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Supporting Information

Insights into the mechanism and regioselectivity in Ni-catalysed redox-relay migratory hydroarylation of alkenes with arylborons

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Computational Details

All of the calculations were performed with Gaussian 09 package. The B3LYP functional with a mixed basis set of SDD for Ni and 6-31G(d,p) for other atoms was used for geometry optimizations and frequency calculations. Frequency outcomes were scrutinized to confirm stationary points as minima (no imaginary frequencies) or transition states (one imaginary frequency). Because M06-L functional can give refined energies for transition-metal systems,[1] single-point energies were calculated using M06-L functional with a mixed basis set of SDD for Ni and 6-311++G(2d,p) for other atoms. The solvation effects were considered using the SMD model with Toluene (ε = 2.3741) as the solvent.

It should be emphasized that the thermal corrections based on the ideal gas phase model inevitably overestimate entropy contributions to free energies for reactions in solvent, in particular for reactions involving multicomponent change due to ignoring the suppressing effect of solvent on the rotational and transitional freedoms of substrates. Since no standard quantum mechanics-based approach is available to accurately calculate entropy in solution, we adopted the approximate approach proposed by Martin et al.[2] According to their approach, a correction of 4.3 kcal/mol applies to per component change for a reaction at 298.15 K and 1 atm (i.e., a reaction from m- to n-components has an additional correction of (n – m) × 4.3 kcal/mol). This approach has been validated through a number of computational and experimental studies of transition metal-catalyzed reactions by Yu group,[3] Wang group[4] and Hong group.[5] In this paper, we discuss the mechanism in terms of the corrected free energies in the relevant figures.

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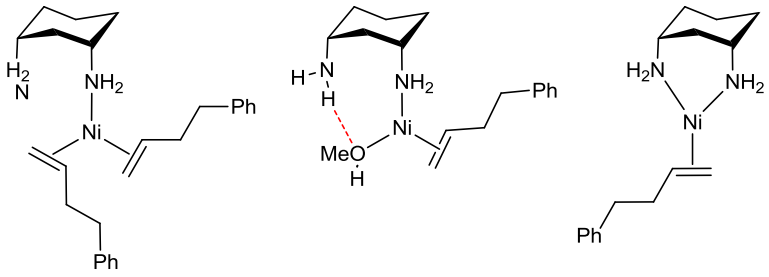

Fig. S1 Possible complexes generated by initiation [Values are free energies in kcal/mol relative to **IM1**].

Energies and Cartesian Coordinates (Å) for the Optimized Structures

IM1 (SCF energy in toluene: -1294.338972 a.u; Free energy in toluene: -1293.813811 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.118292	-0.995191	-0.720783
2	6	0	2.967503	6.154496	1.326962
3	6	0	1.628970	5.981402	0.968073
4	6	0	1.267606	4.972489	0.074641
5	6	0	2.231378	4.116225	-0.478222
6	6	0	3.570953	4.303408	-0.109104
7	6	0	3.938542	5.311405	0.783951
8	1	0	3.251251	6.942253	2.019144
9	1	0	0.865883	6.636236	1.380219
10	1	0	0.223604	4.848398	-0.204350
11	1	0	4.334770	3.655414	-0.533765
12	1	0	4.983944	5.441842	1.051032
13	6	0	1.828762	2.994755	-1.409449
14	1	0	1.001864	3.316132	-2.053538
15	1	0	2.665365	2.745929	-2.074361
16	6	0	1.389489	1.709682	-0.658266
17	1	0	0.533632	1.953997	-0.016411
18	1	0	2.209680	1.422130	0.016596
19	6	0	1.028539	0.570249	-1.591013
20	6	0	-0.270268	0.392738	-2.094464
21	1	0	1.862454	0.199710	-2.193787
22	1	0	-0.430903	-0.083587	-3.060166
23	1	0	-1.072143	1.058901	-1.778513
24	6	0	-7.396814	1.154646	1.030279
25	6	0	-6.651224	0.424052	1.957472
26	6	0	-5.646499	-0.441426	1.522517
27	6	0	-5.365155	-0.595904	0.157520
28	6	0	-6.123289	0.143780	-0.761430
29	6	0	-7.129122	1.010913	-0.332494
30	1	0	-8.181825	1.826338	1.366185
31	1	0	-6.855077	0.524365	3.020273
32	1	0	-5.073539	-1.011564	2.250549
33	1	0	-5.924817	0.033207	-1.825242
34	1	0	-7.707161	1.570869	-1.062845
35	6	0	-4.246577	-1.501724	-0.307447
36	1	0	-4.137825	-2.347406	0.381655
37	1	0	-4.497440	-1.926218	-1.287896

38	6	0	-2.881966	-0.771437	-0.415268
39	1	0	-2.621923	-0.363263	0.569601
40	1	0	-3.003983	0.087493	-1.085947
41	6	0	-1.776177	-1.682254	-0.907640
42	6	0	-1.016675	-2.476500	-0.035205
43	1	0	-1.906362	-2.031825	-1.933578
44	1	0	-0.597885	-3.424867	-0.370664
45	1	0	-1.166074	-2.396519	1.043123
46	6	0	3.056728	-1.713028	-0.087174
47	6	0	3.013041	-2.788972	-1.185214
48	6	0	4.087195	-2.089225	1.001967
49	6	0	2.795794	-4.202584	-0.625382
50	1	0	3.969487	-2.760196	-1.725328
51	1	0	2.226806	-2.530974	-1.902217
52	6	0	3.906342	-3.510070	1.574024
53	1	0	5.092360	-2.023343	0.566110
54	1	0	4.059105	-1.351709	1.816498
55	6	0	3.849772	-4.546473	0.437957
56	1	0	2.838858	-4.933946	-1.440455
57	1	0	1.792628	-4.280152	-0.191912
58	1	0	3.664908	-5.543987	0.858494
59	1	0	4.842027	-4.590259	-0.030576
60	1	0	4.789179	-3.737948	2.195503
61	1	0	3.364787	-0.768117	-0.546047
62	7	0	1.696226	-1.475963	0.475450
63	1	0	1.473768	-2.276157	1.072416
64	1	0	1.755019	-0.679237	1.110636
65	7	0	2.657417	-3.571969	2.363283
66	1	0	2.496372	-4.524353	2.684167
67	1	0	2.750438	-3.000567	3.200632

IM2 (SCF energy in toluene: -1021.730212 a.u; Free energy in toluene: -1021.334793 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.998354	-1.455364	-0.283922
2	6	0	0.805934	-1.698387	-0.815481
3	6	0	0.349587	-2.788710	0.026947
4	1	0	0.761900	-2.864598	1.039362
5	1	0	0.184231	-3.768633	-0.431580
6	6	0	-3.586921	1.661810	1.256928
7	6	0	-4.067823	2.899386	0.475999
8	6	0	-2.057112	1.514398	1.143457

9	6	0	-3.590919	2.893721	-0.984445
10	1	0	-3.684824	3.794712	0.983992
11	1	0	-5.163105	2.963857	0.520671
12	6	0	-1.538330	1.509285	-0.305794
13	1	0	-1.594589	2.357693	1.670728
14	1	0	-1.723584	0.600719	1.649451
15	6	0	-2.064111	2.741110	-1.071371
16	1	0	-3.901188	3.819034	-1.483321
17	1	0	-4.080701	2.072799	-1.520775
18	1	0	-1.740791	2.692373	-2.119672
19	1	0	-1.586726	3.634419	-0.645205
20	1	0	-0.444598	1.549521	-0.281635
21	1	0	-3.827311	1.818988	2.322592
22	7	0	-4.245038	0.451036	0.724532
23	1	0	-3.905468	-0.374396	1.216424
24	1	0	-5.249241	0.506575	0.879068
25	7	0	-1.893338	0.218938	-0.967096
26	1	0	-2.909604	0.108218	-0.892008
27	1	0	-1.653262	0.274953	-1.955884
28	8	0	-2.697565	-2.291685	0.843389
29	6	0	-3.577618	-3.133182	0.084448
30	1	0	-4.310122	-2.477333	-0.390571
31	1	0	-3.033707	-3.681526	-0.691388
32	1	0	-4.101916	-3.839239	0.739893
33	6	0	1.861527	-0.711619	-0.346222
34	1	0	1.745013	0.252429	-0.862869
35	1	0	1.737083	-0.503728	0.724513
36	6	0	3.310765	-1.212641	-0.586670
37	1	0	3.441023	-2.160632	-0.051341
38	1	0	3.430472	-1.436362	-1.654424
39	6	0	4.366821	-0.221975	-0.152376
40	6	0	4.846316	-0.209422	1.165720
41	6	0	4.865534	0.739025	-1.044042
42	6	0	5.791006	0.730200	1.580578
43	1	0	4.477028	-0.950442	1.871257
44	6	0	5.810355	1.681394	-0.635245
45	1	0	4.512079	0.742038	-2.072938
46	6	0	6.277159	1.680840	0.680605
47	1	0	6.151840	0.716925	2.605749
48	1	0	6.186322	2.412798	-1.345986
49	1	0	7.015808	2.410681	1.000184
50	1	0	0.884550	-1.911853	-1.889161
51	1	0	-1.926566	-2.817547	1.127316

TS1 (SCF energy in toluene: -1544.627881 a.u; Free energy in toluene: -1544.087746 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.593404	0.292331	0.362129
2	6	0	2.233607	-0.165091	1.150412
3	6	0	1.205438	-1.072298	1.689381
4	1	0	1.021933	-0.986491	2.765573
5	1	0	1.293168	-2.122874	1.390191
6	6	0	-0.700250	4.268385	0.393107
7	6	0	-0.425128	5.311954	-0.705066
8	6	0	0.613914	3.611293	0.864002
9	6	0	0.422381	4.762864	-1.861569
10	1	0	0.102920	6.157272	-0.243835
11	1	0	-1.375571	5.712875	-1.080985
12	6	0	1.512929	3.080838	-0.268352
13	1	0	1.187418	4.366535	1.416242
14	1	0	0.397400	2.797682	1.565477
15	6	0	1.739429	4.164015	-1.341727
16	1	0	0.637020	5.561434	-2.580585
17	1	0	-0.148057	4.004708	-2.412284
18	1	0	2.332101	3.752349	-2.169187
19	1	0	2.346617	4.963928	-0.896542
20	1	0	2.477327	2.797978	0.165711
21	1	0	-1.122865	4.805142	1.258368
22	7	0	-1.647790	3.236877	-0.088357
23	1	0	-1.987857	2.692278	0.711431
24	1	0	-2.466354	3.695031	-0.485756
25	7	0	0.950013	1.825762	-0.849379
26	1	0	0.059806	2.059574	-1.290688
27	1	0	1.572723	1.497030	-1.587529
28	5	0	-2.324250	-0.167879	0.842258
29	8	0	-1.343720	0.272827	-0.189407
30	1	0	-1.573940	1.180019	-0.453670
31	8	0	-1.480515	-1.271341	1.537771
32	6	0	-3.678413	-0.820042	0.251323
33	6	0	-3.738599	-2.147898	-0.197677
34	6	0	-4.860706	-0.066629	0.113120
35	6	0	-4.895712	-2.708544	-0.747948
36	1	0	-2.851235	-2.770828	-0.114756
37	6	0	-6.027008	-0.595503	-0.430817
38	1	0	-4.870430	0.974362	0.433781
39	6	0	-6.050669	-1.926909	-0.865974

40	1	0	-4.885441	-3.741674	-1.077302
41	1	0	-6.930367	-0.001255	-0.531416
42	8	0	-2.549264	0.960042	1.740198
43	1	0	-3.415778	0.898466	2.155641
44	6	0	-1.884612	-1.714312	2.831024
45	1	0	-1.173236	-2.468521	3.176379
46	1	0	-1.916184	-0.881220	3.541372
47	1	0	-2.877838	-2.166961	2.755153
48	8	0	-7.240615	-2.364204	-1.385524
49	6	0	-7.312955	-3.699226	-1.852129
50	1	0	-7.123985	-4.423695	-1.048580
51	1	0	-8.330133	-3.836389	-2.224018
52	1	0	-6.603513	-3.884972	-2.669598
53	1	0	-0.313013	-0.994001	1.449187
54	6	0	3.341773	-0.707352	0.261361
55	1	0	3.779683	0.102853	-0.340673
56	1	0	2.932125	-1.433598	-0.453130
57	6	0	4.489078	-1.388824	1.053528
58	1	0	4.896360	-0.666786	1.772712
59	1	0	4.062594	-2.209984	1.642187
60	6	0	5.598969	-1.910943	0.169428
61	6	0	5.516732	-3.185283	-0.410866
62	6	0	6.719586	-1.121777	-0.126365
63	6	0	6.519358	-3.656405	-1.259146
64	1	0	4.658217	-3.815383	-0.189092
65	6	0	7.726001	-1.587779	-0.973917
66	1	0	6.805791	-0.133262	0.319724
67	6	0	7.629151	-2.858230	-1.544441
68	1	0	6.436878	-4.649221	-1.693415
69	1	0	8.588459	-0.960757	-1.184196
70	1	0	8.413042	-3.224892	-2.201150
71	1	0	2.601740	0.592481	1.854074

TS1a (SCF energy in toluene: -633.33712 a.u; Free energy in toluene: -633.121076 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.548839	1.111675	-1.020353
2	6	0	-1.856254	1.743002	0.349338
3	6	0	-2.131919	-0.313083	-1.111963
4	6	0	-1.425522	0.852832	1.523043
5	1	0	-2.937893	1.926608	0.402972
6	1	0	-1.374451	2.727298	0.413781

7	6	0	-1.796644	-1.234084	0.076653
8	1	0	-3.224362	-0.228218	-1.166346
9	1	0	-1.814683	-0.786914	-2.050671
10	6	0	-2.069826	-0.535960	1.419626
11	1	0	-1.708545	1.322380	2.472090
12	1	0	-0.333244	0.745065	1.525705
13	1	0	-1.735202	-1.179431	2.243182
14	1	0	-3.159110	-0.441130	1.525655
15	1	0	-2.462296	-2.108316	0.012946
16	1	0	-2.047365	1.722331	-1.791883
17	7	0	-0.091379	1.065285	-1.236530
18	1	0	0.330750	1.979259	-1.087372
19	1	0	0.124803	0.797639	-2.194734
20	7	0	-0.388184	-1.722889	0.007212
21	1	0	-0.181481	-2.293073	0.826408
22	1	0	-0.281602	-2.347583	-0.795183
23	28	0	1.146488	-0.555774	-0.185590
24	8	0	2.925343	0.097720	-0.270773
25	1	0	2.619625	-0.997088	0.145098
26	6	0	3.399577	0.903618	0.800641
27	1	0	4.459248	1.134731	0.627205
28	1	0	2.848886	1.851656	0.869383
29	1	0	3.306009	0.389947	1.767794

TS1b (SCF energy in toluene: -1021.700706 a.u; Free energy in toluene: -1021.307407 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-1.018070	-0.170181	-0.263213
2	6	0	0.631651	-0.771006	0.599423
3	6	0	-0.000880	-1.830833	-0.120691
4	1	0	0.485249	-0.749637	1.686444
5	1	0	-0.541789	-2.616311	0.412299
6	1	0	0.445812	-2.173070	-1.055339
7	6	0	1.977207	-0.208379	0.181608
8	1	0	2.072259	0.840976	0.487585
9	1	0	2.061121	-0.222332	-0.911679
10	6	0	3.164305	-1.003721	0.785391
11	1	0	3.079371	-0.990545	1.879792
12	1	0	3.072014	-2.052037	0.476557
13	6	0	4.514925	-0.462039	0.373653
14	6	0	5.165800	0.516005	1.139026
15	6	0	5.133476	-0.896360	-0.807641

16	6	0	6.393792	1.044893	0.738543
17	1	0	4.705441	0.862007	2.061945
18	6	0	6.361129	-0.371376	-1.213185
19	1	0	4.647078	-1.658901	-1.412055
20	6	0	6.996542	0.602820	-0.440556
21	1	0	6.882066	1.799212	1.349887
22	1	0	6.823912	-0.726176	-2.130293
23	1	0	7.954015	1.010605	-0.752332
24	6	0	-4.719201	0.752396	-1.064543
25	6	0	-4.305222	1.480972	0.221108
26	6	0	-4.558600	0.589127	1.443248
27	6	0	-3.847461	-0.770666	1.348603
28	6	0	-4.176808	-1.482000	0.020288
29	6	0	-4.028981	-0.611308	-1.243789
30	1	0	-4.253238	1.096807	2.368027
31	1	0	-3.248225	1.761179	0.154986
32	1	0	-4.882652	2.408066	0.316547
33	1	0	-5.803008	0.571272	-1.049736
34	1	0	-4.523531	1.379529	-1.943348
35	1	0	-4.231863	-1.404109	2.163660
36	1	0	-3.562977	-2.386157	-0.078723
37	1	0	-5.219921	-1.819035	0.072554
38	1	0	-4.546825	-1.135049	-2.061408
39	1	0	-5.635794	0.396490	1.542203
40	7	0	-2.597415	-0.444679	-1.622310
41	1	0	-2.290202	-1.255712	-2.152676
42	1	0	-2.495562	0.364747	-2.232818
43	7	0	-2.380909	-0.600861	1.495044
44	1	0	-2.183173	0.081210	2.224759
45	1	0	-1.968511	-1.477524	1.806041
46	8	0	-1.160007	1.799628	-0.673758
47	1	0	-0.358193	0.740314	-1.182834
48	6	0	-0.307319	2.746477	-0.072363
49	1	0	-0.698066	3.757242	-0.265176
50	1	0	-0.234588	2.621660	1.020905
51	1	0	0.717930	2.712090	-0.473647

TS1c (SCF energy in toluene: -1021.70899 a.u; Free energy in toluene: -1021.31457 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	1.057104	1.316539	-0.395797
2	6	0	-0.743328	1.598315	-0.893142

3	6	0	-0.301775	2.681419	0.028728
4	1	0	-0.797312	2.699903	1.004859
5	1	0	-0.234071	3.682838	-0.405506
6	6	0	3.488195	-1.437367	1.323354
7	6	0	4.158893	-2.667873	0.682520
8	6	0	1.969408	-1.470384	1.063354
9	6	0	3.841327	-2.791814	-0.815905
10	1	0	3.808874	-3.565946	1.209470
11	1	0	5.244792	-2.621678	0.836660
12	6	0	1.609491	-1.574847	-0.429474
13	1	0	1.549134	-2.343018	1.578008
14	1	0	1.493363	-0.583336	1.496734
15	6	0	2.324895	-2.778920	-1.074888
16	1	0	4.273874	-3.715754	-1.216636
17	1	0	4.321141	-1.966863	-1.354574
18	1	0	2.117797	-2.802170	-2.153265
19	1	0	1.878921	-3.692433	-0.658406
20	1	0	0.527044	-1.712734	-0.521930
21	1	0	3.638467	-1.497016	2.415130
22	7	0	4.058035	-0.203577	0.753725
23	1	0	3.565709	0.623711	1.106514
24	1	0	5.038696	-0.118301	1.008716
25	7	0	1.926256	-0.283365	-1.117377
26	1	0	2.931605	-0.111827	-0.978340
27	1	0	1.743645	-0.379267	-2.115170
28	8	0	2.320099	2.289922	0.893493
29	1	0	1.036330	2.603265	0.559575
30	6	0	3.208873	3.237544	0.337013
31	1	0	4.036340	2.749502	-0.204137
32	1	0	2.710794	3.917064	-0.374492
33	1	0	3.651108	3.860651	1.129214
34	6	0	-1.820231	0.622681	-0.449365
35	1	0	-1.760253	-0.298044	-1.046320
36	1	0	-1.655551	0.323882	0.594205
37	6	0	-3.260290	1.187120	-0.576454
38	1	0	-3.328021	2.106356	0.017759
39	1	0	-3.433960	1.474992	-1.621013
40	6	0	-4.322136	0.206997	-0.130517
41	6	0	-4.727114	0.146357	1.210826
42	6	0	-4.898117	-0.695252	-1.036293
43	6	0	-5.675358	-0.785234	1.635429
44	1	0	-4.297117	0.842354	1.927802
45	6	0	-5.847160	-1.629028	-0.617474
46	1	0	-4.603133	-0.659453	-2.082803

47	6	0	-6.239129	-1.677866	0.721639
48	1	0	-5.977857	-0.810632	2.678920
49	1	0	-6.284575	-2.315037	-1.338011
50	1	0	-6.980457	-2.401322	1.049090
51	1	0	-0.863736	1.905346	-1.938217

TS1d (SCF energy in toluene: -1544.625592 a.u; Free energy in toluene: -1544.08528 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.524934	-1.571045	0.021455
2	6	0	-0.511852	-3.035153	0.560102
3	6	0	-1.197400	-1.822512	1.025801
4	1	0	-1.256090	-1.749897	2.121023
5	6	0	4.761736	-1.509511	0.413820
6	6	0	5.739225	-2.121676	-0.606792
7	6	0	3.694095	-2.538481	0.839680
8	6	0	5.036679	-2.795983	-1.794304
9	1	0	6.348524	-2.869028	-0.081070
10	1	0	6.436794	-1.350554	-0.959288
11	6	0	2.989540	-3.250577	-0.329317
12	1	0	4.188586	-3.307630	1.446316
13	1	0	2.945983	-2.057611	1.479640
14	6	0	4.021334	-3.843173	-1.308863
15	1	0	5.778264	-3.271107	-2.446298
16	1	0	4.535550	-2.036601	-2.407605
17	1	0	3.505222	-4.306779	-2.159932
18	1	0	4.556488	-4.652979	-0.794506
19	1	0	2.373935	-4.057779	0.079289
20	1	0	5.345676	-1.255209	1.313876
21	7	0	4.105939	-0.299867	-0.135381
22	1	0	3.627503	0.185855	0.630918
23	1	0	4.819329	0.340511	-0.480105
24	7	0	2.040937	-2.325341	-1.017677
25	1	0	2.586293	-1.543005	-1.383273
26	1	0	1.629504	-2.809853	-1.815283
27	5	0	0.976971	1.276825	0.783705
28	8	0	1.136842	0.312180	-0.340569
29	1	0	2.075698	0.284049	-0.585385
30	8	0	-0.364137	0.746603	1.372083
31	6	0	0.785933	2.817988	0.343288
32	6	0	-0.438520	3.314836	-0.128606
33	6	0	1.853988	3.736002	0.376288

34	6	0	-0.608517	4.640200	-0.540494
35	1	0	-1.294319	2.645814	-0.174554
36	6	0	1.716257	5.060546	-0.026884
37	1	0	2.832857	3.405419	0.721844
38	6	0	0.477023	5.522295	-0.489081
39	1	0	-1.578994	4.969847	-0.894406
40	1	0	2.549627	5.756076	0.004927
41	8	0	2.079057	1.055894	1.712362
42	1	0	2.257912	1.851621	2.224518
43	6	0	-0.706167	1.100632	2.710235
44	1	0	-1.664329	0.637065	2.956732
45	1	0	0.061582	0.766219	3.415539
46	1	0	-0.809694	2.188267	2.770203
47	8	0	0.431323	6.839631	-0.861552
48	6	0	-0.796998	7.352662	-1.345339
49	1	0	-1.591558	7.290679	-0.589669
50	1	0	-0.614264	8.401770	-1.585538
51	1	0	-1.129293	6.828952	-2.251516
52	1	0	-0.493309	-0.410395	1.102307
53	1	0	-0.066112	-3.693300	1.310878
54	6	0	-2.522335	-1.437489	0.361824
55	1	0	-2.750938	-0.377277	0.532573
56	1	0	-2.427984	-1.551787	-0.725510
57	6	0	-3.718445	-2.288252	0.851682
58	1	0	-3.483540	-3.346812	0.688277
59	1	0	-3.828042	-2.156054	1.936108
60	1	0	-0.975258	-3.595773	-0.258847
61	6	0	-5.017480	-1.937128	0.160737
62	6	0	-5.878367	-0.963931	0.687468
63	6	0	-5.374331	-2.548907	-1.049723
64	6	0	-7.056278	-0.610454	0.027332
65	1	0	-5.623172	-0.481722	1.628639
66	6	0	-6.550397	-2.199693	-1.714505
67	1	0	-4.722911	-3.311195	-1.471569
68	6	0	-7.396731	-1.227345	-1.177841
69	1	0	-7.710393	0.143881	0.456577
70	1	0	-6.808407	-2.690016	-2.649467
71	1	0	-8.314510	-0.955915	-1.691869

IM3 (SCF energy in toluene: -1544.663468 a.u; Free energy in toluene: -1544.11863 a.u.)

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

1	28	0	0.338226	0.971493	-0.021015
2	6	0	2.182338	1.044547	0.568843
3	6	0	2.332808	1.435190	2.044247
4	1	0	3.384997	1.511319	2.357980
5	1	0	1.855590	0.707449	2.709217
6	6	0	-1.804764	4.485281	0.459888
7	6	0	-1.796441	5.654300	-0.542612
8	6	0	-0.369920	4.108598	0.882139
9	6	0	-0.842313	5.433600	-1.724765
10	1	0	-1.492086	6.560869	-0.002519
11	1	0	-2.816963	5.839792	-0.901845
12	6	0	0.636787	3.935189	-0.271790
13	1	0	0.012241	4.913836	1.522190
14	1	0	-0.389357	3.200564	1.494395
15	6	0	0.583504	5.138608	-1.232417
16	1	0	-0.834115	6.319731	-2.369166
17	1	0	-1.209638	4.609383	-2.349033
18	1	0	1.261992	4.972822	-2.079505
19	1	0	0.968607	6.017015	-0.697559
20	1	0	1.638895	3.863051	0.160859
21	1	0	-2.323350	4.835655	1.367625
22	7	0	-2.496063	3.307168	-0.108353
23	1	0	-2.633457	2.611761	0.632717
24	1	0	-3.426925	3.583389	-0.416556
25	7	0	0.425684	2.646880	-1.003728
26	1	0	-0.486080	2.685187	-1.462119
27	1	0	1.128967	2.569714	-1.739401
28	5	0	-1.841692	-0.245001	0.488948
29	8	0	-1.490122	0.581155	-0.725858
30	1	0	-2.037559	1.383741	-0.750825
31	8	0	-0.388212	-0.588033	0.882573
32	6	0	-2.701782	-1.573481	0.188686
33	6	0	-4.097829	-1.591137	0.313602
34	6	0	-2.103850	-2.768162	-0.261665
35	6	0	-4.874499	-2.717951	0.018132
36	1	0	-4.615144	-0.690191	0.641865
37	6	0	-2.847471	-3.903604	-0.560800
38	1	0	-1.023406	-2.801921	-0.377789
39	6	0	-4.242952	-3.885065	-0.421964
40	1	0	-5.952074	-2.672568	0.130713
41	1	0	-2.375057	-4.818863	-0.905153
42	8	0	-2.454939	0.667606	1.450160
43	1	0	-3.065281	0.196805	2.026374
44	6	0	-0.173532	-1.101304	2.186300

45	1	0	-0.416257	-0.359251	2.956583
46	1	0	-0.805205	-1.985673	2.332539
47	1	0	0.871957	-1.400028	2.288482
48	8	0	-4.889989	-5.050646	-0.740126
49	6	0	-6.300626	-5.079184	-0.630068
50	1	0	-6.776924	-4.343116	-1.291811
51	1	0	-6.609364	-6.082136	-0.931169
52	1	0	-6.634295	-4.895415	0.400302
53	6	0	2.852912	-0.292257	0.210874
54	1	0	2.616774	-0.561304	-0.827442
55	1	0	2.443739	-1.103472	0.825651
56	6	0	4.398865	-0.302840	0.357297
57	1	0	4.816062	0.505066	-0.258272
58	1	0	4.669895	-0.077667	1.395013
59	6	0	5.016778	-1.622237	-0.048488
60	6	0	5.204366	-2.648990	0.887982
61	6	0	5.378947	-1.869068	-1.380562
62	6	0	5.733962	-3.882886	0.507652
63	1	0	4.935193	-2.475735	1.927675
64	6	0	5.909231	-3.100666	-1.766854
65	1	0	5.247068	-1.083458	-2.121502
66	6	0	6.088320	-4.113733	-0.822913
67	1	0	5.873473	-4.662959	1.251351
68	1	0	6.186264	-3.268010	-2.804313
69	1	0	6.503146	-5.072577	-1.120688
70	1	0	2.673098	1.825865	-0.038095
71	1	0	1.874446	2.409054	2.253027

TS2 (SCF energy in toluene: -1544.643897 a.u; Free energy in toluene: -1544.098301 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	1.038141	-0.061273	-0.233276
2	6	0	-0.089815	-1.397549	0.646819
3	6	0	0.055971	-1.360535	2.175348
4	1	0	-0.431272	-2.214935	2.669693
5	1	0	-0.390602	-0.451851	2.591493
6	6	0	5.114449	-0.448233	0.777938
7	6	0	6.096566	-1.365139	0.026664
8	6	0	3.876025	-1.227685	1.263967
9	6	0	5.427760	-2.228652	-1.051654
10	1	0	6.568535	-2.026365	0.765624
11	1	0	6.906655	-0.763982	-0.406477

12	6	0	3.220964	-2.167091	0.231999
13	1	0	4.191239	-1.855510	2.107049
14	1	0	3.128004	-0.528893	1.652032
15	6	0	4.278113	-3.055012	-0.453055
16	1	0	6.167474	-2.896055	-1.507595
17	1	0	5.058517	-1.589026	-1.864110
18	1	0	3.802738	-3.676585	-1.222834
19	1	0	4.685950	-3.747358	0.295505
20	1	0	2.510598	-2.800987	0.770866
21	1	0	5.635556	-0.081733	1.676811
22	7	0	4.698099	0.701258	-0.060882
23	1	0	4.226907	1.382788	0.541991
24	1	0	5.524500	1.166007	-0.433591
25	7	0	2.397410	-1.429930	-0.773353
26	1	0	3.018772	-0.931862	-1.409595
27	1	0	1.899954	-2.117092	-1.340420
28	5	0	1.678405	2.333297	-0.223431
29	8	0	2.156770	1.332241	-1.161928
30	1	0	3.098199	1.110727	-0.967151
31	6	0	-0.170909	1.512301	0.112860
32	6	0	-0.600650	1.937802	1.395172
33	6	0	-1.114980	1.686869	-0.924850
34	6	0	-1.853217	2.485707	1.627490
35	1	0	0.088802	1.849473	2.231072
36	6	0	-2.389260	2.225702	-0.722823
37	1	0	-0.859865	1.371897	-1.935113
38	6	0	-2.763668	2.624742	0.565890
39	1	0	-2.161705	2.811710	2.616673
40	1	0	-3.074166	2.320046	-1.558111
41	8	0	2.388929	2.313834	1.012077
42	1	0	2.320358	3.187861	1.414970
43	8	0	-3.974912	3.160922	0.891651
44	6	0	-4.957003	3.269511	-0.126694
45	1	0	-5.212412	2.288557	-0.547094
46	1	0	-5.840113	3.697967	0.350507
47	1	0	-4.629445	3.932811	-0.937714
48	6	0	-1.559927	-1.380032	0.198785
49	1	0	-1.617880	-1.288440	-0.893769
50	1	0	-2.064157	-0.494265	0.600306
51	6	0	-2.378144	-2.634867	0.606250
52	1	0	-1.882918	-3.531195	0.209371
53	1	0	-2.377365	-2.734718	1.697839
54	6	0	-3.806138	-2.585176	0.110755
55	6	0	-4.795379	-1.903770	0.835930

56	6	0	-4.172649	-3.179121	-1.105234
57	6	0	-6.105337	-1.818396	0.363218
58	1	0	-4.532417	-1.437777	1.782884
59	6	0	-5.481766	-3.097700	-1.583335
60	1	0	-3.421466	-3.716182	-1.680457
61	6	0	-6.454467	-2.416020	-0.850058
62	1	0	-6.855802	-1.290143	0.945671
63	1	0	-5.742993	-3.570919	-2.526363
64	1	0	-7.475205	-2.355102	-1.217356
65	1	0	0.328943	-2.361607	0.299783
66	1	0	1.106100	-1.377444	2.490676
67	8	0	1.431241	3.632997	-0.675921
68	6	0	1.025470	3.912750	-1.996321
69	1	0	-0.042825	3.701650	-2.136433
70	1	0	1.194121	4.978124	-2.184760
71	1	0	1.593868	3.327892	-2.730747

IM4 (SCF energy in toluene: -1252.815445 a.u; Free energy in toluene: -1252.341014 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.882898	0.963832	0.764149
2	6	0	0.540026	0.102914	1.807295
3	6	0	0.145699	-1.020099	2.774628
4	1	0	0.965637	-1.296724	3.455134
5	1	0	-0.158348	-1.924168	2.237845
6	6	0	-2.283650	3.176870	-1.000218
7	6	0	-1.455517	3.011690	-2.285913
8	6	0	-1.649510	4.217163	-0.062376
9	6	0	0.024649	2.713257	-2.008524
10	1	0	-1.540996	3.944251	-2.859389
11	1	0	-1.897681	2.224239	-2.908764
12	6	0	-0.158619	3.967738	0.220591
13	1	0	-1.748926	5.206073	-0.525353
14	1	0	-2.208453	4.261819	0.882380
15	6	0	0.634150	3.776190	-1.084033
16	1	0	0.580728	2.680364	-2.951837
17	1	0	0.122385	1.723212	-1.547359
18	1	0	1.677079	3.529568	-0.848026
19	1	0	0.657048	4.744015	-1.602335
20	1	0	0.241063	4.854884	0.733154
21	1	0	-3.282856	3.538976	-1.283383
22	7	0	-2.412374	1.875007	-0.298215

23	1	0	-3.151596	1.927358	0.403144
24	1	0	-2.709931	1.144967	-0.944695
25	7	0	0.006677	2.783589	1.106676
26	1	0	0.999012	2.587737	1.231937
27	1	0	-0.342153	3.006515	2.039830
28	6	0	-1.760774	-0.688471	0.427869
29	6	0	-2.845051	-1.141148	1.214937
30	6	0	-1.477740	-1.465343	-0.709531
31	6	0	-3.585171	-2.278585	0.896108
32	1	0	-3.113093	-0.602581	2.123502
33	6	0	-2.204133	-2.617906	-1.052478
34	1	0	-0.649904	-1.186640	-1.361189
35	6	0	-3.266830	-3.027919	-0.244098
36	1	0	-4.410445	-2.611362	1.520080
37	1	0	-1.927450	-3.177171	-1.940305
38	8	0	-4.052012	-4.133257	-0.476553
39	6	0	-3.743114	-4.935959	-1.598179
40	1	0	-2.727528	-5.351125	-1.538295
41	1	0	-4.464110	-5.756228	-1.595557
42	1	0	-3.838599	-4.379473	-2.541223
43	6	0	1.659252	-0.321076	0.839548
44	1	0	1.913155	0.507855	0.160458
45	1	0	1.293800	-1.130374	0.194244
46	6	0	2.983165	-0.791922	1.502843
47	1	0	3.347031	-0.003345	2.175224
48	1	0	2.780113	-1.667264	2.129479
49	6	0	4.054591	-1.131877	0.492093
50	6	0	4.080488	-2.388307	-0.132467
51	6	0	5.024088	-0.190947	0.116585
52	6	0	5.039363	-2.693395	-1.098754
53	1	0	3.340871	-3.134908	0.147780
54	6	0	5.986843	-0.490454	-0.849200
55	1	0	5.028284	0.786256	0.595332
56	6	0	5.997714	-1.744456	-1.462132
57	1	0	5.041791	-3.675070	-1.565283
58	1	0	6.731884	0.253804	-1.118586
59	1	0	6.747640	-1.982135	-2.211451
60	1	0	0.943773	0.921960	2.439405
61	1	0	-0.701618	-0.724433	3.403581

IM5 (SCF energy in toluene: -1252.786212 a.u; Free energy in toluene: -1252.314984 a.u.)

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

1	28	0	-0.265015	-0.186900	0.079624
2	6	0	2.818647	2.624555	-0.987129
3	6	0	1.795218	1.660964	-1.008374
4	6	0	1.156446	1.173789	0.148914
5	6	0	1.616577	1.748517	1.359051
6	6	0	2.631149	2.703679	1.416611
7	6	0	3.242108	3.149028	0.237675
8	1	0	3.261647	2.957147	-1.920555
9	1	0	1.497060	1.281289	-1.986686
10	1	0	2.963374	3.124560	2.361986
11	6	0	-2.026249	-1.012175	0.156332
12	6	0	-2.284613	0.415292	0.476405
13	1	0	-1.253606	1.033271	0.498416
14	1	0	1.168452	1.439790	2.304177
15	8	0	4.232506	4.089851	0.391017
16	6	0	4.853193	4.592416	-0.775553
17	1	0	4.133938	5.087623	-1.442309
18	1	0	5.589556	5.325091	-0.438736
19	1	0	5.368051	3.802397	-1.340301
20	6	0	3.869655	-2.060715	0.105883
21	6	0	4.056441	-3.535898	-0.294267
22	6	0	2.723765	-1.913960	1.128276
23	6	0	2.752894	-4.176251	-0.794063
24	1	0	4.422417	-4.085937	0.582986
25	1	0	4.840306	-3.617236	-1.058937
26	6	0	1.402430	-2.556311	0.669349
27	1	0	3.030305	-2.404290	2.060327
28	1	0	2.561108	-0.856850	1.357864
29	6	0	1.628953	-4.020254	0.241950
30	1	0	2.913697	-5.238739	-1.009560
31	1	0	2.457659	-3.707443	-1.739911
32	1	0	0.690060	-4.447429	-0.135764
33	1	0	1.884553	-4.594769	1.142673
34	1	0	0.694736	-2.545277	1.503908
35	1	0	4.798008	-1.720513	0.594718
36	7	0	3.558059	-1.258338	-1.093527
37	1	0	3.483411	-0.270114	-0.854249
38	1	0	4.303255	-1.345170	-1.780831
39	7	0	0.781048	-1.746304	-0.433284
40	1	0	1.544587	-1.476129	-1.068491
41	1	0	0.144046	-2.347163	-0.953439
42	1	0	-2.398033	-1.308003	-0.831247
43	1	0	-2.609942	0.572628	1.511714

44	6	0	-2.315004	-2.057238	1.222785
45	1	0	-1.871747	-3.027416	0.964567
46	1	0	-1.905381	-1.764663	2.197775
47	1	0	-3.392620	-2.230275	1.364966
48	6	0	-3.140145	1.248382	-0.504666
49	1	0	-2.982832	2.315949	-0.307518
50	1	0	-2.785209	1.061265	-1.523991
51	6	0	-4.616258	0.925354	-0.402182
52	6	0	-5.231430	0.043231	-1.300354
53	6	0	-5.399624	1.493223	0.613101
54	6	0	-6.587789	-0.267369	-1.186711
55	1	0	-4.642805	-0.398359	-2.100581
56	6	0	-6.755012	1.184986	0.731958
57	1	0	-4.942910	2.189764	1.312910
58	6	0	-7.354243	0.301742	-0.168713
59	1	0	-7.045962	-0.950815	-1.896453
60	1	0	-7.344747	1.639143	1.523542
61	1	0	-8.410449	0.063653	-0.080584

TS3 (SCF energy in toluene: -1252.779463 a.u; Free energy in toluene: -1252.310737 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.352798	-0.109605	0.252058
2	6	0	2.661086	2.635069	-0.958334
3	6	0	1.581671	1.734936	-0.922664
4	6	0	1.054057	1.214342	0.272301
5	6	0	1.659989	1.690754	1.457588
6	6	0	2.736042	2.577019	1.452303
7	6	0	3.247138	3.056311	0.239150
8	1	0	3.018675	3.001614	-1.915196
9	1	0	1.151109	1.435542	-1.877693
10	1	0	3.189508	2.922936	2.377240
11	6	0	-2.058310	-1.240302	0.309413
12	6	0	-2.415489	0.100059	0.517796
13	1	0	-0.975544	1.125031	0.650971
14	1	0	1.282239	1.358111	2.423255
15	8	0	4.305926	3.927719	0.333400
16	6	0	4.818783	4.475829	-0.864767
17	1	0	4.058565	5.051103	-1.410803
18	1	0	5.630537	5.145006	-0.572230
19	1	0	5.218603	3.700254	-1.533307
20	6	0	3.931256	-1.895187	-0.095841

21	6	0	4.117652	-3.360023	-0.532027
22	6	0	2.878739	-1.789232	1.026568
23	6	0	2.790631	-4.034971	-0.908607
24	1	0	4.584432	-3.907920	0.297498
25	1	0	4.824447	-3.410720	-1.370989
26	6	0	1.537723	-2.465602	0.687360
27	1	0	3.283648	-2.277827	1.921564
28	1	0	2.710751	-0.739867	1.284545
29	6	0	1.770067	-3.921423	0.234602
30	1	0	2.961135	-5.090231	-1.150865
31	1	0	2.389070	-3.568019	-1.815628
32	1	0	0.813885	-4.379924	-0.052848
33	1	0	2.132908	-4.490484	1.101599
34	1	0	0.918988	-2.479453	1.590529
35	1	0	4.891432	-1.539102	0.314422
36	7	0	3.498239	-1.085566	-1.251519
37	1	0	3.428032	-0.101913	-0.993624
38	1	0	4.181679	-1.149473	-2.002628
39	7	0	0.786688	-1.672594	-0.342924
40	1	0	1.481732	-1.351451	-1.028653
41	1	0	0.161813	-2.308599	-0.835369
42	1	0	-2.208646	-1.635409	-0.698576
43	1	0	-2.673059	0.391280	1.536978
44	6	0	-2.091936	-2.268492	1.421169
45	1	0	-1.374947	-3.081715	1.259798
46	1	0	-1.863050	-1.814533	2.391472
47	1	0	-3.084588	-2.733445	1.503987
48	6	0	-3.119117	0.934128	-0.552563
49	1	0	-2.847886	1.989149	-0.438238
50	1	0	-2.766350	0.622824	-1.541725
51	6	0	-4.627963	0.783805	-0.468443
52	6	0	-5.306111	-0.173112	-1.235376
53	6	0	-5.374678	1.586694	0.405155
54	6	0	-6.689502	-0.326110	-1.132355
55	1	0	-4.744619	-0.800231	-1.923799
56	6	0	-6.757747	1.435897	0.513812
57	1	0	-4.866732	2.341830	1.000918
58	6	0	-7.420418	0.477612	-0.255395
59	1	0	-7.196932	-1.070461	-1.740056
60	1	0	-7.318217	2.070918	1.194488
61	1	0	-8.497552	0.361483	-0.175814

IM6 (SCF energy in toluene: -1252.78052 a.u; Free energy in toluene: -1252.312661 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.381709	-0.047451	0.439136
2	6	0	2.597921	2.634791	-0.911190
3	6	0	1.481020	1.786872	-0.812465
4	6	0	1.048676	1.230909	0.403746
5	6	0	1.782657	1.620067	1.546991
6	6	0	2.898289	2.452482	1.475801
7	6	0	3.317368	2.966005	0.241197
8	1	0	2.880440	3.032548	-1.880523
9	1	0	0.945207	1.556574	-1.732196
10	1	0	3.453864	2.730882	2.367133
11	6	0	-2.054378	-1.308397	0.544943
12	6	0	-2.484423	0.007402	0.604313
13	1	0	-0.849473	1.223768	0.905877
14	1	0	1.477387	1.259520	2.527629
15	8	0	4.424804	3.779203	0.270990
16	6	0	4.851937	4.358267	-0.946213
17	1	0	4.075716	4.995372	-1.391723
18	1	0	5.721984	4.972045	-0.704341
19	1	0	5.145630	3.596706	-1.682526
20	6	0	3.900049	-1.863356	-0.284684
21	6	0	4.041404	-3.311573	-0.787165
22	6	0	2.937188	-1.794847	0.917626
23	6	0	2.683760	-3.965395	-1.084843
24	1	0	4.565326	-3.891822	-0.015803
25	1	0	4.681749	-3.335167	-1.678961
26	6	0	1.567467	-2.450344	0.658970
27	1	0	3.405128	-2.321262	1.759014
28	1	0	2.801255	-0.755754	1.229572
29	6	0	1.755169	-3.889542	0.137073
30	1	0	2.826656	-5.011783	-1.378181
31	1	0	2.217842	-3.462689	-1.940440
32	1	0	0.776827	-4.334124	-0.091814
33	1	0	2.180381	-4.491762	0.951827
34	1	0	1.025274	-2.495960	1.609285
35	1	0	4.891449	-1.528476	0.065013
36	7	0	3.388227	-1.007961	-1.373011
37	1	0	3.351746	-0.033723	-1.075592
38	1	0	4.010053	-1.050962	-2.177291
39	7	0	0.740735	-1.617694	-0.277748

40	1	0	1.384143	-1.259719	-0.994430
41	1	0	0.093772	-2.239656	-0.759087
42	1	0	-2.101845	-1.806811	-0.425907
43	1	0	-2.769124	0.407179	1.576253
44	6	0	-2.026597	-2.220981	1.751182
45	1	0	-1.223240	-2.963681	1.696195
46	1	0	-1.892280	-1.651632	2.676512
47	1	0	-2.969416	-2.778513	1.841096
48	6	0	-3.093101	0.745951	-0.580431
49	1	0	-2.756213	1.787234	-0.580196
50	1	0	-2.733101	0.295401	-1.512532
51	6	0	-4.612486	0.705911	-0.539535
52	6	0	-5.321362	-0.385996	-1.059350
53	6	0	-5.337409	1.752151	0.046273
54	6	0	-6.714273	-0.431887	-0.996635
55	1	0	-4.775251	-1.205137	-1.521246
56	6	0	-6.731212	1.710023	0.113465
57	1	0	-4.803520	2.610539	0.447521
58	6	0	-7.424607	0.616939	-0.408352
59	1	0	-7.245868	-1.284534	-1.410494
60	1	0	-7.274769	2.533486	0.568615
61	1	0	-8.509376	0.583802	-0.360969

IM7 (SCF energy in toluene: -1252.785766 a.u; Free energy in toluene: -1252.317111 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.085839	-0.979793	0.452836
2	6	0	4.069074	-1.668730	0.589136
3	6	0	2.708776	-1.531654	0.905396
4	6	0	1.715773	-1.319207	-0.065959
5	6	0	2.165547	-1.287200	-1.404016
6	6	0	3.514117	-1.407511	-1.744501
7	6	0	4.478372	-1.599146	-0.745649
8	1	0	4.787014	-1.829246	1.386534
9	1	0	2.432442	-1.591722	1.957087
10	1	0	3.840983	-1.373704	-2.780317
11	6	0	-2.216537	-0.658334	0.627314
12	6	0	-1.825379	-1.547775	1.595896
13	1	0	-0.142886	-2.342920	-0.005582
14	1	0	1.446177	-1.166466	-2.211892
15	8	0	5.779010	-1.709537	-1.177260
16	6	0	6.777801	-1.954925	-0.206575

17	1	0	6.602257	-2.895510	0.333070
18	1	0	7.721747	-2.026727	-0.750779
19	1	0	6.848910	-1.138424	0.525856
20	6	0	2.097819	2.851134	-0.856153
21	6	0	1.965493	4.202352	-0.130739
22	6	0	0.704885	2.243239	-1.121881
23	6	0	1.142600	4.088353	1.160773
24	1	0	1.485169	4.917168	-0.812467
25	1	0	2.963622	4.605223	0.086045
26	6	0	-0.178595	2.133811	0.135244
27	1	0	0.185680	2.881915	-1.847158
28	1	0	0.811845	1.256336	-1.583456
29	6	0	-0.241709	3.485257	0.877676
30	1	0	1.028639	5.075134	1.624096
31	1	0	1.683250	3.463481	1.880496
32	1	0	-0.813225	3.370425	1.808872
33	1	0	-0.816298	4.183400	0.252988
34	1	0	-1.194955	1.880199	-0.185839
35	1	0	2.571871	3.035477	-1.835778
36	7	0	2.885576	1.925054	-0.025070
37	1	0	3.038197	1.045420	-0.516248
38	1	0	3.803200	2.318350	0.170042
39	7	0	0.291991	1.010578	1.003245
40	1	0	1.312439	1.099719	1.077694
41	1	0	-0.086783	1.144004	1.940508
42	1	0	-2.348144	0.385670	0.910095
43	1	0	-1.912770	-2.611680	1.391290
44	6	0	-2.827113	-1.048664	-0.704699
45	1	0	-2.332542	-0.501627	-1.517027
46	1	0	-2.636648	-2.111771	-0.885798
47	6	0	-1.590112	-1.191895	3.042337
48	1	0	-0.669095	-1.644031	3.425731
49	1	0	-1.536533	-0.109455	3.197737
50	1	0	-2.415349	-1.569696	3.661006
51	6	0	-4.321143	-0.764098	-0.757177
52	6	0	-5.225719	-1.569662	-0.050285
53	6	0	-4.826036	0.311896	-1.497115
54	6	0	-6.594945	-1.308731	-0.084702
55	1	0	-4.850948	-2.410782	0.528070
56	6	0	-6.196673	0.579194	-1.532615
57	1	0	-4.139831	0.941663	-2.059082
58	6	0	-7.085903	-0.230908	-0.826223
59	1	0	-7.280464	-1.948611	0.464279
60	1	0	-6.568277	1.416971	-2.116395

61	1	0	-8.152622	-0.027857	-0.855143

TS4 (SCF energy in toluene: -1252.779594 a.u; Free energy in toluene: -1252.311221 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.120812	-0.867378	-0.182167
2	6	0	-4.033905	-1.470173	-0.836881
3	6	0	-2.647748	-1.294067	-0.991797
4	6	0	-1.754502	-1.238590	0.092595
5	6	0	-2.339399	-1.415464	1.367354
6	6	0	-3.710909	-1.584860	1.551250
7	6	0	-4.571450	-1.612397	0.446008
8	1	0	-4.668493	-1.505572	-1.716506
9	1	0	-2.268960	-1.191476	-2.008123
10	1	0	-4.138029	-1.711829	2.542324
11	6	0	2.147856	-0.829321	-0.457534
12	6	0	1.748913	-2.171260	-0.360615
13	1	0	0.029618	-2.277648	0.094333
14	1	0	-1.705183	-1.418929	2.252546
15	8	0	-5.905799	-1.787371	0.725253
16	6	0	-6.802022	-1.881532	-0.364293
17	1	0	-6.558126	-2.725723	-1.023669
18	1	0	-7.792441	-2.040312	0.067172
19	1	0	-6.818046	-0.960898	-0.964785
20	6	0	-2.524021	2.934095	0.283474
21	6	0	-1.967148	4.311460	-0.119419
22	6	0	-1.522871	2.185968	1.187353
23	6	0	-0.568182	4.220677	-0.746977
24	1	0	-1.923930	4.939310	0.780634
25	1	0	-2.663820	4.807613	-0.808111
26	6	0	-0.105692	2.082112	0.593624
27	1	0	-1.448691	2.729631	2.137442
28	1	0	-1.902678	1.187272	1.419847
29	6	0	0.406340	3.476446	0.179444
30	1	0	-0.185126	5.225862	-0.957244
31	1	0	-0.634513	3.704968	-1.711987
32	1	0	1.395143	3.386112	-0.291089
33	1	0	0.556881	4.065442	1.094671
34	1	0	0.562324	1.684452	1.364746
35	1	0	-3.442960	3.099007	0.871146
36	7	0	-2.786680	2.130675	-0.926359
37	1	0	-3.214413	1.239035	-0.679009

38	1	0	-3.440379	2.615807	-1.536854
39	7	0	-0.077874	1.111868	-0.552150
40	1	0	-0.938947	1.272883	-1.090019
41	1	0	0.698507	1.364960	-1.161143
42	1	0	2.329984	-0.442324	-1.463518
43	1	0	1.967882	-2.686061	0.575424
44	6	0	2.931469	-0.129640	0.646493
45	1	0	2.658850	0.932057	0.694692
46	1	0	2.655436	-0.565653	1.614507
47	6	0	1.677491	-3.084099	-1.569351
48	1	0	0.971621	-3.906151	-1.420852
49	1	0	1.372775	-2.535157	-2.465037
50	1	0	2.668596	-3.515515	-1.760537
51	6	0	4.437318	-0.229148	0.454733
52	6	0	5.142014	-1.370056	0.864741
53	6	0	5.152400	0.804687	-0.163331
54	6	0	6.517726	-1.475860	0.660587
55	1	0	4.606542	-2.181015	1.352813
56	6	0	6.529366	0.703401	-0.372493
57	1	0	4.625230	1.702445	-0.479610
58	6	0	7.217304	-0.438732	0.038956
59	1	0	7.045399	-2.366492	0.991079
60	1	0	7.064350	1.518854	-0.851835
61	1	0	8.289043	-0.519109	-0.118753

IM8 (SCF energy in toluene: -1252.787279 a.u; Free energy in toluene: -1252.316076 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.168063	-0.476690	-0.345098
2	6	0	-3.917888	-1.719234	-0.859919
3	6	0	-2.606051	-1.255030	-1.057491
4	6	0	-1.652999	-1.146631	-0.026179
5	6	0	-2.113605	-1.563505	1.246505
6	6	0	-3.408705	-2.026541	1.478059
7	6	0	-4.323695	-2.106603	0.420673
8	1	0	-4.597470	-1.780930	-1.703921
9	1	0	-2.334259	-0.964554	-2.073159
10	1	0	-3.733038	-2.338027	2.467471
11	6	0	2.098683	-0.452344	-0.588215
12	6	0	1.791755	-1.885118	-0.324940
13	1	0	0.620597	-2.023984	-0.106665
14	1	0	-1.436929	-1.526323	2.100926

15	8	0	-5.576402	-2.572452	0.741315
16	6	0	-6.518369	-2.708450	-0.304425
17	1	0	-6.172604	-3.406309	-1.079275
18	1	0	-7.427569	-3.104588	0.152535
19	1	0	-6.748102	-1.743906	-0.778794
20	6	0	-2.749145	2.879326	0.524441
21	6	0	-2.407905	4.331789	0.144700
22	6	0	-1.572194	2.223051	1.275642
23	6	0	-1.093131	4.437786	-0.642222
24	1	0	-2.331028	4.919662	1.069172
25	1	0	-3.234163	4.769348	-0.431105
26	6	0	-0.232066	2.317090	0.523746
27	1	0	-1.453260	2.732950	2.239636
28	1	0	-1.803928	1.175917	1.492067
29	6	0	0.064259	3.775622	0.121590
30	1	0	-0.854377	5.489754	-0.835917
31	1	0	-1.216557	3.961433	-1.621676
32	1	0	0.991945	3.819631	-0.465096
33	1	0	0.260169	4.340877	1.043029
34	1	0	0.568642	1.972987	1.185633
35	1	0	-3.612249	2.900462	1.210866
36	7	0	-3.040700	2.105182	-0.697786
37	1	0	-3.321114	1.153362	-0.464443
38	1	0	-3.811779	2.528215	-1.209222
39	7	0	-0.233148	1.398887	-0.666029
40	1	0	-1.152761	1.501629	-1.116944
41	1	0	0.472704	1.723526	-1.324903
42	1	0	2.406260	-0.263098	-1.623453
43	1	0	2.190957	-2.241018	0.631933
44	6	0	2.979271	0.298683	0.414607
45	1	0	2.905745	1.377316	0.217885
46	1	0	2.596521	0.145258	1.432120
47	6	0	2.054336	-2.893549	-1.448305
48	1	0	1.605652	-3.869490	-1.235476
49	1	0	1.644810	-2.533258	-2.396956
50	1	0	3.132971	-3.029727	-1.574217
51	6	0	4.445217	-0.103733	0.375639
52	6	0	4.981690	-0.986993	1.322405
53	6	0	5.292924	0.376257	-0.634194
54	6	0	6.318799	-1.386216	1.259981
55	1	0	4.347369	-1.359053	2.123968
56	6	0	6.629111	-0.017407	-0.700570
57	1	0	4.899449	1.069353	-1.374855
58	6	0	7.147984	-0.903345	0.247072

59	1	0	6.712991	-2.069817	2.007253
60	1	0	7.268005	0.370783	-1.489448
61	1	0	8.189132	-1.209362	0.198351

IM9 (SCF energy in toluene: -1252.789657 a.u; Free energy in toluene: -1252.319684 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.513166	0.159850	-0.670291
2	6	0	-2.922035	-2.301527	-1.373229
3	6	0	-1.814636	-1.448817	-1.498469
4	6	0	-0.966474	-1.108701	-0.426635
5	6	0	-1.308414	-1.708477	0.808946
6	6	0	-2.407403	-2.554982	0.970010
7	6	0	-3.223970	-2.858007	-0.126899
8	1	0	-3.531205	-2.519240	-2.244493
9	1	0	-1.621827	-1.034511	-2.488743
10	1	0	-2.645631	-3.001081	1.932066
11	6	0	2.279650	0.897745	-0.999487
12	6	0	2.504595	-0.580096	-0.929119
13	1	0	1.457040	-1.156687	-0.771180
14	1	0	-0.697054	-1.514350	1.690919
15	8	0	-4.282086	-3.698757	0.124195
16	6	0	-5.107486	-4.064454	-0.964478
17	1	0	-4.542057	-4.582912	-1.750787
18	1	0	-5.862298	-4.742821	-0.561351
19	1	0	-5.610060	-3.194475	-1.409951
20	6	0	-2.672163	2.200441	1.641782
21	6	0	-3.090841	3.659464	1.383203
22	6	0	-1.136578	2.092364	1.750140
23	6	0	-2.394535	4.252931	0.149498
24	1	0	-2.839854	4.255098	2.271208
25	1	0	-4.181450	3.717140	1.270940
26	6	0	-0.387297	2.693159	0.546515
27	1	0	-0.816793	2.628261	2.652167
28	1	0	-0.845230	1.044537	1.879340
29	6	0	-0.867500	4.131507	0.265607
30	1	0	-2.673006	5.306257	0.030327
31	1	0	-2.745159	3.733502	-0.749499
32	1	0	-0.376869	4.517059	-0.638196
33	1	0	-0.518048	4.763011	1.094012
34	1	0	0.682205	2.724348	0.775060
35	1	0	-3.097065	1.889611	2.611661

36	7	0	-3.144176	1.352088	0.533228
37	1	0	-2.912159	0.374183	0.703437
38	1	0	-4.155978	1.409969	0.446948
39	7	0	-0.535941	1.797990	-0.646642
40	1	0	-1.533921	1.561730	-0.725815
41	1	0	-0.263238	2.316888	-1.481362
42	1	0	2.793648	-1.010525	-1.894349
43	6	0	3.369617	-1.114500	0.189947
44	6	0	4.640196	-1.633943	-0.089600
45	6	0	2.939337	-1.074501	1.523121
46	6	0	5.467134	-2.088262	0.938561
47	1	0	4.984936	-1.680656	-1.119854
48	6	0	3.764644	-1.527761	2.552719
49	1	0	1.946467	-0.692459	1.748434
50	6	0	5.032982	-2.035211	2.264334
51	1	0	6.449619	-2.487647	0.702289
52	1	0	3.412874	-1.492440	3.580186
53	1	0	5.674488	-2.392411	3.064760
54	1	0	2.703090	1.438005	-0.146084
55	6	0	2.542502	1.602341	-2.323404
56	1	0	2.035722	2.579620	-2.323211
57	1	0	2.089431	1.029877	-3.145538
58	6	0	4.031881	1.835430	-2.636144
59	1	0	4.575223	0.885714	-2.694833
60	1	0	4.167760	2.358416	-3.589979
61	1	0	4.506011	2.435810	-1.851570

TS5 (SCF energy in toluene: -1252.784747 a.u; Free energy in toluene: -1252.316963 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.620185	0.030119	-0.755889
2	6	0	-3.009423	-2.077725	-1.411865
3	6	0	-1.821741	-1.347664	-1.570467
4	6	0	-0.901754	-1.139260	-0.527664
5	6	0	-1.232896	-1.750357	0.702822
6	6	0	-2.411609	-2.474804	0.891863
7	6	0	-3.311459	-2.641922	-0.169078
8	1	0	-3.678744	-2.197546	-2.257409
9	1	0	-1.624493	-0.925213	-2.555280
10	1	0	-2.647764	-2.933322	1.848464
11	6	0	2.398932	0.908333	-1.101804
12	6	0	2.627113	-0.488640	-0.977695

13	1	0	1.176176	-1.303716	-0.891959
14	1	0	-0.551066	-1.663291	1.547530
15	8	0	-4.443506	-3.369884	0.111155
16	6	0	-5.354755	-3.606399	-0.944104
17	1	0	-4.888895	-4.158522	-1.771741
18	1	0	-6.161071	-4.209853	-0.522058
19	1	0	-5.777431	-2.672196	-1.339967
20	6	0	-2.481854	2.142249	1.747813
21	6	0	-2.872076	3.615969	1.531964
22	6	0	-0.946386	1.994322	1.799439
23	6	0	-2.202841	4.216970	0.287093
24	1	0	-2.575858	4.187298	2.422018
25	1	0	-3.964140	3.702632	1.458675
26	6	0	-0.221476	2.604916	0.584936
27	1	0	-0.584231	2.501432	2.702277
28	1	0	-0.676767	0.937136	1.896199
29	6	0	-0.676173	4.060588	0.353381
30	1	0	-2.462428	5.277844	0.194849
31	1	0	-2.591390	3.720114	-0.608948
32	1	0	-0.205272	4.455857	-0.556763
33	1	0	-0.288347	4.666086	1.184396
34	1	0	0.854425	2.612889	0.788569
35	1	0	-2.879035	1.824181	2.727308
36	7	0	-3.015498	1.327771	0.642631
37	1	0	-2.814670	0.339862	0.793027
38	1	0	-4.026878	1.421223	0.588790
39	7	0	-0.418922	1.738466	-0.619305
40	1	0	-1.420349	1.512799	-0.665970
41	1	0	-0.184702	2.277823	-1.452686
42	1	0	2.838263	-1.024836	-1.904033
43	6	0	3.293293	-1.108776	0.210026
44	6	0	4.148638	-2.203682	0.021109
45	6	0	3.111467	-0.625515	1.516038
46	6	0	4.814205	-2.791218	1.097953
47	1	0	4.295364	-2.597360	-0.981830
48	6	0	3.775301	-1.210459	2.592570
49	1	0	2.435942	0.207272	1.689789
50	6	0	4.631638	-2.295881	2.389052
51	1	0	5.473660	-3.637367	0.925979
52	1	0	3.618917	-0.822255	3.595393
53	1	0	5.145430	-2.753053	3.229713
54	1	0	2.684360	1.530691	-0.251565
55	6	0	2.505328	1.596435	-2.451415
56	1	0	1.855113	2.483906	-2.478952

57	1	0	2.134305	0.925246	-3.237181
58	6	0	3.938020	2.040412	-2.797864
59	1	0	4.613422	1.179468	-2.841999
60	1	0	3.975236	2.551230	-3.766772
61	1	0	4.329787	2.728283	-2.040109

IM10 (SCF energy in toluene: -1252.79115 a.u; Free energy in toluene: -1252.323551 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.416330	-1.126845	-0.551405
2	6	0	-3.797722	-1.368457	-0.635774
3	6	0	-2.436647	-1.416471	-0.972086
4	6	0	-1.412220	-1.234350	-0.028340
5	6	0	-1.831988	-1.038090	1.305660
6	6	0	-3.180129	-0.979830	1.664208
7	6	0	-4.175185	-1.142579	0.690832
8	1	0	-4.542144	-1.511592	-1.411862
9	1	0	-2.184312	-1.602789	-2.014755
10	1	0	-3.484789	-0.824310	2.695753
11	6	0	2.365833	-1.242999	-1.458253
12	6	0	2.447577	-1.740742	-0.176503
13	1	0	0.203918	-2.481116	-0.117008
14	1	0	-1.088326	-0.926100	2.092467
15	8	0	-5.473082	-1.068879	1.138542
16	6	0	-6.508322	-1.269624	0.196170
17	1	0	-6.452300	-2.263503	-0.268543
18	1	0	-7.445872	-1.187139	0.749872
19	1	0	-6.494165	-0.510002	-0.598027
20	6	0	-1.081709	3.063658	0.543420
21	6	0	-0.920353	4.306053	-0.351549
22	6	0	0.264712	2.323062	0.683159
23	6	0	-0.335747	3.950512	-1.726131
24	1	0	-0.259931	5.020448	0.158333
25	1	0	-1.889990	4.808317	-0.466393
26	6	0	0.925257	1.971388	-0.663009
27	1	0	0.954156	2.965794	1.243829
28	1	0	0.134893	1.410607	1.275156
29	6	0	1.002828	3.212011	-1.577898
30	1	0	-0.192628	4.858875	-2.322820
31	1	0	-1.050728	3.324690	-2.271697
32	1	0	1.396896	2.922636	-2.561949
33	1	0	1.743538	3.898729	-1.144281

34	1	0	1.947169	1.638113	-0.458985
35	1	0	-1.379501	3.404699	1.550387
36	7	0	-2.080359	2.163588	-0.056894
37	1	0	-2.252200	1.358010	0.543073
38	1	0	-2.969270	2.644956	-0.169536
39	7	0	0.213364	0.816963	-1.291872
40	1	0	-0.790755	1.028571	-1.254239
41	1	0	0.470223	0.769307	-2.278132
42	1	0	2.659624	-0.209543	-1.639010
43	1	0	2.371605	-2.815804	-0.041722
44	6	0	2.890949	-0.998234	1.027709
45	6	0	2.498939	-1.452063	2.300929
46	6	0	3.736342	0.122890	0.955900
47	6	0	2.911088	-0.791665	3.456269
48	1	0	1.852185	-2.322194	2.371743
49	6	0	4.148303	0.785005	2.112878
50	1	0	4.099318	0.458934	-0.010926
51	6	0	3.733579	0.334835	3.367599
52	1	0	2.591289	-1.157029	4.428172
53	1	0	4.807839	1.645003	2.033847
54	1	0	4.058333	0.848055	4.268095
55	6	0	2.277931	-2.121106	-2.685151
56	1	0	1.877275	-3.100513	-2.401055
57	1	0	1.564816	-1.692523	-3.403062
58	6	0	3.639597	-2.296523	-3.383375
59	1	0	4.362603	-2.775101	-2.714840
60	1	0	3.542474	-2.917117	-4.280423
61	1	0	4.057640	-1.330628	-3.689078

IM11 (SCF energy in toluene: -1252.795164 a.u; Free energy in toluene: -1252.326394 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.474198	-0.938986	-0.361491
2	6	0	3.263899	-1.327035	1.564301
3	6	0	1.891946	-1.279641	1.275970
4	6	0	1.391364	-1.222463	-0.035701
5	6	0	2.356282	-1.263064	-1.065267
6	6	0	3.727128	-1.302812	-0.804171
7	6	0	4.191087	-1.333244	0.517918
8	1	0	3.589112	-1.361557	2.598698
9	1	0	1.200929	-1.279864	2.117178
10	1	0	4.455882	-1.327708	-1.609823

11	6	0	-2.531726	-0.869752	-0.668946
12	6	0	-2.056172	-2.146514	-0.984292
13	1	0	-0.161045	-2.333077	-0.480383
14	1	0	2.035451	-1.261408	-2.105635
15	8	0	5.555540	-1.374339	0.675270
16	6	0	6.066943	-1.458209	1.991626
17	1	0	5.717427	-2.361692	2.509456
18	1	0	7.153704	-1.500145	1.894777
19	1	0	5.795388	-0.580565	2.594806
20	6	0	1.872509	2.905584	-1.171457
21	6	0	1.377612	4.291685	-0.719249
22	6	0	0.744154	2.137281	-1.890954
23	6	0	0.111999	4.201211	0.145629
24	1	0	1.170909	4.895013	-1.613541
25	1	0	2.178126	4.810046	-0.175092
26	6	0	-0.562558	2.044708	-1.080633
27	1	0	0.524808	2.655870	-2.832453
28	1	0	1.086899	1.130674	-2.152801
29	6	0	-1.001159	3.440537	-0.589780
30	1	0	-0.237568	5.206261	0.408584
31	1	0	0.351303	3.695624	1.087803
32	1	0	-1.891277	3.343445	0.044999
33	1	0	-1.311571	4.021575	-1.469678
34	1	0	-1.348079	1.656467	-1.738359
35	1	0	2.687856	3.056442	-1.900361
36	7	0	2.316825	2.137961	0.004543
37	1	0	2.707238	1.240569	-0.279009
38	1	0	3.052027	2.639260	0.497401
39	7	0	-0.412725	1.059519	0.034350
40	1	0	0.477963	1.265568	0.500954
41	1	0	-1.161251	1.213890	0.710945
42	1	0	-2.697126	-0.185994	-1.502335
43	6	0	-3.192690	-0.478084	0.591450
44	6	0	-3.915071	0.730624	0.644680
45	6	0	-3.118723	-1.244092	1.773274
46	6	0	-4.540564	1.153857	1.818194
47	1	0	-4.000346	1.334121	-0.256442
48	6	0	-3.744660	-0.821051	2.943680
49	1	0	-2.560212	-2.175159	1.776877
50	6	0	-4.459273	0.380202	2.976573
51	1	0	-5.097136	2.087293	1.823310
52	1	0	-3.671657	-1.433281	3.838574
53	1	0	-4.945274	0.705805	3.891454
54	1	0	-2.228028	-2.949825	-0.269316

55	6	0	-1.935937	-2.617423	-2.422726
56	1	0	-1.123261	-3.347068	-2.506832
57	1	0	-1.661952	-1.771252	-3.064313
58	6	0	-3.244446	-3.247701	-2.929409
59	1	0	-3.133415	-3.601796	-3.959775
60	1	0	-3.535414	-4.105080	-2.312055
61	1	0	-4.067537	-2.526126	-2.904557

TS6 (SCF energy in toluene: -1252.794666 a.u; Free energy in toluene: -1252.325385 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.461801	-0.918841	-0.356468
2	6	0	3.286034	-1.308323	1.561366
3	6	0	1.913634	-1.253353	1.275705
4	6	0	1.409072	-1.192260	-0.034409
5	6	0	2.372729	-1.232088	-1.065447
6	6	0	3.744161	-1.278929	-0.807861
7	6	0	4.210821	-1.316129	0.512967
8	1	0	3.613379	-1.346825	2.594984
9	1	0	1.225297	-1.251180	2.119330
10	1	0	4.471120	-1.303692	-1.615180
11	6	0	-2.508042	-0.912795	-0.671677
12	6	0	-2.001918	-2.192273	-0.949396
13	1	0	-0.199604	-2.324409	-0.502657
14	1	0	2.050790	-1.224115	-2.105655
15	8	0	5.575525	-1.363928	0.667307
16	6	0	6.089133	-1.454307	1.982299
17	1	0	5.736164	-2.357588	2.498179
18	1	0	7.175498	-1.501369	1.883187
19	1	0	5.823185	-0.577179	2.588739
20	6	0	1.837330	2.932558	-1.172414
21	6	0	1.331116	4.314644	-0.720368
22	6	0	0.713876	2.153491	-1.888021
23	6	0	0.068923	4.213687	0.148408
24	1	0	1.116323	4.914903	-1.614805
25	1	0	2.128403	4.840997	-0.179178
26	6	0	-0.588796	2.048996	-1.072812
27	1	0	0.486299	2.669864	-2.828768
28	1	0	1.065114	1.150083	-2.150898
29	6	0	-1.039340	3.440824	-0.581815
30	1	0	-0.289577	5.215854	0.410308
31	1	0	0.315987	3.712713	1.091031

32	1	0	-1.926270	3.335684	0.056077
33	1	0	-1.358595	4.017463	-1.461410
34	1	0	-1.373232	1.650623	-1.725597
35	1	0	2.649345	3.089812	-1.903639
36	7	0	2.291631	2.170195	0.003263
37	1	0	2.686370	1.274495	-0.279815
38	1	0	3.025311	2.677337	0.492367
39	7	0	-0.423800	1.067502	0.043617
40	1	0	0.464243	1.286776	0.509555
41	1	0	-1.175405	1.210883	0.719414
42	1	0	-2.693364	-0.262027	-1.527220
43	6	0	-3.188406	-0.506117	0.572907
44	6	0	-3.939359	0.686392	0.591915
45	6	0	-3.103856	-1.239460	1.774904
46	6	0	-4.581655	1.124204	1.750782
47	1	0	-4.032949	1.265021	-0.324546
48	6	0	-3.746933	-0.801908	2.930721
49	1	0	-2.524039	-2.157040	1.805634
50	6	0	-4.489807	0.382415	2.929213
51	1	0	-5.159962	2.044128	1.728859
52	1	0	-3.665162	-1.389646	3.841175
53	1	0	-4.989237	0.719462	3.832628
54	1	0	-2.174588	-2.977814	-0.214369
55	6	0	-1.893702	-2.703028	-2.376673
56	1	0	-1.084581	-3.438219	-2.447310
57	1	0	-1.620161	-1.874962	-3.041478
58	6	0	-3.208522	-3.339714	-2.856475
59	1	0	-3.106638	-3.721510	-3.877800
60	1	0	-3.499197	-4.178985	-2.214574
61	1	0	-4.027824	-2.613617	-2.844980

IM12 (SCF energy in toluene: -1252.802446 a.u; Free energy in toluene: -1252.331008 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.414572	-0.711808	-0.352447
2	6	0	3.392023	-1.326037	1.498403
3	6	0	2.023163	-1.154252	1.241477
4	6	0	1.489784	-1.012198	-0.053550
5	6	0	2.440390	-1.063933	-1.099847
6	6	0	3.808955	-1.227141	-0.876643
7	6	0	4.294079	-1.360396	0.430750
8	1	0	3.735074	-1.429971	2.522574

9	1	0	1.357439	-1.127135	2.104117
10	1	0	4.518876	-1.262847	-1.698757
11	6	0	-2.333041	-1.019650	-0.701758
12	6	0	-1.698545	-2.347203	-0.901760
13	1	0	-0.517382	-2.302928	-0.685069
14	1	0	2.109437	-0.973045	-2.134928
15	8	0	5.653777	-1.515485	0.554789
16	6	0	6.183816	-1.685249	1.855254
17	1	0	5.778048	-2.578496	2.349418
18	1	0	7.262232	-1.804450	1.732322
19	1	0	5.990923	-0.812425	2.494532
20	6	0	1.750258	3.125879	-0.993046
21	6	0	1.184181	4.483116	-0.536896
22	6	0	0.682728	2.331157	-1.773705
23	6	0	-0.111428	4.328217	0.273256
24	1	0	0.991811	5.095084	-1.428472
25	1	0	1.940384	5.020994	0.049816
26	6	0	-0.644400	2.165509	-1.011607
27	1	0	0.472670	2.865537	-2.708295
28	1	0	1.076992	1.347264	-2.048381
29	6	0	-1.162602	3.529887	-0.512968
30	1	0	-0.514307	5.314140	0.531805
31	1	0	0.111760	3.823961	1.220102
32	1	0	-2.070035	3.382654	0.086486
33	1	0	-1.467696	4.109206	-1.395481
34	1	0	-1.390401	1.741564	-1.690949
35	1	0	2.590148	3.320228	-1.682077
36	7	0	2.171437	2.348346	0.185841
37	1	0	2.582700	1.460267	-0.097893
38	1	0	2.881188	2.853918	0.710509
39	7	0	-0.482396	1.177886	0.103802
40	1	0	0.367579	1.437986	0.620169
41	1	0	-1.284093	1.258475	0.732215
42	1	0	-2.674875	-0.541751	-1.623049
43	6	0	-3.157597	-0.689677	0.471478
44	6	0	-4.044717	0.409086	0.414905
45	6	0	-3.062503	-1.370469	1.706345
46	6	0	-4.793045	0.803983	1.522765
47	1	0	-4.154628	0.946097	-0.525152
48	6	0	-3.814873	-0.976386	2.811534
49	1	0	-2.388753	-2.217286	1.803805
50	6	0	-4.685115	0.114030	2.732413
51	1	0	-5.470900	1.649637	1.437106
52	1	0	-3.718711	-1.526715	3.744052

53	1	0	-5.270036	0.417236	3.595561
54	1	0	-1.983373	-3.091315	-0.148988
55	6	0	-1.773423	-2.943922	-2.316701
56	1	0	-1.034231	-3.748606	-2.414946
57	1	0	-1.488479	-2.171809	-3.042105
58	6	0	-3.168669	-3.483255	-2.648361
59	1	0	-3.195916	-3.903780	-3.658793
60	1	0	-3.462166	-4.274829	-1.949586
61	1	0	-3.923276	-2.692574	-2.589364

IM13 (SCF energy in toluene: -1252.826971 a.u; Free energy in toluene: -1252.351793 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.170279	0.468487	-0.347745
2	6	0	-0.544663	-3.166681	2.008769
3	6	0	-0.298264	-3.382640	3.505848
4	1	0	-1.039558	-2.847357	4.112048
5	1	0	0.692128	-3.016421	3.801221
6	6	0	1.658187	-0.077050	-0.449320
7	6	0	2.188992	-0.813151	-1.533038
8	6	0	2.596108	0.326664	0.518950
9	6	0	3.544196	-1.115944	-1.646036
10	1	0	1.521635	-1.174956	-2.313940
11	6	0	3.965935	0.023178	0.438621
12	1	0	2.263055	0.886340	1.394259
13	6	0	4.444335	-0.701338	-0.654955
14	1	0	3.929848	-1.681936	-2.489710
15	1	0	4.633395	0.352053	1.228280
16	8	0	5.758184	-1.053926	-0.851554
17	6	0	6.696264	-0.684029	0.139376
18	1	0	6.457896	-1.127735	1.115904
19	1	0	7.663084	-1.063524	-0.197764
20	1	0	6.761673	0.406881	0.256424
21	6	0	-0.444336	-1.687295	1.585533
22	1	0	-1.139760	-1.095569	2.202217
23	6	0	-0.673680	-1.424183	0.088512
24	1	0	0.556313	-1.325230	1.847475
25	1	0	0.048934	-2.015888	-0.481241
26	6	0	-2.037062	-1.752003	-0.433718
27	6	0	-2.218965	-2.014894	-1.811750
28	6	0	-3.204105	-1.760481	0.363130
29	6	0	-3.476407	-2.251721	-2.359060

30	1	0	-1.341305	-2.034469	-2.454449
31	6	0	-4.469897	-1.998521	-0.184696
32	1	0	-3.120213	-1.604275	1.435482
33	6	0	-4.619000	-2.240014	-1.549155
34	1	0	-3.568598	-2.455948	-3.423214
35	1	0	-5.340845	-2.005124	0.466669
36	1	0	-5.600221	-2.429509	-1.974515
37	1	0	-1.528764	-3.567815	1.737100
38	1	0	-0.354404	-4.442780	3.776848
39	1	0	0.188747	-3.743692	1.429711
40	6	0	-0.194677	3.614509	-0.418314
41	6	0	0.000629	3.830807	1.092116
42	6	0	-1.686226	3.555716	-0.778940
43	6	0	-0.758748	2.803470	1.943585
44	1	0	-0.354501	4.842081	1.330651
45	1	0	1.071116	3.814557	1.331570
46	6	0	-2.476199	2.538771	0.059595
47	1	0	-2.121322	4.549268	-0.619129
48	1	0	-1.807151	3.335558	-1.848733
49	6	0	-2.245602	2.761314	1.564839
50	1	0	-0.652460	3.049932	3.005876
51	1	0	-0.316539	1.809281	1.801972
52	1	0	-2.765846	1.982230	2.135518
53	1	0	-2.721654	3.713019	1.836265
54	1	0	-3.545850	2.689383	-0.146632
55	1	0	0.253865	4.467813	-0.947679
56	7	0	0.477394	2.362300	-0.851975
57	1	0	0.508443	2.320607	-1.871207
58	1	0	1.452963	2.355801	-0.553469
59	7	0	-2.106035	1.151474	-0.325831
60	1	0	-2.657879	0.487287	0.218394
61	1	0	-2.404313	0.980580	-1.287647

TS7 (SCF energy in toluene: -1252.781713 a.u; Free energy in toluene: -1252.306843 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.506609	-0.270509	-0.266221
2	6	0	0.860255	4.234283	0.748686
3	6	0	0.614976	5.151855	1.951266
4	1	0	1.025222	4.718357	2.871161
5	1	0	-0.456627	5.315236	2.114719
6	6	0	-1.068164	0.760813	-0.427468

7	6	0	-1.781438	0.837360	-1.662026
8	6	0	-1.879579	0.635915	0.730196
9	6	0	-3.159692	0.706329	-1.735280
10	1	0	-1.227059	0.997196	-2.585994
11	6	0	-3.274537	0.496954	0.667547
12	1	0	-1.413238	0.649129	1.712004
13	6	0	-3.924479	0.524410	-0.567574
14	1	0	-3.678439	0.753280	-2.689054
15	1	0	-3.834305	0.386148	1.590444
16	8	0	-5.282351	0.408818	-0.753467
17	6	0	-6.092000	0.261112	0.395474
18	1	0	-6.003989	1.122518	1.072234
19	1	0	-7.121639	0.191996	0.038498
20	1	0	-5.845908	-0.651446	0.956929
21	6	0	0.195191	2.855211	0.904611
22	1	0	0.549820	2.377390	1.827796
23	6	0	0.420877	1.938123	-0.295052
24	1	0	-0.882648	2.999100	1.042325
25	1	0	0.110770	2.451936	-1.206832
26	6	0	1.801557	1.416530	-0.498058
27	6	0	2.186777	0.953707	-1.799963
28	6	0	2.844703	1.495210	0.477967
29	6	0	3.475489	0.483168	-2.051850
30	1	0	1.472311	1.026217	-2.616348
31	6	0	4.126338	1.033778	0.204559
32	1	0	2.632295	1.916948	1.455500
33	6	0	4.455308	0.492857	-1.051497
34	1	0	3.726127	0.130109	-3.049965
35	1	0	4.892028	1.110738	0.973853
36	1	0	5.463145	0.146020	-1.257991
37	1	0	1.938587	4.113852	0.591336
38	1	0	1.083246	6.131788	1.809938
39	1	0	0.470315	4.711788	-0.160461
40	6	0	-0.098330	-3.365595	-0.612913
41	6	0	-0.968802	-3.611834	0.631123
42	6	0	1.391668	-3.604971	-0.309895
43	6	0	-0.479355	-2.857502	1.874720
44	1	0	-0.959167	-4.691875	0.831492
45	1	0	-2.010260	-3.347911	0.408208
46	6	0	1.910840	-2.887317	0.949980
47	1	0	1.540456	-4.683144	-0.172181
48	1	0	2.000237	-3.318534	-1.177998
49	6	0	0.998016	-3.160850	2.157504
50	1	0	-1.088750	-3.141060	2.740793

51	1	0	-0.616315	-1.781636	1.725443
52	1	0	1.351759	-2.584537	3.022456
53	1	0	1.109641	-4.219644	2.428006
54	1	0	2.903877	-3.304873	1.180743
55	1	0	-0.403560	-4.092642	-1.381403
56	7	0	-0.301490	-1.988747	-1.134132
57	1	0	0.088937	-1.926219	-2.073781
58	1	0	-1.296559	-1.789521	-1.233643
59	7	0	2.031735	-1.431231	0.701155
60	1	0	2.291873	-0.952595	1.561732
61	1	0	2.816134	-1.257844	0.070466

IM14 (SCF energy in toluene: -1252.823928 a.u; Free energy in toluene: -1252.347965 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-1.047263	-0.354825	0.558372
2	6	0	1.974336	-2.005325	-0.869056
3	6	0	1.842886	-0.855832	0.158247
4	1	0	0.968862	-2.392801	-1.086279
5	6	0	3.183865	-0.148217	0.365981
6	6	0	3.895462	-0.309283	1.563144
7	6	0	3.746006	0.671513	-0.625919
8	6	0	5.127345	0.317776	1.766669
9	1	0	3.477201	-0.936632	2.347327
10	6	0	4.975630	1.298839	-0.428618
11	1	0	3.203264	0.837708	-1.551676
12	6	0	5.674373	1.123839	0.768742
13	1	0	5.656813	0.175926	2.705407
14	1	0	5.387703	1.931568	-1.210512
15	1	0	6.631350	1.615015	0.922279
16	1	0	1.591059	-1.322874	1.119588
17	1	0	2.363798	-1.614467	-1.818181
18	6	0	0.022139	1.843252	-1.830511
19	6	0	0.547022	0.614666	-1.529326
20	6	0	0.697939	0.128310	-0.171028
21	6	0	0.230791	1.046896	0.885608
22	6	0	-0.194087	2.394829	0.529228
23	6	0	-0.330542	2.759998	-0.784226
24	1	0	-0.096331	2.173610	-2.858186
25	1	0	0.877169	-0.016793	-2.352839
26	1	0	0.695285	0.959622	1.872632
27	1	0	-0.373921	3.107102	1.329044

28	8	0	-0.758437	3.989845	-1.240286
29	6	0	-1.051057	4.972285	-0.271690
30	1	0	-0.171504	5.218209	0.340179
31	1	0	-1.368130	5.863464	-0.818128
32	1	0	-1.862324	4.655414	0.400953
33	6	0	2.867531	-3.166187	-0.411956
34	1	0	3.867782	-2.784991	-0.174674
35	1	0	2.470460	-3.580866	0.525665
36	6	0	2.979565	-4.282247	-1.455847
37	1	0	3.411464	-3.907381	-2.390919
38	1	0	3.615716	-5.100621	-1.102088
39	1	0	1.996710	-4.706443	-1.695363
40	6	0	-3.322467	-2.227378	-0.354955
41	6	0	-3.950949	-1.297875	-1.407852
42	6	0	-3.935662	-1.987291	1.037893
43	6	0	-3.934596	0.180619	-0.996502
44	1	0	-4.988527	-1.624820	-1.560136
45	1	0	-3.441189	-1.436460	-2.369978
46	6	0	-3.986538	-0.510680	1.473315
47	1	0	-4.963296	-2.370545	1.023196
48	1	0	-3.398062	-2.580230	1.790477
49	6	0	-4.600957	0.371923	0.372863
50	1	0	-4.459294	0.779378	-1.749531
51	1	0	-2.900679	0.545104	-0.961171
52	1	0	-4.555976	1.424819	0.679286
53	1	0	-5.667118	0.117458	0.301239
54	1	0	-4.636652	-0.445821	2.359713
55	1	0	-3.550426	-3.265202	-0.644015
56	7	0	-1.847061	-2.040768	-0.312024
57	1	0	-1.422644	-2.804715	0.214075
58	1	0	-1.469120	-2.104962	-1.255548
59	7	0	-2.622923	-0.032205	1.821780
60	1	0	-2.637336	0.973154	1.986194
61	1	0	-2.319589	-0.460340	2.696350

IM15 (SCF energy in toluene: -1252.812426 a.u; Free energy in toluene: -1252.338819 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.758328	-0.654535	-0.324959
2	6	0	1.115664	-0.758190	0.260420
3	6	0	2.092326	0.051223	-0.629529
4	1	0	1.929241	1.118542	-0.453091

5	6	0	-3.742925	-1.580736	-0.815794
6	6	0	-4.205345	-1.662282	0.648984
7	6	0	-3.169032	-2.924724	-1.292719
8	6	0	-3.116779	-2.194538	1.591242
9	1	0	-5.079923	-2.325374	0.686374
10	1	0	-4.552643	-0.675540	0.979718
11	6	0	-2.088965	-3.499779	-0.361766
12	1	0	-3.989447	-3.649576	-1.354486
13	1	0	-2.771325	-2.822620	-2.311712
14	6	0	-2.574616	-3.543076	1.097165
15	1	0	-3.523336	-2.307320	2.602364
16	1	0	-2.297367	-1.468640	1.657553
17	1	0	-1.762037	-3.894059	1.745866
18	1	0	-3.366684	-4.301094	1.159409
19	1	0	-1.881949	-4.531606	-0.681115
20	1	0	-4.620034	-1.345523	-1.436362
21	7	0	-2.724723	-0.512425	-0.976781
22	1	0	-2.601848	-0.293758	-1.965796
23	1	0	-3.044204	0.356767	-0.550362
24	7	0	-0.836256	-2.702685	-0.468786
25	1	0	-0.152198	-3.052066	0.201118
26	1	0	-0.414573	-2.858538	-1.385513
27	6	0	-0.757057	1.249447	-0.261687
28	6	0	-0.546950	2.037770	-1.417334
29	6	0	-1.145210	1.961516	0.887503
30	6	0	-0.709028	3.422526	-1.426789
31	1	0	-0.225910	1.561742	-2.343415
32	6	0	-1.314132	3.355916	0.907288
33	1	0	-1.310988	1.426842	1.822198
34	6	0	-1.095551	4.092970	-0.259156
35	1	0	-0.535645	4.007367	-2.326212
36	1	0	-1.607423	3.844486	1.830833
37	8	0	-1.231781	5.457258	-0.366005
38	6	0	-1.595940	6.176130	0.795423
39	1	0	-0.856526	6.058325	1.599623
40	1	0	-1.640107	7.227487	0.503384
41	1	0	-2.580112	5.869489	1.176822
42	6	0	1.221325	-0.442890	1.769033
43	1	0	0.278011	-0.720010	2.264177
44	1	0	1.300723	0.643867	1.899870
45	6	0	2.360125	-1.138921	2.537639
46	1	0	2.289606	-2.229957	2.438153
47	1	0	3.346042	-0.842877	2.172576
48	1	0	1.394542	-1.823699	0.130942

49	1	0	1.820696	-0.120932	-1.680741
50	1	0	2.312456	-0.903754	3.608429
51	6	0	3.574190	-0.251594	-0.480379
52	6	0	4.449174	0.672922	0.108417
53	6	0	4.116828	-1.461133	-0.942291
54	6	0	5.811076	0.395958	0.247695
55	1	0	4.053314	1.621712	0.463066
56	6	0	5.475825	-1.744540	-0.808161
57	1	0	3.461976	-2.188846	-1.417799
58	6	0	6.330731	-0.816322	-0.208386
59	1	0	6.466588	1.129968	0.709455
60	1	0	5.870864	-2.688172	-1.176411
61	1	0	7.390112	-1.033873	-0.103970

IM16 (SCF energy in toluene: -1252.815202 a.u; Free energy in toluene: -1252.343767 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-1.462711	-0.600505	-0.221085
2	6	0	1.289003	-0.910862	-1.084799
3	6	0	-1.196652	1.279019	-0.156531
4	6	0	-1.186956	2.057990	-1.336890
5	6	0	-1.089607	2.004588	1.043546
6	6	0	-1.080878	3.449077	-1.323521
7	1	0	-1.245956	1.567872	-2.309573
8	6	0	-0.992244	3.403599	1.087030
9	1	0	-1.065657	1.469971	1.992200
10	6	0	-0.986322	4.132712	-0.105640
11	1	0	-1.065000	4.026076	-2.244362
12	1	0	-0.913115	3.902934	2.047147
13	8	0	-0.892027	5.502500	-0.190372
14	6	0	-0.764178	6.230685	1.014415
15	1	0	0.140246	5.948305	1.570866
16	1	0	-0.693160	7.282730	0.730004
17	1	0	-1.635483	6.096092	1.670725
18	6	0	0.415786	-0.878268	0.179138
19	1	0	0.778681	-0.107705	0.867146
20	1	0	1.213913	0.055545	-1.601556
21	1	0	0.531374	-1.842302	0.715892
22	6	0	2.781076	-1.239099	-0.861180
23	1	0	2.871702	-2.197256	-0.329689
24	1	0	3.275518	-1.381089	-1.832567
25	6	0	3.552202	-0.158517	-0.075598

26	1	0	3.451761	0.799025	-0.602676
27	1	0	3.085843	-0.023953	0.906397
28	6	0	5.017789	-0.492283	0.098918
29	6	0	5.965126	-0.105011	-0.859716
30	6	0	5.462610	-1.230277	1.205187
31	6	0	7.311710	-0.444428	-0.721045
32	1	0	5.641069	0.473857	-1.721791
33	6	0	6.807777	-1.573212	1.349459
34	1	0	4.744111	-1.534014	1.963354
35	6	0	7.738578	-1.181631	0.385244
36	1	0	8.028632	-0.129053	-1.474622
37	1	0	7.130207	-2.142110	2.217673
38	1	0	8.786910	-1.444096	0.497255
39	1	0	0.897257	-1.656697	-1.796097
40	6	0	-4.528975	-1.229740	-0.522082
41	6	0	-4.889792	-1.314075	0.970683
42	6	0	-4.115792	-2.604902	-1.072685
43	6	0	-3.791701	-1.974040	1.816435
44	1	0	-5.817409	-1.895574	1.055417
45	1	0	-5.118203	-0.310501	1.350641
46	6	0	-3.030770	-3.306447	-0.238411
47	1	0	-5.002487	-3.249715	-1.092720
48	1	0	-3.784106	-2.507732	-2.115574
49	6	0	-3.415378	-3.350454	1.250379
50	1	0	-4.135511	-2.081416	2.851273
51	1	0	-2.905104	-1.328227	1.841680
52	1	0	-2.595883	-3.795065	1.829199
53	1	0	-4.268814	-4.034144	1.351066
54	1	0	-2.944858	-4.342347	-0.597793
55	1	0	-5.423970	-0.899927	-1.069679
56	7	0	-3.433636	-0.249527	-0.735541
57	1	0	-3.365780	-0.014822	-1.726039
58	1	0	-3.644432	0.631099	-0.267766
59	7	0	-1.722047	-2.621851	-0.415825
60	1	0	-1.029164	-3.038027	0.204561
61	1	0	-1.375687	-2.790495	-1.361086

TS8 (SCF energy in toluene: -1252.769126 a.u; Free energy in toluene: -1252.296576 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.482163	-0.731781	-0.263144
2	6	0	1.187311	0.407266	0.347152

3	6	0	2.210082	1.048912	-0.620924
4	1	0	2.177683	2.139277	-0.503392
5	6	0	-3.201280	-2.171328	-0.898764
6	6	0	-3.706857	-2.369472	0.540666
7	6	0	-2.367389	-3.379724	-1.365125
8	6	0	-2.582184	-2.725067	1.521835
9	1	0	-4.450566	-3.177461	0.526929
10	1	0	-4.236610	-1.467019	0.870391
11	6	0	-1.266415	-3.823928	-0.383176
12	1	0	-3.049362	-4.226412	-1.511122
13	1	0	-1.925647	-3.169817	-2.348881
14	6	0	-1.816032	-3.966471	1.046671
15	1	0	-2.999438	-2.904473	2.519135
16	1	0	-1.891836	-1.876817	1.608052
17	1	0	-0.993143	-4.200675	1.734379
18	1	0	-2.485255	-4.837128	1.061142
19	1	0	-0.914217	-4.815450	-0.707996
20	1	0	-4.079946	-2.097396	-1.557489
21	7	0	-2.395825	-0.927969	-0.995492
22	1	0	-2.267393	-0.667537	-1.973707
23	1	0	-2.887699	-0.143731	-0.566467
24	7	0	-0.133528	-2.860157	-0.406570
25	1	0	0.568662	-3.154468	0.272008
26	1	0	0.324986	-2.907336	-1.316638
27	6	0	-0.433172	1.123526	-0.097888
28	6	0	-0.508044	1.874210	-1.326990
29	6	0	-1.179097	1.715468	0.975812
30	6	0	-1.245602	3.042439	-1.460006
31	1	0	0.021576	1.515999	-2.205559
32	6	0	-1.923244	2.892854	0.841487
33	1	0	-1.189872	1.231940	1.947945
34	6	0	-1.961376	3.574346	-0.377743
35	1	0	-1.281395	3.567976	-2.411132
36	1	0	-2.466149	3.265687	1.704624
37	8	0	-2.655407	4.743813	-0.620188
38	6	0	-3.355454	5.320039	0.460257
39	1	0	-2.686775	5.577236	1.294570
40	1	0	-3.815209	6.234578	0.078458
41	1	0	-4.146301	4.657218	0.841997
42	6	0	1.492208	0.709962	1.821872
43	1	0	1.077820	1.693336	2.082359
44	1	0	2.578730	0.789657	1.948706
45	6	0	0.984696	-0.339303	2.817839
46	1	0	-0.097875	-0.487075	2.744484

47	1	0	1.460563	-1.311311	2.637475
48	1	0	1.332959	-0.694664	0.222679
49	1	0	1.900414	0.842354	-1.649312
50	1	0	1.214751	-0.046054	3.848360
51	6	0	3.633144	0.552437	-0.453469
52	6	0	4.591540	1.289581	0.256481
53	6	0	4.031766	-0.670199	-1.017220
54	6	0	5.896104	0.815225	0.415489
55	1	0	4.312175	2.249901	0.683002
56	6	0	5.332612	-1.148752	-0.864156
57	1	0	3.311621	-1.244682	-1.597022
58	6	0	6.271291	-0.407578	-0.141254
59	1	0	6.620226	1.405784	0.970476
60	1	0	5.618013	-2.095459	-1.315735
61	1	0	7.286162	-0.776372	-0.021843

TS9 (SCF energy in toluene: -1252.767195 a.u; Free energy in toluene: -1252.294542 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	1.319186	-0.514314	0.727375
2	6	0	-0.772847	0.533117	2.902556
3	6	0	0.558335	1.181606	0.627536
4	6	0	1.154868	2.189584	1.464347
5	6	0	0.158336	1.668157	-0.660836
6	6	0	1.354249	3.499707	1.047593
7	1	0	1.476543	1.925482	2.467741
8	6	0	0.352185	2.988381	-1.078145
9	1	0	-0.314575	0.989263	-1.364882
10	6	0	0.952513	3.921726	-0.226803
11	1	0	1.821846	4.225433	1.708429
12	1	0	0.025840	3.272001	-2.074011
13	8	0	1.188844	5.247191	-0.535263
14	6	0	0.758473	5.708122	-1.797022
15	1	0	-0.327358	5.594755	-1.929116
16	1	0	1.012880	6.769639	-1.841663
17	1	0	1.264225	5.186744	-2.623309
18	6	0	-0.564646	0.007460	1.479573
19	1	0	-1.060000	1.591332	2.893936
20	1	0	-0.249973	-1.061671	1.591042
21	1	0	0.140912	0.447017	3.497966
22	6	0	3.874496	-1.199159	-0.958254
23	6	0	3.148580	-1.715874	-2.212944

24	6	0	4.162299	-2.346077	0.027923
25	6	0	1.899490	-2.543609	-1.881945
26	1	0	3.858434	-2.334265	-2.778711
27	1	0	2.890098	-0.869842	-2.861833
28	6	0	2.951582	-3.243242	0.347520
29	1	0	4.943371	-2.980711	-0.408289
30	1	0	4.582722	-1.940336	0.958469
31	6	0	2.246325	-3.704232	-0.940055
32	1	0	1.455197	-2.933372	-2.804806
33	1	0	1.148449	-1.897264	-1.408287
34	1	0	1.345099	-4.275005	-0.680838
35	1	0	2.916743	-4.405964	-1.454238
36	1	0	3.331487	-4.139287	0.863099
37	1	0	4.842116	-0.781817	-1.276582
38	7	0	3.067599	-0.146010	-0.293214
39	1	0	3.630975	0.339352	0.405655
40	1	0	2.786353	0.570137	-0.963827
41	7	0	1.992572	-2.525524	1.228752
42	1	0	1.199338	-3.136084	1.423607
43	1	0	2.432761	-2.348815	2.132006
44	1	0	-1.553027	-0.025715	3.433153
45	6	0	-1.853795	-0.036301	0.647806
46	1	0	-2.243869	0.982478	0.521724
47	1	0	-1.624407	-0.396583	-0.360860
48	6	0	-2.974260	-0.938880	1.219373
49	1	0	-2.584373	-1.957190	1.349502
50	1	0	-3.265611	-0.586130	2.214812
51	6	0	-4.196279	-0.976772	0.327144
52	6	0	-5.189631	0.008121	0.427512
53	6	0	-4.349831	-1.972662	-0.647438
54	6	0	-6.299207	0.000234	-0.418305
55	1	0	-5.091272	0.787633	1.179606
56	6	0	-5.458052	-1.986271	-1.496114
57	1	0	-3.593296	-2.749485	-0.737107
58	6	0	-6.437772	-0.998188	-1.384731
59	1	0	-7.058160	0.771853	-0.320268
60	1	0	-5.558287	-2.771190	-2.241158
59	1	0	-7.058160	0.771853	-0.320268
60	1	0	-5.558287	-2.771190	-2.241158
61	1	0	-7.302797	-1.008057	-2.041882

TS10 (SCF energy in toluene: -1252.767907 a.u; Free energy in toluene: -1252.296979 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-1.311494	-0.746942	-0.501501
2	6	0	1.597572	1.045021	-0.968099
3	6	0	-0.942419	1.066411	-0.306574
4	6	0	-1.231570	1.909426	-1.438966
5	6	0	-1.200186	1.680012	0.961131
6	6	0	-1.766414	3.181601	-1.306953
7	1	0	-1.031482	1.535710	-2.441046
8	6	0	-1.740076	2.964168	1.093421
9	1	0	-0.962090	1.128987	1.868867
10	6	0	-2.031907	3.727797	-0.040264
11	1	0	-1.991337	3.783756	-2.183804
12	1	0	-1.918470	3.356123	2.089946
13	8	0	-2.563333	5.002648	-0.029483
14	6	0	-2.819334	5.589926	1.227058
15	1	0	-1.904454	5.692153	1.828691
16	1	0	-3.225324	6.584175	1.026784
17	1	0	-3.554855	5.015671	1.809751
18	6	0	0.560366	0.117556	-0.316451
19	1	0	0.814986	-0.064765	0.732942
20	1	0	1.573346	2.018978	-0.461031
21	1	0	0.645798	-0.854404	-0.858456
22	6	0	3.040239	0.508861	-0.970993
23	1	0	3.075284	-0.470635	-1.467825
24	1	0	3.662975	1.180057	-1.577509
25	6	0	3.679577	0.387426	0.428499
26	1	0	3.609032	1.360304	0.932026
27	1	0	3.101944	-0.319581	1.035112
28	6	0	5.125925	-0.055922	0.380256
29	6	0	6.160656	0.880623	0.244311
30	6	0	5.467402	-1.414483	0.434821
31	6	0	7.493331	0.474938	0.163751
32	1	0	5.916436	1.939873	0.205906
33	6	0	6.798480	-1.826621	0.354193
34	1	0	4.679414	-2.156183	0.546718
35	6	0	7.817465	-0.882164	0.217888
36	1	0	8.279167	1.218826	0.063328
37	1	0	7.040347	-2.885088	0.402725
38	1	0	8.854549	-1.200254	0.158809
39	1	0	1.299916	1.238420	-2.004836
40	6	0	-4.221966	-1.861289	-0.282583

41	6	0	-4.293637	-1.964657	1.250985
42	6	0	-3.693558	-3.168450	-0.903482
43	6	0	-2.976430	-2.434287	1.882511
44	1	0	-5.093186	-2.675153	1.500364
45	1	0	-4.598285	-0.997104	1.669063
46	6	0	-2.405016	-3.717506	-0.261000
47	1	0	-4.473189	-3.932994	-0.798728
48	1	0	-3.542443	-3.032740	-1.983191
49	6	0	-2.522944	-3.766931	1.272186
50	1	0	-3.101367	-2.544514	2.965717
51	1	0	-2.202195	-1.672986	1.721397
52	1	0	-1.564763	-4.084573	1.703753
53	1	0	-3.248275	-4.551878	1.525255
54	1	0	-2.269579	-4.749281	-0.621340
55	1	0	-5.245293	-1.704067	-0.656945
56	7	0	-3.360186	-0.721159	-0.683908
57	1	0	-3.491936	-0.513626	-1.674109
58	1	0	-3.629987	0.125920	-0.184418
59	7	0	-1.236299	-2.889597	-0.661740
60	1	0	-0.397631	-3.250827	-0.206825
61	1	0	-1.076501	-2.998534	-1.663529

IM2' (SCF energy in toluene: -905.991947 a.u; Free energy in toluene: -905.642382 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.998354	-1.455364	-0.283922
2	6	0	0.805934	-1.698387	-0.815481
3	6	0	0.349587	-2.788710	0.026947
4	1	0	0.761900	-2.864598	1.039362
5	1	0	0.184231	-3.768633	-0.431580
6	6	0	-3.586921	1.661810	1.256928
7	6	0	-4.067823	2.899386	0.475999
8	6	0	-2.057112	1.514398	1.143457
9	6	0	-3.590919	2.893721	-0.984445
10	1	0	-3.684824	3.794712	0.983992
11	1	0	-5.163105	2.963857	0.520671
12	6	0	-1.538330	1.509285	-0.305794
13	1	0	-1.594589	2.357693	1.670728
14	1	0	-1.723584	0.600719	1.649451
15	6	0	-2.064111	2.741110	-1.071371
16	1	0	-3.901188	3.819034	-1.483321
17	1	0	-4.080701	2.072799	-1.520775

18	1	0	-1.740791	2.692373	-2.119672
19	1	0	-1.586726	3.634419	-0.645205
20	1	0	-0.444598	1.549521	-0.281635
21	1	0	-3.827311	1.818988	2.322592
22	7	0	-4.245038	0.451036	0.724532
23	1	0	-3.905468	-0.374396	1.216424
24	1	0	-5.249241	0.506575	0.879068
25	7	0	-1.893338	0.218938	-0.967096
26	1	0	-2.909604	0.108218	-0.892008
27	1	0	-1.653262	0.274953	-1.955884
28	8	0	-2.697565	-2.291685	0.843389
29	6	0	-3.577618	-3.133182	0.084448
30	1	0	-4.310122	-2.477333	-0.390571
31	1	0	-3.033707	-3.681526	-0.691388
32	1	0	-4.101916	-3.839239	0.739893
33	6	0	1.861527	-0.711619	-0.346222
34	1	0	1.745013	0.252429	-0.862869
35	1	0	1.737083	-0.503728	0.724513
36	6	0	3.310765	-1.212641	-0.586670
37	1	0	3.441023	-2.160632	-0.051341
38	1	0	3.430472	-1.436362	-1.654424
39	6	0	4.366821	-0.221975	-0.152376
40	6	0	4.846316	-0.209422	1.165720
41	6	0	4.865534	0.739025	-1.044042
42	6	0	5.791006	0.730200	1.580578
43	1	0	4.477028	-0.950442	1.871257
44	6	0	5.810355	1.681394	-0.635245
45	1	0	4.512079	0.742038	-2.072938
46	6	0	6.277159	1.680840	0.680605
47	1	0	6.151840	0.716925	2.605749
48	1	0	6.186322	2.412798	-1.345986
49	1	0	7.015808	2.410681	1.000184
50	1	0	0.884550	-1.911853	-1.889161
51	1	0	-1.926566	-2.817547	1.127316

1a (SCF energy in toluene: -388.321755 a.u; Free energy in toluene: -388.167277 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.245616	0.173257	-0.365113
2	6	0	-2.487414	1.307143	-0.069536
3	6	0	-1.151783	1.176391	0.312109
4	6	0	-0.548396	-0.084952	0.405833

5	6	0	-1.322279	-1.214665	0.107435
6	6	0	-2.658287	-1.089672	-0.274640
7	1	0	-4.286426	0.272559	-0.659143
8	1	0	-2.936956	2.294246	-0.131771
9	1	0	-0.568887	2.064229	0.546148
10	1	0	-0.873654	-2.202739	0.181276
11	1	0	-3.241715	-1.978758	-0.497096
12	6	0	0.911536	-0.219953	0.780171
13	1	0	1.201753	0.592749	1.455766
14	1	0	1.067717	-1.155775	1.331103
15	6	0	1.851534	-0.200323	-0.451112
16	1	0	1.714682	0.739387	-0.998741
17	1	0	1.543352	-1.006833	-1.131298
18	6	0	3.297789	-0.374690	-0.079288
19	6	0	4.265355	0.511461	-0.314600
20	1	0	3.547305	-1.305187	0.433604
21	1	0	5.293606	0.329141	-0.016623
22	1	0	4.064591	1.452995	-0.820777

2a (SCF energy in toluene: -522.888236 a.u; Free energy in toluene: -522.76702 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.085549	0.023679	0.000023
2	6	0	0.464652	1.289490	-0.000182
3	6	0	0.247589	-1.101392	0.000276
4	6	0	-0.915684	1.424379	-0.000116
5	1	0	1.084632	2.181266	-0.000402
6	6	0	-1.143524	-0.990942	0.000333
7	1	0	0.694235	-2.091602	0.000445
8	6	0	-1.730037	0.281052	0.000144
9	1	0	-1.393303	2.398912	-0.000281
10	1	0	-1.752958	-1.886992	0.000542
11	8	0	-3.074727	0.514175	0.000204
12	6	0	-3.951321	-0.601541	-0.000325
13	1	0	-3.815703	-1.224304	0.893056
14	1	0	-4.961948	-0.190475	-0.000769
15	1	0	-3.814819	-1.224135	-0.893683
16	5	0	2.635537	-0.120430	-0.000040
17	8	0	3.395637	1.026925	0.000201
18	1	0	4.348896	0.885643	0.000444
19	8	0	3.173291	-1.387661	-0.000326
20	1	0	4.136330	-1.422020	-0.000702

MeOH (SCF energy in toluene: -115.743891 a.u; Free energy in toluene: -115.71522 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.749330	-0.122046	-0.000067
2	6	0	-0.661572	0.019398	-0.000013
3	1	0	-1.037892	0.542800	0.891984
4	1	0	-1.038584	0.543340	-0.891511
5	1	0	-1.082431	-0.989421	-0.000029
6	1	0	1.133699	0.763265	0.000172

MeOB(OH)$_2$ (SCF energy in toluene: -291.850897 a.u; Free energy in toluene: -291.803582 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.519363	-0.004493	0.000259
2	8	0	-1.703488	-0.701193	0.002737
3	1	0	-1.544228	-1.652312	0.001144
4	8	0	-0.541158	1.366507	0.000014
5	1	0	-1.446926	1.696073	-0.008362
6	8	0	0.659427	-0.694784	-0.005384
7	6	0	1.917425	-0.030000	0.002049
8	1	0	2.384972	-0.135667	0.987424
9	1	0	2.565008	-0.503136	-0.742500
10	1	0	1.815193	1.033264	-0.230237

3a (SCF energy in toluene: -735.181125 a.u; Free energy in toluene: -734.900417 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.724835	2.394992	0.032340
2	6	0	-3.079290	3.664902	-0.747498
3	1	0	-3.000419	3.501349	-1.828416
4	1	0	-2.406593	4.491130	-0.490536
5	6	0	0.630750	0.405843	0.413843
6	6	0	1.533031	0.993689	1.315414
7	6	0	1.165078	-0.356275	-0.627554
8	6	0	2.906061	0.832731	1.182601
9	1	0	1.149967	1.589387	2.141014
10	6	0	2.543932	-0.530024	-0.780049

11	1	0	0.499574	-0.843732	-1.333370
12	6	0	3.423266	0.067344	0.128533
13	1	0	3.598467	1.284569	1.885444
14	1	0	2.913594	-1.133684	-1.600609
15	8	0	4.785866	-0.037942	0.081453
16	6	0	5.360084	-0.806570	-0.962463
17	1	0	5.117009	-0.395610	-1.951016
18	1	0	6.439828	-0.761536	-0.812109
19	1	0	5.034337	-1.854112	-0.922453
20	6	0	-1.292227	1.915869	-0.234447
21	1	0	-1.149605	1.734408	-1.307971
22	6	0	-0.871163	0.660126	0.569325
23	1	0	-0.590411	2.720381	0.019098
24	1	0	-1.033122	0.903264	1.628272
25	6	0	-1.709660	-0.583687	0.282807
26	6	0	-1.969691	-1.489010	1.321974
27	6	0	-2.214326	-0.884803	-0.990194
28	6	0	-2.701727	-2.654672	1.101675
29	1	0	-1.588037	-1.275165	2.317459
30	6	0	-2.947692	-2.051770	-1.216954
31	1	0	-2.043235	-0.201807	-1.816759
32	6	0	-3.194498	-2.942037	-0.172546
33	1	0	-2.890149	-3.336964	1.925869
34	1	0	-3.329681	-2.260688	-2.212409
35	1	0	-3.768028	-3.847545	-0.347691
36	1	0	-3.434654	1.598540	-0.219179
37	1	0	-4.102675	3.991184	-0.535676
38	1	0	-2.845657	2.580281	1.108580
