2.251003
69	6	0	2.519342	2.762803	-0.263907
70	1	0	3.365543	2.708283	0.430019
71	1	0	1.666208	3.042576	0.362582
72	6	0	0.905074	5.393015	-0.292424
73	1	0	0.792834	4.856660	0.657650
74	1	0	0.766127	6.447190	-0.027433
75	6	0	2.742978	3.856639	-1.307716
76	1	0	3.792971	3.873986	-1.621969
77	1	0	2.180371	3.614455	-2.217151
78	6	0	2.337527	5.246775	-0.818019
79	1	0	3.024654	5.565974	-0.023480
80	1	0	2.485183	5.960566	-1.638409

Nine BC Free Energy = -2332.310518

1	6	0	0.303881	-3.167296	1.961360
2	1	0	1.077795	-3.819453	1.544974
3	1	0	-0.554767	-3.312420	1.304204
4	6	0	-2.136094	-1.429063	0.880430

5	1	0	-1.854754	-2.292011	0.269828
6	1	0	-2.614551	-0.762593	0.148961
7	6	0	-0.006141	-3.608373	3.393995
8	1	0	0.925985	-3.545709	3.968725
9	1	0	-0.275171	-4.672239	3.387768
10	6	0	-3.175358	-1.790065	1.951919
11	1	0	-4.161748	-1.660093	1.494635
12	1	0	-3.139871	-1.049142	2.763320
13	6	0	-1.090907	-2.815765	4.130272
14	1	0	-1.032756	-1.752663	3.860173
15	1	0	-0.871766	-2.840773	5.203336
16	6	0	-3.095019	-3.213118	2.531038
17	1	0	-4.103462	-3.640387	2.558936
18	1	0	-2.536932	-3.860632	1.843927
19	6	0	-2.518114	-3.314507	3.938794
20	1	0	-3.173923	-2.754931	4.618922
21	1	0	-2.573910	-4.359658	4.270430
22	6	0	0.282439	1.309071	-1.135961
23	7	0	-0.822881	1.885311	-1.634646
24	7	0	1.361213	1.911715	-1.674571
25	6	0	-0.499023	3.041336	-2.487125
26	1	0	-1.098381	3.027389	-3.401049
27	1	0	-0.720225	3.974569	-1.953071
28	6	0	0.995010	2.855101	-2.736298
29	1	0	1.204033	2.416713	-3.721707
30	1	0	1.566765	3.782693	-2.648153
31	6	0	2.664502	1.342426	-1.498579
32	6	0	5.094918	0.079467	-0.982955
33	6	0	3.544069	1.915045	-0.566100
34	6	0	3.014577	0.203792	-2.244889
35	6	0	4.228774	-0.416731	-1.954680
36	6	0	4.747653	1.256803	-0.321744
37	1	0	4.501894	-1.312647	-2.507522
38	1	0	5.428158	1.674176	0.417051
39	6	0	-2.161836	1.554777	-1.258691
40	6	0	-4.761483	0.864915	-0.530018
41	6	0	-2.884740	0.674015	-2.074122
42	6	0	-2.710576	2.112085	-0.096190
43	6	0	-4.009286	1.741019	0.252065
44	6	0	-4.185273	0.347258	-1.690109
45	1	0	-4.444051	2.152169	1.160621
46	1	0	-4.754324	-0.344769	-2.306847
47	6	0	-2.255035	0.055868	-3.281823
48	1	0	-1.790470	0.801634	-3.934900
49	1	0	-2.991102	-0.493152	-3.871371
50	1	0	-1.466289	-0.645390	-2.982963
51	6	0	-1.921198	3.054116	0.755844
52	1	0	-1.067739	2.558236	1.232572
53	1	0	-2.543392	3.485482	1.541704
54	1	0	-1.506780	3.880576	0.169391
55	6	0	2.173837	-0.294768	-3.380184
56	1	0	2.512987	0.156649	-4.321006
57	1	0	1.113384	-0.072133	-3.257913
58	1	0	2.255086	-1.377204	-3.484052
59	6	0	3.242341	3.212393	0.116463
60	1	0	2.176676	3.439751	0.118487
61	1	0	3.771970	4.032772	-0.383217
62	1	0	3.568737	3.193063	1.157325

63	6	0	-6.163233	0.502183	-0.143231
64	1	0	-6.311508	0.564178	0.937177
65	1	0	-6.421217	-0.509914	-0.463906
66	1	0	-6.889391	1.178578	-0.606737
67	6	0	6.360556	-0.644434	-0.639443
68	1	0	6.212668	-1.296615	0.228453
69	1	0	7.166059	0.047295	-0.381964
70	1	0	6.702488	-1.276132	-1.461707
71	17	0	0.158755	-1.962061	-1.366289
72	44	0	0.529855	-0.180755	0.239223
73	6	0	1.958187	-1.387787	1.153021
74	1	0	2.685327	-0.705186	1.586648
75	1	0	2.326277	-2.124407	0.439837
76	6	0	-0.934374	-0.648620	1.298716
77	1	0	-1.048971	-0.080634	2.237391
78	6	0	0.809467	-1.736927	1.929937
79	1	0	0.752540	-1.192221	2.872610
80	17	0	1.110679	1.461560	1.941091

Nine C Free Energy = -2332.320467

1	6	0	0.068793	-3.304046	1.860887
2	1	0	0.860997	-3.896149	1.395015
3	1	0	-0.828773	-3.522050	1.281151
4	6	0	-2.224858	-1.429779	1.128694
5	1	0	-2.127799	-2.274183	0.443358
6	1	0	-2.662569	-0.635745	0.513031
7	6	0	-0.064302	-3.744963	3.320629
8	1	0	0.931656	-3.670061	3.775232
9	1	0	-0.316337	-4.813301	3.344087
10	6	0	-3.224181	-1.752842	2.250705
11	1	0	-4.222346	-1.541162	1.852150
12	1	0	-3.093900	-1.047483	3.084220
13	6	0	-1.050170	-2.973245	4.200871
14	1	0	-0.970256	-1.895490	4.003336
15	1	0	-0.734740	-3.087110	5.244121
16	6	0	-3.209339	-3.198026	2.774059
17	1	0	-4.242979	-3.542933	2.890612
18	1	0	-2.779705	-3.858864	2.011285
19	6	0	-2.509039	-3.405567	4.112469
20	1	0	-3.072970	-2.861228	4.881583
21	1	0	-2.581125	-4.465354	4.390539
22	6	0	0.379002	1.194081	-1.243661
23	7	0	-0.696082	1.897040	-1.631617
24	7	0	1.455674	1.608369	-1.926914
25	6	0	-0.378250	2.853626	-2.701917
26	1	0	-0.912591	2.580464	-3.618478
27	1	0	-0.694977	3.862227	-2.417596
28	6	0	1.140068	2.715376	-2.842015
29	1	0	1.456945	2.468362	-3.860100
30	1	0	1.675765	3.619599	-2.534183
31	6	0	2.794523	1.218041	-1.594551
32	6	0	5.340393	0.377877	-0.842837
33	6	0	3.531778	2.004487	-0.696425
34	6	0	3.320155	0.053149	-2.167296
35	6	0	4.594474	-0.349365	-1.766697
36	6	0	4.798340	1.557956	-0.332572
37	1	0	5.013129	-1.257509	-2.194501

38	1	0	5.372554	2.144212	0.381481
39	6	0	-2.035887	1.593312	-1.227248
40	6	0	-4.631162	0.985905	-0.407455
41	6	0	-2.821352	0.748976	-2.025690
42	6	0	-2.529535	2.168699	-0.046028
43	6	0	-3.826804	1.840573	0.346001
44	6	0	-4.112443	0.456392	-1.588328
45	1	0	-4.218020	2.268821	1.266221
46	1	0	-4.724553	-0.215083	-2.186167
47	6	0	-2.322344	0.197205	-3.325183
48	1	0	-2.620135	0.843371	-4.160271
49	1	0	-2.742653	-0.791675	-3.513779
50	1	0	-1.236819	0.088741	-3.341620
51	6	0	-1.697690	3.112710	0.764084
52	1	0	-0.854182	2.610057	1.249975
53	1	0	-2.298095	3.588768	1.541014
54	1	0	-1.267511	3.903436	0.140805
55	6	0	2.548034	-0.740576	-3.173332
56	1	0	2.098246	-0.098761	-3.937375
57	1	0	1.722945	-1.296430	-2.713919
58	1	0	3.196521	-1.458986	-3.678038
59	6	0	2.996051	3.294040	-0.154001
60	1	0	1.911852	3.268255	-0.024590
61	1	0	3.246751	4.132363	-0.816180
62	1	0	3.427318	3.512280	0.823897
63	6	0	-6.027273	0.661746	0.029517
64	1	0	-6.307923	-0.358718	-0.241721
65	1	0	-6.754966	1.328873	-0.444985
66	1	0	-6.147356	0.771064	1.109462
67	6	0	6.692960	-0.090647	-0.400415
68	1	0	6.680130	-0.397220	0.650269
69	1	0	7.441954	0.701444	-0.486732
70	1	0	7.036956	-0.943843	-0.987711
71	17	0	-0.389994	-1.899088	-1.480055
72	44	0	0.359677	-0.269670	0.146579
73	6	0	1.648738	-1.557372	0.812786
74	1	0	2.518487	-1.152367	1.332198
75	1	0	1.847900	-2.400278	0.148043
76	6	0	-0.877296	-0.890064	1.544995
77	1	0	-0.945978	-0.162704	2.362971
78	6	0	0.416073	-1.806946	1.777240
79	1	0	0.796598	-1.416764	2.726886
80	17	0	1.234121	1.243903	1.828955

Nine CD Free Energy = -2332.305059

1	6	0	-1.503604	3.323639	0.707070
2	1	0	-0.642366	3.678678	1.278965
3	1	0	-2.120828	2.779212	1.422983
4	6	0	-3.003929	0.697608	0.013022
5	1	0	-2.854305	0.798596	1.090278
6	1	0	-3.030348	-0.381460	-0.178170
7	6	0	-2.230453	4.547315	0.124426
8	1	0	-1.475710	5.173306	-0.368174
9	1	0	-2.618978	5.151543	0.953914
10	6	0	-4.368256	1.297787	-0.378574
11	1	0	-5.117736	0.513755	-0.227253
12	1	0	-4.393456	1.513446	-1.455389

13	6	0	-3.350079	4.278632	-0.883788
14	1	0	-3.019811	3.529073	-1.615094
15	1	0	-3.500375	5.192947	-1.468859
16	6	0	-4.789560	2.541648	0.424321
17	1	0	-5.829457	2.417100	0.746673
18	1	0	-4.213312	2.582776	1.355827
19	6	0	-4.704802	3.875689	-0.311577
20	1	0	-5.427592	3.856980	-1.138107
21	1	0	-5.052786	4.669553	0.362650
22	6	0	1.158641	-1.327094	0.091385
23	7	0	0.608716	-2.556526	0.122885
24	7	0	2.494759	-1.462371	0.003711
25	6	0	1.596269	-3.612140	-0.129223
26	1	0	1.447572	-4.456019	0.549144
27	1	0	1.499141	-3.980714	-1.159569
28	6	0	2.907347	-2.871296	0.102577
29	1	0	3.330749	-3.066394	1.097256
30	1	0	3.671743	-3.101988	-0.642835
31	6	0	3.440659	-0.393018	0.006587
32	6	0	5.254745	1.723288	0.000688
33	6	0	4.106184	-0.073165	-1.182552
34	6	0	3.693655	0.290935	1.206081
35	6	0	4.598830	1.348411	1.174313
36	6	0	5.003227	0.995378	-1.159109
37	1	0	4.802707	1.889343	2.096147
38	1	0	5.514707	1.267075	-2.079749
39	6	0	-0.801778	-2.776486	0.216275
40	6	0	-3.554011	-3.127538	0.478671
40	6	0	-3.554011	-3.127538	0.478671
41	6	0	-1.351457	-2.941603	1.500379
42	6	0	-1.588798	-2.845607	-0.940394
43	6	0	-2.967506	-3.016166	-0.777622
44	6	0	-2.727096	-3.102735	1.605315
45	1	0	-3.595606	-3.055006	-1.664887
46	1	0	-3.167762	-3.209132	2.593771
47	6	0	-0.470849	-2.953102	2.709465
48	1	0	0.311542	-3.715651	2.627741
49	1	0	-1.048913	-3.161453	3.610958
50	1	0	0.021507	-1.986015	2.844182
51	6	0	-0.993970	-2.797408	-2.313573
52	1	0	-0.042764	-2.265226	-2.345093
53	1	0	-1.662122	-2.293064	-3.015104
54	1	0	-0.834173	-3.812642	-2.695982
55	6	0	3.010192	-0.096836	2.479312
56	1	0	3.002874	-1.181872	2.625490
57	1	0	1.961399	0.220764	2.495684
58	1	0	3.508122	0.353388	3.339978
59	6	0	3.886856	-0.859818	-2.436797
60	1	0	2.844312	-1.168693	-2.538840
61	1	0	4.518172	-1.756824	-2.456503
62	1	0	4.143076	-0.269138	-3.317686
63	6	0	-5.038180	-3.258682	0.632458
64	1	0	-5.304251	-4.125912	1.243369
65	1	0	-5.538317	-3.360293	-0.332325
66	1	0	-5.459544	-2.381684	1.134768
67	6	0	6.205435	2.881615	-0.003509
68	1	0	6.951747	2.792421	0.791009
69	1	0	5.680576	3.827611	0.164247

70	1	0	6.735787	2.965183	-0.953781
71	17	0	-0.559903	0.482664	2.278260
72	44	0	0.032236	0.354186	-0.070291
73	6	0	1.014309	1.891935	0.070568
74	1	0	1.574960	2.305031	-0.777939
75	1	0	1.118886	2.408068	1.033522
76	6	0	-1.828260	1.247601	-0.754831
77	1	0	-1.814521	0.988549	-1.815079
78	6	0	-1.090812	2.408290	-0.415579
79	1	0	-0.616950	2.896909	-1.268577
80	17	0	0.599888	0.335598	-2.439381

Nine D Free Energy = -2332.312897

1	6	0	-2.693087	-3.008494	1.538120
2	6	0	-3.490211	-3.069105	0.391646
3	6	0	-2.871618	-2.998922	-0.852216
4	6	0	-1.488269	-2.839471	-0.985236
5	6	0	-0.732105	-2.717982	0.189460
6	6	0	-1.316020	-2.843888	1.463723
7	7	0	0.680818	-2.506328	0.128572
8	6	0	1.233968	-1.274738	0.026769
9	7	0	2.576742	-1.427332	-0.030612
10	6	0	2.970541	-2.827330	0.188460
11	6	0	1.666074	-3.574939	-0.045326
12	44	0	0.049923	0.292683	-0.191916
13	17	0	0.408117	0.232785	-2.588352
14	6	0	3.543488	-0.381768	0.058041
15	6	0	4.250619	-0.020204	-1.097742
16	6	0	5.194729	0.997699	-0.992545
17	6	0	5.446992	1.647793	0.216789
18	6	0	4.735461	1.248985	1.346173
19	6	0	3.783842	0.230001	1.296490
20	6	0	6.482202	2.727724	0.301078
21	6	0	3.963928	-0.683894	-2.406821
22	6	0	3.025211	-0.176018	2.520536
23	6	0	-4.979146	-3.181989	0.508217
24	6	0	-0.468022	-2.815793	2.695243
25	6	0	-0.857615	-2.886601	-2.342297
26	17	0	-0.534904	0.587354	2.132732
27	6	0	1.321977	1.566601	-0.049124
28	6	0	-2.224794	1.144906	-0.814844
29	6	0	-1.500235	2.293836	-0.750056
30	6	0	-1.669682	3.357514	0.283367
31	6	0	-2.434098	4.554750	-0.313859
32	6	0	-3.721648	4.235191	-1.075034
33	6	0	-4.955420	3.918977	-0.235876
34	6	0	-4.923671	2.665142	0.634937
35	6	0	-4.671286	1.331821	-0.093279
36	6	0	-3.284720	0.699674	0.149667
37	1	0	-0.694535	3.710271	0.633501
38	1	0	-2.171268	2.952154	1.164742
39	1	0	-2.972714	0.897942	1.178939
40	1	0	-3.371132	-0.388544	0.070427
41	1	0	-1.754187	5.072186	-1.001709
42	1	0	-2.645784	5.271486	0.489571
43	1	0	-5.418429	0.605867	0.242883
44	1	0	-4.849722	1.447867	-1.170778

45	1	0	-3.536437	3.419592	-1.786746
46	1	0	-3.964904	5.102682	-1.698878
47	1	0	-5.892156	2.606559	1.144224
48	1	0	-4.194501	2.782345	1.444224
49	1	0	-5.813787	3.840900	-0.916430
50	1	0	-5.172072	4.781513	0.408368
51	1	0	1.495550	-4.384941	0.668601
52	1	0	1.599319	-3.993553	-1.059172
53	1	0	3.346404	-2.955013	1.213173
54	1	0	3.766969	-3.117923	-0.500791
55	1	0	4.925459	1.739968	2.297906
56	1	0	5.742409	1.297147	-1.883331
57	1	0	-3.475303	-3.078676	-1.753804
58	1	0	-3.159085	-3.089293	2.517362
59	1	0	0.334155	-3.560290	2.647517
60	1	0	-1.065380	-3.021964	3.584636
61	1	0	-0.002498	-1.834859	2.824234
62	1	0	0.143253	-2.456753	-2.360348
63	1	0	-1.448152	-2.331973	-3.074645
64	1	0	-0.798298	-3.924336	-2.691434
65	1	0	3.024038	-1.262058	2.660245
66	1	0	1.974016	0.131195	2.466376
67	1	0	3.458619	0.273579	3.415525
68	1	0	2.926045	-0.510020	-2.711870
69	1	0	4.100683	-1.769208	-2.353512
70	1	0	4.622217	-0.305753	-3.190642
71	1	0	-5.271230	-3.904805	1.274329
72	1	0	-5.439269	-3.481488	-0.435339
73	1	0	-5.420656	-2.221680	0.797201
74	1	0	6.355760	3.339023	1.196581
75	1	0	6.446471	3.388800	-0.568308
76	1	0	7.492246	2.305299	0.335470
77	1	0	1.969882	1.844987	-0.892942
78	1	0	1.455936	2.141438	0.880396
79	1	0	-2.138396	0.573036	-1.741562
80	1	0	-0.884070	2.536878	-1.616253

Z-Cyclodecene formation

Ten A Free Energy = -2371.609026

1	6	0	-1.003562	-2.441011	0.053532
2	7	0	-2.160446	-3.065208	0.412970
3	7	0	0.016828	-3.274368	0.387454
4	6	0	-1.948893	-4.422167	0.909983
5	1	0	-2.512442	-4.587360	1.833353
6	1	0	-2.293969	-5.156947	0.169760
7	6	0	-0.439805	-4.463877	1.112501
8	1	0	-0.155450	-4.395607	2.171174
9	1	0	0.026447	-5.365261	0.703589
10	6	0	1.405944	-2.974290	0.312114
11	6	0	4.117040	-2.365425	0.124719
12	6	0	2.111455	-3.367952	-0.829007
13	6	0	2.014907	-2.264356	1.354816
14	6	0	3.373051	-1.975733	1.239909
15	6	0	3.468140	-3.053393	-0.900692
16	1	0	3.859237	-1.415882	2.035903
17	1	0	4.028815	-3.342286	-1.786615
18	6	0	-3.468244	-2.538014	0.185578
19	6	0	-5.987743	-1.431131	-0.260041
20	6	0	-4.091456	-1.818180	1.218375
21	6	0	-4.121874	-2.797704	-1.029106
22	6	0	-5.374196	-2.218993	-1.231158
23	6	0	-5.342421	-1.263528	0.964824
24	1	0	-5.882464	-2.392362	-2.177113
25	1	0	-5.824896	-0.682019	1.747004
26	6	0	-3.473390	-1.699401	2.577812
27	1	0	-3.802558	-2.527400	3.218223
28	1	0	-3.773962	-0.770639	3.065256
29	1	0	-2.383468	-1.711259	2.542607
30	6	0	-3.555280	-3.733643	-2.052632
31	1	0	-2.474378	-3.848052	-1.966295
32	1	0	-3.758660	-3.382473	-3.065418
33	1	0	-4.014364	-4.724469	-1.948734
34	6	0	1.206358	-1.751485	2.505214
35	1	0	0.653032	-2.546916	3.014424
36	1	0	0.461036	-1.021712	2.165706
37	1	0	1.840821	-1.263090	3.246477
38	6	0	1.396022	-4.028601	-1.966122
39	1	0	0.636872	-3.359502	-2.388548
40	1	0	0.869038	-4.934262	-1.648923
41	1	0	2.087862	-4.304330	-2.763391
42	6	0	-7.303941	-0.768852	-0.528633
43	1	0	-7.891232	-0.648098	0.384413
44	1	0	-7.902411	-1.332770	-1.247441
45	1	0	-7.157191	0.231717	-0.949014
46	6	0	5.581408	-2.060274	0.039877
47	1	0	5.813669	-1.077604	0.457614
48	1	0	5.940286	-2.084645	-0.990826
49	1	0	6.169683	-2.791543	0.604640
50	44	0	-1.021404	-0.705539	-0.782514
51	17	0	-1.605190	0.566845	1.091772
52	17	0	-1.521509	-1.360839	-2.961714
53	6	0	0.708090	-0.234886	-0.966980
54	1	0	1.603011	-0.834000	-0.773366

55	6	0	4.060143	7.855703	0.520884
56	6	0	0.934689	1.166646	-1.421751
57	1	0	1.500553	1.152200	-2.366164
58	1	0	-0.015869	1.674336	-1.648388
59	6	0	3.745933	6.428696	0.942027
60	1	0	3.152875	6.442476	1.867245
61	1	0	4.680522	5.911851	1.202234
62	6	0	1.699359	1.961377	-0.357759
63	1	0	2.649902	1.451768	-0.147244
64	1	0	1.126233	1.935582	0.577696
65	6	0	3.006631	5.630818	-0.120577
66	1	0	3.591387	5.633196	-1.051197
67	1	0	2.063424	6.137882	-0.367462
68	6	0	1.964498	3.401801	-0.767066
69	1	0	2.529515	3.417843	-1.709780
70	1	0	1.009667	3.898391	-0.986824
71	6	0	2.716365	4.195254	0.289982
72	1	0	2.140371	4.190471	1.225559
73	1	0	3.661678	3.685911	0.525487
74	1	0	4.663248	7.847106	-0.396443
75	1	0	3.128560	8.374197	0.255365
76	6	0	4.794028	8.653522	1.597069
77	1	0	4.179898	8.654364	2.509355
78	1	0	5.730650	8.147664	1.862761
79	6	0	5.079786	10.060244	1.189202
80	1	0	4.209787	10.662625	0.922652
81	6	0	6.288094	10.607908	1.111721
82	1	0	7.182344	10.043609	1.363915
83	1	0	6.434915	11.636026	0.798856

Ten B Free Energy = -2371.616096

1	6	0	-0.007179	0.016864	-0.006458
2	6	0	0.002163	-0.010439	1.400952
3	6	0	1.202943	-0.017657	2.130185
4	6	0	2.395599	-0.123306	1.416146
5	6	0	2.419598	-0.198423	0.023714
6	6	0	1.213631	-0.098514	-0.668440
7	7	0	-1.240972	-0.028612	2.107492
8	6	0	-1.958296	-1.177270	2.224729
9	7	0	-3.135402	-0.864525	2.805301
10	6	0	-3.195575	0.552042	3.199054
11	6	0	-2.022197	1.159930	2.439905
12	6	0	-4.213388	-1.744350	3.115494
13	6	0	-5.178231	-1.986036	2.128830
14	6	0	-6.279229	-2.769575	2.469280
15	6	0	-6.435172	-3.301109	3.749786
16	6	0	-5.447041	-3.048128	4.700692
17	6	0	-4.324136	-2.274667	4.407768
18	6	0	-5.005495	-1.432634	0.750333
19	6	0	-3.251842	-2.039148	5.424954
20	6	0	-7.605161	-4.177768	4.075890
21	44	0	-1.055544	-2.821212	1.616507
22	17	0	-1.900714	-2.924807	-0.655370
23	6	0	1.226911	0.141401	3.618127
24	6	0	3.707712	-0.407887	-0.710471
25	6	0	-1.265404	0.260071	-0.781212
26	6	0	-2.335878	-3.981156	2.222723

27	6	0	-3.248224	-4.891094	1.475535
28	6	0	-4.093557	-5.801482	2.369882
29	6	0	-3.334548	-6.784066	3.264284
30	6	0	-2.924334	-8.103472	2.611427
31	6	0	-1.878930	-8.016267	1.504415
32	6	0	-0.521465	-7.508659	1.976892
33	6	0	0.446775	-7.237795	0.828122
34	6	0	0.206961	-5.884082	0.162911
35	6	0	0.650408	-4.744680	1.028066
36	6	0	0.966441	-3.513090	0.563464
37	17	0	0.073825	-2.948417	3.764057
38	1	0	-2.679217	-5.446892	0.721498
39	1	0	-3.901116	-4.258951	0.855087
40	1	0	-0.856632	-5.761584	-0.089813
41	1	0	0.722018	-5.821531	-0.802007
42	1	0	-0.643868	-6.590060	2.568194
43	1	0	-0.093916	-8.242236	2.671061
44	1	0	-3.972352	-7.026816	4.122260
45	1	0	-2.459368	-6.282767	3.700528
46	1	0	-3.825528	-8.590765	2.216709
47	1	0	-2.544946	-8.775078	3.393225
48	1	0	-2.251008	-7.393750	0.681284
49	1	0	-1.742440	-9.012432	1.064284
50	1	0	0.361430	-8.036354	0.081399
51	1	0	1.481884	-7.274361	1.187834
52	1	0	-4.698334	-5.148782	3.007498
53	1	0	-4.809159	-6.351896	1.743758
54	1	0	-1.434764	1.858503	3.042049
55	1	0	-2.339917	1.680762	1.525192
56	1	0	-3.079896	0.645739	4.286466
57	1	0	-4.161285	0.984082	2.923899
58	1	0	-5.545681	-3.470729	5.698176
59	1	0	-7.036256	-2.967328	1.713528
60	1	0	1.217574	-0.110911	-1.756017
61	1	0	3.332183	-0.157467	1.968272
62	1	0	1.463530	1.180469	3.878247
63	1	0	1.989770	-0.493724	4.071248
64	1	0	0.274150	-0.122540	4.076190
65	1	0	-2.152318	-0.137329	-0.286343
66	1	0	-1.217658	-0.204126	-1.766459
67	1	0	-1.407032	1.338632	-0.925823
68	1	0	-3.247728	-1.002767	5.781117
69	1	0	-2.255065	-2.239214	5.014116
70	1	0	-3.393621	-2.677751	6.298411
71	1	0	-4.124816	-1.864663	0.257532
72	1	0	-4.849628	-0.348200	0.765747
73	1	0	-5.877971	-1.638966	0.128388
74	1	0	4.561904	-0.018924	-0.152302
75	1	0	3.696280	0.066139	-1.694444
76	1	0	3.890151	-1.476330	-0.872974
77	1	0	-7.854326	-4.143939	5.138498
78	1	0	-7.388835	-5.223926	3.829910
79	1	0	-8.494316	-3.895411	3.508069
80	1	0	-2.434247	-4.034261	3.322475
81	1	0	1.444390	-2.779287	1.215432
82	1	0	0.893709	-3.275097	-0.494626
83	1	0	0.805217	-4.942644	2.089180

Ten BC Free Energy = -2371.602570

1	6	0	2.700233	0.387983	-0.209409
2	1	0	2.848832	1.083214	-1.041420
3	1	0	2.512697	-0.560569	-0.729855
4	6	0	1.306393	3.287386	-1.007640
5	1	0	1.962497	2.581275	-1.522044
6	1	0	0.589018	3.583889	-1.777759
7	6	0	3.951700	0.234652	0.666135
8	6	0	2.105541	4.506182	-0.541550
9	6	0	3.251954	4.166648	0.405496
10	1	0	2.851103	3.614926	1.264403
11	1	0	3.660944	5.088631	0.835041
12	6	0	4.420349	1.435480	1.488914
13	1	0	5.075488	1.054465	2.280656
14	1	0	3.565190	1.866040	2.025628
15	6	0	5.188813	2.530405	0.748797
16	1	0	6.038863	2.071641	0.227239
17	1	0	5.631595	3.202467	1.496126
18	6	0	4.384177	3.368111	-0.241576
19	1	0	3.989492	2.722397	-1.032811
20	1	0	5.060099	4.059341	-0.759198
21	1	0	2.500787	5.021913	-1.425727
22	1	0	1.428653	5.219861	-0.055619
23	1	0	3.758791	-0.593184	1.359903
24	1	0	4.772060	-0.113827	0.023789
25	6	0	-1.174593	-1.363394	-0.132090
26	7	0	-0.599978	-2.568619	-0.281665
27	7	0	-2.508140	-1.529121	-0.089242
28	6	0	-1.585339	-3.659245	-0.197078
29	1	0	-1.405499	-4.404865	-0.974823
30	1	0	-1.504555	-4.160444	0.776437
31	6	0	-2.904220	-2.916193	-0.363670
32	1	0	-3.307260	-2.992590	-1.382881
33	1	0	-3.678678	-3.244475	0.333882
34	6	0	-3.438629	-0.448284	0.012831
35	6	0	-5.179756	1.712004	0.296067
36	6	0	-4.069576	-0.234379	1.251604
37	6	0	-3.707006	0.358127	-1.100761
38	6	0	-4.573705	1.441734	-0.924266
39	6	0	-4.926186	0.851341	1.368166
40	1	0	-4.782513	2.083511	-1.777768
41	1	0	-5.400557	1.041807	2.328169
42	6	0	0.806139	-2.815168	-0.344490
43	6	0	3.546941	-3.294771	-0.502894
44	6	0	1.384981	-3.043451	-1.599545
45	6	0	1.557761	-2.854362	0.838729
46	6	0	2.924904	-3.101960	0.730288
47	6	0	2.760359	-3.266586	-1.653436
48	1	0	3.522557	-3.132510	1.638906
49	1	0	3.227165	-3.419102	-2.623600
50	6	0	0.553448	-3.034937	-2.843177
51	1	0	-0.191026	-3.839111	-2.837344
52	1	0	1.174591	-3.170962	-3.729752
53	1	0	0.018965	-2.086411	-2.947652
54	6	0	0.923534	-2.613504	2.172710
55	1	0	0.597127	-1.573520	2.291077
56	1	0	1.619137	-2.842823	2.982007

57	1	0	0.028496	-3.226721	2.319571
58	6	0	-3.151553	0.078819	-2.464688
59	1	0	-2.486351	-0.784345	-2.490083
60	1	0	-2.567716	0.921585	-2.844161
61	1	0	-3.967869	-0.095626	-3.173255
62	6	0	-3.841553	-1.158385	2.406380
63	1	0	-2.796591	-1.467743	2.471745
64	1	0	-4.462710	-2.058719	2.320289
65	1	0	-4.101492	-0.674342	3.348942
66	6	0	5.021928	-3.546536	-0.578866
67	1	0	5.572007	-2.913981	0.123036
68	1	0	5.412424	-3.359791	-1.581085
69	1	0	5.261532	-4.584505	-0.324581
70	6	0	-6.079728	2.896742	0.468931
71	1	0	-5.615305	3.654355	1.108404
72	1	0	-7.023832	2.619515	0.946136
73	1	0	-6.311579	3.370861	-0.486561
74	17	0	0.243218	0.479744	-2.366790
75	44	0	-0.306741	0.490482	-0.016643
76	6	0	-0.877242	2.469752	0.022776
77	1	0	-1.499842	2.640616	0.897756
78	1	0	-1.318861	2.711617	-0.945445
79	6	0	1.458524	0.738856	0.546651
80	1	0	1.586555	0.898249	1.627810
81	6	0	0.549939	2.628079	0.127080
82	1	0	0.875772	2.890728	1.133853
83	17	0	-0.906453	0.564433	2.353733

Ten C

Free Energy = -2371.609275

1	6	0	2.777466	0.539617	-0.143126
2	1	0	3.077738	1.148807	-0.996495
3	1	0	2.542202	-0.427952	-0.605313
4	6	0	1.456546	3.264255	-1.002094
5	1	0	2.144373	2.651406	-1.585912
6	1	0	0.712799	3.598199	-1.728918
7	6	0	3.932897	0.302298	0.838813
8	6	0	2.167315	4.486803	-0.420972
9	6	0	3.269558	4.152907	0.577064
10	1	0	2.836938	3.545735	1.381113
11	1	0	3.613119	5.069325	1.071040
12	6	0	4.448797	1.472975	1.674245
13	1	0	5.097765	1.054866	2.452690
14	1	0	3.611810	1.917846	2.226870
15	6	0	5.243447	2.563025	0.954493
16	1	0	6.093233	2.099701	0.436423
17	1	0	5.686836	3.217469	1.716960
18	6	0	4.465172	3.425495	-0.036597
19	1	0	4.133685	2.808817	-0.876820
20	1	0	5.145121	4.161181	-0.482651
21	1	0	2.581673	5.074462	-1.250111
22	1	0	1.424208	5.134508	0.062214
23	1	0	3.604581	-0.478338	1.537846
24	1	0	4.764820	-0.145688	0.277911
25	6	0	-1.229074	-1.328263	-0.184767
26	7	0	-0.655486	-2.542329	-0.222123
27	7	0	-2.562790	-1.475511	-0.166109
28	6	0	-1.645194	-3.620831	-0.080961

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52	1	0	0.993165	-3.117603	-3.734567
53	1	0	-0.200751	-2.126052	-2.898443
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56	1	0	1.719900	-2.652582	2.948996
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58	6	0	-3.198743	0.171988	-2.458488
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64	1	0	-4.526081	-1.999270	2.395366
65	1	0	-3.959376	-0.622470	3.336657
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75	44	0	-0.233823	0.431802	-0.110771
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78	1	0	-1.046214	2.641611	-1.207228
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80	1	0	1.569056	1.031961	1.612646
81	6	0	0.768057	2.426298	0.089658
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Ten CD

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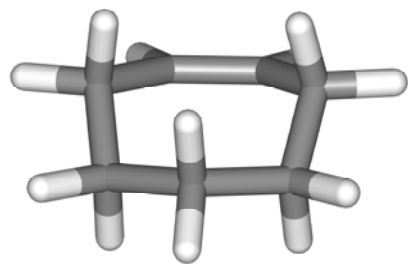
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25	6	0	1.233871	1.349214	-0.205076
26	7	0	0.633479	2.554815	-0.245157
27	7	0	2.563326	1.539163	-0.152108
28	6	0	1.582413	3.655285	-0.038099
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32	1	0	3.336178	3.163645	-1.260751
33	1	0	3.676167	3.226948	0.478089
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37	6	0	3.869755	-0.236908	-1.201202
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61	1	0	3.720247	-0.485153	-3.325347
62	6	0	3.886888	1.136035	2.372056
63	1	0	2.852382	1.484098	2.378184
64	1	0	4.549511	2.009565	2.414714
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66	6	0	-5.038447	3.141817	-0.631836
67	1	0	-5.322307	4.162961	-0.906903
68	1	0	-5.539134	2.904199	0.308946
69	1	0	-5.442471	2.483624	-1.405772
70	6	0	6.437030	-2.640299	0.255684
71	1	0	5.930359	-3.606404	0.353580
72	1	0	7.080797	-2.523888	1.129730
73	1	0	7.074905	-2.707013	-0.629182
74	44	0	0.187626	-0.389624	-0.045399
75	17	0	-0.416281	-0.492318	-2.388994
76	17	0	0.772294	-0.373240	2.323055
77	6	0	1.175662	-1.928625	-0.170112
78	1	0	1.718429	-2.350708	0.684924
79	1	0	1.313067	-2.426562	-1.137945
80	6	0	-1.639902	-1.280088	0.628309
81	1	0	-1.617886	-1.063889	1.698433
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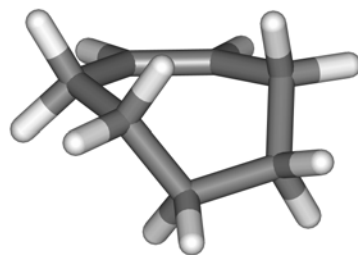
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12	6	0	-5.150233	-1.193038	1.087329
13	1	0	-5.966795	-0.727163	1.651183
14	1	0	-4.482459	-1.606721	1.854090
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17	1	0	-6.416515	-2.910330	0.901639
18	6	0	-4.770670	-3.266856	-0.430484
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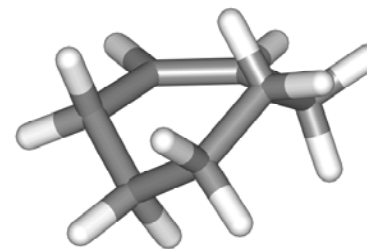
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35	6	0	5.513272	-1.958946	-0.150523
36	6	0	4.376928	-0.231061	1.139583
37	6	0	3.952173	-0.455068	-1.265105
38	6	0	4.850186	-1.521290	-1.295759
39	6	0	5.267485	-1.298552	1.053761
40	1	0	5.035694	-2.020623	-2.244136
41	1	0	5.777173	-1.628377	1.956324
42	6	0	-0.428253	2.726073	-0.269288
43	6	0	-3.153626	3.266860	-0.529296
44	6	0	-0.971284	2.916932	-1.553995
45	6	0	-1.207980	2.859603	0.888606
46	6	0	-2.574079	3.116047	0.725352
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63	1	0	3.042304	0.345266	2.716511
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72	1	0	6.528319	-3.651276	0.717656
73	1	0	7.509013	-2.719446	-0.405229
74	44	0	0.195502	-0.331470	0.136150
75	17	0	-0.366109	-0.554147	-2.203273
76	17	0	0.509573	-0.325078	2.541458
77	6	0	1.406380	-1.665910	0.013196
78	1	0	2.021399	-1.986180	0.866389
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(a)

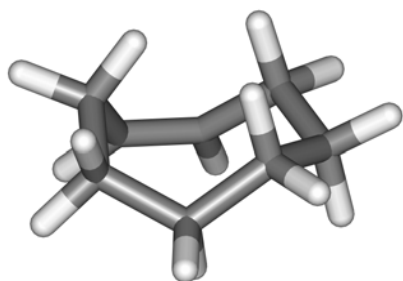


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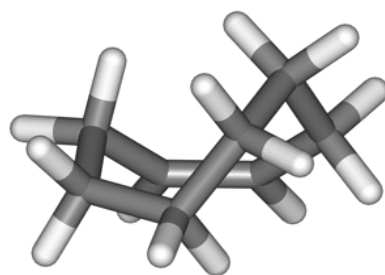


(c)

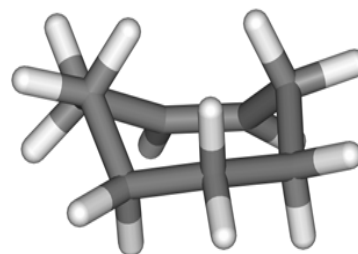
Fig. S1 Conformers found for cycloheptene: **(a)** Chair, **(b)** twist-chair and **(c)** twist-boat.



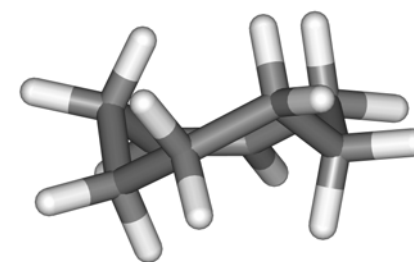
(a)



(b)



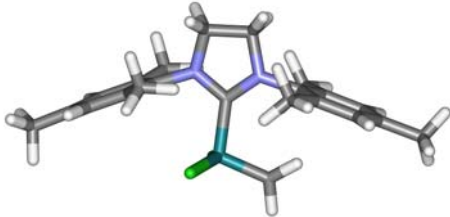
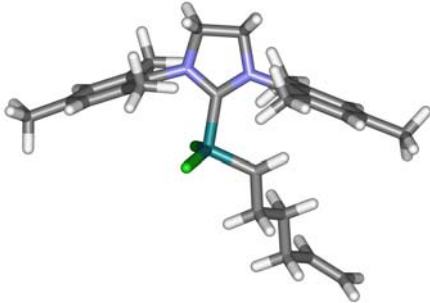
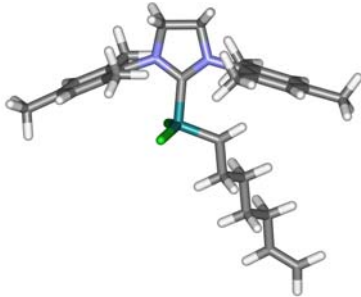
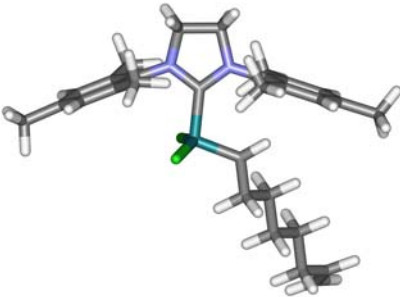
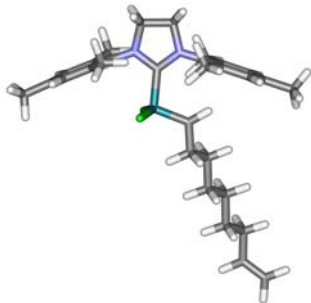
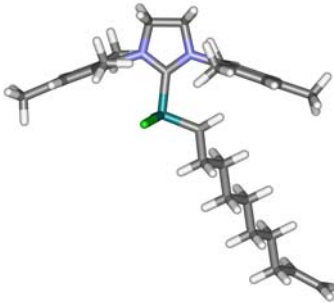
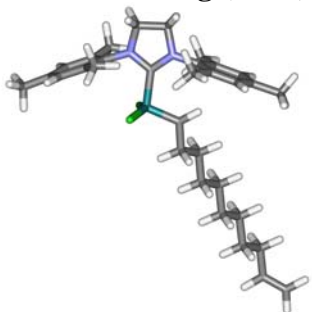
(c)



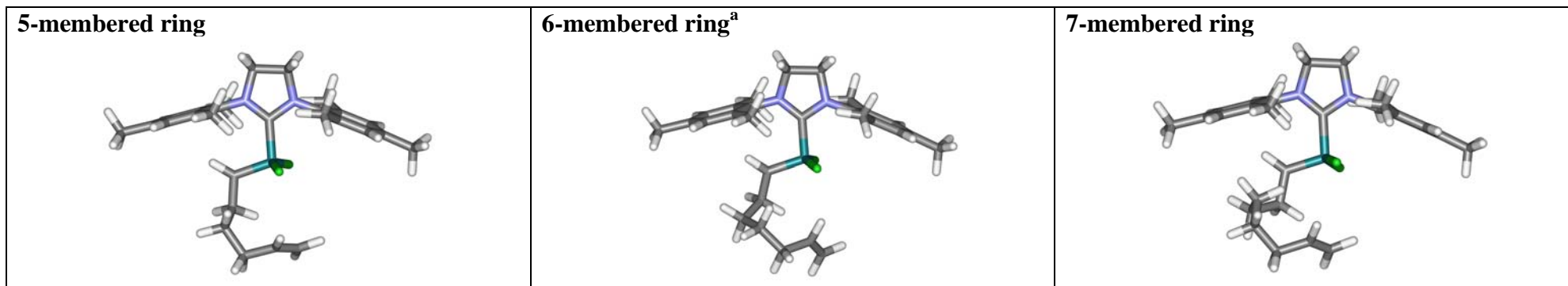
(d)

Fig. S2. Conformers found for cyclooctene; **(a)** boat-chair, **(b)** boat-boat/chair-boat, **(c)** twist-chair-chair, **(d)** chair-chair.

A-Complexes (initial 14e alkylidene complexes)

<p>Template structure (2)</p> 	<p>5-membered ring (-4.05)</p> 	<p>6-membered ring (-4.54)</p> 
<p>7-membered ring (-4.38)</p> 	<p>8-membered ring (-4.30)</p> 	<p>9-membered ring (-4.45)</p> 
<p>10-membered ring (-3.98)</p> 	<p>Individual complexes (M06L/B2 geometries)</p> <p>All energies (G_{rel}) given are free energies (kcal mol^{-1}, dichloromethane, 298K) normalised in each case to the sum of the precursor diene and methylidene complex (2) (see manuscript Table 1). Only the complexes referred to explicitly in the text, or located on the full reaction profiles based on the lowest energy conformers are included.</p>	

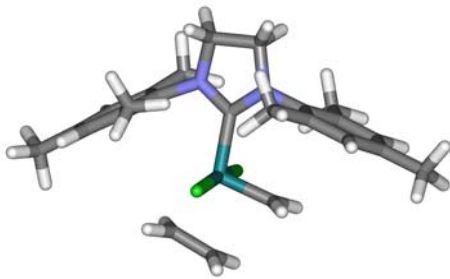
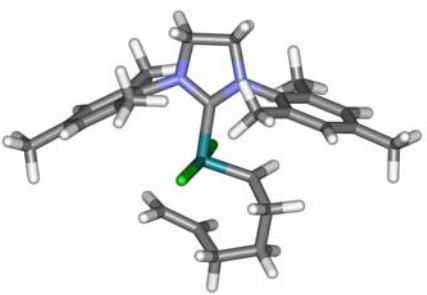
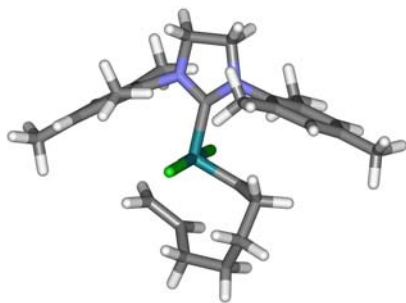
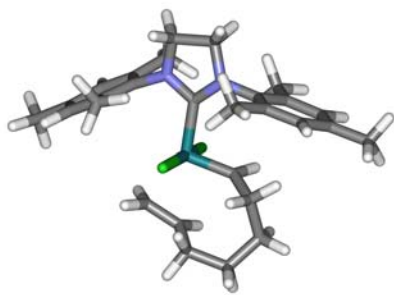
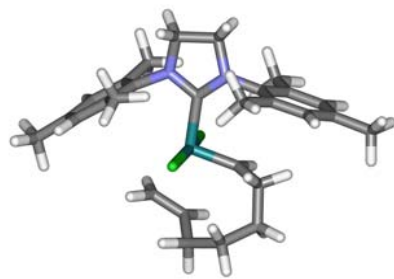
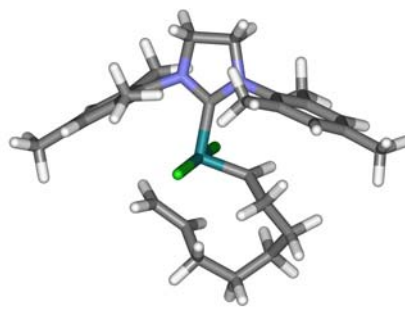
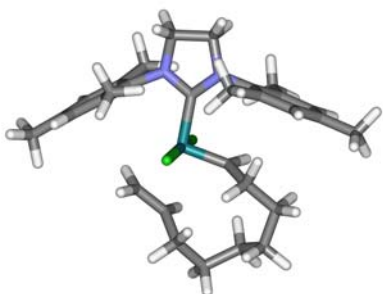
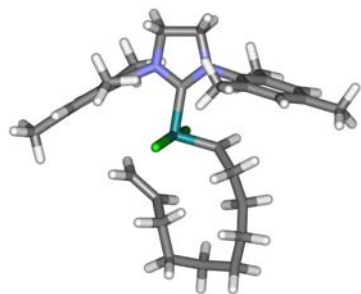
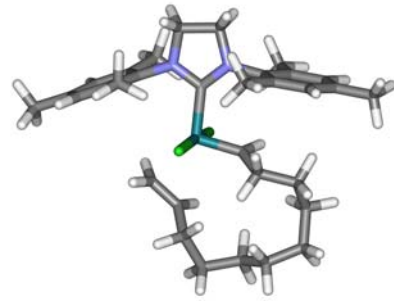
AB[‡]-Transition structures (initial cyclisation transition structures)^a



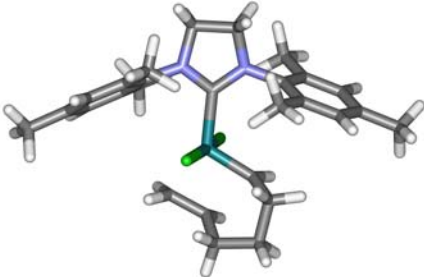
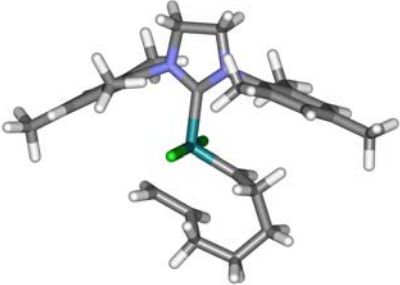
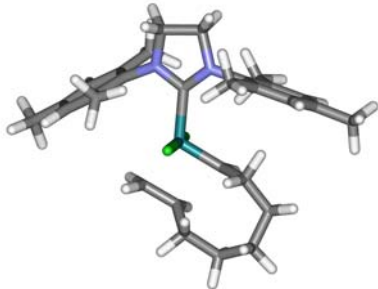
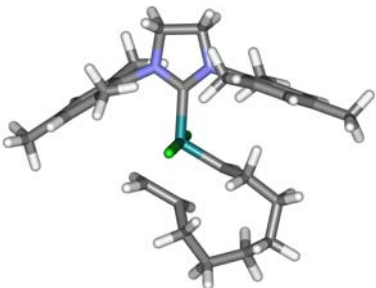
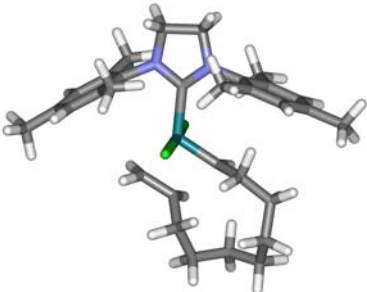
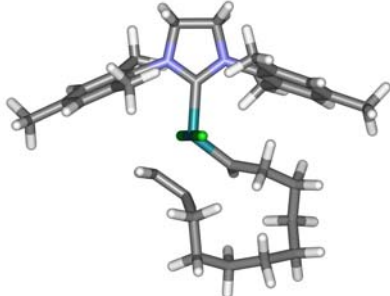
^aThe Structures are displayed in the opposite convention to the **A** complexes so that the tether can be seen more clearly.

^bThe conformation (half-chair or twisted boat) cannot be assigned.

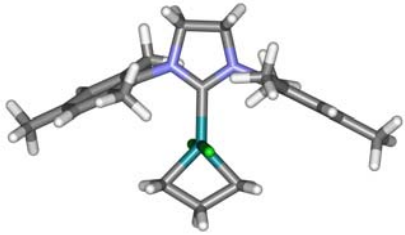
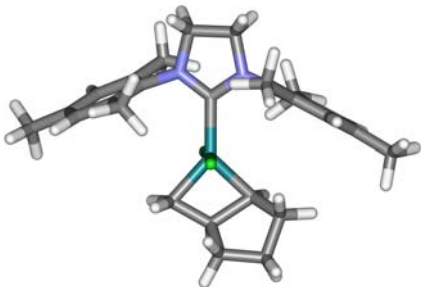
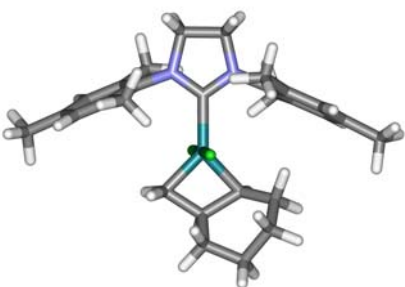
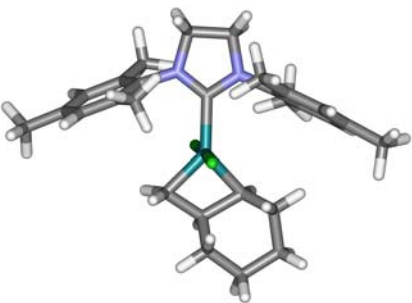
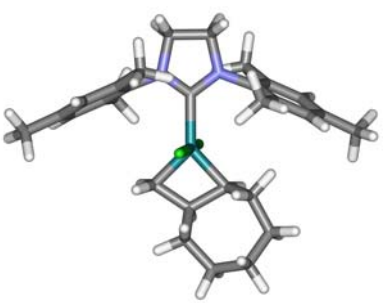
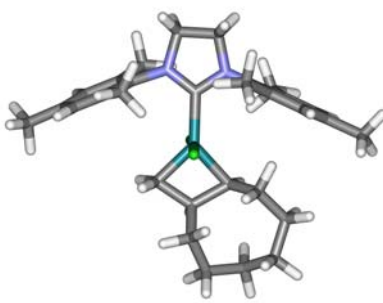
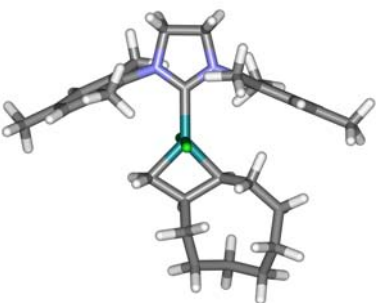
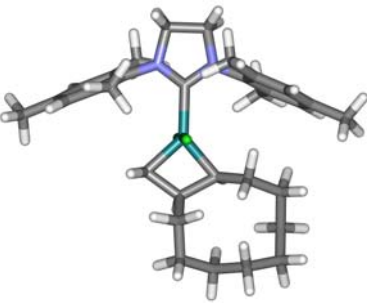
B-Complexes (initial η^2 -complexes)

Template structure 	5-membered ring (-15.53) 	6-membered ring (half-chair) (-9.1) 
6-membered ring (twisted boat) (-11.13) 	6-membered ring (alternate half-chair) (-7.51) 	7-membered ring (-12.04) 
8-membered ring (-9.45) 	9-membered ring (-5.20) 	10-membered ring (-8.42) 

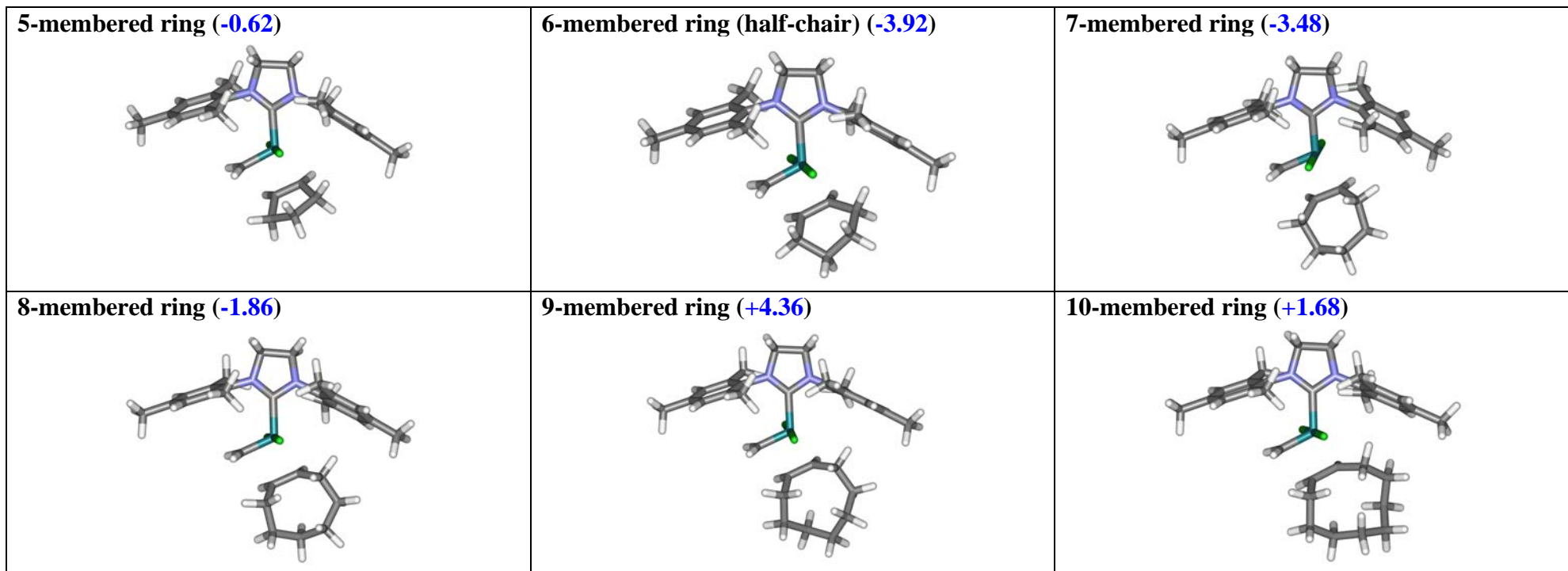
BC[‡]-Transition structures (metallocyclobutane transition structures)

<p>5-membered ring (-12.10)</p> 	<p>6-membered ring (boat) (-8.67)</p> 	<p>7-membered ring (-6.55)</p> 
<p>8-membered ring (-4.07)</p> 	<p>9-membered ring (+0.94)</p> 	<p>10-membered ring (+0.07)</p> 

C-Complex structures (metallocyclobutane structures)

<p>Template structure</p>  The template structure shows a central metal atom (green) coordinated to two nitrogen atoms (blue) of a five-membered ring. Two ethyl groups are attached to the ring. A cyclobutane ring is positioned below the metal center, with one carbon atom coordinated to the metal.	<p>5-membered ring (-14.13)</p>  The structure shows the cyclobutane ring fused to the five-membered ring, sharing two carbon atoms. The metal center is coordinated to the two nitrogen atoms and one carbon of the cyclobutane ring.	<p>6-membered ring (half-chair) (-12.65)</p>  The structure shows the cyclobutane ring fused to the five-membered ring, sharing two carbon atoms. The metal center is coordinated to the two nitrogen atoms and two carbon atoms of the cyclobutane ring, forming a six-membered ring.
<p>6-membered ring (boat) (-14.75)</p>  The structure shows the cyclobutane ring fused to the five-membered ring, sharing two carbon atoms. The metal center is coordinated to the two nitrogen atoms and two carbon atoms of the cyclobutane ring, forming a six-membered ring in a boat conformation.	<p>7-membered ring (-12.98)</p>  The structure shows the cyclobutane ring fused to the five-membered ring, sharing two carbon atoms. The metal center is coordinated to the two nitrogen atoms and three carbon atoms of the cyclobutane ring, forming a seven-membered ring.	<p>8-membered ring (-8.96)</p>  The structure shows the cyclobutane ring fused to the five-membered ring, sharing two carbon atoms. The metal center is coordinated to the two nitrogen atoms and four carbon atoms of the cyclobutane ring, forming an eight-membered ring.
<p>9-membered ring (-5.3)</p>  The structure shows the cyclobutane ring fused to the five-membered ring, sharing two carbon atoms. The metal center is coordinated to the two nitrogen atoms and five carbon atoms of the cyclobutane ring, forming a nine-membered ring.	<p>10-membered ring (-4.14)</p>  The structure shows the cyclobutane ring fused to the five-membered ring, sharing two carbon atoms. The metal center is coordinated to the two nitrogen atoms and six carbon atoms of the cyclobutane ring, forming a ten-membered ring.	

CD[‡]-Transition structures (metallocyclobutane transition structures)



D-Complex structures (product η^2 -complexes)

