Conformational complexity of morphine and morphinum in the gas phase and in water. A DFT and MP2 study

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Electronic supplementary information

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Table 1S. MP2/cc-pVTZ Cartesian Coordinates of M_{equ}-3*syn*-6g^+

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.024594	-1.483969	-0.864399
2	6	0	1.467407	-2.389266	0.296046
3	6	0	1.024611	-1.870108	1.636714
4	6	0	-0.209930	-1.376580	1.800623
5	6	0	-1.117223	-1.249879	0.613455
6	6	0	-0.299648	-0.748225	-0.587812
7	8	0	2.857430	-2.642699	0.228532
8	6	0	1.539727	0.704564	-0.526676
9	8	0	2.047909	-0.449066	-1.079028
10	6	0	0.284080	2.700488	0.890632
11	6	0	1.601905	2.861427	0.452694
12	6	0	2.270221	1.850471	-0.245867
13	8	0	3.587011	1.998950	-0.574972
14	6	0	-2.269388	-0.249039	0.810715
15	6	0	-1.776250	1.175239	1.183577
16	6	0	-0.441626	1.539937	0.588813
17	6	0	0.210849	0.597451	-0.184708
18	6	0	-1.184350	-0.675103	-1.833612
19	6	0	-2.422554	0.165125	-1.573401
20	7	0	-3.114962	-0.317277	-0.385787
21	6	0	-4.386918	0.360141	-0.215919
22	1	0	1.005651	-2.058856	-1.788780
23	1	0	0.978410	-3.355082	0.130720
24	1	0	1.715148	-1.984250	2.462142
25	1	0	-0.554334	-1.055097	2.777203
26	1	0	-1.580582	-2.213643	0.372156
27	1	0	3.256068	-1.794815	-0.005831
28	1	0	-0.165321	3.480851	1.492214
29	1	0	2.154171	3.759674	0.693600
30	1	0	3.845509	1.222921	-1.086210
31	1	0	-2.889274	-0.609952	1.636093
32	1	0	-1.690026	1.242736	2.271395
33	1	0	-2.545112	1.899385	0.903450
34	1	0	-1.487956	-1.689022	-2.107746
35	1	0	-0.611387	-0.252967	-2.662789
36	1	0	-3.109688	0.085373	-2.417306
37	1	0	-2.143143	1.227555	-1.484250
38	1	0	-4.876089	-0.003842	0.686899
39	1	0	-5.026877	0.132263	-1.067491
40	1	0	-4.302276	1.454167	-0.146460

E(MP2) -938.18991634 a.u.

Table 2S. MP2/cc-pVTZ Cartesian Coordinates of M_{equ}-3*anti*-6g^+

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.998345	-1.505839	-0.871465
2	6	0	1.456584	-2.398324	0.295389
3	6	0	1.003274	-1.883791	1.634644
4	6	0	-0.231586	-1.390885	1.798080
5	6	0	-1.136514	-1.249149	0.610599
6	6	0	-0.313892	-0.754713	-0.588937
7	8	0	2.851426	-2.619639	0.230969
8	6	0	1.549977	0.669081	-0.545571
9	8	0	2.023908	-0.485497	-1.110925
10	6	0	0.314094	2.681121	0.894288
11	6	0	1.632035	2.822476	0.448415
12	6	0	2.291849	1.809075	-0.257963
13	8	0	3.603633	1.859313	-0.631918
14	6	0	-2.274403	-0.233923	0.813136
15	6	0	-1.757293	1.179504	1.192085
16	6	0	-0.420486	1.528804	0.592537
17	6	0	0.220812	0.582767	-0.187075
18	6	0	-1.198792	-0.663219	-1.833433
19	6	0	-2.424148	0.194244	-1.568933
20	7	0	-3.122486	-0.282040	-0.382296
21	6	0	-4.382817	0.414789	-0.207050
22	1	0	0.962068	-2.093174	-1.787502
23	1	0	0.985525	-3.374496	0.137554
24	1	0	1.689501	-2.004200	2.462929
25	1	0	-0.578902	-1.078807	2.776823
26	1	0	-1.612491	-2.205731	0.365748
27	1	0	3.226704	-1.780926	-0.071603
28	1	0	-0.122154	3.465486	1.500208
29	1	0	2.183599	3.722482	0.696063
30	1	0	3.973320	2.685795	-0.303182
31	1	0	-2.898919	-0.588537	1.637832
32	1	0	-1.663698	1.237981	2.279799
33	1	0	-2.515474	1.918144	0.920861
34	1	0	-1.517984	-1.671524	-2.110343
35	1	0	-0.619901	-0.247577	-2.661701
36	1	0	-3.113436	0.128156	-2.412301
37	1	0	-2.129289	1.252304	-1.476157
38	1	0	-4.877376	0.053292	0.693880
39	1	0	-5.027158	0.203060	-1.059519
40	1	0	-4.280506	1.507025	-0.130791

E(MP2) -937.80789044 a.u.

Table 3S. MP2/cc-pVTZ Cartesian Coordinates of M_{equ}-3*syn*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.046625	-1.459810	-0.858057
2	6	0	1.432066	-2.373170	0.306747
3	6	0	1.083972	-1.774507	1.641448
4	6	0	-0.138894	-1.258379	1.825169
5	6	0	-1.077734	-1.204290	0.656320
6	6	0	-0.291732	-0.735548	-0.583272
7	8	0	2.800817	-2.708416	0.162842
8	6	0	1.538867	0.724539	-0.555197
9	8	0	2.054770	-0.430833	-1.077391
10	6	0	0.276365	2.747643	0.819678
11	6	0	1.602885	2.893390	0.401195
12	6	0	2.274840	1.866395	-0.269386
13	8	0	3.599913	1.985122	-0.569715
14	6	0	-2.248869	-0.222579	0.833553
15	6	0	-1.784901	1.230481	1.130066
16	6	0	-0.450115	1.584661	0.528836
17	6	0	0.204580	0.629634	-0.228374
18	6	0	-1.201201	-0.728698	-1.811966
19	6	0	-2.453655	0.092246	-1.559465
20	7	0	-3.113611	-0.363963	-0.343138
21	6	0	-4.400723	0.284698	-0.175879
22	1	0	1.025356	-2.046672	-1.775460
23	1	0	0.804583	-3.266843	0.166866
24	1	0	1.821413	-1.810268	2.433549
25	1	0	-0.437223	-0.849453	2.783668
26	1	0	-1.521270	-2.189011	0.465523
27	1	0	2.992713	-3.404866	0.798421
28	1	0	-0.175880	3.537572	1.406633
29	1	0	2.158842	3.788762	0.644626
30	1	0	3.881541	1.137561	-0.937380
31	1	0	-2.845384	-0.560530	1.685458
32	1	0	-1.714600	1.364028	2.212782
33	1	0	-2.564797	1.920840	0.799076
34	1	0	-1.486850	-1.758549	-2.043531
35	1	0	-0.653127	-0.325101	-2.666625
36	1	0	-3.153494	-0.031860	-2.387409
37	1	0	-2.196356	1.162859	-1.511633
38	1	0	-4.865692	-0.060369	0.747004
39	1	0	-5.047305	0.010037	-1.008463
40	1	0	-4.345440	1.382394	-0.145523

E(MP2) -937.80456739 a.u.

Table 4S. MP2/cc-pVTZ Cartesian Coordinates of M_{equ}-3*anti*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.035603	-1.468795	-0.867743
2	6	0	1.382567	-2.426173	0.273539
3	6	0	1.046530	-1.848196	1.620542
4	6	0	-0.164841	-1.307224	1.810045
5	6	0	-1.093947	-1.210643	0.636050
6	6	0	-0.289375	-0.727551	-0.585503
7	8	0	2.736362	-2.811524	0.128586
8	6	0	1.570411	0.699651	-0.531976
9	8	0	2.066904	-0.459278	-1.047697
10	6	0	0.293476	2.734986	0.851351
11	6	0	1.615033	2.878541	0.416958
12	6	0	2.293628	1.858278	-0.260990
13	8	0	3.607791	1.922821	-0.621676
14	6	0	-2.251263	-0.216243	0.824674
15	6	0	-1.764960	1.221026	1.152891
16	6	0	-0.427238	1.572768	0.555915
17	6	0	0.230882	0.621260	-0.204094
18	6	0	-1.188779	-0.676937	-1.821015
19	6	0	-2.432593	0.154739	-1.561794
20	7	0	-3.109232	-0.318168	-0.361021
21	6	0	-4.386847	0.347329	-0.188908
22	1	0	1.010187	-2.030359	-1.801051
23	1	0	0.720193	-3.290299	0.107641
24	1	0	1.781216	-1.916081	2.413087
25	1	0	-0.459266	-0.909606	2.774531
26	1	0	-1.549721	-2.184185	0.418280
27	1	0	2.899733	-3.523653	0.754578
28	1	0	-0.155546	3.523715	1.442129
29	1	0	2.156339	3.788068	0.653056
30	1	0	3.958326	2.762017	-0.304760
31	1	0	-2.859935	-0.560836	1.665316
32	1	0	-1.687183	1.326149	2.238333
33	1	0	-2.535174	1.931824	0.843309
34	1	0	-1.486062	-1.697245	-2.078763
35	1	0	-0.626914	-0.262288	-2.661261
36	1	0	-3.126744	0.057291	-2.398127
37	1	0	-2.162835	1.220924	-1.489004
38	1	0	-4.864711	-0.010493	0.722492
39	1	0	-5.031245	0.102000	-1.032304
40	1	0	-4.314203	1.443189	-0.133683

E(MP2) -937.79925898 a.u.

Table 5S. MP2/cc-pVTZ Cartesian Coordinates of M_{ax}-3*syn*-6g^+

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.636800	1.586954	-0.831921
2	6	0	-0.892418	2.543634	0.344077
3	6	0	-0.612528	1.909818	1.679477
4	6	0	0.478734	1.152790	1.856223
5	6	0	1.360054	0.846594	0.682134
6	6	0	0.479593	0.565174	-0.547574
7	8	0	-2.186249	3.108186	0.255596
8	6	0	-1.642960	-0.432302	-0.555506
9	8	0	-1.861541	0.815936	-1.093729
10	6	0	-0.907301	-2.685707	0.841432
11	6	0	-2.216230	-2.535177	0.373617
12	6	0	-2.620995	-1.386891	-0.315029
13	8	0	-3.928856	-1.226825	-0.673510
14	6	0	2.253553	-0.403049	0.878744
15	6	0	1.440300	-1.676183	1.204651
16	6	0	0.069698	-1.715381	0.580861
17	6	0	-0.333683	-0.635530	-0.183608
18	6	0	1.358129	0.308750	-1.776895
19	6	0	2.339018	-0.830230	-1.498809
20	7	0	3.120737	-0.649685	-0.277295
21	6	0	4.161006	0.353957	-0.429983
22	1	0	-0.464980	2.162485	-1.740149
23	1	0	-0.192788	3.376318	0.214295
24	1	0	-1.283956	2.154843	2.492203
25	1	0	0.718741	0.741627	2.830485
26	1	0	2.015237	1.702724	0.480120
27	1	0	-2.760546	2.378953	-0.011359
28	1	0	-0.661114	-3.558865	1.432774
29	1	0	-2.963380	-3.288717	0.582964
30	1	0	-3.992122	-0.404437	-1.173553
31	1	0	2.919993	-0.213254	1.724711
32	1	0	2.052351	-2.529852	0.905697
33	1	0	1.314697	-1.746887	2.287877
34	1	0	0.725112	0.054721	-2.631272
35	1	0	1.892223	1.230146	-2.027281
36	1	0	3.033634	-0.951353	-2.331182
37	1	0	1.777701	-1.762736	-1.410934
38	1	0	4.725544	0.424825	0.499264
39	1	0	3.804864	1.360740	-0.685094
40	1	0	4.843774	0.034820	-1.216715

E(MP2) -937.80727550 a.u.

Table 6S. MP2/cc-pVTZ Cartesian Coordinates of M_{ax}-3*anti*-6g^+

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.611227	1.599956	-0.839272
2	6	0	-0.887700	2.548182	0.341294
3	6	0	-0.596562	1.918324	1.676457
4	6	0	0.496696	1.164416	1.854206
5	6	0	1.374167	0.845388	0.680511
6	6	0	0.492098	0.568831	-0.547883
7	8	0	-2.194469	3.079919	0.253072
8	6	0	-1.644884	-0.399743	-0.573754
9	8	0	-1.832461	0.841027	-1.125161
10	6	0	-0.927529	-2.662307	0.846359
11	6	0	-2.232131	-2.496062	0.370361
12	6	0	-2.630503	-1.348470	-0.326515
13	8	0	-3.910559	-1.096399	-0.728026
14	6	0	2.253254	-0.412618	0.883595
15	6	0	1.422406	-1.671784	1.215321
16	6	0	0.053862	-1.699514	0.586005
17	6	0	-0.340149	-0.620025	-0.184946
18	6	0	1.368147	0.295319	-1.775390
19	6	0	2.334741	-0.854078	-1.491857
20	7	0	3.118116	-0.677764	-0.270267
21	6	0	4.170694	0.312438	-0.427559
22	1	0	-0.421188	2.183148	-1.738990
23	1	0	-0.204791	3.395970	0.218458
24	1	0	-1.263831	2.167409	2.491506
25	1	0	0.741770	0.762783	2.831339
26	1	0	2.038359	1.693500	0.474677
27	1	0	-2.740620	2.354130	-0.079883
28	1	0	-0.693207	-3.535687	1.442047
29	1	0	-2.977381	-3.253324	0.586536
30	1	0	-4.463483	-1.825861	-0.428074
31	1	0	2.921485	-0.227724	1.729305
32	1	0	2.023568	-2.536322	0.925627
33	1	0	1.290823	-1.731777	2.298484
34	1	0	0.732064	0.046342	-2.628930
35	1	0	1.913705	1.208981	-2.029125
36	1	0	3.028737	-0.987532	-2.322913
37	1	0	1.762622	-1.779684	-1.400280
38	1	0	4.735782	0.380948	0.501564
39	1	0	3.826718	1.322063	-0.687658
40	1	0	4.849708	-0.018917	-1.212504

E(MP2) -937.80481094 a.u.

Table 7S. MP2/cc-pVTZ Cartesian Coordinates of M_{ax}-3*syn*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.651000	1.570483	-0.834354
2	6	0	-0.836526	2.528735	0.343970
3	6	0	-0.664272	1.844824	1.671925
4	6	0	0.405146	1.060788	1.866573
5	6	0	1.324680	0.803212	0.709388
6	6	0	0.474231	0.548395	-0.551362
7	8	0	-2.085174	3.177887	0.184843
8	6	0	-1.649155	-0.439590	-0.578451
9	8	0	-1.866696	0.810593	-1.092902
10	6	0	-0.926466	-2.719441	0.784749
11	6	0	-2.240956	-2.543813	0.340027
12	6	0	-2.638807	-1.379552	-0.324861
13	8	0	-3.948108	-1.179887	-0.650781
14	6	0	2.230854	-0.439411	0.888885
15	6	0	1.429016	-1.735285	1.153243
16	6	0	0.058897	-1.756730	0.526975
17	6	0	-0.337652	-0.664969	-0.225277
18	6	0	1.382838	0.335330	-1.765803
19	6	0	2.372100	-0.797873	-1.496167
20	7	0	3.126648	-0.637728	-0.254710
21	6	0	4.151688	0.387071	-0.358004
22	1	0	-0.473071	2.151715	-1.738393
23	1	0	-0.014374	3.252856	0.232681
24	1	0	-1.391572	2.034977	2.451454
25	1	0	0.582978	0.579984	2.821728
26	1	0	1.970427	1.676001	0.550144
27	1	0	-2.127401	3.881262	0.840118
28	1	0	-0.684871	-3.601334	1.365101
29	1	0	-2.996584	-3.286431	0.558151
30	1	0	-4.014924	-0.285980	-1.010305
31	1	0	2.876015	-0.267484	1.755018
32	1	0	2.051795	-2.566195	0.814523
33	1	0	1.305150	-1.860660	2.231629
34	1	0	0.771299	0.095768	-2.639600
35	1	0	1.910251	1.269391	-1.981835
36	1	0	3.084905	-0.891092	-2.316760
37	1	0	1.820042	-1.738387	-1.441349
38	1	0	4.696550	0.440891	0.584167
39	1	0	3.783627	1.394819	-0.591951
40	1	0	4.855335	0.102205	-1.139570

E(MP2) -937.80133948 a.u.

Table 8S. MP2/cc-pVTZ Cartesian Coordinates of M_{ax}-3*anti*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.616382	1.584851	-0.843693
2	6	0	-0.744186	2.579038	0.312388
3	6	0	-0.591196	1.915920	1.653335
4	6	0	0.450164	1.096610	1.855754
5	6	0	1.349536	0.788335	0.694977
6	6	0	0.477275	0.534992	-0.550599
7	8	0	-1.957049	3.289072	0.150224
8	6	0	-1.679380	-0.386522	-0.557962
9	8	0	-1.859618	0.864792	-1.066656
10	6	0	-0.979450	-2.690601	0.816440
11	6	0	-2.284672	-2.496811	0.352603
12	6	0	-2.673407	-1.332436	-0.321225
13	8	0	-3.953638	-1.064976	-0.709718
14	6	0	2.221970	-0.474839	0.888030
15	6	0	1.384475	-1.739719	1.181653
16	6	0	0.013433	-1.740176	0.556255
17	6	0	-0.370971	-0.646060	-0.200201
18	6	0	1.365518	0.269897	-1.770345
19	6	0	2.327413	-0.883787	-1.490536
20	7	0	3.100004	-0.720931	-0.260199
21	6	0	4.151011	0.273606	-0.394447
22	1	0	-0.429990	2.138584	-1.763481
23	1	0	0.114641	3.255726	0.177345
24	1	0	-1.307666	2.146085	2.432080
25	1	0	0.618151	0.625362	2.817472
26	1	0	2.017007	1.639607	0.510494
27	1	0	-1.959749	4.002487	0.795816
28	1	0	-0.753775	-3.573594	1.401251
29	1	0	-3.039686	-3.246571	0.561889
30	1	0	-4.508386	-1.795135	-0.415266
31	1	0	2.880514	-0.307817	1.745100
32	1	0	1.982409	-2.596767	0.864048
33	1	0	1.256135	-1.834531	2.262732
34	1	0	0.736713	0.030973	-2.631945
35	1	0	1.915206	1.184889	-2.011155
36	1	0	3.028569	-1.010601	-2.316715
37	1	0	1.752411	-1.808788	-1.412632
38	1	0	4.706244	0.332342	0.541400
39	1	0	3.807587	1.285683	-0.646131
40	1	0	4.839170	-0.046309	-1.176268

E(MP2) -937.79611423 a.u.

Table 9S. B3LYP/cc-pVTZ Cartesian Coordinates of M_{equ}-3*syn*-6g^+

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.043284	-1.458524	-0.887900
2	6	0	1.468271	-2.448276	0.223798
3	6	0	0.956255	-2.067143	1.592369
4	6	0	-0.254969	-1.547749	1.765166
5	6	0	-1.132937	-1.257718	0.578665
6	6	0	-0.286941	-0.716212	-0.593932
7	8	0	2.867536	-2.672962	0.197880
8	6	0	1.560758	0.740913	-0.495038
9	8	0	2.073316	-0.415443	-1.040045
10	6	0	0.299300	2.724644	0.922269
11	6	0	1.611647	2.894098	0.487871
12	6	0	2.283974	1.887178	-0.209869
13	8	0	3.602014	2.043525	-0.538610
14	6	0	-2.269637	-0.230723	0.812447
15	6	0	-1.753404	1.184599	1.220967
16	6	0	-0.418416	1.561372	0.618662
17	6	0	0.233139	0.627432	-0.159665
18	6	0	-1.179020	-0.628502	-1.848461
19	6	0	-2.446963	0.183143	-1.599086
20	7	0	-3.126255	-0.256200	-0.383984
21	6	0	-4.417432	0.380424	-0.209420
22	1	0	1.029440	-1.978944	-1.842969
23	1	0	1.016811	-3.411345	-0.041030
24	1	0	1.603506	-2.306983	2.426393
25	1	0	-0.628000	-1.336053	2.760937
26	1	0	-1.633453	-2.181055	0.267210
27	1	0	3.283451	-1.815646	0.046710
28	1	0	-0.155724	3.500997	1.524508
29	1	0	2.158104	3.795521	0.729967
30	1	0	3.887968	1.276995	-1.047172
31	1	0	-2.891377	-0.598873	1.631492
32	1	0	-1.652710	1.216889	2.309602
33	1	0	-2.521241	1.923860	0.980963
34	1	0	-1.453410	-1.644892	-2.143890
35	1	0	-0.619573	-0.184574	-2.674373
36	1	0	-3.134303	0.048190	-2.436539
37	1	0	-2.200499	1.257091	-1.569428
38	1	0	-4.906706	-0.014201	0.682018
39	1	0	-5.050767	0.154057	-1.068479
40	1	0	-4.372092	1.477676	-0.114882

E(RB3LYP) -939.95593244 a.u.

Table 10S. B3LYP/cc-pVTZ Cartesian Coordinates of M_{equ}-3*anti*-6g^+

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.015749	-1.481206	-0.894789
2	6	0	1.449627	-2.462273	0.223266
3	6	0	0.933842	-2.079410	1.590178
4	6	0	-0.274817	-1.554210	1.763390
5	6	0	-1.151015	-1.252332	0.578273
6	6	0	-0.301231	-0.721464	-0.595514
7	8	0	2.851268	-2.666694	0.200383
8	6	0	1.573393	0.704032	-0.513012
9	8	0	2.052171	-0.455127	-1.066841
10	6	0	0.332530	2.708084	0.920212
11	6	0	1.645909	2.856195	0.479373
12	6	0	2.309210	1.844729	-0.222653
13	8	0	3.624096	1.903950	-0.591356
14	6	0	-2.272876	-0.211192	0.816418
15	6	0	-1.733082	1.194695	1.225161
16	6	0	-0.395337	1.553803	0.617819
17	6	0	0.244498	0.614019	-0.164879
18	6	0	-1.195676	-0.617295	-1.847425
19	6	0	-2.450775	0.212089	-1.592896
20	7	0	-3.133295	-0.220641	-0.377271
21	6	0	-4.414497	0.433835	-0.197410
22	1	0	0.985230	-2.012608	-1.843558
23	1	0	1.006486	-3.431834	-0.033383
24	1	0	1.578593	-2.323808	2.424916
25	1	0	-0.647994	-1.344858	2.759755
26	1	0	-1.664039	-2.168594	0.266456
27	1	0	3.252403	-1.818493	-0.030204
28	1	0	-0.109231	3.489959	1.524996
29	1	0	2.192671	3.759149	0.727576
30	1	0	4.002478	2.731474	-0.278542
31	1	0	-2.897703	-0.570695	1.637011
32	1	0	-1.626358	1.222384	2.313306
33	1	0	-2.489987	1.946859	0.990433
34	1	0	-1.485946	-1.628968	-2.143627
35	1	0	-0.631627	-0.180783	-2.674058
36	1	0	-3.142233	0.089959	-2.428983
37	1	0	-2.188652	1.282380	-1.560678
38	1	0	-4.907134	0.043840	0.694254
39	1	0	-5.053393	0.219211	-1.055420
40	1	0	-4.353490	1.530277	-0.099938

E(RB3LYP) -939.95340720 a.u.

Table 11S. B3LYP/cc-pVTZ Cartesian Coordinates of M_{equ}-3*syn*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.070292	-1.430207	-0.883100
2	6	0	1.454042	-2.427167	0.228969
3	6	0	1.009003	-1.989424	1.603874
4	6	0	-0.198095	-1.465706	1.790862
5	6	0	-1.100001	-1.232406	0.609408
6	6	0	-0.276934	-0.706706	-0.589785
7	8	0	2.846905	-2.688434	0.132973
8	6	0	1.555261	0.765796	-0.515369
9	8	0	2.075951	-0.384733	-1.045961
10	6	0	0.279365	2.763046	0.872777
11	6	0	1.597569	2.927308	0.451975
12	6	0	2.277543	1.912320	-0.225751
13	8	0	3.600929	2.051568	-0.534361
14	6	0	-2.254937	-0.222403	0.827583
15	6	0	-1.764991	1.216410	1.186617
16	6	0	-0.432719	1.593866	0.578506
17	6	0	0.225280	0.654008	-0.187519
18	6	0	-1.184860	-0.669919	-1.833893
19	6	0	-2.466921	0.121459	-1.591243
20	7	0	-3.124211	-0.302049	-0.357995
21	6	0	-4.427120	0.310816	-0.185526
22	1	0	1.056849	-1.962174	-1.832441
23	1	0	0.892554	-3.341199	-0.022135
24	1	0	1.691479	-2.162188	2.427437
25	1	0	-0.538082	-1.192685	2.783159
26	1	0	-1.583510	-2.175782	0.332011
27	1	0	3.050774	-3.450517	0.682655
28	1	0	-0.181259	3.544577	1.464097
29	1	0	2.142678	3.829050	0.696315
30	1	0	3.912340	1.221677	-0.914389
31	1	0	-2.860054	-0.578789	1.664201
32	1	0	-1.673677	1.291842	2.273931
33	1	0	-2.545351	1.931150	0.914403
34	1	0	-1.441931	-1.698848	-2.100833
35	1	0	-0.643645	-0.236139	-2.677040
36	1	0	-3.160218	-0.048163	-2.417409
37	1	0	-2.242707	1.200467	-1.589473
38	1	0	-4.899045	-0.072356	0.720280
39	1	0	-5.063702	0.049935	-1.032354
40	1	0	-4.404938	1.410728	-0.117960

E(RB3LYP) -939.94986195 a.u.

Table 12S. B3LYP/cc-pVTZ Cartesian Coordinates of M_{equ}-3*anti*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.056172	-1.443863	-0.889307
2	6	0	1.406923	-2.472828	0.205019
3	6	0	0.970464	-2.045426	1.586141
4	6	0	-0.226505	-1.500219	1.777276
5	6	0	-1.117124	-1.234100	0.593993
6	6	0	-0.277444	-0.702503	-0.590604
7	8	0	2.788584	-2.780275	0.107988
8	6	0	1.584228	0.736001	-0.500145
9	8	0	2.082120	-0.419184	-1.025641
10	6	0	0.302859	2.747635	0.898275
11	6	0	1.616982	2.905903	0.462231
12	6	0	2.299224	1.895693	-0.222900
13	8	0	3.612771	1.977701	-0.589896
14	6	0	-2.257561	-0.211208	0.820743
15	6	0	-1.744294	1.211641	1.204530
16	6	0	-0.407813	1.581885	0.600338
17	6	0	0.249578	0.642926	-0.169078
18	6	0	-1.177271	-0.627666	-1.839608
19	6	0	-2.448710	0.178565	-1.592213
20	7	0	-3.120808	-0.255833	-0.370796
21	6	0	-4.414140	0.375723	-0.195434
22	1	0	1.037903	-1.958869	-1.848190
23	1	0	0.813985	-3.362272	-0.063421
24	1	0	1.648632	-2.241826	2.407936
25	1	0	-0.565186	-1.232681	2.771581
26	1	0	-1.611840	-2.165649	0.296902
27	1	0	2.964903	-3.557549	0.645712
28	1	0	-0.151881	3.529527	1.493395
29	1	0	2.150692	3.819191	0.701745
30	1	0	3.972434	2.815636	-0.283143
31	1	0	-2.873840	-0.569875	1.648278
32	1	0	-1.647620	1.263997	2.292799
33	1	0	-2.513205	1.944735	0.949087
34	1	0	-1.448002	-1.647681	-2.126431
35	1	0	-0.622977	-0.188170	-2.671128
36	1	0	-3.138840	0.033730	-2.425804
37	1	0	-2.208775	1.254098	-1.570461
38	1	0	-4.898069	-0.014620	0.700940
39	1	0	-5.049864	0.140232	-1.050338
40	1	0	-4.374015	1.473990	-0.109039

E(RB3LYP) -939.94473560 a.u.

Table 13S. B3LYP/cc-pVTZ Cartesian Coordinates of M_{ax}-3*syn*-6g^+

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.674798	1.566483	-0.863556
2	6	0	-0.896087	2.606299	0.261267
3	6	0	-0.512271	2.099254	1.631072
4	6	0	0.553339	1.326557	1.816467
5	6	0	1.370604	0.864979	0.640917
6	6	0	0.451978	0.543040	-0.560368
7	8	0	-2.210068	3.135513	0.214119
8	6	0	-1.675823	-0.468137	-0.523031
9	8	0	-1.906392	0.780724	-1.056659
10	6	0	-0.917980	-2.701418	0.881694
11	6	0	-2.226091	-2.567419	0.422435
12	6	0	-2.642414	-1.427223	-0.269763
13	8	0	-3.955496	-1.280111	-0.622407
14	6	0	2.249169	-0.402157	0.875427
15	6	0	1.423992	-1.668323	1.233822
16	6	0	0.047196	-1.724487	0.610310
17	6	0	-0.363946	-0.657685	-0.161846
18	6	0	1.333565	0.270947	-1.799700
19	6	0	2.360098	-0.838283	-1.522882
20	7	0	3.118759	-0.664520	-0.282173
21	6	0	4.249305	0.241950	-0.399596
22	1	0	-0.524294	2.086697	-1.807061
23	1	0	-0.237580	3.450408	0.025395
24	1	0	-1.113110	2.459224	2.456728
25	1	0	0.848372	1.022885	2.814770
26	1	0	2.055755	1.673917	0.362386
27	1	0	-2.801217	2.393967	0.036526
28	1	0	-0.659935	-3.567660	1.477863
29	1	0	-2.964782	-3.326725	0.640564
30	1	0	-4.052752	-0.462255	-1.121988
31	1	0	2.914868	-0.201785	1.717181
32	1	0	2.030023	-2.536933	0.969169
33	1	0	1.299598	-1.706280	2.319350
34	1	0	0.707091	-0.015650	-2.647788
35	1	0	1.838177	1.201670	-2.075618
36	1	0	3.066766	-0.913083	-2.349958
37	1	0	1.837117	-1.795314	-1.474253
38	1	0	4.807339	0.247865	0.537768
39	1	0	3.995320	1.285955	-0.641324
40	1	0	4.918559	-0.120546	-1.180929

E(RB3LYP) -939.95201368 a.u.

Table 14S. B3LYP/cc-pVTZ Cartesian Coordinates of M_{ax}-3*anti*-6g^+

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.647328	1.580198	-0.871331
2	6	0	-0.882454	2.614111	0.258234
3	6	0	-0.493544	2.107718	1.627038
4	6	0	0.570579	1.333259	1.813709
5	6	0	1.384134	0.860195	0.639954
6	6	0	0.464721	0.545586	-0.561697
7	8	0	-2.204906	3.119818	0.213226
8	6	0	-1.679594	-0.433359	-0.540159
9	8	0	-1.878940	0.809647	-1.084087
10	6	0	-0.942761	-2.677757	0.884336
11	6	0	-2.246910	-2.526641	0.417325
12	6	0	-2.655347	-1.386262	-0.281469
13	8	0	-3.942817	-1.149052	-0.675135
14	6	0	2.246946	-0.415702	0.880550
15	6	0	1.403288	-1.667812	1.242038
16	6	0	0.028354	-1.710378	0.613029
17	6	0	-0.371803	-0.642610	-0.165387
18	6	0	1.345047	0.257089	-1.798161
19	6	0	2.356458	-0.864204	-1.515561
20	7	0	3.115365	-0.695607	-0.273906
21	6	0	4.257171	0.196489	-0.393430
22	1	0	-0.478904	2.106771	-1.808416
23	1	0	-0.233481	3.467962	0.029318
24	1	0	-1.091736	2.471370	2.453099
25	1	0	0.867231	1.034209	2.813069
26	1	0	2.078739	1.660221	0.359336
27	1	0	-2.775491	2.383709	-0.044077
28	1	0	-0.697533	-3.544743	1.484653
29	1	0	-2.984605	-3.289006	0.641939
30	1	0	-4.501731	-1.873873	-0.378371
31	1	0	2.913541	-0.221399	1.723122
32	1	0	1.997880	-2.546545	0.984926
33	1	0	1.273255	-1.697395	2.327143
34	1	0	0.716487	-0.023352	-2.646634
35	1	0	1.862400	1.180212	-2.075717
36	1	0	3.063702	-0.952051	-2.340919
37	1	0	1.821092	-1.814290	-1.463922
38	1	0	4.814061	0.199418	0.544688
39	1	0	4.016175	1.242467	-0.639573
40	1	0	4.922927	-0.177259	-1.172484

E(RB3LYP) -939.94954485 a.u.

Table 15S. B3LYP/cc-pVTZ Cartesian Coordinates of M_{ax}-3*syn*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.692204	1.550088	-0.862048
2	6	0	-0.857265	2.589020	0.264893
3	6	0	-0.560682	2.034276	1.637788
4	6	0	0.492499	1.247930	1.836042
5	6	0	1.341863	0.832971	0.665386
6	6	0	0.446044	0.530485	-0.561428
7	8	0	-2.146205	3.173379	0.147355
8	6	0	-1.679590	-0.478045	-0.541795
9	8	0	-1.908765	0.768765	-1.061404
10	6	0	-0.928032	-2.732956	0.834884
11	6	0	-2.240958	-2.580177	0.393560
12	6	0	-2.654045	-1.427594	-0.279184
13	8	0	-3.968407	-1.250876	-0.607287
14	6	0	2.233156	-0.428334	0.881848
15	6	0	1.419051	-1.715690	1.191715
16	6	0	0.041860	-1.759560	0.567558
17	6	0	-0.366222	-0.682900	-0.192987
18	6	0	1.350371	0.296556	-1.790908
19	6	0	2.386199	-0.805675	-1.523145
20	7	0	3.124544	-0.648955	-0.267949
21	6	0	4.241064	0.278024	-0.347150
22	1	0	-0.537241	2.080170	-1.799974
23	1	0	-0.090093	3.349201	0.045582
24	1	0	-1.209970	2.338699	2.450128
25	1	0	0.737207	0.884980	2.827706
26	1	0	2.018290	1.660651	0.421523
27	1	0	-2.182478	3.946138	0.718420
28	1	0	-0.672296	-3.606841	1.420962
29	1	0	-2.985427	-3.332133	0.617876
30	1	0	-4.071731	-0.367273	-0.979663
31	1	0	2.882948	-0.241950	1.739307
32	1	0	2.034608	-2.566475	0.892849
33	1	0	1.297890	-1.798678	2.275025
34	1	0	0.739986	0.021335	-2.654227
35	1	0	1.847975	1.238931	-2.039574
36	1	0	3.105913	-0.854494	-2.340987
37	1	0	1.874334	-1.769653	-1.502141
38	1	0	4.785423	0.270504	0.598307
39	1	0	3.973896	1.323561	-0.567860
40	1	0	4.927306	-0.054636	-1.127101

E(RB3LYP) -939.94592878 a.u.

Table 16S. B3LYP/cc-pVTZ Cartesian Coordinates of M_{ax}-3*anti*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.658785	1.566566	-0.868457
2	6	0	-0.777732	2.631074	0.241260
3	6	0	-0.492380	2.087858	1.621347
4	6	0	0.538108	1.273183	1.825287
5	6	0	1.365985	0.818353	0.653809
6	6	0	0.450960	0.522008	-0.559762
7	8	0	-2.040897	3.265566	0.122217
8	6	0	-1.705211	-0.425790	-0.528706
9	8	0	-1.897489	0.821641	-1.044671
10	6	0	-0.978390	-2.701780	0.862490
11	6	0	-2.282936	-2.531370	0.402637
12	6	0	-2.685870	-1.379517	-0.280021
13	8	0	-3.972825	-1.136001	-0.669364
14	6	0	2.225720	-0.461476	0.881318
15	6	0	1.378090	-1.718853	1.216288
16	6	0	-0.000109	-1.741584	0.592669
17	6	0	-0.394973	-0.662555	-0.173245
18	6	0	1.337680	0.243235	-1.793139
19	6	0	2.346490	-0.881570	-1.518295
20	7	0	3.100823	-0.725222	-0.271964
21	6	0	4.239979	0.171505	-0.376521
22	1	0	-0.495242	2.077446	-1.815870
23	1	0	0.019148	3.355214	0.004887
24	1	0	-1.129055	2.422499	2.431763
25	1	0	0.778639	0.916088	2.820184
26	1	0	2.060581	1.624692	0.390315
27	1	0	-2.039944	4.051315	0.676315
28	1	0	-0.738948	-3.576499	1.453940
29	1	0	-3.026976	-3.289662	0.621048
30	1	0	-4.531917	-1.861579	-0.375158
31	1	0	2.887770	-0.281150	1.730773
32	1	0	1.969770	-2.592633	0.936279
33	1	0	1.253481	-1.774899	2.301034
34	1	0	0.711887	-0.027875	-2.646562
35	1	0	1.857529	1.168222	-2.060692
36	1	0	3.057109	-0.962381	-2.341596
37	1	0	1.810072	-1.831462	-1.477119
38	1	0	4.792379	0.166235	0.564333
39	1	0	3.997244	1.219462	-0.612965
40	1	0	4.910636	-0.191851	-1.156368

E(RB3LYP) -939.94083006 a.u.

Table 17S. PBE0/cc-pVTZ Cartesian Coordinates of M_{equ}-3*syn*-6g^+

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.039042	-1.453678	-0.879549
2	6	0	1.467893	-2.423148	0.237027
3	6	0	0.967516	-2.018684	1.596180
4	6	0	-0.247361	-1.510176	1.765115
5	6	0	-1.125467	-1.254541	0.579771
6	6	0	-0.287218	-0.722593	-0.590183
7	8	0	2.855468	-2.646521	0.201644
8	6	0	1.550094	0.727952	-0.497003
9	8	0	2.055977	-0.420387	-1.043295
10	6	0	0.290074	2.708040	0.916009
11	6	0	1.598686	2.876091	0.480615
12	6	0	2.272308	1.872798	-0.215491
13	8	0	3.580589	2.028790	-0.544527
14	6	0	-2.261295	-0.238684	0.803633
15	6	0	-1.756678	1.170492	1.208210
16	6	0	-0.426676	1.547719	0.615055
17	6	0	0.225811	0.616430	-0.159702
18	6	0	-1.172379	-0.635462	-1.837393
19	6	0	-2.424774	0.182495	-1.584082
20	7	0	-3.107705	-0.268385	-0.387037
21	6	0	-4.385208	0.375465	-0.214925
22	1	0	1.020855	-1.988331	-1.829500
23	1	0	1.005346	-3.388461	-0.008035
24	1	0	1.624518	-2.232135	2.431947
25	1	0	-0.617864	-1.278098	2.759075
26	1	0	-1.619350	-2.187621	0.279562
27	1	0	3.261558	-1.790673	0.030490
28	1	0	-0.164551	3.486653	1.518596
29	1	0	2.145998	3.779224	0.722037
30	1	0	3.860304	1.262652	-1.052363
31	1	0	-2.884671	-0.609996	1.623127
32	1	0	-1.662252	1.210354	2.298418
33	1	0	-2.527473	1.906521	0.959400
34	1	0	-1.456100	-1.652362	-2.128137
35	1	0	-0.608406	-0.197685	-2.665355
36	1	0	-3.111332	0.071662	-2.427746
37	1	0	-2.164224	1.254469	-1.532904
38	1	0	-4.880779	-0.015745	0.676242
39	1	0	-5.020065	0.156562	-1.076521
40	1	0	-4.330058	1.473548	-0.119368

E(RPBE1PBE) -938.88727501 a.u.

Table 18S. PBE0/cc-pVTZ Cartesian Coordinates of M_{equ}-3*anti*-6g^+

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.010511	-1.477546	-0.886673
2	6	0	1.449435	-2.437143	0.236586
3	6	0	0.944396	-2.031618	1.593923
4	6	0	-0.268300	-1.517926	1.763126
5	6	0	-1.144579	-1.249476	0.579079
6	6	0	-0.302131	-0.728108	-0.591556
7	8	0	2.839654	-2.638258	0.203733
8	6	0	1.562781	0.689940	-0.515819
9	8	0	2.033962	-0.461506	-1.071787
10	6	0	0.324498	2.690673	0.914684
11	6	0	1.633932	2.836509	0.472153
12	6	0	2.297977	1.828663	-0.228715
13	8	0	3.603161	1.891525	-0.596181
14	6	0	-2.264951	-0.218756	0.807566
15	6	0	-1.735612	1.180493	1.213243
16	6	0	-0.402806	1.539532	0.614849
17	6	0	0.237635	0.602284	-0.164504
18	6	0	-1.189171	-0.623336	-1.836369
19	6	0	-2.428380	0.212445	-1.577986
20	7	0	-3.115037	-0.231521	-0.380565
21	6	0	-4.382091	0.430711	-0.203147
22	1	0	0.974840	-2.023812	-1.829600
23	1	0	0.996655	-3.409627	0.000111
24	1	0	1.598573	-2.250146	2.430695
25	1	0	-0.639298	-1.289291	2.757871
26	1	0	-1.651688	-2.175032	0.277892
27	1	0	3.229572	-1.791979	-0.043933
28	1	0	-0.116208	3.474928	1.520087
29	1	0	2.182043	3.740953	0.719985
30	1	0	3.973056	2.719339	-0.281926
31	1	0	-2.891832	-0.581299	1.628300
32	1	0	-1.634472	1.214871	2.303008
33	1	0	-2.494976	1.930341	0.970548
34	1	0	-1.488958	-1.635077	-2.128684
35	1	0	-0.620074	-0.192703	-2.664475
36	1	0	-3.118671	0.114351	-2.420233
37	1	0	-2.152127	1.280472	-1.524347
38	1	0	-4.881285	0.044309	0.688128
39	1	0	-5.022401	0.224151	-1.063796
40	1	0	-4.310567	1.527757	-0.104415

E(RPBE1PBE) -938.88496750 a.u.

Table 19S. PBE0/cc-pVTZ Cartesian Coordinates of M_{equ}-3*syn*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.064331	-1.426305	-0.872349
2	6	0	1.441810	-2.405596	0.245044
3	6	0	1.026084	-1.928484	1.608723
4	6	0	-0.180514	-1.406622	1.795353
5	6	0	-1.087731	-1.219378	0.618664
6	6	0	-0.277205	-0.711071	-0.584842
7	8	0	2.814415	-2.699749	0.132284
8	6	0	1.547290	0.752358	-0.520123
9	8	0	2.062309	-0.394097	-1.042733
10	6	0	0.273747	2.753718	0.853305
11	6	0	1.589803	2.912207	0.434683
12	6	0	2.270493	1.896572	-0.235400
13	8	0	3.586050	2.029873	-0.539237
14	6	0	-2.243473	-0.222059	0.822598
15	6	0	-1.767674	1.215097	1.162720
16	6	0	-0.439166	1.588178	0.563453
17	6	0	0.218985	0.647112	-0.195081
18	6	0	-1.182268	-0.684609	-1.818769
19	6	0	-2.450050	0.111829	-1.573942
20	7	0	-3.106004	-0.317667	-0.353734
21	6	0	-4.396973	0.299648	-0.184547
22	1	0	1.046861	-1.971926	-1.816758
23	1	0	0.846372	-3.308034	0.020323
24	1	0	1.724982	-2.066706	2.427217
25	1	0	-0.509567	-1.097054	2.782359
26	1	0	-1.561914	-2.175906	0.362385
27	1	0	3.013763	-3.427104	0.724252
28	1	0	-0.186099	3.540114	1.441796
29	1	0	2.137251	3.815034	0.677345
30	1	0	3.889893	1.197909	-0.914523
31	1	0	-2.846504	-0.575589	1.664854
32	1	0	-1.686692	1.311871	2.250365
33	1	0	-2.551053	1.921334	0.870237
34	1	0	-1.446658	-1.716437	-2.073537
35	1	0	-0.639984	-0.261032	-2.668210
36	1	0	-3.145212	-0.040868	-2.403908
37	1	0	-2.214012	1.190420	-1.558135
38	1	0	-4.871669	-0.075995	0.724632
39	1	0	-5.036591	0.038695	-1.030807
40	1	0	-4.368271	1.401159	-0.123199

E(RPBE1PBE) -938.88124467 a.u.

Table 20S. PBE0/cc-pVTZ Cartesian Coordinates of M_{equ}-3*anti*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.049860	-1.440123	-0.879333
2	6	0	1.392324	-2.454049	0.218849
3	6	0	0.986409	-1.989732	1.590092
4	6	0	-0.209395	-1.444977	1.781406
5	6	0	-1.105360	-1.221647	0.602168
6	6	0	-0.277525	-0.705933	-0.585816
7	8	0	2.752063	-2.796080	0.104688
8	6	0	1.577552	0.722131	-0.503546
9	8	0	2.069399	-0.429363	-1.021017
10	6	0	0.297806	2.738834	0.879826
11	6	0	1.609604	2.890603	0.445530
12	6	0	2.292939	1.879742	-0.231588
13	8	0	3.598776	1.960704	-0.591445
14	6	0	-2.246055	-0.210597	0.815419
15	6	0	-1.745944	1.210393	1.181898
16	6	0	-0.413378	1.576385	0.586381
17	6	0	0.244644	0.636220	-0.175201
18	6	0	-1.174058	-0.639224	-1.825157
19	6	0	-2.431162	0.171732	-1.575051
20	7	0	-3.102488	-0.269607	-0.367506
21	6	0	-4.383642	0.366485	-0.195010
22	1	0	1.027015	-1.966919	-1.834579
23	1	0	0.764029	-3.329424	-0.024978
24	1	0	1.681184	-2.154454	2.407167
25	1	0	-0.536440	-1.142318	2.771288
26	1	0	-1.591761	-2.165909	0.324041
27	1	0	2.923738	-3.538456	0.686509
28	1	0	-0.156202	3.525801	1.471767
29	1	0	2.145804	3.805176	0.682962
30	1	0	3.949317	2.800706	-0.287892
31	1	0	-2.860773	-0.566974	1.648047
32	1	0	-1.658419	1.282530	2.271032
33	1	0	-2.517809	1.936367	0.907704
34	1	0	-1.452349	-1.661793	-2.101513
35	1	0	-0.618090	-0.208894	-2.662182
36	1	0	-3.122510	0.044732	-2.412589
37	1	0	-2.179530	1.246385	-1.538102
38	1	0	-4.870651	-0.017135	0.704285
39	1	0	-5.022199	0.132049	-1.049821
40	1	0	-4.336559	1.466231	-0.113627

E(RPBE1PBE) -938.87626272 a.u.

Table 21S. PBE0/cc-pVTZ Cartesian Coordinates of M_{ax}-3*syn*-6g^+

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.662684	1.562734	-0.851643
2	6	0	-0.888436	2.581199	0.280299
3	6	0	-0.530297	2.045704	1.639154
4	6	0	0.537643	1.277878	1.821535
5	6	0	1.364955	0.853420	0.648284
6	6	0	0.458143	0.545933	-0.553659
7	8	0	-2.186705	3.117269	0.220615
8	6	0	-1.662443	-0.451976	-0.526977
9	8	0	-1.882198	0.790121	-1.058946
10	6	0	-0.915899	-2.688372	0.868161
11	6	0	-2.219105	-2.546750	0.407494
12	6	0	-2.632052	-1.406132	-0.280397
13	8	0	-3.934775	-1.254446	-0.633388
14	6	0	2.241225	-0.404613	0.869705
15	6	0	1.423976	-1.667036	1.218143
16	6	0	0.052041	-1.717667	0.602601
17	6	0	-0.355432	-0.649564	-0.163607
18	6	0	1.334522	0.275608	-1.784592
19	6	0	2.339445	-0.839865	-1.505217
20	7	0	3.103986	-0.659039	-0.281381
21	6	0	4.200967	0.270733	-0.412652
22	1	0	-0.501418	2.097922	-1.787832
23	1	0	-0.211156	3.419713	0.069836
24	1	0	-1.149394	2.379379	2.464539
25	1	0	0.820086	0.947625	2.816804
26	1	0	2.047039	1.673600	0.387094
27	1	0	-2.773053	2.380691	0.019599
28	1	0	-0.663135	-3.559598	1.462318
29	1	0	-2.962478	-3.304829	0.622422
30	1	0	-4.022345	-0.436975	-1.130535
31	1	0	2.908287	-0.207018	1.714227
32	1	0	2.031843	-2.532533	0.940612
33	1	0	1.303337	-1.718308	2.304821
34	1	0	0.705789	0.000503	-2.636542
35	1	0	1.850883	1.203890	-2.053595
36	1	0	3.039220	-0.940267	-2.337824
37	1	0	1.799333	-1.788594	-1.435897
38	1	0	4.764627	0.301642	0.522560
39	1	0	3.917686	1.306205	-0.663657
40	1	0	4.876959	-0.080728	-1.195317

E(RPBE1PBE) -938.88355585 a.u.

Table 22S. PBE0/cc-pVTZ Cartesian Coordinates of M_{ax}-3*anti*-6g^+

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.634646	1.577147	-0.860065
2	6	0	-0.878040	2.588360	0.276972
3	6	0	-0.511217	2.055542	1.634748
4	6	0	0.556880	1.288090	1.818139
5	6	0	1.379824	0.850466	0.646453
6	6	0	0.471441	0.549282	-0.554762
7	8	0	-2.187250	3.095148	0.219605
8	6	0	-1.665205	-0.416924	-0.545213
9	8	0	-1.853143	0.818503	-1.089730
10	6	0	-0.940165	-2.662991	0.873107
11	6	0	-2.238832	-2.504598	0.403513
12	6	0	-2.643754	-1.364670	-0.292429
13	8	0	-3.921299	-1.127383	-0.685391
14	6	0	2.239795	-0.416708	0.874941
15	6	0	1.403177	-1.663650	1.229383
16	6	0	0.033527	-1.701492	0.607563
17	6	0	-0.362955	-0.633169	-0.165886
18	6	0	1.345484	0.260632	-1.783217
19	6	0	2.334439	-0.867128	-1.497559
20	7	0	3.100226	-0.690964	-0.273374
21	6	0	4.209577	0.223617	-0.408943
22	1	0	-0.454589	2.119312	-1.788898
23	1	0	-0.214461	3.439970	0.073448
24	1	0	-1.126503	2.393693	2.461279
25	1	0	0.843060	0.965489	2.815023
26	1	0	2.071845	1.661052	0.381795
27	1	0	-2.748575	2.362837	-0.060281
28	1	0	-0.700431	-3.534405	1.472188
29	1	0	-2.981276	-3.265751	0.625479
30	1	0	-4.475293	-1.852744	-0.389036
31	1	0	2.908652	-0.224422	1.719356
32	1	0	1.999036	-2.540737	0.962427
33	1	0	1.275879	-1.703062	2.315806
34	1	0	0.713861	-0.008648	-2.634790
35	1	0	1.875053	1.180498	-2.055173
36	1	0	3.034026	-0.981575	-2.328569
37	1	0	1.781543	-1.808250	-1.424314
38	1	0	4.772702	0.252715	0.526694
39	1	0	3.939796	1.261042	-0.666284
40	1	0	4.881632	-0.141255	-1.188887

E(RPBE1PBE) -938.88130750 a.u.

Table 23S. PBE0/cc-pVTZ Cartesian Coordinates of M_{ax}-3*syn*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.677608	1.546475	-0.851033
2	6	0	-0.838472	2.565774	0.282531
3	6	0	-0.579820	1.978743	1.642352
4	6	0	0.471226	1.191459	1.839949
5	6	0	1.333214	0.815541	0.674486
6	6	0	0.452099	0.530977	-0.555632
7	8	0	-2.098523	3.180099	0.150682
8	6	0	-1.668462	-0.460266	-0.547006
9	8	0	-1.886270	0.781750	-1.060577
10	6	0	-0.931910	-2.721276	0.816793
11	6	0	-2.240225	-2.557541	0.376034
12	6	0	-2.647921	-1.402675	-0.290169
13	8	0	-3.951974	-1.216513	-0.615634
14	6	0	2.221792	-0.436799	0.877310
15	6	0	1.414947	-1.721082	1.171300
16	6	0	0.042632	-1.756166	0.554902
17	6	0	-0.359788	-0.676745	-0.198879
18	6	0	1.354348	0.300966	-1.774838
19	6	0	2.367850	-0.808562	-1.504938
20	7	0	3.109041	-0.647033	-0.264112
21	6	0	4.191824	0.303624	-0.352688
22	1	0	-0.511817	2.089563	-1.782544
23	1	0	-0.040441	3.305009	0.090975
24	1	0	-1.250860	2.256334	2.448842
25	1	0	0.697248	0.796166	2.825413
26	1	0	2.006338	1.655018	0.451902
27	1	0	-2.138334	3.915980	0.764018
28	1	0	-0.682861	-3.600927	1.400168
29	1	0	-2.990744	-3.306670	0.597843
30	1	0	-4.043092	-0.332237	-0.983135
31	1	0	2.870638	-0.255572	1.739684
32	1	0	2.032148	-2.566803	0.855486
33	1	0	1.297596	-1.823045	2.254640
34	1	0	0.743781	0.039418	-2.643954
35	1	0	1.864361	1.241344	-2.013082
36	1	0	3.083101	-0.880958	-2.327336
37	1	0	1.838351	-1.764979	-1.466899
38	1	0	4.737419	0.321684	0.593567
39	1	0	3.895627	1.340064	-0.584692
40	1	0	4.888037	-0.017519	-1.130705

E(RPBE1PBE) -938.87755547 a.u.

Table 24S. PBE0/cc-pVTZ Cartesian Coordinates of M_{ax}-3*anti*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.641338	1.563877	-0.857474
2	6	0	-0.751005	2.609958	0.258130
3	6	0	-0.509780	2.034147	1.626074
4	6	0	0.515365	1.214737	1.830246
5	6	0	1.357270	0.797828	0.663848
6	6	0	0.457476	0.520838	-0.554062
7	8	0	-1.979209	3.281805	0.122523
8	6	0	-1.695510	-0.404925	-0.533771
9	8	0	-1.874525	0.838648	-1.041602
10	6	0	-0.987036	-2.690231	0.842246
11	6	0	-2.286386	-2.505487	0.383555
12	6	0	-2.682392	-1.350024	-0.291028
13	8	0	-3.959877	-1.098704	-0.673613
14	6	0	2.212627	-0.474490	0.877045
15	6	0	1.370253	-1.728544	1.194028
16	6	0	-0.002803	-1.739669	0.577976
17	6	0	-0.390550	-0.656627	-0.180147
18	6	0	1.342412	0.245437	-1.776907
19	6	0	2.327510	-0.887120	-1.499790
20	7	0	3.084450	-0.727643	-0.267643
21	6	0	4.190887	0.192991	-0.380509
22	1	0	-0.466333	2.085955	-1.799616
23	1	0	0.081516	3.306129	0.049994
24	1	0	-1.169705	2.343809	2.430037
25	1	0	0.733402	0.823708	2.819289
26	1	0	2.049861	1.615815	0.421847
27	1	0	-1.982486	4.025444	0.727611
28	1	0	-0.755598	-3.571512	1.430115
29	1	0	-3.038112	-3.259596	0.599270
30	1	0	-4.515645	-1.824913	-0.383115
31	1	0	2.873230	-0.301024	1.732183
32	1	0	1.962535	-2.598156	0.896018
33	1	0	1.248561	-1.804931	2.279100
34	1	0	0.716772	-0.011044	-2.636674
35	1	0	1.875735	1.167848	-2.033572
36	1	0	3.033154	-0.991930	-2.327063
37	1	0	1.772731	-1.828150	-1.442188
38	1	0	4.745008	0.211848	0.560832
39	1	0	3.919404	1.232743	-0.626806
40	1	0	4.871709	-0.158702	-1.158983

E(RPBE1PBE) -938.87259918 a.u.

Table 25S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M_{equ}-3*syn*-6*g*$^{+}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.040440	-1.468131	-0.889731
2	6	0	1.480028	-2.429694	0.239126
3	6	0	0.978249	-2.030496	1.604544
4	6	0	-0.238600	-1.520445	1.775708
5	6	0	-1.124248	-1.262673	0.587632
6	6	0	-0.288778	-0.729139	-0.596118
7	8	0	2.892011	-2.637339	0.207670
8	6	0	1.557180	0.737743	-0.515735
9	8	0	2.063113	-0.417804	-1.072676
10	6	0	0.286393	2.713992	0.917910
11	6	0	1.599458	2.887360	0.484894
12	6	0	2.274346	1.885882	-0.219247
13	8	0	3.603383	2.061874	-0.542053
14	6	0	-2.272992	-0.250306	0.815586
15	6	0	-1.763612	1.170886	1.203552
16	6	0	-0.426487	1.548096	0.608269
17	6	0	0.228965	0.619733	-0.174411
18	6	0	-1.190248	-0.658887	-1.843461
19	6	0	-2.460628	0.142956	-1.591816
20	7	0	-3.151192	-0.301381	-0.376532
21	6	0	-4.398843	0.430857	-0.200509
22	1	0	1.018059	-2.008184	-1.832109
23	1	0	1.041258	-3.400894	-0.007691
24	1	0	1.627382	-2.251555	2.443266
25	1	0	-0.611955	-1.297011	2.768683
26	1	0	-1.591631	-2.207218	0.294970
27	1	0	3.301877	-1.765363	0.125746
28	1	0	-0.171302	3.485791	1.523889
29	1	0	2.141858	3.789653	0.735851
30	1	0	3.919392	1.288239	-1.025635
31	1	0	-2.879549	-0.609057	1.647617
32	1	0	-1.669791	1.213947	2.291590
33	1	0	-2.526954	1.908776	0.951507
34	1	0	-1.451148	-1.681320	-2.127496
35	1	0	-0.642277	-0.216046	-2.677153
36	1	0	-3.142673	0.016500	-2.433829
37	1	0	-2.224010	1.216930	-1.549275
38	1	0	-4.890642	0.112338	0.719076
39	1	0	-5.066891	0.211582	-1.034513
40	1	0	-4.274455	1.522300	-0.159457

E(RB3LYP) -939.97621252 a.u.

Table 26S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M_{equ}-3*anti*-6*g*$^{+}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.020375	-1.485798	-0.894690
2	6	0	1.454889	-2.450459	0.234128
3	6	0	0.957394	-2.048229	1.600178
4	6	0	-0.254299	-1.526708	1.773328
5	6	0	-1.138470	-1.256830	0.586862
6	6	0	-0.298757	-0.731594	-0.597323
7	8	0	2.866098	-2.664827	0.201327
8	6	0	1.565232	0.713045	-0.523387
9	8	0	2.053649	-0.448732	-1.082646
10	6	0	0.318558	2.702353	0.919719
11	6	0	1.632144	2.861791	0.480500
12	6	0	2.294200	1.855348	-0.229760
13	8	0	3.617308	1.926700	-0.606280
14	6	0	-2.274437	-0.231375	0.818156
15	6	0	-1.746849	1.182652	1.207740
16	6	0	-0.406489	1.545220	0.610215
17	6	0	0.237424	0.610438	-0.175919
18	6	0	-1.201377	-0.647916	-1.843220
19	6	0	-2.460380	0.170186	-1.587848
20	7	0	-3.154443	-0.269657	-0.373036
21	6	0	-4.394027	0.475258	-0.193221
22	1	0	0.987597	-2.027569	-1.835846
23	1	0	1.010351	-3.419390	-0.011249
24	1	0	1.604671	-2.277228	2.438245
25	1	0	-0.624599	-1.301971	2.767172
26	1	0	-1.618114	-2.195073	0.293439
27	1	0	3.278060	-1.795809	0.098761
28	1	0	-0.127743	3.477820	1.529520
29	1	0	2.183238	3.760440	0.731291
30	1	0	3.988520	2.760057	-0.290037
31	1	0	-2.884639	-0.584139	1.650107
32	1	0	-1.650385	1.222259	2.295646
33	1	0	-2.501666	1.930327	0.958653
34	1	0	-1.476625	-1.666372	-2.128029
35	1	0	-0.648745	-0.211571	-2.677270
36	1	0	-3.145378	0.055702	-2.429168
37	1	0	-2.209117	1.240663	-1.541923
38	1	0	-4.888825	0.157746	0.725098
39	1	0	-5.064882	0.267199	-1.027828
40	1	0	-4.257847	1.565083	-0.147277

E(RB3LYP) -939.97592590 a.u.

Table 27S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M_{equ}-3*syn*-6*g*$^-$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.069722	-1.440773	-0.883064
2	6	0	1.473196	-2.429462	0.238345
3	6	0	1.002117	-2.015653	1.604678
4	6	0	-0.210347	-1.497753	1.781236
5	6	0	-1.101386	-1.256499	0.593905
6	6	0	-0.272202	-0.717709	-0.593603
7	8	0	2.880423	-2.663346	0.285346
8	6	0	1.558095	0.767551	-0.509135
9	8	0	2.080390	-0.382829	-1.054844
10	6	0	0.255449	2.740380	0.903299
11	6	0	1.568656	2.926136	0.475382
12	6	0	2.258692	1.927817	-0.218171
13	8	0	3.587128	2.117549	-0.538204
14	6	0	-2.263629	-0.259102	0.816406
15	6	0	-1.775532	1.172957	1.192040
16	6	0	-0.441434	1.563495	0.598370
17	6	0	0.228249	0.638721	-0.176399
18	6	0	-1.175159	-0.665462	-1.840295
19	6	0	-2.459334	0.116053	-1.592736
20	7	0	-3.142625	-0.332022	-0.374441
21	6	0	-4.401234	0.381807	-0.201518
22	1	0	1.054611	-1.972405	-1.831497
23	1	0	0.962981	-3.366923	-0.019695
24	1	0	1.663688	-2.224082	2.436469
25	1	0	-0.571265	-1.254347	2.773700
26	1	0	-1.555430	-2.209080	0.305950
27	1	0	3.149861	-3.055794	-0.553805
28	1	0	-0.214104	3.510264	1.502599
29	1	0	2.099173	3.836517	0.722665
30	1	0	3.923051	1.327240	-0.979752
31	1	0	-2.863735	-0.619886	1.652215
32	1	0	-1.686736	1.228473	2.279929
33	1	0	-2.548737	1.896889	0.929839
34	1	0	-1.419175	-1.692838	-2.121619
35	1	0	-0.634584	-0.216241	-2.675479
36	1	0	-3.138945	-0.027367	-2.434030
37	1	0	-2.241659	1.194247	-1.556724
38	1	0	-4.887778	0.060500	0.719912
39	1	0	-5.066034	0.147701	-1.034113
40	1	0	-4.293849	1.475278	-0.166306

E(RB3LYP) -939.97429688 a.u.

Table 28S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M_{equ}-3*anti*-6*g*⁻

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.051316	-1.457613	-0.889397
2	6	0	1.446636	-2.453322	0.229550
3	6	0	0.977416	-2.041932	1.597175
4	6	0	-0.229789	-1.512554	1.775404
5	6	0	-1.116919	-1.253984	0.588870
6	6	0	-0.280711	-0.719741	-0.595344
7	8	0	2.852159	-2.697406	0.278046
8	6	0	1.567885	0.743189	-0.512693
9	8	0	2.073196	-0.412506	-1.062765
10	6	0	0.287714	2.725243	0.915184
11	6	0	1.600108	2.900299	0.478033
12	6	0	2.277836	1.899978	-0.225820
13	8	0	3.600098	1.991157	-0.603519
14	6	0	-2.266147	-0.242967	0.816529
15	6	0	-1.758164	1.179306	1.201751
16	6	0	-0.420389	1.557162	0.607628
17	6	0	0.238466	0.628331	-0.173139
18	6	0	-1.182739	-0.648771	-1.842066
19	6	0	-2.455093	0.150015	-1.590408
20	7	0	-3.144889	-0.296502	-0.375391
21	6	0	-4.394209	0.432774	-0.199156
22	1	0	1.026565	-1.988440	-1.838158
23	1	0	0.930311	-3.386487	-0.031989
24	1	0	1.635224	-2.262572	2.428844
25	1	0	-0.589448	-1.271960	2.769027
26	1	0	-1.583324	-2.199085	0.295834
27	1	0	3.122411	-3.077615	-0.566451
28	1	0	-0.170567	3.496933	1.520858
29	1	0	2.137904	3.808118	0.724920
30	1	0	3.957095	2.833184	-0.294162
31	1	0	-2.872235	-0.601001	1.649248
32	1	0	-1.666124	1.224859	2.289824
33	1	0	-2.521982	1.915807	0.947000
34	1	0	-1.441794	-1.671195	-2.127990
35	1	0	-0.635360	-0.203791	-2.675080
36	1	0	-3.136679	0.022373	-2.432657
37	1	0	-2.221215	1.224536	-1.547119
38	1	0	-4.885630	0.112543	0.720052
39	1	0	-5.061485	0.212384	-1.033503
40	1	0	-4.272371	1.524482	-0.157463

E(RB3LYP) -939.97383009 a.u.

Table 29S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M_{equ}-3*syn*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.070656	-1.435630	-0.893915
2	6	0	1.473221	-2.424459	0.216645
3	6	0	1.009046	-2.014703	1.592335
4	6	0	-0.204281	-1.501357	1.776843
5	6	0	-1.098056	-1.258820	0.591178
6	6	0	-0.271550	-0.715576	-0.596427
7	8	0	2.884028	-2.640028	0.141919
8	6	0	1.556336	0.772634	-0.509840
9	8	0	2.079925	-0.374851	-1.059969
10	6	0	0.253937	2.738290	0.911862
11	6	0	1.566364	2.927261	0.482890
12	6	0	2.256479	1.932197	-0.215147
13	8	0	3.584426	2.123883	-0.535755
14	6	0	-2.261431	-0.263583	0.818144
15	6	0	-1.774815	1.167856	1.197820
16	6	0	-0.442200	1.561894	0.603334
17	6	0	0.227302	0.640588	-0.175764
18	6	0	-1.176801	-0.661020	-1.841385
19	6	0	-2.461196	0.118447	-1.589484
20	7	0	-3.142208	-0.333576	-0.371454
21	6	0	-4.401057	0.378793	-0.194614
22	1	0	1.056147	-1.961237	-1.844944
23	1	0	0.956478	-3.357445	-0.043004
24	1	0	1.676279	-2.222265	2.420663
25	1	0	-0.563993	-1.260367	2.770552
26	1	0	-1.551207	-2.211145	0.301034
27	1	0	3.088810	-3.415185	0.677192
28	1	0	-0.215636	3.505336	1.514768
29	1	0	2.096219	3.837228	0.733091
30	1	0	3.919126	1.337346	-0.984944
31	1	0	-2.859688	-0.627949	1.653714
32	1	0	-1.684456	1.220062	2.285735
33	1	0	-2.549334	1.891610	0.939036
34	1	0	-1.420003	-1.687957	-2.125051
35	1	0	-0.638243	-0.208963	-2.676333
36	1	0	-3.141961	-0.023215	-2.430146
37	1	0	-2.244520	1.196788	-1.550908
38	1	0	-4.885586	0.055150	0.727047
39	1	0	-5.067263	0.146057	-1.026476
40	1	0	-4.294468	1.472288	-0.157240

E(RB3LYP) -939.97365367 a.u.

Table 30S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M_{equ}-3*anti*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.052836	-1.452171	-0.899745
2	6	0	1.446316	-2.448297	0.208338
3	6	0	0.985554	-2.039371	1.585367
4	6	0	-0.222377	-1.514163	1.771752
5	6	0	-1.112789	-1.255765	0.586961
6	6	0	-0.279674	-0.717512	-0.597945
7	8	0	2.855197	-2.676859	0.133931
8	6	0	1.566191	0.748963	-0.513632
9	8	0	2.073397	-0.404188	-1.066984
10	6	0	0.285381	2.724247	0.922082
11	6	0	1.597113	2.902550	0.484426
12	6	0	2.275392	1.905308	-0.223208
13	8	0	3.597295	1.998419	-0.601393
14	6	0	-2.263654	-0.247330	0.818589
15	6	0	-1.757760	1.174846	1.206628
16	6	0	-0.421621	1.556265	0.611361
17	6	0	0.237446	0.630720	-0.173086
18	6	0	-1.184324	-0.645532	-1.842713
19	6	0	-2.457240	0.150731	-1.587038
20	7	0	-3.144423	-0.299166	-0.371828
21	6	0	-4.394022	0.428751	-0.191962
22	1	0	1.028974	-1.976864	-1.851183
23	1	0	0.921438	-3.375935	-0.054070
24	1	0	1.649764	-2.258185	2.413259
25	1	0	-0.580129	-1.274488	2.766502
26	1	0	-1.577805	-2.201099	0.292517
27	1	0	3.051738	-3.456734	0.665403
28	1	0	-0.173374	3.493234	1.530821
29	1	0	2.134085	3.810084	0.734100
30	1	0	3.952900	2.841744	-0.293977
31	1	0	-2.867548	-0.608660	1.651463
32	1	0	-1.664121	1.218028	2.294655
33	1	0	-2.523197	1.910649	0.954779
34	1	0	-1.442111	-1.667871	-2.130152
35	1	0	-0.639367	-0.198034	-2.675954
36	1	0	-3.140052	0.023904	-2.428420
37	1	0	-2.224885	1.225544	-1.542010
38	1	0	-4.883175	0.106954	0.727893
39	1	0	-5.062909	0.208968	-1.025179
40	1	0	-4.272988	1.520510	-0.149131

E(RB3LYP) -939.97313006 a.u.

Table 31S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M_{ax}-3*syn*-6g^+

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.637610	1.577016	-0.861642
2	6	0	-0.854502	2.598007	0.279070
3	6	0	-0.492949	2.069013	1.644886
4	6	0	0.562741	1.279728	1.827145
5	6	0	1.381073	0.826971	0.650151
6	6	0	0.467986	0.533123	-0.561634
7	8	0	-2.172705	3.144269	0.229318
8	6	0	-1.680836	-0.443660	-0.543396
9	8	0	-1.880970	0.809658	-1.081343
10	6	0	-0.958360	-2.695151	0.863507
11	6	0	-2.266200	-2.534468	0.409414
12	6	0	-2.662997	-1.384829	-0.279617
13	8	0	-3.989535	-1.218537	-0.619289
14	6	0	2.244366	-0.447924	0.878815
15	6	0	1.399590	-1.704215	1.214949
16	6	0	0.022659	-1.733039	0.590857
17	6	0	-0.370802	-0.658104	-0.180519
18	6	0	1.358348	0.264807	-1.793223
19	6	0	2.372612	-0.851562	-1.522186
20	7	0	3.137794	-0.704915	-0.273082
21	6	0	4.211065	0.280618	-0.384305
22	1	0	-0.466756	2.110010	-1.792817
23	1	0	-0.189068	3.437639	0.058166
24	1	0	-1.087946	2.428346	2.476013
25	1	0	0.851629	0.961756	2.822779
26	1	0	2.067584	1.636935	0.387475
27	1	0	-2.780795	2.399404	0.130086
28	1	0	-0.714490	-3.566100	1.458793
29	1	0	-3.016877	-3.281000	0.633749
30	1	0	-4.096025	-0.382391	-1.091085
31	1	0	2.895452	-0.260612	1.732775
32	1	0	1.980133	-2.588407	0.946342
33	1	0	1.271161	-1.750898	2.299014
34	1	0	0.739945	-0.012435	-2.649877
35	1	0	1.869842	1.194950	-2.051966
36	1	0	3.079533	-0.919433	-2.348934
37	1	0	1.846524	-1.807033	-1.487056
38	1	0	4.761537	0.324553	0.555990
39	1	0	3.885822	1.300023	-0.627341
40	1	0	4.906815	-0.032009	-1.163647

E(RB3LYP) -939.97294990 a.u.

Table 32S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M_{ax}-3*anti*-6*g+*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.611571	1.589574	-0.866387
2	6	0	-0.818139	2.614733	0.272766
3	6	0	-0.467593	2.082254	1.640136
4	6	0	0.577283	1.279471	1.825816
5	6	0	1.391919	0.814364	0.650982
6	6	0	0.477468	0.530882	-0.562112
7	8	0	-2.129951	3.176163	0.218235
8	6	0	-1.686028	-0.414634	-0.548967
9	8	0	-1.864704	0.841470	-1.088740
10	6	0	-0.992447	-2.675539	0.864593
11	6	0	-2.297136	-2.498740	0.405666
12	6	0	-2.679888	-1.346106	-0.287763
13	8	0	-3.972901	-1.076803	-0.679470
14	6	0	2.238070	-0.470892	0.882995
15	6	0	1.376521	-1.716173	1.216826
16	6	0	-0.000438	-1.726546	0.591942
17	6	0	-0.380261	-0.647110	-0.181489
18	6	0	1.365909	0.246825	-1.791672
19	6	0	2.364820	-0.882196	-1.516095
20	7	0	3.130371	-0.740719	-0.266647
21	6	0	4.213625	0.233701	-0.380812
22	1	0	-0.429504	2.119911	-1.797086
23	1	0	-0.141206	3.445707	0.053822
24	1	0	-1.060037	2.450165	2.469350
25	1	0	0.859612	0.958585	2.822408
26	1	0	2.089219	1.615014	0.388144
27	1	0	-2.743424	2.439563	0.092228
28	1	0	-0.761867	-3.548248	1.462604
29	1	0	-3.055217	-3.239396	0.630348
30	1	0	-4.548645	-1.796854	-0.391975
31	1	0	2.889633	-0.291513	1.738304
32	1	0	1.946181	-2.606829	0.945859
33	1	0	1.247396	-1.763797	2.300707
34	1	0	0.744913	-0.024306	-2.648400
35	1	0	1.890354	1.169130	-2.052578
36	1	0	3.071758	-0.962748	-2.341738
37	1	0	1.826249	-1.830585	-1.478086
38	1	0	4.759585	0.280580	0.561978
39	1	0	3.899728	1.253946	-0.634658
40	1	0	4.910429	-0.093149	-1.153435

E(RB3LYP) -939.97273148 a.u.

Table 33S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M_{ax}-3*syn*-6*g*⁻

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.650825	1.566540	-0.856466
2	6	0	-0.816370	2.602595	0.281487
3	6	0	-0.496498	2.058117	1.645989
4	6	0	0.544900	1.251502	1.832222
5	6	0	1.369146	0.808931	0.655582
6	6	0	0.458575	0.521528	-0.561405
7	8	0	-2.119431	3.184746	0.310184
8	6	0	-1.691645	-0.450998	-0.540619
9	8	0	-1.892690	0.803448	-1.069475
10	6	0	-0.966327	-2.713854	0.849581
11	6	0	-2.275614	-2.548648	0.401023
12	6	0	-2.673165	-1.394385	-0.279497
13	8	0	-4.000865	-1.224165	-0.614451
14	6	0	2.234799	-0.464839	0.877504
15	6	0	1.391784	-1.725319	1.202997
16	6	0	0.014411	-1.750626	0.579451
17	6	0	-0.379842	-0.671798	-0.186232
18	6	0	1.352696	0.261798	-1.791792
19	6	0	2.369659	-0.853184	-1.525438
20	7	0	3.131902	-0.712016	-0.274045
21	6	0	4.201980	0.278026	-0.376517
22	1	0	-0.481581	2.094663	-1.791881
23	1	0	-0.080409	3.385350	0.054757
24	1	0	-1.104737	2.411347	2.469652
25	1	0	0.812474	0.910820	2.825851
26	1	0	2.052894	1.623825	0.400287
27	1	0	-2.252762	3.666923	-0.514613
28	1	0	-0.721548	-3.587749	1.440194
29	1	0	-3.026636	-3.295318	0.623948
30	1	0	-4.111888	-0.367491	-1.046766
31	1	0	2.883442	-0.282010	1.734336
32	1	0	1.973512	-2.606633	0.927821
33	1	0	1.263504	-1.781119	2.286642
34	1	0	0.736940	-0.012150	-2.651459
35	1	0	1.862332	1.194683	-2.044517
36	1	0	3.078459	-0.913789	-2.351188
37	1	0	1.846382	-1.810460	-1.497237
38	1	0	4.751229	0.316601	0.564730
39	1	0	3.873346	1.298110	-0.612019
40	1	0	4.899648	-0.026045	-1.157501

E(RB3LYP) -939.97101430 a.u.

Table 34S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M_{ax}-3*anti*-6*g*'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.622920	1.579342	-0.862342
2	6	0	-0.767743	2.625594	0.269762
3	6	0	-0.458452	2.083006	1.637405
4	6	0	0.567168	1.257415	1.828081
5	6	0	1.382699	0.794367	0.653401
6	6	0	0.466956	0.516712	-0.561705
7	8	0	-2.058954	3.233825	0.296256
8	6	0	-1.700753	-0.417921	-0.540776
9	8	0	-1.878096	0.839660	-1.071056
10	6	0	-1.007390	-2.690817	0.857796
11	6	0	-2.312507	-2.508813	0.401914
12	6	0	-2.694402	-1.352055	-0.284844
13	8	0	-3.988121	-1.081398	-0.675402
14	6	0	2.227171	-0.492187	0.880827
15	6	0	1.364075	-1.738174	1.208415
16	6	0	-0.014281	-1.742610	0.586278
17	6	0	-0.393542	-0.659399	-0.182239
18	6	0	1.355652	0.234188	-1.791239
19	6	0	2.354432	-0.895804	-1.519036
20	7	0	3.120183	-0.758210	-0.269341
21	6	0	4.202737	0.217459	-0.380008
22	1	0	-0.443095	2.099711	-1.800282
23	1	0	-0.016822	3.392613	0.038244
24	1	0	-1.060286	2.451788	2.458939
25	1	0	0.828005	0.916361	2.823383
26	1	0	2.079723	1.596322	0.393234
27	1	0	-2.184726	3.711637	-0.532246
28	1	0	-0.777459	-3.566284	1.452032
29	1	0	-3.071589	-3.249457	0.623489
30	1	0	-4.562870	-1.803934	-0.392399
31	1	0	2.878285	-0.317136	1.737406
32	1	0	1.932048	-2.628087	0.931561
33	1	0	1.236690	-1.792134	2.292206
34	1	0	0.734538	-0.034669	-2.648631
35	1	0	1.880647	1.156725	-2.050442
36	1	0	3.061271	-0.974061	-2.345027
37	1	0	1.815746	-1.844235	-1.483608
38	1	0	4.749241	0.260571	0.562668
39	1	0	3.888042	1.238598	-0.629145
40	1	0	4.899300	-0.105380	-1.154517

E(RB3LYP) -939.97062073 a.u.

Table 35S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M_{ax}-3*syn*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.649003	1.562929	-0.865399
2	6	0	-0.807199	2.601826	0.259928
3	6	0	-0.500678	2.059732	1.634494
4	6	0	0.538701	1.252224	1.829904
5	6	0	1.366465	0.807335	0.655728
6	6	0	0.458049	0.517679	-0.562592
7	8	0	-2.109469	3.182494	0.162244
8	6	0	-1.693199	-0.452884	-0.539665
9	8	0	-1.893964	0.800849	-1.069934
10	6	0	-0.970217	-2.713909	0.854104
11	6	0	-2.279508	-2.548056	0.405763
12	6	0	-2.675956	-1.394292	-0.276111
13	8	0	-4.003572	-1.222649	-0.610604
14	6	0	2.231675	-0.466503	0.880740
15	6	0	1.388303	-1.726565	1.206737
16	6	0	0.011498	-1.752227	0.582064
17	6	0	-0.381573	-0.674344	-0.185604
18	6	0	1.353847	0.255310	-1.791087
19	6	0	2.369537	-0.859675	-1.521235
20	7	0	3.130202	-0.716029	-0.269117
21	6	0	4.200879	0.273261	-0.372303
22	1	0	-0.481492	2.083370	-1.804646
23	1	0	-0.058128	3.371162	0.032375
24	1	0	-1.116487	2.412913	2.453355
25	1	0	0.800946	0.910084	2.824663
26	1	0	2.050803	1.621525	0.399794
27	1	0	-2.107952	3.993058	0.684143
28	1	0	-0.726261	-3.587038	1.446174
29	1	0	-3.031304	-3.293470	0.630253
30	1	0	-4.113620	-0.366441	-1.044137
31	1	0	2.879242	-0.282483	1.738124
32	1	0	1.970299	-2.608099	0.932787
33	1	0	1.258951	-1.781416	2.290294
34	1	0	0.739100	-0.019460	-2.651190
35	1	0	1.864440	1.187502	-2.044470
36	1	0	3.079331	-0.922567	-2.345935
37	1	0	1.845585	-1.816527	-1.491525
38	1	0	4.749783	0.312519	0.569129
39	1	0	3.873052	1.293267	-0.609180
40	1	0	4.898624	-0.032293	-1.152637

E(RB3LYP) -939.97034232 a.u.

Table 36S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M_{ax}-3*anti*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.619864	1.576380	-0.870147
2	6	0	-0.753705	2.624904	0.249667
3	6	0	-0.463672	2.081125	1.627128
4	6	0	0.558025	1.252471	1.827295
5	6	0	1.378887	0.789518	0.655306
6	6	0	0.466580	0.512089	-0.562928
7	8	0	-2.040213	3.238860	0.147222
8	6	0	-1.703214	-0.418275	-0.540332
9	8	0	-1.879726	0.839989	-1.068693
10	6	0	-1.013930	-2.692175	0.857972
11	6	0	-2.319189	-2.507285	0.403670
12	6	0	-2.699107	-1.349444	-0.282193
13	8	0	-3.992788	-1.074728	-0.670043
14	6	0	2.222662	-0.497360	0.884202
15	6	0	1.358770	-1.743667	1.208658
16	6	0	-0.018895	-1.746392	0.585066
17	6	0	-0.396037	-0.662767	-0.184060
18	6	0	1.358300	0.229006	-1.789980
19	6	0	2.355730	-0.901232	-1.515241
20	7	0	3.118565	-0.763336	-0.263792
21	6	0	4.201311	0.212465	-0.372069
22	1	0	-0.442292	2.089057	-1.812004
23	1	0	0.015343	3.373728	0.019982
24	1	0	-1.075243	2.448284	2.442980
25	1	0	0.810137	0.906109	2.823204
26	1	0	2.076496	1.591543	0.396958
27	1	0	-2.019513	4.049234	0.669057
28	1	0	-0.785368	-3.567800	1.452499
29	1	0	-3.079833	-3.245921	0.626552
30	1	0	-4.569198	-1.795594	-0.386191
31	1	0	2.871675	-0.322885	1.742492
32	1	0	1.926851	-2.633263	0.931048
33	1	0	1.229915	-1.799519	2.292159
34	1	0	0.739197	-0.039203	-2.649013
35	1	0	1.884381	1.151369	-2.047656
36	1	0	3.064420	-0.980078	-2.339571
37	1	0	1.816551	-1.849419	-1.480675
38	1	0	4.746878	0.254105	0.571226
39	1	0	3.886990	1.233945	-0.620147
40	1	0	4.898551	-0.109465	-1.146332

E(RB3LYP) -939.96990039 a.u.

Table 37S. MP2/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*syn*-6g^{+}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.070549	-1.468224	-0.878038
2	6	0	1.514122	-2.391948	0.268790
3	6	0	1.052167	-1.910281	1.618058
4	6	0	-0.186797	-1.434821	1.794170
5	6	0	-1.081222	-1.283720	0.597126
6	6	0	-0.263554	-0.748836	-0.589881
7	8	0	2.895100	-2.645508	0.205577
8	6	0	1.553749	0.723569	-0.514451
9	8	0	2.069837	-0.417052	-1.077639
10	6	0	0.262404	2.700566	0.916146
11	6	0	1.574088	2.880751	0.471664
12	6	0	2.264076	1.885673	-0.233095
13	8	0	3.563994	2.075161	-0.558707
14	6	0	-2.218158	-0.281582	0.855223
15	6	0	-1.754462	1.133591	1.228657
16	6	0	-0.439242	1.528622	0.608043
17	6	0	0.227780	0.597525	-0.167157
18	6	0	-1.137779	-0.659032	-1.843441
19	6	0	-2.351278	0.213420	-1.600230
20	7	0	-3.093673	-0.279278	-0.390880
21	6	0	-4.391304	0.431339	-0.214606
22	1	0	1.057894	-2.031140	-1.809764
23	1	0	1.028561	-3.356646	0.084056
24	1	0	1.731857	-2.043257	2.449358
25	1	0	-0.547797	-1.157312	2.777111
26	1	0	-1.536083	-2.253820	0.343443
27	1	0	3.325229	-1.797338	0.039959
28	1	0	-0.194163	3.470990	1.524133
29	1	0	2.111805	3.787174	0.713763
30	1	0	3.869169	1.322266	-1.079970
31	1	0	-2.871964	-0.665743	1.640452
32	1	0	-1.638525	1.140069	2.314993
33	1	0	-2.544850	1.859246	1.025635
34	1	0	-1.449857	-1.661576	-2.154246
35	1	0	-0.565376	-0.227466	-2.666099
36	1	0	-3.050960	0.196688	-2.434134
37	1	0	-2.068968	1.243990	-1.388687
38	1	0	-3.312709	-1.264748	-0.563633
39	1	0	-4.857418	0.094156	0.706488
40	1	0	-5.025737	0.200252	-1.065347
41	1	0	-4.206685	1.498679	-0.177045

E(MP2) -938.18991634 a.u.

Table 38S. MP2/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*anti*-6g^{+}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.045629	-1.488247	-0.883293
2	6	0	1.508569	-2.393107	0.272844
3	6	0	1.034602	-1.914126	1.619211
4	6	0	-0.206052	-1.442665	1.794164
5	6	0	-1.099260	-1.281509	0.597427
6	6	0	-0.278426	-0.755671	-0.590099
7	8	0	2.895958	-2.606583	0.214913
8	6	0	1.559728	0.691742	-0.533713
9	8	0	2.045050	-0.448393	-1.110836
10	6	0	0.292562	2.683783	0.917126
11	6	0	1.606405	2.844896	0.467051
12	6	0	2.285371	1.845363	-0.243961
13	8	0	3.581823	1.906080	-0.624987
14	6	0	-2.223117	-0.266190	0.858545
15	6	0	-1.738708	1.141239	1.233693
16	6	0	-0.420212	1.520863	0.609701
17	6	0	0.234317	0.584749	-0.171187
18	6	0	-1.152789	-0.652700	-1.842370
19	6	0	-2.354553	0.234870	-1.596436
20	7	0	-3.100627	-0.250349	-0.386113
21	6	0	-4.388965	0.475360	-0.205903
22	1	0	1.017327	-2.066097	-1.805489
23	1	0	1.045536	-3.371045	0.099033
24	1	0	1.710889	-2.049741	2.452947
25	1	0	-0.570719	-1.174029	2.778341
26	1	0	-1.566182	-2.245640	0.343328
27	1	0	3.296175	-1.764566	-0.041099
28	1	0	-0.150764	3.458864	1.528909
29	1	0	2.141665	3.752437	0.719045
30	1	0	3.963349	2.738493	-0.321886
31	1	0	-2.880913	-0.642240	1.644393
32	1	0	-1.619033	1.142643	2.319566
33	1	0	-2.519036	1.878829	1.034855
34	1	0	-1.478476	-1.650751	-2.153592
35	1	0	-0.574799	-0.228548	-2.665022
36	1	0	-3.056308	0.227910	-2.428760
37	1	0	-2.059502	1.261703	-1.384241
38	1	0	-3.331394	-1.232923	-0.560183
39	1	0	-4.858602	0.140297	0.714183
40	1	0	-5.027035	0.255927	-1.057010
41	1	0	-4.191058	1.540176	-0.164055

E(MP2) -938.18912862 a.u.

Table 39S. MP2/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*syn*-6*g*$^{-}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.016328	-1.449924	1.070932
2	6	0	-1.627892	-2.286899	-0.100973
3	6	0	-0.727985	-2.480929	-1.282901
4	6	0	0.558759	-2.132374	-1.360930
5	6	0	1.269876	-1.466216	-0.229101
6	6	0	0.304498	-0.756511	0.708652
7	8	0	-2.807163	-1.711139	-0.628195
8	6	0	-1.530402	0.652150	0.512239
9	8	0	-1.912638	-0.343002	1.387437
10	6	0	-0.412575	2.332837	-1.382710
11	6	0	-1.676419	2.590868	-0.843427
12	6	0	-2.276896	1.750956	0.105794
13	8	0	-3.524876	2.029363	0.549096
14	6	0	2.263953	-0.403886	-0.737226
15	6	0	1.624211	0.733832	-1.538369
16	6	0	0.329087	1.226897	-0.949832
17	6	0	-0.264224	0.438526	0.014586
18	6	0	1.072326	-0.295702	1.954269
19	6	0	2.163132	0.678925	1.558316
20	7	0	3.037297	0.088791	0.482374
21	6	0	4.158118	1.009408	0.142277
22	1	0	-0.949546	-2.048517	1.977959
23	1	0	-1.848243	-3.281939	0.302679
24	1	0	-1.202456	-2.970611	-2.123870
25	1	0	1.122778	-2.363866	-2.257585
26	1	0	1.850793	-2.220338	0.322562
27	1	0	-3.453404	-1.648880	0.084022
28	1	0	-0.027412	2.991506	-2.150433
29	1	0	-2.247549	3.442903	-1.186007
30	1	0	-3.783387	1.355355	1.189455
31	1	0	3.027062	-0.885203	-1.353158
32	1	0	1.425751	0.312473	-2.528597
33	1	0	2.341214	1.538769	-1.707531
34	1	0	1.496379	-1.157472	2.478966
35	1	0	0.398053	0.213482	2.644659
36	1	0	2.820770	0.931180	2.388863
37	1	0	1.743836	1.592466	1.140460
38	1	0	3.452888	-0.757347	0.881940
39	1	0	4.728730	0.586626	-0.679444
40	1	0	4.787711	1.122641	1.020034
41	1	0	3.744931	1.971714	-0.137873

E(MP2) -938.18815407 a.u.

Table 40S. MP2/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*anti*-6g^{-}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.983853	-1.474518	1.071947
2	6	0	-1.602207	-2.296262	-0.105929
3	6	0	-0.698193	-2.494848	-1.284201
4	6	0	0.583458	-2.128259	-1.367039
5	6	0	1.291034	-1.450253	-0.239522
6	6	0	0.322943	-0.759242	0.708408
7	8	0	-2.768643	-1.697359	-0.635372
8	6	0	-1.538112	0.619699	0.541340
9	8	0	-1.892756	-0.386666	1.407969
10	6	0	-0.458146	2.322605	-1.368351
11	6	0	-1.726276	2.552032	-0.822176
12	6	0	-2.310269	1.701053	0.128614
13	8	0	-3.556280	1.842797	0.636408
14	6	0	2.265300	-0.371539	-0.749250
15	6	0	1.601895	0.760919	-1.538058
16	6	0	0.303371	1.231750	-0.938095
17	6	0	-0.270749	0.433991	0.031252
18	6	0	1.092152	-0.296750	1.952410
19	6	0	2.167120	0.694797	1.555162
20	7	0	3.040836	0.124134	0.467915
21	6	0	4.146460	1.061764	0.125733
22	1	0	-0.901832	-2.086675	1.968364
23	1	0	-1.842373	-3.288802	0.293057
24	1	0	-1.166434	-2.993739	-2.123394
25	1	0	1.149318	-2.357282	-2.263309
26	1	0	1.887563	-2.196106	0.306832
27	1	0	-3.339480	-1.457298	0.105470
28	1	0	-0.090907	2.988845	-2.138263
29	1	0	-2.303082	3.398008	-1.176358
30	1	0	-3.983697	2.600799	0.220411
31	1	0	3.030751	-0.836824	-1.374534
32	1	0	1.401369	0.341355	-2.528539
33	1	0	2.304739	1.577964	-1.708675
34	1	0	1.531258	-1.156245	2.468244
35	1	0	0.415074	0.198124	2.650505
36	1	0	2.828189	0.950015	2.382083
37	1	0	1.733120	1.605947	1.147241
38	1	0	3.470377	-0.719226	0.858545
39	1	0	4.717422	0.651532	-0.702099
40	1	0	4.780359	1.179022	0.999852
41	1	0	3.718279	2.019844	-0.146325

E(MP2) -938.18791493 a.u.

Table 41S. MP2/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*syn*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.087904	-1.448827	-0.879528
2	6	0	1.523504	-2.359045	0.277610
3	6	0	1.089378	-1.845873	1.624072
4	6	0	-0.154168	-1.385501	1.807199
5	6	0	-1.062370	-1.275589	0.615644
6	6	0	-0.260748	-0.749458	-0.587352
7	8	0	2.914793	-2.544060	0.156908
8	6	0	1.540556	0.737129	-0.539619
9	8	0	2.053408	-0.390820	-1.115613
10	6	0	0.249744	2.713520	0.894966
11	6	0	1.564014	2.891145	0.455156
12	6	0	2.254811	1.894168	-0.246190
13	8	0	3.556171	2.070604	-0.566037
14	6	0	-2.210784	-0.283942	0.866029
15	6	0	-1.762555	1.142320	1.217680
16	6	0	-0.450514	1.539296	0.591615
17	6	0	0.216653	0.608826	-0.184318
18	6	0	-1.144077	-0.688883	-1.835435
19	6	0	-2.362505	0.177051	-1.595874
20	7	0	-3.092290	-0.308628	-0.375776
21	6	0	-4.397430	0.388159	-0.201390
22	1	0	1.069901	-2.034642	-1.797276
23	1	0	0.989098	-3.304851	0.101654
24	1	0	1.789316	-1.916802	2.446680
25	1	0	-0.499402	-1.070079	2.784159
26	1	0	-1.504846	-2.257247	0.385070
27	1	0	3.164393	-3.313162	0.679847
28	1	0	-0.207055	3.484836	1.501758
29	1	0	2.103063	3.795048	0.703673
30	1	0	3.885382	1.256795	-0.970062
31	1	0	-2.856828	-0.665345	1.659048
32	1	0	-1.651290	1.169281	2.304158
33	1	0	-2.560891	1.855011	0.999566
34	1	0	-1.450360	-1.698490	-2.129306
35	1	0	-0.579944	-0.265046	-2.667732
36	1	0	-3.068158	0.145229	-2.424297
37	1	0	-2.086040	1.211826	-1.397408
38	1	0	-3.300041	-1.298727	-0.535120
39	1	0	-4.854241	0.057923	0.726859
40	1	0	-5.033694	0.137994	-1.045340
41	1	0	-4.225793	1.458063	-0.179142

E(MP2) -938.18660330 a.u.

Table 42S. MP2/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*anti*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.081757	-1.453063	-0.884385
2	6	0	1.482155	-2.403540	0.252145
3	6	0	1.064226	-1.898929	1.607233
4	6	0	-0.169431	-1.414280	1.795971
5	6	0	-1.071542	-1.276157	0.602596
6	6	0	-0.257461	-0.741191	-0.587952
7	8	0	2.863060	-2.643345	0.128613
8	6	0	1.565728	0.721103	-0.520249
9	8	0	2.068830	-0.410296	-1.082588
10	6	0	0.259595	2.708097	0.915158
11	6	0	1.571371	2.885363	0.464632
12	6	0	2.268123	1.893827	-0.240537
13	8	0	3.560030	1.984165	-0.627290
14	6	0	-2.211567	-0.278089	0.859651
15	6	0	-1.750022	1.138482	1.229211
16	6	0	-0.434891	1.534517	0.608033
17	6	0	0.236776	0.605676	-0.167758
18	6	0	-1.132879	-0.651989	-1.839964
19	6	0	-2.346430	0.219197	-1.595757
20	7	0	-3.086659	-0.278759	-0.386861
21	6	0	-4.387467	0.424613	-0.209181
22	1	0	1.062305	-2.016193	-1.816488
23	1	0	0.907768	-3.322329	0.056507
24	1	0	1.765150	-1.992164	2.426690
25	1	0	-0.509661	-1.100399	2.775176
26	1	0	-1.521317	-2.250229	0.354113
27	1	0	3.081174	-3.430265	0.638756
28	1	0	-0.195831	3.478520	1.523944
29	1	0	2.092398	3.802867	0.710791
30	1	0	3.922041	2.825368	-0.325073
31	1	0	-2.865618	-0.661577	1.645094
32	1	0	-1.636400	1.148306	2.315751
33	1	0	-2.541752	1.861931	1.022907
34	1	0	-1.444932	-1.654588	-2.151364
35	1	0	-0.559175	-0.220674	-2.661811
36	1	0	-3.047536	0.203820	-2.428534
37	1	0	-2.064697	1.249281	-1.381187
38	1	0	-3.299923	-1.265092	-0.561614
39	1	0	-4.852940	0.082246	0.710334
40	1	0	-5.020119	0.193816	-1.061321
41	1	0	-4.207915	1.492659	-0.167604

E(MP2) -938.18304434 a.u.

Table 43S. MP2/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*syn*-6g^{+}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.675139	1.587204	-0.840319
2	6	0	-0.931962	2.554695	0.327657
3	6	0	-0.634459	1.941783	1.670113
4	6	0	0.460135	1.194389	1.858421
5	6	0	1.334635	0.886116	0.674840
6	6	0	0.450642	0.575871	-0.543325
7	8	0	-2.215618	3.120291	0.240119
8	6	0	-1.656654	-0.442370	-0.553365
9	8	0	-1.880117	0.797198	-1.099697
10	6	0	-0.900275	-2.687713	0.864166
11	6	0	-2.203618	-2.553131	0.380877
12	6	0	-2.623703	-1.413818	-0.317989
13	8	0	-3.921827	-1.291909	-0.680558
14	6	0	2.202064	-0.354132	0.930958
15	6	0	1.413285	-1.632001	1.262518
16	6	0	0.061213	-1.704313	0.601766
17	6	0	-0.348326	-0.631001	-0.169323
18	6	0	1.319790	0.317426	-1.777643
19	6	0	2.270142	-0.836909	-1.537387
20	7	0	3.082116	-0.614317	-0.285383
21	6	0	4.149266	0.410074	-0.475705
22	1	0	-0.506426	2.158535	-1.751594
23	1	0	-0.232919	3.386921	0.187766
24	1	0	-1.293909	2.198898	2.488440
25	1	0	0.718296	0.812103	2.838576
26	1	0	1.987284	1.743180	0.469931
27	1	0	-2.822512	2.398788	0.032959
28	1	0	-0.652161	-3.552869	1.465445
29	1	0	-2.942912	-3.314645	0.587945
30	1	0	-4.029352	-0.479958	-1.191322
31	1	0	2.909396	-0.152179	1.737315
32	1	0	1.272728	-1.647677	2.345394
33	1	0	2.034019	-2.508932	1.042478
34	1	0	1.857734	1.226099	-2.058301
35	1	0	0.686035	0.047458	-2.624376
36	1	0	2.977586	-0.977771	-2.352619
37	1	0	1.712949	-1.759533	-1.382051
38	1	0	3.557628	-1.497744	-0.089164
39	1	0	4.820896	0.062269	-1.255270
40	1	0	3.700524	1.350314	-0.769650
41	1	0	4.688591	0.529295	0.459306

E(MP2) -938.18843469 a.u.

Table 44S. MP2/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*anti*-6g^{+}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.654552	1.597693	-0.845027
2	6	0	-0.939182	2.550532	0.330393
3	6	0	-0.628086	1.938739	1.670631
4	6	0	0.471980	1.199408	1.859043
5	6	0	1.345724	0.885798	0.676169
6	6	0	0.462909	0.580869	-0.542986
7	8	0	-2.240371	3.073446	0.245219
8	6	0	-1.653908	-0.417430	-0.571887
9	8	0	-1.852846	0.814061	-1.130924
10	6	0	-0.915093	-2.668689	0.865191
11	6	0	-2.216614	-2.520965	0.376517
12	6	0	-2.629821	-1.381706	-0.328349
13	8	0	-3.894308	-1.140083	-0.743252
14	6	0	2.203225	-0.360176	0.935166
15	6	0	1.401885	-1.629520	1.267783
16	6	0	0.050768	-1.692389	0.603367
17	6	0	-0.349961	-0.618957	-0.173318
18	6	0	1.331188	0.313627	-1.775826
19	6	0	2.271831	-0.847870	-1.532791
20	7	0	3.083145	-0.629838	-0.279330
21	6	0	4.158005	0.386370	-0.469365
22	1	0	-0.469962	2.179720	-1.746413
23	1	0	-0.262628	3.403135	0.201763
24	1	0	-1.285645	2.194780	2.490925
25	1	0	0.736078	0.825750	2.841062
26	1	0	2.004713	1.737928	0.471549
27	1	0	-2.811518	2.350736	-0.048359
28	1	0	-0.677183	-3.534150	1.470070
29	1	0	-2.950639	-3.287597	0.593528
30	1	0	-4.463319	-1.869230	-0.469471
31	1	0	2.911059	-0.163644	1.742477
32	1	0	1.258100	-1.640180	2.350220
33	1	0	2.014372	-2.513122	1.051691
34	1	0	1.876865	1.217517	-2.056801
35	1	0	0.695489	0.048738	-2.622766
36	1	0	2.979961	-0.995712	-2.346223
37	1	0	1.707350	-1.765996	-1.377260
38	1	0	3.551833	-1.516350	-0.080896
39	1	0	4.828485	0.032535	-1.247207
40	1	0	3.716477	1.329269	-0.765588
41	1	0	4.696504	0.503336	0.466407

E(MP2) -938.18765105 a.u.

Table 45S. MP2/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*syn*-6*g*$^{-}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.656546	1.537401	-1.037604
2	6	0	-1.163722	2.457541	0.123007
3	6	0	-0.357589	2.399092	1.384495
4	6	0	0.829139	1.805070	1.532063
5	6	0	1.491945	1.078869	0.405588
6	6	0	0.478886	0.591607	-0.619372
7	8	0	-2.488583	2.160118	0.516538
8	6	0	-1.607125	-0.430741	-0.575381
9	8	0	-1.729586	0.636195	-1.440573
10	6	0	-0.962445	-2.337412	1.325264
11	6	0	-2.218781	-2.324086	0.712552
12	6	0	-2.581755	-1.362790	-0.242151
13	8	0	-3.831673	-1.375377	-0.760051
14	6	0	2.235851	-0.164934	0.922060
15	6	0	1.346145	-1.195348	1.630509
16	6	0	0.009665	-1.395666	0.966586
17	6	0	-0.355140	-0.485312	-0.004034
18	6	0	1.233147	0.025063	-1.829809
19	6	0	2.069309	-1.166792	-1.406829
20	7	0	2.972196	-0.822592	-0.242279
21	6	0	4.168258	-0.046740	-0.681889
22	1	0	-0.417140	2.128000	-1.920506
23	1	0	-1.107072	3.488676	-0.245576
24	1	0	-0.803663	2.924972	2.219120
25	1	0	1.348038	1.871105	2.481762
26	1	0	2.222063	1.747547	-0.064506
27	1	0	-3.059097	2.256110	-0.254125
28	1	0	-0.762024	-3.075881	2.090788
29	1	0	-2.968463	-3.049022	0.998794
30	1	0	-3.915501	-0.643441	-1.383305
31	1	0	3.032141	0.139030	1.604203
32	1	0	1.191445	-0.821727	2.646387
33	1	0	1.897799	-2.135034	1.746947
34	1	0	1.844415	0.801054	-2.296858
35	1	0	0.522672	-0.325834	-2.580401
36	1	0	2.715500	-1.533336	-2.202522
37	1	0	1.424914	-1.974495	-1.065122
38	1	0	3.318324	-1.711970	0.124323
39	1	0	4.726519	-0.651079	-1.390852
40	1	0	3.845765	0.871647	-1.156601
41	1	0	4.781284	0.175404	0.186357

E(MP2) -938.18638501 a.u.

Table 46S. MP2/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*anti*-6*g*$^{-}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.626388	1.548035	-1.046862
2	6	0	-1.146954	2.458407	0.114150
3	6	0	-0.322469	2.428540	1.365046
4	6	0	0.856912	1.820768	1.517283
5	6	0	1.508163	1.067383	0.401673
6	6	0	0.493053	0.588694	-0.624112
7	8	0	-2.455598	2.118444	0.527348
8	6	0	-1.608034	-0.403343	-0.600489
9	8	0	-1.704872	0.662184	-1.463790
10	6	0	-1.001035	-2.305492	1.329434
11	6	0	-2.254769	-2.273099	0.708469
12	6	0	-2.601502	-1.314192	-0.255762
13	8	0	-3.818007	-1.201688	-0.836709
14	6	0	2.229605	-0.183662	0.930023
15	6	0	1.319315	-1.195307	1.638721
16	6	0	-0.015185	-1.382834	0.966368
17	6	0	-0.361480	-0.476583	-0.015745
18	6	0	1.245359	0.009184	-1.829575
19	6	0	2.062975	-1.192403	-1.397782
20	7	0	2.962669	-0.858064	-0.227272
21	6	0	4.173642	-0.102644	-0.661942
22	1	0	-0.372491	2.144647	-1.921337
23	1	0	-1.131700	3.488205	-0.262355
24	1	0	-0.754722	2.974787	2.193992
25	1	0	1.383711	1.900086	2.461776
26	1	0	2.251277	1.718083	-0.073252
27	1	0	-2.992671	1.992079	-0.265049
28	1	0	-0.818125	-3.040485	2.102586
29	1	0	-3.007241	-2.991278	1.011460
30	1	0	-4.411422	-1.862398	-0.460367
31	1	0	3.026627	0.110529	1.615597
32	1	0	1.161095	-0.809579	2.649476
33	1	0	1.855728	-2.141974	1.768261
34	1	0	1.869563	0.775629	-2.295130
35	1	0	0.533897	-0.333712	-2.582994
36	1	0	2.710013	-1.569773	-2.187722
37	1	0	1.405854	-1.990953	-1.058917
38	1	0	3.292674	-1.751276	0.144672
39	1	0	4.728475	-0.719720	-1.362568
40	1	0	3.868415	0.817191	-1.145169
41	1	0	4.782947	0.116131	0.209766

E(MP2) -938.18613056 a.u.

Table 47S. MP2/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*syn*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.695315	1.572143	-0.844668
2	6	0	-0.946255	2.525374	0.332876
3	6	0	-0.679824	1.889986	1.670928
4	6	0	0.422686	1.156172	1.865923
5	6	0	1.317278	0.882341	0.688503
6	6	0	0.448929	0.576467	-0.543229
7	8	0	-2.254415	3.027174	0.187017
8	6	0	-1.645896	-0.457261	-0.576883
9	8	0	-1.868302	0.768754	-1.137829
10	6	0	-0.890116	-2.701029	0.846059
11	6	0	-2.196035	-2.562914	0.368918
12	6	0	-2.616492	-1.422023	-0.327194
13	8	0	-3.913461	-1.286293	-0.682288
14	6	0	2.197481	-0.350929	0.937673
15	6	0	1.421010	-1.641566	1.250616
16	6	0	0.070881	-1.716237	0.586215
17	6	0	-0.338981	-0.643839	-0.186157
18	6	0	1.330865	0.341934	-1.772425
19	6	0	2.287474	-0.807557	-1.535997
20	7	0	3.088009	-0.589316	-0.275595
21	6	0	4.145363	0.447593	-0.447823
22	1	0	-0.517348	2.163128	-1.741863
23	1	0	-0.205139	3.328255	0.200300
24	1	0	-1.370798	2.092811	2.479036
25	1	0	0.658903	0.742563	2.838664
26	1	0	1.960211	1.751682	0.504678
27	1	0	-2.339666	3.814066	0.735516
28	1	0	-0.641835	-3.566677	1.446673
29	1	0	-2.936579	-3.320947	0.584183
30	1	0	-4.033481	-0.411604	-1.075322
31	1	0	2.898148	-0.149593	1.750068
32	1	0	1.281637	-1.676148	2.333181
33	1	0	2.052042	-2.507888	1.017041
34	1	0	1.863876	1.257756	-2.039240
35	1	0	0.705216	0.076315	-2.626524
36	1	0	3.002693	-0.937155	-2.346316
37	1	0	1.734635	-1.734642	-1.391875
38	1	0	3.570697	-1.469961	-0.084622
39	1	0	4.824205	0.116891	-1.228606
40	1	0	3.688343	1.386803	-0.732098
41	1	0	4.679280	0.560540	0.491074

E(MP2) -938.18514099 a.u.

Table 48S. MP2/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*anti*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.670246	1.581717	-0.850925
2	6	0	-0.868570	2.570043	0.306851
3	6	0	-0.624833	1.945411	1.654534
4	6	0	0.454017	1.178715	1.856604
5	6	0	1.334805	0.867759	0.677853
6	6	0	0.450334	0.564063	-0.542777
7	8	0	-2.147814	3.136369	0.157487
8	6	0	-1.671512	-0.418502	-0.558655
9	8	0	-1.869846	0.809707	-1.107757
10	6	0	-0.930154	-2.682083	0.870087
11	6	0	-2.230771	-2.530928	0.379466
12	6	0	-2.644576	-1.390647	-0.323473
13	8	0	-3.907170	-1.159892	-0.746726
14	6	0	2.191224	-0.379083	0.936239
15	6	0	1.389118	-1.648197	1.267808
16	6	0	0.036189	-1.707306	0.606529
17	6	0	-0.365508	-0.632262	-0.168233
18	6	0	1.316877	0.292345	-1.775367
19	6	0	2.254142	-0.871156	-1.531128
20	7	0	3.068343	-0.650476	-0.279827
21	6	0	4.142537	0.364885	-0.474308
22	1	0	-0.487800	2.147871	-1.763394
23	1	0	-0.085742	3.329558	0.154960
24	1	0	-1.310270	2.178656	2.459069
25	1	0	0.679806	0.766532	2.832418
26	1	0	1.993337	1.721396	0.476186
27	1	0	-2.191091	3.934031	0.695047
28	1	0	-0.693550	-3.548224	1.474523
29	1	0	-2.965419	-3.298292	0.592247
30	1	0	-4.471179	-1.892509	-0.472468
31	1	0	2.901362	-0.184149	1.742004
32	1	0	1.249785	-1.662768	2.350836
33	1	0	2.001404	-2.531093	1.047235
34	1	0	1.864472	1.194000	-2.060378
35	1	0	0.678075	0.027212	-2.619836
36	1	0	2.960730	-1.024521	-2.344907
37	1	0	1.686292	-1.786307	-1.370385
38	1	0	3.536757	-1.536825	-0.080214
39	1	0	4.811024	0.009913	-1.253369
40	1	0	3.700186	1.307174	-0.771225
41	1	0	4.683622	0.483560	0.459777

E(MP2) -938.18157332 a.u.

Table 49S. B3LYP/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*syn*-6g^{+}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.090770	-1.443550	-0.896544
2	6	0	1.520409	-2.443861	0.205662
3	6	0	0.998464	-2.087008	1.577881
4	6	0	-0.217466	-1.586007	1.764350
5	6	0	-1.090203	-1.287319	0.572800
6	6	0	-0.250918	-0.719277	-0.594167
7	8	0	2.908661	-2.673598	0.177687
8	6	0	1.572791	0.759744	-0.488462
9	8	0	2.095361	-0.385660	-1.038802
10	6	0	0.275206	2.726590	0.936883
11	6	0	1.582153	2.914500	0.498767
12	6	0	2.276381	1.921877	-0.202736
13	8	0	3.577584	2.116264	-0.525468
14	6	0	-2.214590	-0.265107	0.864773
15	6	0	-1.737887	1.149196	1.249517
16	6	0	-0.419034	1.552499	0.626836
17	6	0	0.247592	0.628512	-0.150456
18	6	0	-1.135898	-0.625437	-1.855145
19	6	0	-2.383248	0.212079	-1.624584
20	7	0	-3.119475	-0.255915	-0.386178
21	6	0	-4.422234	0.456820	-0.201755
22	1	0	1.082926	-1.957584	-1.854934
23	1	0	1.067502	-3.404499	-0.067225
24	1	0	1.642553	-2.333264	2.411881
25	1	0	-0.600513	-1.402834	2.760723
26	1	0	-1.579583	-2.221700	0.258036
27	1	0	3.355207	-1.822626	0.095963
28	1	0	-0.187389	3.493751	1.543897
29	1	0	2.114247	3.823522	0.742258
30	1	0	3.909674	1.372731	-1.041422
31	1	0	-2.864245	-0.649855	1.650443
32	1	0	-1.619980	1.143465	2.335795
33	1	0	-2.526658	1.881135	1.064199
34	1	0	-1.415887	-1.631907	-2.181249
35	1	0	-0.579618	-0.172361	-2.676107
36	1	0	-3.082033	0.141301	-2.455998
37	1	0	-2.140000	1.259350	-1.461948
38	1	0	-3.347385	-1.239055	-0.541958
39	1	0	-4.895524	0.103370	0.710254
40	1	0	-5.057328	0.241909	-1.057195
41	1	0	-4.246224	1.525023	-0.141223

E(RB3LYP) -940.33757425 a.u.

Table 50S. B3LYP/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*anti*-6g^{+}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.064978	-1.464424	-0.901759
2	6	0	1.507387	-2.450890	0.209188
3	6	0	0.980851	-2.090283	1.578950
4	6	0	-0.234230	-1.586964	1.765276
5	6	0	-1.106661	-1.281291	0.575119
6	6	0	-0.265447	-0.724782	-0.594991
7	8	0	2.899487	-2.652934	0.185995
8	6	0	1.581233	0.726853	-0.506165
9	8	0	2.074183	-0.420074	-1.065815
10	6	0	0.307002	2.713014	0.932140
11	6	0	1.617225	2.880556	0.489755
12	6	0	2.300594	1.881817	-0.214122
13	8	0	3.600382	1.951081	-0.586318
14	6	0	-2.217698	-0.246304	0.869393
15	6	0	-1.721112	1.161943	1.250725
16	6	0	-0.398802	1.548542	0.623958
17	6	0	0.255739	0.617160	-0.157156
18	6	0	-1.152746	-0.619743	-1.853413
19	6	0	-2.388798	0.233013	-1.619480
20	7	0	-3.126512	-0.226922	-0.378776
21	6	0	-4.420823	0.499387	-0.190129
22	1	0	1.042122	-1.991158	-1.853093
23	1	0	1.066677	-3.420823	-0.052118
24	1	0	1.623874	-2.337368	2.413568
25	1	0	-0.617882	-1.405405	2.761839
26	1	0	-1.607656	-2.210234	0.262634
27	1	0	3.325710	-1.806367	0.000642
28	1	0	-0.142496	3.486200	1.541215
29	1	0	2.147348	3.790888	0.742009
30	1	0	3.990310	2.783167	-0.296957
31	1	0	-2.869874	-0.621261	1.657704
32	1	0	-1.599904	1.155229	2.336530
33	1	0	-2.500374	1.904333	1.066737
34	1	0	-1.446443	-1.622800	-2.177873
35	1	0	-0.592446	-0.174852	-2.676096
36	1	0	-3.091173	0.170955	-2.448549
37	1	0	-2.132733	1.277243	-1.457109
38	1	0	-3.364815	-1.207683	-0.534084
39	1	0	-4.895747	0.149756	0.722493
40	1	0	-5.060391	0.292885	-1.044304
41	1	0	-4.233078	1.565534	-0.128401

E(RB3LYP) -940.33674806 a.u.

Table 51S. B3LYP/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*syn*-6*g*$^{-}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.084115	-1.426751	0.961457
2	6	0	-1.608716	-2.379837	-0.166931
3	6	0	-0.937648	-2.206631	-1.500625
4	6	0	0.310001	-1.784818	-1.657141
5	6	0	1.137702	-1.366283	-0.474003
6	6	0	0.266036	-0.733176	0.626909
7	8	0	-2.997348	-2.258482	-0.386415
8	6	0	-1.545534	0.750416	0.510571
9	8	0	-2.017270	-0.336724	1.205214
10	6	0	-0.301461	2.615483	-1.093918
11	6	0	-1.592664	2.831363	-0.622071
12	6	0	-2.260098	1.891134	0.173128
13	8	0	-3.542132	2.115851	0.543824
14	6	0	2.232117	-0.333762	-0.837219
15	6	0	1.710980	1.018146	-1.359191
16	6	0	0.400985	1.457476	-0.743195
17	6	0	-0.243755	0.582575	0.103909
18	6	0	1.128762	-0.534923	1.892671
19	6	0	2.345795	0.333351	1.619362
20	7	0	3.117392	-0.182115	0.420696
21	6	0	4.380445	0.587564	0.195086
22	1	0	-1.039610	-1.978594	1.898781
23	1	0	-1.371103	-3.399401	0.172755
24	1	0	-1.530233	-2.519281	-2.350505
25	1	0	0.757501	-1.752967	-2.643110
26	1	0	1.653717	-2.254331	-0.079032
27	1	0	-3.477786	-2.427674	0.430263
28	1	0	0.139652	3.345578	-1.759859
29	1	0	-2.134033	3.723111	-0.905760
30	1	0	-3.888892	1.348060	1.012955
31	1	0	2.908958	-0.763471	-1.575473
32	1	0	1.566681	0.886852	-2.434842
33	1	0	2.485879	1.782892	-1.278522
34	1	0	1.440242	-1.508231	2.284188
35	1	0	0.546048	-0.050442	2.676547
36	1	0	3.037545	0.345307	2.459554
37	1	0	2.062227	1.356172	1.384544
38	1	0	3.397071	-1.137178	0.649509
39	1	0	4.883551	0.197321	-0.685479
40	1	0	5.016982	0.471117	1.068382
41	1	0	4.144855	1.636843	0.056445

E(RB3LYP) -940.33530879 a.u.

Table 52S. B3LYP/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*syn*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.111031	-1.420637	-0.902101
2	6	0	1.544950	-2.408494	0.208369
3	6	0	1.031202	-2.042545	1.581313
4	6	0	-0.193519	-1.565251	1.769824
5	6	0	-1.075399	-1.292315	0.579083
6	6	0	-0.246852	-0.721061	-0.594275
7	8	0	2.949805	-2.533246	0.145678
8	6	0	1.556161	0.777323	-0.508082
9	8	0	2.076508	-0.349216	-1.083075
10	6	0	0.254626	2.730956	0.934299
11	6	0	1.561865	2.924357	0.496878
12	6	0	2.259006	1.937109	-0.209118
13	8	0	3.559234	2.127634	-0.531211
14	6	0	-2.210275	-0.280619	0.870115
15	6	0	-1.746971	1.138965	1.252508
16	6	0	-0.433861	1.553211	0.625222
17	6	0	0.235195	0.635926	-0.158001
18	6	0	-1.136203	-0.645373	-1.852482
19	6	0	-2.387345	0.185977	-1.622528
20	7	0	-3.116916	-0.282675	-0.379799
21	6	0	-4.424311	0.421044	-0.195074
22	1	0	1.098009	-1.956026	-1.849037
23	1	0	1.070095	-3.363048	-0.066295
24	1	0	1.688165	-2.240911	2.418777
25	1	0	-0.568803	-1.365629	2.765830
26	1	0	-1.554502	-2.235439	0.274503
27	1	0	3.217063	-3.359679	0.559331
28	1	0	-0.209701	3.494136	1.545086
29	1	0	2.091891	3.832418	0.748456
30	1	0	3.915408	1.331607	-0.944437
31	1	0	-2.855832	-0.670588	1.656713
32	1	0	-1.628715	1.136180	2.338839
33	1	0	-2.544297	1.861695	1.066967
34	1	0	-1.411330	-1.656011	-2.170395
35	1	0	-0.585180	-0.194687	-2.678256
36	1	0	-3.088956	0.108114	-2.450937
37	1	0	-2.148929	1.234933	-1.463698
38	1	0	-3.337716	-1.267939	-0.531869
39	1	0	-4.892445	0.068708	0.720035
40	1	0	-5.060096	0.197344	-1.047728
41	1	0	-4.255902	1.490744	-0.140136

E(RB3LYP) -940.33413514 a.u.

Table 53S. B3LYP/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*anti*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.102075	-1.429177	-0.905350
2	6	0	1.507470	-2.446597	0.189192
3	6	0	1.003147	-2.084763	1.567021
4	6	0	-0.213455	-1.588344	1.759540
5	6	0	-1.087095	-1.291968	0.568204
6	6	0	-0.246248	-0.716559	-0.594109
7	8	0	2.905811	-2.615866	0.124802
8	6	0	1.578761	0.756284	-0.494714
9	8	0	2.085254	-0.373547	-1.060105
10	6	0	0.270072	2.721216	0.952815
11	6	0	1.575620	2.911609	0.503848
12	6	0	2.274615	1.929201	-0.207220
13	8	0	3.566239	2.034515	-0.595561
14	6	0	-2.212154	-0.272550	0.864760
15	6	0	-1.733100	1.136396	1.263650
16	6	0	-0.416077	1.546741	0.640758
17	6	0	0.254128	0.629287	-0.144147
18	6	0	-1.128491	-0.613308	-1.855744
19	6	0	-2.372465	0.227256	-1.622185
20	7	0	-3.112782	-0.250389	-0.389230
21	6	0	-4.414397	0.462572	-0.201776
22	1	0	1.086807	-1.948672	-1.861336
23	1	0	1.000368	-3.380666	-0.099485
24	1	0	1.658175	-2.300434	2.401646
25	1	0	-0.587138	-1.389801	2.756404
26	1	0	-1.574093	-2.226400	0.249413
27	1	0	3.145967	-3.460058	0.518448
28	1	0	-0.189945	3.484492	1.566541
29	1	0	2.090231	3.831229	0.754962
30	1	0	3.938441	2.872454	-0.300321
31	1	0	-2.866065	-0.662641	1.644419
32	1	0	-1.612686	1.117143	2.349579
33	1	0	-2.522311	1.870698	1.089462
34	1	0	-1.411875	-1.616788	-2.188738
35	1	0	-0.567355	-0.158008	-2.672095
36	1	0	-3.070636	0.166771	-2.454971
37	1	0	-2.125137	1.271747	-1.448509
38	1	0	-3.341135	-1.231721	-0.555051
39	1	0	-4.890520	0.102721	0.706260
40	1	0	-5.047993	0.256189	-1.060411
41	1	0	-4.236497	1.529878	-0.131953

E(RB3LYP) -940.33071552 a.u.

Table 54S. B3LYP/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*syn*-6*g*$^{+}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.708622	1.567513	-0.869824
2	6	0	-0.935880	2.613796	0.249998
3	6	0	-0.536341	2.124399	1.622700
4	6	0	0.533173	1.362151	1.820455
5	6	0	1.345956	0.899599	0.637013
6	6	0	0.426435	0.553430	-0.555003
7	8	0	-2.239947	3.141526	0.202867
8	6	0	-1.686543	-0.476295	-0.526433
9	8	0	-1.919904	0.765252	-1.066815
10	6	0	-0.915981	-2.700353	0.902826
11	6	0	-2.217473	-2.580938	0.426256
12	6	0	-2.645126	-1.449375	-0.277901
13	8	0	-3.946460	-1.336155	-0.636153
14	6	0	2.193899	-0.355315	0.934943
15	6	0	1.391819	-1.623215	1.296334
16	6	0	0.036592	-1.713415	0.630063
17	6	0	-0.376769	-0.653561	-0.151501
18	6	0	1.304067	0.285028	-1.796505
19	6	0	2.291050	-0.846777	-1.564433
20	7	0	3.094646	-0.651787	-0.285395
21	6	0	4.228521	0.314389	-0.451436
22	1	0	-0.557300	2.087198	-1.813190
23	1	0	-0.278822	3.458154	0.009524
24	1	0	-1.128373	2.493663	2.449888
25	1	0	0.842866	1.081889	2.819790
26	1	0	2.029965	1.708376	0.356228
27	1	0	-2.858098	2.410522	0.085724
28	1	0	-0.659271	-3.557500	1.511405
29	1	0	-2.950349	-3.345722	0.642375
30	1	0	-4.084621	-0.529839	-1.146196
31	1	0	2.900468	-0.143906	1.736540
32	1	0	1.246652	-1.603239	2.378848
33	1	0	2.008869	-2.511764	1.117086
34	1	0	1.821060	1.202628	-2.087301
35	1	0	0.681451	-0.003003	-2.644407
36	1	0	3.008419	-0.945305	-2.376341
37	1	0	1.766032	-1.791682	-1.447781
38	1	0	3.520436	-1.555216	-0.082522
39	1	0	4.899294	-0.070350	-1.215090
40	1	0	3.849279	1.282694	-0.754870
41	1	0	4.757338	0.403545	0.493537

E(RB3LYP) -940.33545544 a.u.

Table 55S. B3LYP/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*anti*-6g^{+}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.685948	1.578413	-0.875613
2	6	0	-0.932013	2.615041	0.250489
3	6	0	-0.526402	2.124922	1.621390
4	6	0	0.544558	1.364733	1.819943
5	6	0	1.356608	0.896072	0.638177
6	6	0	0.438397	0.556588	-0.555675
7	8	0	-2.247549	3.112293	0.207255
8	6	0	-1.686528	-0.448858	-0.542327
9	8	0	-1.895114	0.786220	-1.092492
10	6	0	-0.934932	-2.681864	0.901841
11	6	0	-2.235134	-2.547851	0.420250
12	6	0	-2.655059	-1.415463	-0.287533
13	8	0	-3.925497	-1.186909	-0.695136
14	6	0	2.192913	-0.365206	0.939389
15	6	0	1.377133	-1.623978	1.300441
16	6	0	0.022905	-1.703626	0.629991
17	6	0	-0.380894	-0.641928	-0.156463
18	6	0	1.315919	0.278403	-1.794831
19	6	0	2.292292	-0.861666	-1.559344
20	7	0	3.094118	-0.671784	-0.278144
21	6	0	4.236114	0.285043	-0.442720
22	1	0	-0.519387	2.105994	-1.812129
23	1	0	-0.288068	3.472588	0.019589
24	1	0	-1.118058	2.494266	2.448858
25	1	0	0.856526	1.088778	2.819890
26	1	0	2.047773	1.698829	0.357895
27	1	0	-2.840559	2.381948	-0.010958
28	1	0	-0.689239	-3.540100	1.513310
29	1	0	-2.963455	-3.317448	0.645217
30	1	0	-4.502210	-1.909403	-0.423796
31	1	0	2.899471	-0.160097	1.742678
32	1	0	1.228339	-1.599194	2.382291
33	1	0	1.985413	-2.519284	1.125407
34	1	0	1.841736	1.191041	-2.085229
35	1	0	0.692039	-0.004153	-2.643635
36	1	0	3.011262	-0.967544	-2.368912
37	1	0	1.759183	-1.802082	-1.442881
38	1	0	3.512153	-1.578224	-0.072886
39	1	0	4.905673	-0.106146	-1.204142
40	1	0	3.865130	1.255772	-0.748496
41	1	0	4.763161	0.371467	0.503492

E(RB3LYP) -940.33462843 a.u.

Table 56S. B3LYP/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*syn*-6*g*$^{-}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.718966	1.537514	-0.954085
2	6	0	-1.101541	2.551805	0.183009
3	6	0	-0.464073	2.281532	1.516914
4	6	0	0.671533	1.619813	1.692868
5	6	0	1.404927	1.008852	0.530498
6	6	0	0.439336	0.572361	-0.583073
7	8	0	-2.493563	2.625702	0.407209
8	6	0	-1.647747	-0.491907	-0.552389
9	8	0	-1.840205	0.664153	-1.271467
10	6	0	-0.905289	-2.563644	1.109497
11	6	0	-2.187392	-2.507217	0.571547
12	6	0	-2.601347	-1.455183	-0.255896
13	8	0	-3.880758	-1.412937	-0.694850
14	6	0	2.220936	-0.239691	0.935798
15	6	0	1.388095	-1.424744	1.465588
16	6	0	0.041656	-1.582643	0.796169
17	6	0	-0.362269	-0.597271	-0.078213
18	6	0	1.274957	0.185712	-1.823727
19	6	0	2.226802	-0.960013	-1.521156
20	7	0	3.066533	-0.698662	-0.275131
21	6	0	4.247279	0.183336	-0.549318
22	1	0	-0.517827	2.088668	-1.870869
23	1	0	-0.725961	3.530562	-0.150601
24	1	0	-0.977375	2.731479	2.356982
25	1	0	1.101523	1.529355	2.683185
26	1	0	2.109210	1.753955	0.143341
27	1	0	-2.946390	2.857960	-0.409733
28	1	0	-0.660990	-3.365038	1.794346
29	1	0	-2.917858	-3.262817	0.825014
30	1	0	-4.033518	-0.599180	-1.188840
31	1	0	2.963434	0.030655	1.685512
32	1	0	1.235660	-1.242941	2.532435
33	1	0	1.986846	-2.342128	1.422632
34	1	0	1.815746	1.059788	-2.194053
35	1	0	0.622518	-0.145903	-2.632298
36	1	0	2.923959	-1.148515	-2.334769
37	1	0	1.669525	-1.871570	-1.320924
38	1	0	3.446610	-1.603583	-0.000977
39	1	0	4.870161	-0.297618	-1.298732
40	1	0	3.912830	1.146029	-0.917252
41	1	0	4.810987	0.314465	0.370191

E(RB3LYP) -940.33320655 a.u.

Table 57S. B3LYP/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*syn*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.731180	1.550614	-0.875876
2	6	0	-0.964357	2.584724	0.252750
3	6	0	-0.578713	2.084560	1.625441
4	6	0	0.503655	1.342026	1.825908
5	6	0	1.332742	0.905730	0.644095
6	6	0	0.424182	0.555597	-0.555428
7	8	0	-2.305100	3.018957	0.165710
8	6	0	-1.673715	-0.494905	-0.546199
9	8	0	-1.906737	0.728454	-1.111436
10	6	0	-0.898151	-2.709209	0.898623
11	6	0	-2.201290	-2.593211	0.423474
12	6	0	-2.632161	-1.465300	-0.284537
13	8	0	-3.931749	-1.347734	-0.641409
14	6	0	2.193690	-0.341521	0.939922
15	6	0	1.403431	-1.618667	1.296212
16	6	0	0.050586	-1.718320	0.626610
17	6	0	-0.366017	-0.663458	-0.160053
18	6	0	1.310166	0.304004	-1.793743
19	6	0	2.302640	-0.822581	-1.562485
20	7	0	3.100016	-0.625897	-0.279363
21	6	0	4.225937	0.349993	-0.438150
22	1	0	-0.569923	2.090476	-1.806547
23	1	0	-0.284242	3.416690	0.012954
24	1	0	-1.195451	2.407646	2.454625
25	1	0	0.799708	1.043832	2.824009
26	1	0	2.007907	1.726308	0.375777
27	1	0	-2.394056	3.872828	0.599892
28	1	0	-0.639563	-3.563629	1.510322
29	1	0	-2.932951	-3.356867	0.647700
30	1	0	-4.084457	-0.485567	-1.047212
31	1	0	2.897004	-0.125459	1.743233
32	1	0	1.258734	-1.605234	2.378932
33	1	0	2.030624	-2.499612	1.113229
34	1	0	1.822591	1.226733	-2.076870
35	1	0	0.692973	0.016815	-2.645861
36	1	0	3.024369	-0.914892	-2.371271
37	1	0	1.782040	-1.770336	-1.449628
38	1	0	3.531952	-1.526760	-0.078212
39	1	0	4.901271	-0.024836	-1.202702
40	1	0	3.838934	1.316547	-0.737294
41	1	0	4.752430	0.438713	0.508159

E(RB3LYP) -940.33203476 a.u.

Table 58S. B3LYP/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*anti*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.706460	1.562857	-0.879296
2	6	0	-0.895374	2.622208	0.233713
3	6	0	-0.526187	2.124566	1.612244
4	6	0	0.536757	1.355644	1.818180
5	6	0	1.350292	0.890917	0.636142
6	6	0	0.427095	0.547388	-0.554069
7	8	0	-2.214197	3.113424	0.143478
8	6	0	-1.695802	-0.454978	-0.533878
9	8	0	-1.903783	0.770230	-1.089021
10	6	0	-0.937593	-2.687655	0.918567
11	6	0	-2.236228	-2.558133	0.430043
12	6	0	-2.658966	-1.431323	-0.284758
13	8	0	-3.926170	-1.221715	-0.708907
14	6	0	2.188274	-0.369041	0.938537
15	6	0	1.373161	-1.624988	1.310364
16	6	0	0.017362	-1.708213	0.643507
17	6	0	-0.389747	-0.649916	-0.146320
18	6	0	1.299706	0.264059	-1.795060
19	6	0	2.272498	-0.878398	-1.559045
20	7	0	3.081463	-0.683571	-0.282691
21	6	0	4.224121	0.269684	-0.458761
22	1	0	-0.540908	2.084650	-1.819772
23	1	0	-0.178303	3.419141	-0.019281
24	1	0	-1.136077	2.469626	2.437561
25	1	0	0.826664	1.055702	2.817593
26	1	0	2.038801	1.695767	0.354343
27	1	0	-2.262677	3.981060	0.555911
28	1	0	-0.691632	-3.542725	1.534372
29	1	0	-2.962618	-3.330206	0.653393
30	1	0	-4.497468	-1.945978	-0.431475
31	1	0	2.900496	-0.160691	1.736091
32	1	0	1.229185	-1.593970	2.392814
33	1	0	1.981942	-2.520853	1.138607
34	1	0	1.827393	1.173922	-2.091438
35	1	0	0.670751	-0.019512	-2.639714
36	1	0	2.987606	-0.992182	-2.371023
37	1	0	1.735604	-1.815485	-1.433701
38	1	0	3.498048	-1.590006	-0.074611
39	1	0	4.888175	-0.126047	-1.222669
40	1	0	3.852987	1.239652	-0.766801
41	1	0	4.757537	0.359555	0.483579

E(RB3LYP) -940.32858184 a.u.

Table 59S. PBE0/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*syn*-6*g*$^{+}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.083037	-1.439803	-0.889499
2	6	0	1.512979	-2.421959	0.217119
3	6	0	1.001913	-2.042840	1.580318
4	6	0	-0.216789	-1.550546	1.762391
5	6	0	-1.086782	-1.282447	0.570734
6	6	0	-0.252462	-0.723854	-0.591178
7	8	0	2.889611	-2.654358	0.181155
8	6	0	1.564245	0.744384	-0.488793
9	8	0	2.077827	-0.393611	-1.041814
10	6	0	0.271112	2.709653	0.933000
11	6	0	1.574563	2.893928	0.493506
12	6	0	2.268318	1.904127	-0.206775
13	8	0	3.560310	2.097040	-0.530571
14	6	0	-2.209453	-0.268557	0.851056
15	6	0	-1.738485	1.137281	1.238925
16	6	0	-0.423773	1.539447	0.625622
17	6	0	0.242396	0.617196	-0.148123
18	6	0	-1.129871	-0.623312	-1.844642
19	6	0	-2.359290	0.222945	-1.604957
20	7	0	-3.095485	-0.257444	-0.389975
21	6	0	-4.388207	0.446929	-0.209320
22	1	0	1.071050	-1.967223	-1.843386
23	1	0	1.047284	-3.383812	-0.037578
24	1	0	1.653765	-2.266263	2.417018
25	1	0	-0.598291	-1.349467	2.757786
26	1	0	-1.569672	-2.226105	0.265912
27	1	0	3.330602	-1.804915	0.082596
28	1	0	-0.189647	3.480053	1.540332
29	1	0	2.108928	3.803983	0.736109
30	1	0	3.885800	1.352912	-1.045105
31	1	0	-2.861182	-0.656031	1.637186
32	1	0	-1.623908	1.131126	2.327052
33	1	0	-2.528345	1.870534	1.052512
34	1	0	-1.420759	-1.628356	-2.171969
35	1	0	-0.567986	-0.174201	-2.665940
36	1	0	-3.056772	0.182380	-2.441862
37	1	0	-2.097569	1.264649	-1.418162
38	1	0	-3.315751	-1.240743	-0.556019
39	1	0	-4.865622	0.093788	0.702579
40	1	0	-5.022957	0.234567	-1.067649
41	1	0	-4.213267	1.517229	-0.148049

E(RPBE1PBE) -939.26928903 a.u.

Table 60S. PBE0/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*anti*-6g^{+}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.056325	-1.461856	-0.895058
2	6	0	1.500764	-2.428308	0.220794
3	6	0	0.983163	-2.047052	1.581194
4	6	0	-0.235332	-1.553808	1.762873
5	6	0	-1.104594	-1.277115	0.572470
6	6	0	-0.267690	-0.729872	-0.591923
7	8	0	2.881933	-2.629097	0.189973
8	6	0	1.572461	0.710270	-0.507552
9	8	0	2.055352	-0.428946	-1.071379
10	6	0	0.304266	2.694651	0.929723
11	6	0	1.610778	2.857920	0.485210
12	6	0	2.292847	1.862177	-0.218360
13	8	0	3.583268	1.933068	-0.590672
14	6	0	-2.213278	-0.249686	0.855484
15	6	0	-1.721050	1.149211	1.241502
16	6	0	-0.402721	1.534401	0.624028
17	6	0	0.250761	0.604897	-0.154319
18	6	0	-1.146737	-0.616574	-1.843170
19	6	0	-2.364255	0.245391	-1.599888
20	7	0	-3.102694	-0.226932	-0.383079
21	6	0	-4.386422	0.491933	-0.198163
22	1	0	1.028572	-2.002762	-1.841125
23	1	0	1.050285	-3.400895	-0.022279
24	1	0	1.633338	-2.272021	2.418841
25	1	0	-0.618228	-1.356385	2.758604
26	1	0	-1.599868	-2.214803	0.269049
27	1	0	3.299065	-1.784715	-0.013706
28	1	0	-0.142660	3.470970	1.539722
29	1	0	2.143507	3.769040	0.737213
30	1	0	3.966982	2.764289	-0.299029
31	1	0	-2.868197	-0.627457	1.643748
32	1	0	-1.602715	1.140573	2.329121
33	1	0	-2.500639	1.894059	1.057766
34	1	0	-1.451974	-1.617591	-2.169766
35	1	0	-0.580000	-0.175648	-2.665577
36	1	0	-3.064771	0.214489	-2.434675
37	1	0	-2.089151	1.283632	-1.413082
38	1	0	-3.334198	-1.207690	-0.549191
39	1	0	-4.866426	0.142223	0.713705
40	1	0	-5.025411	0.289573	-1.055780
41	1	0	-4.198805	1.559972	-0.134457

E(RPBE1PBE) -939.26868124 a.u.

Table 61S. PBE0/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*syn*-6*g*$^{-}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.079293	-1.422873	0.948486
2	6	0	-1.598434	-2.356749	-0.184383
3	6	0	-0.950990	-2.140725	-1.516602
4	6	0	0.298986	-1.728637	-1.670476
5	6	0	1.129177	-1.356874	-0.482172
6	6	0	0.266056	-0.738265	0.620625
7	8	0	-2.982157	-2.263183	-0.374173
8	6	0	-1.536675	0.737679	0.512152
9	8	0	-2.003235	-0.345159	1.199387
10	6	0	-0.290814	2.608802	-1.075078
11	6	0	-1.580002	2.819421	-0.605082
12	6	0	-2.250251	1.877948	0.181026
13	8	0	-3.524932	2.098411	0.547632
14	6	0	2.226131	-0.333632	-0.825305
15	6	0	1.715980	1.015564	-1.339550
16	6	0	0.410156	1.452067	-0.731485
17	6	0	-0.237130	0.574967	0.106115
18	6	0	1.122269	-0.543803	1.878693
19	6	0	2.325146	0.328067	1.600533
20	7	0	3.093731	-0.194524	0.422552
21	6	0	4.351016	0.561573	0.205538
22	1	0	-1.033123	-1.987291	1.881243
23	1	0	-1.324833	-3.379028	0.126803
24	1	0	-1.557854	-2.417531	-2.371029
25	1	0	0.739076	-1.665157	-2.660091
26	1	0	1.635074	-2.260830	-0.104363
27	1	0	-3.438824	-2.470932	0.444070
28	1	0	0.150924	3.345162	-1.736457
29	1	0	-2.122199	3.713879	-0.885466
30	1	0	-3.867522	1.326338	1.007595
31	1	0	2.902899	-0.763128	-1.567522
32	1	0	1.575785	0.892193	-2.418188
33	1	0	2.494224	1.778705	-1.251375
34	1	0	1.440581	-1.518375	2.266850
35	1	0	0.535594	-0.064799	2.665193
36	1	0	3.014863	0.361786	2.444208
37	1	0	2.028720	1.346214	1.348693
38	1	0	3.361008	-1.152281	0.655296
39	1	0	4.855639	0.175270	-0.677893
40	1	0	4.986995	0.438714	1.080315
41	1	0	4.121489	1.615020	0.073272

E(RPBE1PBE) -939.26687176 a.u.

Table 62S. PBE0/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*syn*-anti

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.103334	-1.416973	-0.893302
2	6	0	1.532256	-2.387815	0.221464
3	6	0	1.038460	-1.989838	1.585664
4	6	0	-0.187611	-1.518566	1.771710
5	6	0	-1.069185	-1.283285	0.581637
6	6	0	-0.247799	-0.724921	-0.590301
7	8	0	2.922294	-2.536875	0.142206
8	6	0	1.548819	0.762582	-0.509375
9	8	0	2.061495	-0.358516	-1.081903
10	6	0	0.250456	2.718566	0.922951
11	6	0	1.554981	2.906823	0.485768
12	6	0	2.252323	1.920182	-0.215168
13	8	0	3.544399	2.106914	-0.535692
14	6	0	-2.203673	-0.280714	0.858106
15	6	0	-1.747855	1.132796	1.237042
16	6	0	-0.438639	1.544211	0.618342
17	6	0	0.230389	0.626756	-0.158849
18	6	0	-1.131271	-0.647372	-1.840206
19	6	0	-2.365476	0.191723	-1.602397
20	7	0	-3.092763	-0.286961	-0.380809
21	6	0	-4.391532	0.406166	-0.200970
22	1	0	1.087275	-1.965381	-1.835603
23	1	0	1.030068	-3.337263	-0.031594
24	1	0	1.706507	-2.159064	2.423018
25	1	0	-0.557709	-1.292326	2.765834
26	1	0	-1.539991	-2.237861	0.292058
27	1	0	3.180665	-3.343330	0.592956
28	1	0	-0.212589	3.486456	1.531812
29	1	0	2.087202	3.816271	0.735361
30	1	0	3.893828	1.309251	-0.945622
31	1	0	-2.849726	-0.671147	1.647575
32	1	0	-1.633981	1.135451	2.325305
33	1	0	-2.546868	1.854989	1.045879
34	1	0	-1.416161	-1.657969	-2.156094
35	1	0	-0.575944	-0.202239	-2.668108
36	1	0	-3.066875	0.140598	-2.435476
37	1	0	-2.109709	1.236198	-1.422801
38	1	0	-3.303977	-1.273326	-0.539739
39	1	0	-4.861898	0.056630	0.715985
40	1	0	-5.027482	0.180119	-1.054894
41	1	0	-4.226651	1.478556	-0.149771

E(RPBE1PBE) -939.26584701 a.u.

Table 63S. PBE0/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*anti*-anti

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.093966	-1.425801	-0.896614
2	6	0	1.492160	-2.428280	0.201355
3	6	0	1.010280	-2.034290	1.571225
4	6	0	-0.206898	-1.541839	1.761853
5	6	0	-1.080720	-1.282121	0.571033
6	6	0	-0.247101	-0.719604	-0.590011
7	8	0	2.874288	-2.625675	0.119042
8	6	0	1.572501	0.741276	-0.495653
9	8	0	2.071257	-0.383922	-1.057449
10	6	0	0.266714	2.710005	0.940648
11	6	0	1.569481	2.894218	0.492005
12	6	0	2.268813	1.911922	-0.213286
13	8	0	3.552536	2.016588	-0.597309
14	6	0	-2.205219	-0.271354	0.852880
15	6	0	-1.733545	1.131944	1.247254
16	6	0	-0.420176	1.538734	0.633105
17	6	0	0.250164	0.620772	-0.145102
18	6	0	-1.123467	-0.614617	-1.843206
19	6	0	-2.350812	0.233041	-1.601841
20	7	0	-3.088571	-0.254094	-0.389912
21	6	0	-4.381552	0.448429	-0.207321
22	1	0	1.075195	-1.957186	-1.848857
23	1	0	0.954707	-3.354683	-0.066395
24	1	0	1.677152	-2.221918	2.405512
25	1	0	-0.574178	-1.315880	2.757111
26	1	0	-1.559828	-2.228072	0.266739
27	1	0	3.104256	-3.448355	0.555432
28	1	0	-0.192076	3.478346	1.551927
29	1	0	2.086552	3.815283	0.740955
30	1	0	3.916968	2.855603	-0.303785
31	1	0	-2.859539	-0.661439	1.635726
32	1	0	-1.617885	1.119090	2.335246
33	1	0	-2.524295	1.865757	1.066396
34	1	0	-1.416366	-1.618085	-2.174208
35	1	0	-0.558025	-0.164871	-2.661689
36	1	0	-3.048482	0.198566	-2.438927
37	1	0	-2.086894	1.272887	-1.408071
38	1	0	-3.307318	-1.236593	-0.562201
39	1	0	-4.859987	0.091078	0.702416
40	1	0	-5.015254	0.240143	-1.067410
41	1	0	-4.206891	1.518448	-0.140753

E(RPBE1PBE) -939.26257433 a.u.

Table 64S. PBE0/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*syn*-6*g*$^{+}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.699414	1.563473	-0.859372
2	6	0	-0.931053	2.589086	0.266771
3	6	0	-0.553041	2.074201	1.629100
4	6	0	0.520320	1.318695	1.823024
5	6	0	1.341056	0.893277	0.640484
6	6	0	0.430882	0.557999	-0.549347
7	8	0	-2.220788	3.122060	0.209235
8	6	0	-1.673230	-0.461952	-0.528409
9	8	0	-1.898358	0.771808	-1.068708
10	6	0	-0.908444	-2.687310	0.892316
11	6	0	-2.205330	-2.563326	0.414043
12	6	0	-2.632265	-1.432654	-0.286399
13	8	0	-3.924049	-1.318718	-0.645770
14	6	0	2.190109	-0.353466	0.923752
15	6	0	1.395134	-1.615900	1.283388
16	6	0	0.044355	-1.704066	0.625223
17	6	0	-0.368026	-0.644024	-0.150493
18	6	0	1.301604	0.287295	-1.782661
19	6	0	2.268709	-0.849198	-1.542102
20	7	0	3.074840	-0.641763	-0.285989
21	6	0	4.178529	0.335861	-0.467619
22	1	0	-0.539969	2.097430	-1.796283
23	1	0	-0.257488	3.429445	0.049561
24	1	0	-1.161227	2.418624	2.457579
25	1	0	0.820512	1.015834	2.820523
26	1	0	2.019499	1.714872	0.375163
27	1	0	-2.834958	2.394640	0.070025
28	1	0	-0.655100	-3.548901	1.499064
29	1	0	-2.941109	-3.328754	0.626954
30	1	0	-4.055134	-0.512373	-1.152798
31	1	0	2.897858	-0.141534	1.727743
32	1	0	1.252338	-1.600418	2.367831
33	1	0	2.012640	-2.505330	1.099688
34	1	0	1.827101	1.201854	-2.074428
35	1	0	0.675909	0.003524	-2.631683
36	1	0	2.977662	-0.975232	-2.360226
37	1	0	1.724644	-1.783641	-1.403948
38	1	0	3.514980	-1.537904	-0.081834
39	1	0	4.852753	-0.040833	-1.234518
40	1	0	3.777433	1.295142	-0.777943
41	1	0	4.713959	0.446743	0.473213

E(RPBE1PBE) -939.26716703 a.u.

Table 65S. PBE0/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*anti*-6g^{+}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.676131	1.575146	-0.865468
2	6	0	-0.929847	2.589149	0.267788
3	6	0	-0.543241	2.074460	1.627988
4	6	0	0.532868	1.322796	1.822386
5	6	0	1.352620	0.890657	0.641409
6	6	0	0.443549	0.561858	-0.549945
7	8	0	-2.233101	3.087015	0.214069
8	6	0	-1.672265	-0.434092	-0.545785
9	8	0	-1.871999	0.792710	-1.097413
10	6	0	-0.927520	-2.667448	0.892342
11	6	0	-2.222727	-2.528691	0.408403
12	6	0	-2.641424	-1.397626	-0.296580
13	8	0	-3.902948	-1.171293	-0.703684
14	6	0	2.189613	-0.362750	0.928331
15	6	0	1.380317	-1.615369	1.288679
16	6	0	0.030691	-1.692976	0.626045
17	6	0	-0.371746	-0.631508	-0.155308
18	6	0	1.313669	0.280755	-1.781096
19	6	0	2.269735	-0.864096	-1.536958
20	7	0	3.074363	-0.662004	-0.278752
21	6	0	4.186890	0.305725	-0.459357
22	1	0	-0.500660	2.118096	-1.794401
23	1	0	-0.272796	3.445572	0.060863
24	1	0	-1.150462	2.418965	2.457201
25	1	0	0.836753	1.026105	2.820762
26	1	0	2.038673	1.705831	0.376149
27	1	0	-2.817892	2.359945	-0.026467
28	1	0	-0.685618	-3.529797	1.502543
29	1	0	-2.954055	-3.298807	0.630900
30	1	0	-4.473569	-1.895275	-0.432494
31	1	0	2.897703	-0.157027	1.733688
32	1	0	1.233620	-1.593848	2.372425
33	1	0	1.988576	-2.512101	1.110151
34	1	0	1.848198	1.189953	-2.073004
35	1	0	0.686236	0.002416	-2.630651
36	1	0	2.980050	-0.997727	-2.352730
37	1	0	1.717352	-1.793691	-1.399091
38	1	0	3.506255	-1.561473	-0.071950
39	1	0	4.859619	-0.077980	-1.224090
40	1	0	3.794567	1.267811	-0.772126
41	1	0	4.720996	0.413654	0.482578

E(RPBE1PBE) -939.26655283 a.u.

Table 66S. PBE0/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*syn*-6*g*$^{-}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.716775	1.536536	-0.923905
2	6	0	-1.079446	2.531006	0.220442
3	6	0	-0.514810	2.176565	1.560726
4	6	0	0.619630	1.514959	1.736603
5	6	0	1.384093	0.987050	0.561624
6	6	0	0.440176	0.577480	-0.569591
7	8	0	-2.460639	2.692371	0.382779
8	6	0	-1.636960	-0.482575	-0.554584
9	8	0	-1.832826	0.680829	-1.241622
10	6	0	-0.884945	-2.587902	1.050621
11	6	0	-2.167558	-2.517133	0.524262
12	6	0	-2.588737	-1.448849	-0.272868
13	8	0	-3.863850	-1.392574	-0.695266
14	6	0	2.215074	-0.253462	0.924174
15	6	0	1.401365	-1.456733	1.417233
16	6	0	0.058684	-1.603589	0.754549
17	6	0	-0.350984	-0.601996	-0.093742
18	6	0	1.278957	0.221483	-1.804058
19	6	0	2.223172	-0.922351	-1.511468
20	7	0	3.057039	-0.663592	-0.281480
21	6	0	4.195382	0.253172	-0.548342
22	1	0	-0.515968	2.100624	-1.836128
23	1	0	-0.615373	3.490540	-0.062905
24	1	0	-1.069052	2.568089	2.406096
25	1	0	1.014241	1.358036	2.735011
26	1	0	2.074131	1.768039	0.215244
27	1	0	-2.853986	2.984595	-0.442513
28	1	0	-0.637701	-3.406089	1.717023
29	1	0	-2.898392	-3.278360	0.767232
30	1	0	-4.015071	-0.563974	-1.159469
31	1	0	2.951452	0.008580	1.686605
32	1	0	1.251249	-1.313045	2.491631
33	1	0	2.008994	-2.368206	1.341330
34	1	0	1.819730	1.105098	-2.156869
35	1	0	0.629785	-0.097598	-2.622462
36	1	0	2.916287	-1.113828	-2.330478
37	1	0	1.658035	-1.832175	-1.310180
38	1	0	3.464537	-1.561371	-0.024008
39	1	0	4.831889	-0.195087	-1.308876
40	1	0	3.825359	1.209611	-0.903421
41	1	0	4.761190	0.394692	0.370316

E(RPBE1PBE) -939.26470766 a.u.

Table 67S. PBE0/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*syn*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.719670	1.547574	-0.862919
2	6	0	-0.944865	2.562460	0.271515
3	6	0	-0.598314	2.025335	1.633572
4	6	0	0.483005	1.283024	1.832445
5	6	0	1.324137	0.891023	0.652663
6	6	0	0.428141	0.557623	-0.549388
7	8	0	-2.258674	3.034602	0.163595
8	6	0	-1.663745	-0.478207	-0.548449
9	8	0	-1.888574	0.741454	-1.104650
10	6	0	-0.896131	-2.701557	0.876917
11	6	0	-2.195566	-2.576017	0.403683
12	6	0	-2.624564	-1.444710	-0.294265
13	8	0	-3.915533	-1.320184	-0.647058
14	6	0	2.186474	-0.348528	0.929340
15	6	0	1.403544	-1.623249	1.273727
16	6	0	0.054619	-1.715689	0.612246
17	6	0	-0.359744	-0.656942	-0.164530
18	6	0	1.310324	0.308742	-1.778335
19	6	0	2.283734	-0.822455	-1.541003
20	7	0	3.080424	-0.617122	-0.278192
21	6	0	4.174136	0.373550	-0.445421
22	1	0	-0.551946	2.100227	-1.787864
23	1	0	-0.227516	3.374075	0.059701
24	1	0	-1.237613	2.317569	2.459345
25	1	0	0.760784	0.949859	2.826545
26	1	0	1.992749	1.726768	0.406220
27	1	0	-2.338017	3.862156	0.642296
28	1	0	-0.641648	-3.563224	1.483176
29	1	0	-2.931406	-3.339436	0.623606
30	1	0	-4.059150	-0.456598	-1.047120
31	1	0	2.888402	-0.136072	1.738386
32	1	0	1.261641	-1.623808	2.358394
33	1	0	2.031321	-2.503333	1.078633
34	1	0	1.830801	1.230040	-2.058132
35	1	0	0.691908	0.028351	-2.633794
36	1	0	2.999151	-0.938227	-2.355036
37	1	0	1.744761	-1.761071	-1.411537
38	1	0	3.528271	-1.510431	-0.078620
39	1	0	4.855891	0.011511	-1.212697
40	1	0	3.763787	1.331079	-0.748923
41	1	0	4.704016	0.481586	0.498868

E(RPBE1PBE) -939.26377546 a.u.

Table 68S. PBE0/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*anti*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.693649	1.560118	-0.867330
2	6	0	-0.874910	2.600804	0.251297
3	6	0	-0.544549	2.068793	1.619725
4	6	0	0.516785	1.299334	1.824260
5	6	0	1.342498	0.876505	0.644052
6	6	0	0.431608	0.549054	-0.548216
7	8	0	-2.165849	3.127506	0.140559
8	6	0	-1.685794	-0.437290	-0.536582
9	8	0	-1.884397	0.783941	-1.083869
10	6	0	-0.937339	-2.678884	0.898358
11	6	0	-2.231678	-2.538805	0.411185
12	6	0	-2.651747	-1.408769	-0.294436
13	8	0	-3.911034	-1.194967	-0.712033
14	6	0	2.180808	-0.376703	0.928104
15	6	0	1.371805	-1.629373	1.289217
16	6	0	0.020198	-1.704964	0.630152
17	6	0	-0.383968	-0.643012	-0.150360
18	6	0	1.299871	0.267093	-1.779932
19	6	0	2.252723	-0.880155	-1.537252
20	7	0	3.061415	-0.676991	-0.281514
21	6	0	4.173331	0.289931	-0.466574
22	1	0	-0.520324	2.094152	-1.802435
23	1	0	-0.122621	3.376911	0.025404
24	1	0	-1.176530	2.385501	2.442047
25	1	0	0.788186	0.966403	2.820226
26	1	0	2.025561	1.695901	0.382774
27	1	0	-2.206578	3.967395	0.602090
28	1	0	-0.696248	-3.540955	1.509279
29	1	0	-2.962940	-3.310019	0.630717
30	1	0	-4.476939	-1.921427	-0.438200
31	1	0	2.892014	-0.171894	1.731070
32	1	0	1.230079	-1.610928	2.373748
33	1	0	1.980401	-2.525307	1.106503
34	1	0	1.836248	1.174814	-2.073697
35	1	0	0.669224	-0.009649	-2.627573
36	1	0	2.960830	-1.018258	-2.354243
37	1	0	1.697011	-1.807078	-1.394816
38	1	0	3.492929	-1.576602	-0.074692
39	1	0	4.842645	-0.093510	-1.234426
40	1	0	3.779745	1.252111	-0.777445
41	1	0	4.711670	0.397467	0.473009

E(RPBE1PBE) -939.26046081 a.u.

Table 69S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*syn*-6*g*$^{+}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.056896	-1.466314	-0.891771
2	6	0	1.489409	-2.440813	0.229502
3	6	0	0.986448	-2.054514	1.597509
4	6	0	-0.225721	-1.539404	1.777537
5	6	0	-1.103900	-1.258223	0.588955
6	6	0	-0.267302	-0.718874	-0.592175
7	8	0	2.897810	-2.656631	0.198644
8	6	0	1.585286	0.735259	-0.510104
9	8	0	2.082485	-0.421559	-1.068798
10	6	0	0.320810	2.722229	0.920337
11	6	0	1.633737	2.887492	0.485530
12	6	0	2.305944	1.882307	-0.216555
13	8	0	3.632002	2.055428	-0.541553
14	6	0	-2.222425	-0.227934	0.864466
15	6	0	-1.732625	1.192871	1.210847
16	6	0	-0.393409	1.558254	0.612200
17	6	0	0.257535	0.625030	-0.166315
18	6	0	-1.162766	-0.639713	-1.843645
19	6	0	-2.416753	0.187600	-1.619310
20	7	0	-3.131925	-0.245053	-0.365550
21	6	0	-4.421197	0.484953	-0.182376
22	1	0	1.026979	-1.999714	-1.837292
23	1	0	1.044482	-3.406692	-0.026205
24	1	0	1.630864	-2.289600	2.435610
25	1	0	-0.602870	-1.327513	2.770635
26	1	0	-1.592535	-2.193207	0.291561
27	1	0	3.317806	-1.787127	0.150083
28	1	0	-0.134477	3.496950	1.523620
29	1	0	2.179642	3.788342	0.733271
30	1	0	3.950648	1.277575	-1.016840
31	1	0	-2.857428	-0.588935	1.669724
32	1	0	-1.643542	1.233957	2.297829
33	1	0	-2.497997	1.927048	0.960475
34	1	0	-1.439055	-1.655133	-2.135571
35	1	0	-0.614298	-0.197552	-2.675367
36	1	0	-3.120903	0.068550	-2.438748
37	1	0	-2.199420	1.246795	-1.507031
38	1	0	-3.382463	-1.227803	-0.495533
39	1	0	-4.879559	0.152428	0.744331
40	1	0	-5.063411	0.244664	-1.024833
41	1	0	-4.237193	1.553201	-0.154997

E(RB3LYP) -940.44535394 a.u.

Table 70S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*anti*-6*g*$^{+}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.036329	-1.484322	-0.895618
2	6	0	1.463255	-2.461138	0.226197
3	6	0	0.967089	-2.068293	1.594867
4	6	0	-0.239234	-1.540420	1.777223
5	6	0	-1.117009	-1.250246	0.590535
6	6	0	-0.277402	-0.721236	-0.592936
7	8	0	2.870181	-2.686243	0.192181
8	6	0	1.593431	0.710186	-0.518386
9	8	0	2.073279	-0.453340	-1.077620
10	6	0	0.353509	2.712112	0.918664
11	6	0	1.667449	2.862284	0.478742
12	6	0	2.326592	1.850955	-0.227846
13	8	0	3.646997	1.914945	-0.604858
14	6	0	-2.223171	-0.207686	0.868000
15	6	0	-1.716372	1.207823	1.211564
16	6	0	-0.373526	1.557197	0.610983
17	6	0	0.265855	0.616581	-0.169712
18	6	0	-1.174928	-0.631414	-1.842406
19	6	0	-2.417596	0.211472	-1.614546
20	7	0	-3.135041	-0.215809	-0.360386
21	6	0	-4.417404	0.525266	-0.174604
22	1	0	0.996471	-2.019733	-1.839672
23	1	0	1.010143	-3.424086	-0.026085
24	1	0	1.610797	-2.309348	2.431810
25	1	0	-0.612124	-1.324106	2.770996
26	1	0	-1.616922	-2.179816	0.294867
27	1	0	3.293936	-1.819928	0.120213
28	1	0	-0.090316	3.491277	1.524786
29	1	0	2.222320	3.759255	0.726298
30	1	0	4.024203	2.747483	-0.293141
31	1	0	-2.860700	-0.560669	1.674764
32	1	0	-1.626005	1.249622	2.298371
33	1	0	-2.473562	1.950218	0.960276
34	1	0	-1.465197	-1.643360	-2.132920
35	1	0	-0.622825	-0.196927	-2.675710
36	1	0	-3.124745	0.103334	-2.432915
37	1	0	-2.186660	1.267526	-1.499956
38	1	0	-3.393917	-1.196359	-0.490885
39	1	0	-4.877991	0.194505	0.751630
40	1	0	-5.062458	0.292383	-1.016980
41	1	0	-4.224015	1.591779	-0.144983

E(RB3LYP) -940.44512064 a.u.

Table 71S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*syn*-6*g*$^{-}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.085157	-1.440232	-0.886274
2	6	0	1.487708	-2.438046	0.229110
3	6	0	1.008055	-2.042319	1.597107
4	6	0	-0.201885	-1.524117	1.780890
5	6	0	-1.083718	-1.256536	0.592126
6	6	0	-0.251821	-0.709633	-0.590215
7	8	0	2.893996	-2.662151	0.281146
8	6	0	1.584577	0.763697	-0.503762
9	8	0	2.097121	-0.386633	-1.055929
10	6	0	0.290063	2.743405	0.912655
11	6	0	1.602137	2.922806	0.480272
12	6	0	2.288643	1.922771	-0.214969
13	8	0	3.613314	2.111214	-0.539166
14	6	0	-2.215119	-0.239427	0.863716
15	6	0	-1.743731	1.188551	1.205791
16	6	0	-0.408225	1.568857	0.608005
17	6	0	0.255999	0.641148	-0.165846
18	6	0	-1.147507	-0.645248	-1.841990
19	6	0	-2.413515	0.165167	-1.622092
20	7	0	-3.124113	-0.271265	-0.366898
21	6	0	-4.421720	0.444439	-0.186363
22	1	0	1.062063	-1.967232	-1.836597
23	1	0	0.982813	-3.375292	-0.038775
24	1	0	1.662702	-2.265744	2.430044
25	1	0	-0.570077	-1.297774	2.773771
26	1	0	-1.559758	-2.198609	0.296482
27	1	0	3.169851	-3.057178	-0.554770
28	1	0	-0.176276	3.514802	1.511731
29	1	0	2.135965	3.831731	0.724965
30	1	0	3.948637	1.323110	-0.985350
31	1	0	-2.846122	-0.605828	1.669669
32	1	0	-1.656813	1.234498	2.292765
33	1	0	-2.518175	1.911879	0.952106
34	1	0	-1.409415	-1.665106	-2.131746
35	1	0	-0.604588	-0.197549	-2.674400
36	1	0	-3.115179	0.032044	-2.441522
37	1	0	-2.211692	1.227944	-1.514800
38	1	0	-3.363884	-1.257063	-0.493404
39	1	0	-4.876933	0.109386	0.741002
40	1	0	-5.060666	0.194904	-1.028629
41	1	0	-4.249717	1.514783	-0.161621

E(RB3LYP) -940.44351579 a.u.

Table 72S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*anti*-6*g*$^{-}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.065993	-1.457277	-0.891871
2	6	0	1.458958	-2.462202	0.221271
3	6	0	0.983080	-2.066550	1.590520
4	6	0	-0.220692	-1.534963	1.776229
5	6	0	-1.098883	-1.251384	0.588652
6	6	0	-0.260517	-0.710864	-0.591704
7	8	0	2.863092	-2.699744	0.273759
8	6	0	1.595045	0.738788	-0.507586
9	8	0	2.090165	-0.417441	-1.062759
10	6	0	0.324128	2.729791	0.921589
11	6	0	1.636147	2.896698	0.481649
12	6	0	2.309672	1.893500	-0.222750
13	8	0	3.628260	1.978924	-0.604130
14	6	0	-2.216962	-0.221348	0.864625
15	6	0	-1.726745	1.199080	1.211367
16	6	0	-0.386549	1.564687	0.614342
17	6	0	0.266638	0.631634	-0.163963
18	6	0	-1.155795	-0.628734	-1.843048
19	6	0	-2.410053	0.197978	-1.618312
20	7	0	-3.125890	-0.237626	-0.365955
21	6	0	-4.416102	0.490409	-0.182502
22	1	0	1.033355	-1.983455	-1.842445
23	1	0	0.945527	-3.394147	-0.049037
24	1	0	1.634367	-2.301643	2.422910
25	1	0	-0.586769	-1.309241	2.770048
26	1	0	-1.587481	-2.186002	0.289514
27	1	0	3.138013	-3.084174	-0.567377
28	1	0	-0.130690	3.503874	1.526052
29	1	0	2.178081	3.802393	0.726363
30	1	0	3.990360	2.821514	-0.301844
31	1	0	-2.852582	-0.582353	1.669378
32	1	0	-1.639264	1.240137	2.298463
33	1	0	-2.491704	1.933336	0.959879
34	1	0	-1.432157	-1.643540	-2.137203
35	1	0	-0.606750	-0.185123	-2.673611
36	1	0	-3.113682	0.080556	-2.438456
37	1	0	-2.193107	1.256969	-1.503479
38	1	0	-3.375003	-1.220486	-0.497694
39	1	0	-4.875090	0.155485	0.743034
40	1	0	-5.057213	0.251107	-1.026098
41	1	0	-4.233306	1.558806	-0.152717

E(RB3LYP) -940.44311805 a.u.

Table 73S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*syn*-anti

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.086206	-1.435508	-0.896145
2	6	0	1.487497	-2.432873	0.208393
3	6	0	1.015072	-2.040460	1.585864
4	6	0	-0.195802	-1.526898	1.777233
5	6	0	-1.080433	-1.258697	0.589969
6	6	0	-0.251074	-0.707784	-0.592583
7	8	0	2.897896	-2.638282	0.138063
8	6	0	1.582860	0.768624	-0.504313
9	8	0	2.096885	-0.378886	-1.060225
10	6	0	0.288109	2.741799	0.920174
11	6	0	1.599508	2.924267	0.487015
12	6	0	2.286327	1.927193	-0.212069
13	8	0	3.610624	2.117485	-0.536570
14	6	0	-2.212960	-0.243800	0.865415
15	6	0	-1.743280	1.183787	1.211049
16	6	0	-0.409265	1.567519	0.612346
17	6	0	0.255006	0.642954	-0.165251
18	6	0	-1.148808	-0.641594	-1.842816
19	6	0	-2.414831	0.167381	-1.618988
20	7	0	-3.123562	-0.273124	-0.364089
21	6	0	-4.421485	0.441108	-0.180027
22	1	0	1.063996	-1.956588	-1.849010
23	1	0	0.975605	-3.365671	-0.060257
24	1	0	1.675238	-2.262779	2.415554
25	1	0	-0.562791	-1.302497	2.771211
26	1	0	-1.555538	-2.200689	0.292676
27	1	0	3.104687	-3.424007	0.657108
28	1	0	-0.178481	3.510592	1.522385
29	1	0	2.132615	3.832898	0.734355
30	1	0	3.944971	1.332894	-0.989691
31	1	0	-2.842432	-0.613417	1.671081
32	1	0	-1.654777	1.226699	2.298015
33	1	0	-2.519050	1.906793	0.960555
34	1	0	-1.410313	-1.661074	-2.134283
35	1	0	-0.607604	-0.191721	-2.675178
36	1	0	-3.117454	0.036369	-2.437932
37	1	0	-2.213420	1.229942	-1.508807
38	1	0	-3.362626	-1.258790	-0.493009
39	1	0	-4.874612	0.104630	0.747828
40	1	0	-5.061850	0.192076	-1.021354
41	1	0	-4.250360	1.511569	-0.154379

E(RB3LYP) -940.44286999 a.u.

Table 74S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M^{+}_{equ}-3*anti*-anti

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.067616	-1.452294	-0.901204
2	6	0	1.458107	-2.457216	0.200980
3	6	0	0.991412	-2.063003	1.579780
4	6	0	-0.213046	-1.535463	1.773419
5	6	0	-1.094721	-1.252880	0.587429
6	6	0	-0.259375	-0.708835	-0.593824
7	8	0	2.865992	-2.679581	0.129698
8	6	0	1.593451	0.744334	-0.508261
9	8	0	2.090747	-0.409524	-1.065846
10	6	0	0.321365	2.729436	0.927258
11	6	0	1.632863	2.899393	0.486977
12	6	0	2.307174	1.898845	-0.220320
13	8	0	3.625526	1.986297	-0.601959
14	6	0	-2.214453	-0.225451	0.866629
15	6	0	-1.726579	1.195095	1.215716
16	6	0	-0.388018	1.564223	0.617397
17	6	0	0.265633	0.633994	-0.163950
18	6	0	-1.157018	-0.626103	-1.843428
19	6	0	-2.411748	0.198570	-1.615167
20	7	0	-3.125260	-0.240464	-0.362638
21	6	0	-4.415975	0.485846	-0.175856
22	1	0	1.036130	-1.972307	-1.854481
23	1	0	0.935232	-3.383437	-0.069314
24	1	0	1.649140	-2.295952	2.408506
25	1	0	-0.576965	-1.309835	2.768260
26	1	0	-1.581840	-2.188000	0.287541
27	1	0	3.062925	-3.469506	0.646173
28	1	0	-0.134103	3.501154	1.534244
29	1	0	2.173826	3.805017	0.734066
30	1	0	3.986894	2.828868	-0.298745
31	1	0	-2.848255	-0.589385	1.671487
32	1	0	-1.637404	1.234002	2.302751
33	1	0	-2.493243	1.928484	0.966972
34	1	0	-1.432450	-1.640865	-2.138630
35	1	0	-0.610062	-0.180513	-2.674320
36	1	0	-3.116393	0.082097	-2.434576
37	1	0	-2.195864	1.257577	-1.498442
38	1	0	-3.373419	-1.223350	-0.496007
39	1	0	-4.872626	0.149852	0.750434
40	1	0	-5.058600	0.246429	-1.018262
41	1	0	-4.234347	1.554435	-0.145784

E(RB3LYP) -940.44241459 a.u.

Table 75S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*syn*-6*g*$^{+}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.686667	1.571983	-0.872040
2	6	0	-0.924739	2.602324	0.258623
3	6	0	-0.523490	2.112906	1.627495
4	6	0	0.546448	1.347144	1.816840
5	6	0	1.354707	0.882596	0.635582
6	6	0	0.434313	0.548985	-0.558487
7	8	0	-2.259831	3.100214	0.222121
8	6	0	-1.693230	-0.464170	-0.537003
9	8	0	-1.909524	0.777412	-1.092021
10	6	0	-0.937151	-2.688987	0.900966
11	6	0	-2.240832	-2.560444	0.427134
12	6	0	-2.656277	-1.426629	-0.277981
13	8	0	-3.978983	-1.299351	-0.637471
14	6	0	2.199365	-0.374878	0.925593
15	6	0	1.389018	-1.641070	1.272112
16	6	0	0.022987	-1.707581	0.628589
17	6	0	-0.383992	-0.649083	-0.156613
18	6	0	1.315039	0.279823	-1.794870
19	6	0	2.316151	-0.837745	-1.561207
20	7	0	3.102125	-0.651142	-0.279823
21	6	0	4.226374	0.325169	-0.424830
22	1	0	-0.518670	2.098760	-1.806686
23	1	0	-0.293306	3.461698	0.016233
24	1	0	-1.107485	2.482560	2.461368
25	1	0	0.859590	1.059604	2.813232
26	1	0	2.037431	1.688020	0.353544
27	1	0	-2.847319	2.334302	0.172680
28	1	0	-0.680647	-3.548406	1.506766
29	1	0	-2.977012	-3.322301	0.647100
30	1	0	-4.102629	-0.476193	-1.127723
31	1	0	2.890117	-0.172498	1.739632
32	1	0	1.256543	-1.644589	2.355503
33	1	0	1.990485	-2.526026	1.052012
34	1	0	1.826378	1.204513	-2.067069
35	1	0	0.697468	-0.012146	-2.644660
36	1	0	3.041134	-0.903541	-2.367700
37	1	0	1.819624	-1.800096	-1.473482
38	1	0	3.541721	-1.552251	-0.090185
39	1	0	4.914888	-0.070050	-1.166110
40	1	0	3.848485	1.287388	-0.750144
41	1	0	4.726878	0.420996	0.534002

E(RB3LYP) -940.44321167 a.u.

Table 76S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*anti*-6g^{+}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.664748	1.584245	-0.878454
2	6	0	-0.895524	2.619260	0.249853
3	6	0	-0.497049	2.131242	1.620109
4	6	0	0.565547	1.355936	1.811979
5	6	0	1.367147	0.875641	0.632509
6	6	0	0.442496	0.548895	-0.559852
7	8	0	-2.228565	3.123146	0.212559
8	6	0	-1.697842	-0.438204	-0.542086
9	8	0	-1.896020	0.805138	-1.100672
10	6	0	-0.966467	-2.669056	0.905959
11	6	0	-2.267320	-2.528548	0.425817
12	6	0	-2.670576	-1.393067	-0.284846
13	8	0	-3.961304	-1.164005	-0.698566
14	6	0	2.195204	-0.391365	0.928567
15	6	0	1.367250	-1.644077	1.281235
16	6	0	0.002436	-1.698016	0.633942
17	6	0	-0.392552	-0.636926	-0.155424
18	6	0	1.320224	0.263254	-1.794674
19	6	0	2.306330	-0.866621	-1.556054
20	7	0	3.094373	-0.685652	-0.275071
21	6	0	4.233414	0.272792	-0.423778
22	1	0	-0.486992	2.107994	-1.813096
23	1	0	-0.258977	3.474478	0.006005
24	1	0	-1.075869	2.510924	2.453124
25	1	0	0.877031	1.070664	2.809559
26	1	0	2.060769	1.670142	0.346008
27	1	0	-2.816754	2.360191	0.131934
28	1	0	-0.721344	-3.529165	1.515498
29	1	0	-3.009220	-3.286528	0.645887
30	1	0	-4.521120	-1.899218	-0.417455
31	1	0	2.888454	-0.194225	1.741812
32	1	0	1.231359	-1.637717	2.364218
33	1	0	1.957541	-2.538789	1.069976
34	1	0	1.844010	1.179986	-2.070150
35	1	0	0.699506	-0.023732	-2.643879
36	1	0	3.030608	-0.946090	-2.361901
37	1	0	1.796773	-1.821765	-1.464512
38	1	0	3.521002	-1.592132	-0.081307
39	1	0	4.915928	-0.136315	-1.163091
40	1	0	3.871042	1.239560	-0.753444
41	1	0	4.734931	0.364740	0.534928

E(RB3LYP) -940.44309407 a.u.

Table 77S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*syn*-6*g*$^{-}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.699076	1.562430	-0.864087
2	6	0	-0.896999	2.601555	0.268763
3	6	0	-0.536774	2.089520	1.635149
4	6	0	0.523620	1.311679	1.826762
5	6	0	1.341797	0.865884	0.645155
6	6	0	0.426868	0.539762	-0.556965
7	8	0	-2.224338	3.119855	0.307164
8	6	0	-1.700842	-0.472139	-0.536971
9	8	0	-1.917844	0.769920	-1.085501
10	6	0	-0.940192	-2.708020	0.884350
11	6	0	-2.245829	-2.575092	0.416888
12	6	0	-2.662755	-1.436963	-0.280111
13	8	0	-3.986922	-1.306446	-0.634591
14	6	0	2.192323	-0.389363	0.924696
15	6	0	1.387667	-1.664360	1.253345
16	6	0	0.019287	-1.725362	0.613941
17	6	0	-0.389668	-0.662501	-0.164377
18	6	0	1.312499	0.283112	-1.792254
19	6	0	2.318976	-0.830895	-1.564396
20	7	0	3.100832	-0.647937	-0.280213
21	6	0	4.216316	0.339761	-0.415359
22	1	0	-0.531314	2.089977	-1.799388
23	1	0	-0.200318	3.414760	0.027907
24	1	0	-1.136520	2.445722	2.463255
25	1	0	0.816341	0.998695	2.821287
26	1	0	2.019386	1.679948	0.375453
27	1	0	-2.387664	3.594488	-0.516694
28	1	0	-0.682212	-3.570481	1.485205
29	1	0	-2.982125	-3.337078	0.636190
30	1	0	-4.115919	-0.464893	-1.091163
31	1	0	2.878996	-0.192492	1.743521
32	1	0	1.259707	-1.687383	2.336951
33	1	0	1.991447	-2.543155	1.015382
34	1	0	1.819779	1.212105	-2.057410
35	1	0	0.698310	-0.006087	-2.645473
36	1	0	3.046071	-0.886960	-2.369783
37	1	0	1.827540	-1.796542	-1.484288
38	1	0	3.548145	-1.546347	-0.096151
39	1	0	4.910915	-0.044195	-1.156858
40	1	0	3.830235	1.300258	-0.735837
41	1	0	4.712890	0.434537	0.545641

E(RB3LYP) -940.44132199 a.u.

Table 78S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*anti*-6*g*$^{-}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.677766	1.574094	-0.873063
2	6	0	-0.863420	2.623873	0.253009
3	6	0	-0.498206	2.122968	1.622137
4	6	0	0.554216	1.335064	1.816287
5	6	0	1.358652	0.862670	0.635754
6	6	0	0.433556	0.538918	-0.558505
7	8	0	-2.187613	3.149855	0.296047
8	6	0	-1.707780	-0.444703	-0.536513
9	8	0	-1.905900	0.797353	-1.092414
10	6	0	-0.971454	-2.682700	0.902435
11	6	0	-2.272823	-2.541273	0.423782
12	6	0	-2.677707	-1.404481	-0.283722
13	8	0	-3.969194	-1.179411	-0.699186
14	6	0	2.189171	-0.403514	0.926346
15	6	0	1.363189	-1.659075	1.273994
16	6	0	-0.003782	-1.710355	0.630703
17	6	0	-0.400939	-0.647510	-0.155176
18	6	0	1.310882	0.256537	-1.794179
19	6	0	2.299268	-0.872080	-1.559075
20	7	0	3.088330	-0.691519	-0.278794
21	6	0	4.223255	0.271899	-0.426520
22	1	0	-0.500793	2.094279	-1.810903
23	1	0	-0.164017	3.431609	0.001619
24	1	0	-1.086815	2.497027	2.450421
25	1	0	0.850208	1.032090	2.812973
26	1	0	2.049402	1.661206	0.353171
27	1	0	-2.360675	3.602922	-0.537908
28	1	0	-0.725128	-3.543961	1.509874
29	1	0	-3.013877	-3.300773	0.641703
30	1	0	-4.526056	-1.917714	-0.420507
31	1	0	2.882486	-0.208619	1.740088
32	1	0	1.230859	-1.659654	2.357409
33	1	0	1.953694	-2.551854	1.055328
34	1	0	1.832968	1.174468	-2.069012
35	1	0	0.689603	-0.029944	-2.643170
36	1	0	3.022801	-0.948770	-2.365896
37	1	0	1.791613	-1.828339	-1.468514
38	1	0	3.518562	-1.596822	-0.087579
39	1	0	4.906843	-0.132761	-1.167293
40	1	0	3.856480	1.237769	-0.753847
41	1	0	4.725329	0.364108	0.531863

E(RB3LYP) -940.44105548 a.u.

Table 79S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*syn*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.695548	1.559949	-0.869142
2	6	0	-0.874850	2.602597	0.250708
3	6	0	-0.543622	2.082247	1.627716
4	6	0	0.508914	1.295879	1.829822
5	6	0	1.335361	0.855118	0.651044
6	6	0	0.426113	0.533573	-0.557564
7	8	0	-2.192505	3.142464	0.157385
8	6	0	-1.705424	-0.471621	-0.536101
9	8	0	-1.922088	0.773825	-1.076129
10	6	0	-0.949160	-2.714344	0.875946
11	6	0	-2.255846	-2.575221	0.413328
12	6	0	-2.670550	-1.432945	-0.277937
13	8	0	-3.995634	-1.294511	-0.625959
14	6	0	2.185835	-0.400597	0.927921
15	6	0	1.381834	-1.679383	1.244291
16	6	0	0.013190	-1.734634	0.605121
17	6	0	-0.393406	-0.668420	-0.170054
18	6	0	1.317185	0.281277	-1.789682
19	6	0	2.324319	-0.831899	-1.561532
20	7	0	3.100606	-0.651406	-0.273735
21	6	0	4.213710	0.340112	-0.400897
22	1	0	-0.530916	2.078442	-1.809404
23	1	0	-0.148403	3.390151	0.013884
24	1	0	-1.156217	2.435013	2.448580
25	1	0	0.787631	0.970027	2.824405
26	1	0	2.013067	1.671240	0.387888
27	1	0	-2.208921	3.963329	0.662825
28	1	0	-0.692498	-3.579070	1.474102
29	1	0	-2.994469	-3.334791	0.633160
30	1	0	-4.122301	-0.450747	-1.079166
31	1	0	2.868048	-0.207733	1.751394
32	1	0	1.254277	-1.713834	2.327582
33	1	0	1.985707	-2.555596	0.996875
34	1	0	1.824125	1.211851	-2.049974
35	1	0	0.706665	-0.005724	-2.646261
36	1	0	3.054566	-0.883875	-2.364346
37	1	0	1.834137	-1.798616	-1.486656
38	1	0	3.550136	-1.548931	-0.090927
39	1	0	4.913225	-0.040057	-1.139711
40	1	0	3.826346	1.300078	-0.721288
41	1	0	4.705032	0.434331	0.562880

E(RB3LYP) -940.44066215 a.u.

Table 80S. B3LYP/SMD/cc-pVTZ Cartesian Coordinates of M^{+}_{ax}-3*anti*-6*anti*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.673600	1.571945	-0.877247
2	6	0	-0.839279	2.624569	0.236486
3	6	0	-0.506033	2.113073	1.616224
4	6	0	0.537590	1.315615	1.820971
5	6	0	1.351518	0.850090	0.643125
6	6	0	0.432979	0.532393	-0.558853
7	8	0	-2.153086	3.174458	0.145505
8	6	0	-1.712524	-0.443670	-0.536257
9	8	0	-1.909759	0.802661	-1.082418
10	6	0	-0.981687	-2.689866	0.891514
11	6	0	-2.284177	-2.540986	0.418406
12	6	0	-2.686456	-1.399193	-0.282323
13	8	0	-3.978614	-1.164541	-0.689989
14	6	0	2.181993	-0.416790	0.929783
15	6	0	1.356623	-1.676915	1.262882
16	6	0	-0.010551	-1.720984	0.619709
17	6	0	-0.404860	-0.653996	-0.162192
18	6	0	1.316453	0.255670	-1.791221
19	6	0	2.305651	-0.872180	-1.556730
20	7	0	3.088459	-0.695228	-0.272292
21	6	0	4.220204	0.273377	-0.410146
22	1	0	-0.499691	2.083595	-1.819713
23	1	0	-0.108075	3.404979	-0.009099
24	1	0	-1.108538	2.482673	2.437201
25	1	0	0.817772	0.997620	2.817718
26	1	0	2.042307	1.651436	0.368759
27	1	0	-2.161119	3.997560	0.647455
28	1	0	-0.737025	-3.553907	1.495674
29	1	0	-3.028029	-3.297564	0.636900
30	1	0	-4.538855	-1.900503	-0.411902
31	1	0	2.870348	-0.226850	1.748858
32	1	0	1.224591	-1.691087	2.346156
33	1	0	1.947196	-2.566803	1.032932
34	1	0	1.838246	1.175573	-2.060033
35	1	0	0.699225	-0.027940	-2.644104
36	1	0	3.032798	-0.943513	-2.360831
37	1	0	1.799487	-1.829855	-1.472798
38	1	0	3.521387	-1.599707	-0.083369
39	1	0	4.909358	-0.125451	-1.148926
40	1	0	3.851129	1.238948	-0.735606
41	1	0	4.716893	0.363842	0.551218

E(RB3LYP) -940.44034606 a.u.

Table 81S. B3LYP/cc-pVTZ Cartesian Coordinates of the Transition State of Morphine with the OH Groups in the 3*syn*-6g^+ Positions

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.861875	1.524024	-0.881932
2	6	0	-1.187456	2.548508	0.232868
3	6	0	-0.721069	2.114992	1.601964
4	6	0	0.423217	1.462616	1.779223
5	6	0	1.268560	1.065379	0.599737
6	6	0	0.371183	0.630328	-0.580847
7	8	0	-2.556355	2.915215	0.205151
8	6	0	-1.635439	-0.602126	-0.507982
9	8	0	-2.001727	0.606699	-1.057707
10	6	0	-0.640735	-2.718910	0.926569
11	6	0	-1.956003	-2.734235	0.469309
12	6	0	-2.493358	-1.654951	-0.236802
13	8	0	-3.815823	-1.653216	-0.585635
14	6	0	2.269544	-0.106190	0.835629
15	6	0	1.567369	-1.426730	1.275402
16	6	0	0.213676	-1.647635	0.638721
17	6	0	-0.309240	-0.643705	-0.150789
18	6	0	1.245868	0.437665	-1.840669
19	6	0	2.397081	-0.545681	-1.595560
20	7	0	3.083673	-0.279145	-0.352431
21	6	0	4.504601	-0.063330	-0.279239
22	1	0	-0.775526	2.046248	-1.832149
23	1	0	-0.640093	3.461904	-0.027229
24	1	0	-1.337834	2.429975	2.434350
25	1	0	0.767303	1.216586	2.777737
26	1	0	1.880215	1.922810	0.294999
27	1	0	-3.056413	2.106449	0.041403
28	1	0	-0.289867	-3.542345	1.535852
29	1	0	-2.608426	-3.565299	0.700526
30	1	0	-3.999426	-0.859835	-1.100250
31	1	0	2.944176	0.185001	1.642119
32	1	0	1.425299	-1.409606	2.360262
33	1	0	2.253433	-2.251695	1.072263
34	1	0	1.650438	1.414168	-2.123751
35	1	0	0.627115	0.083825	-2.668952
36	1	0	3.112720	-0.478005	-2.414663
37	1	0	1.994095	-1.568483	-1.622480
38	1	0	4.774532	0.963872	0.009075
39	1	0	4.952880	-0.252456	-1.254045
40	1	0	4.995367	-0.738792	0.433879

E(RB3LYP) -939.94540192 a.u.

Table 82S. B3LYP/cc-pVTZ Cartesian Coordinates of the Transition State of Morphine with the OH Groups in the 3*anti*-6g^+ Positions

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.835421	1.541317	-0.889592
2	6	0	-1.172961	2.558289	0.230613
3	6	0	-0.701204	2.125513	1.598312
4	6	0	0.441367	1.470231	1.776259
5	6	0	1.283625	1.061175	0.598364
6	6	0	0.383944	0.634461	-0.582602
7	8	0	-2.547364	2.900932	0.206331
8	6	0	-1.642886	-0.567348	-0.525978
9	8	0	-1.977384	0.639417	-1.085049
10	6	0	-0.667743	-2.698471	0.926692
11	6	0	-1.981305	-2.695478	0.462493
12	6	0	-2.510930	-1.614385	-0.248925
13	8	0	-3.818077	-1.519916	-0.638146
14	6	0	2.269408	-0.121030	0.839943
15	6	0	1.547028	-1.428777	1.282407
16	6	0	0.193807	-1.635934	0.639483
17	6	0	-0.318238	-0.629491	-0.155634
18	6	0	1.259281	0.426499	-1.839608
19	6	0	2.397455	-0.570474	-1.589905
20	7	0	3.084223	-0.310836	-0.345098
21	6	0	4.507610	-0.114543	-0.268423
22	1	0	-0.731988	2.072096	-1.833517
23	1	0	-0.635500	3.479968	-0.022601
24	1	0	-1.315077	2.444716	2.431337
25	1	0	0.786944	1.228680	2.775518
26	1	0	1.905662	1.910452	0.291974
27	1	0	-3.028780	2.100495	-0.041145
28	1	0	-0.329377	-3.524417	1.539452
29	1	0	-2.632730	-3.529175	0.700139
30	1	0	-4.297097	-2.292880	-0.323666
31	1	0	2.945956	0.163273	1.647349
32	1	0	1.398391	-1.403091	2.366214
33	1	0	2.221890	-2.264958	1.087888
34	1	0	1.676831	1.397179	-2.123632
35	1	0	0.637754	0.079358	-2.668522
36	1	0	3.116236	-0.512726	-2.407079
37	1	0	1.982671	-1.588676	-1.616775
38	1	0	4.790758	0.908867	0.020708
39	1	0	4.955630	-0.309468	-1.242224
40	1	0	4.987822	-0.796651	0.445778

E(RB3LYP) -939.94290068 a.u.

Table 83S. B3LYP/cc-pVTZ Cartesian Coordinates of the Transition State of Morphine with the OH Groups in the 3*syn*-6*anti* Positions

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.884867	1.502581	-0.878628
2	6	0	-1.163336	2.530664	0.237315
3	6	0	-0.769714	2.046775	1.612228
4	6	0	0.368556	1.387568	1.801593
5	6	0	1.240430	1.039995	0.625117
6	6	0	0.363461	0.619914	-0.579315
7	8	0	-2.520785	2.938011	0.140273
8	6	0	-1.635079	-0.619856	-0.526058
9	8	0	-2.004459	0.584699	-1.064194
10	6	0	-0.634146	-2.755188	0.880392
11	6	0	-1.955401	-2.759268	0.438039
12	6	0	-2.496128	-1.669387	-0.248521
13	8	0	-3.822106	-1.646095	-0.576825
14	6	0	2.257820	-0.120546	0.844542
15	6	0	1.572188	-1.464367	1.241231
16	6	0	0.219378	-1.681077	0.600219
17	6	0	-0.306524	-0.669029	-0.177205
18	6	0	1.256133	0.467565	-1.830924
19	6	0	2.418330	-0.503936	-1.592589
20	7	0	3.088230	-0.249311	-0.337685
21	6	0	4.503534	-0.008988	-0.244411
22	1	0	-0.796525	2.036098	-1.823005
23	1	0	-0.508796	3.381983	-0.009108
24	1	0	-1.426001	2.301871	2.436028
25	1	0	0.674067	1.083873	2.796411
26	1	0	1.839193	1.917303	0.351340
27	1	0	-2.645066	3.712140	0.696869
28	1	0	-0.281071	-3.585612	1.478984
29	1	0	-2.609674	-3.588020	0.672781
30	1	0	-4.025154	-0.782677	-0.955482
31	1	0	2.918604	0.160599	1.666051
32	1	0	1.433612	-1.485530	2.326453
33	1	0	2.270009	-2.272001	1.009749
34	1	0	1.650331	1.455372	-2.089278
35	1	0	0.651936	0.122658	-2.673496
36	1	0	3.141476	-0.412677	-2.402817
37	1	0	2.029289	-1.531238	-1.639917
38	1	0	4.751919	1.017119	0.067154
39	1	0	4.965787	-0.170149	-1.217769
40	1	0	4.999432	-0.689358	0.460663

E(RB3LYP) -939.93914903 a.u.

Table 84S. B3LYP/cc-pVTZ Cartesian Coordinates of the Transition State of Morphine with the OH Groups in the 3*anti*-6*anti* Positions

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.860571	1.519759	-0.882574
2	6	0	-1.090556	2.577832	0.215708
3	6	0	-0.719091	2.094925	1.597410
4	6	0	0.399190	1.403963	1.793330
5	6	0	1.258790	1.027103	0.616514
6	6	0	0.365986	0.612423	-0.578443
7	8	0	-2.423182	3.053285	0.111570
8	6	0	-1.665519	-0.577326	-0.512856
9	8	0	-2.005409	0.633620	-1.039465
10	6	0	-0.674437	-2.737620	0.898011
11	6	0	-1.990925	-2.726469	0.441479
12	6	0	-2.527616	-1.635753	-0.249393
13	8	0	-3.836049	-1.547143	-0.633609
14	6	0	2.254189	-0.149243	0.842362
15	6	0	1.541530	-1.472983	1.253775
16	6	0	0.184396	-1.672086	0.615392
17	6	0	-0.334390	-0.655931	-0.163325
18	6	0	1.248838	0.424730	-1.832626
19	6	0	2.395242	-0.564155	-1.590430
20	7	0	3.076503	-0.308071	-0.341830
21	6	0	4.496450	-0.094556	-0.257791
22	1	0	-0.766212	2.034730	-1.836992
23	1	0	-0.390917	3.389125	-0.043729
24	1	0	-1.372157	2.373356	2.416145
25	1	0	0.695357	1.095481	2.789519
26	1	0	1.871405	1.890439	0.329126
27	1	0	-2.508688	3.839123	0.658904
28	1	0	-0.332526	-3.570859	1.498898
29	1	0	-2.640714	-3.564242	0.670067
30	1	0	-4.306424	-2.327827	-0.325558
31	1	0	2.924226	0.125386	1.658641
32	1	0	1.401113	-1.477602	2.339024
33	1	0	2.221783	-2.298391	1.033158
34	1	0	1.659154	1.401812	-2.106131
35	1	0	0.632425	0.081164	-2.666751
36	1	0	3.115376	-0.493369	-2.405454
37	1	0	1.989552	-1.585638	-1.625380
38	1	0	4.766284	0.929365	0.042950
39	1	0	4.950396	-0.273505	-1.231971
40	1	0	4.983124	-0.777823	0.451131

E(RB3LYP) -939.93402638 a.u.

Table 85S. B3LYP/SMD(water)/cc-pVTZ Cartesian Coordinates of the Transition State of Morphine with the OH Groups in the 3*syn*-6g^+ Positions

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.858454	1.530822	-0.888970
2	6	0	-1.203652	2.535524	0.237382
3	6	0	-0.723354	2.111083	1.602377
4	6	0	0.431524	1.473181	1.773667
5	6	0	1.272921	1.078762	0.591381
6	6	0	0.373427	0.640881	-0.584869
7	8	0	-2.593974	2.861120	0.220407
8	6	0	-1.632252	-0.600540	-0.521994
9	8	0	-1.990679	0.602783	-1.091965
10	6	0	-0.633887	-2.700687	0.947502
11	6	0	-1.946602	-2.726275	0.480892
12	6	0	-2.483892	-1.656864	-0.241050
13	8	0	-3.817113	-1.677420	-0.594455
14	6	0	2.274985	-0.089924	0.831884
15	6	0	1.563145	-1.393058	1.299880
16	6	0	0.216116	-1.626131	0.653972
17	6	0	-0.307008	-0.632971	-0.150925
18	6	0	1.246396	0.449784	-1.844529
19	6	0	2.397008	-0.532324	-1.607102
20	7	0	3.083065	-0.280898	-0.359097
21	6	0	4.512104	-0.110031	-0.278385
22	1	0	-0.762308	2.066020	-1.829231
23	1	0	-0.688917	3.465142	-0.022075
24	1	0	-1.328797	2.426177	2.444098
25	1	0	0.789474	1.240306	2.770433
26	1	0	1.872474	1.941829	0.284759
27	1	0	-3.073767	2.026801	0.128131
28	1	0	-0.282825	-3.515207	1.568592
29	1	0	-2.594657	-3.559666	0.718966
30	1	0	-4.022892	-0.886176	-1.108229
31	1	0	2.952838	0.209003	1.631164
32	1	0	1.404354	-1.337779	2.380874
33	1	0	2.239241	-2.234622	1.140357
34	1	0	1.647530	1.428829	-2.119341
35	1	0	0.627821	0.100011	-2.674176
36	1	0	3.113805	-0.452337	-2.423667
37	1	0	1.998271	-1.557611	-1.652453
38	1	0	4.804637	0.886954	0.080723
39	1	0	4.951580	-0.237547	-1.267390
40	1	0	4.993677	-0.843099	0.383567

E(RB3LYP) -939.96055472 a.u.

Table 86S. B3LYP/SMD(water)/cc-pVTZ Cartesian Coordinates of the Transition State of Morphine with the OH Groups in the 3*anti*-6g^+ Positions

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.836690	1.545839	-0.893554
2	6	0	-1.175418	2.553339	0.232672
3	6	0	-0.704327	2.122561	1.598856
4	6	0	0.442153	1.470633	1.773788
5	6	0	1.283269	1.067986	0.594083
6	6	0	0.383205	0.641508	-0.585921
7	8	0	-2.563062	2.890724	0.211762
8	6	0	-1.638042	-0.575378	-0.531861
9	8	0	-1.978549	0.633413	-1.101230
10	6	0	-0.664685	-2.689860	0.939600
11	6	0	-1.977354	-2.699015	0.469970
12	6	0	-2.502162	-1.622968	-0.252186
13	8	0	-3.817650	-1.537526	-0.652898
14	6	0	2.272001	-0.111267	0.836580
15	6	0	1.544469	-1.407748	1.298731
16	6	0	0.196460	-1.624818	0.648836
17	6	0	-0.314483	-0.624750	-0.156742
18	6	0	1.259135	0.442121	-1.842334
19	6	0	2.398773	-0.551996	-1.602055
20	7	0	3.082923	-0.309254	-0.351347
21	6	0	4.513034	-0.152381	-0.265180
22	1	0	-0.729739	2.081618	-1.832446
23	1	0	-0.651347	3.478630	-0.023640
24	1	0	-1.309058	2.444063	2.438690
25	1	0	0.793708	1.232693	2.771648
26	1	0	1.892715	1.925270	0.290889
27	1	0	-3.048043	2.061258	0.102554
28	1	0	-0.325007	-3.508714	1.561304
29	1	0	-2.633123	-3.528120	0.707319
30	1	0	-4.292302	-2.317921	-0.339248
31	1	0	2.949657	0.178906	1.639255
32	1	0	1.383699	-1.354100	2.379470
33	1	0	2.211599	-2.256181	1.137721
34	1	0	1.671498	1.417191	-2.114677
35	1	0	0.640093	0.099655	-2.674691
36	1	0	3.119051	-0.478047	-2.416131
37	1	0	1.989880	-1.573175	-1.650335
38	1	0	4.815488	0.844974	0.085158
39	1	0	4.955881	-0.294882	-1.250618
40	1	0	4.982945	-0.884050	0.406457

E(RB3LYP) -939.96043274 a.u.

Table 87S. B3LYP/SMD(water)/cc-pVTZ Cartesian Coordinates of the Transition State of Morphine with the OH Groups in the 3*syn*-6*g*¯ Positions

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.881004	1.511735	-0.886087
2	6	0	-1.195838	2.535088	0.236043
3	6	0	-0.733773	2.107359	1.600777
4	6	0	0.418527	1.466031	1.773864
5	6	0	1.261059	1.076967	0.590846
6	6	0	0.361916	0.632594	-0.584038
7	8	0	-2.582643	2.867823	0.304939
8	6	0	-1.635132	-0.620803	-0.517295
9	8	0	-2.000851	0.576022	-1.090187
10	6	0	-0.618157	-2.717347	0.948292
11	6	0	-1.931033	-2.752068	0.482374
12	6	0	-2.476768	-1.686256	-0.238384
13	8	0	-3.809373	-1.718642	-0.594750
14	6	0	2.271300	-0.084850	0.830001
15	6	0	1.568950	-1.392524	1.299661
16	6	0	0.222647	-1.635228	0.655688
17	6	0	-0.308868	-0.645654	-0.147943
18	6	0	1.234101	0.446867	-1.844834
19	6	0	2.392159	-0.526990	-1.609216
20	7	0	3.078652	-0.270283	-0.362447
21	6	0	4.506614	-0.088962	-0.284407
22	1	0	-0.787763	2.044388	-1.829102
23	1	0	-0.628125	3.434155	-0.037480
24	1	0	-1.345457	2.417432	2.439505
25	1	0	0.769792	1.224969	2.770702
26	1	0	1.854136	1.944195	0.282581
27	1	0	-2.844667	3.247325	-0.542498
28	1	0	-0.260436	-3.529788	1.568327
29	1	0	-2.572602	-3.590796	0.719478
30	1	0	-4.027599	-0.911509	-1.077689
31	1	0	2.948698	0.218646	1.627974
32	1	0	1.411260	-1.337365	2.380852
33	1	0	2.250583	-2.229659	1.140462
34	1	0	1.627878	1.428497	-2.121230
35	1	0	0.616501	0.092236	-2.673174
36	1	0	3.107147	-0.442432	-2.426943
37	1	0	2.000591	-1.555073	-1.653325
38	1	0	4.791549	0.907307	0.082367
39	1	0	4.944209	-0.204443	-1.275738
40	1	0	4.996467	-0.823487	0.369998

E(RB3LYP) -939.95856790 a.u.

Table 88S. B3LYP/SMD(water)/cc-pVTZ Cartesian Coordinates of the Transition State of Morphine with the OH Groups in the 3*anti*-6*g*⁻ Positions

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.858908	1.527153	-0.891187
2	6	0	-1.161741	2.557143	0.228366
3	6	0	-0.709586	2.125194	1.595017
4	6	0	0.432744	1.467332	1.772063
5	6	0	1.272915	1.066315	0.591370
6	6	0	0.370923	0.632186	-0.585148
7	8	0	-2.544052	2.909302	0.293929
8	6	0	-1.643590	-0.594138	-0.523764
9	8	0	-1.990706	0.608616	-1.095558
10	6	0	-0.651691	-2.704204	0.946376
11	6	0	-1.963806	-2.723539	0.475311
12	6	0	-2.497062	-1.652279	-0.247753
13	8	0	-3.812368	-1.582473	-0.654118
14	6	0	2.268488	-0.106988	0.833606
15	6	0	1.549106	-1.406106	1.300887
16	6	0	0.200713	-1.632347	0.654753
17	6	0	-0.318653	-0.636668	-0.150650
18	6	0	1.244095	0.433771	-1.843496
19	6	0	2.389933	-0.553491	-1.604313
20	7	0	3.076740	-0.303239	-0.356505
21	6	0	4.506307	-0.138248	-0.275328
22	1	0	-0.755490	2.057600	-1.834555
23	1	0	-0.581079	3.447951	-0.045300
24	1	0	-1.319279	2.445061	2.431530
25	1	0	0.777832	1.222179	2.770059
26	1	0	1.876511	1.926522	0.284037
27	1	0	-2.803128	3.276246	-0.559926
28	1	0	-0.305741	-3.520228	1.568370
29	1	0	-2.612687	-3.558593	0.710945
30	1	0	-4.279145	-2.367704	-0.340855
31	1	0	2.947282	0.188406	1.633437
32	1	0	1.390840	-1.350409	2.381921
33	1	0	2.220758	-2.251165	1.140766
34	1	0	1.650486	1.410143	-2.120284
35	1	0	0.624093	0.085584	-2.672791
36	1	0	3.107379	-0.478201	-2.420796
37	1	0	1.986601	-1.577073	-1.648059
38	1	0	4.803472	0.859131	0.079138
39	1	0	4.946035	-0.272531	-1.263338
40	1	0	4.983975	-0.870321	0.390536

E(RB3LYP) -939.95827868 a.u.

Table 89S. B3LYP/SMD(water)/cc-pVTZ Cartesian Coordinates of the Transition State of Morphine with the OH Groups in the 3*syn*-6*anti* Positions

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.881635	1.507405	-0.893324
2	6	0	-1.183507	2.534344	0.216653
3	6	0	-0.743744	2.098967	1.591980
4	6	0	0.405803	1.455161	1.775103
5	6	0	1.254984	1.072140	0.593897
6	6	0	0.360298	0.627956	-0.585463
7	8	0	-2.570192	2.876950	0.156155
8	6	0	-1.637173	-0.625273	-0.517195
9	8	0	-2.005675	0.572789	-1.085311
10	6	0	-0.619332	-2.722706	0.945945
11	6	0	-1.932858	-2.756916	0.481845
12	6	0	-2.479132	-1.690197	-0.236988
13	8	0	-3.812545	-1.720621	-0.590438
14	6	0	2.267479	-0.087535	0.833296
15	6	0	1.566850	-1.397862	1.298197
16	6	0	0.221548	-1.640955	0.652306
17	6	0	-0.310128	-0.651101	-0.151107
18	6	0	1.236637	0.444829	-1.843604
19	6	0	2.395991	-0.526676	-1.605488
20	7	0	3.078764	-0.268583	-0.357070
21	6	0	4.505942	-0.082904	-0.275107
22	1	0	-0.790833	2.031454	-1.840724
23	1	0	-0.590415	3.417256	-0.053769
24	1	0	-1.366915	2.404851	2.424565
25	1	0	0.748303	1.204476	2.772794
26	1	0	1.846306	1.941768	0.288866
27	1	0	-2.692567	3.680910	0.673901
28	1	0	-0.261134	-3.535077	1.565798
29	1	0	-2.574478	-3.595378	0.719747
30	1	0	-4.029784	-0.914445	-1.075467
31	1	0	2.941812	0.215909	1.633874
32	1	0	1.407480	-1.345842	2.379281
33	1	0	2.250040	-2.233497	1.138019
34	1	0	1.629173	1.427498	-2.118136
35	1	0	0.622007	0.089820	-2.674001
36	1	0	3.112682	-0.440579	-2.421538
37	1	0	2.006611	-1.555554	-1.650495
38	1	0	4.786577	0.913426	0.094717
39	1	0	4.946322	-0.194574	-1.265647
40	1	0	4.996627	-0.817357	0.378788

E(RB3LYP) -939.95784916 a.u.

Table 90S. B3LYP/SMD(water)/cc-pVTZ Cartesian Coordinates of the Transition State of Morphine with the OH Groups in the 3*anti*-6*anti* Positions

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.858689	1.523681	-0.896505
2	6	0	-1.144405	2.557631	0.211059
3	6	0	-0.721409	2.112424	1.588549
4	6	0	0.416361	1.449169	1.776169
5	6	0	1.265409	1.057980	0.597401
6	6	0	0.369227	0.626774	-0.585886
7	8	0	-2.523156	2.929584	0.142518
8	6	0	-1.646946	-0.597610	-0.523910
9	8	0	-1.996679	0.608362	-1.086971
10	6	0	-0.654369	-2.712871	0.937952
11	6	0	-1.967711	-2.729326	0.470342
12	6	0	-2.501454	-1.654967	-0.247546
13	8	0	-3.818311	-1.581148	-0.648096
14	6	0	2.263713	-0.113240	0.837472
15	6	0	1.546212	-1.416868	1.295249
16	6	0	0.198666	-1.641450	0.646734
17	6	0	-0.320700	-0.643448	-0.156075
18	6	0	1.247711	0.433793	-1.841184
19	6	0	2.395241	-0.550940	-1.600662
20	7	0	3.077222	-0.300791	-0.350363
21	6	0	4.505845	-0.130679	-0.263663
22	1	0	-0.758097	2.045242	-1.844483
23	1	0	-0.531001	3.427472	-0.056436
24	1	0	-1.345272	2.425449	2.417937
25	1	0	0.749072	1.188917	2.774718
26	1	0	1.866941	1.921869	0.296170
27	1	0	-2.632090	3.736078	0.659267
28	1	0	-0.308021	-3.530397	1.557746
29	1	0	-2.617291	-3.563864	0.705901
30	1	0	-4.284908	-2.367074	-0.336316
31	1	0	2.938445	0.180049	1.641490
32	1	0	1.386204	-1.368061	2.376331
33	1	0	2.219420	-2.259902	1.131380
34	1	0	1.652639	1.411976	-2.113789
35	1	0	0.631419	0.086696	-2.673713
36	1	0	3.114880	-0.472256	-2.414870
37	1	0	1.994718	-1.575510	-1.647327
38	1	0	4.797382	0.865475	0.098617
39	1	0	4.949122	-0.256084	-1.251267
40	1	0	4.984828	-0.865240	0.398593

E(RB3LYP) -939.95751558 a.u.

Table 91S. Relative energies of fully optimized conformers[a,b] of morphine

Method:	MP2	B3LYP			PBE0			B3LYP/SMD(water)
Relative energy:	ΔE/kJ mol^{-1}	ΔE/kJ mol^{-1}	ΔH^{o}/kJ mol^{-1}	ΔG^{o}/kJ mol^{-1}	ΔE/kJ mol^{-1}	ΔH^{o}/kJ mol^{-1}	ΔG^{o}/kJ mol^{-1}	ΔE/kJ mol^{-1}
M_{ax}-3*anti*-6*anti*	37.6	39.6	38.1	35.8	38.5	36.9	34.8	16.6
M_{equ}-3*anti*-6*anti*	29.4	29.4	27.8	25.9	28.9	27.2	25.3	8.1
M_{ax}-3*syn*-6*anti*	23.9	26.3	25.5	23.9	25.5	24.7	23.3	15.4
M_{ax}-3*anti*-6g^-	[c]							14.7
M_{ax}-3*syn*-6g^-	[c]							13.6
M_{ax}-3*anti*-6g^+	14.8	16.8	16.5	16.1	15.7	15.4	15.1	9.1
M_{equ}-3*syn*-6*anti*	15.4	15.9	15.1	13.5	15.8	14.9	13.1	6.7
M_{ax}-3*syn*-6g^+	8.3	10.3	10.4	10.2	9.8	9.8	9.6	8.6
M_{equ}-3*anti*-6g^-	[c]							6.3
M_{equ}-3*syn*-6g^-	[c]							5.0
M_{equ}-3*anti*-6g^+	6.7	6.6	6.3	6.3	6.1	5.7	5.8	0.8
M_{equ}-3*syn*-6g^+	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

[a] The cc-pVTZ basis set was used in all calculations; see text. [b] Enthalpies and Gibbs energies refer to 298.15 K and 1 atm. [c] This form was not found as a minimum on the conformational energy hypersurface in the isolated state; see article.

Table 92S. Relative energies of fully optimized conformers[a,b] of morphinum

Method:	MP2	B3LYP			PBE0			B3LYP/SMD(water)
Relative energy:	ΔE/kJ mol^{-1}	ΔE/kJ mol^{-1}	ΔH^{o}/kJ mol^{-1}	ΔG^{o}/kJ mol^{-1}	ΔE/kJ mol^{-1}	ΔH^{o}/kJ mol^{-1}	ΔG^{o}/kJ mol^{-1}	ΔE/kJ mol^{-1}
M^{+}_{ax}-3*anti*-6*anti*	21.9	23.6	22.8	21.0	23.2	22.5	21.1	13.2
M^{+}_{equ}-3*anti*-6*anti*	18.0	18.0	16.9	15.6	17.6	16.6	15.3	7.7
M^{+}_{ax}-3*syn*-6*anti*	12.5	14.5	14.2	12.5	14.5	14.2	13.0	12.3
M^{+}_{ax}-3*anti*-6g^{-}	9.9	–[c]			–[c]			11.3
M^{+}_{ax}-3*syn*-6g^{-}	9.3	11.5	11.7	8.3[d]	12.0	12.1	7.4[e]	10.6
M^{+}_{equ}-3*syn*-6*anti*	8.7	9.0	8.4	7.2	9.0	8.5	7.2	6.5
M^{+}_{ax}-3*anti*-6g^{+}	5.9	7.7	7.9	8.4	7.8	7.4	7.6	5.9
M^{+}_{equ}-3*anti*-6g^{-}	5.3	-[f]	-	-	-[g]	-	-	5.9
M^{+}_{equ}-3*syn*-6g^{-}	4.6	5.9	5.9	2.4[h]	6.3	6.4	3.3[i]	4.8
M^{+}_{ax}-3*syn*-6g^{+}	3.9	5.6	5.9	5.8	5.6	6.0	5.9	5.6
M^{+}_{equ}-3*anti*-6g^{+}	2.1	2.2	1.9	2.0	1.6	1.4	1.6	0.6
M^{+}_{equ}-3*syn*-6g^{+}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

(Table 92S continues next page)

(Table 92S continued)

[a] The cc-pVTZ basis set was used in all calculations; see text. [b] Enthalpies and Gibbs energies refer to 298.15 K and 1 atm. [c] This conformer was not found in both the B3LYP and in the PBE0 calculations. Calculations refined to M^{+}_{ax}-3*anti*–6g^{+}; see text. [d] Lowest torsional frequency is 19 cm^{-1}. [e] Lowest torsional frequency is 13 cm^{-1}. [f] Imaginary vibrational frequency. Relative electronic energy of stationary point: 7.6 kJ/mol. [g]Imaginary vibrational frequency. Relative electronic energy of stationary point: 7.3 kJ/mol. [h] Lowest torsional frequency is 20 cm^{-1}. [i] Lowest torsional frequency is 23 cm^{-1}.

Table 93S. Comparison of MP2 bond distances of the low-energy conformers of morphine and morphinum with experimental values from X-ray studies[a]

Compound:	Morphine[b]		Morphinum[c]	
Method:	X-Ray[1]	MP2[2]	X-ray[3]	MP2[2]
	(Å)	(Å)	(Å)	(Å)
O-C3	1.380(7)	1.365	1.375(2)	1.353
O-C4	1.385(7)	1.370	1.3770(17)	1.373
O-C5	1.483(7)	1.466	1.4196(19)	1.464
O-C6	1.442(8)	1.414	1.4665(18)	1.405
N17-C9	1.474(8)	1.466	1.517(2)	1.522
N17-C15	1.456(8)	1.457	1.497(2)	1.502
N17-CH_3	1.460(8)	1.451	1.492(2)	1.490
C1-C2	1.387(9)	1.398	1.388(2)	1.401
C1-C11	1.397(8)	1.399	1.395(2)	1.402
C2-C3	1.390(8)	1.400	1.395(2)	1.401
C3-C4	1.374(8)	1.390	1.390(2)	1.391
C4-C12	1.371(8)	1.383	1.370(2)	1.376
C5-C6	1.542(8)	1.539	1.536(2)	1.538
C5-C13	1.563(9)	1.538	1.549(2)	1.543
C6-C7	1.486(9)	1.505	1.504(2)	1.505
C7-C8	1.331(9)	1.340	1.320(2)	1.339
C8-C14	1.512(9)	1.500	–[d]	1.502
C9-C10	1.566(9)	1.552	1.540(2)	1.537
C9-C14	1.538(9)	1.538	1.535(2)	1.514
C10-C11	1.516(8)	1.506	1.511(2)	1.507
C11-C12	1.387(8)	1.379	1.380(2)	1.383
C12-C13	1.507(8)	1.495	1.503(2)	1.494

C13-C14	1.511(9)	1.536	1.538(2)	1.537
C13-C16	1.535(8)	1.530	1.543(2)	1.537
C15-16	1.512(8)	1.519	1.516(2)	1.514

[a] Uncertainties represent one standard deviation. [b] M_{equ}-3*anti*-6g^+ conformer; see text. [c] M^+_{equ}-3*syni*-6g^+ conformer; see article. [d] Not given.

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REFERENCES

1. T. Gelbrich, D. E. Braun and U. J. Griesser, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2013, **69**, o2.
2. *This work*
3. T. Gelbrich, D. E. Braun and U. J. Griesser, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2012, **68**, o3358-o3359.