

Supporting Information

On the Enhanced Reactivity and Selectivity of Triazole Formation in Molecular Flasks. A Theoretical Rationale

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Complete reference 12

Gaussian 09, Revision A.1, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

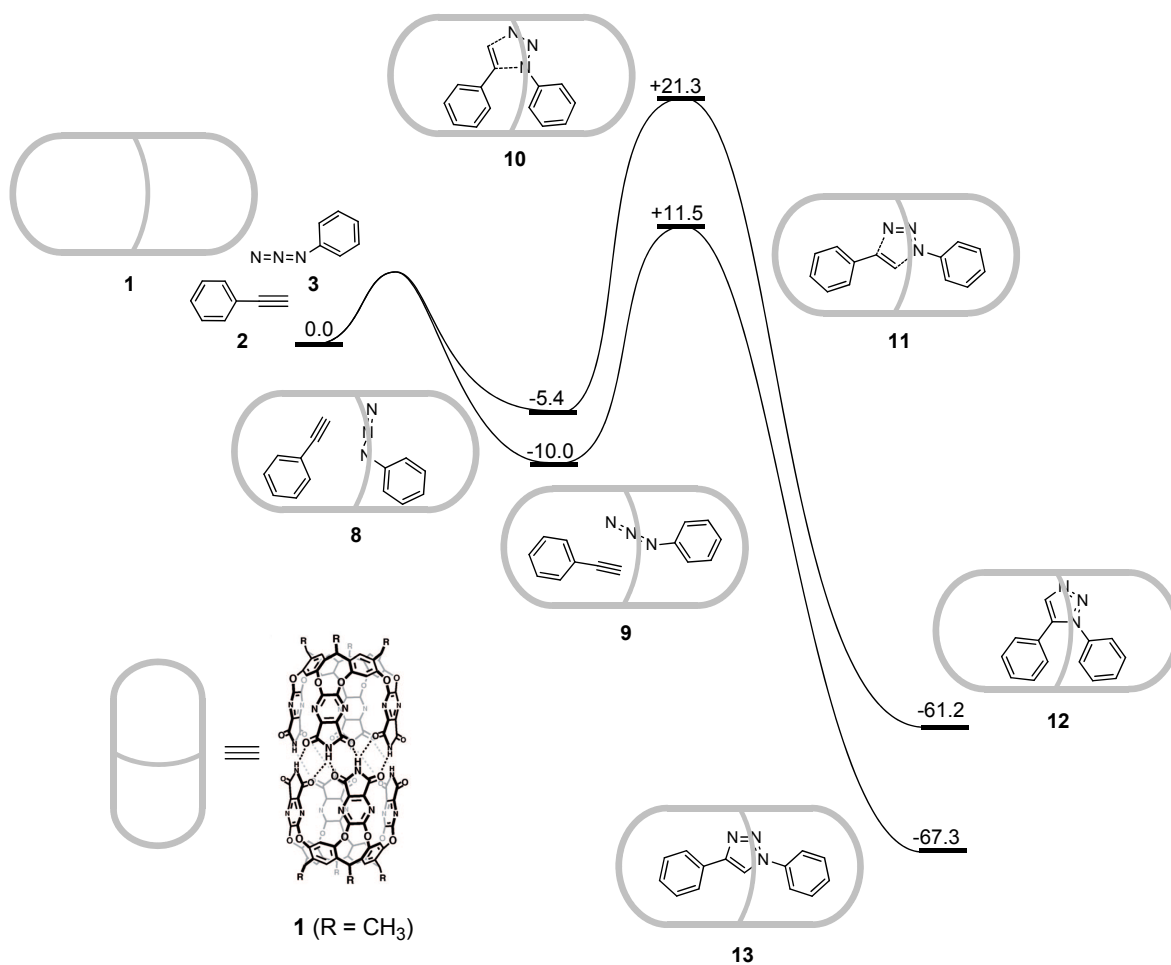


Figure S1 Energy profile for the 1,3-dipolar cycloaddition of phenylacetylene (**2**) and phenylazide (**3**) assisted by the self-assembled molecular flask **1**, calculated at the ONIOM[B3LYP/6-311G(d,p):PM6] level

Cartesian coordinates, energy, and imaginary frequency (TSs) for all calculations

Structure 1

E(RPM6) = -0.499641311915

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-9.106229	-1.320686	-2.248840
2	6	0	-8.569295	-2.593413	-1.978385
3	6	0	-7.454630	-2.985790	-2.738442
4	6	0	-6.846635	-2.142997	-3.672541
5	6	0	-7.405895	-0.882938	-3.869936
6	6	0	-8.555430	-0.438129	-3.190548
7	6	0	-8.555492	3.190526	-0.438110
8	6	0	-9.106247	2.248794	-1.320669
9	6	0	-8.569294	1.978350	-2.593390
10	6	0	-7.454646	2.738425	-2.985763
11	6	0	-6.846685	3.672549	-2.142969
12	6	0	-7.405964	3.869944	-0.882918
13	6	0	-6.846582	-3.672585	2.142935
14	6	0	-7.405883	-3.870003	0.882896
15	6	0	-8.555415	-3.190595	0.438095
16	6	0	-9.106178	-2.248870	1.320658
17	6	0	-8.569210	-1.978411	2.593369
18	6	0	-7.454539	-2.738459	2.985728
19	6	0	-7.405893	0.882896	3.869944
20	6	0	-8.555405	0.438058	3.190542
21	6	0	-9.106221	1.320602	2.248833
22	6	0	-8.569321	2.593345	1.978384
23	6	0	-7.454655	2.985742	2.738436
24	6	0	-6.846651	2.142962	3.672544
25	6	0	-9.237636	-3.426769	-0.899413
26	6	0	-9.237615	0.899386	-3.426762
27	6	0	-9.237710	3.426670	0.899411
28	6	0	-9.237549	-0.899474	3.426758
29	8	0	-6.954952	-4.309515	-2.630839
30	8	0	-6.855109	-0.052185	-4.871954
31	8	0	-6.954959	2.630830	-4.309485
32	8	0	-6.855186	4.871972	-0.052168
33	8	0	-6.855127	-4.872053	0.052158
34	8	0	-6.954851	-2.630862	4.309450
35	8	0	-6.855128	0.052152	4.871984
36	8	0	-6.954976	4.309467	2.630835
37	6	0	-3.413760	-0.637905	4.385191
38	6	0	-3.452824	-2.070056	4.328943
39	7	0	-4.598023	-2.765679	4.283969
40	6	0	-5.724994	-2.000843	4.361448
41	6	0	-5.679939	-0.581474	4.544841
42	7	0	-4.510472	0.122647	4.512944
43	7	0	-4.510476	-4.512947	0.122581
44	6	0	-3.413797	-4.385084	-0.637999
45	6	0	-3.452909	-4.328787	-2.070149
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48	6	0	-5.679963	-4.544887	-0.581504

49	7	0	-4.510466	-0.122596	-4.512739
50	6	0	-5.679956	0.581483	-4.544762
51	6	0	-5.725075	2.000858	-4.361446
52	7	0	-4.598139	2.765742	-4.283943
53	6	0	-3.452914	2.070156	-4.328787
54	6	0	-3.413791	0.638000	-4.384924
55	7	0	-4.598153	4.283945	2.765711
56	6	0	-5.725102	4.361447	2.000847
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59	6	0	-3.413840	4.385063	0.637957
60	6	0	-3.452938	4.328853	2.070111
61	6	0	-1.968624	-0.186152	4.266270
62	6	0	-2.029977	-2.601768	4.287663
63	6	0	-1.968651	-4.266129	-0.186285
64	6	0	-2.030089	-4.287192	-2.601904
65	6	0	-2.030097	2.601931	-4.287284
66	6	0	-1.968637	0.186315	-4.265905
67	6	0	-1.968691	4.266140	0.186240
68	6	0	-2.030112	4.287357	2.601858
69	8	0	-1.586816	3.708773	-4.286740
70	7	0	-1.226302	1.402129	-4.246773
71	8	0	-1.507469	-0.915353	-4.147295
72	8	0	-1.586790	-4.286397	-3.708740
73	7	0	-1.226305	-4.246787	-1.402089
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82	1	0	-0.192479	-4.242504	-1.434853
83	1	0	-0.192406	-1.434640	4.242779
84	1	0	-0.192508	4.242691	1.434794
85	6	0	9.106730	2.523217	0.660425
86	6	0	8.555476	2.562791	1.950299
87	6	0	7.405767	3.357283	2.117125
88	6	0	6.847426	4.111105	1.087835
89	6	0	7.455801	4.048653	-0.168505
90	6	0	8.570090	3.233718	-0.429744
91	6	0	8.570083	-0.429703	-3.233649
92	6	0	9.106723	0.660479	-2.523167
93	6	0	8.555453	1.950346	-2.562734
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96	6	0	7.455740	-0.168483	-4.048527
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98	6	0	7.455790	0.168529	4.048554
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101	6	0	8.555506	-1.950274	2.562725
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127	7	0	4.599118	1.060720	4.983271
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130	7	0	4.508909	3.265179	3.103152
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133	7	0	4.599165	4.983517	-1.060742
134	6	0	5.725272	4.500164	-1.660045
135	6	0	5.678712	3.626495	-2.793464
136	7	0	4.508888	3.103347	-3.265155
137	6	0	3.413085	3.547680	-2.633177
138	6	0	3.453467	4.520554	-1.580575
139	7	0	4.508959	-3.265363	-3.103219
140	6	0	5.678738	-2.793564	-3.626368
141	6	0	5.725207	-1.660072	-4.499945
142	7	0	4.599050	-1.060764	-4.983178
143	6	0	3.453395	-1.580685	-4.520204
144	6	0	3.413107	-2.633387	-3.547437
145	6	0	2.031606	-4.862560	1.168719
146	6	0	1.967991	-3.139979	2.862559
147	6	0	2.031483	1.168805	4.862291
148	6	0	1.967960	2.862725	3.139789
149	6	0	1.967931	3.140165	-2.862772
150	6	0	2.031521	4.862708	-1.168897
151	6	0	2.031416	-1.168955	-4.862168
152	6	0	1.967975	-2.863169	-3.139955
153	8	0	1.504667	2.276756	-3.555644
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158	8	0	1.588902	0.382666	5.642058
159	7	0	1.227243	-3.983736	1.985367
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186	1	0	10.299673	1.589456	2.727962
187	1	0	9.993399	-0.491995	1.907217
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193	6	0	-9.354841	1.258902	-4.906473
194	1	0	-9.880629	0.477889	-5.467521
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199	1	0	-9.897557	5.045579	2.201515
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201	6	0	-9.354711	-1.259008	4.906467
202	1	0	-9.880486	-0.478009	5.467546
203	1	0	-9.896939	-2.201620	5.045809
204	1	0	-8.369503	-1.388351	5.386729
205	6	0	-9.355009	-4.906470	-1.258939
206	1	0	-9.880838	-5.467472	-0.477921
207	1	0	-9.897294	-5.045742	-2.201529
208	1	0	-8.369879	-5.386885	-1.388317
209	6	0	9.354145	2.572949	4.363576
210	1	0	9.895230	2.003712	5.128518
211	1	0	9.880649	3.521809	4.209759
212	1	0	8.368595	2.821139	4.793858
213	6	0	9.354200	-4.363537	2.572935
214	1	0	9.895288	-5.128489	2.003713
215	1	0	9.880704	-4.209696	3.521791
216	1	0	8.368651	-4.793820	2.821133
217	6	0	9.354380	-2.572831	-4.363579
218	1	0	9.895508	-2.003543	-5.128452
219	1	0	9.880942	-3.521652	-4.209721
220	1	0	8.368902	-2.821095	-4.793985
221	6	0	9.354072	4.363626	-2.572943
222	1	0	9.895145	5.128593	-2.003729
223	1	0	9.880556	4.209810	-3.521813
224	1	0	8.368499	4.793871	-2.821112

Monomer precursor of 1

E(RPM6) = -0.226889219121

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.849316	-3.534161	1.831761

2	6	0	1.256468	-2.863112	2.914822
3	6	0	1.915543	-1.709830	3.375660
4	6	0	3.133159	-1.272084	2.855744
5	6	0	3.691216	-2.003919	1.806552
6	6	0	3.048629	-3.115257	1.231055
7	6	0	1.256227	-2.865166	-2.912907
8	6	0	1.849149	-3.535396	-1.829363
9	6	0	3.048497	-3.116068	-1.229048
10	6	0	3.691017	-2.005111	-1.805376
11	6	0	3.132901	-1.274083	-2.855087
12	6	0	1.915278	-1.712250	-3.374673
13	6	0	-3.132927	-1.271873	2.855955
14	6	0	-1.915316	-1.709685	3.375874
15	6	0	-1.256309	-2.862972	2.914984
16	6	0	-1.849258	-3.534010	1.831953
17	6	0	-3.048588	-3.115098	1.231317
18	6	0	-3.691069	-2.003680	1.806803
19	6	0	-3.691294	-2.005230	-1.805106
20	6	0	-3.048725	-3.116142	-1.228781
21	6	0	-1.849415	-3.535522	-1.829172
22	6	0	-1.256551	-2.865286	-2.912724
23	6	0	-1.915609	-1.712327	-3.374417
24	6	0	-3.133224	-1.274182	-2.854845
25	6	0	0.000087	-3.454707	3.528039
26	6	0	3.536308	-3.863818	0.001228
27	6	0	-0.000178	-3.457341	-3.525517
28	6	0	-3.536424	-3.863762	0.001612
29	8	0	1.373205	-0.987318	4.471058
30	8	0	4.995108	-1.678401	1.375906
31	8	0	4.994919	-1.679253	-1.375020
32	8	0	1.373085	-0.990531	-4.470688
33	8	0	-1.373096	-0.987179	4.471349
34	8	0	-4.994967	-1.678116	1.376215
35	8	0	-4.995185	-1.679373	-1.374706
36	8	0	-1.373222	-0.990622	-4.470326
37	6	0	-5.617445	1.744238	-0.718028
38	6	0	-5.617270	1.744910	0.716520
39	7	0	-5.363663	0.651141	1.448742
40	6	0	-5.119880	-0.473923	0.715262
41	6	0	-5.120041	-0.474591	-0.714813
42	7	0	-5.364003	0.649789	-1.449285
43	7	0	-1.447578	1.270566	3.770063
44	6	0	-0.716069	2.354471	3.472485
45	6	0	0.716376	2.354315	3.472023
46	7	0	1.447839	1.270291	3.769278
47	6	0	0.716286	0.161956	4.084755
48	6	0	-0.716077	0.162060	4.085044
49	7	0	5.363982	0.650808	1.448700
50	6	0	5.119997	-0.474127	0.715090
51	6	0	5.119852	-0.474565	-0.714986
52	7	0	5.363667	0.649936	-1.449321
53	6	0	5.617299	1.744259	-0.717942
54	6	0	5.617453	1.744692	0.716609
55	7	0	-1.447803	1.267454	-3.770031
56	6	0	-0.716275	0.158905	-4.084829
57	6	0	0.716085	0.158996	-4.085188
58	7	0	1.447615	1.267712	-3.771017
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60	6	0	-0.716314	2.351667	-3.473538
61	6	0	-5.944817	3.142039	-1.216620
62	6	0	-5.944531	3.143177	1.213873
63	6	0	-1.213948	3.725820	3.055509
64	6	0	1.214293	3.725505	3.054562

65	6	0	5.944613	3.142133	-1.216367
66	6	0	5.944865	3.142866	1.214126
67	6	0	1.214045	3.723444	-3.058086
68	6	0	-1.214196	3.723121	-3.056901
69	8	0	6.075272	3.590232	-2.314234
70	7	0	6.109388	3.895889	-0.001365
71	8	0	6.075756	3.591625	2.311695
72	8	0	2.311323	4.165441	2.886530
73	7	0	0.000199	4.469015	2.839129
74	8	0	-2.310970	4.166107	2.888404
75	7	0	-6.109204	3.896025	-0.001707
76	8	0	-6.075605	3.589982	-2.314535
77	8	0	-6.075050	3.592154	2.311396
78	7	0	-0.000085	4.466780	-2.842084
79	8	0	2.311080	4.163850	-2.891384
80	8	0	-2.311212	4.163157	-2.889030
81	1	0	6.323250	4.892852	-0.001691
82	1	0	0.000223	5.454385	2.577303
83	1	0	-6.322915	4.893020	-0.002151
84	1	0	-0.000089	5.452327	-2.580925
85	1	0	3.639266	-0.390191	-3.269812
86	1	0	1.350927	-4.422347	-1.430844
87	1	0	3.037818	-4.876506	0.001587
88	1	0	3.639547	-0.387883	3.269780
89	1	0	1.351080	-4.421411	1.433930
90	1	0	0.000012	-4.556065	3.271685
91	1	0	-1.351070	-4.421287	1.434117
92	1	0	-3.639256	-0.387648	3.270018
93	1	0	-3.037971	-4.876469	0.002011
94	1	0	-3.639606	-0.390287	-3.269538
95	1	0	-1.351203	-4.422490	-1.430681
96	1	0	-0.000114	-4.558507	-3.268346
97	6	0	0.000192	-3.391714	5.055426
98	1	0	-0.886540	-3.880405	5.475449
99	1	0	0.887083	-3.880223	5.475327
100	1	0	0.000113	-2.354338	5.432458
101	6	0	-5.036453	-4.141690	0.001826
102	1	0	-5.336861	-4.710890	-0.885586
103	1	0	-5.336728	-4.710251	0.889696
104	1	0	-5.635938	-3.215489	0.001541
105	6	0	-0.000284	-3.395492	-5.052951
106	1	0	0.886441	-3.884512	-5.472611
107	1	0	-0.887184	-3.884299	-5.472487
108	1	0	-0.000178	-2.358400	-5.430761
109	6	0	5.036326	-4.141814	0.001247
110	1	0	5.336695	-4.710358	0.889097
111	1	0	5.336588	-4.711059	-0.886184
112	1	0	5.635855	-3.215641	0.000855

Structure 2 (B3LYP)

E(RB3LYP) = -308.473532621

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.593602	0.000005	-0.000156
2	6	0	-0.119509	1.210535	-0.000085
3	6	0	-0.119505	-1.210531	-0.000085

4	6	0	-1.509479	1.206101	0.000045
5	1	0	0.427223	2.145662	-0.000125
6	6	0	-1.509473	-1.206105	0.000045
7	1	0	0.427235	-2.145654	-0.000125
8	6	0	-2.208661	-0.000003	0.000104
9	1	0	-2.048728	2.146590	0.000104
10	1	0	-2.048717	-2.146596	0.000103
11	1	0	-3.292689	-0.000005	0.000210
12	6	0	2.021751	-0.000003	-0.000190
13	6	0	3.225872	0.000004	0.000231
14	1	0	4.288089	-0.000007	0.000387

Structure 2 (M06-2X)

E(RM062X) = -308.334329561

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.585761	0.000002	-0.000115
2	6	0	-0.118959	1.208480	-0.000058
3	6	0	-0.118961	-1.208477	-0.000058
4	6	0	-1.506787	1.204513	0.000027
5	1	0	0.432243	2.140628	-0.000086
6	6	0	-1.506788	-1.204512	0.000027
7	1	0	0.432244	-2.140623	-0.000085
8	6	0	-2.203064	0.000002	0.000063
9	1	0	-2.046622	2.143671	0.000070
10	1	0	-2.046623	-2.143669	0.000070
11	1	0	-3.286302	0.000003	0.000143
12	6	0	2.019823	-0.000018	-0.000099
13	6	0	3.220782	-0.000004	0.000214
14	1	0	4.284216	0.000074	-0.000109

Structure 3 (B3LYP)

E(RB3LYP) = -395.937058902

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.471982	-0.878193	-0.000137
2	7	0	2.415393	-0.085982	-0.000036
3	7	0	3.367263	0.529525	0.000207
4	6	0	0.148962	-0.361936	-0.000086
5	6	0	-0.154353	1.003707	-0.000102
6	6	0	-0.880572	-1.307146	0.000010
7	6	0	-1.484514	1.412522	-0.000027
8	1	0	0.640244	1.741639	-0.000173
9	6	0	-2.204868	-0.885746	0.000085
10	1	0	-0.623681	-2.359197	0.000026
11	6	0	-2.514362	0.474056	0.000065
12	1	0	-1.714058	2.472034	-0.000043
13	1	0	-2.998801	-1.623790	0.000159
14	1	0	-3.547931	0.799126	0.000123

Structure 3 (M06-2X)

E(RM062X) = -395.768451702

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.469681	-0.913723	-0.000063
2	7	0	2.392024	-0.096936	-0.000033
3	7	0	3.299755	0.563009	0.000115
4	6	0	0.153850	-0.377077	-0.000040
5	6	0	-0.127682	0.988927	-0.000053
6	6	0	-0.883960	-1.306964	0.000006
7	6	0	-1.450233	1.415107	-0.000016
8	1	0	0.676945	1.716076	-0.000096
9	6	0	-2.199439	-0.868782	0.000044
10	1	0	-0.636704	-2.361104	0.000013
11	6	0	-2.489902	0.492885	0.000033
12	1	0	-1.664805	2.477004	-0.000027
13	1	0	-3.003283	-1.594953	0.000083
14	1	0	-3.518173	0.831953	0.000062

Structure 4 (B3LYP)

E(RB3LYP) = -704.505364405

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.025746	0.490083	0.071591
2	6	0	1.076010	-0.328998	-0.065238
3	7	0	-1.096206	-0.337069	-0.071524
4	1	0	-0.130978	1.538518	0.283940
5	7	0	-0.675839	-1.610938	-0.285617
6	7	0	0.616780	-1.602775	-0.280549
7	6	0	2.508204	-0.018646	-0.001087
8	6	0	3.450976	-1.051808	-0.099127
9	6	0	2.966096	1.296798	0.157172
10	6	0	4.811834	-0.773136	-0.038515
11	1	0	3.098669	-2.067805	-0.223437
12	6	0	4.327910	1.571748	0.218852
13	1	0	2.257285	2.114647	0.228545
14	6	0	5.257464	0.537836	0.121538
15	1	0	5.527876	-1.583704	-0.116008
16	1	0	4.664124	2.595312	0.341311
17	1	0	6.318981	0.752663	0.168933
18	6	0	-2.484497	-0.030737	-0.020343
19	6	0	-2.933882	1.247118	-0.354994
20	6	0	-3.387762	-1.022488	0.366006
21	6	0	-4.293797	1.535643	-0.284346
22	1	0	-2.234571	2.003487	-0.689010
23	6	0	-4.744760	-0.724419	0.417552
24	1	0	-3.015730	-2.007235	0.612499
25	6	0	-5.203023	0.553533	0.100481
26	1	0	-4.641256	2.528736	-0.544271
27	1	0	-5.446257	-1.494968	0.715378
28	1	0	-6.261439	0.780640	0.148694

Structure 4 (M06-2X)

E(RM062X) = -704.215580233

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.028262	0.485706	0.068386
2	6	0	1.068215	-0.333383	-0.066112
3	7	0	-1.089275	-0.345177	-0.076346
4	1	0	-0.141769	1.534009	0.279929
5	7	0	-0.675222	-1.604264	-0.285339
6	7	0	0.610131	-1.601598	-0.279967
7	6	0	2.500762	-0.021846	-0.000103
8	6	0	3.440311	-1.047916	-0.123256
9	6	0	2.945191	1.288951	0.184799
10	6	0	4.797759	-0.763296	-0.061098
11	1	0	3.088700	-2.061848	-0.267461
12	6	0	4.303115	1.569955	0.248059
13	1	0	2.227899	2.096990	0.278333
14	6	0	5.234636	0.544205	0.125103
15	1	0	5.518524	-1.566372	-0.158898
16	1	0	4.635305	2.591092	0.392049
17	1	0	6.294483	0.763132	0.173545
18	6	0	-2.475742	-0.037189	-0.025000
19	6	0	-2.915506	1.230363	-0.390421
20	6	0	-3.372554	-1.014624	0.394200
21	6	0	-4.270625	1.527126	-0.315000
22	1	0	-2.211065	1.968573	-0.753530
23	6	0	-4.725136	-0.708493	0.449271
24	1	0	-2.998689	-1.992818	0.664419
25	6	0	-5.177907	0.560999	0.103478
26	1	0	-4.616367	2.513163	-0.599517
27	1	0	-5.427841	-1.466005	0.773960
28	1	0	-6.234152	0.794005	0.154910

Transition structure 5 (B3LYP)

Imaginary Freq: -404.0534 cm⁻¹
E(RB3LYP) = -704.374748903

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.276070	1.171559	-0.485452
2	6	0	1.287808	0.484891	-0.299978
3	7	0	-1.357066	-0.239636	-0.613504
4	1	0	-0.349859	2.012426	-0.668870
5	7	0	-0.671408	-1.263563	-0.330712
6	7	0	0.453509	-1.522753	-0.183966
7	6	0	2.699332	0.281641	-0.069937
8	6	0	3.382265	-0.838782	-0.565860
9	6	0	3.420623	1.249477	0.650905
10	6	0	4.750258	-0.977816	-0.357602

11	1	0	2.831401	-1.595652	-1.107474
12	6	0	4.785464	1.098107	0.865607
13	1	0	2.898074	2.114649	1.040911
14	6	0	5.456475	-0.014040	0.359366
15	1	0	5.265272	-1.846577	-0.751950
16	1	0	5.326626	1.851223	1.427391
17	1	0	6.521601	-0.129569	0.525130
18	6	0	-2.703100	-0.118859	-0.218721
19	6	0	-3.443835	0.913579	-0.806308
20	6	0	-3.304393	-0.943796	0.742067
21	6	0	-4.764974	1.124367	-0.427225
22	1	0	-2.977832	1.531276	-1.564680
23	6	0	-4.631520	-0.734804	1.097816
24	1	0	-2.730666	-1.743696	1.194789
25	6	0	-5.366902	0.301348	0.522742
26	1	0	-5.329733	1.927703	-0.886469
27	1	0	-5.091950	-1.382885	1.835067
28	1	0	-6.399591	0.461536	0.808915

Transition structure 5 (M06-2X)

Imaginary Freq: -480.4700 cm⁻¹
E(RM062X) = -704.069578001

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.165879	-0.988335	-0.793536
2	6	0	-1.201337	-0.408618	-0.458274
3	7	0	1.353863	0.482373	-0.792287
4	1	0	0.489819	-1.762406	-1.123724
5	7	0	0.645009	1.397875	-0.295638
6	7	0	-0.457462	1.610084	-0.053488
7	6	0	-2.605431	-0.286314	-0.130786
8	6	0	-3.345930	0.843615	-0.490278
9	6	0	-3.244149	-1.335987	0.540317
10	6	0	-4.701361	0.912971	-0.198036
11	1	0	-2.849348	1.661465	-0.996311
12	6	0	-4.596081	-1.254212	0.843100
13	1	0	-2.667536	-2.209231	0.820333
14	6	0	-5.329591	-0.131957	0.471441
15	1	0	-5.267690	1.790017	-0.487916
16	1	0	-5.079462	-2.070427	1.366811
17	1	0	-6.385907	-0.071570	0.704375
18	6	0	2.638747	0.223082	-0.269858
19	6	0	3.423945	-0.678005	-0.988557
20	6	0	3.117332	0.776190	0.919493
21	6	0	4.676449	-1.035952	-0.510414
22	1	0	3.042713	-1.076151	-1.921438
23	6	0	4.379762	0.425107	1.376712
24	1	0	2.503554	1.478092	1.471711
25	6	0	5.161390	-0.484575	0.671082
26	1	0	5.281060	-1.738595	-1.070889
27	1	0	4.752585	0.861858	2.295496
28	1	0	6.143154	-0.757433	1.037004

Transition structure 6 (B3LYP)

Imaginary Freq: -428.6075 cm⁻¹
E(RB3LYP) = -704.376592509

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.389844	1.729952	0.169135
2	6	0	1.167242	2.943563	0.252951
3	7	0	-0.855930	1.156288	-0.372647
4	7	0	-1.242261	2.348601	-0.242009
5	7	0	-0.740028	3.391722	-0.046943
6	6	0	-1.748040	0.080099	-0.224526
7	6	0	-1.273340	-1.188360	-0.582186
8	6	0	-3.049086	0.213991	0.283445
9	6	0	-2.088733	-2.304067	-0.428518
10	1	0	-0.269018	-1.282292	-0.975442
11	6	0	-3.858052	-0.907881	0.417686
12	1	0	-3.416301	1.195553	0.558538
13	6	0	-3.384342	-2.172253	0.068021
14	1	0	-1.710073	-3.281321	-0.706177
15	1	0	-4.865553	-0.792873	0.802034
16	1	0	-4.019680	-3.043105	0.178603
17	6	0	2.008985	0.442013	0.137858
18	6	0	2.067467	-0.350554	1.296568
19	6	0	2.596036	-0.035807	-1.046700
20	6	0	2.704605	-1.585550	1.268956
21	1	0	1.610002	0.011528	2.209070
22	6	0	3.228026	-1.273311	-1.065373
23	1	0	2.548447	0.571576	-1.942276
24	6	0	3.285386	-2.052142	0.090540
25	1	0	2.745400	-2.187044	2.169891
26	1	0	3.679555	-1.630556	-1.983988
27	1	0	3.780006	-3.016501	0.072692
28	1	0	1.508764	3.940601	0.421111

Transition structure 6 (M06-2X)

Imaginary Freq: -499.2939 cm⁻¹
E(RM062X) = -704.073513950

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.954710	1.883745	0.360323
2	6	0	0.642785	3.052837	0.599526
3	7	0	-0.881539	1.213209	-0.684967
4	7	0	-1.510484	2.277477	-0.447803
5	7	0	-1.292794	3.336000	-0.038603
6	6	0	-1.487438	-0.032587	-0.428040
7	6	0	-0.811855	-1.161091	-0.894560
8	6	0	-2.666547	-0.176447	0.307957
9	6	0	-1.308974	-2.425725	-0.612092
10	1	0	0.102377	-1.029552	-1.461319
11	6	0	-3.163650	-1.445816	0.565507

12	1	0	-3.187640	0.704994	0.663568
13	6	0	-2.486271	-2.574763	0.113349
14	1	0	-0.774754	-3.298306	-0.968340
15	1	0	-4.084980	-1.552920	1.125489
16	1	0	-2.877410	-3.562932	0.321554
17	6	0	1.683317	0.644052	0.281034
18	6	0	1.506457	-0.335640	1.262685
19	6	0	2.537085	0.392659	-0.797891
20	6	0	2.180924	-1.546023	1.168232
21	1	0	0.828272	-0.144113	2.085665
22	6	0	3.203827	-0.821426	-0.887760
23	1	0	2.662133	1.151415	-1.560827
24	6	0	3.027544	-1.794048	0.093530
25	1	0	2.035828	-2.300720	1.931893
26	1	0	3.864589	-1.009958	-1.725526
27	1	0	3.549176	-2.740615	0.019219
28	1	0	0.804634	4.037539	0.977438

Structure 7 (B3LYP)

E(RB3LYP) = -704.499218546

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.659359	1.324706	-0.006726
2	6	0	0.896651	2.684809	-0.013120
3	7	0	-0.709730	1.244519	0.011216
4	7	0	-1.257276	2.494438	0.014408
5	7	0	-0.286595	3.351066	-0.005520
6	6	0	-1.578560	0.114925	0.093550
7	6	0	-1.313132	-0.920139	0.989517
8	6	0	-2.717229	0.085997	-0.711600
9	6	0	-2.187717	-2.000498	1.062395
10	1	0	-0.438654	-0.875590	1.625391
11	6	0	-3.591133	-0.992728	-0.619756
12	1	0	-2.909992	0.911541	-1.383749
13	6	0	-3.326182	-2.040526	0.260169
14	1	0	-1.982383	-2.806434	1.757275
15	1	0	-4.478842	-1.014743	-1.241116
16	1	0	-4.006940	-2.881351	0.325078
17	6	0	1.608969	0.205255	-0.084868
18	6	0	1.424251	-0.856683	-0.982064
19	6	0	2.760467	0.221441	0.714851
20	6	0	2.365729	-1.876455	-1.070209
21	1	0	0.548841	-0.876205	-1.619723
22	6	0	3.701786	-0.799499	0.621188
23	1	0	2.907066	1.032533	1.418787
24	6	0	3.506614	-1.852411	-0.269635
25	1	0	2.211119	-2.688675	-1.771338
26	1	0	4.585625	-0.773726	1.248412
27	1	0	4.238977	-2.648361	-0.341256
28	1	0	1.841150	3.201678	-0.060638

Structure 7 (M06-2X)

E(RM062X) = -704.213025694

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.647992	1.350468	0.005487
2	6	0	-0.874919	2.706883	0.024290
3	7	0	0.712546	1.261902	-0.023842
4	7	0	1.267613	2.489396	-0.020637
5	7	0	0.316292	3.355276	0.011775
6	6	0	1.556818	0.117201	-0.108600
7	6	0	1.231848	-0.932263	-0.961294
8	6	0	2.713309	0.087116	0.662251
9	6	0	2.073678	-2.035397	-1.024963
10	1	0	0.334307	-0.880666	-1.565214
11	6	0	3.553562	-1.015536	0.578195
12	1	0	2.942734	0.930140	1.300832
13	6	0	3.232920	-2.080108	-0.257500
14	1	0	1.825719	-2.857331	-1.685101
15	1	0	4.458531	-1.043112	1.172623
16	1	0	3.887761	-2.940893	-0.314927
17	6	0	-1.587569	0.223927	0.088281
18	6	0	-1.365858	-0.838655	0.968743
19	6	0	-2.745281	0.236518	-0.692141
20	6	0	-2.286020	-1.873441	1.058857
21	1	0	-0.474307	-0.846808	1.585534
22	6	0	-3.666624	-0.799503	-0.595279
23	1	0	-2.911298	1.055847	-1.382204
24	6	0	-3.438007	-1.856786	0.277573
25	1	0	-2.107535	-2.691403	1.746148
26	1	0	-4.561157	-0.782012	-1.206202
27	1	0	-4.155649	-2.664840	0.351645
28	1	0	-1.813461	3.232522	0.082399

Structure 8 (B3LYP) (atoms treated at DFT level are marked in bold)

ONIOM: extrapolated energy = -704.922467518229

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	9.115306	-2.595510	-0.185213
2	6	0	8.626846	-2.784983	-1.488870
3	6	0	7.491559	-3.603926	-1.627003
4	6	0	6.857303	-4.205518	-0.538712
5	6	0	7.392726	-3.982174	0.730793
6	6	0	8.520142	-3.170239	0.950139
7	6	0	8.384762	0.729370	3.325798
8	6	0	8.963232	-0.428479	2.781597
9	6	0	8.422694	-1.713960	2.960198
10	6	0	7.258313	-1.808682	3.742884
11	6	0	6.631070	-0.694025	4.303230
12	6	0	7.214603	0.553251	4.085503
13	6	0	7.031495	0.632390	-4.083702
14	6	0	7.615688	-0.612026	-3.838404
15	6	0	8.699420	-0.783980	-2.959388
16	6	0	9.206993	0.374166	-2.345276

17	6	0	8.671301	1.654204	-2.559677
18	6	0	7.578827	1.742552	-3.441439
19	6	0	7.432053	3.969527	-0.453194
20	6	0	8.557798	3.134257	-0.565430
21	6	0	9.027419	2.546193	0.620600
22	6	0	8.426461	2.748600	1.874476
23	6	0	7.299149	3.588710	1.906202
24	6	0	6.781557	4.197895	0.761251
25	6	0	9.362439	-2.111290	-2.634827
26	6	0	9.138726	-2.884160	2.307929
27	6	0	9.059383	2.066255	3.074802
28	6	0	9.311406	2.834232	-1.849516
29	8	0	7.041729	-3.923909	-2.927974
30	8	0	6.847056	-4.688862	1.826631
31	8	0	6.753834	-3.088728	4.071877
32	8	0	6.673514	1.680692	4.744617
33	8	0	7.159749	-1.721300	-4.589184
34	8	0	7.094594	3.025938	-3.778946
35	8	0	7.005507	4.705471	-1.584141
36	8	0	6.730261	3.941270	3.154534
37	6	0	3.561918	4.396620	-2.343465
38	6	0	3.600283	3.448438	-3.417222
39	7	0	4.739634	2.923296	-3.888578
40	6	0	5.867052	3.362326	-3.255333
41	6	0	5.824314	4.266833	-2.146357
42	7	0	4.656336	4.801303	-1.684244
43	7	0	4.809876	-1.642000	-4.757138
44	6	0	3.657961	-2.221358	-4.392112
45	6	0	3.593788	-3.316888	-3.471079
46	7	0	4.680781	-3.883541	-2.928428
47	6	0	5.863490	-3.321942	-3.315066
48	6	0	5.924953	-2.201363	-4.202465
49	7	0	4.496173	-4.670675	1.631040
50	6	0	5.622147	-4.236449	2.268233
51	6	0	5.571615	-3.420161	3.442444
52	7	0	4.395430	-3.037040	4.020623
53	6	0	3.297507	-3.487075	3.396962
54	6	0	3.349511	-4.285323	2.208106
55	7	0	4.378522	3.979300	3.028047
56	6	0	5.518065	3.345582	3.432154
57	6	0	5.489507	2.155459	4.229812
58	7	0	4.325333	1.544087	4.596223
59	6	0	3.216092	2.174109	4.186302
60	6	0	3.242050	3.389779	3.428096
61	6	0	2.116840	4.802142	-2.092115
62	6	0	2.177587	3.168434	-3.867888
63	6	0	2.245071	-1.849896	-4.817282
64	6	0	2.133287	-3.656613	-3.215341
65	6	0	1.840446	-3.243713	3.761197
66	6	0	1.931052	-4.549524	1.730207
67	6	0	1.772430	1.760411	4.407671
68	6	0	1.812566	3.825247	3.157865
69	8	0	1.341448	-2.641039	4.664110
70	7	0	1.113499	-3.918587	2.720251
71	8	0	1.531730	-5.095509	0.742718
72	8	0	1.642422	-4.446493	-2.460967
73	7	0	1.416986	-2.754088	-4.061301
74	8	0	1.842676	-1.021804	-5.575749
75	7	0	1.380470	4.041022	-3.065235
76	8	0	1.638418	5.540127	-1.285652
77	8	0	1.747763	2.384726	-4.667608
78	7	0	1.017857	2.821371	3.798233
79	8	0	1.296282	0.785933	4.909489

80	8	0	1.371974	4.746890	2.529698
81	1	0	0.079486	-3.953101	2.695582
82	1	0	0.385909	-2.766480	-4.143955
83	1	0	0.352972	4.106538	-3.161860
84	1	0	-0.012638	2.886791	3.859706
85	6	0	-9.167322	1.166347	2.090680
86	6	0	-8.655921	2.438600	1.793731
87	6	0	-7.574295	2.880055	2.577798
88	6	0	-7.034682	2.128402	3.618778
89	6	0	-7.598064	0.875522	3.877888
90	6	0	-8.652078	0.347723	3.113017
91	6	0	-8.436076	-3.369324	0.384081
92	6	0	-9.041973	-2.407153	1.212173
93	6	0	-8.536875	-2.054247	2.473182
94	6	0	-7.367034	-2.715988	2.890824
95	6	0	-6.739717	-3.702535	2.133046
96	6	0	-7.297900	-4.019204	0.892541
97	6	0	-6.797929	3.569509	-2.259156
98	6	0	-7.449860	3.811190	-1.047973
99	6	0	-8.553096	3.053224	-0.617127
100	6	0	-9.002191	2.044071	-1.485392
101	6	0	-8.399935	1.764055	-2.723349
102	6	0	-7.290382	2.551962	-3.078483
103	6	0	-7.136735	-1.088201	-3.909725
104	6	0	-8.321606	-0.656537	-3.287359
105	6	0	-8.898013	-1.530317	-2.351339
106	6	0	-8.339241	-2.776751	-2.020574
107	6	0	-7.157808	-3.139607	-2.692096
108	6	0	-6.533249	-2.312621	-3.627362
109	6	0	-9.307917	3.247763	0.686131
110	6	0	-9.283176	-1.020621	3.300315
111	6	0	-9.050274	-3.627343	-0.981120
112	6	0	-9.014274	0.664075	-3.571780
113	8	0	-7.088512	4.189964	2.365104
114	8	0	-7.118968	0.169801	5.012219
115	8	0	-6.873048	-2.440382	4.184076
116	8	0	-6.744819	-5.100341	0.169318
117	8	0	-7.036706	4.934868	-0.291159
118	8	0	-6.711222	2.402230	-4.360971
119	8	0	-6.601248	-0.290017	-4.945307
120	8	0	-6.634038	-4.436985	-2.494152
121	6	0	-3.156501	0.443746	-4.614146
122	6	0	-3.211434	1.858447	-4.392610
123	7	0	-4.361432	2.532072	-4.243167
124	6	0	-5.485446	1.769005	-4.373977
125	6	0	-5.428951	0.364192	-4.647270
126	7	0	-4.250464	-0.318867	-4.742633
127	7	0	-4.689030	5.102664	-0.248647
128	6	0	-3.582506	4.948283	0.492699
129	6	0	-3.599506	4.386392	1.810002
130	7	0	-4.729173	4.058708	2.453291
131	6	0	-5.869671	4.284863	1.737505
132	6	0	-5.845659	4.748322	0.381956
133	7	0	-4.774633	0.378114	5.183298
134	6	0	-5.857453	-0.360219	4.805238
135	6	0	-5.734011	-1.674302	4.250928
136	7	0	-4.526661	-2.212046	3.907550
137	6	0	-3.473133	-1.448279	4.230081
138	6	0	-3.593048	-0.199334	4.922739
139	7	0	-4.275611	-4.291041	-2.439990
140	6	0	-5.455260	-4.484367	-1.779971
141	6	0	-5.512549	-4.840741	-0.396764
142	7	0	-4.391464	-5.026525	0.360174

143	6	0	-3.240534	-4.852713	-0.303751
144	6	0	-3.183729	-4.484314	-1.687961
145	6	0	-1.700054	0.008403	-4.674702
146	6	0	-1.794475	2.406816	-4.372788
147	6	0	-2.151722	5.309228	0.123021
148	6	0	-2.168194	4.249039	2.297708
149	6	0	-2.001011	-1.707523	3.949287
150	6	0	-2.201150	0.321940	5.243915
151	6	0	-1.821992	-4.980215	0.231384
152	6	0	-1.725570	-4.351244	-2.101577
153	8	0	-1.484869	-2.540563	3.257635
154	7	0	-1.328710	-0.650409	4.627858
155	8	0	-1.832811	1.283296	5.844438
156	8	0	-1.731918	3.725760	3.285416
157	7	0	-1.388012	4.831000	1.255599
158	8	0	-1.694280	5.850624	-0.832352
159	7	0	-0.974763	1.241991	-4.539986
160	8	0	-1.205196	-1.074984	-4.753291
161	8	0	-1.384131	3.521731	-4.230328
162	7	0	-1.001097	-4.677945	-0.908008
163	8	0	-1.420255	-5.235108	1.327211
164	8	0	-1.239379	-4.022883	-3.143195
165	1	0	-0.298933	-0.603797	4.717764
166	1	0	-0.368086	4.978741	1.339171
167	1	0	0.051850	1.304600	-4.674552
168	1	0	0.031312	-4.774204	-0.891637
169	1	0	10.406306	-1.880049	-2.269314
170	1	0	10.058765	0.272966	-1.668611
171	1	0	6.182942	0.736449	-4.776240
172	1	0	10.000733	-1.970079	-0.047713
173	1	0	5.978946	-4.852365	-0.679894
174	1	0	10.205747	-2.560513	2.125314
175	1	0	9.875888	-0.325768	2.189897
176	1	0	5.720009	-0.799495	4.910766
177	1	0	10.134556	1.848340	2.802929
178	1	0	5.906701	4.860864	0.819171
179	1	0	9.907220	1.899929	0.565757
180	1	0	10.355162	2.516996	-1.554383
181	1	0	-5.847769	-4.226151	2.508035
182	1	0	-9.947712	-1.910772	0.855736
183	1	0	-10.333626	-0.960624	2.888632
184	1	0	-6.203873	2.515234	4.227107
185	1	0	-10.005148	0.790769	1.498382
186	1	0	-10.344943	2.824691	0.534145
187	1	0	-9.867929	1.448449	-1.183781
188	1	0	-5.944340	4.186490	-2.575869
189	1	0	-10.089429	0.553018	-3.241323
190	1	0	-5.608947	-2.624973	-4.136614
191	1	0	-9.824579	-1.227814	-1.857738
192	1	0	-10.122422	-3.274422	-0.937827
193	6	0	9.233924	-4.116535	3.204355
194	1	0	9.793811	-4.922743	2.716460
195	1	0	9.730775	-3.882211	4.152972
196	1	0	8.242635	-4.528449	3.459847
197	6	0	9.126092	2.956763	4.313646
198	1	0	9.611398	2.440962	5.150361
199	1	0	9.684372	3.878426	4.112060
200	1	0	8.126802	3.263247	4.666443
201	6	0	9.496216	4.055782	-2.747019
202	1	0	10.012785	4.864912	-2.217724
203	1	0	10.077974	3.808577	-3.642574
204	1	0	8.535529	4.470141	-3.097260
205	6	0	9.547458	-3.015187	-3.851465

206	1	0	10.118459	-2.510837	-4.639712
207	1	0	10.074904	-3.938651	-3.586208
208	1	0	8.586168	-3.316788	-4.301603
209	6	0	-9.516997	4.715323	1.053397
210	1	0	-10.046066	5.253954	0.258369
211	1	0	-10.098211	4.817042	1.977321
212	1	0	-8.565186	5.248969	1.216451
213	6	0	-9.079629	1.008790	-5.057948
214	1	0	-9.554570	0.205581	-5.633508
215	1	0	-9.647665	1.930827	-5.228905
216	1	0	-8.080798	1.166824	-5.499004
217	6	0	-9.120803	-5.107092	-1.349282
218	1	0	-9.678576	-5.679040	-0.598582
219	1	0	-9.607915	-5.254237	-2.320286
220	1	0	-8.122107	-5.570899	-1.422627
221	6	0	-9.439592	-1.425328	4.764511
222	1	0	-10.027201	-0.686072	5.321712
223	1	0	-9.937379	-2.397065	4.860342
224	1	0	-8.469289	-1.511075	5.283308
225	6	0	-5.514469	-0.885870	-0.065109
226	6	0	-4.489224	-1.520405	0.636103
227	6	0	-5.239193	0.280193	-0.775861
228	1	0	-6.520112	-1.293030	-0.054245
229	6	0	-3.201698	-1.000089	0.628779
230	1	0	-4.687850	-2.424932	1.205033
231	6	0	-3.953227	0.814323	-0.791224
232	1	0	-6.032103	0.783547	-1.318997
233	6	0	-2.931179	0.169455	-0.086000
234	1	0	-2.397224	-1.488805	1.169691
235	1	0	-3.750745	1.726702	-1.341917
236	7	0	-1.590901	0.637168	-0.032696
237	6	0	2.931089	1.785657	0.214931
238	7	0	-1.286178	1.633245	-0.689819
239	6	0	2.818932	2.975607	0.362915
240	6	0	3.067595	0.377910	0.024806
241	7	0	-0.873613	2.531898	-1.242594
242	1	0	2.737247	4.032691	0.506752
243	6	0	1.936159	-0.454881	0.003886
244	6	0	4.339301	-0.191997	-0.153466
245	6	0	2.078586	-1.821399	-0.204649
246	1	0	0.951644	-0.029362	0.153478
247	6	0	4.471249	-1.560236	-0.354693
248	1	0	5.213581	0.447089	-0.134367
249	6	0	3.343105	-2.378209	-0.385743
250	1	0	1.197890	-2.455904	-0.230492
251	1	0	5.457667	-1.990634	-0.489124
252	1	0	3.446333	-3.450297	-0.554692

Structure 8 (M06-2X) (atoms treated at DFT level are marked in bold)

ONIOM: extrapolated energy = -704.623836439645

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	9.066371	-0.931858	2.289937
2	6	0	8.511968	-2.220112	2.251903
3	6	0	7.383219	-2.443933	3.061624
4	6	0	6.830881	-1.455972	3.877417

5	6	0	7.440357	-0.197017	3.888860
6	6	0	8.556757	0.106884	3.089520
7	6	0	8.612686	3.202171	-0.319023
8	6	0	9.146092	2.387479	0.696360
9	6	0	8.618112	2.340347	1.995262
10	6	0	7.503969	3.159711	2.252610
11	6	0	6.939709	4.001808	1.296748
12	6	0	7.522165	4.018882	0.026931
13	6	0	6.730501	-4.105633	-1.512517
14	6	0	7.361135	-4.122442	-0.266989
15	6	0	8.479422	-3.324001	0.028220
16	6	0	8.981289	-2.525193	-1.014093
17	6	0	8.402108	-2.476569	-2.292458
18	6	0	7.266074	-3.279269	-2.500462
19	6	0	7.237146	0.121803	-4.067239
20	6	0	8.397725	-0.222376	-3.351953
21	6	0	9.005692	0.799936	-2.603021
22	6	0	8.502270	2.109030	-2.538796
23	6	0	7.334416	2.374513	-3.277228
24	6	0	6.680867	1.402298	-4.035071
25	6	0	9.181711	-3.262737	1.372561
26	6	0	9.277525	1.442579	3.027447
27	6	0	9.250706	3.127367	-1.695019
28	6	0	9.050996	-1.593259	-3.344012
29	8	0	6.878441	-3.760977	3.151025
30	8	0	6.983758	0.739059	4.848607
31	8	0	7.020243	3.201354	3.577427
32	8	0	7.054636	4.976978	-0.904036
33	8	0	6.908148	-5.057214	0.695713
34	8	0	6.699391	-3.332023	-3.795448
35	8	0	6.674574	-0.825909	-4.955028
36	8	0	6.882247	3.710439	-3.352457
37	6	0	3.206928	-1.385850	-4.497404
38	6	0	3.222949	-2.666360	-3.855148
39	7	0	4.353139	-3.323137	-3.559225
40	6	0	5.496014	-2.672822	-3.925641
41	6	0	5.482432	-1.380771	-4.542459
42	7	0	4.322339	-0.723679	-4.836529
43	7	0	4.559055	-5.185012	0.677279
44	6	0	3.428579	-4.883606	1.330696
45	6	0	3.412811	-4.105910	2.533709
46	7	0	4.523352	-3.669025	3.143495
47	6	0	5.685476	-4.007149	2.511449
48	6	0	5.699303	-4.727509	1.273895
49	7	0	4.641123	0.838234	5.045844
50	6	0	5.793079	1.365412	4.535861
51	6	0	5.808073	2.595328	3.802688
52	7	0	4.665541	3.250972	3.443097
53	6	0	3.541281	2.696904	3.914700
54	6	0	3.533267	1.536299	4.756236
55	7	0	4.523786	3.715536	-3.269227
56	6	0	5.719128	3.998485	-2.675064
57	6	0	5.808659	4.700710	-1.430304
58	7	0	4.711450	5.193886	-0.785410
59	6	0	3.546204	4.942932	-1.399598
60	6	0	3.453717	4.185046	-2.611662
61	6	0	1.762459	-0.945326	-4.678482
62	6	0	1.792180	-3.094492	-3.581401
63	6	0	1.998316	-5.244737	0.957828
64	6	0	1.971007	-3.861104	2.936391
65	6	0	2.108690	3.135202	3.672026
66	6	0	2.101520	1.257852	5.189932
67	6	0	2.145832	5.342322	-0.961161

68	6	0	1.986409	3.985979	-2.954580
69	8	0	1.668282	3.973566	2.935672
70	7	0	1.335047	2.263306	4.495941
71	8	0	1.640174	0.431464	5.916276
72	8	0	1.526816	-3.177739	3.818933
73	7	0	1.208675	-4.581284	1.972477
74	8	0	1.548248	-5.903411	0.073161
75	7	0	1.003382	-2.039156	-4.141471
76	8	0	1.296211	0.060186	-5.127253
77	8	0	1.361050	-4.061333	-3.020111
78	7	0	1.294424	4.722206	-1.947736
79	8	0	1.753675	5.997674	-0.045062
80	8	0	1.474998	3.322942	-3.813020
81	1	0	0.306290	2.330838	4.573099
82	1	0	0.178341	-4.667035	2.015392
83	1	0	-0.028899	-2.044591	-4.137063
84	1	0	0.265323	4.812198	-1.926654
85	6	0	-8.969409	2.535978	-0.976980
86	6	0	-8.459393	2.414841	-2.282731
87	6	0	-7.344419	3.207306	-2.602417
88	6	0	-6.718017	4.035481	-1.667476
89	6	0	-7.251391	4.087997	-0.381360
90	6	0	-8.395512	3.363010	0.001270
91	6	0	-8.390265	0.160596	3.250440
92	6	0	-8.949046	1.163737	2.442783
93	6	0	-8.388887	2.447577	2.313069
94	6	0	-7.242758	2.719036	3.079171
95	6	0	-6.624015	1.755373	3.878242
96	6	0	-7.207603	0.491780	3.937971
97	6	0	-6.880005	-1.616831	-3.853046
98	6	0	-7.382615	-0.318222	-3.876448
99	6	0	-8.519962	0.077351	-3.147635
100	6	0	-9.106355	-0.896082	-2.323909
101	6	0	-8.617345	-2.211415	-2.218477
102	6	0	-7.521217	-2.547101	-3.031057
103	6	0	-7.467409	-3.909123	0.427877
104	6	0	-8.586284	-3.124251	0.093329
105	6	0	-9.072268	-2.267313	1.093647
106	6	0	-8.494819	-2.168580	2.372599
107	6	0	-7.401163	-3.009368	2.640388
108	6	0	-6.865357	-3.874797	1.683989
109	6	0	-9.159389	1.453906	-3.226527
110	6	0	-9.057481	3.429595	1.367881
111	6	0	-9.102681	-1.178028	3.349370
112	6	0	-9.304726	-3.153567	-1.245769
113	8	0	-6.850369	3.237243	-3.934151
114	8	0	-6.671743	4.989533	0.541076
115	8	0	-6.728819	4.038388	3.112602
116	8	0	-6.642077	-0.463315	4.811309
117	8	0	-6.784765	0.615385	-4.752647
118	8	0	-7.081578	-3.892781	-3.086716
119	8	0	-6.986367	-4.846704	-0.516167
120	8	0	-6.848636	-3.054886	3.946152
121	6	0	-3.526328	-4.467928	-1.197732
122	6	0	-3.578578	-4.117898	-2.588077
123	7	0	-4.726554	-3.900214	-3.243653
124	6	0	-5.849009	-4.080848	-2.489253
125	6	0	-5.799381	-4.508291	-1.124885
126	7	0	-4.621189	-4.678624	-0.454318
127	7	0	-4.459993	0.449752	-4.278718
128	6	0	-3.353078	1.172723	-4.052454
129	6	0	-3.362572	2.600768	-3.931652
130	7	0	-4.492614	3.320072	-3.881572

131	6	0	-5.632170	2.587857	-4.036320
132	6	0	-5.610690	1.184465	-4.321313
133	7	0	-4.322270	4.692758	0.397820
134	6	0	-5.485122	4.579738	1.106039
135	6	0	-5.509990	4.157904	2.473039
136	7	0	-4.374188	3.926464	3.192619
137	6	0	-3.238826	4.094028	2.501652
138	6	0	-3.215046	4.438201	1.109588
139	7	0	-4.500990	-3.244707	3.783678
140	6	0	-5.598331	-2.466834	4.009758
141	6	0	-5.499397	-1.083286	4.361031
142	7	0	-4.309455	-0.412539	4.369074
143	6	0	-3.242113	-1.179375	4.103199
144	6	0	-3.333815	-2.591101	3.864117
145	6	0	-2.070388	-4.511105	-0.761057
146	6	0	-2.162762	-3.995644	-3.123137
147	6	0	-1.924944	0.684818	-3.866829
148	6	0	-1.931876	3.099741	-3.824587
149	6	0	-1.812106	3.940470	2.999418
150	6	0	-1.769349	4.451045	0.638323
151	6	0	-1.782547	-0.761196	3.998972
152	6	0	-1.934753	-3.155396	3.694566
153	8	0	-1.372414	3.671542	4.077835
154	7	0	-1.018040	4.185876	1.826110
155	8	0	-1.303614	4.587490	-0.456352
156	8	0	-1.478326	4.199230	-3.746788
157	7	0	-1.153022	1.880970	-3.812202
158	8	0	-1.505447	-0.427370	-3.690393
159	7	0	-1.345432	-4.245735	-1.966447
160	8	0	-1.572612	-4.638811	0.319888
161	8	0	-1.739086	-3.724371	-4.206745
162	7	0	-1.089898	-1.997735	3.812050
163	8	0	-1.266491	0.320056	4.007375
164	8	0	-1.537082	-4.264801	3.495695
165	1	0	0.015715	4.231243	1.863699
166	1	0	-0.119779	1.892785	-3.859936
167	1	0	-0.310431	-4.310795	-2.027123
168	1	0	-0.059261	-2.070316	3.816120
169	1	0	10.236553	-2.906037	1.179334
170	1	0	9.862961	-1.910032	-0.818880
171	1	0	5.853084	-4.737241	-1.715815
172	1	0	9.943144	-0.725672	1.670409
173	1	0	5.967195	-1.670765	4.522569
174	1	0	10.327144	1.236503	2.662408
175	1	0	10.009172	1.760797	0.460667
176	1	0	6.079639	4.643098	1.538902
177	1	0	10.301450	2.736922	-1.554744
178	1	0	5.774227	1.642385	-4.607885
179	1	0	9.915337	0.564756	-2.045185
180	1	0	10.127084	-1.446302	-3.031242
181	1	0	-5.717799	1.988049	4.457219
182	1	0	-9.861783	0.936619	1.886802
183	1	0	-10.126784	3.089766	1.235699
184	1	0	-5.838689	4.638283	-1.939384
185	1	0	-9.855193	1.953991	-0.710697
186	1	0	-10.223259	1.346890	-2.861122
187	1	0	-9.983834	-0.619829	-1.734239
188	1	0	-6.017091	-1.901327	-4.472980
189	1	0	-10.346530	-2.752461	-1.072753
190	1	0	-6.002589	-4.516876	1.917181
191	1	0	-9.939767	-1.642941	0.866907
192	1	0	-10.172571	-1.009083	3.027854
193	6	0	9.445520	2.105487	4.392926

194	1	0	10.006910	1.462790	5.081039
195	1	0	9.975721	3.061358	4.310561
196	1	0	8.478619	2.319386	4.879153
197	6	0	9.407295	4.485022	-2.375227
198	1	0	9.989182	5.176611	-1.754772
199	1	0	9.910579	4.390359	-3.344288
200	1	0	8.437134	4.973912	-2.567547
201	6	0	9.113785	-2.240586	-4.725939
202	1	0	9.644868	-1.601988	-5.441309
203	1	0	9.624609	-3.209778	-4.690212
204	1	0	8.111954	-2.425556	-5.149700
205	6	0	9.330703	-4.622369	2.051114
206	1	0	9.851578	-5.336395	1.402314
207	1	0	9.893043	-4.541034	2.988493
208	1	0	8.357702	-5.076962	2.302936
209	6	0	-9.267898	1.976842	-4.657523
210	1	0	-9.826449	1.283098	-5.296246
211	1	0	-9.773561	2.949312	-4.689233
212	1	0	-8.280302	2.120767	-5.128716
213	6	0	-9.494558	-4.565169	-1.796137
214	1	0	-10.039546	-5.200115	-1.087943
215	1	0	-10.051176	-4.554174	-2.740529
216	1	0	-8.534447	-5.069443	-2.000865
217	6	0	-9.183005	-1.706678	4.780059
218	1	0	-9.673205	-0.987215	5.445873
219	1	0	-9.742563	-2.648398	4.826403
220	1	0	-8.186733	-1.910975	5.209109
221	6	0	-9.144060	4.848933	1.924459
222	1	0	-9.686446	5.513553	1.242093
223	1	0	-9.655395	4.866852	2.894142
224	1	0	-8.149391	5.299737	2.083843
225	6	0	-5.398495	-0.148540	-0.395745
226	6	0	-4.865997	0.371378	0.780726
227	6	0	-4.560793	-0.798695	-1.294204
228	1	0	-6.454940	-0.043418	-0.611669
229	6	0	-3.515054	0.234778	1.062294
230	1	0	-5.507155	0.885597	1.487614
231	6	0	-3.206023	-0.941954	-1.025044
232	1	0	-4.954925	-1.192319	-2.225687
233	6	0	-2.684027	-0.431720	0.162616
234	1	0	-3.084196	0.640997	1.970855
235	1	0	-2.557567	-1.425464	-1.751652
236	7	0	-1.320987	-0.544656	0.539710
237	6	0	2.975518	0.795355	-1.339136
238	7	0	-0.578616	-1.153411	-0.239067
239	6	0	3.042800	1.091847	-2.501102
240	6	0	2.865497	0.395485	0.031675
241	7	0	0.196756	-1.671852	-0.859610
242	1	0	3.097032	1.382125	-3.531698
243	6	0	1.668936	0.599985	0.726274
244	6	0	3.932645	-0.242959	0.671112
245	6	0	1.518546	0.118703	2.019278
246	1	0	0.849954	1.113851	0.236034
247	6	0	3.784708	-0.698323	1.972698
248	1	0	4.862969	-0.384335	0.135982
249	6	0	2.574522	-0.541895	2.639936
250	1	0	0.568005	0.250097	2.529185
251	1	0	4.613646	-1.187527	2.471607
252	1	0	2.457934	-0.948728	3.642838

Structure 9 (B3LYP) (atoms treated at DFT level are marked in bold)

ONIOM: extrapolated energy = -704.929912775690

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-9.093286	-0.822701	2.553369
2	6	0	-8.568453	0.297730	3.215123
3	6	0	-7.397463	0.090028	3.968297
4	6	0	-6.789451	-1.155595	4.102157
5	6	0	-7.368149	-2.236256	3.431647
6	6	0	-8.505729	-2.100329	2.617352
7	6	0	-8.476557	-2.712255	-1.942863
8	6	0	-9.014019	-2.651310	-0.643844
9	6	0	-8.456050	-3.327251	0.452869
10	6	0	-7.299788	-4.087782	0.199294
11	6	0	-6.733858	-4.208794	-1.068214
12	6	0	-7.346825	-3.528631	-2.122983
13	6	0	-6.991813	4.078539	1.157607
14	6	0	-7.580392	3.372374	2.210583
15	6	0	-8.649398	2.481217	2.019722
16	6	0	-9.164758	2.379694	0.713549
17	6	0	-8.633738	3.081178	-0.379398
18	6	0	-7.525388	3.907842	-0.117308
19	6	0	-7.448769	2.058716	-3.354803
20	6	0	-8.579118	1.855151	-2.543899
21	6	0	-9.091904	0.546405	-2.483571
22	6	0	-8.510594	-0.539210	-3.156343
23	6	0	-7.359445	-0.262827	-3.917814
24	6	0	-6.814217	1.014894	-4.033653
25	6	0	-9.293826	1.628497	3.098382
26	6	0	-9.141929	-3.214250	1.804783
27	6	0	-9.162623	-1.906361	-3.032183
28	6	0	-9.293456	2.926181	-1.739184
29	8	0	-6.877125	1.176735	4.704686
30	8	0	-6.816198	-3.520809	3.658442
31	8	0	-6.739034	-4.840983	1.257026
32	8	0	-6.842204	-3.757262	-3.428009
33	8	0	-7.101077	3.642567	3.520725
34	8	0	-7.002501	4.682827	-1.175784
35	8	0	-6.986392	3.374742	-3.596753
36	8	0	-6.799691	-1.310589	-4.680499
37	6	0	-3.517142	3.860676	-3.055781
38	6	0	-3.520270	4.349099	-1.707572
39	7	0	-4.643348	4.577342	-1.012244
40	6	0	-5.792280	4.275787	-1.686104
41	6	0	-5.784178	3.676403	-2.986394
42	7	0	-4.633985	3.485125	-3.695928
43	7	0	-4.752830	3.881661	3.486280
44	6	0	-3.578839	3.255029	3.649935
45	6	0	-3.478773	1.860318	3.967745
46	7	0	-4.539260	1.101960	4.281878
47	6	0	-5.735206	1.756065	4.207565
48	6	0	-5.844356	3.100690	3.726254
49	7	0	-4.459766	-3.340821	3.710648
50	6	0	-5.592487	-3.707581	3.042573
51	6	0	-5.558697	-4.342757	1.761569
52	7	0	-4.394505	-4.555414	1.080236
53	6	0	-3.292875	-4.166845	1.736256
54	6	0	-3.320435	-3.594378	3.051377

55	7	0	-4.453114	-1.131102	-4.423573
56	6	0	-5.610304	-1.825262	-4.219181
57	6	0	-5.625994	-3.139894	-3.653187
58	7	0	-4.483775	-3.838336	-3.388278
59	6	0	-3.351689	-3.171854	-3.656389
60	6	0	-3.340995	-1.817078	-4.124254
61	6	0	-2.087184	3.850447	-3.573803
62	6	0	-2.082801	4.547855	-1.261301
63	6	0	-2.181496	3.827052	3.489106
64	6	0	-2.022056	1.444662	3.861934
65	6	0	-1.852381	-4.226937	1.259222
66	6	0	-1.893409	-3.322287	3.498887
67	6	0	-1.916498	-3.653321	-3.509622
68	6	0	-1.903555	-1.340323	-4.204246
69	8	0	-1.396950	-4.571622	0.204611
70	7	0	-1.100985	-3.741804	2.371440
71	8	0	-1.439832	-2.878437	4.510369
72	8	0	-1.520486	0.353302	3.883473
73	7	0	-1.330599	2.664885	3.622806
74	8	0	-1.780103	4.934119	3.307222
75	7	0	-1.314984	4.300142	-2.436780
76	8	0	-1.624003	3.571622	-4.635730
77	8	0	-1.633610	4.797881	-0.175868
78	7	0	-1.133580	-2.484924	-3.849352
79	8	0	-1.453322	-4.709851	-3.211502
80	8	0	-1.470523	-0.250416	-4.462682
81	1	0	-0.071124	-3.670623	2.367131
82	1	0	-0.299855	2.729573	3.573892
83	1	0	-0.287467	4.404248	-2.469620
84	1	0	-0.100457	-2.504277	-3.870663
85	6	0	9.174037	-1.264868	-2.162738
86	6	0	8.614728	-0.447037	-3.162365
87	6	0	7.512292	-0.965088	-3.862770
88	6	0	6.938793	-2.201261	-3.555085
89	6	0	7.518694	-2.948156	-2.533003
90	6	0	8.655854	-2.523502	-1.820716
91	6	0	8.595849	-1.785406	2.666894
92	6	0	9.170569	-2.110721	1.428946
93	6	0	8.678753	-3.132612	0.594401
94	6	0	7.594418	-3.882056	1.080752
95	6	0	6.971488	-3.596833	2.299479
96	6	0	7.469844	-2.536913	3.052228
97	6	0	6.797636	3.676187	-2.221151
98	6	0	7.376579	2.659922	-2.977381
99	6	0	8.536395	1.971534	-2.574642
100	6	0	9.071216	2.322796	-1.325442
101	6	0	8.508432	3.310547	-0.495717
102	6	0	7.388011	3.994700	-0.995960
103	6	0	7.311666	3.074772	2.620778
104	6	0	8.476107	2.707102	1.920452
105	6	0	9.051955	1.475776	2.268185
106	6	0	8.528291	0.632728	3.266546
107	6	0	7.398966	1.097773	3.960733
108	6	0	6.764721	2.301875	3.642208
109	6	0	9.246443	0.912576	-3.402006
110	6	0	9.359188	-3.338346	-0.747514
111	6	0	9.231149	-0.690885	3.508657
112	6	0	9.154076	3.554876	0.856319
113	8	0	6.986074	-0.258902	-4.975117
114	8	0	6.999075	-4.235631	-2.266363
115	8	0	7.127865	-5.010756	0.358475
116	8	0	6.870813	-2.261100	4.302824
117	8	0	6.819691	2.374143	-4.244054

118	8	0	6.853770	5.096207	-0.279758
119	8	0	6.730375	4.334268	2.348548
120	8	0	6.902123	0.376690	5.079642
121	6	0	3.306621	4.135764	1.453636
122	6	0	3.351674	4.733935	0.150813
123	7	0	4.499909	5.049777	-0.464241
124	6	0	5.620127	4.807253	0.275670
125	6	0	5.566403	4.310710	1.617070
126	7	0	4.395465	3.930003	2.207936
127	7	0	4.484641	2.198836	-3.837852
128	6	0	3.406627	1.427657	-4.038320
129	6	0	3.475367	0.127798	-4.643579
130	7	0	4.632333	-0.470975	-4.956404
131	6	0	5.741602	0.283561	-4.707892
132	6	0	5.664106	1.625770	-4.220703
133	7	0	4.648035	-3.908848	-2.142107
134	6	0	5.826489	-4.266760	-1.550087
135	6	0	5.888662	-4.781102	-0.216391
136	7	0	4.770882	-5.086886	0.503183
137	6	0	3.618229	-4.798784	-0.116650
138	6	0	3.560391	-4.160505	-1.400819
139	7	0	4.542052	0.444122	5.079803
140	6	0	5.692125	-0.234158	4.801024
141	6	0	5.689755	-1.559334	4.257232
142	7	0	4.548887	-2.156998	3.802975
143	6	0	3.433107	-1.442880	4.011169
144	6	0	3.420742	-0.193478	4.714363
145	6	0	1.862243	3.805129	1.785850
146	6	0	1.932991	4.895341	-0.367431
147	6	0	1.956924	1.722992	-3.685530
148	6	0	2.066636	-0.417110	-4.804738
149	6	0	2.204225	-5.013555	0.394777
150	6	0	2.110316	-3.819918	-1.706819
151	6	0	2.017138	-1.752243	3.557900
152	6	0	1.980976	0.258362	4.892443
153	8	0	1.776997	-5.553786	1.368471
154	7	0	1.388173	-4.373288	-0.608106
155	8	0	1.623774	-3.166969	-2.587335
156	8	0	1.644342	-1.427524	-5.281144
157	7	0	1.243985	0.607541	-4.217120
158	8	0	1.460220	2.622706	-3.066722
159	7	0	1.124638	4.326216	0.682645
160	8	0	1.398171	3.204748	2.715149
161	8	0	1.493182	5.360127	-1.375779
162	7	0	1.226524	-0.737188	4.158747
163	8	0	1.618927	-2.585245	2.785877
164	8	0	1.492611	1.177024	5.472554
165	1	0	0.349722	-4.396385	-0.569581
166	1	0	0.208734	0.551253	-4.221239
167	1	0	0.090064	4.350238	0.648806
168	1	0	0.191379	-0.722301	4.118356
169	1	0	-10.347480	1.404151	2.758362
170	1	0	-10.017555	1.718527	0.542808
171	1	0	-6.143885	4.757468	1.329659
172	1	0	-9.999068	-0.697495	1.955232
173	1	0	-5.891848	-1.285366	4.724401
174	1	0	-10.213082	-2.914110	1.607952
175	1	0	-9.908897	-2.046024	-0.480900
176	1	0	-5.840722	-4.829923	-1.233651
177	1	0	-10.228375	-1.736544	-2.697848
178	1	0	-5.928241	1.198981	-4.658828
179	1	0	-9.986499	0.367116	-1.882031
180	1	0	-10.346034	2.558580	-1.555532

181	1	0	6.118690	-4.193196	2.656331
182	1	0	10.039976	-1.540524	1.092604
183	1	0	10.408215	-2.929594	-0.654208
184	1	0	6.063047	-2.576807	-4.105334
185	1	0	10.052733	-0.900134	-1.625808
186	1	0	10.310343	0.856589	-3.026240
187	1	0	9.965917	1.801081	-0.977203
188	1	0	5.910423	4.216013	-2.584988
189	1	0	10.224430	3.200858	0.782426
190	1	0	5.869942	2.636462	4.187459
191	1	0	9.951099	1.153764	1.737270
192	1	0	10.295672	-0.572791	3.148675
193	6	0	-9.218868	-4.542613	2.554205
194	1	0	-9.772446	-4.438452	3.494586
195	1	0	-9.713256	-5.313561	1.951973
196	1	0	-8.221167	-4.935252	2.816316
197	6	0	-9.264131	-2.646054	-4.364355
198	1	0	-9.783116	-3.604896	-4.249397
199	1	0	-9.805456	-2.053382	-5.110640
200	1	0	-8.273894	-2.873447	-4.795246
201	6	0	-9.447265	4.247441	-2.489574
202	1	0	-9.984832	4.108556	-3.434825
203	1	0	-9.994733	4.985361	-1.891972
204	1	0	-8.474466	4.702242	-2.743674
205	6	0	-9.438320	2.347079	4.438324
206	1	0	-10.006225	3.278871	4.331398
207	1	0	-9.950642	1.719435	5.176235
208	1	0	-8.462531	2.622237	4.874413
209	6	0	9.351464	1.281084	-4.880421
210	1	0	9.855901	2.244246	-5.018393
211	1	0	9.908775	0.522060	-5.441956
212	1	0	8.362372	1.366820	-5.363117
213	6	0	9.235476	5.032672	1.233162
214	1	0	9.752769	5.174081	2.189085
215	1	0	9.769485	5.610229	0.469355
216	1	0	8.238889	5.495170	1.338447
217	6	0	9.336783	-1.061117	4.986686
218	1	0	9.889470	-1.997188	5.126755
219	1	0	9.847254	-0.276886	5.558308
220	1	0	8.348226	-1.200096	5.457254
221	6	0	9.523150	-4.808718	-1.126474
222	1	0	10.059400	-4.919671	-2.075997
223	1	0	10.076669	-5.360021	-0.357343
224	1	0	8.553478	-5.322295	-1.246440
225	1	0	5.934404	1.497708	-0.813719
226	6	0	5.251370	0.729851	-0.466787
227	6	0	3.888222	0.873626	-0.696776
228	6	0	5.742386	-0.390553	0.202481
229	6	0	3.000608	-0.113548	-0.257025
230	1	0	3.494534	1.742606	-1.212419
231	6	0	4.851680	-1.365929	0.644616
232	1	0	6.806553	-0.501432	0.379162
233	7	0	1.628981	0.100432	-0.544344
234	6	0	3.485740	-1.235682	0.421740
235	1	0	5.213862	-2.238587	1.178561
236	7	0	0.808242	-0.732631	-0.146498
237	1	0	2.802888	-1.998966	0.787008
238	7	0	-0.048482	-1.407100	0.153874
239	6	0	-1.197766	1.368848	-1.548805
240	6	0	-2.216888	0.935436	-1.075848
241	1	0	-0.278351	1.733608	-1.948102
242	6	0	-3.420980	0.428695	-0.501799
243	6	0	-3.433071	-0.037794	0.823798

244	6	0	-4.609085	0.394189	-1.249776
245	6	0	-4.607901	-0.521557	1.385421
246	1	0	-2.515150	-0.023368	1.400300
247	6	0	-5.778912	-0.092652	-0.679091
248	1	0	-4.599107	0.745718	-2.276319
249	6	0	-5.783438	-0.548929	0.637163
250	1	0	-4.605043	-0.865783	2.416100
251	1	0	-6.695204	-0.113054	-1.259257
252	1	0	-6.703392	-0.921034	1.075324

Structure 9 (M06-2X) (atoms treated at DFT level are marked in bold)

ONIOM: extrapolated energy = -704.626976019115
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-9.090789	-0.572451	2.603523
2	6	0	-8.566431	0.602027	3.163947
3	6	0	-7.398405	0.460902	3.936847
4	6	0	-6.794097	-0.768728	4.185448
5	6	0	-7.374441	-1.905041	3.615536
6	6	0	-8.507867	-1.840648	2.786832
7	6	0	-8.471726	-2.863230	-1.699036
8	6	0	-9.013735	-2.684772	-0.412793
9	6	0	-8.458683	-3.257690	0.742242
10	6	0	-7.301652	-4.037717	0.561955
11	6	0	-6.731259	-4.273239	-0.687261
12	6	0	-7.341205	-3.691900	-1.801209
13	6	0	-6.976802	4.177409	0.779565
14	6	0	-7.571171	3.572010	1.890477
15	6	0	-8.641590	2.669389	1.777854
16	6	0	-9.153570	2.451019	0.484748
17	6	0	-8.616694	3.048288	-0.665647
18	6	0	-7.506155	3.891720	-0.476343
19	6	0	-7.427826	1.756369	-3.535052
20	6	0	-8.558449	1.629987	-2.709104
21	6	0	-9.073216	0.333174	-2.529151
22	6	0	-8.496053	-0.809804	-3.103108
23	6	0	-7.345284	-0.606344	-3.887440
24	6	0	-6.795815	0.654079	-4.116785
25	6	0	-9.289938	1.917772	2.926895
26	6	0	-9.146339	-3.021657	2.077199
27	6	0	-9.153407	-2.157974	-2.858412
28	6	0	-9.272341	2.771685	-2.007852
29	8	0	-6.878910	1.608955	4.574318
30	8	0	-6.828147	-3.164580	3.964838
31	8	0	-6.745852	-4.689697	1.686987
32	8	0	-6.834567	-4.038487	-3.078945
33	8	0	-7.095659	3.959158	3.172374
34	8	0	-6.975629	4.563152	-1.599826
35	8	0	-6.961435	3.044055	-3.894782
36	8	0	-6.790997	-1.719477	-4.556124
37	6	0	-3.490798	3.553319	-3.386307
38	6	0	-3.494494	4.153297	-2.084013
39	7	0	-4.617912	4.450471	-1.415755
40	6	0	-5.766969	4.103073	-2.066865
41	6	0	-5.759169	3.393294	-3.310394
42	7	0	-4.608440	3.133360	-3.996672
43	7	0	-4.747202	4.191067	3.123376

44	6	0	-3.574511	3.580656	3.347040
45	6	0	-3.477608	2.220927	3.791628
46	7	0	-4.540100	1.494771	4.168858
47	6	0	-5.734936	2.140398	4.031058
48	6	0	-5.840498	3.436380	3.429981
49	7	0	-4.471021	-2.995663	4.013310
50	6	0	-5.602925	-3.410397	3.372496
51	6	0	-5.566987	-4.148366	2.147960
52	7	0	-4.402333	-4.411948	1.485604
53	6	0	-3.302104	-3.971214	2.109880
54	6	0	-3.330800	-3.302225	3.378516
55	7	0	-4.443549	-1.526065	-4.329902
56	6	0	-5.601519	-2.193309	-4.052987
57	6	0	-5.618040	-3.446073	-3.360954
58	7	0	-4.476020	-4.116025	-3.029326
59	6	0	-3.343552	-3.481045	-3.363894
60	6	0	-3.331678	-2.180579	-3.966735
61	6	0	-2.059320	3.488385	-3.895891
62	6	0	-2.056874	4.374325	-1.649184
63	6	0	-2.175921	4.133452	3.137802
64	6	0	-2.021265	1.796198	3.731993
65	6	0	-1.861878	-4.061192	1.637439
66	6	0	-1.903510	-3.003156	3.808263
67	6	0	-1.908715	-3.945574	-3.168785
68	6	0	-1.893915	-1.716184	-4.098375
69	8	0	-1.409834	-4.470001	0.604277
70	7	0	-1.110322	-3.505052	2.714963
71	8	0	-1.451810	-2.490338	4.787202
72	8	0	-1.521570	0.711338	3.861737
73	7	0	-1.327059	2.987048	3.380464
74	8	0	-1.771398	5.218151	2.856031
75	7	0	-1.287144	4.023697	-2.796489
76	8	0	-1.595466	3.119176	-4.929534
77	8	0	-1.610841	4.707710	-0.584896
78	7	0	-1.125281	-2.819333	-3.627293
79	8	0	-1.444991	-4.965154	-2.761844
80	8	0	-1.458550	-0.660581	-4.469566
81	1	0	-0.079863	-3.441474	2.709139
82	1	0	-0.295981	3.045022	3.327182
83	1	0	-0.258463	4.116961	-2.834651
84	1	0	-0.092238	-2.840550	-3.644980
85	6	0	9.169159	-1.474884	-2.037366
86	6	0	8.623835	-0.745215	-3.110265
87	6	0	7.525546	-1.317689	-3.773740
88	6	0	6.941120	-2.518211	-3.362668
89	6	0	7.505142	-3.173728	-2.271381
90	6	0	8.639501	-2.695014	-1.589677
91	6	0	8.578196	-1.558843	2.820010
92	6	0	9.151048	-1.997196	1.616529
93	6	0	8.646544	-3.080168	0.871578
94	6	0	7.548232	-3.767156	1.415373
95	6	0	6.923631	-3.367088	2.600254
96	6	0	7.439886	-2.257567	3.264160
97	6	0	6.809400	3.437938	-2.523796
98	6	0	7.392412	2.362658	-3.189802
99	6	0	8.552139	1.712916	-2.726968
100	6	0	9.084573	2.171185	-1.511890
101	6	0	8.519831	3.226793	-0.771913
102	6	0	7.398462	3.862475	-1.330579
103	6	0	7.326736	3.279960	2.358779
104	6	0	8.486856	2.845746	1.690248
105	6	0	9.057999	1.647513	2.144890
106	6	0	8.533577	0.899360	3.215901

107	6	0	7.410867	1.431537	3.871458
108	6	0	6.781712	2.605878	3.448810
109	6	0	9.263637	0.586712	-3.458911
110	6	0	9.329496	-3.415116	-0.442692
111	6	0	9.226576	-0.404818	3.567159
112	6	0	9.165372	3.591631	0.552786
113	8	0	7.012976	-0.710316	-4.949093
114	8	0	6.968064	-4.426098	-1.893423
115	8	0	7.072648	-4.950508	0.793528
116	8	0	6.851841	-1.873419	4.490673
117	8	0	6.844759	1.972406	-4.432037
118	8	0	6.863908	5.022741	-0.714205
119	8	0	6.744280	4.509361	1.973381
120	8	0	6.914000	0.816367	5.051904
121	6	0	3.321097	4.212377	1.102175
122	6	0	3.363583	4.688612	-0.250100
123	7	0	4.510152	4.951602	-0.892368
124	6	0	5.631432	4.783497	-0.133721
125	6	0	5.579883	4.414097	1.248152
126	7	0	4.410828	4.083498	1.872101
127	7	0	4.505236	1.833580	-4.036209
128	6	0	3.427643	1.051058	-4.189668
129	6	0	3.499654	-0.291499	-4.692452
130	7	0	4.658569	-0.914825	-4.944363
131	6	0	5.766819	-0.145412	-4.741377
132	6	0	5.687349	1.230654	-4.360419
133	7	0	4.620984	-4.058070	-1.814638
134	6	0	5.791401	-4.374818	-1.184549
135	6	0	5.839762	-4.760317	0.192497
136	7	0	4.714669	-4.978851	0.932088
137	6	0	3.569230	-4.733270	0.281464
138	6	0	3.526611	-4.220982	-1.058443
139	7	0	4.554317	0.906944	5.065429
140	6	0	5.695688	0.197097	4.833449
141	6	0	5.676500	-1.167404	4.398362
142	7	0	4.526433	-1.789628	4.004598
143	6	0	3.418989	-1.050491	4.163662
144	6	0	3.424179	0.252546	4.761960
145	6	0	1.878509	3.904421	1.462314
146	6	0	1.944597	4.794901	-0.780812
147	6	0	1.974791	1.375337	-3.877399
148	6	0	2.091230	-0.844825	-4.827311
149	6	0	2.150779	-4.871569	0.805710
150	6	0	2.083792	-3.888408	-1.402954
151	6	0	1.996383	-1.382871	3.748768
152	6	0	1.990083	0.731973	4.912075
153	8	0	1.711715	-5.303474	1.827187
154	7	0	1.348536	-4.317745	-0.258148
155	8	0	1.610630	-3.319210	-2.346737
156	8	0	1.672140	-1.887562	-5.230691
157	7	0	1.264727	0.223501	-4.328663
158	8	0	1.475479	2.321765	-3.335114
159	7	0	1.138774	4.319014	0.316569
160	8	0	1.416438	3.387834	2.442050
161	8	0	1.503221	5.164615	-1.827094
162	7	0	1.220862	-0.312960	4.268714
163	8	0	1.582961	-2.273743	3.053627
164	8	0	1.514454	1.699752	5.418403
165	1	0	0.309850	-4.329669	-0.224721
166	1	0	0.229646	0.166896	-4.335652
167	1	0	0.104171	4.331430	0.279000
168	1	0	0.185927	-0.289707	4.229218
169	1	0	-10.343036	1.664891	2.605646

170	1	0	-10.007963	1.779531	0.372087
171	1	0	-6.127430	4.866925	0.891816
172	1	0	-9.993200	-0.499818	1.991711
173	1	0	-5.898868	-0.843468	4.819889
174	1	0	-10.216305	-2.737390	1.852324
175	1	0	-9.909385	-2.067820	-0.308431
176	1	0	-5.836953	-4.905667	-0.792695
177	1	0	-10.219278	-1.955069	-2.543424
178	1	0	-5.909502	0.778967	-4.755922
179	1	0	-9.966792	0.210810	-1.912037
180	1	0	-10.326554	2.424864	-1.795303
181	1	0	6.059650	-3.916519	3.002474
182	1	0	10.029885	-1.470949	1.236011
183	1	0	10.382587	-3.010527	-0.382542
184	1	0	6.068460	-2.936679	-3.886171
185	1	0	10.045352	-1.068966	-1.526449
186	1	0	10.324845	0.557994	-3.072752
187	1	0	9.979307	1.682619	-1.118589
188	1	0	5.921683	3.942792	-2.933652
189	1	0	10.235229	3.230755	0.511718
190	1	0	5.891474	2.993445	3.965618
191	1	0	9.953076	1.274183	1.641406
192	1	0	10.291013	-0.326398	3.196528
193	6	0	-9.228418	-4.276860	2.943069
194	1	0	-9.784547	-4.087216	3.868484
195	1	0	-9.722716	-5.098029	2.411275
196	1	0	-8.232406	-4.646143	3.242830
197	6	0	-9.254983	-3.015028	-4.118210
198	1	0	-9.780040	-3.956493	-3.918492
199	1	0	-9.790430	-2.489556	-4.917251
200	1	0	-8.264850	-3.286150	-4.523180
201	6	0	-9.420123	4.019624	-2.875782
202	1	0	-9.953526	3.796324	-3.807135
203	1	0	-9.969018	4.809508	-2.350274
204	1	0	-8.445314	4.448064	-3.165503
205	6	0	-9.436977	2.753551	4.196725
206	1	0	-10.004140	3.672206	4.005437
207	1	0	-9.951347	2.194725	4.986725
208	1	0	-8.462078	3.066303	4.608726
209	6	0	9.379357	0.830840	-4.962017
210	1	0	9.888660	1.777383	-5.176124
211	1	0	9.936939	0.025762	-5.454979
212	1	0	8.393680	0.879759	-5.456648
213	6	0	9.248947	5.097600	0.793160
214	1	0	9.766659	5.324926	1.732141
215	1	0	9.783608	5.602303	-0.020177
216	1	0	8.252985	5.569097	0.855967
217	6	0	9.332681	-0.652120	5.070517
218	1	0	9.876592	-1.578789	5.286731
219	1	0	9.852283	0.171790	5.574048
220	1	0	8.344140	-0.741710	5.552940
221	6	0	9.478966	-4.915770	-0.684079
222	1	0	10.019148	-5.119141	-1.615920
223	1	0	10.022075	-5.400000	0.135944
224	1	0	8.504275	-5.427795	-0.762750
225	1	0	5.860585	1.333687	-0.980615
226	6	0	5.154861	0.631103	-0.551917
227	6	0	3.798939	0.795625	-0.790971
228	6	0	5.611222	-0.425200	0.231625
229	6	0	2.884660	-0.106069	-0.245905
230	1	0	3.427516	1.615602	-1.395400
231	6	0	4.693326	-1.314815	0.777037
232	1	0	6.671195	-0.552178	0.416982

233	7	0	1.520246	0.129596	-0.551484
234	6	0	3.332657	-1.163406	0.544192
235	1	0	5.029533	-2.137084	1.400115
236	7	0	0.698723	-0.647047	-0.053209
237	1	0	2.626536	-1.861337	0.988454
238	7	0	-0.137323	-1.281741	0.338074
239	6	0	-1.133863	1.169166	-1.684225
240	6	0	-2.139738	0.768238	-1.163447
241	1	0	-0.222792	1.511050	-2.125091
242	6	0	-3.342647	0.306696	-0.536030
243	6	0	-3.349787	-0.001230	0.829141
244	6	0	-4.519553	0.174686	-1.280285
245	6	0	-4.519967	-0.429980	1.438464
246	1	0	-2.433110	0.095242	1.400036
247	6	0	-5.684473	-0.258617	-0.663392
248	1	0	-4.505972	0.414556	-2.338216
249	6	0	-5.688260	-0.558819	0.694536
250	1	0	-4.519767	-0.649923	2.501821
251	1	0	-6.597757	-0.355402	-1.239549
252	1	0	-6.605445	-0.887537	1.170037

Transition structure 10 (B3LYP) (atoms treated at DFT level are marked in bold)

Imaginary Freq: -426.4711 cm⁻¹
ONIOM: extrapolated energy = -704.878322117936

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	9.065591	-2.441542	0.499914
2	6	0	8.554709	-3.050217	-0.657544
3	6	0	7.440106	-3.892389	-0.489461
4	6	0	6.865748	-4.137317	0.759447
5	6	0	7.432886	-3.519725	1.878510
6	6	0	8.528221	-2.642850	1.782703
7	6	0	8.368077	1.835751	2.717396
8	6	0	8.984454	0.580600	2.586836
9	6	0	8.462149	-0.588326	3.165173
10	6	0	7.286101	-0.450502	3.924183
11	6	0	6.612727	0.762724	4.071580
12	6	0	7.176693	1.883738	3.464047
13	6	0	6.803194	-0.618162	-4.066655
14	6	0	7.439745	-1.720295	-3.491924
15	6	0	8.572633	-1.602565	-2.667975
16	6	0	9.095269	-0.310791	-2.484651
17	6	0	8.521566	0.833624	-3.060272
18	6	0	7.365792	0.637116	-3.839182
19	6	0	7.404987	3.806229	-1.862109
20	6	0	8.486803	2.922611	-1.709434
21	6	0	8.957581	2.725127	-0.400304
22	6	0	8.385583	3.334555	0.729343
23	6	0	7.284705	4.179633	0.501763
24	6	0	6.785929	4.431444	-0.777613
25	6	0	9.260206	-2.763197	-1.972240
26	6	0	9.185935	-1.904138	2.936720
27	6	0	9.024690	3.045266	2.076195
28	6	0	9.190261	2.178677	-2.830528
29	8	0	6.975431	-4.638819	-1.595532
30	8	0	6.958884	-3.901046	3.156198

31	8	0	6.848069	-1.573800	4.655620
32	8	0	6.607976	3.152507	3.705158
33	8	0	7.015441	-3.016787	-3.854088
34	8	0	6.843752	1.753398	-4.527579
35	8	0	6.954341	4.151450	-3.162930
36	8	0	6.700826	4.897928	1.575280
37	6	0	3.458009	3.711955	-3.514630
38	6	0	3.399456	2.362771	-3.994643
39	7	0	4.489472	1.640967	-4.291202
40	6	0	5.669894	2.287558	-4.059630
41	6	0	5.727211	3.587065	-3.458728
42	7	0	4.608866	4.326153	-3.207588
43	7	0	4.680558	-3.142683	-4.061047
44	6	0	3.559980	-3.704265	-3.587234
45	6	0	3.535380	-4.508292	-2.401714
46	7	0	4.629537	-4.782157	-1.675677
47	6	0	5.785104	-4.242631	-2.163755
48	6	0	5.805256	-3.424441	-3.340004
49	7	0	4.615279	-4.106410	3.219591
50	6	0	5.731038	-3.372922	3.505251
51	6	0	5.668766	-2.146367	4.238205
52	7	0	4.490030	-1.585645	4.639553
53	6	0	3.403225	-2.304778	4.331748
54	6	0	3.467777	-3.564963	3.651927
55	7	0	4.347833	4.922872	1.432044
56	6	0	5.479811	4.397742	1.986498
57	6	0	5.435769	3.438884	3.048870
58	7	0	4.264699	2.914726	3.517117
59	6	0	3.163982	3.431177	2.954803
60	6	0	3.203123	4.454308	1.950809
61	6	0	2.044582	4.261357	-3.394508
62	6	0	1.942225	1.944469	-4.076208
63	6	0	2.153420	-3.616821	-4.160069
64	6	0	2.103709	-4.938909	-2.138765
65	6	0	1.944585	-1.956595	4.587122
66	6	0	2.054204	-4.103266	3.477754
67	6	0	1.712644	3.090934	3.258653
68	6	0	1.778057	4.879894	1.631249
69	8	0	1.450439	-0.991912	5.093417
70	7	0	1.229749	-3.073995	4.047912
71	8	0	1.659724	-5.119473	2.991992
72	8	0	1.631524	-5.560988	-1.225979
73	7	0	1.362707	-4.379502	-3.220534
74	8	0	1.720749	-3.080762	-5.132018
75	7	0	1.221933	3.130639	-3.763745
76	8	0	1.632220	5.336541	-3.094617
77	8	0	1.453212	0.869284	-4.297243
78	7	0	0.975148	4.037793	2.474141
79	8	0	1.234307	2.231279	3.936620
80	8	0	1.344583	5.703219	0.879910
81	1	0	0.197689	-3.129322	4.061851
82	1	0	0.345623	-4.517809	-3.335169
83	1	0	0.191040	3.166273	-3.720781
84	1	0	-0.049870	4.150018	2.549032
85	6	0	-9.200237	1.729123	1.678685
86	6	0	-8.723051	2.880184	1.032701
87	6	0	-7.615514	3.520149	1.619398
88	6	0	-6.997547	3.054660	2.778848
89	6	0	-7.524359	1.909102	3.380010
90	6	0	-8.620587	1.207358	2.848694
91	6	0	-8.449061	-3.080250	1.216641
92	6	0	-9.045925	-1.948775	1.795422
93	6	0	-8.494238	-1.270786	2.895579

94	6	0	-7.294841	-1.784680	3.421166
95	6	0	-6.644502	-2.896293	2.882338
96	6	0	-7.248373	-3.529946	1.797148
97	6	0	-6.898701	2.856118	-3.127000
98	6	0	-7.591795	3.440022	-2.063897
99	6	0	-8.686002	2.813625	-1.441846
100	6	0	-9.114330	1.590458	-1.988692
101	6	0	-8.477309	0.967417	-3.073910
102	6	0	-7.351947	1.626229	-3.600684
103	6	0	-7.267919	-2.191278	-3.550212
104	6	0	-8.399386	-1.543020	-3.024343
105	6	0	-8.967918	-2.114407	-1.873785
106	6	0	-8.460474	-3.269571	-1.251993
107	6	0	-7.359403	-3.888459	-1.867807
108	6	0	-6.745286	-3.363388	-3.006483
109	6	0	-9.429161	3.346848	-0.229346
110	6	0	-9.227430	-0.054994	3.436500
111	6	0	-9.131995	-3.735947	0.027758
112	6	0	-9.068650	-0.318959	-3.623665
113	8	0	-7.196027	4.752654	1.074657
114	8	0	-6.991436	1.515957	4.629952
115	8	0	-6.802054	-1.228897	4.620198
116	8	0	-6.720172	-4.754529	1.338342
117	8	0	-7.228009	4.751829	-1.678242
118	8	0	-6.689401	1.060104	-4.720256
119	8	0	-6.638253	-1.681791	-4.717779
120	8	0	-6.870237	-5.124872	-1.375405
121	6	0	-3.243985	-0.960178	-3.966231
122	6	0	-3.285225	0.471324	-3.925351
123	7	0	-4.401261	1.183277	-4.133381
124	6	0	-5.508118	0.429970	-4.399600
125	6	0	-5.473662	-1.001534	-4.422407
126	7	0	-4.328511	-1.712188	-4.202460
127	7	0	-4.896136	5.079221	-1.758139
128	6	0	-3.773675	5.210510	-1.037157
129	6	0	-3.737286	5.045716	0.386521
130	7	0	-4.832614	4.828289	1.128018
131	6	0	-5.992212	4.756619	0.410528
132	6	0	-6.016408	4.832178	-1.018863
133	7	0	-4.644252	1.742686	4.640346
134	6	0	-5.741422	0.934206	4.560489
135	6	0	-5.643183	-0.492288	4.517670
136	7	0	-4.444938	-1.146027	4.509584
137	6	0	-3.377675	-0.339309	4.587944
138	6	0	-3.475295	1.087764	4.669788
139	7	0	-4.520047	-5.228201	-1.543623
140	6	0	-5.627226	-5.002515	-0.779771
141	6	0	-5.550651	-4.713772	0.620949
142	7	0	-4.361033	-4.546587	1.269633
143	6	0	-3.281311	-4.749386	0.500983
144	6	0	-3.358782	-5.122772	-0.881087
145	6	0	-1.824597	-1.418378	-3.676110
146	6	0	-1.898789	0.992958	-3.605333
147	6	0	-2.371515	5.529146	-1.536525
148	6	0	-2.295271	5.156922	0.851457
149	6	0	-1.908377	-0.730571	4.593341
150	6	0	-2.073445	1.672026	4.773598
151	6	0	-1.818576	-4.648083	0.903822
152	6	0	-1.952316	-5.339970	-1.412113
153	8	0	-1.403396	-1.812446	4.484838
154	7	0	-1.219423	0.511496	4.717704
155	8	0	-1.698077	2.798795	4.878059
156	8	0	-1.806297	4.970172	1.930671

157	7	0	-1.572523	5.481059	-0.334822
158	8	0	-1.953956	5.770413	-2.625489
159	7	0	-1.096996	-0.184844	-3.515101
160	8	0	-1.344684	-2.503551	-3.537750
161	8	0	-1.512693	2.111172	-3.402112
162	7	0	-1.116016	-5.063715	-0.274771
163	8	0	-1.306285	-4.265802	1.913781
164	8	0	-1.538446	-5.643625	-2.491722
165	1	0	-0.187151	0.578344	4.773592
166	1	0	-0.552197	5.655316	-0.334914
167	1	0	-0.066663	-0.148295	-3.456057
168	1	0	-0.097251	-5.237522	-0.289481
169	1	0	10.308925	-2.426239	-1.719327
170	1	0	9.990475	-0.193265	-1.869627
171	1	0	5.909686	-0.736803	-4.695936
172	1	0	9.929107	-1.778614	0.398708
173	1	0	6.018471	-4.828688	0.864588
174	1	0	10.239415	-1.653912	2.614186
175	1	0	9.910602	0.510274	2.012206
176	1	0	5.687224	0.837140	4.661759
177	1	0	10.102976	2.771687	1.876599
178	1	0	5.945582	5.124905	-0.926893
179	1	0	9.811446	2.058790	-0.252385
180	1	0	10.243665	1.971487	-2.477778
181	1	0	-5.709490	-3.276115	3.318999
182	1	0	-9.983979	-1.580400	1.373436
183	1	0	-10.292793	-0.115111	3.065341
184	1	0	-6.139623	3.584297	3.219201
185	1	0	-10.062903	1.212266	1.251511
186	1	0	-10.455654	2.875493	-0.232250
187	1	0	-9.984562	1.100579	-1.545035
188	1	0	-6.034480	3.356878	-3.587059
189	1	0	-10.150795	-0.347251	-3.297199
190	1	0	-5.878060	-3.860858	-3.466036
191	1	0	-9.843380	-1.631248	-1.432711
192	1	0	-10.196744	-3.360233	0.000798
193	6	0	9.336446	-2.749162	4.198932
194	1	0	9.928697	-3.651339	4.006056
195	1	0	9.826200	-2.184916	5.001103
196	1	0	8.365453	-3.088823	4.597441
197	6	0	9.077456	4.262151	2.997675
198	1	0	9.567427	4.022542	3.948452
199	1	0	9.624288	5.090820	2.532644
200	1	0	8.073305	4.646828	3.245250
201	6	0	9.342242	2.997920	-4.110295
202	1	0	9.866801	3.941717	-3.919334
203	1	0	9.902305	2.446105	-4.873910
204	1	0	8.369703	3.264168	-4.558046
205	6	0	9.433117	-3.996734	-2.854795
206	1	0	9.962950	-3.751695	-3.782854
207	1	0	9.997919	-4.780905	-2.337119
208	1	0	8.469113	-4.443690	-3.149838
209	6	0	-9.670395	4.853580	-0.269575
210	1	0	-10.219650	5.145861	-1.172205
211	1	0	-10.244398	5.189185	0.601991
212	1	0	-8.730120	5.430846	-0.271465
213	6	0	-9.101774	-0.347748	-5.151505
214	1	0	-9.593177	-1.254390	-5.523452
215	1	0	-9.638330	0.518249	-5.556249
216	1	0	-8.090665	-0.330797	-5.593800
217	6	0	-9.234694	-5.253796	0.153631
218	1	0	-9.766479	-5.543615	1.067261
219	1	0	-9.764455	-5.690164	-0.701417

220	1	0	-8.245402	-5.740804	0.193014
221	6	0	-9.326329	-0.034228	4.959934
222	1	0	-9.903855	0.829354	5.310104
223	1	0	-9.806461	-0.942591	5.341603
224	1	0	-8.337279	0.030262	5.444971
225	6	0	-3.918852	-1.041094	0.838366
226	6	0	-2.733987	-1.374569	1.492162
227	6	0	-3.931241	0.032998	-0.050674
228	1	0	-4.823680	-1.606555	1.031888
229	6	0	-1.573933	-0.639145	1.269036
230	1	0	-2.710349	-2.206158	2.197905
231	6	0	-2.773328	0.762107	-0.297856
232	1	0	-4.849991	0.308553	-0.555936
233	6	0	-1.584157	0.433517	0.369967
234	1	0	-0.658303	-0.882106	1.795999
235	1	0	-2.783247	1.599441	-0.986131
236	7	0	-0.370223	1.127194	0.156491
237	6	0	1.987571	0.978913	-0.254440
238	7	0	-0.391713	2.310441	-0.271209
239	6	0	2.103944	2.164969	-0.591116
240	6	0	2.363930	-0.369123	0.053266
241	7	0	0.402082	3.093818	-0.642222
242	1	0	2.695355	2.990628	-0.918173
243	6	0	1.503757	-1.462916	-0.113454
244	6	0	3.685474	-0.601998	0.479319
245	6	0	1.948462	-2.750794	0.154387
246	1	0	0.489751	-1.293437	-0.445448
247	6	0	4.130363	-1.896158	0.714325
248	1	0	4.354987	0.238778	0.612491
249	6	0	3.262692	-2.975860	0.556911
250	1	0	1.263123	-3.587416	0.058116
251	1	0	5.157464	-2.061362	1.019306
252	1	0	3.604531	-3.993586	0.743360

Transition structure 10 (M06-2X) (atoms treated at DFT level are marked in bold)

Imaginary Freq: -463.8365 cm⁻¹
ONIOM: extrapolated energy = -704.573716976385

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	9.043765	-2.462307	0.547756
2	6	0	8.544347	-3.071144	-0.614544
3	6	0	7.428240	-3.913261	-0.457727
4	6	0	6.835033	-4.153461	0.782750
5	6	0	7.391109	-3.535459	1.906496
6	6	0	8.489744	-2.661546	1.823888
7	6	0	8.314971	1.815206	2.754060
8	6	0	8.932374	0.559965	2.633542
9	6	0	8.401848	-0.608239	3.206644
10	6	0	7.215856	-0.469124	3.949656
11	6	0	6.540781	0.744850	4.085828
12	6	0	7.113492	1.864382	3.484452
13	6	0	6.802725	-0.637706	-4.029322
14	6	0	7.435438	-1.741457	-3.452496
15	6	0	8.565566	-1.624785	-2.624369
16	6	0	9.087613	-0.333103	-2.437275
17	6	0	8.518385	0.811912	-3.015294

18	6	0	7.366732	0.616685	-3.800683
19	6	0	7.396158	3.790058	-1.832244
20	6	0	8.473197	2.902563	-1.668267
21	6	0	8.929443	2.703635	-0.354440
22	6	0	8.349800	3.317092	0.769248
23	6	0	7.254830	4.166732	0.530736
24	6	0	6.768827	4.418077	-0.754001
25	6	0	9.255052	-2.782977	-1.925942
26	6	0	9.130317	-1.923179	2.987584
27	6	0	8.978124	3.025195	2.120625
28	6	0	9.186902	2.156218	-2.781249
29	8	0	6.980199	-4.658428	-1.570770
30	8	0	6.899174	-3.909785	3.179527
31	8	0	6.764864	-1.589432	4.679023
32	8	0	6.547414	3.135332	3.716132
33	8	0	7.011756	-3.035558	-3.824668
34	8	0	6.857023	1.733329	-4.496657
35	8	0	6.963405	4.139568	-3.137718
36	8	0	6.666434	4.894642	1.595666
37	6	0	3.472576	3.727574	-3.560206
38	6	0	3.410931	2.373587	-4.026346
39	7	0	4.499773	1.639368	-4.295046
40	6	0	5.681233	2.277860	-4.046964
41	6	0	5.738749	3.580971	-3.453739
42	7	0	4.622549	4.332971	-3.233030
43	7	0	4.677659	-3.183619	-4.038397
44	6	0	3.561474	-3.756093	-3.566377
45	6	0	3.540761	-4.556582	-2.378397
46	7	0	4.635526	-4.819856	-1.649768
47	6	0	5.786732	-4.272558	-2.138685
48	6	0	5.803281	-3.453010	-3.314052
49	7	0	4.552656	-4.107812	3.181558
50	6	0	5.664464	-3.382495	3.502328
51	6	0	5.591613	-2.160723	4.242222
52	7	0	4.406662	-1.602030	4.627868
53	6	0	3.324727	-2.315882	4.291773
54	6	0	3.398650	-3.566495	3.595571
55	7	0	4.315146	4.955172	1.460172
56	6	0	5.440273	4.403951	2.002986
57	6	0	5.382760	3.430730	3.052016
58	7	0	4.205423	2.907638	3.505330
59	6	0	3.111594	3.446188	2.950301
60	6	0	3.164314	4.492955	1.971436
61	6	0	2.062736	4.292756	-3.479052
62	6	0	1.952120	1.966880	-4.129530
63	6	0	2.155698	-3.686401	-4.143551
64	6	0	2.112584	-4.997962	-2.114501
65	6	0	1.862669	-1.968841	4.527130
66	6	0	1.987493	-4.097386	3.385482
67	6	0	1.656435	3.113937	3.243032
68	6	0	1.745894	4.949088	1.667687
69	8	0	1.363879	-1.008723	5.037346
70	7	0	1.154714	-3.076300	3.958460
71	8	0	1.601781	-5.102765	2.870816
72	8	0	1.642608	-5.612603	-1.196094
73	7	0	1.370047	-4.452489	-3.203117
74	8	0	1.720856	-3.159692	-5.119870
75	7	0	1.236452	3.163417	-3.847294
76	8	0	1.654924	5.378207	-3.212286
77	8	0	1.457413	0.893388	-4.346582
78	7	0	0.930979	4.091099	2.484422
79	8	0	1.166214	2.241468	3.895838
80	8	0	1.319871	5.802453	0.946328

81	1	0	0.122892	-3.138095	3.966705
82	1	0	0.354282	-4.599509	-3.317631
83	1	0	0.206357	3.206864	-3.818782
84	1	0	-0.091350	4.218734	2.568879
85	6	0	-9.222458	1.712505	1.626391
86	6	0	-8.742012	2.863487	0.982745
87	6	0	-7.644126	3.509584	1.580735
88	6	0	-7.037013	3.048700	2.747779
89	6	0	-7.566339	1.902607	3.345857
90	6	0	-8.654731	1.196170	2.804602
91	6	0	-8.454017	-3.096782	1.190928
92	6	0	-9.060444	-1.964321	1.757642
93	6	0	-8.524570	-1.281876	2.862887
94	6	0	-7.331885	-1.792429	3.406534
95	6	0	-6.672846	-2.905282	2.880974
96	6	0	-7.260958	-3.542981	1.789619
97	6	0	-6.862075	2.831712	-3.150062
98	6	0	-7.572560	3.417008	-2.099238
99	6	0	-8.672893	2.788672	-1.490068
100	6	0	-9.089082	1.562098	-2.038442
101	6	0	-8.435091	0.937913	-3.112861
102	6	0	-7.304559	1.598668	-3.626007
103	6	0	-7.210284	-2.217877	-3.562441
104	6	0	-8.350821	-1.571716	-3.054000
105	6	0	-8.932837	-2.141147	-1.909294
106	6	0	-8.430112	-3.292674	-1.276986
107	6	0	-7.318327	-3.909547	-1.875455
108	6	0	-6.690405	-3.385889	-3.007306
109	6	0	-9.434409	3.322945	-0.289482
110	6	0	-9.266184	-0.065159	3.389941
111	6	0	-9.118659	-3.757258	-0.005611
112	6	0	-9.015587	-0.351756	-3.666449
113	8	0	-7.226276	4.744025	1.039475
114	8	0	-7.046099	1.515064	4.602823
115	8	0	-6.855678	-1.230322	4.609440
116	8	0	-6.725403	-4.768177	1.341021
117	8	0	-7.222330	4.732804	-1.715218
118	8	0	-6.626439	1.032497	-4.736103
119	8	0	-6.569309	-1.710528	-4.724639
120	8	0	-6.833229	-5.143937	-1.374222
121	6	0	-3.183665	-0.978614	-3.947607
122	6	0	-3.227860	0.452748	-3.911767
123	7	0	-4.343990	1.161815	-4.129782
124	6	0	-5.447346	0.405583	-4.402044
125	6	0	-5.409713	-1.026152	-4.420272
126	7	0	-4.264981	-1.733662	-4.188966
127	7	0	-4.894258	5.085492	-1.765165
128	6	0	-3.783403	5.235664	-1.029944
129	6	0	-3.763534	5.077829	0.394745
130	7	0	-4.865565	4.847940	1.122592
131	6	0	-6.014570	4.757858	0.390370
132	6	0	-6.020994	4.827236	-1.039762
133	7	0	-4.699056	1.742557	4.636493
134	6	0	-5.795361	0.933243	4.549960
135	6	0	-5.696222	-0.493288	4.517473
136	7	0	-4.497710	-1.146852	4.528169
137	6	0	-3.431815	-0.339648	4.614903
138	6	0	-3.530523	1.088171	4.684526
139	7	0	-4.480951	-5.249013	-1.504998
140	6	0	-5.599893	-5.020030	-0.759518
141	6	0	-5.545030	-4.729207	0.642001
142	7	0	-4.365611	-4.562999	1.309289
143	6	0	-3.274159	-4.770960	0.558779

144	6	0	-3.330314	-5.146024	-0.823543
145	6	0	-1.765467	-1.433720	-3.647823
146	6	0	-1.844071	0.977916	-3.585542
147	6	0	-2.380125	5.573827	-1.512503
148	6	0	-2.330077	5.213692	0.878555
149	6	0	-1.962709	-0.731008	4.642561
150	6	0	-2.129681	1.673192	4.799432
151	6	0	-1.817672	-4.676612	0.985625
152	6	0	-1.915928	-5.369420	-1.330728
153	8	0	-1.457063	-1.814232	4.551653
154	7	0	-1.275374	0.512468	4.761340
155	8	0	-1.755748	2.800763	4.900769
156	8	0	-1.851344	5.039454	1.964329
157	7	0	-1.596000	5.541872	-0.300108
158	8	0	-1.951624	5.816274	-2.596808
159	7	0	-1.040500	-0.198252	-3.486372
160	8	0	-1.285451	-2.517566	-3.500824
161	8	0	-1.461673	2.097221	-3.381065
162	7	0	-1.096783	-5.098754	-0.179232
163	8	0	-1.323869	-4.291199	2.003883
164	8	0	-1.488594	-5.671577	-2.405483
165	1	0	-0.243243	0.579493	4.817362
166	1	0	-0.580616	5.742386	-0.286888
167	1	0	-0.010102	-0.158822	-3.434715
168	1	0	-0.079185	-5.280331	-0.175135
169	1	0	10.301439	-2.442516	-1.668489
170	1	0	9.979759	-0.216695	-1.817523
171	1	0	5.911823	-0.755331	-4.662302
172	1	0	9.909104	-1.800679	0.456036
173	1	0	5.981920	-4.839559	0.877879
174	1	0	10.188049	-1.671880	2.680373
175	1	0	9.866051	0.488275	2.071357
176	1	0	5.607627	0.820502	4.663448
177	1	0	10.057637	2.750740	1.928934
178	1	0	5.933405	5.115097	-0.912285
179	1	0	9.778470	2.033092	-0.197526
180	1	0	10.236328	1.948056	-2.417297
181	1	0	-5.743343	-3.282326	3.331710
182	1	0	-9.993091	-1.598653	1.321623
183	1	0	-10.326888	-0.128778	3.006149
184	1	0	-6.186439	3.582729	3.196911
185	1	0	-10.078391	1.191445	1.190782
186	1	0	-10.458559	2.846688	-0.303923
187	1	0	-9.963604	1.070516	-1.605166
188	1	0	-5.993625	3.334107	-3.600019
189	1	0	-10.101902	-0.382112	-3.354225
190	1	0	-5.815619	-3.882134	-3.453538
191	1	0	-9.815860	-1.659560	-1.481730
192	1	0	-10.183747	-3.383941	-0.048526
193	6	0	9.262958	-2.768610	4.251552
194	1	0	9.852765	-3.673774	4.065322
195	1	0	9.746738	-2.206566	5.058831
196	1	0	8.285889	-3.103225	4.639427
197	6	0	9.025303	4.240256	3.044785
198	1	0	9.504527	3.997407	4.000184
199	1	0	9.579779	5.067793	2.586773
200	1	0	8.020050	4.628169	3.282281
201	6	0	9.353660	2.973053	-4.060694
202	1	0	9.877191	3.916580	-3.865660
203	1	0	9.921246	2.419141	-4.817192
204	1	0	8.386414	3.239665	-4.519404
205	6	0	9.435571	-4.015222	-2.808704
206	1	0	9.981308	-3.770507	-3.727537

207	1	0	9.987849	-4.803729	-2.284174
208	1	0	8.473939	-4.456129	-3.120213
209	6	0	-9.682423	4.828276	-0.338092
210	1	0	-10.221332	5.114724	-1.248824
211	1	0	-10.269479	5.163966	0.524736
212	1	0	-8.745223	5.410332	-0.329705
213	6	0	-9.028686	-0.385398	-5.194460
214	1	0	-9.511360	-1.295301	-5.569924
215	1	0	-9.563726	0.477006	-5.608820
216	1	0	-8.012117	-0.365408	-5.623817
217	6	0	-9.220027	-5.274997	0.122483
218	1	0	-9.762392	-5.563730	1.030247
219	1	0	-9.738601	-5.714293	-0.737915
220	1	0	-8.230474	-5.760148	0.175058
221	6	0	-9.383762	-0.038108	4.911954
222	1	0	-9.968966	0.824643	5.251244
223	1	0	-9.864954	-0.946722	5.291749
224	1	0	-8.401015	0.032368	5.408815
225	6	0	-3.548036	-1.045490	0.899193
226	6	0	-2.331714	-1.310398	1.520379
227	6	0	-3.644524	0.015720	0.005079
228	1	0	-4.414562	-1.655823	1.125591
229	6	0	-1.221375	-0.517917	1.261674
230	1	0	-2.247059	-2.134350	2.229082
231	6	0	-2.535262	0.800342	-0.281745
232	1	0	-4.590146	0.237586	-0.474299
233	6	0	-1.319530	0.537429	0.354682
234	1	0	-0.275589	-0.699750	1.759313
235	1	0	-2.603524	1.629766	-0.976601
236	7	0	-0.148796	1.287151	0.095993
237	6	0	2.056600	1.138731	-0.319670
238	7	0	-0.227873	2.462351	-0.325437
239	6	0	2.256435	2.311794	-0.645703
240	6	0	2.359566	-0.242760	-0.037671
241	7	0	0.504853	3.276241	-0.707987
242	1	0	2.845068	3.149883	-0.945972
243	6	0	1.475473	-1.275992	-0.353261
244	6	0	3.609075	-0.552196	0.512479
245	6	0	1.820616	-2.592015	-0.086638
246	1	0	0.517395	-1.041110	-0.797206
247	6	0	3.960342	-1.873858	0.745095
248	1	0	4.296305	0.250988	0.748030
249	6	0	3.063137	-2.897597	0.457635
250	1	0	1.108358	-3.382273	-0.295502
251	1	0	4.938738	-2.104477	1.148731
252	1	0	3.330482	-3.935066	0.652663

Transition structure 11 (B3LYP) (atoms treated at DFT level are marked in bold)

Imaginary Freq: -385.0963 cm⁻¹
ONIOM: extrapolated energy = -704.894067660566

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-9.086878	-0.475822	2.582181
2	6	0	-8.543361	0.685626	3.152027
3	6	0	-7.381064	0.518894	3.927812

4	6	0	-6.798296	-0.723066	4.168031
5	6	0	-7.395196	-1.844479	3.586782
6	6	0	-8.527883	-1.755090	2.759788
7	6	0	-8.563158	-2.785392	-1.728999
8	6	0	-9.082692	-2.591871	-0.435152
9	6	0	-8.524103	-3.172482	0.713769
10	6	0	-7.382980	-3.973517	0.521705
11	6	0	-6.843015	-4.232608	-0.735767
12	6	0	-7.458098	-3.645160	-1.844574
13	6	0	-6.890865	4.205584	0.747323
14	6	0	-7.489916	3.617293	1.864527
15	6	0	-8.590318	2.749692	1.762988
16	6	0	-9.126161	2.550981	0.476427
17	6	0	-8.584500	3.132191	-0.680109
18	6	0	-7.445104	3.938648	-0.501757
19	6	0	-7.475450	1.832716	-3.583016
20	6	0	-8.590665	1.725485	-2.734773
21	6	0	-9.124554	0.436635	-2.544864
22	6	0	-8.570349	-0.717203	-3.119115
23	6	0	-7.422958	-0.532559	-3.912953
24	6	0	-6.868354	0.718905	-4.169510
25	6	0	-9.243781	2.014539	2.919713
26	6	0	-9.193665	-2.923228	2.054873
27	6	0	-9.243138	-2.058404	-2.875650
28	6	0	-9.264887	2.880126	-2.015373
29	8	0	-6.837854	1.652561	4.572160
30	8	0	-6.870364	-3.115317	3.927326
31	8	0	-6.816952	-4.626664	1.639968
32	8	0	-6.963660	-4.006308	-3.126677
33	8	0	-6.989742	3.987059	3.140688
34	8	0	-6.898417	4.587501	-1.632348
35	8	0	-6.972937	3.109935	-3.939610
36	8	0	-6.863302	-1.661810	-4.551245
37	6	0	-3.473833	3.371155	-3.411266
38	6	0	-3.446379	3.942496	-2.096519
39	7	0	-4.550410	4.316300	-1.434171
40	6	0	-5.715091	4.069814	-2.102673
41	6	0	-5.747477	3.386414	-3.360713
42	7	0	-4.613824	3.056066	-4.043799
43	7	0	-4.634323	4.144089	3.058345
44	6	0	-3.478516	3.510510	3.302766
45	6	0	-3.417210	2.167926	3.804096
46	7	0	-4.499307	1.481128	4.196803
47	6	0	-5.677535	2.150326	4.028398
48	6	0	-5.747924	3.430854	3.392872
49	7	0	-4.511601	-3.008101	3.984399
50	6	0	-5.651071	-3.379457	3.330735
51	6	0	-5.629549	-4.099270	2.095053
52	7	0	-4.469340	-4.373781	1.428424
53	6	0	-3.360180	-3.974428	2.065619
54	6	0	-3.377231	-3.337245	3.350961
55	7	0	-4.533070	-1.432702	-4.155004
56	6	0	-5.694005	-2.134969	-4.005010
57	6	0	-5.734617	-3.423911	-3.383095
58	7	0	-4.604810	-4.115217	-3.057025
59	6	0	-3.463951	-3.449996	-3.288277
60	6	0	-3.436610	-2.097806	-3.764337
61	6	0	-2.046768	3.188305	-3.900170
62	6	0	-2.003418	4.029975	-1.634930
63	6	0	-2.064981	4.015731	3.072146
64	6	0	-1.969711	1.709147	3.785207
65	6	0	-1.918013	-4.099895	1.605398
66	6	0	-1.944654	-3.114253	3.809296

67	6	0	-2.037551	-3.921810	-3.065012
68	6	0	-2.003946	-1.600217	-3.727867
69	8	0	-1.469306	-4.475473	0.557582
70	7	0	-1.157527	-3.630027	2.716865
71	8	0	-1.487332	-2.649810	4.808937
72	8	0	-1.495119	0.624498	3.986959
73	7	0	-1.245597	2.866258	3.382261
74	8	0	-1.632644	5.073636	2.732476
75	7	0	-1.249017	3.611811	-2.770722
76	8	0	-1.594588	2.810257	-4.936224
77	8	0	-1.545996	4.314007	-0.562092
78	7	0	-1.247247	-2.741142	-3.347227
79	8	0	-1.576372	-4.975294	-2.753842
80	8	0	-1.570104	-0.493899	-3.914121
81	1	0	-0.125494	-3.613840	2.728322
82	1	0	-0.212809	2.897010	3.332698
83	1	0	-0.216494	3.639321	-2.805514
84	1	0	-0.215295	-2.748481	-3.290938
85	6	0	9.108224	-1.472949	-2.162352
86	6	0	8.559587	-0.715614	-3.214698
87	6	0	7.450394	-1.263868	-3.880091
88	6	0	6.858659	-2.467092	-3.486755
89	6	0	7.425496	-3.149564	-2.413565
90	6	0	8.571961	-2.696944	-1.734121
91	6	0	8.592785	-1.659833	2.705926
92	6	0	9.142559	-2.077880	1.484389
93	6	0	8.609986	-3.133483	0.720134
94	6	0	7.507188	-3.814381	1.262487
95	6	0	6.903356	-3.432427	2.463478
96	6	0	7.449487	-2.350803	3.149340
97	6	0	6.809352	3.473918	-2.495296
98	6	0	7.363692	2.401644	-3.188714
99	6	0	8.526903	1.732371	-2.763921
100	6	0	9.087903	2.160784	-1.551098
101	6	0	8.548221	3.207052	-0.778976
102	6	0	7.426165	3.868391	-1.305244
103	6	0	7.403154	3.204934	2.369350
104	6	0	8.547676	2.770831	1.674718
105	6	0	9.108589	1.555112	2.094767
106	6	0	8.586836	0.788927	3.154269
107	6	0	7.477239	1.318566	3.834173
108	6	0	6.860618	2.511867	3.448529
109	6	0	9.210865	0.617108	-3.537598
110	6	0	9.268619	-3.448417	-0.611301
111	6	0	9.267097	-0.531371	3.468796
112	6	0	9.218761	3.533271	0.543637
113	8	0	6.928046	-0.631361	-5.039587
114	8	0	6.875813	-4.401858	-2.053338
115	8	0	7.004485	-4.975165	0.619876
116	8	0	6.885944	-1.991380	4.393968
117	8	0	6.784424	2.032973	-4.423323
118	8	0	6.913720	5.021524	-0.656501
119	8	0	6.831034	4.450089	2.018637
120	8	0	6.983786	0.680447	5.002903
121	6	0	3.395800	4.165763	1.187092
122	6	0	3.418911	4.675596	-0.153339
123	7	0	4.556003	4.960537	-0.803101
124	6	0	5.687484	4.777746	-0.063260
125	6	0	5.654744	4.377584	1.310249
126	7	0	4.495130	4.027501	1.941198
127	7	0	4.458185	1.879981	-3.949431
128	6	0	3.372975	1.111628	-4.122667
129	6	0	3.422195	-0.189866	-4.724990

130	7	0	4.571471	-0.805620	-5.035693
131	6	0	5.689739	-0.061118	-4.799924
132	6	0	5.627265	1.294598	-4.344896
133	7	0	4.535386	-4.007512	-1.941729
134	6	0	5.708440	-4.345808	-1.329114
135	6	0	5.766851	-4.752123	0.041895
136	7	0	4.648148	-4.962596	0.793135
137	6	0	3.498259	-4.694533	0.158880
138	6	0	3.447908	-4.169071	-1.174905
139	7	0	4.624655	0.802545	5.044008
140	6	0	5.754372	0.082537	4.786812
141	6	0	5.713187	-1.276006	4.336989
142	7	0	4.549491	-1.887678	3.967230
143	6	0	3.451630	-1.142747	4.161507
144	6	0	3.482711	0.160159	4.760060
145	6	0	1.962520	3.821697	1.550715
146	6	0	1.994177	4.775000	-0.669299
147	6	0	1.934322	1.405575	-3.730774
148	6	0	2.006415	-0.718861	-4.875183
149	6	0	2.082993	-4.830985	0.691733
150	6	0	2.004414	-3.835783	-1.509862
151	6	0	2.013906	-1.471275	3.796300
152	6	0	2.056835	0.653563	4.942051
153	8	0	1.647725	-5.263478	1.714484
154	7	0	1.272965	-4.275519	-0.367176
155	8	0	1.533827	-3.269956	-2.457483
156	8	0	1.561734	-1.704697	-5.376324
157	7	0	1.201266	0.304610	-4.246183
158	8	0	1.470816	2.302469	-3.075325
159	7	0	1.207274	4.236116	0.414140
160	8	0	1.517598	3.280206	2.524558
161	8	0	1.536731	5.175096	-1.696395
162	7	0	1.262811	-0.387045	4.324598
163	8	0	1.569516	-2.374259	3.138239
164	8	0	1.603180	1.627637	5.456905
165	1	0	0.235604	-4.298192	-0.329267
166	1	0	0.168551	0.234598	-4.183936
167	1	0	0.172495	4.224540	0.384376
168	1	0	0.227717	-0.349809	4.303207
169	1	0	-10.304479	1.781092	2.609128
170	1	0	-10.003970	1.908690	0.374006
171	1	0	-6.016357	4.864771	0.850007
172	1	0	-9.986240	-0.383101	1.968739
173	1	0	-5.906529	-0.818349	4.805291
174	1	0	-10.260476	-2.619170	1.840730
175	1	0	-9.962823	-1.954745	-0.320226
176	1	0	-5.966107	-4.887120	-0.850412
177	1	0	-10.303281	-1.843055	-2.550047
178	1	0	-5.987130	0.826630	-4.818810
179	1	0	-10.011532	0.330473	-1.915616
180	1	0	-10.324825	2.559509	-1.791412
181	1	0	6.031508	-3.973192	2.860873
182	1	0	10.024287	-1.556173	1.104539
183	1	0	10.327462	-3.057989	-0.558788
184	1	0	5.978084	-2.867578	-4.010565
185	1	0	9.992820	-1.085354	-1.651493
186	1	0	10.277917	0.564119	-3.170527
187	1	0	9.984697	1.655290	-1.184897
188	1	0	5.921866	3.998371	-2.879656
189	1	0	10.282907	3.159640	0.478077
190	1	0	5.980398	2.897403	3.984048
191	1	0	9.992582	1.182058	1.572018
192	1	0	10.327523	-0.459228	3.085932

193	6	0	-9.290678	-4.178062	2.920086
194	1	0	-9.825973	-3.977207	3.855382
195	1	0	-9.813410	-4.986134	2.395641
196	1	0	-8.298528	-4.571140	3.202110
197	6	0	-9.365662	-2.902529	-4.142631
198	1	0	-9.904245	-3.837454	-3.947780
199	1	0	-9.897581	-2.362467	-4.934085
200	1	0	-8.381855	-3.186433	-4.554642
201	6	0	-9.389056	4.138527	-2.871966
202	1	0	-9.936688	3.936733	-3.799958
203	1	0	-9.912817	4.937796	-2.335128
204	1	0	-8.405998	4.544048	-3.167336
205	6	0	-9.362697	2.857444	4.187674
206	1	0	-9.917305	3.784248	3.999533
207	1	0	-9.876484	2.309691	4.985852
208	1	0	-8.378031	3.155442	4.587483
209	6	0	9.304567	0.901422	-5.035247
210	1	0	9.820441	1.848180	-5.231899
211	1	0	9.845721	0.104576	-5.559069
212	1	0	8.311668	0.973278	-5.512051
213	6	0	9.325242	5.032344	0.815997
214	1	0	9.857197	5.232039	1.753310
215	1	0	9.856554	5.548081	0.007492
216	1	0	8.336235	5.514893	0.901761
217	6	0	9.388611	-0.811600	4.965183
218	1	0	9.921761	-1.750176	5.155059
219	1	0	9.925922	-0.005797	5.479167
220	1	0	8.404695	-0.897715	5.457876
221	6	0	9.395477	-4.945631	-0.885410
222	1	0	9.918830	-5.136766	-1.829316
223	1	0	9.944830	-5.453049	-0.083744
224	1	0	8.413202	-5.443735	-0.959045
225	1	0	5.216883	1.898515	-1.116404
226	6	0	4.736705	1.064683	-0.614467
227	6	0	3.350907	0.966759	-0.643478
228	6	0	5.503331	0.103765	0.041600
229	6	0	2.708849	-0.106224	-0.012167
230	1	0	2.760224	1.719635	-1.156234
231	6	0	4.861803	-0.960302	0.673644
232	1	0	6.584180	0.182727	0.061409
233	7	0	1.308174	-0.152778	-0.089700
234	6	0	3.477044	-1.073636	0.652448
235	1	0	5.442043	-1.714352	1.195473
236	7	0	0.622474	-1.029916	0.502051
237	1	0	2.982718	-1.899327	1.155743
238	7	0	-0.511586	-1.250899	0.653700
239	6	0	-0.386338	1.010039	-0.813350
240	6	0	-1.372856	0.408566	-0.373582
241	1	0	0.224406	1.726476	-1.315272
242	6	0	-2.785383	0.189829	-0.168664
243	6	0	-3.292632	-0.155329	1.092965
244	6	0	-3.679005	0.351166	-1.239661
245	6	0	-4.660111	-0.315050	1.280710
246	1	0	-2.606252	-0.297424	1.919694
247	6	0	-5.044755	0.175892	-1.045600
248	1	0	-3.291700	0.599992	-2.223237
249	6	0	-5.542332	-0.152168	0.214187
250	1	0	-5.034464	-0.566191	2.268172
251	1	0	-5.722750	0.297698	-1.883295
252	1	0	-6.609014	-0.281930	0.362537

Transition structure 11 (M06-2X) (atoms treated at DFT level are marked in bold)

Imaginary Freq: -453.4175 cm⁻¹
ONIOM: extrapolated energy = -704.588176708918

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	9.082396	-0.083758	-2.640982
2	6	0	8.542726	1.155976	-3.016546
3	6	0	7.369299	1.120503	-3.792792
4	6	0	6.767467	-0.064316	-4.209698
5	6	0	7.362272	-1.266120	-3.818734
6	6	0	8.508468	-1.315381	-3.006990
7	6	0	8.557720	-3.042696	1.253742
8	6	0	9.071204	-2.649998	0.003471
9	6	0	8.509833	-3.047614	-1.219800
10	6	0	7.373822	-3.875042	-1.150026
11	6	0	6.839937	-4.326943	0.054619
12	6	0	7.455073	-3.913307	1.239162
13	6	0	6.923747	4.282859	-0.104048
14	6	0	7.520653	3.872559	-1.299325
15	6	0	8.610189	2.986346	-1.334079
16	6	0	9.140559	2.583409	-0.093870
17	6	0	8.601581	2.981012	1.139139
18	6	0	7.469243	3.815144	1.088565
19	6	0	7.481968	1.240532	3.791384
20	6	0	8.601130	1.263616	2.942030
21	6	0	9.132677	0.018729	2.555009
22	6	0	8.572684	-1.208505	2.940516
23	6	0	7.422044	-1.146161	3.748623
24	6	0	6.867762	0.051464	4.193247
25	6	0	9.256274	2.428728	-2.589978
26	6	0	9.172448	-2.585784	-2.506809
27	6	0	9.241906	-2.498704	2.495395
28	6	0	9.279726	2.516164	2.417136
29	8	0	6.838944	2.345157	-4.254376
30	8	0	6.826183	-2.466066	-4.345978
31	8	0	6.800083	-4.348961	-2.352600
32	8	0	6.961068	-4.466353	2.451128
33	8	0	7.026462	4.444438	-2.501419
34	8	0	6.918583	4.281431	2.304383
35	8	0	6.985484	2.449427	4.341246
36	8	0	6.863036	-2.359956	4.205576
37	6	0	3.488537	2.797657	3.857167
38	6	0	3.463081	3.578928	2.654958
39	7	0	4.569000	4.053751	2.064019
40	6	0	5.732750	3.697656	2.683418
41	6	0	5.761812	2.818187	3.813034
42	7	0	4.626823	2.381541	4.431016
43	7	0	4.673482	4.624644	-2.395737
44	6	0	3.508673	4.046276	-2.721262
45	6	0	3.428365	2.786638	-3.402740
46	7	0	4.499643	2.147717	-3.893553
47	6	0	5.686724	2.772533	-3.639656
48	6	0	5.776161	3.949836	-2.830476
49	7	0	4.467937	-2.329479	-4.338867
50	6	0	5.614463	-2.822437	-3.785226
51	6	0	5.606832	-3.756264	-2.702067
52	7	0	4.453822	-4.154076	-2.087319
53	6	0	3.337690	-3.642818	-2.624364

54	6	0	3.340765	-2.767699	-3.761244
55	7	0	4.531515	-2.074653	3.854583
56	6	0	5.692257	-2.745793	3.598301
57	6	0	5.731970	-3.929248	2.793553
58	7	0	4.601535	-4.567123	2.374414
59	6	0	3.460935	-3.945542	2.707062
60	6	0	3.434014	-2.677814	3.376200
61	6	0	2.061495	2.535138	4.307362
62	6	0	2.019657	3.744905	2.215410
63	6	0	2.102523	4.532304	-2.416392
64	6	0	1.975636	2.345842	-3.436490
65	6	0	1.901473	-3.858108	-2.179956
66	6	0	1.903836	-2.447523	-4.140202
67	6	0	2.033608	-4.385085	2.429455
68	6	0	1.999552	-2.185402	3.424881
69	8	0	1.461779	-4.444621	-1.230361
70	7	0	1.128984	-3.163854	-3.159149
71	8	0	1.434804	-1.785894	-5.016373
72	8	0	1.487912	1.302016	-3.774757
73	7	0	1.267586	3.446988	-2.878181
74	8	0	1.685126	5.538360	-1.931355
75	7	0	1.265160	3.144102	3.265848
76	8	0	1.608756	1.986483	5.263986
77	8	0	1.560186	4.207831	1.207471
78	7	0	1.242234	-3.263639	2.891183
79	8	0	1.574252	-5.383355	1.968909
80	8	0	1.565840	-1.119247	3.772219
81	1	0	0.097200	-3.143550	-3.153605
82	1	0	0.235289	3.483778	-2.823365
83	1	0	0.232693	3.157902	3.302619
84	1	0	0.209768	-3.272505	2.854395
85	6	0	-9.100872	-1.778180	1.895764
86	6	0	-8.544648	-1.189439	3.046989
87	6	0	-7.432516	-1.833362	3.614974
88	6	0	-6.850518	-2.968720	3.045260
89	6	0	-7.428984	-3.484535	1.888108
90	6	0	-8.573219	-2.927373	1.287240
91	6	0	-8.574403	-1.223233	-2.938612
92	6	0	-9.134684	-1.820376	-1.798941
93	6	0	-8.612008	-2.983646	-1.202781
94	6	0	-7.510103	-3.580700	-1.838028
95	6	0	-6.895041	-3.021791	-2.961409
96	6	0	-7.430610	-1.843632	-3.474871
97	6	0	-6.802520	3.067849	2.978300
98	6	0	-7.352302	1.899790	3.499415
99	6	0	-8.513789	1.299535	2.977777
100	6	0	-9.077041	1.905767	1.844484
101	6	0	-8.541841	3.059982	1.241748
102	6	0	-7.423080	3.638240	1.863954
103	6	0	-7.387289	3.540574	-1.864132
104	6	0	-8.532581	3.002093	-1.248192
105	6	0	-9.086629	1.861832	-1.849528
106	6	0	-8.557885	1.266017	-3.010173
107	6	0	-7.444887	1.893221	-3.594976
108	6	0	-6.835032	3.017059	-3.030644
109	6	0	-9.194030	0.077853	3.573138
110	6	0	-9.276230	-3.493499	0.064029
111	6	0	-9.238507	0.010927	-3.526373
112	6	0	-9.211829	3.580662	-0.017299
113	8	0	-6.901783	-1.382139	4.852296
114	8	0	-6.897134	-4.679389	1.350254
115	8	0	-7.023807	-4.831954	-1.380631
116	8	0	-6.854662	-1.297025	-4.643687

117	8	0	-6.771210	1.348142	4.662826
118	8	0	-6.921455	4.882160	1.401683
119	8	0	-6.828541	4.725526	-1.331445
120	8	0	-6.941366	1.439744	-4.843274
121	6	0	-3.389921	4.377851	-0.542089
122	6	0	-3.422137	4.671148	0.861297
123	7	0	-4.564255	4.832444	1.543873
124	6	0	-5.692276	4.748036	0.781239
125	6	0	-5.652452	4.564376	-0.637579
126	7	0	-4.486611	4.337671	-1.311643
127	7	0	-4.443984	1.284123	4.182085
128	6	0	-3.354927	0.503579	4.231479
129	6	0	-3.398469	-0.880550	4.606570
130	7	0	-4.545172	-1.544631	4.808496
131	6	0	-5.667093	-0.776454	4.698592
132	6	0	-5.610907	0.635537	4.470532
133	7	0	-4.548015	-4.334765	1.306061
134	6	0	-5.725369	-4.539107	0.644585
135	6	0	-5.785278	-4.720975	-0.773693
136	7	0	-4.667636	-4.829591	-1.547902
137	6	0	-3.515413	-4.692945	-0.877037
138	6	0	-3.460221	-4.397134	0.525373
139	7	0	-4.581554	1.553909	-4.847594
140	6	0	-5.716350	0.809463	-4.708890
141	6	0	-5.683155	-0.600650	-4.464073
142	7	0	-4.525825	-1.262750	-4.167421
143	6	0	-3.424773	-0.500735	-4.232360
144	6	0	-3.444897	0.872824	-4.644815
145	6	0	-1.950886	4.121947	-0.951600
146	6	0	-1.999547	4.711613	1.391285
147	6	0	-1.915800	0.868748	3.904918
148	6	0	-1.979463	-1.419061	4.670125
149	6	0	-2.100822	-4.768273	-1.424184
150	6	0	-2.011121	-4.161465	0.914372
151	6	0	-1.994425	-0.877761	-3.884934
152	6	0	-2.014872	1.378141	-4.743803
153	8	0	-1.671503	-5.024751	-2.507107
154	7	0	-1.283812	-4.422215	-0.285398
155	8	0	-1.531747	-3.770300	1.941714
156	8	0	-1.531382	-2.475828	4.992056
157	7	0	-1.177747	-0.297723	4.234045
158	8	0	-1.459932	1.867880	3.412378
159	7	0	-1.203016	4.359749	0.239252
160	8	0	-1.497386	3.752179	-1.998950
161	8	0	-1.548967	4.953802	2.469057
162	7	0	-1.232239	0.259390	-4.262479
163	8	0	-1.566163	-1.856052	-3.330810
164	8	0	-1.553063	2.410092	-5.119343
165	1	0	-0.246704	-4.462831	-0.323752
166	1	0	-0.145114	-0.352707	4.161401
167	1	0	-0.168002	4.358275	0.270676
168	1	0	-0.197100	0.286017	-4.230037
169	1	0	10.315202	2.142403	-2.320662
170	1	0	10.011485	1.923728	-0.092498
171	1	0	6.056891	4.959829	-0.102493
172	1	0	9.990832	-0.094157	-2.034096
173	1	0	5.864971	-0.052937	-4.838697
174	1	0	10.242106	-2.325484	-2.252836
175	1	0	9.948314	-1.998654	-0.014745
176	1	0	5.966586	-4.996056	0.070048
177	1	0	10.301838	-2.238989	2.203287
178	1	0	5.983350	0.059377	4.847081
179	1	0	10.022252	0.009140	1.920687

180	1	0	10.338887	2.232126	2.145237
181	1	0	-6.023361	-3.500189	-3.432106
182	1	0	-10.016422	-1.358108	-1.348739
183	1	0	-10.331416	-3.090080	0.071764
184	1	0	-5.969665	-3.446252	3.499588
185	1	0	-9.985218	-1.314386	1.452386
186	1	0	-10.262566	0.081442	3.206316
187	1	0	-9.971808	1.458431	1.405050
188	1	0	-5.916723	3.530387	3.438460
189	1	0	-10.273777	3.195215	-0.012823
190	1	0	-5.953500	3.480999	-3.497461
191	1	0	-9.971945	1.411834	-1.393667
192	1	0	-10.301990	0.028406	-3.145336
193	6	0	9.257813	-3.681995	-3.566824
194	1	0	9.788060	-3.332491	-4.460284
195	1	0	9.780051	-4.567047	-3.185633
196	1	0	8.262018	-4.020166	-3.902051
197	6	0	9.364925	-3.524738	3.620107
198	1	0	9.902774	-4.419717	3.285696
199	1	0	9.897699	-3.110793	4.483688
200	1	0	8.381190	-3.867218	3.985155
201	6	0	9.406933	3.621062	3.463948
202	1	0	9.947417	3.269954	4.350722
203	1	0	9.939302	4.491625	3.063899
204	1	0	8.424731	3.981809	3.815026
205	6	0	9.380454	3.450959	-3.717704
206	1	0	9.944224	4.334041	-3.394716
207	1	0	9.887230	3.024405	-4.590788
208	1	0	8.397801	3.814601	-4.064619
209	6	0	-9.282588	0.127649	5.097077
210	1	0	-9.795161	1.033895	5.439330
211	1	0	-9.824515	-0.739259	5.493257
212	1	0	-8.288148	0.122672	5.576048
213	6	0	-9.327346	5.102940	-0.059110
214	1	0	-9.860000	5.439380	-0.956062
215	1	0	-9.862386	5.486654	0.817557
216	1	0	-8.341499	5.599100	-0.069020
217	6	0	-9.348703	-0.038249	-5.048874
218	1	0	-9.880758	-0.936235	-5.383262
219	1	0	-9.881950	0.837111	-5.438264
220	1	0	-8.361218	-0.049801	-5.541746
221	6	0	-9.416881	-5.013667	0.106273
222	1	0	-9.944716	-5.341615	1.009213
223	1	0	-9.968155	-5.387967	-0.764292
224	1	0	-8.439297	-5.526122	0.105085
225	1	0	-5.250482	1.783023	1.240658
226	6	0	-4.751497	1.002669	0.677075
227	6	0	-3.383453	0.831497	0.826128
228	6	0	-5.479844	0.176454	-0.172180
229	6	0	-2.725594	-0.174526	0.116266
230	1	0	-2.817158	1.473495	1.492963
231	6	0	-4.818458	-0.821979	-0.879127
232	1	0	-6.549530	0.307924	-0.280972
233	7	0	-1.343483	-0.306914	0.331670
234	6	0	-3.449112	-1.001533	-0.746491
235	1	0	-5.371357	-1.474137	-1.546286
236	7	0	-0.644715	-1.118429	-0.321790
237	1	0	-2.934280	-1.775451	-1.308471
238	7	0	0.469050	-1.309289	-0.539072
239	6	0	0.272395	0.960051	0.918057
240	6	0	1.278621	0.407683	0.470204
241	1	0	-0.351458	1.659973	1.430362
242	6	0	2.687660	0.207323	0.215801

243	6	0	3.161260	0.041848	-1.088998
244	6	0	3.592197	0.192291	1.281591
245	6	0	4.520250	-0.108523	-1.323347
246	1	0	2.454750	0.035175	-1.912582
247	6	0	4.949186	0.023899	1.039795
248	1	0	3.219060	0.297171	2.295676
249	6	0	5.419111	-0.119823	-0.261345
250	1	0	4.876083	-0.214185	-2.342885
251	1	0	5.641501	0.006565	1.873639
252	1	0	6.479941	-0.242705	-0.446602

Structure 12 (B3LYP) (atoms treated at DFT level are marked in bold)

ONIOM: extrapolated energy = -705.007725896795

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	9.147523	-2.041667	-1.266327
2	6	0	8.640945	-1.634889	-2.510736
3	6	0	7.544659	-2.360615	-3.011961
4	6	0	7.001782	-3.465115	-2.358567
5	6	0	7.565919	-3.836455	-1.136053
6	6	0	8.615842	-3.120189	-0.536469
7	6	0	8.142644	-0.672926	3.297290
8	6	0	8.825041	-1.440694	2.337977
9	6	0	8.370488	-2.689607	1.885858
10	6	0	7.176131	-3.170241	2.454272
11	6	0	6.438273	-2.443968	3.390219
12	6	0	6.944342	-1.209259	3.801456
13	6	0	6.894191	2.558798	-3.254593
14	6	0	7.499420	1.348752	-3.605820
15	6	0	8.606428	0.825586	-2.915432
16	6	0	9.113135	1.595483	-1.852613
17	6	0	8.559864	2.823833	-1.461878
18	6	0	7.445727	3.275861	-2.194184
19	6	0	7.304360	3.995649	1.425838
20	6	0	8.424681	3.279721	0.969093
21	6	0	8.854303	2.199006	1.759944
22	6	0	8.195579	1.794623	2.931716
23	6	0	7.050861	2.526198	3.293827
24	6	0	6.593126	3.626566	2.570634
25	6	0	9.313303	-0.480182	-3.233212
26	6	0	9.197286	-3.413853	0.835509
27	6	0	8.774236	0.638970	3.728090
28	6	0	9.198834	3.572661	-0.304026
29	8	0	7.032657	-2.012525	-4.282479
30	8	0	7.113340	-5.028568	-0.523797
31	8	0	6.781314	-4.493578	2.160940
32	8	0	6.285547	-0.548290	4.865753
33	8	0	7.032164	0.698609	-4.775903
34	8	0	6.964627	4.572572	-1.919319
35	8	0	6.925307	5.192516	0.771316
36	8	0	6.387612	2.188463	4.498146
37	6	0	3.483257	5.402589	-0.036839
38	6	0	3.485036	4.882775	-1.372234
39	7	0	4.602321	4.527264	-2.021615
40	6	0	5.747003	4.677109	-1.292371
41	6	0	5.733758	5.093119	0.077867

42	7	0	4.590921	5.483529	0.713524
43	7	0	4.675361	0.736602	-4.849994
44	6	0	3.553723	0.019027	-4.693618
45	6	0	3.556166	-1.341171	-4.243068
46	7	0	4.678798	-2.044870	-4.040230
47	6	0	5.829098	-1.345440	-4.267886
48	6	0	5.827171	0.045566	-4.607691
49	7	0	4.787145	-5.247386	-0.832956
50	6	0	5.834069	-4.945619	-0.010513
51	6	0	5.659876	-4.632580	1.374386
52	7	0	4.429651	-4.584628	1.965335
53	6	0	3.411554	-4.882440	1.146949
54	6	0	3.588165	-5.220276	-0.235935
55	7	0	4.074694	2.284763	4.066899
56	6	0	5.187360	1.536694	4.323598
57	6	0	5.130014	0.119601	4.525466
58	7	0	3.953161	-0.574442	4.510278
59	6	0	2.864407	0.178447	4.296898
60	6	0	2.928673	1.591317	4.065007
61	6	0	2.060135	5.796139	0.340171
62	6	0	2.049029	4.812125	-1.865730
63	6	0	2.115361	0.463530	-4.908241
64	6	0	2.118684	-1.785852	-4.029498
65	6	0	1.927520	-4.902543	1.472149
66	6	0	2.227022	-5.484101	-0.858996
67	6	0	1.407484	-0.256503	4.247078
68	6	0	1.525073	2.120291	3.832368
69	8	0	1.333793	-4.645783	2.476930
70	7	0	1.314519	-5.277241	0.229921
71	8	0	1.902138	-5.767516	-1.973365
72	8	0	1.688729	-2.786053	-3.522125
73	7	0	1.343697	-0.682029	-4.482347
74	8	0	1.649742	1.480288	-5.319914
75	7	0	1.290442	5.406008	-0.817167
76	8	0	1.617302	6.305599	1.320879
77	8	0	1.602736	4.321570	-2.865897
78	7	0	0.695658	0.960383	3.974250
79	8	0	0.895982	-1.332303	4.355892
80	8	0	1.141054	3.218147	3.550875
81	1	0	0.296920	-5.425266	0.126645
82	1	0	0.309934	-0.694671	-4.513761
83	1	0	0.259826	5.505686	-0.859983
84	1	0	-0.339816	1.025994	3.993226
85	6	0	-9.407644	0.412685	2.083899
86	6	0	-8.882373	1.697148	2.298350
87	6	0	-7.801082	1.797093	3.193324
88	6	0	-7.264807	0.700468	3.866827
89	6	0	-7.847471	-0.544880	3.629131
90	6	0	-8.903322	-0.734303	2.720391
91	6	0	-8.420219	-3.148948	-1.121205
92	6	0	-9.091370	-2.580149	-0.026058
93	6	0	-8.684397	-2.753791	1.306621
94	6	0	-7.542434	-3.547564	1.520447
95	6	0	-6.818081	-4.120484	0.471694
96	6	0	-7.280566	-3.920867	-0.831256
97	6	0	-6.975717	4.388706	-0.930125
98	6	0	-7.653813	4.122518	0.260602
99	6	0	-8.728679	3.218938	0.331776
100	6	0	-9.107330	2.593841	-0.868676
101	6	0	-8.458351	2.813945	-2.095889
102	6	0	-7.390327	3.727624	-2.087083
103	6	0	-7.021877	0.586406	-4.126065
104	6	0	-8.261037	0.743716	-3.478173

105	6	0	-8.866525	-0.423468	-2.984931
106	6	0	-8.291515	-1.698852	-3.122630
107	6	0	-7.078010	-1.775907	-3.826738
108	6	0	-6.413052	-0.652452	-4.318891
109	6	0	-9.518391	2.876850	1.583040
110	6	0	-9.517739	-2.081633	2.385288
111	6	0	-8.998754	-2.890213	-2.502615
112	6	0	-8.981473	2.070906	-3.312372
113	8	0	-7.318960	3.086548	3.506796
114	8	0	-7.449157	-1.645977	4.415617
115	8	0	-7.199564	-3.911956	2.840837
116	8	0	-6.665168	-4.657441	-1.870360
117	8	0	-7.263868	4.860064	1.407941
118	8	0	-6.728738	4.065457	-3.298072
119	8	0	-6.421085	1.728144	-4.702130
120	8	0	-6.568819	-3.058192	-4.130823
121	6	0	-3.099427	2.249964	-3.587927
122	6	0	-3.227269	3.563609	-3.027473
123	7	0	-4.406211	4.186924	-2.890061
124	6	0	-5.472669	3.493715	-3.383904
125	6	0	-5.327486	2.227282	-4.035954
126	7	0	-4.131912	1.570970	-4.107019
127	7	0	-4.907420	4.976466	1.502499
128	6	0	-3.800493	4.494898	2.084023
129	6	0	-3.825254	3.429719	3.045056
130	7	0	-4.958173	2.889475	3.512728
131	6	0	-6.096018	3.419406	2.973674
132	6	0	-6.068932	4.409696	1.942509
133	7	0	-5.129841	-1.575962	4.809747
134	6	0	-6.191588	-2.146675	4.167845
135	6	0	-6.068022	-3.327828	3.368898
136	7	0	-4.883449	-3.993473	3.233164
137	6	0	-3.861330	-3.450622	3.909837
138	6	0	-3.975128	-2.240488	4.669707
139	7	0	-4.219797	-3.011361	-4.081578
140	6	0	-5.393476	-3.386542	-3.494624
141	6	0	-5.445586	-4.205188	-2.319353
142	7	0	-4.315685	-4.680208	-1.716243
143	6	0	-3.171067	-4.330019	-2.322528
144	6	0	-3.122213	-3.496669	-3.486428
145	6	0	-1.645787	1.817450	-3.493584
146	6	0	-1.849163	4.065745	-2.631731
147	6	0	-2.356807	4.923096	1.859571
148	6	0	-2.394227	3.063018	3.398103
149	6	0	-2.432784	-3.960046	4.007686
150	6	0	-2.610505	-1.882700	5.239068
151	6	0	-1.750088	-4.701863	-1.933428
152	6	0	-1.671444	-3.276726	-3.881661
153	8	0	-1.921425	-4.949826	3.574278
154	7	0	-1.765551	-2.952652	4.778966
155	8	0	-2.242419	-0.966983	5.909820
156	8	0	-1.964990	2.150920	4.051880
157	7	0	-1.611443	4.045288	2.729958
158	8	0	-1.877149	5.769182	1.171268
159	7	0	-0.979798	2.970144	-2.980873
160	8	0	-1.127114	0.758989	-3.714610
161	8	0	-1.483612	5.091693	-2.142157
162	7	0	-0.937970	-4.046412	-2.909627
163	8	0	-1.342389	-5.363258	-1.020168
164	8	0	-1.178646	-2.625529	-4.752748
165	1	0	-0.752290	-2.964275	4.951887
166	1	0	-0.579962	4.059986	2.772667
167	1	0	0.046932	3.052249	-2.925465

168	1	0	0.091728	-4.135251	-2.943564
169	1	0	10.361714	-0.399053	-2.818736
170	1	0	9.982493	1.219409	-1.307763
171	1	0	6.029077	2.944624	-3.813704
172	1	0	9.990500	-1.491582	-0.841511
173	1	0	6.169815	-4.032431	-2.800993
174	1	0	10.235572	-2.969864	0.860728
175	1	0	9.759625	-1.048697	1.928514
176	1	0	5.505329	-2.844074	3.814165
177	1	0	9.872638	0.579808	3.466561
178	1	0	5.716099	4.199613	2.905057
179	1	0	9.741985	1.645337	1.444361
180	1	0	10.238160	3.151955	-0.165889
181	1	0	-5.938596	-4.747602	0.669886
182	1	0	-9.981190	-1.975399	-0.221139
183	1	0	-10.538048	-1.882221	1.942922
184	1	0	-6.428368	0.817619	4.571511
185	1	0	-10.245025	0.299563	1.391947
186	1	0	-10.544804	2.547154	1.244830
187	1	0	-9.946255	1.893746	-0.845120
188	1	0	-6.144955	5.110186	-0.957594
189	1	0	-10.068215	1.835218	-3.110991
190	1	0	-5.455703	-0.738583	-4.852675
191	1	0	-9.825305	-0.336718	-2.468806
192	1	0	-10.081418	-2.598831	-2.362410
193	6	0	9.380975	-4.901172	1.123982
194	1	0	10.002647	-5.381925	0.359383
195	1	0	9.854867	-5.063072	2.099159
196	1	0	8.423436	-5.448842	1.142070
197	6	0	8.728882	0.858530	5.239073
198	1	0	9.232670	0.045699	5.775144
199	1	0	9.212401	1.801467	5.520530
200	1	0	7.697555	0.903055	5.628295
201	6	0	9.394241	5.061361	-0.579099
202	1	0	9.893655	5.559749	0.260217
203	1	0	9.997096	5.225303	-1.479812
204	1	0	8.438899	5.590477	-0.735580
205	6	0	9.485431	-0.724968	-4.731053
206	1	0	10.036891	0.094165	-5.207529
207	1	0	10.028092	-1.657413	-4.924618
208	1	0	8.519364	-0.803045	-5.258653
209	6	0	-9.754637	4.075675	2.499503
210	1	0	-10.267781	4.887221	1.970546
211	1	0	-10.360396	3.800158	3.370241
212	1	0	-8.812191	4.499172	2.887971
213	6	0	-8.974680	2.914782	-4.585842
214	1	0	-9.398041	2.364100	-5.433474
215	1	0	-9.553948	3.836590	-4.455979
216	1	0	-7.956397	3.221987	-4.880595
217	6	0	-9.023144	-4.129402	-3.393689
218	1	0	-9.624949	-4.929216	-2.946403
219	1	0	-9.439706	-3.902114	-4.382069
220	1	0	-8.016921	-4.547736	-3.562796
221	6	0	-9.768427	-2.966148	3.603822
222	1	0	-10.379977	-2.449142	4.352591
223	1	0	-10.282544	-3.893086	3.324486
224	1	0	-8.833835	-3.262691	4.109002
225	6	0	-2.299128	-3.077939	0.780790
226	6	0	-1.058999	-2.923773	1.396771
227	6	0	-2.826801	-2.034209	0.023154
228	1	0	-2.845902	-4.013475	0.888939
229	6	0	-0.352432	-1.731874	1.275690
230	1	0	-0.637687	-3.733947	1.993932

231	6	0	-2.115972	-0.849711	-0.135074
232	1	0	-3.795784	-2.140157	-0.448283
233	6	0	-0.880160	-0.703585	0.495964
234	1	0	0.588875	-1.606735	1.795921
235	1	0	-2.508506	-0.033351	-0.723324
236	7	0	-0.194873	0.543508	0.368977
237	6	0	1.138196	0.842932	0.284208
238	7	0	-0.933846	1.685731	0.408189
239	6	0	1.152359	2.225092	0.278239
240	6	0	2.278004	-0.071563	0.124415
241	7	0	-0.115716	2.693051	0.344981
242	1	0	2.004171	2.878971	0.203663
243	6	0	2.236187	-1.178905	-0.733899
244	6	0	3.483434	0.232794	0.774954
245	6	0	3.373380	-1.953444	-0.939266
246	1	0	1.319247	-1.425433	-1.258417
247	6	0	4.618411	-0.543579	0.566069
248	1	0	3.526409	1.085984	1.440382
249	6	0	4.567602	-1.636867	-0.295141
250	1	0	3.328967	-2.793978	-1.630045
251	1	0	5.544185	-0.293680	1.072469
252	1	0	5.457469	-2.229287	-0.475337

Structure 12 (M06-2X) (atoms treated at DFT level are marked in bold)

ONIOM: extrapolated energy = -704.721292840170
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	9.151226	-1.961601	-1.367220
2	6	0	8.639899	-1.490721	-2.586929
3	6	0	7.541311	-2.189068	-3.120808
4	6	0	6.998305	-3.324293	-2.522216
5	6	0	7.567915	-3.759090	-1.323686
6	6	0	8.621900	-3.076458	-0.692616
7	6	0	8.151660	-0.841653	3.265309
8	6	0	8.832331	-1.554464	2.263102
9	6	0	8.383992	-2.782012	1.750405
10	6	0	7.197198	-3.300273	2.301127
11	6	0	6.462262	-2.629058	3.279441
12	6	0	6.961682	-1.412866	3.750243
13	6	0	6.891436	2.736165	-3.118673
14	6	0	7.495517	1.544660	-3.529868
15	6	0	8.602816	0.987148	-2.867362
16	6	0	9.109501	1.702230	-1.767027
17	6	0	8.556424	2.909375	-1.314501
18	6	0	7.443229	3.399035	-2.023576
19	6	0	7.293526	3.913324	1.626247
20	6	0	8.420551	3.230374	1.136496
21	6	0	8.856157	2.112387	1.870435
22	6	0	8.196322	1.641760	3.016402
23	6	0	7.044394	2.344638	3.411215
24	6	0	6.580201	3.478346	2.746383
25	6	0	9.310116	-0.300477	-3.251401
26	6	0	9.209467	-3.443909	0.658768
27	6	0	8.779163	0.451036	3.756200
28	6	0	9.194433	3.595583	-0.117982
29	8	0	7.028170	-1.778090	-4.371731
30	8	0	7.121024	-4.982656	-0.772910
31	8	0	6.805507	-4.608381	1.941212

32	8	0	6.300116	-0.814237	4.850169
33	8	0	7.026120	0.953256	-4.729802
34	8	0	6.962286	4.680751	-1.685312
35	8	0	6.912508	5.142413	1.036875
36	8	0	6.382005	1.935201	4.593295
37	6	0	3.474283	5.407648	0.229270
38	6	0	3.481576	4.977750	-1.137727
39	7	0	4.601004	4.658178	-1.801940
40	6	0	5.742139	4.753698	-1.058076
41	6	0	5.723311	5.083295	0.335316
42	7	0	4.578148	5.435607	0.989029
43	7	0	4.669044	0.995211	-4.795286
44	6	0	3.548035	0.269767	-4.675531
45	6	0	3.551393	-1.112734	-4.298817
46	7	0	4.674378	-1.825231	-4.132537
47	6	0	5.824038	-1.113749	-4.323362
48	6	0	5.821395	0.292698	-4.591566
49	7	0	4.793297	-5.186836	-1.081326
50	6	0	5.845018	-4.933436	-0.248601
51	6	0	5.679786	-4.707605	1.154269
52	7	0	4.453770	-4.704739	1.755780
53	6	0	3.431169	-4.956647	0.927606
54	6	0	3.598615	-5.203410	-0.475405
55	7	0	4.073052	2.031477	4.137178
56	6	0	5.188142	1.283714	4.383520
57	6	0	5.139284	-0.139547	4.540245
58	7	0	3.966280	-0.839061	4.505690
59	6	0	2.873595	-0.086637	4.310296
60	6	0	2.931731	1.330934	4.108803
61	6	0	2.050380	5.780431	0.624220
62	6	0	2.048455	4.950400	-1.644594
63	6	0	2.109299	0.724593	-4.864738
64	6	0	2.114158	-1.570370	-4.113206
65	6	0	1.950009	-5.006426	1.262074
66	6	0	2.233510	-5.431148	-1.104426
67	6	0	1.418744	-0.526389	4.251215
68	6	0	1.527838	1.856816	3.873559
69	8	0	1.363627	-4.820031	2.286384
70	7	0	1.328557	-5.300504	0.002145
71	8	0	1.901874	-5.640403	-2.233182
72	8	0	1.684841	-2.598629	-3.665151
73	7	0	1.338530	-0.443522	-4.504764
74	8	0	1.644127	1.763520	-5.217634
75	7	0	1.285782	5.472835	-0.560585
76	8	0	1.604206	6.223193	1.635497
77	8	0	1.605546	4.535141	-2.679321
78	7	0	0.702447	0.692306	3.992701
79	8	0	0.909526	-1.604185	4.347033
80	8	0	1.143520	2.957327	3.601842
81	1	0	0.310469	-5.442804	-0.103842
82	1	0	0.304808	-0.455237	-4.538206
83	1	0	0.255887	5.580023	-0.602893
84	1	0	-0.333018	0.753824	4.009655
85	6	0	-9.403305	0.304721	2.109679
86	6	0	-8.875599	1.576236	2.386151
87	6	0	-7.793768	1.630039	3.284399
88	6	0	-7.261637	0.501385	3.906096
89	6	0	-7.847342	-0.729791	3.609100
90	6	0	-8.901638	-0.872850	2.690200
91	6	0	-8.414987	-3.092218	-1.267368
92	6	0	-9.088064	-2.579415	-0.146003
93	6	0	-8.681876	-2.818118	1.176772
94	6	0	-7.538733	-3.619667	1.351962

95	6	0	-6.812730	-4.139147	0.276978
96	6	0	-7.274617	-3.876139	-1.014908
97	6	0	-6.976906	4.431221	-0.709991
98	6	0	-7.649840	4.102904	0.468047
99	6	0	-8.723406	3.195515	0.497019
100	6	0	-9.104629	2.631186	-0.732344
101	6	0	-8.459953	2.914225	-1.948916
102	6	0	-7.394257	3.829263	-1.897909
103	6	0	-7.020588	0.791637	-4.081212
104	6	0	-8.261333	0.913806	-3.428609
105	6	0	-8.864805	-0.277460	-2.994214
106	6	0	-8.286378	-1.543167	-3.193369
107	6	0	-7.071232	-1.582520	-3.897737
108	6	0	-6.407885	-0.434718	-4.332716
109	6	0	-9.510366	2.791199	1.731305
110	6	0	-9.516467	-2.201217	2.287084
111	6	0	-8.992206	-2.765408	-2.634830
112	6	0	-8.984473	2.229961	-3.198803
113	8	0	-7.304721	2.901472	3.656365
114	8	0	-7.452101	-1.867743	4.343275
115	8	0	-7.196547	-4.047406	2.653311
116	8	0	-6.656742	-4.559440	-2.088363
117	8	0	-7.253565	4.779434	1.650789
118	8	0	-6.738446	4.231473	-3.092059
119	8	0	-6.425260	1.961854	-4.602064
120	8	0	-6.559333	-2.847323	-4.264139
121	6	0	-3.100581	2.452828	-3.484750
122	6	0	-3.231698	3.742064	-2.870672
123	7	0	-4.413554	4.350885	-2.697681
124	6	0	-5.479578	3.671411	-3.211258
125	6	0	-5.331406	2.435062	-3.917922
126	7	0	-4.132682	1.789330	-4.024165
127	7	0	-4.895670	4.877985	1.734965
128	6	0	-3.787497	4.357395	2.279376
129	6	0	-3.812258	3.241331	3.180745
130	7	0	-4.945285	2.685804	3.630011
131	6	0	-6.083556	3.253170	3.131550
132	6	0	-6.057604	4.296561	2.153961
133	7	0	-5.134605	-1.820428	4.750600
134	6	0	-6.193456	-2.355090	4.073942
135	6	0	-6.065955	-3.489796	3.210804
136	7	0	-4.878963	-4.142287	3.037512
137	6	0	-3.858951	-3.635518	3.744742
138	6	0	-3.977982	-2.473170	4.575033
139	7	0	-4.210565	-2.799044	-4.208331
140	6	0	-5.384564	-3.205530	-3.643395
141	6	0	-5.436943	-4.083160	-2.511539
142	7	0	-4.307318	-4.585911	-1.930787
143	6	0	-3.162104	-4.202594	-2.515598
144	6	0	-3.113281	-3.311777	-3.636137
145	6	0	-1.643223	2.026962	-3.420758
146	6	0	-1.852429	4.238598	-2.470535
147	6	0	-2.342769	4.786150	2.064538
148	6	0	-2.381317	2.843476	3.497856
149	6	0	-2.427940	-4.143337	3.811886
150	6	0	-2.615953	-2.146638	5.168671
151	6	0	-1.740642	-4.589528	-2.142621
152	6	0	-1.662647	-3.069690	-4.018195
153	8	0	-1.911315	-5.100262	3.315457
154	7	0	-1.766302	-3.183767	4.646086
155	8	0	-2.252132	-1.272279	5.894671
156	8	0	-1.953675	1.891509	4.093559
157	7	0	-1.596664	3.855091	2.877883

158	8	0	-1.861759	5.665146	1.419954
159	7	0	-0.978905	3.166703	-2.878744
160	8	0	-1.121767	0.979040	-3.682234
161	8	0	-1.488658	5.245955	-1.942783
162	7	0	-0.928841	-3.885472	-3.084971
163	8	0	-1.331771	-5.292219	-1.261388
164	8	0	-1.171145	-2.374061	-4.855007
165	1	0	-0.753712	-3.204845	4.823753
166	1	0	-0.565116	3.861967	2.914353
167	1	0	0.047418	3.252288	-2.826877
168	1	0	0.100834	-3.972977	-3.124193
169	1	0	10.359125	-0.239205	-2.835051
170	1	0	9.978585	1.298784	-1.241649
171	1	0	6.026979	3.150324	-3.658249
172	1	0	9.996472	-1.434893	-0.918049
173	1	0	6.163414	-3.866741	-2.989629
174	1	0	10.246304	-2.998233	0.705281
175	1	0	9.760725	-1.134534	1.867355
176	1	0	5.536168	-3.058202	3.689753
177	1	0	9.877414	0.407526	3.490945
178	1	0	5.696938	4.025510	3.106584
179	1	0	9.749333	1.583228	1.529493
180	1	0	10.234823	3.170525	-0.003464
181	1	0	-5.932301	-4.773887	0.444661
182	1	0	-9.978625	-1.967068	-0.311762
183	1	0	-10.536188	-1.979296	1.854265
184	1	0	-6.425554	0.582884	4.616125
185	1	0	-10.240380	0.226825	1.412511
186	1	0	-10.538003	2.480415	1.379101
187	1	0	-9.942115	1.929033	-0.741649
188	1	0	-6.147671	5.154964	-0.703503
189	1	0	-10.070346	1.982795	-3.006967
190	1	0	-5.449272	-0.492274	-4.868038
191	1	0	-9.824751	-0.218434	-2.476384
192	1	0	-10.075561	-2.483327	-2.481608
193	6	0	9.399462	-4.944319	0.863060
194	1	0	10.019313	-5.379428	0.070170
195	1	0	9.878345	-5.158600	1.825624
196	1	0	8.443896	-5.495633	0.854849
197	6	0	8.735013	0.599393	5.275917
198	1	0	9.244580	-0.234631	5.772586
199	1	0	9.213403	1.530929	5.600680
200	1	0	7.704076	0.619009	5.668222
201	6	0	9.385981	5.097647	-0.310256
202	1	0	9.884207	5.550143	0.555331
203	1	0	9.988345	5.312627	-1.200530
204	1	0	8.429322	5.632151	-0.437531
205	6	0	9.479947	-0.469642	-4.759925
206	1	0	10.030249	0.372669	-5.195563
207	1	0	10.022696	-1.390908	-5.000946
208	1	0	8.513019	-0.521672	-5.289181
209	6	0	-9.742823	3.942834	2.707444
210	1	0	-10.255628	4.780776	2.220996
211	1	0	-10.347414	3.624939	3.564429
212	1	0	-8.798840	4.344776	3.114666
213	6	0	-8.981553	3.133740	-4.430439
214	1	0	-9.404746	2.623171	-5.302892
215	1	0	-9.562823	4.046861	-4.255862
216	1	0	-7.964426	3.457256	-4.711442
217	6	0	-9.013209	-3.958246	-3.587148
218	1	0	-9.614419	-4.780478	-3.181695
219	1	0	-9.428581	-3.682133	-4.563528
220	1	0	-8.006017	-4.365930	-3.775447

221	6	0	-9.768583	-3.146225	3.458992
222	1	0	-10.380510	-2.667525	4.232523
223	1	0	-10.282945	-4.057530	3.132629
224	1	0	-8.834529	-3.468398	3.949255
225	6	0	-2.233152	-3.130978	0.696171
226	6	0	-0.984984	-2.959909	1.286175
227	6	0	-2.810138	-2.084875	-0.015242
228	1	0	-2.749878	-4.084203	0.790897
229	6	0	-0.316301	-1.748537	1.179916
230	1	0	-0.531112	-3.772919	1.853180
231	6	0	-2.139273	-0.878068	-0.158285
232	1	0	-3.788379	-2.206851	-0.461897
233	6	0	-0.895981	-0.720795	0.444363
234	1	0	0.637160	-1.603975	1.672477
235	1	0	-2.566646	-0.053171	-0.710066
236	7	0	-0.241054	0.540927	0.334001
237	6	0	1.082070	0.851649	0.262906
238	7	0	-0.986363	1.658288	0.386154
239	6	0	1.084199	2.228013	0.279221
240	6	0	2.220594	-0.060951	0.086049
241	7	0	-0.190471	2.673901	0.346773
242	1	0	1.929881	2.890879	0.223286
243	6	0	2.169317	-1.139750	-0.800040
244	6	0	3.417629	0.224928	0.747309
245	6	0	3.301554	-1.911272	-1.023526
246	1	0	1.248140	-1.363470	-1.329217
247	6	0	4.548183	-0.549451	0.520487
248	1	0	3.456957	1.063937	1.431456
249	6	0	4.493263	-1.615965	-0.369028
250	1	0	3.257084	-2.730424	-1.738107
251	1	0	5.474159	-0.316636	1.032649
252	1	0	5.380955	-2.205189	-0.566170

Structure 13 (B3LYP) (atoms treated at DFT level are marked in bold)

ONIOM: extrapolated energy = -705.024831733247

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	9.110531	-1.166355	-2.175932
2	6	0	8.551577	-0.290108	-3.119824
3	6	0	7.463389	-0.782464	-3.861969
4	6	0	6.969134	-2.076756	-3.718010
5	6	0	7.572532	-2.906502	-2.769246
6	6	0	8.633558	-2.471921	-1.956178
7	6	0	8.508115	-1.893505	2.620297
8	6	0	9.097562	-2.153620	1.369953
9	6	0	8.572418	-3.075235	0.451463
10	6	0	7.398708	-3.750565	0.835876
11	6	0	6.769990	-3.543441	2.061782
12	6	0	7.353114	-2.628648	2.941401
13	6	0	6.822149	3.901309	-2.055693
14	6	0	7.365278	2.890052	-2.845840
15	6	0	8.479716	2.128390	-2.450141
16	6	0	9.004726	2.405761	-1.177733
17	6	0	8.477324	3.386538	-0.317160
18	6	0	7.396986	4.140903	-0.804616
19	6	0	7.241742	2.934255	2.716292

20	6	0	8.441435	2.621790	2.050069
21	6	0	9.032631	1.388093	2.364940
22	6	0	8.478862	0.489225	3.294541
23	6	0	7.307889	0.900000	3.954771
24	6	0	6.664281	2.107327	3.675613
25	6	0	9.177009	1.081448	-3.301106
26	6	0	9.300185	-3.291246	-0.864959
27	6	0	9.164811	-0.849503	3.508625
28	6	0	9.124403	3.537941	1.048232
29	8	0	6.873329	0.046095	-4.850988
30	8	0	7.117343	-4.246297	-2.694996
31	8	0	6.917320	-4.769415	-0.012097
32	8	0	6.814152	-2.534121	4.245635
33	8	0	6.794672	2.689804	-4.130286
34	8	0	6.873738	5.230136	-0.054379
35	8	0	6.660482	4.197352	2.473477
36	8	0	6.802015	0.097302	5.000674
37	6	0	3.280725	4.035210	1.418661
38	6	0	3.357411	4.907497	0.282514
39	7	0	4.520628	5.321859	-0.241139
40	6	0	5.621996	4.925343	0.456303
41	6	0	5.526767	4.224057	1.702718
42	7	0	4.347931	3.711890	2.164375
43	7	0	4.456490	2.600382	-3.774366
44	6	0	3.364878	1.823596	-3.837043
45	6	0	3.412534	0.434200	-4.184119
46	7	0	4.549220	-0.205067	-4.493078
47	6	0	5.665384	0.580160	-4.458591
48	6	0	5.621669	1.964406	-4.092938
49	7	0	4.769738	-4.341208	-2.936433
50	6	0	5.861102	-4.343605	-2.117325
51	6	0	5.757592	-4.506369	-0.700654
52	7	0	4.555956	-4.534118	-0.051420
53	6	0	3.492491	-4.480416	-0.864170
54	6	0	3.597711	-4.443765	-2.294641
55	7	0	4.443500	0.199491	4.903669
56	6	0	5.594604	-0.508726	4.716248
57	6	0	5.600278	-1.884225	4.328026
58	7	0	4.450484	-2.596958	4.138684
59	6	0	3.326060	-1.896898	4.343598
60	6	0	3.324111	-0.510969	4.713061
61	6	0	1.838697	3.580515	1.576698
62	6	0	1.951721	5.205020	-0.208979
63	6	0	1.923997	2.206222	-3.557972
64	6	0	2.009145	-0.136594	-4.122581
65	6	0	2.018827	-4.450576	-0.485328
66	6	0	2.200683	-4.519881	-2.892678
67	6	0	1.885428	-2.372112	4.221466
68	6	0	1.888019	-0.028658	4.817541
69	8	0	1.505420	-4.355170	0.593036
70	7	0	1.340475	-4.532235	-1.736582
71	8	0	1.824724	-4.581841	-4.022747
72	8	0	1.596961	-1.249783	-4.274350
73	7	0	1.192591	0.995792	-3.781928
74	8	0	1.436050	3.241091	-3.199225
75	7	0	1.125180	4.361335	0.625622
76	8	0	1.361115	2.705708	2.249842
77	8	0	1.533332	5.940141	-1.048270
78	7	0	1.114475	-1.191789	4.516845
79	8	0	1.423158	-3.438959	3.952019
80	8	0	1.447696	1.058317	5.062789
81	1	0	0.311272	-4.554192	-1.818310
82	1	0	0.159150	0.942759	-3.763715

83	1	0	0.094504	4.356879	0.552761
84	1	0	0.079126	-1.198950	4.543675
85	6	0	-9.054119	-0.778584	2.597567
86	6	0	-8.516062	0.302435	3.319061
87	6	0	-7.363195	0.047055	4.081105
88	6	0	-6.724771	-1.194410	4.093959
89	6	0	-7.291712	-2.216438	3.336502
90	6	0	-8.468013	-2.054025	2.581221
91	6	0	-8.515808	-2.589283	-1.946448
92	6	0	-9.027232	-2.560586	-0.638327
93	6	0	-8.483137	-3.304593	0.423619
94	6	0	-7.387574	-4.130873	0.118308
95	6	0	-6.830715	-4.195655	-1.161020
96	6	0	-7.402893	-3.419593	-2.168906
97	6	0	-6.788234	3.913956	1.178913
98	6	0	-7.373777	3.230762	2.248094
99	6	0	-8.540533	2.457819	2.106454
100	6	0	-9.137113	2.434557	0.833294
101	6	0	-8.609690	3.116004	-0.274084
102	6	0	-7.422836	3.842441	-0.060103
103	6	0	-7.651007	2.249273	-3.392399
104	6	0	-8.699234	2.004097	-2.490692
105	6	0	-9.168798	0.679537	-2.407566
106	6	0	-8.602029	-0.383419	-3.127211
107	6	0	-7.505038	-0.069437	-3.950885
108	6	0	-7.027959	1.228312	-4.115705
109	6	0	-9.202323	1.653353	3.213446
110	6	0	-9.137205	-3.163285	1.787294
111	6	0	-9.224513	-1.763007	-3.004605
112	6	0	-9.354170	3.042595	-1.597777
113	8	0	-6.874010	1.061575	4.936338
114	8	0	-6.719476	-3.506009	3.404789
115	8	0	-6.846029	-4.995347	1.105610
116	8	0	-6.869549	-3.551572	-3.477375
117	8	0	-6.842295	3.433088	3.540914
118	8	0	-6.944340	4.641351	-1.119601
119	8	0	-7.225247	3.580604	-3.643500
120	8	0	-6.909613	-1.099776	-4.717164
121	6	0	-3.700765	3.858770	-3.396187
122	6	0	-3.552947	4.124826	-1.995864
123	7	0	-4.590985	4.336800	-1.172936
124	6	0	-5.811819	4.225552	-1.772678
125	6	0	-5.958093	3.812889	-3.137476
126	7	0	-4.893819	3.664061	-3.976414
127	7	0	-4.480171	3.427731	3.443315
128	6	0	-3.366451	2.800953	3.849059
129	6	0	-3.385191	1.580361	4.601006
130	7	0	-4.516757	0.957031	4.954626
131	6	0	-5.657881	1.585356	4.546755
132	6	0	-5.641794	2.806898	3.803848
133	7	0	-4.393472	-3.116775	3.124696
134	6	0	-5.558891	-3.682982	2.690839
135	6	0	-5.613691	-4.555227	1.558433
136	7	0	-4.490380	-5.003359	0.926758
137	6	0	-3.346055	-4.504130	1.413406
138	6	0	-3.304566	-3.522627	2.458482
139	7	0	-4.579908	-0.808249	-4.394734
140	6	0	-5.708787	-1.560001	-4.225868
141	6	0	-5.680896	-2.866440	-3.642459
142	7	0	-4.515291	-3.490001	-3.300712
143	6	0	-3.410676	-2.766638	-3.528139
144	6	0	-3.446265	-1.424293	-4.032940
145	6	0	-2.324363	3.788636	-4.036203

146	6	0	-2.073906	4.101180	-1.653922
147	6	0	-1.919450	3.191180	3.583607
148	6	0	-1.954197	1.135230	4.858807
149	6	0	-1.923760	-4.812217	0.969746
150	6	0	-1.865700	-3.056741	2.629003
151	6	0	-1.961161	-3.168213	-3.303169
152	6	0	-2.025639	-0.887097	-4.067364
153	8	0	-1.494327	-5.597084	0.181936
154	7	0	-1.127040	-3.894382	1.744611
155	8	0	-1.416242	-2.152455	3.274914
156	8	0	-1.517120	0.186064	5.437967
157	7	0	-1.165616	2.141513	4.203515
158	8	0	-1.452300	4.116893	2.988390
159	7	0	-1.427344	3.931541	-2.908238
160	8	0	-1.967445	3.663382	-5.165275
161	8	0	-1.528826	4.136580	-0.583919
162	7	0	-1.220276	-2.014023	-3.738759
163	8	0	-1.475984	-4.167829	-2.865501
164	8	0	-1.614374	0.226371	-4.262156
165	1	0	-0.091096	-3.892470	1.697077
166	1	0	-0.129528	2.134803	4.226421
167	1	0	-0.398189	3.939347	-3.015971
168	1	0	-0.185786	-1.972792	-3.695918
169	1	0	10.240032	1.008244	-2.923195
170	1	0	9.864825	1.825448	-0.834063
171	1	0	5.969847	4.498035	-2.412651
172	1	0	9.954281	-0.815642	-1.576645
173	1	0	6.135114	-2.437576	-4.338792
174	1	0	10.347552	-2.887601	-0.739487
175	1	0	10.008742	-1.613439	1.102893
176	1	0	5.856238	-4.093426	2.333253
177	1	0	10.233361	-0.737245	3.161222
178	1	0	5.741883	2.398872	4.199282
179	1	0	9.962031	1.110513	1.862624
180	1	0	10.193712	3.187826	0.948880
181	1	0	-5.975465	-4.855321	-1.373480
182	1	0	-9.892523	-1.924690	-0.434283
183	1	0	-10.206705	-2.845546	1.608845
184	1	0	-5.813481	-1.364048	4.687181
185	1	0	-9.967430	-0.616203	2.020848
186	1	0	-10.269903	1.461847	2.898430
187	1	0	-10.058401	1.861372	0.701846
188	1	0	-5.878939	4.515419	1.318489
189	1	0	-10.399651	2.677254	-1.375292
190	1	0	-6.194263	1.439939	-4.800883
191	1	0	-10.011854	0.469095	-1.745138
192	1	0	-10.286594	-1.613495	-2.647352
193	6	0	9.467969	-4.766251	-1.222241
194	1	0	10.033971	-4.889978	-2.152843
195	1	0	9.991969	-5.312332	-0.429524
196	1	0	8.499626	-5.274518	-1.372471
197	6	0	9.250231	-1.266285	4.974652
198	1	0	9.807315	-2.203255	5.090625
199	1	0	9.744555	-0.498501	5.580783
200	1	0	8.255261	-1.432787	5.422389
201	6	0	9.207388	4.985503	1.527999
202	1	0	9.718191	5.058053	2.494926
203	1	0	9.748456	5.613130	0.809962
204	1	0	8.211309	5.442901	1.656880
205	6	0	9.292082	1.492415	-4.768748
206	1	0	9.812534	2.451205	-4.875624
207	1	0	9.839676	0.742970	-5.352015
208	1	0	8.305752	1.610949	-5.249795

209	6	0	-9.294623	2.404620	4.538774
210	1	0	-9.857408	3.338909	4.429607
211	1	0	-9.787535	1.798137	5.307794
212	1	0	-8.302928	2.676548	4.938939
213	6	0	-9.528246	4.406643	-2.261118
214	1	0	-10.092463	4.325138	-3.197959
215	1	0	-10.058957	5.105809	-1.604730
216	1	0	-8.563476	4.877330	-2.515893
217	6	0	-9.342973	-2.483236	-4.347029
218	1	0	-9.851895	-3.448284	-4.238671
219	1	0	-9.903208	-1.884562	-5.074460
220	1	0	-8.358384	-2.694585	-4.799039
221	6	0	-9.223408	-4.479497	2.557363
222	1	0	-9.735364	-4.348737	3.517616
223	1	0	-9.764616	-5.242038	1.984890
224	1	0	-8.228297	-4.901506	2.781207
225	6	0	-3.911556	1.788425	0.746021
226	6	0	-2.581080	1.430422	0.550918
227	6	0	-4.918380	0.829143	0.670331
228	1	0	-4.153854	2.833533	0.932505
229	6	0	-2.263741	0.101253	0.278260
230	1	0	-1.805671	2.192787	0.577279
231	6	0	-4.589014	-0.497185	0.395112
232	1	0	-5.954223	1.114872	0.815670
233	7	0	-0.911316	-0.274256	0.036085
234	6	0	-3.263387	-0.869236	0.199305
235	1	0	-5.368423	-1.247287	0.335871
236	6	0	0.239709	0.234112	0.544147
237	7	0	-0.636063	-1.238769	-0.879067
238	1	0	-2.990775	-1.890425	-0.021570
239	6	0	1.245963	-0.461962	-0.098851
240	1	0	0.253466	1.008250	1.300940
241	7	0	0.654007	-1.346552	-0.957987
242	6	0	2.703758	-0.355149	0.022491
243	6	0	3.531943	-0.972561	-0.925894
244	6	0	3.298195	0.357451	1.072346
245	6	0	4.915101	-0.873839	-0.825564
246	1	0	3.076851	-1.527882	-1.735350
247	6	0	4.681679	0.453500	1.168577
248	1	0	2.679101	0.839830	1.827735
249	6	0	5.498099	-0.161064	0.220856
250	1	0	5.541391	-1.353545	-1.569982
251	1	0	5.118516	1.013212	1.990345
252	1	0	6.577600	-0.087970	0.299517

Structure 13 (M06-2X) (atoms treated at DFT level are marked in bold)

ONIOM: extrapolated energy = -704.735051943503

Standard orientation:					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	9.109731	-1.104773	-2.209307
2	6	0	8.550741	-0.201598	-3.127450
3	6	0	7.461625	-0.671811	-3.882473
4	6	0	6.966288	-1.969148	-3.774753
5	6	0	7.570026	-2.826190	-2.850792
6	6	0	8.632050	-2.415784	-2.026545
7	6	0	8.508297	-1.969727	2.564766

8	6	0	9.097370	-2.193771	1.307231
9	6	0	8.571895	-3.088484	0.362764
10	6	0	7.398396	-3.774726	0.728100
11	6	0	6.770163	-3.603058	1.959675
12	6	0	7.353450	-2.713799	2.865019
13	6	0	6.823150	3.958229	-1.944386
14	6	0	7.366060	2.970077	-2.763397
15	6	0	8.480075	2.196824	-2.389669
16	6	0	9.005077	2.437259	-1.109758
17	6	0	8.477941	3.392969	-0.221278
18	6	0	7.397807	4.161371	-0.686784
19	6	0	7.242290	2.853150	2.797200
20	6	0	8.442282	2.560034	2.122819
21	6	0	9.033533	1.317911	2.402552
22	6	0	8.479441	0.392851	3.305857
23	6	0	7.307965	0.784336	3.976861
24	6	0	6.664083	1.998843	3.731755
25	6	0	9.176866	1.174184	-3.270096
26	6	0	9.298974	-3.266424	-0.959734
27	6	0	9.165279	-0.951411	3.482209
28	6	0	9.125243	3.504693	1.147843
29	8	0	6.872043	0.184834	-4.847544
30	8	0	7.114501	-4.167460	-2.815314
31	8	0	6.916589	-4.768386	-0.149025
32	8	0	6.814529	-2.656913	4.171491
33	8	0	6.795430	2.807260	-4.053148
34	8	0	6.874515	5.228642	0.094338
35	8	0	6.661851	4.123077	2.591015
36	8	0	6.802454	-0.047733	4.999673
37	6	0	3.281531	3.993328	1.533913
38	6	0	3.358128	4.897595	0.423039
39	7	0	4.521317	5.326219	-0.089094
40	6	0	5.622802	4.909438	0.596278
41	6	0	5.527734	4.172758	1.822076
42	7	0	4.348861	3.648286	2.269613
43	7	0	4.457105	2.709897	-3.700556
44	6	0	3.364916	1.935948	-3.784744
45	6	0	3.411526	0.556638	-4.170012
46	7	0	4.547742	-0.074693	-4.496595
47	6	0	5.664451	0.708467	-4.440390
48	6	0	5.621808	2.082078	-4.036465
49	7	0	4.766552	-4.254583	-3.057611
50	6	0	5.858589	-4.281200	-2.239841
51	6	0	5.756223	-4.485121	-0.828450
52	7	0	4.555195	-4.531086	-0.179188
53	6	0	3.491071	-4.453271	-0.989114
54	6	0	3.595038	-4.375154	-2.417992
55	7	0	4.443905	0.056923	4.907062
56	6	0	5.594947	-0.645609	4.699051
57	6	0	5.600590	-2.009734	4.272607
58	7	0	4.450751	-2.717092	4.064291
59	6	0	3.326359	-2.023226	4.289525
60	6	0	3.324488	-0.648161	4.697590
61	6	0	1.839347	3.535006	1.679792
62	6	0	1.952256	5.209899	-0.058712
63	6	0	1.924417	2.311857	-3.494971
64	6	0	2.007732	-0.014566	-4.123851
65	6	0	2.017853	-4.433740	-0.608151
66	6	0	2.197403	-4.433148	-3.016635
67	6	0	1.885648	-2.495016	4.155431
68	6	0	1.888428	-0.169225	4.816828
69	8	0	1.505503	-4.369342	0.473011
70	7	0	1.338285	-4.479207	-1.860622

71	8	0	1.820353	-4.461788	-4.147699
72	8	0	1.594742	-1.122996	-4.305548
73	7	0	1.192010	1.108531	-3.752049
74	8	0	1.437296	3.336708	-3.107590
75	7	0	1.125723	4.343153	0.751821
76	8	0	1.361764	2.641557	2.327870
77	8	0	1.533855	5.968945	-0.876463
78	7	0	1.114759	-1.323556	4.484490
79	8	0	1.423114	-3.553895	3.856621
80	8	0	1.448248	0.910381	5.093043
81	1	0	0.309045	-4.498507	-1.942003
82	1	0	0.158534	1.055899	-3.735867
83	1	0	0.095029	4.341470	0.679761
84	1	0	0.079400	-1.331436	4.511224
85	6	0	-9.054103	-0.852267	2.576020
86	6	0	-8.515996	0.207164	3.328894
87	6	0	-7.363715	-0.070716	4.083881
88	6	0	-6.725921	-1.312397	4.060903
89	6	0	-7.292618	-2.311635	3.273509
90	6	0	-8.468480	-2.126897	2.522705
91	6	0	-8.516995	-2.530445	-2.019195
92	6	0	-9.028173	-2.539503	-0.710686
93	6	0	-8.483892	-3.313860	0.329246
94	6	0	-7.388357	-4.130951	0.000006
95	6	0	-6.831844	-4.158899	-1.280808
96	6	0	-7.404199	-3.354071	-2.265746
97	6	0	-6.785213	3.874766	1.291519
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99	6	0	-8.539986	2.395698	2.177390
100	6	0	-9.137283	2.410350	0.904505
101	6	0	-8.609084	3.122740	-0.182888
102	6	0	-7.420943	3.840684	0.051480
103	6	0	-7.651537	2.347533	-3.325660
104	6	0	-8.699528	2.076621	-2.431067
105	6	0	-9.169407	0.750334	-2.386124
106	6	0	-8.603075	-0.291577	-3.136263
107	6	0	-7.506367	0.045854	-3.950959
108	6	0	-7.029157	1.347729	-4.078505
109	6	0	-9.201864	1.560737	3.261504
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112	6	0	-9.353800	3.088912	-1.508037
113	8	0	-6.873537	0.917859	4.968564
114	8	0	-6.720025	-3.602550	3.303910
115	8	0	-6.846230	-5.023236	0.961904
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117	8	0	-6.840276	3.325932	3.638809
118	8	0	-6.942162	4.669774	-0.984369
119	8	0	-7.224869	3.685294	-3.538055
120	8	0	-6.910871	-0.962047	-4.746613
121	6	0	-3.700071	3.954065	-3.284348
122	6	0	-3.551372	4.177483	-1.876664
123	7	0	-4.588893	4.365115	-1.047137
124	6	0	-5.809984	4.272785	-1.649558
125	6	0	-5.957221	3.901484	-3.026083
126	7	0	-4.893472	3.777491	-3.869663
127	7	0	-4.478126	3.321338	3.538655
128	6	0	-3.364789	2.683305	3.927687
129	6	0	-3.384231	1.443721	4.647776
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131	6	0	-5.656920	1.451404	4.593763
132	6	0	-5.639983	2.692273	3.883546
133	7	0	-4.394371	-3.203422	3.034804

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135	6	0	-5.613990	-4.595629	1.426861
136	7	0	-4.490580	-5.023522	0.781485
137	6	0	-3.346486	-4.538001	1.282341
138	6	0	-3.305375	-3.588276	2.356399
139	7	0	-4.581307	-0.679203	-4.414611
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141	6	0	-5.682220	-2.758434	-3.722428
142	7	0	-4.516694	-3.391092	-3.397621
143	6	0	-3.412158	-2.661120	-3.603312
144	6	0	-3.447724	-1.304935	-4.069562
145	6	0	-2.324146	3.903468	-3.927128
146	6	0	-2.072045	4.144154	-1.536671
147	6	0	-1.917613	3.079662	3.672399
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149	6	0	-1.924152	-4.831639	0.829301
150	6	0	-1.866748	-3.127156	2.540912
151	6	0	-1.962824	-3.068518	-3.388186
152	6	0	-2.027290	-0.766387	-4.086833
153	8	0	-1.494264	-5.591741	0.017774
154	7	0	-1.127769	-3.937222	1.631402
155	8	0	-1.417398	-2.242974	3.214155
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157	7	0	-1.164305	2.014353	4.265350
158	8	0	-1.450466	4.020409	3.101169
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163	8	0	-1.477703	-4.080116	-2.979015
164	8	0	-1.616199	0.352339	-4.249283
165	1	0	-0.091791	-3.934323	1.584611
166	1	0	-0.128192	2.006828	4.289109
167	1	0	-0.397318	4.025775	-2.904397
168	1	0	-0.187418	-1.861823	-3.744387
169	1	0	10.239929	1.089897	-2.894629
170	1	0	9.864930	1.846946	-0.782898
171	1	0	5.971099	4.565344	-2.284031
172	1	0	9.954119	-0.771841	-1.600848
173	1	0	6.131339	-2.311495	-4.404689
174	1	0	10.346488	-2.866802	-0.823099
175	1	0	10.008430	-1.646057	1.055545
176	1	0	5.856594	-4.160744	2.215632
177	1	0	10.233847	-0.829608	3.138110
178	1	0	5.741283	2.275132	4.262923
179	1	0	9.963206	1.054933	1.892946
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181	1	0	-5.976656	-4.812218	-1.512343
182	1	0	-9.893408	-1.909736	-0.488198
183	1	0	-10.207249	-2.889332	1.527573
184	1	0	-5.815108	-1.499671	4.649537
185	1	0	-9.967080	-0.672778	2.003847
186	1	0	-10.269578	1.378524	2.941529
187	1	0	-10.059649	1.842867	0.756967
188	1	0	-5.874715	4.470259	1.447892
189	1	0	-10.399521	2.717944	-1.296363
190	1	0	-6.195754	1.578885	-4.757716
191	1	0	-10.012327	0.521060	-1.729790
192	1	0	-10.287732	-1.534627	-2.691471
193	6	0	9.466175	-4.730508	-1.359634
194	1	0	10.032365	-4.827438	-2.293284
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198	1	0	9.807867	-2.349066	5.025502
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201	6	0	9.208340	4.937779	1.669220
202	1	0	9.718717	4.982278	2.638060
203	1	0	9.749815	5.585751	0.969799
204	1	0	8.212291	5.391481	1.810807
205	6	0	9.291766	1.626358	-4.725572
206	1	0	9.812757	2.587479	-4.805482
207	1	0	9.838702	0.893327	-5.329934
208	1	0	8.305376	1.759024	-5.202786
209	6	0	-9.293449	2.274546	4.607420
210	1	0	-9.854648	3.212468	4.524424
211	1	0	-9.787615	1.647443	5.358899
212	1	0	-8.301455	2.533436	5.015440
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214	1	0	-10.091039	4.418498	-3.069855
215	1	0	-10.056983	5.151964	-1.454340
216	1	0	-8.561663	4.949215	-2.371846
217	6	0	-9.344527	-2.355468	-4.415561
218	1	0	-9.853393	-3.323245	-4.334786
219	1	0	-9.904958	-1.736193	-5.125386
220	1	0	-8.360054	-2.553729	-4.873716
221	6	0	-9.224057	-4.550500	2.427757
222	1	0	-9.735879	-4.447839	3.391492
223	1	0	-9.765399	-5.295898	1.833272
224	1	0	-8.228957	-4.978972	2.639069
225	6	0	-3.894158	1.757244	0.790941
226	6	0	-2.565729	1.406912	0.585921
227	6	0	-4.898600	0.803118	0.677176
228	1	0	-4.136420	2.794147	1.015042
229	6	0	-2.254732	0.091724	0.265905
230	1	0	-1.786797	2.164245	0.640620
231	6	0	-4.571118	-0.509998	0.353271
232	1	0	-5.933914	1.083483	0.830721
233	7	0	-0.902706	-0.274722	0.016357
234	6	0	-3.248028	-0.875293	0.147579
235	1	0	-5.350940	-1.255518	0.261992
236	6	0	0.239774	0.226741	0.539101
237	7	0	-0.630387	-1.210126	-0.905861
238	1	0	-2.970143	-1.886545	-0.111048
239	6	0	1.240933	-0.456719	-0.114850
240	1	0	0.246995	0.985891	1.311832
241	7	0	0.651114	-1.320453	-0.988634
242	6	0	2.699315	-0.354409	0.009755
243	6	0	3.520473	-0.941495	-0.955869
244	6	0	3.284496	0.323754	1.080327
245	6	0	4.901264	-0.845893	-0.850703
246	1	0	3.061485	-1.469866	-1.781523
247	6	0	4.665472	0.417768	1.180972
248	1	0	2.659238	0.779245	1.847100
249	6	0	5.480020	-0.166481	0.216572
250	1	0	5.529178	-1.302062	-1.607258
251	1	0	5.102382	0.950466	2.019404
252	1	0	6.558748	-0.095712	0.298660