BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

On the aromaticity and photophysics of 1-arylbenzo[*a*]imidazo[5,1,2-*cd*]indolizines as bicolor fluorescent molecules for barium tagging in the study of double-beta decay of ^{136}Xe

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Beilstein J. Org. Chem. **2025,** *21,* 1627–1638. doi:10.3762/bjoc.21.126

Cartesian coordinates of the optimized structures

Cartesian coordinates of all the stationary points discussed in the main text

1 (S_0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.313815	2.199899	0.000000
2	6	0	1.163644	2.989069	0.000000
3	6	0	-0.082170	2.343002	-0.000000
4	7	0	0.000000	0.976132	-0.000000
5	6	0	1.078281	0.135525	0.000000
6	6	0	2.299495	0.780334	0.000000
7	7	0	-1.390766	2.686558	-0.000000
8	6	0	-2.090172	1.518370	-0.000000
9	6	0	-1.236701	0.398700	-0.000000
10	6	0	0.470554	-1.188346	0.000000
11	6	0	-0.962957	-1.023604	-0.000000
12	6	0	-1.787372	-2.151083	-0.000000
13	6	0	-1.201987	-3.411203	-0.000000
14	6	0	0.193169	-3.569839	0.000000
15	6	0	1.034407	-2.464391	0.000000
16	1	0	3.276797	2.695792	0.000000
17	1	0	1.220977	4.068804	-0.000000
18	1	0	3.227602	0.225334	0.000000
19	1	0	-3.169530	1.526633	-0.000000
20	1	0	-2.865400	-2.044957	-0.000000
21	1	0	-1.835019	-4.290818	-0.000000
22	1	0	0.617157	-4.566654	0.000000
23	1	0	2.110737	-2.591556	0.000000

1 (S_1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.269672	2.271280	0.000000
2	6	0	1.090943	3.045375	-0.000000
3	6	0	-0.128685	2.317132	-0.000000
4	7	0	0.000000	0.986054	-0.000000
5	6	0	1.086460	0.161220	0.000000
6	6	0	2.321799	0.866821	0.000000
7	7	0	-1.483437	2.612683	-0.000000
8	6	0	-2.152273	1.448329	-0.000000
9	6	0	-1.244906	0.343410	-0.000000
10	6	0	0.521343	-1.160690	0.000000
11	6	0	-0.942584	-1.049966	-0.000000
12	6	0	-1.746055	-2.188483	-0.000000
13	6	0	-1.140056	-3.453175	0.000000
14	6	0	0.256477	-3.559238	0.000000
15	6	0	1.094482	-2.431997	0.000000
16	1	0	3.214578	2.803749	0.000000
17	1	0	1.107755	4.123410	-0.000000
18	1	0	3.267700	0.346361	0.000000
19	1	0	-3.230091	1.416707	-0.000000
20	1	0	-2.825657	-2.095135	-0.000000
21	1	0	-1.750117	-4.346723	0.000000
22	1	0	0.709587	-4.544079	0.000000
23	1	0	2.170606	-2.555543	0.000000

2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.652359	-1.788447	-0.238304
2	6	0	3.189395	-0.416717	0.273562
3	6	0	2.191741	0.674667	0.027304
4	7	0	0.913866	0.258206	-0.077769
5	6	0	0.327442	-1.009882	-0.002331
6	6	0	1.167281	-2.053911	-0.020053
7	7	0	2.222661	1.997933	0.045604
8	6	0	0.896538	2.419786	-0.030178
9	6	0	0.048994	1.326120	-0.090234
10	6	0	-1.116487	-0.702186	0.022694
11	6	0	-1.282476	0.718559	-0.049866
12	6	0	-2.559655	1.265847	-0.055552
13	6	0	-3.661778	0.410225	0.009492
14	6	0	-3.498062	-0.974546	0.076883
15	6	0	-2.220450	-1.539518	0.081256
16	1	0	2.837325	-1.853562	-1.320180
17	1	0	3.243973	-2.586727	0.214891
18	1	0	4.149406	-0.194076	-0.193910
19	1	0	3.367566	-0.470208	1.355392
20	1	0	0.809077	-3.074335	0.016729
21	1	0	0.653108	3.469589	-0.031775
22	1	0	-2.699377	2.338667	-0.110328
23	1	0	-4.661193	0.829332	0.006244
24	1	0	-4.369074	-1.616699	0.126472
25	1	0	-2.095551	-2.614930	0.133577

3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.604477	-1.838988	-0.110322
2	6	0	3.134131	-0.577777	-0.134364
3	6	0	2.227311	0.543335	-0.015627
4	7	0	1.002189	0.179081	0.556918
5	6	0	0.389686	-1.021864	0.275220
6	6	0	1.192397	-2.092782	0.004162
7	7	0	2.287023	1.760975	-0.432826
8	6	0	0.912199	2.321542	-0.338246
9	6	0	0.104090	1.333832	0.563111
10	6	0	-1.039619	-0.722075	0.147729
11	6	0	-1.212378	0.680437	0.210911
12	6	0	-2.470720	1.239166	0.045375
13	6	0	-3.554945	0.394544	-0.205174
14	6	0	-3.383503	-0.991018	-0.268136
15	6	0	-2.124627	-1.561411	-0.091456
16	1	0	3.264247	-2.683334	-0.277569
17	1	0	4.174858	-0.398580	-0.366297
18	1	0	0.783256	-3.070152	-0.206847
19	1	0	0.930353	3.319361	0.100048
20	1	0	0.495188	2.404770	-1.349315
21	1	0	0.044415	1.739001	1.581143
22	1	0	-2.613535	2.312377	0.101313
23	1	0	-4.541624	0.817979	-0.351648
24	1	0	-4.239623	-1.627604	-0.457482
25	1	0	-1.993013	-2.635850	-0.141080

4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.714009	-1.733111	0.178623
2	6	0	3.085500	-0.364276	-0.454494
3	6	0	2.040973	0.676391	-0.159197
4	7	0	0.994452	0.260217	0.695068
5	6	0	0.413656	-0.989507	0.318577
6	6	0	1.236379	-2.011763	0.047491
7	7	0	1.932049	1.839603	-0.665793
8	6	0	0.640771	2.408345	-0.232034
9	6	0	-0.014767	1.342042	0.706054
10	6	0	-1.019617	-0.749267	0.138733
11	6	0	-1.278149	0.623687	0.296554
12	6	0	-2.559840	1.125571	0.117909
13	6	0	-3.586758	0.244200	-0.226167
14	6	0	-3.331392	-1.121760	-0.377418
15	6	0	-2.046755	-1.629211	-0.196029
16	1	0	3.309741	-2.523472	-0.280569
17	1	0	2.986399	-1.705655	1.241703
18	1	0	3.165118	-0.450799	-1.540912
19	1	0	4.058258	-0.023673	-0.089410
20	1	0	0.865014	-2.964344	-0.304639
21	1	0	0.805578	3.348640	0.298001
22	1	0	0.031124	2.626491	-1.113909
23	1	0	-0.121452	1.742194	1.718558
24	1	0	-2.764883	2.183284	0.241522
25	1	0	-4.592070	0.621107	-0.373357
26	1	0	-4.141711	-1.792109	-0.638892
27	1	0	-1.850697	-2.688441	-0.314630

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.319264	-2.093397	-0.000162
2	1	0	0.976485	-3.119199	-0.009772
3	6	0	0.420001	-1.032843	-0.042763
4	7	0	1.029385	0.192998	-0.020776
5	6	0	0.190222	1.268633	-0.053852
6	6	0	-0.983739	-0.707256	-0.095680
7	6	0	-1.117190	0.692637	-0.099079
8	6	0	-2.471042	1.318731	-0.235196
9	1	0	-2.498539	2.312937	0.216821
10	1	0	-2.682732	1.453419	-1.305531
11	6	0	-3.550320	0.414588	0.390997
12	1	0	-4.541430	0.763046	0.090556
13	1	0	-3.509611	0.510896	1.486200
14	6	0	2.699267	-1.805148	0.058418
15	1	0	3.389371	-2.639808	0.089234
16	6	0	3.234689	-0.506660	0.081325
17	1	0	4.301461	-0.338555	0.128307
18	6	0	2.341211	0.563564	0.041544
19	7	0	2.390582	1.927026	0.046208
20	6	0	1.109279	2.352251	-0.009592
21	1	0	0.881704	3.407933	-0.015831
22	6	0	-2.150614	-1.567807	-0.159681
23	1	0	-2.021955	-2.625529	-0.361615
24	6	0	-3.371663	-1.044981	0.038911
25	1	0	-4.250711	-1.679178	0.012462

6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.263396	-2.095408	-0.031503
2	1	0	0.895276	-3.112263	-0.055088
3	6	0	0.387408	-1.011415	-0.059530
4	7	0	1.030778	0.200913	-0.024915
5	6	0	0.222825	1.295462	-0.044265
6	6	0	-0.999573	-0.658209	-0.103820
7	6	0	-1.105012	0.744059	-0.098223
8	6	0	2.648687	-1.842480	0.034315
9	1	0	3.317779	-2.694415	0.056333
10	6	0	3.217413	-0.557842	0.077642
11	1	0	4.287922	-0.418403	0.132611
12	6	0	2.352464	0.536183	0.049512
13	7	0	2.436791	1.896373	0.075363
14	6	0	1.165424	2.354739	0.022696
15	1	0	0.964113	3.415635	0.031941
16	6	0	-2.223410	-1.512831	-0.246753
17	1	0	-2.080163	-2.496537	0.207467
18	1	0	-2.419313	-1.684675	-1.314697
19	6	0	-3.439709	-0.811700	0.387646
20	1	0	-3.383473	-0.905955	1.482355
21	1	0	-4.360057	-1.316970	0.084517
22	6	0	-3.511743	0.659641	0.051623
23	1	0	-4.486410	1.135535	0.042755
24	6	0	-2.402876	1.389996	-0.152691
25	1	0	-2.460433	2.455883	-0.341243

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.343277	-2.091345	-0.041480
2	1	0	-0.982776	-3.111057	-0.062388
3	6	0	-0.462617	-1.015923	-0.020851
4	7	0	-1.093351	0.198277	0.004696
5	6	0	-0.271870	1.282148	0.025115
6	6	0	0.938864	-0.673160	-0.014376
7	6	0	1.053989	0.719582	0.011465
8	6	0	2.114746	-1.604430	-0.038237
9	1	0	2.235132	-2.027714	-1.044245
10	1	0	1.944077	-2.453455	0.631808
11	6	0	2.370428	1.434538	0.031740
12	1	0	2.342360	2.299261	-0.638677
13	1	0	2.548700	1.835390	1.038118
14	6	0	3.515747	0.486607	-0.359742
15	1	0	4.477041	0.957151	-0.136660
16	1	0	3.488513	0.316132	-1.442292
17	6	0	3.399871	-0.861612	0.363397
18	1	0	4.271346	-1.485219	0.146669
19	1	0	3.392776	-0.688414	1.445883
20	6	0	-2.731199	-1.826687	-0.036383
21	1	0	-3.407462	-2.673107	-0.053075
22	6	0	-3.288775	-0.539263	-0.011846
23	1	0	-4.359540	-0.390354	-0.009990
24	6	0	-2.413383	0.548925	0.010133
25	7	0	-2.483450	1.908296	0.035394
26	6	0	-1.202830	2.351486	0.044388
27	1	0	-0.990713	3.410180	0.064275

8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.190960	-0.143137	-0.000000
2	1	0	3.260159	0.020412	-0.000000
3	6	0	1.357507	0.934932	-0.000000
4	1	0	1.694185	1.962332	-0.000000
5	7	0	0.000000	0.732933	0.000000
6	6	0	-1.054243	1.623131	0.000000
7	1	0	-0.902634	2.688841	0.000000
8	6	0	-2.190372	0.841619	0.000000
9	1	0	-3.213021	1.187702	0.000000
10	7	0	-1.894056	-0.489018	0.000000
11	6	0	-0.567007	-0.558065	0.000000
12	6	0	1.660525	-1.463965	-0.000000
13	1	0	2.337922	-2.308530	-0.000000
14	6	0	0.305113	-1.668041	-0.000000
15	1	0	-0.133107	-2.657004	-0.000000

9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.987207	0.885130	0.016048
2	1	0	-2.876798	1.499279	-0.041239
3	6	0	-0.790763	1.454235	-0.143832
4	1	0	-0.635970	2.507319	-0.335713
5	7	0	0.373656	0.669981	-0.064024
6	7	0	1.561132	-1.205175	0.033996
7	6	0	0.351834	-0.707579	-0.071081
8	6	0	-2.111620	-0.587099	0.327848
9	1	0	-2.118426	-0.715451	1.419017
10	1	0	-3.067106	-0.974183	-0.033000
11	6	0	-0.954215	-1.401664	-0.281215
12	1	0	-0.903848	-2.405151	0.142172
13	1	0	-1.119142	-1.514138	-1.360809
14	6	0	1.700839	1.054545	0.053352
15	1	0	1.992476	2.090104	0.099293
16	6	0	2.409442	-0.114472	0.115864
17	1	0	3.475451	-0.240008	0.218567

10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.284199	0.082640	0.000000
2	1	0	-3.325314	0.370124	0.000000
3	6	0	-1.308621	1.034667	0.000000
4	1	0	-1.516792	2.097370	0.000000
5	7	0	-0.000000	0.676357	0.000000
6	7	0	1.732339	-0.812172	0.000000
7	6	0	0.453449	-0.660210	0.000000
8	6	0	-1.890041	-1.294608	0.000000
9	1	0	-2.659097	-2.059004	0.000000

10	6	0	-0.580675	-1.664393	0.000000
11	1	0	-0.271036	-2.700386	0.000000
12	6	0	1.168756	1.564095	0.000000
13	1	0	1.161483	2.200860	0.888202
14	1	0	1.161483	2.200860	-0.888202
15	6	0	2.336830	0.528082	0.000000
16	1	0	2.974952	0.649622	-0.880086
17	1	0	2.974952	0.649622	0.880086

11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.040618	0.900817	0.089230
2	1	0	-2.914383	1.539059	0.116237
3	6	0	-0.842066	1.439360	-0.170116
4	1	0	-0.702769	2.499492	-0.344996
5	7	0	0.315462	0.665591	-0.264845
6	7	0	1.392158	-1.297832	0.110697
7	6	0	0.275483	-0.721468	-0.123668
8	6	0	1.659228	1.112317	0.120859
9	1	0	1.636000	1.571700	1.116629
10	1	0	2.059429	1.837855	-0.590128
11	6	0	2.422823	-0.238931	0.118707
12	1	0	3.042394	-0.347498	-0.777636
13	1	0	3.076127	-0.350161	0.985564
14	6	0	-2.183796	-0.576914	0.359448
15	1	0	-2.168199	-0.757606	1.442606
16	1	0	-3.151682	-0.941601	0.005501
17	6	0	-1.055452	-1.381185	-0.316140
18	1	0	-0.998815	-2.405642	0.050525
19	1	0	-1.245053	-1.423889	-1.395178

12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.051076	1.422065	0.110802
2	1	0	0.013601	2.506307	0.112398
3	6	0	-0.051076	0.730563	1.255119
4	1	0	-0.188893	1.243185	2.201101
5	6	0	0.051076	-0.730563	1.255119
6	1	0	0.188893	-1.243185	2.201101
7	6	0	-0.051076	-1.422065	0.110802
8	1	0	-0.013601	-2.506307	0.112398
9	6	0	-0.309576	-0.702356	-1.190108
10	1	0	-1.398855	-0.624178	-1.331274
11	1	0	0.068520	-1.280602	-2.037106
12	6	0	0.309576	0.702356	-1.190108
13	1	0	-0.068520	1.280602	-2.037106
14	1	0	1.398855	0.624178	-1.331274

13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.120665	-0.656064	1.303401
2	1	0	-0.227666	-1.178502	2.250285
3	6	0	0.120665	0.656064	1.303401
4	1	0	0.227666	1.178502	2.250285
5	6	0	0.253305	1.477288	0.046506
6	1	0	1.305887	1.761185	-0.091600
7	1	0	-0.292381	2.420002	0.164946
8	6	0	-0.253305	0.723007	-1.189702
9	1	0	0.056246	1.241425	-2.101754
10	1	0	-1.349605	0.717297	-1.183107
11	6	0	0.253305	-0.723007	-1.189702
12	1	0	1.349605	-0.717297	-1.183107
13	1	0	-0.056246	-1.241425	-2.101754
14	6	0	-0.253305	-1.477288	0.046506
15	1	0	0.292381	-2.420002	0.164946
16	1	0	-1.305887	-1.761185	-0.091600

14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000000	1.394109	0.000000
2	1	0	-0.000000	2.478130	0.000000
3	6	0	1.207334	0.697054	0.000000
4	1	0	2.146124	1.239065	0.000000
5	6	0	1.207334	-0.697054	0.000000
6	1	0	2.146124	-1.239065	0.000000
7	6	0	-0.000000	-1.394109	0.000000
8	1	0	-0.000000	-2.478130	0.000000
9	6	0	-1.207334	0.697054	0.000000
10	1	0	-2.146124	1.239065	0.000000
11	6	0	-1.207334	-0.697054	0.000000
12	1	0	-2.146124	-1.239065	0.000000

15a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.577182	0.000092	-0.700894
2	8	0	-0.000000	-2.150065	0.024390
3	8	0	1.577182	-0.000092	-0.700894
4	8	0	0.000000	2.150065	0.024390
5	6	0	1.251230	-2.394339	-0.660886
6	6	0	1.703784	-1.204248	-1.491455
7	6	0	1.699920	1.202329	-1.494705
8	6	0	1.248635	2.394074	-0.665808
9	6	0	-1.251230	2.394339	-0.660886
10	6	0	-1.703784	1.204248	-1.491455
11	6	0	-1.699920	-1.202329	-1.494705
12	6	0	-1.248635	-2.394074	-0.665808
13	1	0	1.169101	-3.284150	-1.289263
14	1	0	1.971306	-2.614703	0.130057
15	1	0	2.745678	-1.348334	-1.792740
16	1	0	1.098920	-1.091593	-2.394837

17	1	0	2.740743	1.346950	-1.799443
18	1	0	1.092525	1.086585	-2.395996
19	1	0	1.163034	3.281921	-1.296495
20	1	0	1.971130	2.617558	0.121979
21	1	0	-1.169101	3.284150	-1.289263
22	1	0	-1.971306	2.614703	0.130057
23	1	0	-2.745678	1.348334	-1.792740
24	1	0	-1.098920	1.091593	-2.394837
25	1	0	-2.740743	-1.346950	-1.799443
26	1	0	-1.092525	-1.086585	-2.395996
27	1	0	-1.163034	-3.281921	-1.296495
28	1	0	-1.971130	-2.617558	0.121979
29	56	0	-0.000000	0.000000	1.500210

15b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.035764	-2.029192	0.308120
2	8	0	-2.416115	0.384164	-0.096724
3	8	0	-0.379781	2.069781	0.471399
4	8	0	2.139603	1.106290	0.176220
5	8	0	1.594125	-1.516150	0.284950
6	6	0	-2.611364	1.390389	0.923705
7	6	0	-1.727875	2.573133	0.590713
8	6	0	0.697561	3.030804	0.436023
9	6	0	1.946680	2.328772	0.925082
10	6	0	3.116788	0.234814	0.792951
11	6	0	2.989399	-1.158169	0.208087
12	6	0	1.210635	-2.898474	0.431588
13	6	0	-0.164872	-2.900213	1.067144
14	6	0	-2.323810	-1.838867	0.935878
15	6	0	-3.128607	-0.859593	0.103551
16	1	0	-3.659589	1.700511	0.936203
17	1	0	-2.341772	0.980319	1.901168
18	1	0	-1.782957	3.308705	1.397429
19	1	0	-2.032849	3.051079	-0.346299
20	1	0	0.478714	3.871418	1.099229
21	1	0	0.812975	3.420690	-0.582169
22	1	0	2.814661	2.983152	0.803762
23	1	0	1.834917	2.072992	1.982630
24	1	0	4.124610	0.624854	0.625074
25	1	0	2.918759	0.200706	1.867953
26	1	0	3.596691	-1.852151	0.793984
27	1	0	3.327499	-1.203678	-0.833476
28	1	0	1.912424	-3.421561	1.085812
29	1	0	1.211618	-3.392250	-0.546197
30	1	0	-0.571710	-3.915319	1.076772
31	1	0	-0.105328	-2.525788	2.093578
32	1	0	-2.857235	-2.792948	0.988291
33	1	0	-2.167774	-1.470906	1.955401
34	1	0	-4.096017	-0.669927	0.574346
35	1	0	-3.316776	-1.261603	-0.894137
36	56	0	0.011703	0.013517	-1.136061

15c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	56	0	0.000123	-0.000423	-0.002400
2	6	0	2.204945	2.910899	-0.322293
3	8	0	0.846774	2.623554	0.067138
4	8	0	2.695544	0.578392	-0.066210
5	6	0	3.116775	1.900601	0.326369
6	8	0	1.849036	-2.044770	0.068396
7	6	0	3.204936	-1.749308	-0.322627
8	6	0	3.622553	-0.453815	0.325708
9	8	0	-0.847097	-2.623562	-0.067685
10	6	0	0.087166	-3.649748	0.323456
11	6	0	1.418181	-3.363604	-0.324077
12	6	0	-0.087332	3.649624	-0.324806
13	6	0	-1.418176	3.364432	0.323558
14	8	0	-1.849274	2.044942	-0.066955
15	6	0	-3.204582	1.749118	0.326334
16	6	0	-3.623328	0.454123	-0.321843
17	8	0	-2.694920	-0.578185	0.067581
18	6	0	-3.117629	-1.900373	-0.322205
19	6	0	-2.204409	-2.909486	0.325909
20	1	0	2.287348	2.872319	-1.413985
21	1	0	2.482932	3.913407	0.016377
22	1	0	3.083782	1.984363	1.418147
23	1	0	4.143036	2.077180	-0.009183
24	1	0	3.262895	-1.680116	-1.414396
25	1	0	3.870404	-2.549357	0.015084
26	1	0	4.630487	-0.193651	-0.011038
27	1	0	3.628195	-0.543554	1.417498
28	1	0	0.175532	-3.665486	1.415242
29	1	0	-0.272638	-4.626150	-0.014465
30	1	0	2.147129	-4.106674	0.012753
31	1	0	1.343631	-3.412944	-1.415908
32	1	0	-0.176014	3.664287	-1.416599
33	1	0	0.272784	4.626297	0.011980
34	1	0	-2.147246	4.106978	-0.014186
35	1	0	-1.343316	3.415292	1.415279
36	1	0	-3.260484	1.679192	1.418162
37	1	0	-3.870634	2.549468	-0.009528
38	1	0	-4.630393	0.193476	0.017078
39	1	0	-3.631362	0.544382	-1.413565
40	1	0	-3.087610	-1.985882	-1.413928
41	1	0	-4.143018	-2.076145	0.016408
42	1	0	-2.483714	-3.912696	-0.009534
43	1	0	-2.283712	-2.868016	1.417696

15d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.688775	-2.474166	-0.736065
2	8	0	2.370419	-1.275457	1.107103
3	8	0	2.589161	1.309724	0.072627
4	8	0	0.360413	2.654847	-0.842766
5	8	0	-2.013046	1.893595	0.387504
6	8	0	-2.258792	-0.670904	1.440460
7	8	0	-1.790124	-1.321739	-1.258996
8	6	0	1.596309	-3.277431	0.042473
9	6	0	2.803774	-2.443226	0.386350
10	6	0	-1.197727	-2.266241	-2.170885

11	6	0	-0.300918	-3.242389	-1.440707
12	6	0	-3.316449	1.448260	0.795363
13	6	0	-3.128748	0.395829	1.870357
14	6	0	3.444309	-0.394524	1.493530
15	6	0	3.787543	0.578046	0.383937
16	6	0	-0.718223	3.597733	-0.684663
17	6	0	-2.035528	2.865089	-0.673869
18	6	0	2.740140	2.291461	-0.968350
19	6	0	1.641830	3.314315	-0.820448
20	6	0	-2.874352	-1.834905	0.860457
21	6	0	-3.038693	-1.711140	-0.647006
22	1	0	1.920058	-4.145934	-0.538858
23	1	0	1.087468	-3.629730	0.946520
24	1	0	3.483805	-3.029918	1.011641
25	1	0	3.328530	-2.147198	-0.527794
26	1	0	-1.970920	-2.796994	-2.731029
27	1	0	-0.614751	-1.676739	-2.881995
28	1	0	0.186405	-3.908755	-2.160228
29	1	0	-0.867274	-3.855306	-0.729697
30	1	0	-3.884600	2.288892	1.207996
31	1	0	-3.858515	1.059039	-0.072225
32	1	0	-4.096184	-0.005894	2.181726
33	1	0	-2.647579	0.837250	2.745052
34	1	0	4.325413	-0.973539	1.782322
35	1	0	3.091695	0.145858	2.374032
36	1	0	4.566219	1.266844	0.727153
37	1	0	4.150344	0.064657	-0.513403
38	1	0	-0.707529	4.312639	-1.513580
39	1	0	-0.579925	4.142697	0.255130
40	1	0	-2.836103	3.590971	-0.502998
41	1	0	-2.223540	2.358374	-1.627732
42	1	0	3.704887	2.798249	-0.872983
43	1	0	2.703747	1.797727	-1.946292
44	1	0	1.701392	4.034002	-1.643143
45	1	0	1.748782	3.850875	0.128258
46	1	0	-3.842708	-2.024858	1.332322
47	1	0	-2.213199	-2.668450	1.106240
48	1	0	-3.378725	-2.668072	-1.051610
49	1	0	-3.779509	-0.955678	-0.912467
50	56	0	0.098362	0.090831	0.223383

16a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.055502	2.893191	0.096623
2	8	0	-1.533061	0.262840	-0.311448
3	8	0	0.055502	-2.893191	0.096623
4	8	0	1.533061	-0.262840	-0.311448
5	6	0	-1.434968	-0.967307	0.387210
6	6	0	-0.862130	-2.023379	-0.567337
7	6	0	1.434968	-2.646554	-0.136722
8	6	0	1.968830	-1.360393	0.475089
9	6	0	1.434968	0.967307	0.387210
10	6	0	0.862130	2.023379	-0.567337
11	6	0	-1.434968	2.646554	-0.136722
12	6	0	-1.968830	1.360393	0.475089
13	1	0	-2.418870	-1.267795	0.773858
14	1	0	-0.762253	-0.861657	1.247055
15	1	0	-1.657731	-2.657661	-0.965542
16	1	0	-0.376941	-1.500954	-1.394028
17	1	0	1.957914	-3.495785	0.309517
18	1	0	1.644685	-2.639726	-1.215000
19	1	0	3.068340	-1.395370	0.507118

20	1	0	1.602850	-1.266691	1.506176
21	1	0	2.418870	1.267795	0.773858
22	1	0	0.762253	0.861657	1.247055
23	1	0	1.657731	2.657661	-0.965542
24	1	0	0.376941	1.500954	-1.394028
25	1	0	-1.957914	3.495785	0.309517
26	1	0	-1.644685	2.639726	-1.215000
27	1	0	-3.068340	1.395370	0.507118
28	1	0	-1.602850	1.266691	1.506176

16b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.230866	-0.764654	0.391304
2	8	0	0.150509	-1.213400	-0.140602
3	8	0	-3.086856	-1.245829	-0.178425
4	8	0	-2.000489	2.198378	0.442816
5	8	0	1.501583	2.298676	-0.598505
6	6	0	-0.855897	-1.992169	0.539592
7	6	0	-2.033847	-2.193058	-0.419125
8	6	0	-2.791548	0.125599	-0.524353
9	6	0	-2.486128	0.885026	0.774381
10	6	0	-0.578731	2.394453	0.539786
11	6	0	0.128440	1.859938	-0.710500
12	6	0	2.499223	1.267599	-0.660488
13	6	0	2.582629	0.499668	0.664976
14	6	0	2.389095	-1.925568	0.472858
15	6	0	1.307435	-1.931257	-0.611479
16	1	0	-0.450772	-2.938811	0.923525
17	1	0	-1.146323	-1.338753	1.391080
18	1	0	-2.561813	-3.149853	-0.242267
19	1	0	-1.705791	-2.131434	-1.472342
20	1	0	-3.729183	0.473165	-0.995604
21	1	0	-1.966010	0.198929	-1.249850
22	1	0	-3.407005	1.097398	1.349309
23	1	0	-1.778511	0.326441	1.412499
24	1	0	-0.505994	3.498886	0.602461
25	1	0	-0.179600	1.950515	1.465029
26	1	0	-0.250652	2.339891	-1.630251
27	1	0	0.042747	0.761618	-0.801502
28	1	0	3.414311	1.857193	-0.861417
29	1	0	2.311780	0.586392	-1.508501
30	1	0	3.257880	0.984978	1.391154
31	1	0	1.585934	0.361219	1.117048
32	1	0	3.128345	-2.737488	0.327979
33	1	0	1.949763	-1.992977	1.483411
34	1	0	1.041287	-2.946937	-0.940023
35	1	0	1.620682	-1.327136	-1.488340

16c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.381351	-1.927326	0.155572
2	8	0	0.137799	-1.904565	-0.535633
3	8	0	3.736658	-1.454777	-0.252961
4	6	0	2.461351	-1.608218	-0.869786
5	8	0	2.509214	0.920697	1.080786
6	6	0	3.903139	0.690430	0.953308

7	6	0	4.287600	-0.147306	-0.263067
8	8	0	-0.167855	2.643570	-0.602329
9	6	0	0.465702	1.621201	0.163004
10	6	0	1.955723	1.906773	0.218857
11	6	0	-0.987686	-1.967192	0.326301
12	6	0	-2.232431	-1.955131	-0.549928
13	8	0	-3.411754	-1.918088	0.253257
14	6	0	-4.151568	-0.709151	0.238159
15	6	0	-3.529545	0.414265	1.059903
16	8	0	-2.348777	0.941308	0.464090
17	6	0	-2.559042	2.031146	-0.422688
18	6	0	-1.329351	2.225328	-1.294588
19	1	0	1.398933	-1.172328	0.947116
20	1	0	1.553983	-2.914497	0.605199
21	1	0	2.176384	-0.698623	-1.408357
22	1	0	2.534893	-2.420002	-1.599957
23	1	0	4.194214	0.154295	1.859120
24	1	0	4.455880	1.642117	0.923235
25	1	0	5.375915	-0.267090	-0.256436
26	1	0	4.020741	0.366382	-1.195520
27	1	0	0.054488	1.583609	1.175291
28	1	0	0.298999	0.645137	-0.301434
29	1	0	2.380105	1.848329	-0.790324
30	1	0	2.148506	2.914088	0.611008
31	1	0	-0.998723	-1.102979	0.999853
32	1	0	-0.963193	-2.883055	0.932652
33	1	0	-2.269473	-2.866387	-1.153775
34	1	0	-2.188174	-1.095051	-1.223185
35	1	0	-4.315465	-0.375250	-0.796603
36	1	0	-5.126893	-0.956734	0.667009
37	1	0	-4.269814	1.211349	1.216754
38	1	0	-3.239123	0.023274	2.038095
39	1	0	-2.767860	2.944778	0.151035
40	1	0	-3.415550	1.838267	-1.085635
41	1	0	-1.545942	3.012528	-2.021782
42	1	0	-1.126561	1.293766	-1.841309

16d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.589853	2.558905	0.086766
2	8	0	3.346817	-0.137810	-1.027724
3	8	0	2.878462	-1.751762	1.368902
4	8	0	-0.555131	-2.268125	0.291659
5	8	0	-3.928943	-1.854001	-1.012800
6	8	0	-3.597425	0.820928	0.345932
7	8	0	-0.983415	2.161859	0.103650
8	6	0	3.703019	2.217559	-0.721709
9	6	0	4.233164	0.818481	-0.463243
10	6	0	0.294401	2.477092	0.630367
11	6	0	1.326310	2.161721	-0.435281
12	6	0	-4.903715	-1.081196	-0.333983
13	6	0	-4.698027	0.417200	-0.449133
14	6	0	3.778303	-1.483051	-0.931936
15	6	0	3.962466	-2.001649	0.496501
16	6	0	-1.579579	-1.558713	-0.397107
17	6	0	-2.853771	-2.376257	-0.239187
18	6	0	1.668897	-2.445207	1.079322
19	6	0	0.656660	-1.544412	0.382747
20	6	0	-3.361608	2.216714	0.298749
21	6	0	-2.043255	2.534464	0.964270
22	1	0	4.491207	2.932601	-0.469133
23	1	0	3.460883	2.334139	-1.786469

24	1	0	5.231414	0.720803	-0.920150
25	1	0	4.326743	0.671682	0.618592
26	1	0	0.351257	3.541838	0.897348
27	1	0	0.499039	1.889864	1.536256
28	1	0	1.098506	2.725301	-1.350531
29	1	0	1.316612	1.096957	-0.672426
30	1	0	-5.868142	-1.322828	-0.793106
31	1	0	-4.950691	-1.362781	0.725432
32	1	0	-5.616548	0.924664	-0.111823
33	1	0	-4.525307	0.685644	-1.500706
34	1	0	4.732172	-1.622271	-1.466448
35	1	0	3.018852	-2.066067	-1.456714
36	1	0	4.175090	-3.080243	0.433694
37	1	0	4.824941	-1.528087	0.969396
38	1	0	-1.329063	-1.464034	-1.463210
39	1	0	-1.707157	-0.554525	0.015343
40	1	0	-2.669455	-3.394556	-0.592373
41	1	0	-3.129066	-2.429126	0.820158
42	1	0	1.862665	-3.338494	0.473094
43	1	0	1.247593	-2.774115	2.032574
44	1	0	1.008612	-1.248629	-0.612788
45	1	0	0.520624	-0.627794	0.971766
46	1	0	-4.171315	2.752733	0.817148
47	1	0	-3.330566	2.566098	-0.742317
48	1	0	-1.998031	3.614395	1.171486
49	1	0	-1.972209	2.000400	1.922556

17a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.984316	0.381024	-2.448522
2	6	0	3.764462	0.214134	-1.400035
3	6	0	3.318308	-0.217196	1.332061
4	6	0	3.689254	-1.093072	-0.900208
5	6	0	3.616801	1.305345	-0.533517
6	6	0	3.393684	1.089663	0.832921
7	6	0	3.466563	-1.308664	0.466096
8	1	0	3.851167	-1.935972	-1.562607
9	1	0	3.722678	2.315612	-0.912451
10	1	0	3.324148	1.933684	1.509610
11	1	0	3.454388	-2.318383	0.860426
12	1	0	3.195191	-0.384856	2.396012
13	56	0	0.439844	-0.014427	-0.522099
14	8	0	-0.752049	-1.130605	1.628327
15	8	0	-0.891512	1.606152	1.184695
16	8	0	-1.727159	-1.598036	-0.924721
17	8	0	-1.866398	1.137301	-1.370641
18	6	0	-1.910769	-1.978921	1.478181
19	1	0	-2.821036	-1.384317	1.598379
20	1	0	-1.899647	-2.756854	2.246980
21	6	0	-1.844217	-2.609619	0.100210
22	1	0	-2.719532	-3.238388	-0.078844
23	1	0	-0.957588	-3.240144	0.006397
24	6	0	-0.802586	-0.208116	2.738650
25	1	0	-1.271093	-0.677669	3.606773
26	1	0	0.236233	0.009642	2.994682
27	6	0	-1.536378	1.063302	2.356296
28	1	0	-2.589414	0.862943	2.138092
29	1	0	-1.483090	1.786519	3.175172
30	6	0	-1.639885	2.626336	0.486110
31	1	0	-0.901618	3.238060	-0.036639
32	1	0	-2.163545	3.271005	1.195832
33	6	0	-2.615870	2.007208	-0.496123

34	1	0	-3.387959	1.431509	0.022739
35	1	0	-3.102694	2.791063	-1.083487
36	6	0	-2.977738	-1.035922	-1.377234
37	1	0	-3.494290	-1.754970	-2.019481
38	1	0	-3.615951	-0.818211	-0.515868
39	6	0	-2.662461	0.224877	-2.159443
40	1	0	-2.067968	-0.007882	-3.045417
41	1	0	-3.582039	0.709855	-2.495283

17b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.771473	-0.386524	-1.582428
2	6	0	3.581518	-0.152503	-0.541013
3	6	0	3.215107	0.455894	2.167391
4	6	0	3.499605	-1.183737	0.402417
5	6	0	3.479736	1.182568	-0.131529
6	6	0	3.296159	1.486979	1.222807
7	6	0	3.316139	-0.879655	1.756891
8	1	0	3.617955	-2.215273	0.091517
9	1	0	3.584583	1.982515	-0.855405
10	1	0	3.262165	2.521139	1.546040
11	1	0	3.296943	-1.675299	2.492934
12	1	0	3.118599	0.692866	3.220918
13	56	0	0.229373	0.030468	0.450791
14	8	0	-2.123384	-0.974937	1.284984
15	8	0	-1.745790	1.744325	1.175049
16	8	0	-0.464455	-2.502586	-0.309284
17	8	0	-0.540220	1.997294	-1.332535
18	6	0	-2.575924	-2.294904	0.918717
19	1	0	-3.234082	-2.219207	0.047365
20	1	0	-3.135516	-2.745531	1.743605
21	6	0	-1.346441	-3.140255	0.637728
22	1	0	-1.639006	-4.130963	0.280551
23	1	0	-0.761139	-3.271134	1.550061
24	6	0	-3.113005	-0.091925	1.865428
25	1	0	-4.108749	-0.532957	1.785008
26	1	0	-2.871848	0.038603	2.922724
27	6	0	-3.092678	1.232464	1.133226
28	1	0	-3.409167	1.099145	0.093490
29	1	0	-3.770505	1.936755	1.625258
30	6	0	-1.553200	3.042927	0.579208
31	1	0	-0.602790	3.407343	0.974864
32	1	0	-2.336780	3.731417	0.907166
33	6	0	-1.515923	2.980317	-0.936457
34	1	0	-2.489630	2.700525	-1.351838
35	1	0	-1.245088	3.964023	-1.333308
36	6	0	-0.570127	1.720383	-2.746918
37	1	0	-1.603628	1.515664	-3.043643
38	1	0	-0.202464	2.585050	-3.307763
39	6	0	0.295288	0.511721	-3.029982
40	1	0	0.167689	0.215135	-4.074518
41	1	0	1.357091	0.721208	-2.856316
42	8	0	-0.144149	-0.539042	-2.150827
43	6	0	-0.748036	-2.785041	-1.694473
44	1	0	-1.801471	-2.580085	-1.907031
45	1	0	-0.534892	-3.836624	-1.906963
46	6	0	0.130617	-1.895695	-2.545057
47	1	0	1.192343	-2.121250	-2.395508
48	1	0	-0.116005	-2.040398	-3.600478

17c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.835923	2.522496	-2.947190
2	6	0	-0.347601	1.555166	-2.969537
3	6	0	0.920632	-0.934832	-3.124770
4	6	0	-1.106572	0.393714	-3.153342
5	6	0	1.045282	1.472579	-2.864711
6	6	0	1.678924	0.227132	-2.943375
7	6	0	-0.472865	-0.851514	-3.229364
8	1	0	-2.181911	0.463320	-3.264781
9	1	0	1.634677	2.375396	-2.756412
10	1	0	2.760563	0.167459	-2.907566
11	1	0	-1.055921	-1.747849	-3.405886
12	1	0	1.413292	-1.895221	-3.222252
13	56	0	-0.011414	-0.021220	0.127057
14	8	0	-1.584447	-2.273051	0.645914
15	8	0	2.671770	-0.255567	0.818727
16	8	0	-2.793421	0.162735	0.005585
17	8	0	1.452155	2.201779	0.986196
18	6	0	-3.000707	-2.119641	0.844221
19	1	0	-3.199748	-1.815057	1.878332
20	1	0	-3.507759	-3.072436	0.660458
21	6	0	-3.484579	-1.089323	-0.153025
22	1	0	-4.563869	-0.943818	-0.059533
23	1	0	-3.269391	-1.425988	-1.168764
24	6	0	-0.990953	-3.324249	1.427860
25	1	0	-1.629140	-4.213076	1.408046
26	6	0	3.456279	0.933276	0.637007
27	1	0	3.504447	1.188736	-0.427859
28	1	0	4.474074	0.772755	1.005312
29	6	0	2.809677	2.037437	1.435030
30	1	0	2.811800	1.789124	2.501791
31	1	0	3.364046	2.969650	1.286781
32	6	0	0.764905	3.248566	1.693933
33	1	0	0.650985	2.962655	2.745404
34	1	0	1.345797	4.175139	1.643002
35	6	0	-0.579253	3.476316	1.052263
36	1	0	-1.114337	4.247597	1.614862
37	1	0	-0.468997	3.812359	0.014903
38	8	0	-1.324563	2.245689	1.079511
39	6	0	-3.420404	1.102553	0.895170
40	1	0	-3.362503	0.746099	1.929624
41	1	0	-4.473136	1.226094	0.623825
42	6	0	-2.713044	2.425496	0.747391
43	1	0	-2.798582	2.794891	-0.280472
44	1	0	-3.163663	3.156615	1.425805
45	1	0	-0.887132	-2.991859	2.467223
46	6	0	0.352139	-3.667587	0.827297
47	1	0	0.237304	-4.121826	-0.160821
48	1	0	0.860634	-4.377203	1.485149
49	8	0	1.134955	-2.463953	0.691340
50	6	0	3.287943	-1.464335	0.350199
51	1	0	4.334415	-1.504491	0.667502
52	1	0	3.253886	-1.493469	-0.745280
53	6	0	2.542120	-2.633522	0.950004
54	1	0	2.699938	-2.685522	2.031340
55	1	0	2.902208	-3.558728	0.490578

17d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.039696	-2.981625	2.580397
2	6	0	-0.071213	-2.501277	2.528040
3	6	0	2.462243	-1.321043	2.455111
4	6	0	0.191776	-1.365398	3.298156
5	6	0	0.928342	-3.040738	1.712249
6	6	0	2.194516	-2.450874	1.676492
7	6	0	1.461219	-0.774004	3.261898
8	1	0	-0.568375	-0.968932	3.961755
9	1	0	0.733537	-3.942628	1.143364
10	1	0	2.982091	-2.891886	1.077036
11	1	0	1.677734	0.078882	3.895144
12	1	0	3.455707	-0.891165	2.453345
13	56	0	0.182893	0.073831	0.033374
14	8	0	1.243690	2.647654	0.387638
15	8	0	1.670291	-0.800888	-2.173709
16	8	0	-1.504823	2.329059	-0.072434
17	8	0	-1.065720	-1.252621	-2.071620
18	6	0	0.423363	3.791783	0.094440
19	1	0	0.444569	3.988680	-0.983411
20	1	0	0.811612	4.670099	0.620584
21	6	0	-0.979253	3.512097	0.568962
22	1	0	-1.606176	4.375667	0.337836
23	1	0	-0.998034	3.357532	1.652306
24	6	0	2.646449	2.904522	0.201054
25	1	0	2.957973	3.743115	0.832489
26	6	0	1.091235	-1.731364	-3.105118
27	1	0	1.172438	-2.750182	-2.709086
28	1	0	1.627129	-1.687774	-4.058679
29	6	0	-0.347464	-1.314896	-3.315894
30	1	0	-0.387794	-0.307467	-3.733512
31	1	0	-0.847721	-1.995928	-4.009456
32	6	0	-3.636134	0.405391	1.317832
33	1	0	-2.800463	1.090239	1.495003
34	8	0	-4.269046	0.673521	0.074661
35	6	0	-2.817665	2.540232	-0.669682
36	1	0	-2.681746	3.119697	-1.587831
37	1	0	-3.437871	3.115976	0.022206
38	6	0	-3.495434	1.220715	-0.983398
39	1	0	-4.218128	1.396994	-1.781868
40	1	0	-2.758798	0.503340	-1.367184
41	1	0	2.831972	3.173017	-0.844994
42	6	0	3.399388	1.657830	0.607482
43	1	0	3.201513	1.428292	1.655789
44	1	0	4.476225	1.804572	0.486053
45	8	0	2.959843	0.512677	-0.139594
46	6	0	3.095480	-0.935409	-2.025742
47	1	0	3.561262	-1.071757	-3.006069
48	1	0	3.317898	-1.809116	-1.404253
49	6	0	3.625473	0.328331	-1.398036
50	1	0	3.439472	1.183499	-2.056340
51	1	0	4.704086	0.232808	-1.237361
52	1	0	-4.379789	0.591165	2.097702
53	6	0	-1.628508	-2.497742	-1.613958
54	1	0	-0.851197	-3.110681	-1.142527
55	1	0	-2.042675	-3.053063	-2.460044
56	6	0	-2.735477	-2.182690	-0.639523
57	1	0	-3.549987	-1.649376	-1.135723
58	1	0	-3.126640	-3.118673	-0.228151
59	8	0	-2.201433	-1.370174	0.420439
60	6	0	-3.182966	-1.037516	1.432769
61	1	0	-4.036539	-1.710858	1.336251
62	1	0	-2.720237	-1.208545	2.408425

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.670492	-0.250365	-0.305750
2	6	0	-0.967460	0.798483	0.262092
3	6	0	-0.938701	-1.234219	-0.951972
4	6	0	0.397710	0.880428	0.178413
5	1	0	-1.499364	1.567854	0.805680
6	6	0	0.425578	-1.168035	-1.045969
7	1	0	-1.466008	-2.074540	-1.382614
8	6	0	1.140417	-0.100792	-0.487747
9	1	0	0.891909	1.731134	0.622153
10	1	0	0.947509	-1.974397	-1.538409
11	6	0	7.333370	-1.295987	2.672102
12	1	0	7.841939	-2.076783	2.099259
13	1	0	7.565646	-1.470785	3.727748
14	6	0	7.842167	0.052954	2.270423
15	1	0	8.903172	0.140632	2.531592
16	1	0	7.296221	0.818187	2.822948
17	6	0	8.595972	-0.226863	0.069846
18	1	0	8.812976	-1.272973	0.318291
19	1	0	9.535546	0.332859	0.154645
20	6	0	8.086345	-0.175843	-1.332767
21	1	0	7.118433	-0.685769	-1.375017
22	1	0	8.787026	-0.708824	-1.980849
23	6	0	6.680161	1.515365	-2.172330
24	1	0	6.234272	0.757701	-2.828224
25	1	0	6.772687	2.436993	-2.746277
26	6	0	5.794918	1.723234	-0.981864
27	1	0	6.184047	2.539672	-0.361120
28	1	0	5.803237	0.816381	-0.374292
29	6	0	3.597603	2.174548	-0.391881
30	1	0	2.704914	2.630677	-0.820776
31	1	0	4.002233	2.858966	0.364638
32	6	0	3.243509	0.865323	0.262743
33	1	0	2.685260	1.062647	1.176897
34	1	0	4.150181	0.342257	0.571546
35	6	0	3.232136	-0.840056	-1.493741
36	1	0	3.994244	-0.218302	-1.968257
37	1	0	2.571127	-1.175126	-2.289029
38	6	0	3.920443	-2.019976	-0.871502
39	1	0	4.129476	-2.777704	-1.636077
40	1	0	3.275593	-2.476183	-0.110986
41	6	0	5.805307	-2.564090	0.397760
42	1	0	5.567455	-3.558022	0.003604
43	1	0	6.871913	-2.399060	0.233480
44	6	0	5.498738	-2.520897	1.864501
45	1	0	4.418887	-2.550343	2.015964
46	1	0	5.926475	-3.404513	2.352158
47	7	0	2.491832	-0.022155	-0.577768
48	8	0	4.513556	2.028969	-1.433286
49	8	0	7.963110	1.140547	-1.786062
50	8	0	7.638536	0.308308	0.919714
51	8	0	5.955875	-1.353488	2.469409
52	8	0	5.120791	-1.581849	-0.311633
53	6	0	-5.050258	-1.258233	-0.268138
54	6	0	-4.024017	0.682042	0.087879
55	7	0	-5.199792	0.041101	0.049913
56	6	0	-6.306112	0.772734	0.275747
57	6	0	-7.479499	0.080512	0.207806
58	6	0	-7.413802	-1.288450	-0.096343

59	6	0	-6.234154	-1.969362	-0.339611
60	1	0	-8.435393	0.551772	0.372058
61	1	0	-6.260740	-3.021042	-0.580994
62	6	0	-4.374306	2.045337	0.369714
63	6	0	-5.788367	2.096603	0.496703
64	6	0	-3.640517	3.212976	0.506301
65	6	0	-6.435480	3.286148	0.771168
66	6	0	-5.685508	4.425750	0.912080
67	6	0	-4.302409	4.384870	0.774878
68	1	0	-3.734412	5.298997	0.880272
69	1	0	-7.512304	3.316091	0.868428
70	1	0	-2.566458	3.216145	0.392201
71	7	0	-3.751675	-1.499086	-0.432624
72	6	0	-3.106292	-0.339140	-0.217008
73	1	0	-6.171975	5.366897	1.126013
74	6	0	-8.652300	-2.077934	-0.180196
75	8	0	-8.685961	-3.245134	-0.442209
76	8	0	-9.726494	-1.368480	0.063849
77	6	0	-10.952695	-2.058268	0.001911
78	1	0	-11.720356	-1.329141	0.233937
79	1	0	-11.107217	-2.466567	-0.994351
80	1	0	-10.968022	-2.868578	0.727331

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.670601	-0.277856	-0.340993
2	6	0	-0.937972	0.762678	0.250155
3	6	0	-0.943248	-1.257489	-1.037027
4	6	0	0.439523	0.840017	0.143243
5	1	0	-1.451792	1.520082	0.827902
6	6	0	0.433292	-1.194834	-1.154329
7	1	0	-1.477029	-2.083558	-1.489820
8	6	0	1.176377	-0.135975	-0.572649
9	1	0	0.942780	1.675535	0.607648
10	1	0	0.937314	-1.988619	-1.686491
11	6	0	7.227887	-1.300849	2.702754
12	1	0	7.721928	-2.069992	2.100645
13	1	0	7.357031	-1.578490	3.757965
14	6	0	7.875639	0.051127	2.458460
15	1	0	8.909963	0.028975	2.826035
16	1	0	7.334059	0.819826	3.014030
17	6	0	8.793775	-0.162827	0.246055
18	1	0	8.993936	-1.195776	0.555515
19	1	0	9.739987	0.392025	0.297126
20	6	0	8.275218	-0.200494	-1.177424
21	1	0	7.304038	-0.703828	-1.195298
22	1	0	8.977780	-0.779998	-1.787260
23	6	0	6.866120	1.466022	-2.197967
24	1	0	6.410589	0.637572	-2.754252
25	1	0	6.995396	2.304474	-2.885121
26	6	0	5.965776	1.854537	-1.033628
27	1	0	6.331217	2.774382	-0.557922
28	1	0	5.992188	1.061285	-0.285050
29	6	0	3.678069	2.170219	-0.482793
30	1	0	2.788846	2.609185	-0.938583
31	1	0	4.047032	2.858890	0.289570
32	6	0	3.335068	0.824689	0.159894
33	1	0	2.799358	1.000571	1.093530

34	1	0	4.247953	0.293366	0.430989
35	6	0	3.273993	-0.912440	-1.625646
36	1	0	4.087908	-0.324547	-2.052337
37	1	0	2.617092	-1.179318	-2.452377
38	6	0	3.862865	-2.174272	-1.005143
39	1	0	4.032879	-2.933250	-1.780820
40	1	0	3.169388	-2.589218	-0.264567
41	6	0	5.609808	-2.799889	0.518173
42	1	0	5.222865	-3.798008	0.281000
43	1	0	6.693366	-2.830840	0.381214
44	6	0	5.260105	-2.450928	1.959254
45	1	0	4.180094	-2.320861	2.057193
46	1	0	5.564437	-3.273822	2.620168
47	7	0	2.544214	-0.060686	-0.691740
48	8	0	4.643620	2.055227	-1.529427
49	8	0	8.169879	1.110604	-1.745822
50	8	0	7.828351	0.449989	1.093594
51	8	0	5.841749	-1.221082	2.384315
52	8	0	5.107398	-1.829591	-0.396154
53	6	0	-5.108171	-1.271110	-0.254755
54	6	0	-4.034806	0.691823	0.090325
55	7	0	-5.236493	0.053212	0.069342
56	6	0	-6.351043	0.811353	0.295644
57	6	0	-7.544926	0.120539	0.233453
58	6	0	-7.506431	-1.268067	-0.066857
59	6	0	-6.314110	-1.969810	-0.316753
60	1	0	-8.489879	0.614340	0.398206
61	1	0	-6.345826	-3.022214	-0.558109
62	6	0	-4.374543	2.074665	0.361797
63	6	0	-5.812009	2.144721	0.500818
64	6	0	-3.620418	3.248193	0.480657
65	6	0	-6.444918	3.359937	0.768407
66	6	0	-5.669674	4.505480	0.890868
67	6	0	-4.273375	4.446103	0.742678
68	1	0	-3.692174	5.356189	0.833131
69	1	0	-7.522289	3.406775	0.873736
70	1	0	-2.545652	3.234851	0.360395
71	7	0	-3.792865	-1.531069	-0.436535
72	6	0	-3.117366	-0.355285	-0.229171
73	1	0	-6.144572	5.456839	1.097333
74	6	0	-8.768937	-2.052732	-0.143995
75	8	0	-8.823649	-3.240447	-0.397520
76	8	0	-9.856863	-1.304414	0.098234
77	6	0	-11.129420	-1.982109	0.043131
78	1	0	-11.871388	-1.218329	0.259622
79	1	0	-11.289624	-2.402410	-0.949619
80	1	0	-11.166356	-2.775405	0.789620

19·Ba(ClO$_4$)$_2$ (S_0) BHandH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.149897	2.014101	-1.763257
2	6	0	0.200791	2.976041	-0.829467
3	6	0	0.840142	1.527551	-2.596874
4	6	0	1.515950	3.290819	-0.610868
5	1	0	-0.556326	3.378939	-0.171103
6	6	0	2.153851	1.878086	-2.416930
7	1	0	0.589643	0.780022	-3.337758
8	6	0	2.537214	2.670409	-1.336511
9	1	0	1.745846	3.974865	0.190250

10	1	0	2.889094	1.434165	-3.064461
11	6	0	2.929161	-3.082762	1.740062
12	1	0	3.132403	-2.761949	2.769560
13	1	0	3.557418	-3.955880	1.529181
14	6	0	1.503012	-3.477223	1.551046
15	1	0	1.250075	-4.293800	2.234077
16	1	0	1.361500	-3.813151	0.525686
17	6	0	0.189075	-2.152401	3.035681
18	1	0	0.177567	-3.078334	3.618423
19	1	0	-0.827001	-1.782508	2.944108
20	6	0	1.025033	-1.124467	3.739428
21	1	0	1.980211	-1.530275	4.095004
22	1	0	0.459050	-0.761368	4.603572
23	6	0	1.791321	1.049462	3.511333
24	1	0	2.682988	0.759825	4.082352
25	1	0	1.038817	1.448576	4.200788
26	6	0	2.137690	2.090245	2.496475
27	1	0	2.607681	2.937794	3.003206
28	1	0	1.224313	2.439961	2.016167
29	6	0	4.232424	2.175905	1.370133
30	1	0	4.935257	1.402645	1.073529
31	1	0	4.559425	2.606754	2.323466
32	6	0	4.215885	3.256239	0.315672
33	1	0	5.219319	3.685237	0.262889
34	1	0	3.565321	4.075654	0.617501
35	6	0	4.873404	2.167707	-1.776090
36	1	0	5.821865	2.520822	-1.372371
37	1	0	4.825234	2.531473	-2.807788
38	6	0	4.910288	0.651629	-1.829587
39	1	0	5.929677	0.368655	-2.124567
40	1	0	4.234492	0.225600	-2.572960
41	6	0	5.007833	-1.223882	-0.507569
42	1	0	4.567298	-1.816558	-1.313348
43	1	0	6.101581	-1.279782	-0.589464
44	6	0	4.607823	-1.799615	0.802609
45	1	0	5.151303	-2.741652	0.926513
46	1	0	4.894148	-1.129580	1.622828
47	7	0	3.850909	2.796544	-0.991728
48	8	0	2.995841	1.545989	1.532970
49	8	0	1.278488	-0.071194	2.863654
50	8	0	0.631695	-2.404291	1.734813
51	8	0	3.237240	-2.055176	0.851061
52	8	0	4.607708	0.106191	-0.590896
53	56	0	1.089211	-0.239603	0.108641
54	6	0	-2.676090	1.684272	-1.296407
55	6	0	-2.508648	-0.534861	-1.341339
56	6	0	-4.589465	0.582727	-0.702654
57	6	0	-3.092899	-1.768330	-1.118482
58	1	0	-2.551906	-2.694573	-1.243958
59	6	0	-5.176134	-0.624317	-0.476992
60	1	0	-6.190009	-0.718009	-0.122490
61	6	0	-4.407582	-1.781391	-0.699124
62	6	0	-4.835378	2.000354	-0.599913
63	6	0	-3.649045	2.680883	-0.966608
64	6	0	-5.954031	2.705617	-0.209474
65	1	0	-6.859437	2.187980	0.076999
66	6	0	-3.606707	4.060795	-0.938455
67	6	0	-4.730866	4.744485	-0.546978
68	1	0	-4.712617	5.825342	-0.518831
69	6	0	-5.893729	4.076770	-0.185917
70	1	0	-2.706499	4.590223	-1.219529
71	7	0	-3.317464	0.517317	-1.134453
72	1	0	-6.760123	4.645994	0.120044

73	7	0	-1.301876	-0.065526	-1.656715
74	6	0	-1.390395	1.280953	-1.634669
75	6	0	-4.997896	-3.106935	-0.456468
76	8	0	-4.418035	-4.138890	-0.590691
77	8	0	-6.254954	-3.041050	-0.061325
78	6	0	-6.866326	-4.278524	0.192306
79	1	0	-7.881831	-4.057051	0.502577
80	1	0	-6.866471	-4.894655	-0.704921
81	1	0	-6.334739	-4.812196	0.977963
82	17	0	1.952614	-2.502399	-2.283408
83	17	0	-1.673873	0.808913	2.029232
84	8	0	3.040705	-3.401182	-2.008885
85	8	0	2.433322	-1.113991	-2.161787
86	8	0	0.925090	-2.637089	-1.248380
87	8	0	1.403067	-2.721789	-3.578429
88	8	0	-1.459410	-0.460218	1.334304
89	8	0	-0.668081	1.720122	1.476393
90	8	0	-1.448203	0.635123	3.440957
91	8	0	-2.990076	1.300872	1.766184

19·Ba(ClO$_4$)$_2$ (S_1) BHandH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.368426	2.475186	-1.322086
2	6	0	0.007083	3.208431	-0.187168
3	6	0	0.587005	2.292291	-2.327565
4	6	0	1.332887	3.551111	0.025808
5	1	0	-0.718324	3.387760	0.595399
6	6	0	1.905101	2.683499	-2.143247
7	1	0	0.317807	1.756979	-3.229236
8	6	0	2.338264	3.185391	-0.898411
9	1	0	1.589477	4.017927	0.964546
10	1	0	2.606258	2.494443	-2.939017
11	6	0	3.516740	-3.323247	0.977044
12	1	0	3.855573	-3.195775	2.013850
13	1	0	4.148334	-4.087376	0.504955
14	6	0	2.079447	-3.795503	0.902631
15	1	0	1.977693	-4.748327	1.434557
16	1	0	1.800208	-3.935651	-0.141146
17	6	0	0.866924	-2.880523	2.819296
18	1	0	0.993658	-3.898410	3.204028
19	1	0	-0.176652	-2.588473	2.909043
20	6	0	1.729843	-1.918875	3.620258
21	1	0	2.771885	-2.257306	3.697130
22	1	0	1.315194	-1.845492	4.633826
23	6	0	2.262081	0.397521	3.764418
24	1	0	3.304264	0.149590	4.012255
25	1	0	1.694057	0.518451	4.695660
26	6	0	2.187237	1.676462	2.955573
27	1	0	2.611583	2.505268	3.530733
28	1	0	1.145020	1.900331	2.729439
29	6	0	4.163797	2.134724	1.610213
30	1	0	4.819690	1.419633	1.119946
31	1	0	4.553646	2.350954	2.612403
32	6	0	4.122286	3.430723	0.793512
33	1	0	5.134644	3.846883	0.784747
34	1	0	3.496713	4.173981	1.288576
35	6	0	4.699953	2.821544	-1.545685
36	1	0	5.667803	3.084888	-1.115774

37	1	0	4.604288	3.401388	-2.471972
38	6	0	4.742387	1.342782	-1.956631
39	1	0	5.674091	1.208594	-2.526214
40	1	0	3.914408	1.054433	-2.605036
41	6	0	5.136778	-0.838204	-1.172796
42	1	0	4.525351	-1.217013	-1.994984
43	1	0	6.190471	-0.831098	-1.489065
44	6	0	5.008316	-1.756066	0.016156
45	1	0	5.563035	-2.672984	-0.215357
46	1	0	5.453091	-1.301133	0.911453
47	7	0	3.690326	3.266287	-0.589369
48	8	0	2.877575	1.512828	1.711205
49	8	0	1.694542	-0.647551	2.984131
50	8	0	1.153735	-2.842178	1.419565
51	8	0	3.643379	-2.092889	0.268697
52	8	0	4.745021	0.485576	-0.821853
53	56	0	1.157387	-0.358529	0.155087
54	6	0	-2.919030	1.922261	-1.028762
55	6	0	-2.579515	-0.308866	-1.209843
56	6	0	-4.803868	0.622642	-0.627794
57	6	0	-3.082611	-1.603549	-1.089246
58	1	0	-2.453006	-2.471005	-1.223522
59	6	0	-5.306034	-0.654156	-0.506281
60	1	0	-6.326929	-0.836403	-0.208671
61	6	0	-4.433012	-1.752252	-0.747529
62	6	0	-5.162811	2.020662	-0.426225
63	6	0	-3.991216	2.823834	-0.671977
64	6	0	-6.360100	2.623408	-0.044090
65	1	0	-7.242428	2.023611	0.146205
66	6	0	-4.054873	4.210533	-0.526707
67	6	0	-5.260045	4.787955	-0.145947
68	1	0	-5.321801	5.863753	-0.029545
69	6	0	-6.400991	4.005629	0.093637
70	1	0	-3.179479	4.822333	-0.708262
71	7	0	-3.491748	0.684811	-1.000587
72	1	0	-7.324281	4.487617	0.391897
73	7	0	-1.372540	0.278298	-1.402050
74	6	0	-1.569903	1.637069	-1.302241
75	6	0	-4.926981	-3.149285	-0.601598
76	8	0	-4.250614	-4.139999	-0.753656
77	8	0	-6.238199	-3.199459	-0.272753
78	6	0	-6.784196	-4.517769	-0.104180
79	1	0	-7.829933	-4.367763	0.154709
80	1	0	-6.693616	-5.088302	-1.029387
81	1	0	-6.261397	-5.046311	0.693955
82	17	0	1.732565	-1.977750	-2.852297
83	17	0	-1.632866	0.117351	2.289092
84	8	0	2.929309	-2.842321	-2.991287
85	8	0	2.176615	-0.574609	-2.444474
86	8	0	0.878311	-2.465667	-1.697289
87	8	0	0.952136	-1.922026	-4.094278
88	8	0	-1.240104	-1.134499	1.534580
89	8	0	-0.686211	1.197084	1.787130
90	8	0	-1.434920	-0.086913	3.743253
91	8	0	-3.023865	0.488427	1.974072

19 (S_0) BHandHLYP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.740312	-0.251948	-0.107915
2	6	0	-1.061080	0.709329	0.634134
3	6	0	-0.965857	-1.139894	-0.852073
4	6	0	0.313342	0.800380	0.626246
5	1	0	-1.611082	1.394340	1.254983
6	6	0	0.408008	-1.063923	-0.871180
7	1	0	-1.454922	-1.906244	-1.426871
8	6	0	1.099612	-0.082081	-0.136084
9	1	0	0.770447	1.571794	1.215026
10	1	0	0.945073	-1.786734	-1.454547
11	6	0	8.231418	-2.024162	1.372134
12	1	0	8.037370	-2.477395	0.400883
13	1	0	8.797382	-2.740718	1.970196
14	6	0	9.043965	-0.764204	1.198798
15	1	0	10.056082	-1.023418	0.893924
16	1	0	9.103575	-0.247510	2.151370
17	6	0	8.942098	0.027580	-1.040895
18	1	0	9.121277	-1.011804	-1.314729
19	1	0	9.885586	0.566352	-1.131961
20	6	0	7.922141	0.583874	-1.995613
21	1	0	6.989184	0.042514	-1.862772
22	1	0	8.263281	0.419812	-3.017340
23	6	0	6.398932	2.402486	-1.930399
24	1	0	5.911613	1.885871	-2.755659
25	1	0	6.434504	3.458139	-2.173882
26	6	0	5.611730	2.178204	-0.653538
27	1	0	5.938199	2.876871	0.116779
28	1	0	5.804024	1.172594	-0.286049
29	6	0	3.394242	2.310979	0.184051
30	1	0	2.450831	2.734576	-0.140157
31	1	0	3.792317	2.939388	0.981981
32	6	0	3.184335	0.904014	0.728658
33	1	0	2.663482	0.977464	1.677255
34	1	0	4.137430	0.444208	0.954477
35	6	0	3.265161	-0.785318	-1.073870
36	1	0	4.137907	-0.202312	-1.339579
37	1	0	2.717965	-0.943896	-1.996076
38	6	0	3.730737	-2.126362	-0.542167
39	1	0	4.256869	-2.648020	-1.343303
40	1	0	2.888514	-2.746087	-0.233858
41	6	0	5.311642	-3.056674	0.937370
42	1	0	4.631396	-3.877856	1.170442
43	1	0	5.955305	-3.386054	0.121106
44	6	0	6.111418	-2.744195	2.180648
45	1	0	5.432488	-2.434497	2.967662
46	1	0	6.618650	-3.651947	2.509370
47	7	0	2.466624	0.005770	-0.157577
48	8	0	4.247366	2.367435	-0.938344
49	8	0	7.728700	1.964977	-1.778862
50	8	0	8.456939	0.124855	0.276126
51	8	0	7.031480	-1.692410	2.026111
52	8	0	4.594685	-1.914910	0.546948
53	6	0	-5.137749	-1.272564	-0.323714
54	6	0	-4.137787	0.654236	0.211404
55	7	0	-5.313080	0.010625	0.065222
56	6	0	-6.443752	0.729269	0.260813
57	6	0	-7.610284	0.036470	0.074109
58	6	0	-7.523523	-1.322627	-0.308618

59	6	0	-6.317577	-1.984209	-0.514583
60	1	0	-8.567783	0.500656	0.202964
61	1	0	-6.310396	-3.012968	-0.819555
62	6	0	-4.517438	2.007897	0.549016
63	6	0	-5.944498	2.049284	0.590179
64	6	0	-3.795674	3.172286	0.799000
65	6	0	-6.614551	3.227928	0.891676
66	6	0	-5.876670	4.364345	1.143659
67	6	0	-4.480731	4.332736	1.091975
68	1	0	-3.927052	5.235549	1.284022
69	1	0	-7.689961	3.253465	0.923820
70	1	0	-2.722145	3.179924	0.757037
71	7	0	-3.822803	-1.503014	-0.425354
72	6	0	-3.192353	-0.347484	-0.101608
73	1	0	-6.378032	5.286909	1.378023
74	6	0	-8.761458	-2.114605	-0.525198
75	8	0	-8.769424	-3.270314	-0.853370
76	8	0	-9.863074	-1.413036	-0.319157
77	6	0	-11.107142	-2.086949	-0.504531
78	1	0	-11.869306	-1.354530	-0.286827
79	1	0	-11.196851	-2.433575	-1.525854
80	1	0	-11.183834	-2.925911	0.174732

19 (S_1) BHandHLYP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.670601	-0.277856	-0.340993
2	6	0	-0.937972	0.762678	0.250155
3	6	0	-0.943248	-1.257489	-1.037027
4	6	0	0.439523	0.840017	0.143243
5	1	0	-1.451792	1.520082	0.827902
6	6	0	0.433292	-1.194834	-1.154329
7	1	0	-1.477029	-2.083558	-1.489820
8	6	0	1.176377	-0.135975	-0.572649
9	1	0	0.942780	1.675535	0.607648
10	1	0	0.937314	-1.988619	-1.686491
11	6	0	7.227887	-1.300849	2.702754
12	1	0	7.721928	-2.069992	2.100645
13	1	0	7.357031	-1.578490	3.757965
14	6	0	7.875639	0.051127	2.458460
15	1	0	8.909963	0.028975	2.826035
16	1	0	7.334059	0.819826	3.014030
17	6	0	8.793775	-0.162827	0.246055
18	1	0	8.993936	-1.195776	0.555515
19	1	0	9.739987	0.392025	0.297126
20	6	0	8.275218	-0.200494	-1.177424
21	1	0	7.304038	-0.703828	-1.195298
22	1	0	8.977780	-0.779998	-1.787260
23	6	0	6.866120	1.466022	-2.197967
24	1	0	6.410589	0.637572	-2.754252
25	1	0	6.995396	2.304474	-2.885121
26	6	0	5.965776	1.854537	-1.033628
27	1	0	6.331217	2.774382	-0.557922
28	1	0	5.992188	1.061285	-0.285050
29	6	0	3.678069	2.170219	-0.482793
30	1	0	2.788846	2.609185	-0.938583
31	1	0	4.047032	2.858890	0.289570
32	6	0	3.335068	0.824689	0.159894
33	1	0	2.799358	1.000571	1.093530

34	1	0	4.247953	0.293366	0.430989
35	6	0	3.273993	-0.912440	-1.625646
36	1	0	4.087908	-0.324547	-2.052337
37	1	0	2.617092	-1.179318	-2.452377
38	6	0	3.862865	-2.174272	-1.005143
39	1	0	4.032879	-2.933250	-1.780820
40	1	0	3.169388	-2.589218	-0.264567
41	6	0	5.609808	-2.799889	0.518173
42	1	0	5.222865	-3.798008	0.281000
43	1	0	6.693366	-2.830840	0.381214
44	6	0	5.260105	-2.450928	1.959254
45	1	0	4.180094	-2.320861	2.057193
46	1	0	5.564437	-3.273822	2.620168
47	7	0	2.544214	-0.060686	-0.691740
48	8	0	4.643620	2.055227	-1.529427
49	8	0	8.169879	1.110604	-1.745822
50	8	0	7.828351	0.449989	1.093594
51	8	0	5.841749	-1.221082	2.384315
52	8	0	5.107398	-1.829591	-0.396154
53	6	0	-5.108171	-1.271110	-0.254755
54	6	0	-4.034806	0.691823	0.090325
55	7	0	-5.236493	0.053212	0.069342
56	6	0	-6.351043	0.811353	0.295644
57	6	0	-7.544926	0.120539	0.233453
58	6	0	-7.506431	-1.268067	-0.066857
59	6	0	-6.314110	-1.969810	-0.316753
60	1	0	-8.489879	0.614340	0.398206
61	1	0	-6.345826	-3.022214	-0.558109
62	6	0	-4.374543	2.074665	0.361797
63	6	0	-5.812009	2.144721	0.500818
64	6	0	-3.620418	3.248193	0.480657
65	6	0	-6.444918	3.359937	0.768407
66	6	0	-5.669674	4.505480	0.890868
67	6	0	-4.273375	4.446103	0.742678
68	1	0	-3.692174	5.356189	0.833131
69	1	0	-7.522289	3.406775	0.873736
70	1	0	-2.545652	3.234851	0.360395
71	7	0	-3.792865	-1.531069	-0.436535
72	6	0	-3.117366	-0.355285	-0.229171
73	1	0	-6.144572	5.456839	1.097333
74	6	0	-8.768937	-2.052732	-0.143995
75	8	0	-8.823649	-3.240447	-0.397520
76	8	0	-9.856863	-1.304414	0.098234
77	6	0	-11.129420	-1.982109	0.043131
78	1	0	-11.871388	-1.218329	0.259622
79	1	0	-11.289624	-2.402410	-0.949619
80	1	0	-11.166356	-2.775405	0.789620

19·Ba(ClO$_4$)$_2$ (S_0) BHandHLYP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.544642	2.401384	-0.985180
2	6	0	-0.100200	3.086593	0.141253
3	6	0	0.329842	2.285293	-2.055736
4	6	0	1.214767	3.479064	0.256139
5	1	0	-0.759209	3.212102	0.981655
6	6	0	1.638417	2.712906	-1.962380
7	1	0	0.010666	1.785339	-2.953125
8	6	0	2.148669	3.202403	-0.755200

9	1	0	1.524731	3.922542	1.181364
10	1	0	2.273488	2.565121	-2.810526
11	6	0	3.975807	-3.181724	0.530325
12	1	0	4.395114	-3.085724	1.532960
13	1	0	4.599154	-3.884271	-0.024218
14	6	0	2.576455	-3.742922	0.559417
15	1	0	2.591861	-4.725767	1.026801
16	1	0	2.211618	-3.843348	-0.454226
17	6	0	1.455762	-3.090175	2.612327
18	1	0	1.687061	-4.115011	2.894715
19	1	0	0.406356	-2.904110	2.792139
20	6	0	2.283647	-2.133360	3.438580
21	1	0	3.345601	-2.380035	3.408064
22	1	0	1.950733	-2.192668	4.475019
23	6	0	2.691358	0.171597	3.717477
24	1	0	3.762077	-0.022678	3.807429
25	1	0	2.255155	0.182002	4.716511
26	6	0	2.441694	1.498181	3.047380
27	1	0	2.879606	2.296766	3.641855
28	1	0	1.374265	1.665552	2.975816
29	6	0	4.207260	2.162169	1.535839
30	1	0	4.842861	1.499173	0.967240
31	1	0	4.678356	2.363080	2.497401
32	6	0	4.046720	3.476722	0.782160
33	1	0	5.032067	3.928416	0.706760
34	1	0	3.448226	4.170876	1.360562
35	6	0	4.452271	3.107352	-1.632147
36	1	0	5.413450	3.469693	-1.285510
37	1	0	4.188673	3.719701	-2.493665
38	6	0	4.641461	1.682840	-2.150499
39	1	0	5.514140	1.710476	-2.808197
40	1	0	3.801078	1.337461	-2.741482
41	6	0	5.240590	-0.496861	-1.587543
42	1	0	4.557330	-0.834228	-2.360636
43	1	0	6.243837	-0.431122	-2.014424
44	6	0	5.272354	-1.509612	-0.478416
45	1	0	5.834453	-2.368517	-0.842829
46	1	0	5.794198	-1.109466	0.391962
47	7	0	3.508616	3.355896	-0.558541
48	8	0	2.969206	1.499022	1.734297
49	8	0	2.090807	-0.833262	2.938204
50	8	0	1.653413	-2.905365	1.224101
51	8	0	3.974505	-1.931338	-0.116200
52	8	0	4.858972	0.770324	-1.104748
53	56	0	1.141479	-0.376685	0.159731
54	6	0	-3.095291	1.887673	-0.721745
55	6	0	-2.800948	-0.321420	-0.914192
56	6	0	-5.021181	0.643594	-0.492201
57	6	0	-3.348650	-1.600970	-0.895476
58	1	0	-2.745828	-2.477569	-1.036062
59	6	0	-5.570242	-0.607240	-0.470936
60	1	0	-6.615815	-0.766042	-0.296410
61	6	0	-4.712805	-1.716589	-0.677006
62	6	0	-5.366348	2.047880	-0.339550
63	6	0	-4.174745	2.815490	-0.482398
64	6	0	-6.579542	2.673281	-0.094298
65	1	0	-7.481589	2.096651	0.017413
66	6	0	-4.225873	4.199126	-0.379125
67	6	0	-5.443076	4.801003	-0.136736
68	1	0	-5.495826	5.873060	-0.054913
69	6	0	-6.609697	4.048480	0.005852
70	1	0	-3.333268	4.789939	-0.487331
71	7	0	-3.687906	0.675016	-0.718955

72	1	0	-7.542787	4.549178	0.196680
73	7	0	-1.586247	0.232575	-1.051950
74	6	0	-1.755970	1.577822	-0.943488
75	6	0	-5.263147	-3.096854	-0.656695
76	8	0	-4.612224	-4.085131	-0.821988
77	8	0	-6.575797	-3.122715	-0.432875
78	6	0	-7.178575	-4.409281	-0.391207
79	1	0	-8.227763	-4.235193	-0.201800
80	1	0	-7.042464	-4.921490	-1.335617
81	1	0	-6.743137	-5.004803	0.401541
82	17	0	1.681502	-1.769142	-2.990116
83	17	0	-1.419470	-0.247299	2.566290
84	8	0	2.883230	-2.520188	-3.301988
85	8	0	2.058098	-0.402602	-2.527810
86	8	0	0.990171	-2.380296	-1.828526
87	8	0	0.798907	-1.684598	-4.124881
88	8	0	-0.987972	-1.404857	1.745930
89	8	0	-0.566091	0.884493	2.115354
90	8	0	-1.176787	-0.518466	3.968888
91	8	0	-2.808929	0.056394	2.312958

19·Ba(ClO$_4$)$_2$ (S_1) BHandHLYP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.368426	2.475186	-1.322086
2	6	0	0.007083	3.208431	-0.187168
3	6	0	0.587005	2.292291	-2.327565
4	6	0	1.332887	3.551111	0.025808
5	1	0	-0.718324	3.387760	0.595399
6	6	0	1.905101	2.683499	-2.143247
7	1	0	0.317807	1.756979	-3.229236
8	6	0	2.338264	3.185391	-0.898411
9	1	0	1.589477	4.017927	0.964546
10	1	0	2.606258	2.494443	-2.939017
11	6	0	3.516740	-3.323247	0.977044
12	1	0	3.855573	-3.195775	2.013850
13	1	0	4.148334	-4.087376	0.504955
14	6	0	2.079447	-3.795503	0.902631
15	1	0	1.977693	-4.748327	1.434557
16	1	0	1.800208	-3.935651	-0.141146
17	6	0	0.866924	-2.880523	2.819296
18	1	0	0.993658	-3.898410	3.204028
19	1	0	-0.176652	-2.588473	2.909043
20	6	0	1.729843	-1.918875	3.620258
21	1	0	2.771885	-2.257306	3.697130
22	1	0	1.315194	-1.845492	4.633826
23	6	0	2.262081	0.397521	3.764418
24	1	0	3.304264	0.149590	4.012255
25	1	0	1.694057	0.518451	4.695660
26	6	0	2.187237	1.676462	2.955573
27	1	0	2.611583	2.505268	3.530733
28	1	0	1.145020	1.900331	2.729439
29	6	0	4.163797	2.134724	1.610213
30	1	0	4.819690	1.419633	1.119946
31	1	0	4.553646	2.350954	2.612403
32	6	0	4.122286	3.430723	0.793512
33	1	0	5.134644	3.846883	0.784747
34	1	0	3.496713	4.173981	1.288576
35	6	0	4.699953	2.821544	-1.545685

36	1	0	5.667803	3.084888	-1.115774
37	1	0	4.604288	3.401388	-2.471972
38	6	0	4.742387	1.342782	-1.956631
39	1	0	5.674091	1.208594	-2.526214
40	1	0	3.914408	1.054433	-2.605036
41	6	0	5.136778	-0.838204	-1.172796
42	1	0	4.525351	-1.217013	-1.994984
43	1	0	6.190471	-0.831098	-1.489065
44	6	0	5.008316	-1.756066	0.016156
45	1	0	5.563035	-2.672984	-0.215357
46	1	0	5.453091	-1.301133	0.911453
47	7	0	3.690326	3.266287	-0.589369
48	8	0	2.877575	1.512828	1.711205
49	8	0	1.694542	-0.647551	2.984131
50	8	0	1.153735	-2.842178	1.419565
51	8	0	3.643379	-2.092889	0.268697
52	8	0	4.745021	0.485576	-0.821853
53	56	0	1.157387	-0.358529	0.155087
54	6	0	-2.919030	1.922261	-1.028762
55	6	0	-2.579515	-0.308866	-1.209843
56	6	0	-4.803868	0.622642	-0.627794
57	6	0	-3.082611	-1.603549	-1.089246
58	1	0	-2.453006	-2.471005	-1.223522
59	6	0	-5.306034	-0.654156	-0.506281
60	1	0	-6.326929	-0.836403	-0.208671
61	6	0	-4.433012	-1.752252	-0.747529
62	6	0	-5.162811	2.020662	-0.426225
63	6	0	-3.991216	2.823834	-0.671977
64	6	0	-6.360100	2.623408	-0.044090
65	1	0	-7.242428	2.023611	0.146205
66	6	0	-4.054873	4.210533	-0.526707
67	6	0	-5.260045	4.787955	-0.145947
68	1	0	-5.321801	5.863753	-0.029545
69	6	0	-6.400991	4.005629	0.093637
70	1	0	-3.179479	4.822333	-0.708262
71	7	0	-3.491748	0.684811	-1.000587
72	1	0	-7.324281	4.487617	0.391897
73	7	0	-1.372540	0.278298	-1.402050
74	6	0	-1.569903	1.637069	-1.302241
75	6	0	-4.926981	-3.149285	-0.601598
76	8	0	-4.250614	-4.139999	-0.753656
77	8	0	-6.238199	-3.199459	-0.272753
78	6	0	-6.784196	-4.517769	-0.104180
79	1	0	-7.829933	-4.367763	0.154709
80	1	0	-6.693616	-5.088302	-1.029387
81	1	0	-6.261397	-5.046311	0.693955
82	17	0	1.732565	-1.977750	-2.852297
83	17	0	-1.632866	0.117351	2.289092
84	8	0	2.929309	-2.842321	-2.991287
85	8	0	2.176615	-0.574609	-2.444474
86	8	0	0.878311	-2.465667	-1.697289
87	8	0	0.952136	-1.922026	-4.094278
88	8	0	-1.240104	-1.134499	1.534580
89	8	0	-0.686211	1.197084	1.787130
90	8	0	-1.434920	-0.086913	3.743253
91	8	0	-3.023865	0.488427	1.974072

19 (S_0) B3LYP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.568331	-0.256182	-0.395187
2	6	0	-0.825695	0.799472	0.149469
3	6	0	-0.856799	-1.267242	-1.058554
4	6	0	0.552113	0.862001	0.029936
5	1	0	-1.332291	1.580364	0.702110
6	6	0	0.518902	-1.218361	-1.186985
7	1	0	-1.408439	-2.103554	-1.468740
8	6	0	1.273958	-0.147219	-0.649105
9	1	0	1.067421	1.710328	0.456559
10	1	0	1.013865	-2.033519	-1.695529
11	6	0	6.634488	-1.063442	2.895739
12	1	0	7.200463	-1.895954	2.461344
13	1	0	6.589561	-1.229165	3.982687
14	6	0	7.345792	0.250258	2.613423
15	1	0	8.313966	0.261173	3.134305
16	1	0	6.742823	1.074968	2.999606
17	6	0	8.569865	-0.190489	0.589452
18	1	0	8.725477	-1.179789	1.041537
19	1	0	9.500812	0.382152	0.694769
20	6	0	8.244572	-0.401667	-0.878856
21	1	0	7.272122	-0.898615	-0.961262
22	1	0	9.010005	-1.063649	-1.303478
23	6	0	7.016438	1.179442	-2.212682
24	1	0	6.514678	0.301609	-2.639183
25	1	0	7.253191	1.862162	-3.030571
26	6	0	6.093356	1.837715	-1.195519
27	1	0	6.465847	2.835385	-0.926067
28	1	0	6.088364	1.232796	-0.288433
29	6	0	3.786096	2.136551	-0.761377
30	1	0	2.902824	2.507201	-1.285285
31	1	0	4.114057	2.907319	-0.048289
32	6	0	3.451367	0.846529	-0.005525
33	1	0	2.929031	1.086750	0.921391
34	1	0	4.368462	0.340431	0.297904
35	6	0	3.345174	-0.973728	-1.704854
36	1	0	4.198240	-0.427007	-2.108138
37	1	0	2.690510	-1.195810	-2.549340
38	6	0	3.842493	-2.273292	-1.082601
39	1	0	4.037769	-3.021503	-1.864328
40	1	0	3.081141	-2.674800	-0.404655
41	6	0	5.308250	-2.842489	0.736271
42	1	0	4.891205	-3.846485	0.580364
43	1	0	6.394110	-2.950433	0.800572
44	6	0	4.749605	-2.255682	2.029563
45	1	0	3.678312	-2.071528	1.920630
46	1	0	4.886922	-2.975849	2.850160
47	7	0	2.646676	-0.098842	-0.773344
48	8	0	4.786218	1.939639	-1.756439
49	8	0	8.259908	0.811005	-1.625984
50	8	0	7.505071	0.499288	1.228885
51	8	0	5.325084	-0.999268	2.354263
52	8	0	5.053853	-2.002498	-0.377893
53	6	0	-4.997945	-1.246355	-0.263458
54	6	0	-3.929698	0.724983	0.047640
55	7	0	-5.129499	0.083387	0.048488
56	6	0	-6.243560	0.839803	0.280917
57	6	0	-7.435029	0.142635	0.240659
58	6	0	-7.393930	-1.248458	-0.046186

59	6	0	-6.202499	-1.948690	-0.303413
60	1	0	-8.383000	0.628888	0.411435
61	1	0	-6.237714	-3.003743	-0.532801
62	6	0	-4.270175	2.108117	0.306538
63	6	0	-5.706110	2.176420	0.464533
64	6	0	-3.520026	3.286762	0.397477
65	6	0	-6.336484	3.393555	0.726441
66	6	0	-5.564790	4.542796	0.823353
67	6	0	-4.171408	4.485408	0.653673
68	1	0	-3.592104	5.398962	0.721028
69	1	0	-7.412735	3.438931	0.846708
70	1	0	-2.447803	3.273151	0.254817
71	7	0	-3.686353	-1.502987	-0.457136
72	6	0	-3.014373	-0.327899	-0.269487
73	1	0	-6.039730	5.495377	1.024718
74	6	0	-8.650978	-2.042250	-0.101197
75	8	0	-8.709123	-3.226655	-0.342577
76	8	0	-9.747421	-1.291368	0.151021
77	6	0	-11.001663	-1.992452	0.113939
78	1	0	-11.758814	-1.243934	0.336246
79	1	0	-11.166007	-2.425993	-0.873286
80	1	0	-11.014901	-2.787956	0.859980

19 (S_1) B3LYP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.670948	-0.378697	-0.302234
2	6	0	-0.920991	0.814243	-0.359748
3	6	0	-0.945632	-1.591469	-0.365833
4	6	0	0.430462	0.805522	-0.454104
5	1	0	-1.436045	1.761681	-0.359211
6	6	0	0.404222	-1.608349	-0.464788
7	1	0	-1.501089	-2.516469	-0.314024
8	6	0	1.153629	-0.408517	-0.507661
9	1	0	0.949167	1.748567	-0.529431
10	1	0	0.909106	-2.561889	-0.470942
11	6	0	7.098074	0.481832	2.861987
12	1	0	7.617288	-0.481043	2.874303
13	1	0	7.219599	0.923790	3.856764
14	6	0	7.713206	1.381660	1.837444
15	1	0	8.751322	1.599291	2.113584
16	1	0	7.167446	2.325249	1.814673
17	6	0	8.604366	-0.104257	0.253402
18	1	0	8.779909	-0.784275	1.095339
19	1	0	9.557210	0.387215	0.022846
20	6	0	8.143116	-0.917795	-0.911368
21	1	0	7.174654	-1.367927	-0.670128
22	1	0	8.863621	-1.721328	-1.084888
23	6	0	6.767236	-0.079801	-2.626681
24	1	0	6.321236	-1.079519	-2.695341
25	1	0	6.876019	0.304800	-3.640347
26	6	0	5.870160	0.808763	-1.820462
27	1	0	6.256182	1.834855	-1.818557
28	1	0	5.863291	0.459713	-0.786366
29	6	0	3.663831	1.484705	-1.628451
30	1	0	2.787320	1.632533	-2.259733
31	1	0	4.066024	2.470216	-1.364532
32	6	0	3.270906	0.768105	-0.359432
33	1	0	2.719830	1.446277	0.287564

34	1	0	4.161947	0.466683	0.195139
35	6	0	3.224989	-1.606220	-0.932390
36	1	0	3.993052	-1.322687	-1.654858
37	1	0	2.565717	-2.308045	-1.433300
38	6	0	3.894118	-2.264880	0.239407
39	1	0	4.106156	-3.312650	-0.001147
40	1	0	3.228864	-2.246331	1.110250
41	6	0	5.667444	-1.931562	1.723731
42	1	0	5.398543	-2.953949	2.008033
43	1	0	6.749724	-1.909816	1.582319
44	6	0	5.266893	-0.977251	2.807927
45	1	0	4.178986	-0.905803	2.851131
46	1	0	5.613440	-1.352020	3.777563
47	7	0	2.490789	-0.416969	-0.593403
48	8	0	4.594267	0.775868	-2.381323
49	8	0	8.041119	-0.145514	-2.072057
50	8	0	7.636679	0.843013	0.558956
51	8	0	5.746776	0.307744	2.571320
52	8	0	5.083877	-1.590671	0.504540
53	6	0	-5.042632	-1.263696	-0.120475
54	6	0	-3.978284	0.700656	-0.054233
55	7	0	-5.163203	0.082190	-0.022302
56	6	0	-6.258203	0.874194	0.116498
57	6	0	-7.457671	0.194820	0.150708
58	6	0	-7.422381	-1.200377	0.047424
59	6	0	-6.262950	-1.955651	-0.086379
60	1	0	-8.401407	0.704905	0.255521
61	1	0	-6.316137	-3.029460	-0.157453
62	6	0	-4.287284	2.087532	0.087278
63	6	0	-5.717987	2.181179	0.187007
64	6	0	-3.528720	3.249036	0.155798
65	6	0	-6.329357	3.418973	0.335839
66	6	0	-5.548958	4.542227	0.391273
67	6	0	-4.156586	4.458895	0.304214
68	1	0	-3.564866	5.361637	0.357609
69	1	0	-7.406242	3.491953	0.409673
70	1	0	-2.450398	3.224974	0.105213
71	7	0	-3.772572	-1.574595	-0.223877
72	6	0	-3.061375	-0.396508	-0.196225
73	1	0	-6.014999	5.511014	0.508333
74	6	0	-8.686569	-1.949815	0.082838
75	8	0	-8.760766	-3.142954	0.000311
76	8	0	-9.744703	-1.182708	0.215952
77	6	0	-10.985603	-1.843413	0.257885
78	1	0	-11.735810	-1.069509	0.374359
79	1	0	-11.153742	-2.396307	-0.663955
80	1	0	-11.021130	-2.533451	1.098321

19·Ba(ClO$_4$)$_2$ (S_0) B3LYP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.353552	2.431930	-1.417442
2	6	0	0.014407	3.221840	-0.318007
3	6	0	0.614826	2.185729	-2.397477
4	6	0	1.339929	3.566584	-0.107037
5	1	0	-0.718430	3.446547	0.445921
6	6	0	1.933010	2.577065	-2.217764
7	1	0	0.353390	1.602466	-3.271188
8	6	0	2.354226	3.145162	-0.997555

9	1	0	1.588687	4.081002	0.808798
10	1	0	2.642416	2.337651	-2.992059
11	6	0	3.487101	-3.292399	1.118429
12	1	0	3.809799	-3.127316	2.155042
13	1	0	4.124491	-4.074402	0.684958
14	6	0	2.050380	-3.765558	1.038835
15	1	0	1.939232	-4.698448	1.603212
16	1	0	1.787045	-3.943196	-0.003323
17	6	0	0.809727	-2.781609	2.902665
18	1	0	0.926193	-3.785859	3.324676
19	1	0	-0.233801	-2.482961	2.965903
20	6	0	1.664354	-1.795687	3.682995
21	1	0	2.702043	-2.138098	3.793562
22	1	0	1.230318	-1.680622	4.684381
23	6	0	2.206205	0.521627	3.752887
24	1	0	3.243365	0.281175	4.027674
25	1	0	1.621284	0.674456	4.668725
26	6	0	2.147211	1.772550	2.900141
27	1	0	2.567912	2.618676	3.452290
28	1	0	1.109344	1.993008	2.652585
29	6	0	4.143805	2.175166	1.567593
30	1	0	4.802978	1.440969	1.111322
31	1	0	4.520259	2.423923	2.567309
32	6	0	4.119235	3.441988	0.706122
33	1	0	5.133415	3.853527	0.694830
34	1	0	3.490903	4.204342	1.167347
35	6	0	4.722917	2.755911	-1.605750
36	1	0	5.685155	3.042144	-1.177847
37	1	0	4.630439	3.300304	-2.553549
38	6	0	4.779913	1.262584	-1.961522
39	1	0	5.725298	1.111243	-2.503683
40	1	0	3.968676	0.947486	-2.618701
41	6	0	5.149793	-0.890136	-1.092916
42	1	0	4.550818	-1.296371	-1.911186
43	1	0	6.208737	-0.898153	-1.391103
44	6	0	4.997791	-1.764182	0.126030
45	1	0	5.553871	-2.690023	-0.062811
46	1	0	5.428468	-1.278427	1.011975
47	7	0	3.702664	3.228788	-0.674769
48	8	0	2.852629	1.563931	1.670972
49	8	0	1.651597	-0.549231	2.998444
50	8	0	1.117785	-2.793661	1.506885
51	8	0	3.627905	-2.089228	0.367182
52	8	0	4.757537	0.446822	-0.797012
53	56	0	1.148274	-0.356373	0.159304
54	6	0	-2.899719	1.895519	-1.076194
55	6	0	-2.577402	-0.338820	-1.250991
56	6	0	-4.787291	0.611009	-0.642054
57	6	0	-3.087305	-1.629228	-1.115299
58	1	0	-2.465308	-2.501646	-1.253421
59	6	0	-5.296364	-0.661822	-0.507114
60	1	0	-6.314427	-0.835497	-0.195060
61	6	0	-4.434067	-1.766956	-0.753804
62	6	0	-5.133820	2.012233	-0.442834
63	6	0	-3.960348	2.806067	-0.709387
64	6	0	-6.321150	2.625083	-0.046041
65	1	0	-7.204621	2.032310	0.160285
66	6	0	-4.012445	4.193898	-0.569895
67	6	0	-5.207842	4.781424	-0.174320
68	1	0	-5.260516	5.858166	-0.062189
69	6	0	-6.350536	4.008136	0.085672
70	1	0	-3.135794	4.798951	-0.767367
71	7	0	-3.479858	0.662185	-1.032712

72	1	0	-7.265962	4.497914	0.395272
73	7	0	-1.369687	0.238947	-1.466315
74	6	0	-1.556277	1.599374	-1.368165
75	6	0	-4.935331	-3.159685	-0.593137
76	8	0	-4.267299	-4.155825	-0.746918
77	8	0	-6.242960	-3.199271	-0.248771
78	6	0	-6.795556	-4.512880	-0.065809
79	1	0	-7.837165	-4.354390	0.204435
80	1	0	-6.719664	-5.089553	-0.988529
81	1	0	-6.266881	-5.040155	0.729293
82	17	0	1.768408	-2.082016	-2.780226
83	17	0	-1.652564	0.212951	2.260626
84	8	0	2.963156	-2.955629	-2.870566
85	8	0	2.212073	-0.667479	-2.413194
86	8	0	0.893580	-2.526552	-1.623075
87	8	0	1.008106	-2.065432	-4.035715
88	8	0	-1.275708	-1.062792	1.538667
89	8	0	-0.706655	1.271315	1.714240
90	8	0	-1.436229	0.051104	3.718006
91	8	0	-3.045695	0.581792	1.954084

19·Ba(ClO$_4$)$_2$ (S_1) B3LYP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.128717	1.793809	-1.927706
2	6	0	0.221319	2.914295	-1.163325
3	6	0	0.876584	1.193148	-2.692979
4	6	0	1.531649	3.237201	-0.975827
5	1	0	-0.538243	3.424491	-0.586742
6	6	0	2.183030	1.559209	-2.550187
7	1	0	0.619149	0.363201	-3.337087
8	6	0	2.561505	2.498084	-1.585375
9	1	0	1.762560	4.041627	-0.295564
10	1	0	2.923049	1.033069	-3.127097
11	6	0	2.888856	-2.935069	2.023993
12	1	0	3.083868	-2.513046	3.017881
13	1	0	3.516298	-3.826094	1.906968
14	6	0	1.462709	-3.342885	1.865389
15	1	0	1.201804	-4.079451	2.631071
16	1	0	1.326106	-3.786954	0.881615
17	6	0	0.138157	-1.862777	3.188741
18	1	0	0.103428	-2.724289	3.861982
19	1	0	-0.870558	-1.489382	3.044318
20	6	0	0.982303	-0.782181	3.797168
21	1	0	1.925299	-1.164961	4.206024
22	1	0	0.410298	-0.323783	4.609878
23	6	0	1.771492	1.352115	3.371234
24	1	0	2.657487	1.118868	3.975781
25	1	0	1.009342	1.810086	4.011320
26	6	0	2.126540	2.295116	2.268253
27	1	0	2.591049	3.186115	2.699576
28	1	0	1.218961	2.596982	1.746498
29	6	0	4.232133	2.278846	1.165980
30	1	0	4.943738	1.486180	0.954852
31	1	0	4.543898	2.804842	2.075733
32	6	0	4.221774	3.253303	0.011919
33	1	0	5.222559	3.681841	-0.077312
34	1	0	3.558875	4.089181	0.227224

35	6	0	4.903269	1.958450	-1.949024
36	1	0	5.843746	2.366857	-1.580925
37	1	0	4.852585	2.209320	-3.013429
38	6	0	4.960672	0.444634	-1.838804
39	1	0	5.991266	0.148839	-2.076768
40	1	0	4.310246	-0.066763	-2.550313
41	6	0	5.027390	-1.284586	-0.329390
42	1	0	4.615752	-1.955083	-1.087554
43	1	0	6.123422	-1.344100	-0.366161
44	6	0	4.580449	-1.731169	1.015946
45	1	0	5.128628	-2.648001	1.254697
46	1	0	4.827509	-0.978309	1.774796
47	7	0	3.867978	2.655959	-1.241633
48	8	0	2.996633	1.663635	1.369572
49	8	0	1.267229	0.175313	2.824188
50	8	0	0.593912	-2.252940	1.926605
51	8	0	3.211710	-2.001357	1.040515
52	8	0	4.631453	0.029916	-0.558378
53	56	0	1.069255	-0.275473	0.114331
54	6	0	-2.623028	1.579464	-1.293831
55	6	0	-2.575713	-0.649452	-1.360517
56	6	0	-4.586720	0.590503	-0.676997
57	6	0	-3.223161	-1.861693	-1.138765
58	1	0	-2.747235	-2.816431	-1.288794
59	6	0	-5.246464	-0.604342	-0.448403
60	1	0	-6.261253	-0.648182	-0.090320
61	6	0	-4.541157	-1.786121	-0.686282
62	6	0	-4.750606	2.001450	-0.595756
63	6	0	-3.516376	2.624464	-0.992676
64	6	0	-5.810474	2.795622	-0.211157
65	1	0	-6.746628	2.354930	0.103110
66	6	0	-3.390719	4.002131	-1.000781
67	6	0	-4.464220	4.769408	-0.615421
68	1	0	-4.385411	5.846717	-0.614154
69	6	0	-5.657077	4.165671	-0.225479
70	1	0	-2.464141	4.466578	-1.311721
71	7	0	-3.317295	0.440553	-1.113918
72	1	0	-6.486783	4.789909	0.077086
73	7	0	-1.352049	-0.249504	-1.733234
74	6	0	-1.337739	1.096530	-1.709516
75	6	0	-5.208587	-3.076577	-0.444451
76	8	0	-4.689913	-4.138484	-0.597883
77	8	0	-6.456942	-2.947627	-0.034396
78	6	0	-7.129983	-4.152918	0.211519
79	1	0	-8.129086	-3.881855	0.535796
80	1	0	-7.172789	-4.758119	-0.692343
81	1	0	-6.619646	-4.724581	0.984727
82	17	0	2.022878	-2.746003	-2.018601
83	17	0	-1.662734	1.039341	1.952640
84	8	0	3.100065	-3.614628	-1.628345
85	8	0	2.501957	-1.351265	-2.012036
86	8	0	0.963659	-2.781457	-1.008217
87	8	0	1.514035	-3.084371	-3.304435
88	8	0	-1.457099	-0.266390	1.318688
89	8	0	-0.700018	1.933333	1.304282
90	8	0	-1.372586	0.947282	3.360965
91	8	0	-2.998450	1.491334	1.725213

19(S_0) CAM-B3LYP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.742338	-0.261580	-0.106584
2	6	0	-1.063162	0.695902	0.647273
3	6	0	-0.966508	-1.143510	-0.862756
4	6	0	0.315192	0.789403	0.638792
5	1	0	-1.619033	1.377424	1.279216
6	6	0	0.411378	-1.065717	-0.881892
7	1	0	-1.460350	-1.908889	-1.448138
8	6	0	1.103228	-0.087058	-0.135674
9	1	0	0.775890	1.560584	1.238068
10	1	0	0.953618	-1.786979	-1.475514
11	6	0	8.252466	-2.032883	1.362801
12	1	0	8.044503	-2.469760	0.379141
13	1	0	8.818632	-2.770134	1.948306
14	6	0	9.074889	-0.773219	1.205113
15	1	0	10.092488	-1.033951	0.895149
16	1	0	9.135387	-0.264217	2.169342
17	6	0	8.958212	0.023111	-1.042738
18	1	0	9.127595	-1.026731	-1.309878
19	1	0	9.909592	0.558660	-1.152385
20	6	0	7.925059	0.578003	-1.988752
21	1	0	6.983158	0.044913	-1.831331
22	1	0	8.248063	0.399550	-3.021422
23	6	0	6.411372	2.417054	-1.932051
24	1	0	5.919022	1.899072	-2.762791
25	1	0	6.453716	3.478973	-2.176488
26	6	0	5.621110	2.193219	-0.651991
27	1	0	5.942486	2.900648	0.122313
28	1	0	5.818005	1.182670	-0.278452
29	6	0	3.394216	2.316088	0.189441
30	1	0	2.442006	2.736475	-0.136009
31	1	0	3.795003	2.951888	0.989720
32	6	0	3.194371	0.903447	0.732903
33	1	0	2.674490	0.969539	1.690363
34	1	0	4.156403	0.443279	0.954016
35	6	0	3.277157	-0.780265	-1.084964
36	1	0	4.152205	-0.187495	-1.349902
37	1	0	2.725498	-0.934948	-2.013201
38	6	0	3.748501	-2.125304	-0.559485
39	1	0	4.283408	-2.645381	-1.365369
40	1	0	2.903606	-2.754073	-0.251549
41	6	0	5.331258	-3.063616	0.928337
42	1	0	4.643347	-3.889588	1.154810
43	1	0	5.981409	-3.391135	0.106956
44	6	0	6.126573	-2.757267	2.180245
45	1	0	5.440571	-2.447067	2.970132
46	1	0	6.635989	-3.672162	2.509344
47	7	0	2.475092	0.003676	-0.158107
48	8	0	4.248011	2.376863	-0.944272
49	8	0	7.748391	1.972215	-1.780245
50	8	0	8.489249	0.137964	0.288960
51	8	0	7.053176	-1.697585	2.035967
52	8	0	4.614404	-1.910161	0.539521
53	6	0	-5.154620	-1.283447	-0.320273
54	6	0	-4.143897	0.650571	0.213027
55	7	0	-5.326160	0.007526	0.068385
56	6	0	-6.459814	0.733543	0.262646
57	6	0	-7.630455	0.041141	0.075789
58	6	0	-7.548038	-1.323028	-0.305137

59	6	0	-6.341739	-1.991083	-0.509940
60	1	0	-8.593473	0.510956	0.203389
61	1	0	-6.340303	-3.027430	-0.815121
62	6	0	-4.522694	2.010939	0.548568
63	6	0	-5.953094	2.057260	0.589833
64	6	0	-3.795047	3.176015	0.796392
65	6	0	-6.620763	3.241722	0.889338
66	6	0	-5.876695	4.379672	1.139323
67	6	0	-4.477719	4.343334	1.087540
68	1	0	-3.917142	5.250451	1.278709
69	1	0	-7.703120	3.270877	0.921740
70	1	0	-2.714347	3.178514	0.754156
71	7	0	-3.833621	-1.518111	-0.422506
72	6	0	-3.199269	-0.356950	-0.099887
73	1	0	-6.378438	5.310369	1.373089
74	6	0	-8.791850	-2.114240	-0.521704
75	8	0	-8.807171	-3.278374	-0.849969
76	8	0	-9.898691	-1.401241	-0.315476
77	6	0	-11.147823	-2.083621	-0.503920
78	1	0	-11.916532	-1.347797	-0.287626
79	1	0	-11.233394	-2.434707	-1.531300
80	1	0	-11.222837	-2.927307	0.180549

19 (S_1) CAM-B3LYP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.670601	-0.277856	-0.340993
2	6	0	-0.937972	0.762678	0.250155
3	6	0	-0.943248	-1.257489	-1.037027
4	6	0	0.439523	0.840017	0.143243
5	1	0	-1.451792	1.520082	0.827902
6	6	0	0.433292	-1.194834	-1.154329
7	1	0	-1.477029	-2.083558	-1.489820
8	6	0	1.176377	-0.135975	-0.572649
9	1	0	0.942780	1.675535	0.607648
10	1	0	0.937314	-1.988619	-1.686491
11	6	0	7.227887	-1.300849	2.702754
12	1	0	7.721928	-2.069992	2.100645
13	1	0	7.357031	-1.578490	3.757965
14	6	0	7.875639	0.051127	2.458460
15	1	0	8.909963	0.028975	2.826035
16	1	0	7.334059	0.819826	3.014030
17	6	0	8.793775	-0.162827	0.246055
18	1	0	8.993936	-1.195776	0.555515
19	1	0	9.739987	0.392025	0.297126
20	6	0	8.275218	-0.200494	-1.177424
21	1	0	7.304038	-0.703828	-1.195298
22	1	0	8.977780	-0.779998	-1.787260
23	6	0	6.866120	1.466022	-2.197967
24	1	0	6.410589	0.637572	-2.754252
25	1	0	6.995396	2.304474	-2.885121
26	6	0	5.965776	1.854537	-1.033628
27	1	0	6.331217	2.774382	-0.557922
28	1	0	5.992188	1.061285	-0.285050
29	6	0	3.678069	2.170219	-0.482793
30	1	0	2.788846	2.609185	-0.938583
31	1	0	4.047032	2.858890	0.289570
32	6	0	3.335068	0.824689	0.159894
33	1	0	2.799358	1.000571	1.093530
34	1	0	4.247953	0.293366	0.430989

35	6	0	3.273993	-0.912440	-1.625646
36	1	0	4.087908	-0.324547	-2.052337
37	1	0	2.617092	-1.179318	-2.452377
38	6	0	3.862865	-2.174272	-1.005143
39	1	0	4.032879	-2.933250	-1.780820
40	1	0	3.169388	-2.589218	-0.264567
41	6	0	5.609808	-2.799889	0.518173
42	1	0	5.222865	-3.798008	0.281000
43	1	0	6.693366	-2.830840	0.381214
44	6	0	5.260105	-2.450928	1.959254
45	1	0	4.180094	-2.320861	2.057193
46	1	0	5.564437	-3.273822	2.620168
47	7	0	2.544214	-0.060686	-0.691740
48	8	0	4.643620	2.055227	-1.529427
49	8	0	8.169879	1.110604	-1.745822
50	8	0	7.828351	0.449989	1.093594
51	8	0	5.841749	-1.221082	2.384315
52	8	0	5.107398	-1.829591	-0.396154
53	6	0	-5.108171	-1.271110	-0.254755
54	6	0	-4.034806	0.691823	0.090325
55	7	0	-5.236493	0.053212	0.069342
56	6	0	-6.351043	0.811353	0.295644
57	6	0	-7.544926	0.120539	0.233453
58	6	0	-7.506431	-1.268067	-0.066857
59	6	0	-6.314110	-1.969810	-0.316753
60	1	0	-8.489879	0.614340	0.398206
61	1	0	-6.345826	-3.022214	-0.558109
62	6	0	-4.374543	2.074665	0.361797
63	6	0	-5.812009	2.144721	0.500818
64	6	0	-3.620418	3.248193	0.480657
65	6	0	-6.444918	3.359937	0.768407
66	6	0	-5.669674	4.505480	0.890868
67	6	0	-4.273375	4.446103	0.742678
68	1	0	-3.692174	5.356189	0.833131
69	1	0	-7.522289	3.406775	0.873736
70	1	0	-2.545652	3.234851	0.360395
71	7	0	-3.792865	-1.531069	-0.436535
72	6	0	-3.117366	-0.355285	-0.229171
73	1	0	-6.144572	5.456839	1.097333
74	6	0	-8.768937	-2.052732	-0.143995
75	8	0	-8.823649	-3.240447	-0.397520
76	8	0	-9.856863	-1.304414	0.098234
77	6	0	-11.129420	-1.982109	0.043131
78	1	0	-11.871388	-1.218329	0.259622
79	1	0	-11.289624	-2.402410	-0.949619
80	1	0	-11.166356	-2.775405	0.789620

19·Ba(ClO$_4$)$_2$ (S_0) CAM-B3LYP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.514913	2.423466	-0.981545
2	6	0	-0.072595	3.097436	0.157194
3	6	0	0.364647	2.316321	-2.053738
4	6	0	1.247758	3.481773	0.282972
5	1	0	-0.740493	3.217630	1.000333
6	6	0	1.678257	2.738770	-1.950027
7	1	0	0.044062	1.823778	-2.963158
8	6	0	2.186842	3.208945	-0.729957
9	1	0	1.558467	3.917283	1.220027
10	1	0	2.320694	2.599396	-2.803167

11	6	0	3.911764	-3.220547	0.540582
12	1	0	4.321813	-3.129774	1.555073
13	1	0	4.540928	-3.929758	-0.012932
14	6	0	2.503456	-3.768948	0.546907
15	1	0	2.499618	-4.761367	1.010490
16	1	0	2.147853	-3.855194	-0.479064
17	6	0	1.368762	-3.111202	2.602348
18	1	0	1.582713	-4.148474	2.879633
19	1	0	0.314850	-2.905259	2.777026
20	6	0	2.210103	-2.169583	3.439542
21	1	0	3.275536	-2.433072	3.416600
22	1	0	1.865358	-2.224450	4.479857
23	6	0	2.651674	0.138744	3.731610
24	1	0	3.725012	-0.075102	3.831536
25	1	0	2.201036	0.151439	4.731990
26	6	0	2.427297	1.472645	3.058981
27	1	0	2.872143	2.271377	3.660393
28	1	0	1.355712	1.653933	2.972347
29	6	0	4.227647	2.121079	1.564317
30	1	0	4.860657	1.455019	0.982761
31	1	0	4.696847	2.299568	2.538802
32	6	0	4.084183	3.450943	0.826396
33	1	0	5.079796	3.898391	0.762177
34	1	0	3.483373	4.147968	1.411548
35	6	0	4.501302	3.092201	-1.596530
36	1	0	5.471891	3.439278	-1.239264
37	1	0	4.250670	3.718778	-2.460311
38	6	0	4.669341	1.664642	-2.123841
39	1	0	5.549498	1.678641	-2.783616
40	1	0	3.818346	1.329480	-2.719022
41	6	0	5.231778	-0.537517	-1.568128
42	1	0	4.535553	-0.858537	-2.346854
43	1	0	6.241791	-0.486512	-1.999163
44	6	0	5.243225	-1.556904	-0.461221
45	1	0	5.794900	-2.430452	-0.827758
46	1	0	5.769513	-1.166300	0.419648
47	7	0	3.551743	3.347242	-0.523165
48	8	0	2.973484	1.462952	1.743620
49	8	0	2.039139	-0.858352	2.935810
50	8	0	1.574219	-2.920383	1.207180
51	8	0	3.927401	-1.960296	-0.106684
52	8	0	4.871749	0.741005	-1.072142
53	56	0	1.148677	-0.371929	0.160269
54	6	0	-3.075624	1.906390	-0.738692
55	6	0	-2.774372	-0.312892	-0.928150
56	6	0	-5.007036	0.652412	-0.508149
57	6	0	-3.322160	-1.596275	-0.903357
58	1	0	-2.713519	-2.478747	-1.037953
59	6	0	-5.552117	-0.603960	-0.481084
60	1	0	-6.603485	-0.767646	-0.301437
61	6	0	-4.689580	-1.714721	-0.684551
62	6	0	-5.354855	2.060933	-0.351329
63	6	0	-4.161748	2.833062	-0.493543
64	6	0	-6.571877	2.684858	-0.101700
65	1	0	-7.478409	2.102081	0.009694
66	6	0	-4.215336	4.219646	-0.384689
67	6	0	-5.436627	4.820677	-0.137446
68	1	0	-5.491156	5.899284	-0.050784
69	6	0	-6.604447	4.063713	0.004039
70	1	0	-3.317615	4.815594	-0.492650
71	7	0	-3.668607	0.687638	-0.740380
72	1	0	-7.544367	4.565043	0.199276
73	7	0	-1.554455	0.246891	-1.058487

74	6	0	-1.729998	1.597891	-0.951002
75	6	0	-5.236700	-3.100690	-0.657321
76	8	0	-4.581317	-4.097113	-0.816532
77	8	0	-6.560496	-3.127243	-0.433975
78	6	0	-7.154241	-4.427559	-0.387867
79	1	0	-8.211723	-4.260495	-0.200661
80	1	0	-7.008336	-4.945517	-1.335529
81	1	0	-6.710806	-5.018701	0.413048
82	17	0	1.682071	-1.744427	-2.998127
83	17	0	-1.443983	-0.225610	2.537831
84	8	0	2.891479	-2.509953	-3.316973
85	8	0	2.074189	-0.369366	-2.514666
86	8	0	0.974379	-2.367154	-1.830710
87	8	0	0.794530	-1.639087	-4.145764
88	8	0	-1.010828	-1.397618	1.708481
89	8	0	-0.562797	0.911603	2.094961
90	8	0	-1.218566	-0.506998	3.956963
91	8	0	-2.841033	0.098399	2.265322

19·Ba(ClO$_4$)$_2$ (S_1) CAM-B3LYP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.368426	2.475186	-1.322086
2	6	0	0.007083	3.208431	-0.187168
3	6	0	0.587005	2.292291	-2.327565
4	6	0	1.332887	3.551111	0.025808
5	1	0	-0.718324	3.387760	0.595399
6	6	0	1.905101	2.683499	-2.143247
7	1	0	0.317807	1.756979	-3.229236
8	6	0	2.338264	3.185391	-0.898411
9	1	0	1.589477	4.017927	0.964546
10	1	0	2.606258	2.494443	-2.939017
11	6	0	3.516740	-3.323247	0.977044
12	1	0	3.855573	-3.195775	2.013850
13	1	0	4.148334	-4.087376	0.504955
14	6	0	2.079447	-3.795503	0.902631
15	1	0	1.977693	-4.748327	1.434557
16	1	0	1.800208	-3.935651	-0.141146
17	6	0	0.866924	-2.880523	2.819296
18	1	0	0.993658	-3.898410	3.204028
19	1	0	-0.176652	-2.588473	2.909043
20	6	0	1.729843	-1.918875	3.620258
21	1	0	2.771885	-2.257306	3.697130
22	1	0	1.315194	-1.845492	4.633826
23	6	0	2.262081	0.397521	3.764418
24	1	0	3.304264	0.149590	4.012255
25	1	0	1.694057	0.518451	4.695660
26	6	0	2.187237	1.676462	2.955573
27	1	0	2.611583	2.505268	3.530733
28	1	0	1.145020	1.900331	2.729439
29	6	0	4.163797	2.134724	1.610213
30	1	0	4.819690	1.419633	1.119946
31	1	0	4.553646	2.350954	2.612403
32	6	0	4.122286	3.430723	0.793512
33	1	0	5.134644	3.846883	0.784747
34	1	0	3.496713	4.173981	1.288576
35	6	0	4.699953	2.821544	-1.545685
36	1	0	5.667803	3.084888	-1.115774
37	1	0	4.604288	3.401388	-2.471972

38	6	0	4.742387	1.342782	-1.956631
39	1	0	5.674091	1.208594	-2.526214
40	1	0	3.914408	1.054433	-2.605036
41	6	0	5.136778	-0.838204	-1.172796
42	1	0	4.525351	-1.217013	-1.994984
43	1	0	6.190471	-0.831098	-1.489065
44	6	0	5.008316	-1.756066	0.016156
45	1	0	5.563035	-2.672984	-0.215357
46	1	0	5.453091	-1.301133	0.911453
47	7	0	3.690326	3.266287	-0.589369
48	8	0	2.877575	1.512828	1.711205
49	8	0	1.694542	-0.647551	2.984131
50	8	0	1.153735	-2.842178	1.419565
51	8	0	3.643379	-2.092889	0.268697
52	8	0	4.745021	0.485576	-0.821853
53	56	0	1.157387	-0.358529	0.155087
54	6	0	-2.919030	1.922261	-1.028762
55	6	0	-2.579515	-0.308866	-1.209843
56	6	0	-4.803868	0.622642	-0.627794
57	6	0	-3.082611	-1.603549	-1.089246
58	1	0	-2.453006	-2.471005	-1.223522
59	6	0	-5.306034	-0.654156	-0.506281
60	1	0	-6.326929	-0.836403	-0.208671
61	6	0	-4.433012	-1.752252	-0.747529
62	6	0	-5.162811	2.020662	-0.426225
63	6	0	-3.991216	2.823834	-0.671977
64	6	0	-6.360100	2.623408	-0.044090
65	1	0	-7.242428	2.023611	0.146205
66	6	0	-4.054873	4.210533	-0.526707
67	6	0	-5.260045	4.787955	-0.145947
68	1	0	-5.321801	5.863753	-0.029545
69	6	0	-6.400991	4.005629	0.093637
70	1	0	-3.179479	4.822333	-0.708262
71	7	0	-3.491748	0.684811	-1.000587
72	1	0	-7.324281	4.487617	0.391897
73	7	0	-1.372540	0.278298	-1.402050
74	6	0	-1.569903	1.637069	-1.302241
75	6	0	-4.926981	-3.149285	-0.601598
76	8	0	-4.250614	-4.139999	-0.753656
77	8	0	-6.238199	-3.199459	-0.272753
78	6	0	-6.784196	-4.517769	-0.104180
79	1	0	-7.829933	-4.367763	0.154709
80	1	0	-6.693616	-5.088302	-1.029387
81	1	0	-6.261397	-5.046311	0.693955
82	17	0	1.732565	-1.977750	-2.852297
83	17	0	-1.632866	0.117351	2.289092
84	8	0	2.929309	-2.842321	-2.991287
85	8	0	2.176615	-0.574609	-2.444474
86	8	0	0.878311	-2.465667	-1.697289
87	8	0	0.952136	-1.922026	-4.094278
88	8	0	-1.240104	-1.134499	1.534580
89	8	0	-0.686211	1.197084	1.787130
90	8	0	-1.434920	-0.086913	3.743253
91	8	0	-3.023865	0.488427	1.974072

19 (S_0) M06

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.699911	-0.272689	-0.322824
2	6	0	-0.979479	0.778731	0.249547
3	6	0	-0.967506	-1.257946	-0.992075
4	6	0	0.393794	0.863294	0.145700
5	1	0	-1.504357	1.543512	0.815269
6	6	0	0.405504	-1.189363	-1.104018
7	1	0	-1.496549	-2.099133	-1.429536
8	6	0	1.135172	-0.117281	-0.546204
9	1	0	0.893229	1.713660	0.595499
10	1	0	0.919594	-1.994889	-1.615894
11	6	0	7.345356	-1.294471	2.626152
12	1	0	7.813471	-2.074926	2.008197
13	1	0	7.485488	-1.594663	3.677155
14	6	0	8.025288	0.030284	2.383872
15	1	0	9.073994	-0.030559	2.714819
16	1	0	7.532460	0.806529	2.979199
17	6	0	8.844377	-0.177896	0.157905
18	1	0	9.049681	-1.217855	0.457073
19	1	0	9.805828	0.360765	0.162580
20	6	0	8.259802	-0.206046	-1.229277
21	1	0	7.290955	-0.726089	-1.200827
22	1	0	8.932982	-0.778258	-1.883323
23	6	0	6.800421	1.430947	-2.168887
24	1	0	6.343512	0.603499	-2.736183
25	1	0	6.882939	2.287260	-2.846694
26	6	0	5.922117	1.774410	-0.986975
27	1	0	6.315034	2.662093	-0.463369
28	1	0	5.940797	0.940930	-0.272354
29	6	0	3.674765	2.156742	-0.413072
30	1	0	2.792129	2.638402	-0.848592
31	1	0	4.075098	2.824171	0.367908
32	6	0	3.286277	0.826702	0.210086
33	1	0	2.729887	1.012514	1.133660
34	1	0	4.183663	0.272066	0.510318
35	6	0	3.237362	-0.895321	-1.573046
36	1	0	4.049109	-0.310518	-2.021362
37	1	0	2.583627	-1.188401	-2.397230
38	6	0	3.841234	-2.123646	-0.921009
39	1	0	3.952380	-2.938308	-1.654914
40	1	0	3.177517	-2.485817	-0.118623
41	6	0	5.658220	-2.723413	0.483727
42	1	0	5.285423	-3.733558	0.257702
43	1	0	6.742549	-2.736886	0.311865
44	6	0	5.356819	-2.375227	1.925289
45	1	0	4.277004	-2.228754	2.050803
46	1	0	5.657991	-3.206975	2.581938
47	7	0	2.501842	-0.029839	-0.666902
48	8	0	4.615840	2.022236	-1.460438
49	8	0	8.107889	1.100572	-1.757973
50	8	0	7.937241	0.443192	1.039656
51	8	0	5.972998	-1.169816	2.325888
52	8	0	5.111471	-1.773445	-0.405759
53	6	0	-5.112481	-1.271282	-0.237229
54	6	0	-4.058234	0.689307	0.088834
55	7	0	-5.252560	0.048397	0.071388
56	6	0	-6.364723	0.802398	0.286740
57	6	0	-7.551829	0.109487	0.228482
58	6	0	-7.503656	-1.276638	-0.057502

59	6	0	-6.314413	-1.972928	-0.295552
60	1	0	-8.501953	0.602988	0.385977
61	1	0	-6.344234	-3.030609	-0.526886
62	6	0	-4.404551	2.068965	0.345466
63	6	0	-5.831887	2.133101	0.479262
64	6	0	-3.660148	3.245193	0.454461
65	6	0	-6.473506	3.342149	0.733278
66	6	0	-5.710182	4.488925	0.847557
67	6	0	-4.318224	4.436155	0.703269
68	1	0	-3.741813	5.352264	0.786838
69	1	0	-7.554257	3.379012	0.834841
70	1	0	-2.582089	3.238921	0.334536
71	7	0	-3.804976	-1.529554	-0.412113
72	6	0	-3.144758	-0.354660	-0.215288
73	1	0	-6.191618	5.441097	1.044878
74	6	0	-8.756806	-2.070686	-0.132931
75	8	0	-8.800135	-3.252880	-0.379881
76	8	0	-9.842184	-1.332224	0.103613
77	6	0	-11.095114	-2.015255	0.049593
78	1	0	-11.853871	-1.266059	0.266606
79	1	0	-11.256854	-2.440209	-0.943369
80	1	0	-11.128449	-2.813588	0.794055

19 (S_1) M06

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.670601	-0.277856	-0.340993
2	6	0	-0.937972	0.762678	0.250155
3	6	0	-0.943248	-1.257489	-1.037027
4	6	0	0.439523	0.840017	0.143243
5	1	0	-1.451792	1.520082	0.827902
6	6	0	0.433292	-1.194834	-1.154329
7	1	0	-1.477029	-2.083558	-1.489820
8	6	0	1.176377	-0.135975	-0.572649
9	1	0	0.942780	1.675535	0.607648
10	1	0	0.937314	-1.988619	-1.686491
11	6	0	7.227887	-1.300849	2.702754
12	1	0	7.721928	-2.069992	2.100645
13	1	0	7.357031	-1.578490	3.757965
14	6	0	7.875639	0.051127	2.458460
15	1	0	8.909963	0.028975	2.826035
16	1	0	7.334059	0.819826	3.014030
17	6	0	8.793775	-0.162827	0.246055
18	1	0	8.993936	-1.195776	0.555515
19	1	0	9.739987	0.392025	0.297126
20	6	0	8.275218	-0.200494	-1.177424
21	1	0	7.304038	-0.703828	-1.195298
22	1	0	8.977780	-0.779998	-1.787260
23	6	0	6.866120	1.466022	-2.197967
24	1	0	6.410589	0.637572	-2.754252
25	1	0	6.995396	2.304474	-2.885121
26	6	0	5.965776	1.854537	-1.033628
27	1	0	6.331217	2.774382	-0.557922
28	1	0	5.992188	1.061285	-0.285050
29	6	0	3.678069	2.170219	-0.482793
30	1	0	2.788846	2.609185	-0.938583
31	1	0	4.047032	2.858890	0.289570
32	6	0	3.335068	0.824689	0.159894
33	1	0	2.799358	1.000571	1.093530

34	1	0	4.247953	0.293366	0.430989
35	6	0	3.273993	-0.912440	-1.625646
36	1	0	4.087908	-0.324547	-2.052337
37	1	0	2.617092	-1.179318	-2.452377
38	6	0	3.862865	-2.174272	-1.005143
39	1	0	4.032879	-2.933250	-1.780820
40	1	0	3.169388	-2.589218	-0.264567
41	6	0	5.609808	-2.799889	0.518173
42	1	0	5.222865	-3.798008	0.281000
43	1	0	6.693366	-2.830840	0.381214
44	6	0	5.260105	-2.450928	1.959254
45	1	0	4.180094	-2.320861	2.057193
46	1	0	5.564437	-3.273822	2.620168
47	7	0	2.544214	-0.060686	-0.691740
48	8	0	4.643620	2.055227	-1.529427
49	8	0	8.169879	1.110604	-1.745822
50	8	0	7.828351	0.449989	1.093594
51	8	0	5.841749	-1.221082	2.384315
52	8	0	5.107398	-1.829591	-0.396154
53	6	0	-5.108171	-1.271110	-0.254755
54	6	0	-4.034806	0.691823	0.090325
55	7	0	-5.236493	0.053212	0.069342
56	6	0	-6.351043	0.811353	0.295644
57	6	0	-7.544926	0.120539	0.233453
58	6	0	-7.506431	-1.268067	-0.066857
59	6	0	-6.314110	-1.969810	-0.316753
60	1	0	-8.489879	0.614340	0.398206
61	1	0	-6.345826	-3.022214	-0.558109
62	6	0	-4.374543	2.074665	0.361797
63	6	0	-5.812009	2.144721	0.500818
64	6	0	-3.620418	3.248193	0.480657
65	6	0	-6.444918	3.359937	0.768407
66	6	0	-5.669674	4.505480	0.890868
67	6	0	-4.273375	4.446103	0.742678
68	1	0	-3.692174	5.356189	0.833131
69	1	0	-7.522289	3.406775	0.873736
70	1	0	-2.545652	3.234851	0.360395
71	7	0	-3.792865	-1.531069	-0.436535
72	6	0	-3.117366	-0.355285	-0.229171
73	1	0	-6.144572	5.456839	1.097333
74	6	0	-8.768937	-2.052732	-0.143995
75	8	0	-8.823649	-3.240447	-0.397520
76	8	0	-9.856863	-1.304414	0.098234
77	6	0	-11.129420	-1.982109	0.043131
78	1	0	-11.871388	-1.218329	0.259622
79	1	0	-11.289624	-2.402410	-0.949619
80	1	0	-11.166356	-2.775405	0.789620

19·Ba(ClO$_4$)$_2$ (S_0) M06

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.335517	2.279349	-1.393611
2	6	0	0.034963	3.120145	-0.341491
3	6	0	0.624813	1.979976	-2.356679
4	6	0	1.354337	3.484329	-0.160358
5	1	0	-0.701310	3.387735	0.411604
6	6	0	1.937086	2.386106	-2.207997
7	1	0	0.357208	1.350514	-3.200798
8	6	0	2.361344	3.030498	-1.034648

9	1	0	1.605722	4.059394	0.722689
10	1	0	2.642484	2.107244	-2.977092
11	6	0	3.524380	-3.220287	1.156532
12	1	0	3.847601	-3.010687	2.190926
13	1	0	4.176595	-4.015400	0.760033
14	6	0	2.103275	-3.708100	1.095314
15	1	0	2.001898	-4.631855	1.682672
16	1	0	1.846554	-3.924629	0.054016
17	6	0	0.873056	-2.702641	2.919999
18	1	0	1.005408	-3.698013	3.367031
19	1	0	-0.180600	-2.424788	2.989779
20	6	0	1.707977	-1.693313	3.674669
21	1	0	2.752509	-2.024233	3.806622
22	1	0	1.268450	-1.558257	4.676119
23	6	0	2.239544	0.600706	3.692468
24	1	0	3.269776	0.351801	4.005093
25	1	0	1.636091	0.795533	4.593624
26	6	0	2.236938	1.813006	2.800048
27	1	0	2.652416	2.676257	3.337441
28	1	0	1.205260	2.050215	2.516419
29	6	0	4.230498	2.198676	1.499090
30	1	0	4.927016	1.483057	1.056635
31	1	0	4.607251	2.481220	2.494522
32	6	0	4.143555	3.435487	0.616583
33	1	0	5.139744	3.894285	0.575749
34	1	0	3.493945	4.186808	1.076398
35	6	0	4.722526	2.713379	-1.679678
36	1	0	5.683450	3.041498	-1.269220
37	1	0	4.603979	3.242425	-2.637281
38	6	0	4.829151	1.224462	-2.005013
39	1	0	5.812729	1.080158	-2.486547
40	1	0	4.073193	0.878543	-2.721811
41	6	0	5.162587	-0.886795	-1.092239
42	1	0	4.583242	-1.329485	-1.914847
43	1	0	6.228529	-0.886397	-1.378483
44	6	0	5.003323	-1.719783	0.141961
45	1	0	5.588364	-2.641256	0.000399
46	1	0	5.410730	-1.193278	1.022378
47	7	0	3.708329	3.165457	-0.742327
48	8	0	2.980867	1.539108	1.621443
49	8	0	1.690672	-0.474652	2.966698
50	8	0	1.174303	-2.738702	1.536321
51	8	0	3.649266	-2.059810	0.362330
52	8	0	4.744847	0.437749	-0.842431
53	56	0	1.142369	-0.323512	0.121783
54	6	0	-2.882734	1.856113	-1.035527
55	6	0	-2.655190	-0.377158	-1.186994
56	6	0	-4.820084	0.671089	-0.603453
57	6	0	-3.227206	-1.639303	-1.047031
58	1	0	-2.647481	-2.545266	-1.179532
59	6	0	-5.388065	-0.570858	-0.467092
60	1	0	-6.421215	-0.695136	-0.170054
61	6	0	-4.575444	-1.710378	-0.697620
62	6	0	-5.104503	2.083870	-0.437278
63	6	0	-3.904296	2.816244	-0.703395
64	6	0	-6.270317	2.750392	-0.078579
65	1	0	-7.180668	2.194444	0.127038
66	6	0	-3.903095	4.204885	-0.606302
67	6	0	-5.075246	4.847375	-0.249691
68	1	0	-5.087735	5.930310	-0.171559
69	6	0	-6.247701	4.130476	0.013090
70	1	0	-2.999045	4.770640	-0.811217
71	7	0	-3.511800	0.655734	-0.973552

72	1	0	-7.149119	4.666390	0.292669
73	7	0	-1.431285	0.137544	-1.420329
74	6	0	-1.562955	1.494681	-1.329902
75	6	0	-5.140789	-3.076428	-0.548840
76	8	0	-4.522746	-4.095734	-0.706192
77	8	0	-6.442444	-3.053384	-0.215508
78	6	0	-7.051579	-4.328087	-0.051504
79	1	0	-8.089804	-4.134101	0.214905
80	1	0	-6.998182	-4.904207	-0.978776
81	1	0	-6.555334	-4.894129	0.740826
82	17	0	1.769836	-2.178021	-2.706991
83	17	0	-1.620877	0.178206	2.265554
84	8	0	2.909354	-3.093968	-2.733847
85	8	0	2.261634	-0.785368	-2.412824
86	8	0	0.872304	-2.523691	-1.561382
87	8	0	1.035481	-2.190065	-3.956277
88	8	0	-1.255522	-1.055270	1.508590
89	8	0	-0.684404	1.240282	1.769832
90	8	0	-1.410701	-0.034282	3.697076
91	8	0	-2.995306	0.557327	1.972504

19·Ba(ClO$_4$)$_2$ (S$_1$) M06

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.368426	2.475186	-1.322086
2	6	0	0.007083	3.208431	-0.187168
3	6	0	0.587005	2.292291	-2.327565
4	6	0	1.332887	3.551111	0.025808
5	1	0	-0.718324	3.387760	0.595399
6	6	0	1.905101	2.683499	-2.143247
7	1	0	0.317807	1.756979	-3.229236
8	6	0	2.338264	3.185391	-0.898411
9	1	0	1.589477	4.017927	0.964546
10	1	0	2.606258	2.494443	-2.939017
11	6	0	3.516740	-3.323247	0.977044
12	1	0	3.855573	-3.195775	2.013850
13	1	0	4.148334	-4.087376	0.504955
14	6	0	2.079447	-3.795503	0.902631
15	1	0	1.977693	-4.748327	1.434557
16	1	0	1.800208	-3.935651	-0.141146
17	6	0	0.866924	-2.880523	2.819296
18	1	0	0.993658	-3.898410	3.204028
19	1	0	-0.176652	-2.588473	2.909043
20	6	0	1.729843	-1.918875	3.620258
21	1	0	2.771885	-2.257306	3.697130
22	1	0	1.315194	-1.845492	4.633826
23	6	0	2.262081	0.397521	3.764418
24	1	0	3.304264	0.149590	4.012255
25	1	0	1.694057	0.518451	4.695660
26	6	0	2.187237	1.676462	2.955573
27	1	0	2.611583	2.505268	3.530733
28	1	0	1.145020	1.900331	2.729439
29	6	0	4.163797	2.134724	1.610213
30	1	0	4.819690	1.419633	1.119946
31	1	0	4.553646	2.350954	2.612403
32	6	0	4.122286	3.430723	0.793512
33	1	0	5.134644	3.846883	0.784747
34	1	0	3.496713	4.173981	1.288576
35	6	0	4.699953	2.821544	-1.545685

36	1	0	5.667803	3.084888	-1.115774
37	1	0	4.604288	3.401388	-2.471972
38	6	0	4.742387	1.342782	-1.956631
39	1	0	5.674091	1.208594	-2.526214
40	1	0	3.914408	1.054433	-2.605036
41	6	0	5.136778	-0.838204	-1.172796
42	1	0	4.525351	-1.217013	-1.994984
43	1	0	6.190471	-0.831098	-1.489065
44	6	0	5.008316	-1.756066	0.016156
45	1	0	5.563035	-2.672984	-0.215357
46	1	0	5.453091	-1.301133	0.911453
47	7	0	3.690326	3.266287	-0.589369
48	8	0	2.877575	1.512828	1.711205
49	8	0	1.694542	-0.647551	2.984131
50	8	0	1.153735	-2.842178	1.419565
51	8	0	3.643379	-2.092889	0.268697
52	8	0	4.745021	0.485576	-0.821853
53	56	0	1.157387	-0.358529	0.155087
54	6	0	-2.919030	1.922261	-1.028762
55	6	0	-2.579515	-0.308866	-1.209843
56	6	0	-4.803868	0.622642	-0.627794
57	6	0	-3.082611	-1.603549	-1.089246
58	1	0	-2.453006	-2.471005	-1.223522
59	6	0	-5.306034	-0.654156	-0.506281
60	1	0	-6.326929	-0.836403	-0.208671
61	6	0	-4.433012	-1.752252	-0.747529
62	6	0	-5.162811	2.020662	-0.426225
63	6	0	-3.991216	2.823834	-0.671977
64	6	0	-6.360100	2.623408	-0.044090
65	1	0	-7.242428	2.023611	0.146205
66	6	0	-4.054873	4.210533	-0.526707
67	6	0	-5.260045	4.787955	-0.145947
68	1	0	-5.321801	5.863753	-0.029545
69	6	0	-6.400991	4.005629	0.093637
70	1	0	-3.179479	4.822333	-0.708262
71	7	0	-3.491748	0.684811	-1.000587
72	1	0	-7.324281	4.487617	0.391897
73	7	0	-1.372540	0.278298	-1.402050
74	6	0	-1.569903	1.637069	-1.302241
75	6	0	-4.926981	-3.149285	-0.601598
76	8	0	-4.250614	-4.139999	-0.753656
77	8	0	-6.238199	-3.199459	-0.272753
78	6	0	-6.784196	-4.517769	-0.104180
79	1	0	-7.829933	-4.367763	0.154709
80	1	0	-6.693616	-5.088302	-1.029387
81	1	0	-6.261397	-5.046311	0.693955
82	17	0	1.732565	-1.977750	-2.852297
83	17	0	-1.632866	0.117351	2.289092
84	8	0	2.929309	-2.842321	-2.991287
85	8	0	2.176615	-0.574609	-2.444474
86	8	0	0.878311	-2.465667	-1.697289
87	8	0	0.952136	-1.922026	-4.094278
88	8	0	-1.240104	-1.134499	1.534580
89	8	0	-0.686211	1.197084	1.787130
90	8	0	-1.434920	-0.086913	3.743253
91	8	0	-3.023865	0.488427	1.974072

19 (S_0) M06-L

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.689697	-0.175691	-0.401018
2	6	0	-0.978576	0.902888	0.145232
3	6	0	-0.939161	-1.170575	-1.047673
4	6	0	0.395644	0.998360	0.047202
5	1	0	-1.512790	1.678856	0.683215
6	6	0	0.434502	-1.090136	-1.157298
7	1	0	-1.458323	-2.027339	-1.463949
8	6	0	1.152513	0.003321	-0.615143
9	1	0	0.885477	1.864621	0.474157
10	1	0	0.960158	-1.899528	-1.648669
11	6	0	7.272874	-1.392469	2.732408
12	1	0	7.724522	-2.195531	2.135276
13	1	0	7.439741	-1.651675	3.788546
14	6	0	7.938213	-0.072576	2.418502
15	1	0	8.991838	-0.105177	2.732252
16	1	0	7.449168	0.728088	2.981212
17	6	0	8.746885	-0.362999	0.197475
18	1	0	8.861346	-1.426588	0.457342
19	1	0	9.740028	0.103148	0.294311
20	6	0	8.248673	-0.278291	-1.222688
21	1	0	7.252561	-0.733761	-1.285326
22	1	0	8.924586	-0.852231	-1.870328
23	6	0	6.939421	1.492501	-2.150164
24	1	0	6.508167	0.752476	-2.841982
25	1	0	7.107039	2.412794	-2.716505
26	6	0	5.986574	1.730998	-0.997638
27	1	0	6.364504	2.533657	-0.345220
28	1	0	5.928139	0.819786	-0.389457
29	6	0	3.746246	2.269432	-0.502157
30	1	0	2.898453	2.770399	-0.978283
31	1	0	4.145474	2.940813	0.274271
32	6	0	3.294651	0.969352	0.147972
33	1	0	2.709539	1.200526	1.040479
34	1	0	4.162564	0.401715	0.499480
35	6	0	3.270231	-0.809778	-1.580221
36	1	0	4.110622	-0.253250	-2.006006
37	1	0	2.641183	-1.103756	-2.421072
38	6	0	3.822767	-2.039750	-0.879910
39	1	0	3.924880	-2.876365	-1.588511
40	1	0	3.139622	-2.366389	-0.081002
41	6	0	5.641023	-2.707154	0.495285
42	1	0	5.297983	-3.704236	0.185808
43	1	0	6.726931	-2.683649	0.349785
44	6	0	5.298114	-2.472521	1.953040
45	1	0	4.216339	-2.349505	2.068938
46	1	0	5.595831	-3.347736	2.549555
47	7	0	2.519334	0.098743	-0.726968
48	8	0	4.716113	2.084458	-1.524271
49	8	0	8.209775	1.071343	-1.683803
50	8	0	7.820529	0.281831	1.051745
51	8	0	5.881873	-1.285529	2.466542
52	8	0	5.099801	-1.705405	-0.352962
53	6	0	-5.080745	-1.246925	-0.318906
54	6	0	-4.067688	0.732636	0.066723
55	7	0	-5.246855	0.062001	0.038249
56	6	0	-6.377066	0.777188	0.306686
57	6	0	-7.550090	0.049974	0.244955
58	6	0	-7.474256	-1.323739	-0.094649

59	6	0	-6.264430	-1.978794	-0.381931
60	1	0	-8.508451	0.509686	0.442117
61	1	0	-6.272132	-3.027202	-0.649838
62	6	0	-4.444194	2.089473	0.386713
63	6	0	-5.877030	2.110349	0.546429
64	6	0	-3.729932	3.283891	0.533343
65	6	0	-6.544354	3.293948	0.862571
66	6	0	-5.807872	4.458031	1.012997
67	6	0	-4.415518	4.448625	0.843476
68	1	0	-3.861288	5.374684	0.955094
69	1	0	-7.622938	3.299216	0.983033
70	1	0	-2.655425	3.313761	0.395710
71	7	0	-3.766689	-1.470088	-0.521090
72	6	0	-3.128385	-0.282670	-0.287075
73	1	0	-6.310967	5.387061	1.257693
74	6	0	-8.702988	-2.147535	-0.173768
75	8	0	-8.726365	-3.326048	-0.467987
76	8	0	-9.809696	-1.442465	0.120214
77	6	0	-11.038845	-2.176971	0.064130
78	1	0	-11.818924	-1.469154	0.332061
79	1	0	-11.206998	-2.564831	-0.941506
80	1	0	-11.020263	-3.007818	0.770749

19 (S_1) M06-L

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.670601	-0.277856	-0.340993
2	6	0	-0.937972	0.762678	0.250155
3	6	0	-0.943248	-1.257489	-1.037027
4	6	0	0.439523	0.840017	0.143243
5	1	0	-1.451792	1.520082	0.827902
6	6	0	0.433292	-1.194834	-1.154329
7	1	0	-1.477029	-2.083558	-1.489820
8	6	0	1.176377	-0.135975	-0.572649
9	1	0	0.942780	1.675535	0.607648
10	1	0	0.937314	-1.988619	-1.686491
11	6	0	7.227887	-1.300849	2.702754
12	1	0	7.721928	-2.069992	2.100645
13	1	0	7.357031	-1.578490	3.757965
14	6	0	7.875639	0.051127	2.458460
15	1	0	8.909963	0.028975	2.826035
16	1	0	7.334059	0.819826	3.014030
17	6	0	8.793775	-0.162827	0.246055
18	1	0	8.993936	-1.195776	0.555515
19	1	0	9.739987	0.392025	0.297126
20	6	0	8.275218	-0.200494	-1.177424
21	1	0	7.304038	-0.703828	-1.195298
22	1	0	8.977780	-0.779998	-1.787260
23	6	0	6.866120	1.466022	-2.197967
24	1	0	6.410589	0.637572	-2.754252
25	1	0	6.995396	2.304474	-2.885121
26	6	0	5.965776	1.854537	-1.033628
27	1	0	6.331217	2.774382	-0.557922
28	1	0	5.992188	1.061285	-0.285050
29	6	0	3.678069	2.170219	-0.482793
30	1	0	2.788846	2.609185	-0.938583
31	1	0	4.047032	2.858890	0.289570
32	6	0	3.335068	0.824689	0.159894

33	1	0	2.799358	1.000571	1.093530
34	1	0	4.247953	0.293366	0.430989
35	6	0	3.273993	-0.912440	-1.625646
36	1	0	4.087908	-0.324547	-2.052337
37	1	0	2.617092	-1.179318	-2.452377
38	6	0	3.862865	-2.174272	-1.005143
39	1	0	4.032879	-2.933250	-1.780820
40	1	0	3.169388	-2.589218	-0.264567
41	6	0	5.609808	-2.799889	0.518173
42	1	0	5.222865	-3.798008	0.281000
43	1	0	6.693366	-2.830840	0.381214
44	6	0	5.260105	-2.450928	1.959254
45	1	0	4.180094	-2.320861	2.057193
46	1	0	5.564437	-3.273822	2.620168
47	7	0	2.544214	-0.060686	-0.691740
48	8	0	4.643620	2.055227	-1.529427
49	8	0	8.169879	1.110604	-1.745822
50	8	0	7.828351	0.449989	1.093594
51	8	0	5.841749	-1.221082	2.384315
52	8	0	5.107398	-1.829591	-0.396154
53	6	0	-5.108171	-1.271110	-0.254755
54	6	0	-4.034806	0.691823	0.090325
55	7	0	-5.236493	0.053212	0.069342
56	6	0	-6.351043	0.811353	0.295644
57	6	0	-7.544926	0.120539	0.233453
58	6	0	-7.506431	-1.268067	-0.066857
59	6	0	-6.314110	-1.969810	-0.316753
60	1	0	-8.489879	0.614340	0.398206
61	1	0	-6.345826	-3.022214	-0.558109
62	6	0	-4.374543	2.074665	0.361797
63	6	0	-5.812009	2.144721	0.500818
64	6	0	-3.620418	3.248193	0.480657
65	6	0	-6.444918	3.359937	0.768407
66	6	0	-5.669674	4.505480	0.890868
67	6	0	-4.273375	4.446103	0.742678
68	1	0	-3.692174	5.356189	0.833131
69	1	0	-7.522289	3.406775	0.873736
70	1	0	-2.545652	3.234851	0.360395
71	7	0	-3.792865	-1.531069	-0.436535
72	6	0	-3.117366	-0.355285	-0.229171
73	1	0	-6.144572	5.456839	1.097333
74	6	0	-8.768937	-2.052732	-0.143995
75	8	0	-8.823649	-3.240447	-0.397520
76	8	0	-9.856863	-1.304414	0.098234
77	6	0	-11.129420	-1.982109	0.043131
78	1	0	-11.871388	-1.218329	0.259622
79	1	0	-11.289624	-2.402410	-0.949619
80	1	0	-11.166356	-2.775405	0.789620

19·Ba(ClO$_4$)$_2$ (S_0) M06-L

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.322763	2.219036	-1.449290
2	6	0	0.072646	3.088244	-0.423256
3	6	0	0.641452	1.845954	-2.391434
4	6	0	1.404087	3.416090	-0.246613
5	1	0	-0.653967	3.408510	0.315969
6	6	0	1.967958	2.217916	-2.253312
7	1	0	0.361918	1.184340	-3.205231
8	6	0	2.404717	2.916004	-1.110693

9	1	0	1.669647	4.018278	0.612536
10	1	0	2.671018	1.879804	-2.999621
11	6	0	3.391046	-3.225384	1.260765
12	1	0	3.721795	-3.028586	2.293592
13	1	0	4.032093	-4.023567	0.856293
14	6	0	1.958753	-3.684322	1.201977
15	1	0	1.834983	-4.586535	1.815552
16	1	0	1.693825	-3.921277	0.169969
17	6	0	0.771989	-2.592412	3.006679
18	1	0	0.906199	-3.573059	3.481343
19	1	0	-0.275759	-2.303111	3.086673
20	6	0	1.629646	-1.563570	3.710458
21	1	0	2.668061	-1.900728	3.860328
22	1	0	1.195808	-1.364399	4.701464
23	6	0	2.161217	0.732870	3.644048
24	1	0	3.152247	0.474954	4.052762
25	1	0	1.494915	0.991286	4.480460
26	6	0	2.264724	1.891670	2.686723
27	1	0	2.669609	2.769616	3.203838
28	1	0	1.267993	2.146881	2.311197
29	6	0	4.311110	2.242868	1.446269
30	1	0	5.044934	1.534297	1.061460
31	1	0	4.649700	2.593241	2.431954
32	6	0	4.200062	3.428879	0.492630
33	1	0	5.189586	3.892838	0.412480
34	1	0	3.547878	4.199505	0.910636
35	6	0	4.760174	2.603619	-1.780574
36	1	0	5.715322	2.981963	-1.406944
37	1	0	4.603796	3.078362	-2.758743
38	6	0	4.889007	1.096470	-2.020720
39	1	0	5.898525	0.916589	-2.426379
40	1	0	4.180058	0.713639	-2.764023
41	6	0	5.151710	-0.962306	-0.963983
42	1	0	4.628610	-1.448288	-1.796123
43	1	0	6.232560	-0.972774	-1.181441
44	6	0	4.915055	-1.727780	0.303179
45	1	0	5.495561	-2.658444	0.241636
46	1	0	5.277769	-1.166169	1.179197
47	7	0	3.752260	3.080275	-0.845224
48	8	0	3.089598	1.522560	1.578222
49	8	0	1.636175	-0.375715	2.934794
50	8	0	1.042331	-2.678900	1.611211
51	8	0	3.539843	-2.052692	0.471413
52	8	0	4.718551	0.380772	-0.815039
53	56	0	1.151157	-0.269497	0.108547
54	6	0	-2.886832	1.841881	-1.067778
55	6	0	-2.682078	-0.401246	-1.211066
56	6	0	-4.839424	0.675540	-0.631271
57	6	0	-3.263203	-1.657011	-1.061374
58	1	0	-2.692136	-2.568447	-1.184935
59	6	0	-5.418854	-0.567056	-0.487429
60	1	0	-6.451582	-0.680469	-0.188142
61	6	0	-4.618436	-1.717689	-0.709374
62	6	0	-5.110144	2.089033	-0.469192
63	6	0	-3.897245	2.812077	-0.739267
64	6	0	-6.269770	2.771493	-0.108317
65	1	0	-7.185532	2.227239	0.100340
66	6	0	-3.883843	4.203852	-0.642571
67	6	0	-5.051380	4.860560	-0.283537
68	1	0	-5.051888	5.942987	-0.206007
69	6	0	-6.232604	4.154708	-0.017445
70	1	0	-2.976160	4.761822	-0.848569
71	7	0	-3.528785	0.646861	-1.004398

72	1	0	-7.127623	4.699173	0.263682
73	7	0	-1.448031	0.099567	-1.449080
74	6	0	-1.565372	1.462378	-1.364620
75	6	0	-5.191527	-3.075491	-0.547050
76	8	0	-4.582020	-4.108549	-0.696845
77	8	0	-6.501109	-3.036577	-0.205656
78	6	0	-7.106077	-4.317955	-0.028867
79	1	0	-8.142493	-4.123783	0.238927
80	1	0	-7.051885	-4.900697	-0.950386
81	1	0	-6.604467	-4.874787	0.764837
82	17	0	1.864214	-2.279457	-2.600631
83	17	0	-1.606570	0.264658	2.239570
84	8	0	3.008534	-3.195352	-2.504701
85	8	0	2.340712	-0.860006	-2.374497
86	8	0	0.900220	-2.552723	-1.480754
87	8	0	1.196683	-2.378619	-3.889311
88	8	0	-1.236571	-0.990210	1.508206
89	8	0	-0.698825	1.334622	1.683196
90	8	0	-1.354409	0.098349	3.676924
91	8	0	-2.999531	0.613386	1.972534

19·Ba(ClO$_4$)$_2$ (S_1) M06-L

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.368426	2.475186	-1.322086
2	6	0	0.007083	3.208431	-0.187168
3	6	0	0.587005	2.292291	-2.327565
4	6	0	1.332887	3.551111	0.025808
5	1	0	-0.718324	3.387760	0.595399
6	6	0	1.905101	2.683499	-2.143247
7	1	0	0.317807	1.756979	-3.229236
8	6	0	2.338264	3.185391	-0.898411
9	1	0	1.589477	4.017927	0.964546
10	1	0	2.606258	2.494443	-2.939017
11	6	0	3.516740	-3.323247	0.977044
12	1	0	3.855573	-3.195775	2.013850
13	1	0	4.148334	-4.087376	0.504955
14	6	0	2.079447	-3.795503	0.902631
15	1	0	1.977693	-4.748327	1.434557
16	1	0	1.800208	-3.935651	-0.141146
17	6	0	0.866924	-2.880523	2.819296
18	1	0	0.993658	-3.898410	3.204028
19	1	0	-0.176652	-2.588473	2.909043
20	6	0	1.729843	-1.918875	3.620258
21	1	0	2.771885	-2.257306	3.697130
22	1	0	1.315194	-1.845492	4.633826
23	6	0	2.262081	0.397521	3.764418
24	1	0	3.304264	0.149590	4.012255
25	1	0	1.694057	0.518451	4.695660
26	6	0	2.187237	1.676462	2.955573
27	1	0	2.611583	2.505268	3.530733
28	1	0	1.145020	1.900331	2.729439
29	6	0	4.163797	2.134724	1.610213
30	1	0	4.819690	1.419633	1.119946
31	1	0	4.553646	2.350954	2.612403
32	6	0	4.122286	3.430723	0.793512
33	1	0	5.134644	3.846883	0.784747
34	1	0	3.496713	4.173981	1.288576
35	6	0	4.699953	2.821544	-1.545685

36	1	0	5.667803	3.084888	-1.115774
37	1	0	4.604288	3.401388	-2.471972
38	6	0	4.742387	1.342782	-1.956631
39	1	0	5.674091	1.208594	-2.526214
40	1	0	3.914408	1.054433	-2.605036
41	6	0	5.136778	-0.838204	-1.172796
42	1	0	4.525351	-1.217013	-1.994984
43	1	0	6.190471	-0.831098	-1.489065
44	6	0	5.008316	-1.756066	0.016156
45	1	0	5.563035	-2.672984	-0.215357
46	1	0	5.453091	-1.301133	0.911453
47	7	0	3.690326	3.266287	-0.589369
48	8	0	2.877575	1.512828	1.711205
49	8	0	1.694542	-0.647551	2.984131
50	8	0	1.153735	-2.842178	1.419565
51	8	0	3.643379	-2.092889	0.268697
52	8	0	4.745021	0.485576	-0.821853
53	56	0	1.157387	-0.358529	0.155087
54	6	0	-2.919030	1.922261	-1.028762
55	6	0	-2.579515	-0.308866	-1.209843
56	6	0	-4.803868	0.622642	-0.627794
57	6	0	-3.082611	-1.603549	-1.089246
58	1	0	-2.453006	-2.471005	-1.223522
59	6	0	-5.306034	-0.654156	-0.506281
60	1	0	-6.326929	-0.836403	-0.208671
61	6	0	-4.433012	-1.752252	-0.747529
62	6	0	-5.162811	2.020662	-0.426225
63	6	0	-3.991216	2.823834	-0.671977
64	6	0	-6.360100	2.623408	-0.044090
65	1	0	-7.242428	2.023611	0.146205
66	6	0	-4.054873	4.210533	-0.526707
67	6	0	-5.260045	4.787955	-0.145947
68	1	0	-5.321801	5.863753	-0.029545
69	6	0	-6.400991	4.005629	0.093637
70	1	0	-3.179479	4.822333	-0.708262
71	7	0	-3.491748	0.684811	-1.000587
72	1	0	-7.324281	4.487617	0.391897
73	7	0	-1.372540	0.278298	-1.402050
74	6	0	-1.569903	1.637069	-1.302241
75	6	0	-4.926981	-3.149285	-0.601598
76	8	0	-4.250614	-4.139999	-0.753656
77	8	0	-6.238199	-3.199459	-0.272753
78	6	0	-6.784196	-4.517769	-0.104180
79	1	0	-7.829933	-4.367763	0.154709
80	1	0	-6.693616	-5.088302	-1.029387
81	1	0	-6.261397	-5.046311	0.693955
82	17	0	1.732565	-1.977750	-2.852297
83	17	0	-1.632866	0.117351	2.289092
84	8	0	2.929309	-2.842321	-2.991287
85	8	0	2.176615	-0.574609	-2.444474
86	8	0	0.878311	-2.465667	-1.697289
87	8	0	0.952136	-1.922026	-4.094278
88	8	0	-1.240104	-1.134499	1.534580
89	8	0	-0.686211	1.197084	1.787130
90	8	0	-1.434920	-0.086913	3.743253
91	8	0	-3.023865	0.488427	1.974072

19 (S_0) M06-2X

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.695557	-0.185657	-0.298252
2	6	0	-1.018040	0.825519	0.390458
3	6	0	-0.932704	-1.074418	-1.062254
4	6	0	0.356052	0.963864	0.308923
5	1	0	-1.574311	1.507586	1.024226
6	6	0	0.442686	-0.951691	-1.153028
7	1	0	-1.432242	-1.878538	-1.589833
8	6	0	1.132009	0.079977	-0.474822
9	1	0	0.826545	1.778945	0.842289
10	1	0	0.985682	-1.680718	-1.739124
11	6	0	7.470722	-1.861114	2.434299
12	1	0	7.928644	-2.546467	1.713561
13	1	0	7.708303	-2.232906	3.437976
14	6	0	8.037679	-0.463646	2.266604
15	1	0	9.110123	-0.466785	2.499091
16	1	0	7.536943	0.211169	2.964180
17	6	0	8.750014	-0.337775	-0.001223
18	1	0	8.941320	-1.418540	0.035744
19	1	0	9.702477	0.180439	0.171752
20	6	0	8.203489	0.006865	-1.369497
21	1	0	7.221244	-0.463517	-1.489021
22	1	0	8.879439	-0.390009	-2.133718
23	6	0	6.811868	1.895297	-1.848970
24	1	0	6.363557	1.304865	-2.658628
25	1	0	6.933923	2.920430	-2.202734
26	6	0	5.906935	1.861005	-0.629190
27	1	0	6.323567	2.493654	0.165303
28	1	0	5.849485	0.835685	-0.253608
29	6	0	3.692918	2.334751	0.044702
30	1	0	2.830093	2.903963	-0.307228
31	1	0	4.119104	2.847177	0.918080
32	6	0	3.257557	0.929640	0.453233
33	1	0	2.663115	0.995762	1.365315
34	1	0	4.130676	0.321477	0.702658
35	6	0	3.258655	-0.499437	-1.578458
36	1	0	4.080243	0.141040	-1.908187
37	1	0	2.623653	-0.665385	-2.447912
38	6	0	3.862324	-1.818316	-1.106027
39	1	0	3.993695	-2.499447	-1.956751
40	1	0	3.202353	-2.302356	-0.374362
41	6	0	5.797405	-2.664046	-0.010607
42	1	0	5.506597	-3.568930	-0.558327
43	1	0	6.865549	-2.503026	-0.179369
44	6	0	5.526054	-2.858698	1.472726
45	1	0	4.449175	-2.858080	1.656581
46	1	0	5.924901	-3.829811	1.792660
47	7	0	2.497496	0.226376	-0.573283
48	8	0	4.630888	2.341818	-1.019099
49	8	0	8.106951	1.415863	-1.536980
50	8	0	7.802471	0.051016	0.971159
51	8	0	6.063504	-1.814403	2.263738
52	8	0	5.130461	-1.531595	-0.535871
53	6	0	-5.090185	-1.288017	-0.261925
54	6	0	-4.090538	0.694803	0.098080
55	7	0	-5.266788	0.024174	0.062214
56	6	0	-6.402702	0.744718	0.279576
57	6	0	-7.572005	0.022300	0.205285
58	6	0	-7.480269	-1.362005	-0.098341

59	6	0	-6.275712	-2.026112	-0.337515
60	1	0	-8.535503	0.484483	0.362131
61	1	0	-6.273134	-3.079602	-0.580904
62	6	0	-4.474452	2.069624	0.368731
63	6	0	-5.902632	2.095932	0.493775
64	6	0	-3.753444	3.261974	0.491279
65	6	0	-6.578182	3.287619	0.756793
66	6	0	-5.840635	4.453105	0.886014
67	6	0	-4.443730	4.436326	0.747769
68	1	0	-3.891971	5.364051	0.841650
69	1	0	-7.657553	3.298754	0.852335
70	1	0	-2.677531	3.278830	0.375498
71	7	0	-3.771456	-1.508643	-0.429317
72	6	0	-3.146833	-0.319424	-0.210959
73	1	0	-6.345306	5.389478	1.089182
74	6	0	-8.721357	-2.188300	-0.189671
75	8	0	-8.731494	-3.366925	-0.452952
76	8	0	-9.825795	-1.483103	0.052373
77	6	0	-11.061361	-2.207056	-0.016700
78	1	0	-11.837983	-1.482366	0.208044
79	1	0	-11.197822	-2.618789	-1.015997
80	1	0	-11.063893	-3.012870	0.716357

19 (S_1) M06-2X

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.670601	-0.277856	-0.340993
2	6	0	-0.937972	0.762678	0.250155
3	6	0	-0.943248	-1.257489	-1.037027
4	6	0	0.439523	0.840017	0.143243
5	1	0	-1.451792	1.520082	0.827902
6	6	0	0.433292	-1.194834	-1.154329
7	1	0	-1.477029	-2.083558	-1.489820
8	6	0	1.176377	-0.135975	-0.572649
9	1	0	0.942780	1.675535	0.607648
10	1	0	0.937314	-1.988619	-1.686491
11	6	0	7.227887	-1.300849	2.702754
12	1	0	7.721928	-2.069992	2.100645
13	1	0	7.357031	-1.578490	3.757965
14	6	0	7.875639	0.051127	2.458460
15	1	0	8.909963	0.028975	2.826035
16	1	0	7.334059	0.819826	3.014030
17	6	0	8.793775	-0.162827	0.246055
18	1	0	8.993936	-1.195776	0.555515
19	1	0	9.739987	0.392025	0.297126
20	6	0	8.275218	-0.200494	-1.177424
21	1	0	7.304038	-0.703828	-1.195298
22	1	0	8.977780	-0.779998	-1.787260
23	6	0	6.866120	1.466022	-2.197967
24	1	0	6.410589	0.637572	-2.754252
25	1	0	6.995396	2.304474	-2.885121
26	6	0	5.965776	1.854537	-1.033628
27	1	0	6.331217	2.774382	-0.557922
28	1	0	5.992188	1.061285	-0.285050
29	6	0	3.678069	2.170219	-0.482793
30	1	0	2.788846	2.609185	-0.938583
31	1	0	4.047032	2.858890	0.289570
32	6	0	3.335068	0.824689	0.159894
33	1	0	2.799358	1.000571	1.093530

34	1	0	4.247953	0.293366	0.430989
35	6	0	3.273993	-0.912440	-1.625646
36	1	0	4.087908	-0.324547	-2.052337
37	1	0	2.617092	-1.179318	-2.452377
38	6	0	3.862865	-2.174272	-1.005143
39	1	0	4.032879	-2.933250	-1.780820
40	1	0	3.169388	-2.589218	-0.264567
41	6	0	5.609808	-2.799889	0.518173
42	1	0	5.222865	-3.798008	0.281000
43	1	0	6.693366	-2.830840	0.381214
44	6	0	5.260105	-2.450928	1.959254
45	1	0	4.180094	-2.320861	2.057193
46	1	0	5.564437	-3.273822	2.620168
47	7	0	2.544214	-0.060686	-0.691740
48	8	0	4.643620	2.055227	-1.529427
49	8	0	8.169879	1.110604	-1.745822
50	8	0	7.828351	0.449989	1.093594
51	8	0	5.841749	-1.221082	2.384315
52	8	0	5.107398	-1.829591	-0.396154
53	6	0	-5.108171	-1.271110	-0.254755
54	6	0	-4.034806	0.691823	0.090325
55	7	0	-5.236493	0.053212	0.069342
56	6	0	-6.351043	0.811353	0.295644
57	6	0	-7.544926	0.120539	0.233453
58	6	0	-7.506431	-1.268067	-0.066857
59	6	0	-6.314110	-1.969810	-0.316753
60	1	0	-8.489879	0.614340	0.398206
61	1	0	-6.345826	-3.022214	-0.558109
62	6	0	-4.374543	2.074665	0.361797
63	6	0	-5.812009	2.144721	0.500818
64	6	0	-3.620418	3.248193	0.480657
65	6	0	-6.444918	3.359937	0.768407
66	6	0	-5.669674	4.505480	0.890868
67	6	0	-4.273375	4.446103	0.742678
68	1	0	-3.692174	5.356189	0.833131
69	1	0	-7.522289	3.406775	0.873736
70	1	0	-2.545652	3.234851	0.360395
71	7	0	-3.792865	-1.531069	-0.436535
72	6	0	-3.117366	-0.355285	-0.229171
73	1	0	-6.144572	5.456839	1.097333
74	6	0	-8.768937	-2.052732	-0.143995
75	8	0	-8.823649	-3.240447	-0.397520
76	8	0	-9.856863	-1.304414	0.098234
77	6	0	-11.129420	-1.982109	0.043131
78	1	0	-11.871388	-1.218329	0.259622
79	1	0	-11.289624	-2.402410	-0.949619
80	1	0	-11.166356	-2.775405	0.789620

19·Ba(ClO$_4$)$_2$ (S_0) M06-2X

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.263463	2.216085	-1.469542
2	6	0	0.084225	3.069925	-0.417542
3	6	0	0.729456	1.859349	-2.381960
4	6	0	1.406209	3.408228	-0.190106
5	1	0	-0.673564	3.370581	0.296479
6	6	0	2.050704	2.231823	-2.185333
7	1	0	0.484133	1.206085	-3.211889
8	6	0	2.439924	2.916743	-1.018463

9	1	0	1.630607	4.007342	0.680147
10	1	0	2.778744	1.904619	-2.909020
11	6	0	3.239699	-3.303481	1.244500
12	1	0	3.516423	-3.157398	2.297858
13	1	0	3.875206	-4.093943	0.825906
14	6	0	1.794369	-3.717304	1.097467
15	1	0	1.609376	-4.630794	1.673112
16	1	0	1.577930	-3.905925	0.047113
17	6	0	0.567802	-2.634100	2.882019
18	1	0	0.715160	-3.614905	3.347509
19	1	0	-0.486749	-2.374289	2.925444
20	6	0	1.374072	-1.595364	3.644940
21	1	0	2.400536	-1.929080	3.847561
22	1	0	0.870854	-1.408437	4.601678
23	6	0	1.875415	0.705609	3.653746
24	1	0	2.806827	0.434195	4.170208
25	1	0	1.110408	0.972332	4.393282
26	6	0	2.118470	1.874168	2.721191
27	1	0	2.528798	2.713753	3.292164
28	1	0	1.174047	2.186008	2.272637
29	6	0	4.241621	2.184358	1.601701
30	1	0	4.976710	1.480764	1.218301
31	1	0	4.552467	2.515906	2.600757
32	6	0	4.168929	3.395848	0.668356
33	1	0	5.162393	3.852846	0.640214
34	1	0	3.504977	4.156987	1.078763
35	6	0	4.813519	2.593763	-1.593876
36	1	0	5.759806	2.939038	-1.174751
37	1	0	4.706422	3.081447	-2.570006
38	6	0	4.922370	1.078430	-1.843904
39	1	0	5.957135	0.886636	-2.161904
40	1	0	4.267391	0.718687	-2.639990
41	6	0	5.147381	-0.968347	-0.755204
42	1	0	4.724712	-1.486567	-1.621349
43	1	0	6.241395	-0.928978	-0.857775
44	6	0	4.815149	-1.729905	0.500278
45	1	0	5.431492	-2.635783	0.510613
46	1	0	5.054491	-1.134723	1.391594
47	7	0	3.775779	3.078286	-0.696033
48	8	0	3.015324	1.472398	1.688131
49	8	0	1.426707	-0.397890	2.888276
50	8	0	0.911604	-2.685442	1.503864
51	8	0	3.444023	-2.097521	0.523930
52	8	0	4.643008	0.352241	-0.665396
53	56	0	1.185201	-0.261818	0.096774
54	6	0	-2.833034	1.836045	-1.149048
55	6	0	-2.632367	-0.403073	-1.264095
56	6	0	-4.780186	0.675751	-0.678481
57	6	0	-3.213601	-1.662537	-1.087497
58	1	0	-2.639314	-2.572371	-1.197097
59	6	0	-5.359603	-0.556853	-0.503479
60	1	0	-6.383832	-0.665727	-0.179203
61	6	0	-4.556755	-1.710073	-0.723526
62	6	0	-5.046126	2.101620	-0.513004
63	6	0	-3.841412	2.816285	-0.801587
64	6	0	-6.199536	2.784226	-0.134242
65	1	0	-7.111751	2.243139	0.088230
66	6	0	-3.816087	4.207816	-0.707657
67	6	0	-4.974678	4.868434	-0.329569
68	1	0	-4.970411	5.949283	-0.252740
69	6	0	-6.155033	4.166779	-0.044389
70	1	0	-2.909657	4.757980	-0.930271
71	7	0	-3.478994	0.644824	-1.078963

72	1	0	-7.041903	4.714332	0.250058
73	7	0	-1.398831	0.093247	-1.493154
74	6	0	-1.512620	1.452186	-1.424415
75	6	0	-5.137554	-3.071442	-0.526124
76	8	0	-4.529952	-4.099815	-0.665286
77	8	0	-6.432235	-3.030491	-0.170935
78	6	0	-7.043714	-4.303689	0.040132
79	1	0	-8.072959	-4.093974	0.318858
80	1	0	-7.004342	-4.897867	-0.873069
81	1	0	-6.529985	-4.841644	0.837107
82	17	0	2.001261	-2.211552	-2.621255
83	17	0	-1.666077	0.261342	2.118008
84	8	0	3.116767	-3.146606	-2.472651
85	8	0	2.482845	-0.816284	-2.338954
86	8	0	0.972172	-2.483259	-1.575976
87	8	0	1.420777	-2.278097	-3.947340
88	8	0	-1.286173	-0.972201	1.379208
89	8	0	-0.734549	1.324092	1.625476
90	8	0	-1.470317	0.060819	3.555777
91	8	0	-3.041287	0.630239	1.811704

19·Ba(ClO$_4$)$_2$ (S_1) M06-2X

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.368426	2.475186	-1.322086
2	6	0	0.007083	3.208431	-0.187168
3	6	0	0.587005	2.292291	-2.327565
4	6	0	1.332887	3.551111	0.025808
5	1	0	-0.718324	3.387760	0.595399
6	6	0	1.905101	2.683499	-2.143247
7	1	0	0.317807	1.756979	-3.229236
8	6	0	2.338264	3.185391	-0.898411
9	1	0	1.589477	4.017927	0.964546
10	1	0	2.606258	2.494443	-2.939017
11	6	0	3.516740	-3.323247	0.977044
12	1	0	3.855573	-3.195775	2.013850
13	1	0	4.148334	-4.087376	0.504955
14	6	0	2.079447	-3.795503	0.902631
15	1	0	1.977693	-4.748327	1.434557
16	1	0	1.800208	-3.935651	-0.141146
17	6	0	0.866924	-2.880523	2.819296
18	1	0	0.993658	-3.898410	3.204028
19	1	0	-0.176652	-2.588473	2.909043
20	6	0	1.729843	-1.918875	3.620258
21	1	0	2.771885	-2.257306	3.697130
22	1	0	1.315194	-1.845492	4.633826
23	6	0	2.262081	0.397521	3.764418
24	1	0	3.304264	0.149590	4.012255
25	1	0	1.694057	0.518451	4.695660
26	6	0	2.187237	1.676462	2.955573
27	1	0	2.611583	2.505268	3.530733
28	1	0	1.145020	1.900331	2.729439
29	6	0	4.163797	2.134724	1.610213
30	1	0	4.819690	1.419633	1.119946
31	1	0	4.553646	2.350954	2.612403
32	6	0	4.122286	3.430723	0.793512
33	1	0	5.134644	3.846883	0.784747
34	1	0	3.496713	4.173981	1.288576
35	6	0	4.699953	2.821544	-1.545685
36	1	0	5.667803	3.084888	-1.115774

37	1	0	4.604288	3.401388	-2.471972
38	6	0	4.742387	1.342782	-1.956631
39	1	0	5.674091	1.208594	-2.526214
40	1	0	3.914408	1.054433	-2.605036
41	6	0	5.136778	-0.838204	-1.172796
42	1	0	4.525351	-1.217013	-1.994984
43	1	0	6.190471	-0.831098	-1.489065
44	6	0	5.008316	-1.756066	0.016156
45	1	0	5.563035	-2.672984	-0.215357
46	1	0	5.453091	-1.301133	0.911453
47	7	0	3.690326	3.266287	-0.589369
48	8	0	2.877575	1.512828	1.711205
49	8	0	1.694542	-0.647551	2.984131
50	8	0	1.153735	-2.842178	1.419565
51	8	0	3.643379	-2.092889	0.268697
52	8	0	4.745021	0.485576	-0.821853
53	56	0	1.157387	-0.358529	0.155087
54	6	0	-2.919030	1.922261	-1.028762
55	6	0	-2.579515	-0.308866	-1.209843
56	6	0	-4.803868	0.622642	-0.627794
57	6	0	-3.082611	-1.603549	-1.089246
58	1	0	-2.453006	-2.471005	-1.223522
59	6	0	-5.306034	-0.654156	-0.506281
60	1	0	-6.326929	-0.836403	-0.208671
61	6	0	-4.433012	-1.752252	-0.747529
62	6	0	-5.162811	2.020662	-0.426225
63	6	0	-3.991216	2.823834	-0.671977
64	6	0	-6.360100	2.623408	-0.044090
65	1	0	-7.242428	2.023611	0.146205
66	6	0	-4.054873	4.210533	-0.526707
67	6	0	-5.260045	4.787955	-0.145947
68	1	0	-5.321801	5.863753	-0.029545
69	6	0	-6.400991	4.005629	0.093637
70	1	0	-3.179479	4.822333	-0.708262
71	7	0	-3.491748	0.684811	-1.000587
72	1	0	-7.324281	4.487617	0.391897
73	7	0	-1.372540	0.278298	-1.402050
74	6	0	-1.569903	1.637069	-1.302241
75	6	0	-4.926981	-3.149285	-0.601598
76	8	0	-4.250614	-4.139999	-0.753656
77	8	0	-6.238199	-3.199459	-0.272753
78	6	0	-6.784196	-4.517769	-0.104180
79	1	0	-7.829933	-4.367763	0.154709
80	1	0	-6.693616	-5.088302	-1.029387
81	1	0	-6.261397	-5.046311	0.693955
82	17	0	1.732565	-1.977750	-2.852297
83	17	0	-1.632866	0.117351	2.289092
84	8	0	2.929309	-2.842321	-2.991287
85	8	0	2.176615	-0.574609	-2.444474
86	8	0	0.878311	-2.465667	-1.697289
87	8	0	0.952136	-1.922026	-4.094278
88	8	0	-1.240104	-1.134499	1.534580
89	8	0	-0.686211	1.197084	1.787130
90	8	0	-1.434920	-0.086913	3.743253
91	8	0	-3.023865	0.488427	1.974072

19 (S_0) PBE

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.739112	-0.251673	-0.310519
2	6	0	-1.005575	0.752025	0.331707
3	6	0	-1.013477	-1.202228	-1.040633
4	6	0	0.371640	0.822682	0.240977
5	1	0	-1.518264	1.488329	0.941433
6	6	0	0.362330	-1.145544	-1.143428
7	1	0	-1.549642	-2.005358	-1.534662
8	6	0	1.107310	-0.122433	-0.510377
9	1	0	0.876208	1.633296	0.750923
10	1	0	0.864170	-1.921874	-1.707008
11	6	0	7.641569	-1.761316	2.313258
12	1	0	8.052508	-2.344574	1.479413
13	1	0	7.950132	-2.259350	3.244753
14	6	0	8.203544	-0.356639	2.285128
15	1	0	9.275295	-0.386689	2.525295
16	1	0	7.705095	0.245468	3.050517
17	6	0	8.945122	0.013102	0.058835
18	1	0	9.235595	-1.046758	0.076608
19	1	0	9.852129	0.610778	0.232732
20	6	0	8.375434	0.305173	-1.307306
21	1	0	7.445718	-0.261656	-1.433534
22	1	0	9.090567	-0.042285	-2.064549
23	6	0	6.843486	2.018633	-1.948263
24	1	0	6.504829	1.312123	-2.718384
25	1	0	6.907635	3.008231	-2.408157
26	6	0	5.857717	2.028166	-0.793959
27	1	0	6.091322	2.854926	-0.106775
28	1	0	5.960550	1.092711	-0.231845
29	6	0	3.557898	2.192648	-0.302973
30	1	0	2.662130	2.620472	-0.760906
31	1	0	3.870835	2.854063	0.518777
32	6	0	3.250283	0.808622	0.262284
33	1	0	2.728931	0.921057	1.216440
34	1	0	4.182644	0.286856	0.491948
35	6	0	3.205714	-0.869902	-1.560656
36	1	0	4.025644	-0.267868	-1.963053
37	1	0	2.556559	-1.104585	-2.405517
38	6	0	3.797915	-2.154192	-0.998051
39	1	0	3.928653	-2.884787	-1.810262
40	1	0	3.121017	-2.592974	-0.251740
41	6	0	5.693262	-2.942591	0.211611
42	1	0	5.257940	-3.895681	-0.115829
43	1	0	6.739781	-2.939516	-0.111772
44	6	0	5.607163	-2.850003	1.723533
45	1	0	4.559287	-2.791633	2.031979
46	1	0	6.038405	-3.759315	2.167967
47	7	0	2.472579	-0.051920	-0.612126
48	8	0	4.551805	2.183067	-1.313115
49	8	0	8.143783	1.692703	-1.499227
50	8	0	7.980040	0.296008	1.050583
51	8	0	6.231947	-1.691092	2.240091
52	8	0	5.056780	-1.849702	-0.425301
53	6	0	-5.156107	-1.250149	-0.280980
54	6	0	-4.109692	0.698697	0.122684
55	7	0	-5.299304	0.056727	0.073878
56	6	0	-6.415690	0.795038	0.314423
57	6	0	-7.602310	0.098060	0.228015
58	6	0	-7.547669	-1.277111	-0.108406

59	6	0	-6.352325	-1.959276	-0.369109
60	1	0	-8.554913	0.578417	0.402076
61	1	0	-6.374331	-3.007342	-0.637738
62	6	0	-4.459795	2.067426	0.431178
63	6	0	-5.890477	2.122092	0.561574
64	6	0	-3.716059	3.240621	0.589391
65	6	0	-6.536066	3.321263	0.860637
66	6	0	-5.773424	4.465745	1.021927
67	6	0	-4.378791	4.421822	0.881464
68	1	0	-3.804708	5.334600	1.002651
69	1	0	-7.615860	3.356229	0.960528
70	1	0	-2.638592	3.240261	0.475774
71	7	0	-3.845332	-1.499083	-0.457790
72	6	0	-3.186561	-0.332239	-0.214047
73	1	0	-6.258095	5.407940	1.253731
74	6	0	-8.799144	-2.073262	-0.213501
75	8	0	-8.835360	-3.258168	-0.502082
76	8	0	-9.890066	-1.347674	0.044064
77	6	0	-11.140374	-2.038208	-0.035603
78	1	0	-11.899759	-1.296005	0.200120
79	1	0	-11.293089	-2.433274	-1.041171
80	1	0	-11.169774	-2.855721	0.686493

19 (S_1) PBE

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.670601	-0.277856	-0.340993
2	6	0	-0.937972	0.762678	0.250155
3	6	0	-0.943248	-1.257489	-1.037027
4	6	0	0.439523	0.840017	0.143243
5	1	0	-1.451792	1.520082	0.827902
6	6	0	0.433292	-1.194834	-1.154329
7	1	0	-1.477029	-2.083558	-1.489820
8	6	0	1.176377	-0.135975	-0.572649
9	1	0	0.942780	1.675535	0.607648
10	1	0	0.937314	-1.988619	-1.686491
11	6	0	7.227887	-1.300849	2.702754
12	1	0	7.721928	-2.069992	2.100645
13	1	0	7.357031	-1.578490	3.757965
14	6	0	7.875639	0.051127	2.458460
15	1	0	8.909963	0.028975	2.826035
16	1	0	7.334059	0.819826	3.014030
17	6	0	8.793775	-0.162827	0.246055
18	1	0	8.993936	-1.195776	0.555515
19	1	0	9.739987	0.392025	0.297126
20	6	0	8.275218	-0.200494	-1.177424
21	1	0	7.304038	-0.703828	-1.195298
22	1	0	8.977780	-0.779998	-1.787260
23	6	0	6.866120	1.466022	-2.197967
24	1	0	6.410589	0.637572	-2.754252
25	1	0	6.995396	2.304474	-2.885121
26	6	0	5.965776	1.854537	-1.033628
27	1	0	6.331217	2.774382	-0.557922
28	1	0	5.992188	1.061285	-0.285050
29	6	0	3.678069	2.170219	-0.482793
30	1	0	2.788846	2.609185	-0.938583
31	1	0	4.047032	2.858890	0.289570
32	6	0	3.335068	0.824689	0.159894
33	1	0	2.799358	1.000571	1.093530
34	1	0	4.247953	0.293366	0.430989

35	6	0	3.273993	-0.912440	-1.625646
36	1	0	4.087908	-0.324547	-2.052337
37	1	0	2.617092	-1.179318	-2.452377
38	6	0	3.862865	-2.174272	-1.005143
39	1	0	4.032879	-2.933250	-1.780820
40	1	0	3.169388	-2.589218	-0.264567
41	6	0	5.609808	-2.799889	0.518173
42	1	0	5.222865	-3.798008	0.281000
43	1	0	6.693366	-2.830840	0.381214
44	6	0	5.260105	-2.450928	1.959254
45	1	0	4.180094	-2.320861	2.057193
46	1	0	5.564437	-3.273822	2.620168
47	7	0	2.544214	-0.060686	-0.691740
48	8	0	4.643620	2.055227	-1.529427
49	8	0	8.169879	1.110604	-1.745822
50	8	0	7.828351	0.449989	1.093594
51	8	0	5.841749	-1.221082	2.384315
52	8	0	5.107398	-1.829591	-0.396154
53	6	0	-5.108171	-1.271110	-0.254755
54	6	0	-4.034806	0.691823	0.090325
55	7	0	-5.236493	0.053212	0.069342
56	6	0	-6.351043	0.811353	0.295644
57	6	0	-7.544926	0.120539	0.233453
58	6	0	-7.506431	-1.268067	-0.066857
59	6	0	-6.314110	-1.969810	-0.316753
60	1	0	-8.489879	0.614340	0.398206
61	1	0	-6.345826	-3.022214	-0.558109
62	6	0	-4.374543	2.074665	0.361797
63	6	0	-5.812009	2.144721	0.500818
64	6	0	-3.620418	3.248193	0.480657
65	6	0	-6.444918	3.359937	0.768407
66	6	0	-5.669674	4.505480	0.890868
67	6	0	-4.273375	4.446103	0.742678
68	1	0	-3.692174	5.356189	0.833131
69	1	0	-7.522289	3.406775	0.873736
70	1	0	-2.545652	3.234851	0.360395
71	7	0	-3.792865	-1.531069	-0.436535
72	6	0	-3.117366	-0.355285	-0.229171
73	1	0	-6.144572	5.456839	1.097333
74	6	0	-8.768937	-2.052732	-0.143995
75	8	0	-8.823649	-3.240447	-0.397520
76	8	0	-9.856863	-1.304414	0.098234
77	6	0	-11.129420	-1.982109	0.043131
78	1	0	-11.871388	-1.218329	0.259622
79	1	0	-11.289624	-2.402410	-0.949619
80	1	0	-11.166356	-2.775405	0.789620

19·Ba(ClO$_4$)$_2$ (S_0) PBE

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.499092	2.346653	-1.111516
2	6	0	-0.061884	3.107079	-0.021732
3	6	0	0.392546	2.152563	-2.166863
4	6	0	1.261523	3.492088	0.085746
5	1	0	-0.738369	3.297340	0.804250
6	6	0	1.707454	2.579771	-2.085945
7	1	0	0.074409	1.595506	-3.041350
8	6	0	2.210282	3.139980	-0.898116
9	1	0	1.568288	3.998085	0.991020

10	1	0	2.357016	2.377375	-2.924210
11	6	0	3.952487	-3.159138	0.759763
12	1	0	4.346068	-3.002407	1.775666
13	1	0	4.593012	-3.907352	0.268235
14	6	0	2.546599	-3.712421	0.775355
15	1	0	2.541865	-4.678891	1.295983
16	1	0	2.212625	-3.864289	-0.252964
17	6	0	1.381255	-2.946927	2.760575
18	1	0	1.598778	-3.965579	3.105010
19	1	0	0.321690	-2.738791	2.914735
20	6	0	2.203788	-1.950972	3.549505
21	1	0	3.275269	-2.201406	3.548991
22	1	0	1.852660	-1.956989	4.591767
23	6	0	2.616301	0.364293	3.714458
24	1	0	3.691863	0.162014	3.839631
25	1	0	2.156656	0.437367	4.710859
26	6	0	2.394440	1.653052	2.960149
27	1	0	2.823768	2.491880	3.521310
28	1	0	1.319827	1.820799	2.849922
29	6	0	4.212381	2.202694	1.466424
30	1	0	4.855836	1.498510	0.938020
31	1	0	4.668101	2.440089	2.437529
32	6	0	4.091085	3.483678	0.644821
33	1	0	5.093161	3.917938	0.559026
34	1	0	3.490973	4.225572	1.178413
35	6	0	4.522498	2.982847	-1.745600
36	1	0	5.488460	3.369455	-1.409827
37	1	0	4.263745	3.549511	-2.650373
38	6	0	4.713433	1.529270	-2.180865
39	1	0	5.584626	1.522291	-2.857116
40	1	0	3.859825	1.141655	-2.745778
41	6	0	5.283826	-0.624709	-1.506873
42	1	0	4.573171	-0.979824	-2.261677
43	1	0	6.291145	-0.614964	-1.952800
44	6	0	5.290825	-1.586075	-0.349863
45	1	0	5.831951	-2.484761	-0.677771
46	1	0	5.834050	-1.158958	0.506863
47	7	0	3.568892	3.295294	-0.695664
48	8	0	2.953568	1.568938	1.657871
49	8	0	2.015871	-0.676259	2.974356
50	8	0	1.594935	-2.840564	1.361531
51	8	0	3.976160	-1.950972	0.029845
52	8	0	4.946784	0.681196	-1.079512
53	56	0	1.103041	-0.360177	0.160599
54	6	0	-3.057692	1.872700	-0.788151
55	6	0	-2.790929	-0.353260	-0.974204
56	6	0	-5.000026	0.651745	-0.509511
57	6	0	-3.353979	-1.626725	-0.932548
58	1	0	-2.762234	-2.520974	-1.079110
59	6	0	-5.564826	-0.602296	-0.466886
60	1	0	-6.617008	-0.748682	-0.266849
61	6	0	-4.724716	-1.724820	-0.681873
62	6	0	-5.324676	2.059899	-0.358375
63	6	0	-4.118920	2.815854	-0.532650
64	6	0	-6.528248	2.706296	-0.089186
65	1	0	-7.442567	2.138045	0.047060
66	6	0	-4.149968	4.206242	-0.436109
67	6	0	-5.359312	4.827843	-0.169915
68	1	0	-5.396659	5.909665	-0.093085
69	6	0	-6.536672	4.088632	0.003590
70	1	0	-3.244737	4.788808	-0.569164
71	7	0	-3.666147	0.663460	-0.766269
72	1	0	-7.466067	4.607060	0.213618

73	7	0	-1.564300	0.186479	-1.142793
74	6	0	-1.717358	1.539204	-1.039323
75	6	0	-5.286332	-3.101108	-0.638973
76	8	0	-4.645353	-4.107104	-0.811061
77	8	0	-6.604716	-3.107672	-0.384471
78	6	0	-7.204213	-4.399734	-0.322685
79	1	0	-8.257757	-4.225853	-0.110523
80	1	0	-7.085423	-4.923175	-1.273497
81	1	0	-6.746973	-4.996105	0.469351
82	17	0	1.696229	-1.928960	-2.871380
83	17	0	-1.471439	-0.124890	2.507758
84	8	0	2.901052	-2.719677	-3.122600
85	8	0	2.089191	-0.530319	-2.472193
86	8	0	0.967240	-2.471658	-1.680654
87	8	0	0.827049	-1.890825	-4.033800
88	8	0	-1.037633	-1.325891	1.724823
89	8	0	-0.606008	0.998618	2.010133
90	8	0	-1.230678	-0.345101	3.931774
91	8	0	-2.870357	0.175241	2.236983

19·Ba(ClO$_4$)$_2$ (S_1) PBE

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.368426	2.475186	-1.322086
2	6	0	0.007083	3.208431	-0.187168
3	6	0	0.587005	2.292291	-2.327565
4	6	0	1.332887	3.551111	0.025808
5	1	0	-0.718324	3.387760	0.595399
6	6	0	1.905101	2.683499	-2.143247
7	1	0	0.317807	1.756979	-3.229236
8	6	0	2.338264	3.185391	-0.898411
9	1	0	1.589477	4.017927	0.964546
10	1	0	2.606258	2.494443	-2.939017
11	6	0	3.516740	-3.323247	0.977044
12	1	0	3.855573	-3.195775	2.013850
13	1	0	4.148334	-4.087376	0.504955
14	6	0	2.079447	-3.795503	0.902631
15	1	0	1.977693	-4.748327	1.434557
16	1	0	1.800208	-3.935651	-0.141146
17	6	0	0.866924	-2.880523	2.819296
18	1	0	0.993658	-3.898410	3.204028
19	1	0	-0.176652	-2.588473	2.909043
20	6	0	1.729843	-1.918875	3.620258
21	1	0	2.771885	-2.257306	3.697130
22	1	0	1.315194	-1.845492	4.633826
23	6	0	2.262081	0.397521	3.764418
24	1	0	3.304264	0.149590	4.012255
25	1	0	1.694057	0.518451	4.695660
26	6	0	2.187237	1.676462	2.955573
27	1	0	2.611583	2.505268	3.530733
28	1	0	1.145020	1.900331	2.729439
29	6	0	4.163797	2.134724	1.610213
30	1	0	4.819690	1.419633	1.119946
31	1	0	4.553646	2.350954	2.612403
32	6	0	4.122286	3.430723	0.793512
33	1	0	5.134644	3.846883	0.784747
34	1	0	3.496713	4.173981	1.288576
35	6	0	4.699953	2.821544	-1.545685
36	1	0	5.667803	3.084888	-1.115774

37	1	0	4.604288	3.401388	-2.471972
38	6	0	4.742387	1.342782	-1.956631
39	1	0	5.674091	1.208594	-2.526214
40	1	0	3.914408	1.054433	-2.605036
41	6	0	5.136778	-0.838204	-1.172796
42	1	0	4.525351	-1.217013	-1.994984
43	1	0	6.190471	-0.831098	-1.489065
44	6	0	5.008316	-1.756066	0.016156
45	1	0	5.563035	-2.672984	-0.215357
46	1	0	5.453091	-1.301133	0.911453
47	7	0	3.690326	3.266287	-0.589369
48	8	0	2.877575	1.512828	1.711205
49	8	0	1.694542	-0.647551	2.984131
50	8	0	1.153735	-2.842178	1.419565
51	8	0	3.643379	-2.092889	0.268697
52	8	0	4.745021	0.485576	-0.821853
53	56	0	1.157387	-0.358529	0.155087
54	6	0	-2.919030	1.922261	-1.028762
55	6	0	-2.579515	-0.308866	-1.209843
56	6	0	-4.803868	0.622642	-0.627794
57	6	0	-3.082611	-1.603549	-1.089246
58	1	0	-2.453006	-2.471005	-1.223522
59	6	0	-5.306034	-0.654156	-0.506281
60	1	0	-6.326929	-0.836403	-0.208671
61	6	0	-4.433012	-1.752252	-0.747529
62	6	0	-5.162811	2.020662	-0.426225
63	6	0	-3.991216	2.823834	-0.671977
64	6	0	-6.360100	2.623408	-0.044090
65	1	0	-7.242428	2.023611	0.146205
66	6	0	-4.054873	4.210533	-0.526707
67	6	0	-5.260045	4.787955	-0.145947
68	1	0	-5.321801	5.863753	-0.029545
69	6	0	-6.400991	4.005629	0.093637
70	1	0	-3.179479	4.822333	-0.708262
71	7	0	-3.491748	0.684811	-1.000587
72	1	0	-7.324281	4.487617	0.391897
73	7	0	-1.372540	0.278298	-1.402050
74	6	0	-1.569903	1.637069	-1.302241
75	6	0	-4.926981	-3.149285	-0.601598
76	8	0	-4.250614	-4.139999	-0.753656
77	8	0	-6.238199	-3.199459	-0.272753
78	6	0	-6.784196	-4.517769	-0.104180
79	1	0	-7.829933	-4.367763	0.154709
80	1	0	-6.693616	-5.088302	-1.029387
81	1	0	-6.261397	-5.046311	0.693955
82	17	0	1.732565	-1.977750	-2.852297
83	17	0	-1.632866	0.117351	2.289092
84	8	0	2.929309	-2.842321	-2.991287
85	8	0	2.176615	-0.574609	-2.444474
86	8	0	0.878311	-2.465667	-1.697289
87	8	0	0.952136	-1.922026	-4.094278
88	8	0	-1.240104	-1.134499	1.534580
89	8	0	-0.686211	1.197084	1.787130
90	8	0	-1.434920	-0.086913	3.743253
91	8	0	-3.023865	0.488427	1.974072

19 (S_0) wB97XD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.683357	-0.240507	-0.304224
2	6	0	-0.977134	0.747933	0.385299
3	6	0	-0.945056	-1.131547	-1.087379
4	6	0	0.397648	0.861617	0.287703
5	1	0	-1.507894	1.437469	1.032850
6	6	0	0.430156	-1.034218	-1.193152
7	1	0	-1.462775	-1.920370	-1.621141
8	6	0	1.148667	-0.025671	-0.513375
9	1	0	0.885652	1.661472	0.828427
10	1	0	0.948680	-1.766849	-1.797034
11	6	0	7.353967	-1.679164	2.481047
12	1	0	7.824744	-2.373424	1.775840
13	1	0	7.520044	-2.081804	3.489696
14	6	0	8.005337	-0.311955	2.381217
15	1	0	9.057504	-0.392607	2.686940
16	1	0	7.506401	0.377558	3.066153
17	6	0	8.787805	-0.237499	0.125240
18	1	0	8.973741	-1.310069	0.267321
19	1	0	9.753297	0.281119	0.202571
20	6	0	8.196255	-0.055433	-1.255756
21	1	0	7.214405	-0.540654	-1.291063
22	1	0	8.852244	-0.549085	-1.982386
23	6	0	6.787285	1.749061	-1.954335
24	1	0	6.308122	1.034729	-2.637401
25	1	0	6.903303	2.696531	-2.484966
26	6	0	5.920106	1.929889	-0.719341
27	1	0	6.333016	2.720891	-0.078104
28	1	0	5.926952	0.999134	-0.146147
29	6	0	3.672237	2.243434	-0.071166
30	1	0	2.788517	2.774100	-0.432515
31	1	0	4.072876	2.789758	0.794768
32	6	0	3.292630	0.828715	0.361066
33	1	0	2.736187	0.884389	1.298581
34	1	0	4.191059	0.247951	0.582378
35	6	0	3.253984	-0.636508	-1.642502
36	1	0	4.069679	0.001497	-1.990040
37	1	0	2.605573	-0.801195	-2.503112
38	6	0	3.853025	-1.959204	-1.181824
39	1	0	3.984727	-2.635546	-2.037791
40	1	0	3.182122	-2.445530	-0.461572
41	6	0	5.679045	-2.771119	0.117981
42	1	0	5.314985	-3.729162	-0.274091
43	1	0	6.758018	-2.737552	-0.058916
44	6	0	5.381011	-2.691514	1.608023
45	1	0	4.303176	-2.597384	1.763075
46	1	0	5.712181	-3.618700	2.095810
47	7	0	2.515341	0.090445	-0.623423
48	8	0	4.610314	2.269930	-1.134508
49	8	0	8.089382	1.318041	-1.608357
50	8	0	7.891990	0.263364	1.096389
51	8	0	5.967319	-1.561491	2.226003
52	8	0	5.115231	-1.688063	-0.595353
53	6	0	-5.097239	-1.283530	-0.232773
54	6	0	-4.060551	0.681048	0.091586
55	7	0	-5.247807	0.033159	0.069962
56	6	0	-6.367187	0.776530	0.278911
57	6	0	-7.548104	0.076870	0.217823
58	6	0	-7.487226	-1.313670	-0.064336

59	6	0	-6.294210	-2.000439	-0.294613
60	1	0	-8.500676	0.562368	0.370015
61	1	0	-6.308502	-3.057572	-0.521406
62	6	0	-4.416454	2.064240	0.344748
63	6	0	-5.841414	2.120099	0.472295
64	6	0	-3.670293	3.239899	0.453721
65	6	0	-6.490213	3.328181	0.721129
66	6	0	-5.728529	4.478767	0.834895
67	6	0	-4.333898	4.431325	0.696872
68	1	0	-3.762078	5.348484	0.780772
69	1	0	-7.569069	3.364777	0.818930
70	1	0	-2.593566	3.229544	0.340148
71	7	0	-3.783458	-1.531114	-0.400273
72	6	0	-3.137152	-0.348142	-0.203927
73	1	0	-6.213785	5.428356	1.027243
74	6	0	-8.743620	-2.116803	-0.140800
75	8	0	-8.776889	-3.301965	-0.381874
76	8	0	-9.831634	-1.384377	0.086281
77	6	0	-11.089708	-2.068627	0.032554
78	1	0	-11.841182	-1.311209	0.239340
79	1	0	-11.244221	-2.498720	-0.957401
80	1	0	-11.124556	-2.855981	0.786058

19 (S_1) wB97XDYP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.670601	-0.277856	-0.340993
2	6	0	-0.937972	0.762678	0.250155
3	6	0	-0.943248	-1.257489	-1.037027
4	6	0	0.439523	0.840017	0.143243
5	1	0	-1.451792	1.520082	0.827902
6	6	0	0.433292	-1.194834	-1.154329
7	1	0	-1.477029	-2.083558	-1.489820
8	6	0	1.176377	-0.135975	-0.572649
9	1	0	0.942780	1.675535	0.607648
10	1	0	0.937314	-1.988619	-1.686491
11	6	0	7.227887	-1.300849	2.702754
12	1	0	7.721928	-2.069992	2.100645
13	1	0	7.357031	-1.578490	3.757965
14	6	0	7.875639	0.051127	2.458460
15	1	0	8.909963	0.028975	2.826035
16	1	0	7.334059	0.819826	3.014030
17	6	0	8.793775	-0.162827	0.246055
18	1	0	8.993936	-1.195776	0.555515
19	1	0	9.739987	0.392025	0.297126
20	6	0	8.275218	-0.200494	-1.177424
21	1	0	7.304038	-0.703828	-1.195298
22	1	0	8.977780	-0.779998	-1.787260
23	6	0	6.866120	1.466022	-2.197967
24	1	0	6.410589	0.637572	-2.754252
25	1	0	6.995396	2.304474	-2.885121
26	6	0	5.965776	1.854537	-1.033628
27	1	0	6.331217	2.774382	-0.557922
28	1	0	5.992188	1.061285	-0.285050
29	6	0	3.678069	2.170219	-0.482793
30	1	0	2.788846	2.609185	-0.938583
31	1	0	4.047032	2.858890	0.289570
32	6	0	3.335068	0.824689	0.159894
33	1	0	2.799358	1.000571	1.093530

34	1	0	4.247953	0.293366	0.430989
35	6	0	3.273993	-0.912440	-1.625646
36	1	0	4.087908	-0.324547	-2.052337
37	1	0	2.617092	-1.179318	-2.452377
38	6	0	3.862865	-2.174272	-1.005143
39	1	0	4.032879	-2.933250	-1.780820
40	1	0	3.169388	-2.589218	-0.264567
41	6	0	5.609808	-2.799889	0.518173
42	1	0	5.222865	-3.798008	0.281000
43	1	0	6.693366	-2.830840	0.381214
44	6	0	5.260105	-2.450928	1.959254
45	1	0	4.180094	-2.320861	2.057193
46	1	0	5.564437	-3.273822	2.620168
47	7	0	2.544214	-0.060686	-0.691740
48	8	0	4.643620	2.055227	-1.529427
49	8	0	8.169879	1.110604	-1.745822
50	8	0	7.828351	0.449989	1.093594
51	8	0	5.841749	-1.221082	2.384315
52	8	0	5.107398	-1.829591	-0.396154
53	6	0	-5.108171	-1.271110	-0.254755
54	6	0	-4.034806	0.691823	0.090325
55	7	0	-5.236493	0.053212	0.069342
56	6	0	-6.351043	0.811353	0.295644
57	6	0	-7.544926	0.120539	0.233453
58	6	0	-7.506431	-1.268067	-0.066857
59	6	0	-6.314110	-1.969810	-0.316753
60	1	0	-8.489879	0.614340	0.398206
61	1	0	-6.345826	-3.022214	-0.558109
62	6	0	-4.374543	2.074665	0.361797
63	6	0	-5.812009	2.144721	0.500818
64	6	0	-3.620418	3.248193	0.480657
65	6	0	-6.444918	3.359937	0.768407
66	6	0	-5.669674	4.505480	0.890868
67	6	0	-4.273375	4.446103	0.742678
68	1	0	-3.692174	5.356189	0.833131
69	1	0	-7.522289	3.406775	0.873736
70	1	0	-2.545652	3.234851	0.360395
71	7	0	-3.792865	-1.531069	-0.436535
72	6	0	-3.117366	-0.355285	-0.229171
73	1	0	-6.144572	5.456839	1.097333
74	6	0	-8.768937	-2.052732	-0.143995
75	8	0	-8.823649	-3.240447	-0.397520
76	8	0	-9.856863	-1.304414	0.098234
77	6	0	-11.129420	-1.982109	0.043131
78	1	0	-11.871388	-1.218329	0.259622
79	1	0	-11.289624	-2.402410	-0.949619
80	1	0	-11.166356	-2.775405	0.789620

19·Ba(ClO$_4$)$_2$ (S_0) wB97XD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.288031	2.346384	-1.472328
2	6	0	0.100259	3.142130	-0.392548
3	6	0	0.663112	2.062300	-2.449803
4	6	0	1.430624	3.465019	-0.196411
5	1	0	-0.623369	3.393147	0.372678
6	6	0	1.986651	2.431858	-2.287180
7	1	0	0.385988	1.463886	-3.309250
8	6	0	2.426716	3.015172	-1.086229

9	1	0	1.691268	3.990791	0.710527
10	1	0	2.684246	2.166182	-3.064986
11	6	0	3.277397	-3.343218	1.197705
12	1	0	3.616215	-3.197337	2.233099
13	1	0	3.865467	-4.160782	0.759007
14	6	0	1.816284	-3.726720	1.129554
15	1	0	1.649251	-4.644323	1.706495
16	1	0	1.541993	-3.903659	0.089455
17	6	0	0.685436	-2.619665	2.968594
18	1	0	0.771187	-3.610862	3.429620
19	1	0	-0.343968	-2.276022	3.047858
20	6	0	1.593241	-1.645526	3.697722
21	1	0	2.618513	-2.028037	3.802106
22	1	0	1.181628	-1.485009	4.702879
23	6	0	2.198300	0.636984	3.710660
24	1	0	3.208478	0.354515	4.043238
25	1	0	1.582621	0.865514	4.590325
26	6	0	2.257495	1.847374	2.805736
27	1	0	2.708329	2.688579	3.343139
28	1	0	1.244535	2.124535	2.507523
29	6	0	4.264966	2.154359	1.487430
30	1	0	4.929584	1.407703	1.056522
31	1	0	4.654850	2.453374	2.469321
32	6	0	4.216862	3.376635	0.569358
33	1	0	5.228370	3.793239	0.521076
34	1	0	3.596302	4.160280	1.006340
35	6	0	4.768517	2.545192	-1.696479
36	1	0	5.744094	2.805852	-1.280975
37	1	0	4.702952	3.053682	-2.666692
38	6	0	4.759896	1.037896	-1.984051
39	1	0	5.716627	0.815351	-2.480250
40	1	0	3.961615	0.730907	-2.662875
41	6	0	5.057577	-1.053828	-0.988858
42	1	0	4.497809	-1.514298	-1.809142
43	1	0	6.130097	-1.075407	-1.234974
44	6	0	4.845098	-1.850028	0.270686
45	1	0	5.413943	-2.782611	0.170388
46	1	0	5.226652	-1.305669	1.145629
47	7	0	3.776780	3.095580	-0.786324
48	8	0	2.998694	1.530949	1.634031
49	8	0	1.622044	-0.427412	2.982600
50	8	0	0.959161	-2.694462	1.578958
51	8	0	3.473925	-2.156751	0.451590
52	8	0	4.650005	0.286231	-0.793517
53	56	0	1.164543	-0.278641	0.133186
54	6	0	-2.838702	1.858089	-1.120492
55	6	0	-2.542085	-0.366796	-1.228249
56	6	0	-4.730929	0.613698	-0.650129
57	6	0	-3.064451	-1.650172	-1.059533
58	1	0	-2.447597	-2.530227	-1.178078
59	6	0	-5.254750	-0.641789	-0.480530
60	1	0	-6.276309	-0.793626	-0.165304
61	6	0	-4.403369	-1.760538	-0.697242
62	6	0	-5.061959	2.026441	-0.497150
63	6	0	-3.891228	2.791925	-0.784742
64	6	0	-6.243824	2.658822	-0.124514
65	1	0	-7.132607	2.079951	0.099438
66	6	0	-3.925643	4.181394	-0.694397
67	6	0	-5.112043	4.792255	-0.322382
68	1	0	-5.154329	5.873037	-0.246813
69	6	0	-6.260276	4.041475	-0.039740
70	1	0	-3.041204	4.769037	-0.911032
71	7	0	-3.428697	0.640292	-1.036739

72	1	0	-7.171584	4.550746	0.251351
73	7	0	-1.335248	0.183543	-1.463692
74	6	0	-1.509262	1.538773	-1.402043
75	6	0	-4.922726	-3.145522	-0.500283
76	8	0	-4.264956	-4.146589	-0.624899
77	8	0	-6.220779	-3.160840	-0.160482
78	6	0	-6.787760	-4.452345	0.056305
79	1	0	-7.828105	-4.274950	0.320517
80	1	0	-6.719873	-5.056771	-0.849695
81	1	0	-6.268782	-4.965926	0.867257
82	17	0	1.674032	-2.193731	-2.719855
83	17	0	-1.629162	0.391609	2.286719
84	8	0	2.799700	-3.129137	-2.758621
85	8	0	2.194723	-0.812119	-2.429715
86	8	0	0.781951	-2.522370	-1.567197
87	8	0	0.929926	-2.195054	-3.965409
88	8	0	-1.305892	-0.871002	1.562825
89	8	0	-0.670501	1.410966	1.751721
90	8	0	-1.410410	0.213213	3.723578
91	8	0	-2.997626	0.802013	2.001516

19·Ba(ClO$_4$)$_2$ (S_1) wB97XD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.368426	2.475186	-1.322086
2	6	0	0.007083	3.208431	-0.187168
3	6	0	0.587005	2.292291	-2.327565
4	6	0	1.332887	3.551111	0.025808
5	1	0	-0.718324	3.387760	0.595399
6	6	0	1.905101	2.683499	-2.143247
7	1	0	0.317807	1.756979	-3.229236
8	6	0	2.338264	3.185391	-0.898411
9	1	0	1.589477	4.017927	0.964546
10	1	0	2.606258	2.494443	-2.939017
11	6	0	3.516740	-3.323247	0.977044
12	1	0	3.855573	-3.195775	2.013850
13	1	0	4.148334	-4.087376	0.504955
14	6	0	2.079447	-3.795503	0.902631
15	1	0	1.977693	-4.748327	1.434557
16	1	0	1.800208	-3.935651	-0.141146
17	6	0	0.866924	-2.880523	2.819296
18	1	0	0.993658	-3.898410	3.204028
19	1	0	-0.176652	-2.588473	2.909043
20	6	0	1.729843	-1.918875	3.620258
21	1	0	2.771885	-2.257306	3.697130
22	1	0	1.315194	-1.845492	4.633826
23	6	0	2.262081	0.397521	3.764418
24	1	0	3.304264	0.149590	4.012255
25	1	0	1.694057	0.518451	4.695660
26	6	0	2.187237	1.676462	2.955573
27	1	0	2.611583	2.505268	3.530733
28	1	0	1.145020	1.900331	2.729439
29	6	0	4.163797	2.134724	1.610213
30	1	0	4.819690	1.419633	1.119946
31	1	0	4.553646	2.350954	2.612403
32	6	0	4.122286	3.430723	0.793512
33	1	0	5.134644	3.846883	0.784747
34	1	0	3.496713	4.173981	1.288576
35	6	0	4.699953	2.821544	-1.545685

36	1	0	5.667803	3.084888	-1.115774
37	1	0	4.604288	3.401388	-2.471972
38	6	0	4.742387	1.342782	-1.956631
39	1	0	5.674091	1.208594	-2.526214
40	1	0	3.914408	1.054433	-2.605036
41	6	0	5.136778	-0.838204	-1.172796
42	1	0	4.525351	-1.217013	-1.994984
43	1	0	6.190471	-0.831098	-1.489065
44	6	0	5.008316	-1.756066	0.016156
45	1	0	5.563035	-2.672984	-0.215357
46	1	0	5.453091	-1.301133	0.911453
47	7	0	3.690326	3.266287	-0.589369
48	8	0	2.877575	1.512828	1.711205
49	8	0	1.694542	-0.647551	2.984131
50	8	0	1.153735	-2.842178	1.419565
51	8	0	3.643379	-2.092889	0.268697
52	8	0	4.745021	0.485576	-0.821853
53	56	0	1.157387	-0.358529	0.155087
54	6	0	-2.919030	1.922261	-1.028762
55	6	0	-2.579515	-0.308866	-1.209843
56	6	0	-4.803868	0.622642	-0.627794
57	6	0	-3.082611	-1.603549	-1.089246
58	1	0	-2.453006	-2.471005	-1.223522
59	6	0	-5.306034	-0.654156	-0.506281
60	1	0	-6.326929	-0.836403	-0.208671
61	6	0	-4.433012	-1.752252	-0.747529
62	6	0	-5.162811	2.020662	-0.426225
63	6	0	-3.991216	2.823834	-0.671977
64	6	0	-6.360100	2.623408	-0.044090
65	1	0	-7.242428	2.023611	0.146205
66	6	0	-4.054873	4.210533	-0.526707
67	6	0	-5.260045	4.787955	-0.145947
68	1	0	-5.321801	5.863753	-0.029545
69	6	0	-6.400991	4.005629	0.093637
70	1	0	-3.179479	4.822333	-0.708262
71	7	0	-3.491748	0.684811	-1.000587
72	1	0	-7.324281	4.487617	0.391897
73	7	0	-1.372540	0.278298	-1.402050
74	6	0	-1.569903	1.637069	-1.302241
75	6	0	-4.926981	-3.149285	-0.601598
76	8	0	-4.250614	-4.139999	-0.753656
77	8	0	-6.238199	-3.199459	-0.272753
78	6	0	-6.784196	-4.517769	-0.104180
79	1	0	-7.829933	-4.367763	0.154709
80	1	0	-6.693616	-5.088302	-1.029387
81	1	0	-6.261397	-5.046311	0.693955
82	17	0	1.732565	-1.977750	-2.852297
83	17	0	-1.632866	0.117351	2.289092
84	8	0	2.929309	-2.842321	-2.991287
85	8	0	2.176615	-0.574609	-2.444474
86	8	0	0.878311	-2.465667	-1.697289
87	8	0	0.952136	-1.922026	-4.094278
88	8	0	-1.240104	-1.134499	1.534580
89	8	0	-0.686211	1.197084	1.787130
90	8	0	-1.434920	-0.086913	3.743253
91	8	0	-3.023865	0.488427	1.974072