ESI

Table S1. Free energies of solvation (kcal/mol) for all the studied species, in benzene (BZ) and water (WT) solutions. For O_2^-, N=O_2^-, C=O_2, A=O_2^{-2}. For the others, N=neutral; C=cation; A=anion.

G (solv)	BZ			Wt		
	N	C	A	N	C	A
O2-	-42.45	-0.10	-161.98	-75.89	-0.23	-291.07
BC	-3.20	-15.71	-16.52	-9.62	-32.21	-35.72
BCRYP	-5.72	-18.52	-18.64	-16.26	-39.47	-41.57
ZEA	-7.89	-20.71	-20.74	-22.22	-45.29	-47.45
LUTE	-8.47	-22.24	-20.95	-23.59	-48.73	-47.86
3dhLUTE	-8.68	-23.56	-20.60	-23.38	-51.32	-46.16
3HCAR	-8.43	-22.81	-20.80	-22.97	-49.61	-46.98
33CAR	-8.46	-23.97	-19.79	-22.40	-51.85	-43.73
OXO	-6.62	-20.25	-18.87	-18.30	-43.82	-41.19
ECH	-5.20	-18.41	-17.98	-14.36	-38.86	-38.94
3HECH	-6.25	-19.95	-18.65	-17.42	-42.88	-40.34
CAN	-7.17	-20.98	-18.89	-19.21	-45.36	-41.03
ADO	-8.07	-22.46	-19.13	-21.62	-49.13	-41.87
ASTA	-9.22	-24.18	-19.77	-24.77	-53.17	-43.87
DHIR	-6.77	-18.22	-16.89	-19.29	-39.60	-45.24
TORU	-4.23	-15.79	-16.78	-12.41	-29.60	-40.22
LYC	-4.58	-16.75	-17.91	-13.29	-35.27	-39.01
DORA	-9.17	-23.77	-21.33	-24.75	-52.24	-47.31
ANYLUTE	-6.07	-19.20	-19.13	-17.06	-40.94	-42.48

ESI. Optimized structures of neutral, cation and anion CAR.

BC

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	14.144122	1.580893	-0.142018
2	6	0	12.954379	2.118733	-0.934005
3	6	0	11.750293	1.197764	-0.959045
4	6	0	11.594620	0.173051	-0.087997
5	6	0	12.671459	-0.197839	0.960048
6	6	0	13.661090	0.969505	1.168065
7	1	0	14.864264	2.382905	0.051286
8	1	0	12.637940	3.087412	-0.517034
9	1	0	13.166151	1.749449	1.760643
10	6	0	13.437285	-1.458492	0.494224
11	6	0	12.018879	-0.497914	2.326255
12	6	0	10.768574	1.546498	-2.052110
13	6	0	10.414419	-0.710905	-0.089165
14	6	0	9.122202	-0.319457	-0.111759
15	6	0	7.953629	-1.183111	-0.101982
16	6	0	8.164179	-2.675516	-0.093864
17	6	0	6.719577	-0.598555	-0.101790

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18	6	0	5.432698	-1.230694	-0.100106
19	6	0	4.264589	-0.531083	-0.094521
20	6	0	2.930190	-1.076291	-0.097570
21	6	0	2.765430	-2.575561	-0.114630
22	6	0	1.871730	-0.205253	-0.085259
23	6	0	0.476284	-0.504297	-0.089504
24	6	0	-0.500590	0.449750	-0.070428
25	6	0	-1.897063	0.155955	-0.079091
26	6	0	-2.950047	1.033557	-0.058258
27	6	0	-2.774883	2.531281	-0.015694
28	6	0	-4.288912	0.499492	-0.079047
29	6	0	-5.449172	1.211804	-0.061017
30	6	0	-6.745051	0.599331	-0.092518
31	6	0	-7.968735	1.205223	-0.074928
32	6	0	-8.152684	2.699702	-0.004948
33	6	0	-9.153782	0.365825	-0.126544
34	6	0	-10.437264	0.785936	-0.098422
35	6	0	-11.629418	-0.081750	-0.150175
36	6	0	-11.775272	-1.060281	-1.073759
37	6	0	-12.952343	-2.012207	-1.084442
38	6	0	-13.770873	-2.000360	0.202910
39	6	0	-14.009040	-0.557895	0.635595
40	6	0	-12.699106	0.206178	0.930136
41	6	0	-12.147081	-0.204171	2.314477
42	6	0	-13.050046	1.710635	0.977232
43	6	0	-10.829687	-1.297768	-2.226597
44	1	0	11.302729	1.743709	-2.988199
45	1	0	10.036711	0.762783	-2.238110
46	1	0	13.257014	2.341017	-1.964207
47	1	0	14.675090	0.829931	-0.736687
48	1	0	14.506714	0.616375	1.769322
49	1	0	12.768976	-2.312904	0.358962
50	1	0	14.185553	-1.748401	1.239286
51	1	0	13.950712	-1.294654	-0.455643
52	1	0	11.413606	0.345793	2.668788
53	1	0	12.791345	-0.685391	3.079233
54	1	0	11.370205	-1.375844	2.294258
55	1	0	10.624608	-1.775135	-0.004795
56	1	0	8.911198	0.747578	-0.121513
57	1	0	7.229278	-3.233333	-0.105594
58	1	0	8.750146	-2.994734	-0.961954
59	1	0	8.721092	-2.988481	0.795876
60	1	0	6.697673	0.491066	-0.104678
61	1	0	5.392460	-2.315175	-0.104824
62	1	0	4.330249	0.556544	-0.087443
63	1	0	1.722128	-2.886120	-0.116111
64	1	0	3.239410	-3.012200	-0.999827
65	1	0	3.242025	-3.032308	0.758965
66	1	0	2.117944	0.856237	-0.070706
67	1	0	0.164333	-1.545752	-0.109793
68	1	0	-0.186463	1.490475	-0.048492
69	1	0	-2.148891	-0.903946	-0.107092
70	1	0	-3.246660	2.955870	0.876536
71	1	0	-1.729663	2.834940	-0.007309
72	1	0	-3.247451	3.006239	-0.881680
73	1	0	-4.364793	-0.586922	-0.114034
74	1	0	-5.395129	2.294962	-0.023996
75	1	0	-6.741185	-0.489504	-0.138792
76	1	0	-8.712990	2.984034	0.892231
77	1	0	-7.208423	3.241133	0.015927
78	1	0	-8.724658	3.066270	-0.863559
79	1	0	-10.623371	1.849923	0.018513

80	1	0	-12.862034	0.046214	3.105414
81	1	0	-11.945084	-1.276683	2.369532
82	1	0	-11.209939	0.313420	2.533457
83	1	0	-12.234248	2.321120	1.370188
84	1	0	-13.910771	1.867849	1.634490
85	1	0	-13.315148	2.090754	-0.013758
86	1	0	-14.652227	-0.514723	1.521726
87	1	0	-14.551434	-0.037794	-0.164547
88	1	0	-14.722674	-2.520779	0.054054
89	1	0	-13.238749	-2.549128	0.987342
90	1	0	-13.597359	-1.762285	-1.940619
91	1	0	-12.584095	-3.024730	-1.295792
92	1	0	-8.965999	-0.704573	-0.179435
93	1	0	-11.402997	-1.481122	-3.143165
94	1	0	-10.217939	-2.194553	-2.067916
95	1	0	-10.154098	-0.463473	-2.407537
96	1	0	10.217449	2.466354	-1.817678

BC radical cation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	14.200493	1.463456	-0.263088
2	6	0	12.974973	2.129597	-0.884643
3	6	0	11.719208	1.286002	-0.874775
4	6	0	11.588193	0.182087	-0.085545
5	6	0	12.742100	-0.347351	0.804038
6	6	0	13.805414	0.750630	1.023694
7	1	0	14.973182	2.212129	-0.065812
8	1	0	12.747834	3.064799	-0.349585
9	1	0	13.410444	1.489356	1.732202
10	6	0	13.388774	-1.584141	0.138899
11	6	0	12.209891	-0.753242	2.196309
12	6	0	10.664676	1.788328	-1.829725
13	6	0	10.386310	-0.640416	-0.059640
14	6	0	9.086012	-0.228414	-0.090263
15	6	0	7.938906	-1.088553	-0.058461
16	6	0	8.130497	-2.582192	-0.043113
17	6	0	6.686585	-0.490846	-0.045297
18	6	0	5.431341	-1.126163	-0.031702
19	6	0	4.234973	-0.428492	-0.017167
20	6	0	2.941857	-0.994602	-0.016706
21	6	0	2.776924	-2.493735	-0.035683
22	6	0	1.849340	-0.118448	-0.000816
23	6	0	0.492805	-0.443940	-0.010835
24	6	0	-0.522125	0.511384	0.009544
25	6	0	-1.878235	0.184854	-0.010282
26	6	0	-2.972279	1.059256	0.010957
27	6	0	-2.810014	2.557595	0.071431
28	6	0	-4.263780	0.491676	-0.026883
29	6	0	-5.462332	1.186354	-0.007610
30	6	0	-6.714845	0.549127	-0.062657
31	6	0	-7.970220	1.141887	-0.041195
32	6	0	-8.167014	2.630979	0.070735
33	6	0	-9.112358	0.281352	-0.131466
34	6	0	-10.415684	0.685208	-0.073143
35	6	0	-11.604796	-0.149921	-0.158561
36	6	0	-11.684608	-1.235855	-0.980551
37	6	0	-12.880275	-2.157028	-0.991822

38	6	0	-13.814119	-1.982882	0.200105
39	6	0	-14.070591	-0.496236	0.416667
40	6	0	-12.785450	0.297885	0.741816
41	6	0	-12.396215	0.086309	2.222775
42	6	0	-13.112487	1.793804	0.527801
43	6	0	-10.651765	-1.616929	-2.010709
44	1	0	11.133021	2.149450	-2.749496
45	1	0	9.928538	1.033950	-2.101884
46	1	0	13.189660	2.440535	-1.912781
47	1	0	14.636588	0.754813	-0.974299
48	1	0	14.680450	0.302330	1.505556
49	1	0	12.667010	-2.390677	-0.017265
50	1	0	14.183542	-1.984533	0.775209
51	1	0	13.823052	-1.346076	-0.834074
52	1	0	11.673697	0.072043	2.672511
53	1	0	13.043029	-1.029583	2.848793
54	1	0	11.533988	-1.611060	2.157233
55	1	0	10.562576	-1.705490	0.065248
56	1	0	8.878499	0.836577	-0.103856
57	1	0	7.191650	-3.131443	-0.031430
58	1	0	8.694935	-2.913413	-0.919100
59	1	0	8.698636	-2.891304	0.839440
60	1	0	6.669946	0.597631	-0.049991
61	1	0	5.394901	-2.209955	-0.036841
62	1	0	4.292748	0.658220	-0.007961
63	1	0	1.735018	-2.805717	-0.024495
64	1	0	3.236496	-2.927013	-0.928666
65	1	0	3.260929	-2.951352	0.831812
66	1	0	2.088223	0.943505	0.019375
67	1	0	0.192719	-1.487591	-0.037765
68	1	0	-0.222667	1.555077	0.040954
69	1	0	-2.115703	-0.876953	-0.048012
70	1	0	-3.282875	2.966158	0.969177
71	1	0	-1.768479	2.870767	0.084790
72	1	0	-3.282251	3.037875	-0.790229
73	1	0	-4.319145	-0.594080	-0.076485
74	1	0	-5.428988	2.268786	0.048817
75	1	0	-6.694339	-0.537015	-0.133233
76	1	0	-8.733904	2.880965	0.972675
77	1	0	-7.229942	3.181541	0.115910
78	1	0	-8.734889	3.016103	-0.780525
79	1	0	-10.595026	1.736787	0.126067
80	1	0	-13.194155	0.437831	2.883574
81	1	0	-12.210512	-0.966228	2.449564
82	1	0	-11.487100	0.637772	2.478557
83	1	0	-12.348852	2.463124	0.931153
84	1	0	-14.045264	2.039762	1.042452
85	1	0	-13.248677	2.027555	-0.531768
86	1	0	-14.795454	-0.335857	1.220994
87	1	0	-14.524901	-0.083460	-0.492740
88	1	0	-14.753490	-2.514880	0.024691
89	1	0	-13.367858	-2.430844	1.094179
90	1	0	-13.431410	-1.993654	-1.930053
91	1	0	-12.517873	-3.190957	-1.058718
92	1	0	-8.899351	-0.779019	-0.220034
93	1	0	-11.153596	-1.974133	-2.915717
94	1	0	-10.029098	-2.450921	-1.663914
95	1	0	-9.991072	-0.798066	-2.291244
96	1	0	10.125076	2.645548	-1.407548

BC radical anion

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	14.112598	1.663335	-0.132173
2	6	0	12.881657	2.214729	-0.847908
3	6	0	11.712101	1.251058	-0.903376
4	6	0	11.594597	0.177116	-0.080819
5	6	0	12.716559	-0.210109	0.916721
6	6	0	13.688838	0.966449	1.155059
7	1	0	14.823377	2.469796	0.083378
8	1	0	12.556376	3.145538	-0.354905
9	1	0	13.197142	1.701544	1.805518
10	6	0	13.497562	-1.427226	0.367829
11	6	0	12.121302	-0.590556	2.289133
12	6	0	10.699429	1.612249	-1.963739
13	6	0	10.438409	-0.730154	-0.083505
14	6	0	9.124569	-0.369584	-0.125817
15	6	0	7.979279	-1.235400	-0.115067
16	6	0	8.203382	-2.726605	-0.103088
17	6	0	6.716056	-0.670851	-0.112233
18	6	0	5.449223	-1.295570	-0.103378
19	6	0	4.254694	-0.588115	-0.098627
20	6	0	2.944584	-1.107447	-0.095313
21	6	0	2.754356	-2.606448	-0.103778
22	6	0	1.856041	-0.222709	-0.083816
23	6	0	0.489045	-0.500895	-0.083592
24	6	0	-0.516607	0.472671	-0.065677
25	6	0	-1.884225	0.198379	-0.071121
26	6	0	-2.968852	1.088235	-0.051172
27	6	0	-2.770575	2.585806	-0.010128
28	6	0	-4.281835	0.577292	-0.070779
29	6	0	-5.470898	1.294421	-0.053188
30	6	0	-6.743776	0.684385	-0.087773
31	6	0	-8.000344	1.265071	-0.077698
32	6	0	-8.205007	2.757752	-0.010642
33	6	0	-9.156907	0.417553	-0.131221
34	6	0	-10.466095	0.799015	-0.093485
35	6	0	-11.626592	-0.101511	-0.149923
36	6	0	-11.711762	-1.150228	-1.007819
37	6	0	-12.832714	-2.167480	-0.973273
38	6	0	-13.696189	-2.091481	0.282235
39	6	0	-14.021302	-0.631586	0.576020
40	6	0	-12.760765	0.217816	0.855897
41	6	0	-12.262082	-0.043273	2.295239
42	6	0	-13.186038	1.700572	0.755892
43	6	0	-10.730311	-1.412667	-2.124456
44	1	0	11.208676	1.937673	-2.879287
45	1	0	10.043042	0.779795	-2.213889
46	1	0	13.147673	2.516449	-1.869126
47	1	0	14.636394	0.959252	-0.788597
48	1	0	14.562818	0.601767	1.709179
49	1	0	12.840800	-2.285534	0.206702
50	1	0	14.275083	-1.738313	1.075174
51	1	0	13.977482	-1.202222	-0.587536
52	1	0	11.500908	0.218075	2.684872
53	1	0	12.925096	-0.784417	3.008862
54	1	0	11.496425	-1.483390	2.236936
55	1	0	10.667590	-1.787561	0.030906
56	1	0	8.897039	0.694922	-0.143967
57	1	0	7.270405	-3.287537	-0.152476

58	1	0	8.823477	-3.044887	-0.950108
59	1	0	8.729033	-3.047690	0.805664
60	1	0	6.690102	0.420700	-0.118117
61	1	0	5.404871	-2.380861	-0.099247
62	1	0	4.335068	0.500281	-0.097041
63	1	0	1.703692	-2.895333	-0.103788
64	1	0	3.218503	-3.062944	-0.986132
65	1	0	3.220508	-3.072998	0.772295
66	1	0	2.119120	0.836700	-0.073382
67	1	0	0.161733	-1.539412	-0.098299
68	1	0	-0.187599	1.510569	-0.046853
69	1	0	-2.151507	-0.859743	-0.095320
70	1	0	-3.230040	3.024931	0.883462
71	1	0	-1.718530	2.869368	-0.005836
72	1	0	-3.236519	3.074051	-0.874300
73	1	0	-4.369898	-0.509954	-0.105243
74	1	0	-5.416231	2.378472	-0.013530
75	1	0	-6.731177	-0.406506	-0.132063
76	1	0	-8.745397	3.048695	0.899602
77	1	0	-7.264408	3.307929	-0.018241
78	1	0	-8.803783	3.118315	-0.856051
79	1	0	-10.678665	1.854931	0.046166
80	1	0	-13.025719	0.240007	3.029109
81	1	0	-12.016058	-1.096511	2.452887
82	1	0	-11.358431	0.533174	2.503892
83	1	0	-12.413485	2.382405	1.115704
84	1	0	-14.078898	1.873035	1.366805
85	1	0	-13.427509	1.974995	-0.275283
86	1	0	-14.707313	-0.543159	1.427289
87	1	0	-14.548740	-0.210712	-0.290319
88	1	0	-14.614580	-2.675909	0.153563
89	1	0	-13.161393	-2.536904	1.128491
90	1	0	-13.464894	-2.037375	-1.866830
91	1	0	-12.403453	-3.173981	-1.078501
92	1	0	-8.946549	-0.649490	-0.187093
93	1	0	-11.271891	-1.709051	-3.032760
94	1	0	-10.049296	-2.242480	-1.893906
95	1	0	-10.117446	-0.542892	-2.357187
96	1	0	10.058537	2.450351	-1.657894

BCRIP

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	14.419653	0.283478	0.676185
2	6	0	14.192105	1.790332	0.716507
3	6	0	13.103926	-0.525380	0.722587
4	6	0	12.033528	0.095488	-0.206756
5	6	0	12.187619	1.310844	-0.781711
6	6	0	13.373574	2.209079	-0.500558
7	6	0	12.560483	-0.568308	2.168764
8	6	0	13.442682	-1.970433	0.291023
9	6	0	11.241101	1.902899	-1.798207
10	6	0	10.831390	-0.733998	-0.416172
11	6	0	9.552610	-0.315293	-0.299292
12	6	0	8.358996	-1.122741	-0.485910
13	6	0	7.141749	-0.532365	-0.299390
14	6	0	5.841012	-1.122828	-0.421844
15	6	0	4.686182	-0.433304	-0.210692

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16	6	0	3.344357	-0.950858	-0.310623
17	6	0	3.159216	-2.401413	-0.681146
18	6	0	8.526879	-2.570459	-0.871373
19	6	0	2.297087	-0.101031	-0.064661
20	6	0	0.899174	-0.386067	-0.105200
21	6	0	-0.071531	0.538675	0.154076
22	6	0	-1.468726	0.249956	0.112229
23	6	0	-2.520160	1.096429	0.351316
24	6	0	-2.343199	2.549750	0.714338
25	6	0	-3.858742	0.571009	0.249599
26	6	0	-5.019509	1.254251	0.447951
27	6	0	-6.313884	0.650145	0.322847
28	6	0	-7.538917	1.229892	0.488624
29	6	0	-7.727313	2.681219	0.849765
30	6	0	-8.721021	0.405092	0.302657
31	6	0	-10.005751	0.810436	0.391080
32	6	0	-11.201767	-0.025034	0.173642
33	6	0	-11.383212	-1.225073	0.771641
34	6	0	-12.601876	-2.087787	0.507267
35	6	0	-13.288174	-0.450491	-1.224663
36	6	0	-12.261072	0.604891	-0.762216
37	6	0	-10.421882	-1.844288	1.757152
38	6	0	-12.985223	1.759031	-0.028231
39	6	0	-11.590876	1.177558	-2.029673
40	1	0	-10.968906	-2.234187	2.622832
41	1	0	-9.897119	-2.702174	1.317586
42	1	0	-12.288812	2.542366	0.281337
43	1	0	-13.723727	2.225113	-0.688136
44	1	0	-10.918148	2.007188	-1.802402
45	1	0	-12.353107	1.547016	-2.722929
46	1	0	14.302907	-2.333199	0.861960
47	1	0	12.622861	-2.668235	0.474347
48	1	0	13.703509	-2.020274	-0.770237
49	1	0	13.276351	-1.059719	2.836112
50	1	0	11.620310	-1.122856	2.218607
51	1	0	11.813819	2.355941	-2.616160
52	1	0	10.556333	1.171792	-2.224776
53	1	0	15.063787	-0.038826	1.501981
54	1	0	13.664928	2.071088	1.634682
55	1	0	13.014044	3.240039	-0.385144
56	1	0	11.006137	-1.784200	-0.632989
57	1	0	9.094268	-3.115907	-0.109664
58	1	0	7.576916	-3.085812	-1.001428
59	1	0	3.595335	-2.614711	-1.662635
60	1	0	2.112508	-2.697426	-0.718097
61	1	0	-1.297841	2.850316	0.754427
62	1	0	-2.843295	3.198755	-0.011955
63	1	0	-6.784485	3.208405	0.984592
64	1	0	-8.289456	3.209535	0.072187
65	1	0	9.376028	0.721405	-0.020060
66	1	0	7.148186	0.520952	-0.019861
67	1	0	5.779089	-2.170899	-0.695987
68	1	0	4.768826	0.618133	0.062922
69	1	0	2.554747	0.925589	0.194609
70	1	0	0.579501	-1.394248	-0.357024
71	1	0	0.246464	1.547516	0.405443
72	1	0	-1.722170	-0.778599	-0.143575
73	1	0	-3.933691	-0.483158	-0.015664
74	1	0	-6.307048	-0.407053	0.058279
75	1	0	-4.967938	2.305473	0.712143
76	1	0	-8.528036	-0.634207	0.045394
77	1	0	-10.197094	1.865264	0.576443

78	1	0	-12.834935	-1.099153	-1.983071
79	1	0	-12.333335	-2.902965	-0.180273
80	1	0	12.367080	0.433420	2.559999
81	1	0	9.084502	-2.665704	-1.808775
82	1	0	3.660091	-3.056733	0.038851
83	1	0	10.639392	2.711788	-1.365479
84	1	0	-2.785037	2.766949	1.692431
85	1	0	-8.298526	2.784739	1.778136
86	1	0	-13.504304	1.411184	0.867431
87	1	0	-11.007742	0.412068	-2.548504
88	1	0	-9.669023	-1.145854	2.117463
89	1	0	14.957209	0.035880	-0.248349
90	1	0	15.147945	2.324143	0.734524
91	1	0	14.016277	2.232588	-1.393857
92	1	0	-12.909383	-2.579361	1.440289
93	6	0	-13.780906	-1.334899	-0.098485
94	1	0	-14.253549	-0.718525	0.679575
95	1	0	-14.140507	0.042481	-1.702984
96	8	0	-14.755355	-2.224717	-0.648873
97	1	0	-15.086785	-2.785825	0.061738

BCRIP radical cation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-14.501915	0.270579	-0.355100
2	6	0	-14.273369	1.751084	-0.634384
3	6	0	-13.207433	-0.568223	-0.451640
4	6	0	-12.013152	0.161420	0.217903
5	6	0	-12.100594	1.450430	0.658375
6	6	0	-13.316716	2.309690	0.411830
7	6	0	-12.867324	-0.839315	-1.934692
8	6	0	-13.493636	-1.919195	0.243997
9	6	0	-11.053372	2.152982	1.484705
10	6	0	-10.806403	-0.639205	0.351893
11	6	0	-9.508745	-0.220365	0.261657
12	6	0	-8.357451	-1.063419	0.384732
13	6	0	-7.108917	-0.479576	0.211606
14	6	0	-5.852311	-1.104625	0.293027
15	6	0	-4.658431	-0.428414	0.098521
16	6	0	-3.365590	-0.988604	0.172500
17	6	0	-3.196503	-2.454277	0.486178
18	6	0	-8.535902	-2.527946	0.689793
19	6	0	-2.275068	-0.137397	-0.048819
20	6	0	-0.918512	-0.460648	-0.012425
21	6	0	0.093423	0.469244	-0.245380
22	6	0	1.450898	0.149438	-0.200861
23	6	0	2.539353	1.003423	-0.417329
24	6	0	2.367363	2.464036	-0.751646
25	6	0	3.835692	0.452996	-0.312105
26	6	0	5.026498	1.136664	-0.487958
27	6	0	6.288996	0.527756	-0.356553
28	6	0	7.532561	1.125537	-0.496113
29	6	0	7.704031	2.583721	-0.832283
30	6	0	8.693831	0.305377	-0.297881
31	6	0	9.983959	0.744658	-0.325333
32	6	0	11.197272	-0.030619	-0.095715
33	6	0	11.388039	-1.283559	-0.593008
34	6	0	12.647075	-2.074810	-0.313393

35	6	0	13.361391	-0.260502	1.223211
36	6	0	12.290564	0.721084	0.703800
37	6	0	10.409393	-2.016722	-1.475465
38	6	0	12.947631	1.794065	-0.196198
39	6	0	11.678596	1.417943	1.939180
40	1	0	10.943595	-2.528228	-2.281469
41	1	0	9.883184	-2.800820	-0.916462
42	1	0	12.221609	2.527323	-0.557928
43	1	0	13.707121	2.345740	0.365171
44	1	0	10.989944	2.222493	1.670076
45	1	0	12.471314	1.860837	2.548429
46	1	0	-14.435085	-2.329259	-0.131534
47	1	0	-12.727805	-2.674291	0.051968
48	1	0	-13.593896	-1.799733	1.326315
49	1	0	-13.673886	-1.399367	-2.417116
50	1	0	-11.950937	-1.428044	-2.033239
51	1	0	-11.542570	2.780764	2.236198
52	1	0	-10.376057	1.473812	2.000541
53	1	0	-15.244129	-0.149245	-1.041208
54	1	0	-13.857220	1.894046	-1.637178
55	1	0	-12.976109	3.316135	0.136274
56	1	0	-10.966209	-1.706250	0.465941
57	1	0	-9.118845	-3.019606	-0.094805
58	1	0	-7.592724	-3.062970	0.774024
59	1	0	-3.599622	-2.692023	1.474967
60	1	0	-2.156369	-2.771967	0.475618
61	1	0	1.324624	2.771739	-0.780923
62	1	0	2.871287	3.096232	-0.015209
63	1	0	6.758942	3.098144	-0.990954
64	1	0	8.229367	3.108561	-0.028505
65	1	0	-9.309407	0.823261	0.041575
66	1	0	-7.099688	0.585595	-0.012815
67	1	0	-5.811258	-2.163827	0.521394
68	1	0	-4.719030	0.633834	-0.130190
69	1	0	-2.515729	0.900662	-0.271844
70	1	0	-0.616688	-1.480036	0.209963
71	1	0	-0.209152	1.488051	-0.469475
72	1	0	1.693283	-0.886181	0.031350
73	1	0	3.899176	-0.605154	-0.065923
74	1	0	6.285201	-0.532264	-0.108854
75	1	0	4.981539	2.191569	-0.734769
76	1	0	8.503878	-0.737240	-0.062351
77	1	0	10.139219	1.811861	-0.458949
78	1	0	12.961117	-0.837038	2.065027
79	1	0	12.427464	-2.824937	0.460151
80	1	0	-12.718885	0.086764	-2.495341
81	1	0	-9.079091	-2.669612	1.628047
82	1	0	-3.730707	-3.073905	-0.239367
83	1	0	-10.449329	2.833790	0.872168
84	1	0	2.801641	2.695213	-1.728659
85	1	0	8.301403	2.708198	-1.739512
86	1	0	13.429369	1.354752	-1.071918
87	1	0	11.134247	0.707246	2.566571
88	1	0	9.660678	-1.369194	-1.928215
89	1	0	-14.922235	0.165345	0.653007
90	1	0	-15.219679	2.298889	-0.611703
91	1	0	-13.842359	2.445594	1.368927
92	1	0	12.923970	-2.648814	-1.206270
93	6	0	13.833584	-1.245346	0.173474
94	1	0	14.270661	-0.704535	-0.677530
95	1	0	14.218226	0.299243	1.609102
96	8	0	14.830491	-2.062530	0.780989

97	1	0	15.225877	-2.627077	0.106905

BCRIP radical anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	14.420929	0.287194	0.795141
2	6	0	14.135469	1.775158	0.962942
3	6	0	13.135590	-0.570363	0.771158
4	6	0	12.036931	0.077564	-0.108539
5	6	0	12.165408	1.339058	-0.592369
6	6	0	13.307939	2.261674	-0.222998
7	6	0	12.599884	-0.753555	2.209197
8	6	0	13.532614	-1.961138	0.225488
9	6	0	11.217229	1.965427	-1.586116
10	6	0	10.858982	-0.765682	-0.360069
11	6	0	9.557653	-0.363254	-0.294884
12	6	0	8.387471	-1.162684	-0.522302
13	6	0	7.139868	-0.584850	-0.364472
14	6	0	5.859095	-1.159490	-0.519608
15	6	0	4.677981	-0.454103	-0.333922
16	6	0	3.360141	-0.937747	-0.458585
17	6	0	3.148048	-2.386314	-0.833933
18	6	0	8.569130	-2.606484	-0.918633
19	6	0	2.283308	-0.067254	-0.233123
20	6	0	0.913597	-0.325050	-0.293985
21	6	0	-0.085841	0.623998	-0.049866
22	6	0	-1.454183	0.357258	-0.100199
23	6	0	-2.537609	1.219698	0.125399
24	6	0	-2.337576	2.678664	0.464854
25	6	0	-3.849567	0.713027	0.044207
26	6	0	-5.039848	1.399257	0.246702
27	6	0	-6.308683	0.786837	0.158515
28	6	0	-7.567444	1.332366	0.344714
29	6	0	-7.781412	2.786999	0.680878
30	6	0	-8.715327	0.480817	0.222411
31	6	0	-10.027044	0.833479	0.348068
32	6	0	-11.189409	-0.053874	0.217795
33	6	0	-11.256523	-1.295813	0.764036
34	6	0	-12.440329	-2.220630	0.553144
35	6	0	-13.410749	-0.525422	-0.966251
36	6	0	-12.382181	0.555021	-0.564648
37	6	0	-10.178660	-1.893972	1.635250
38	6	0	-13.074831	1.632268	0.304708
39	6	0	-11.894079	1.221312	-1.868546
40	1	0	-10.627314	-2.422961	2.485321
41	1	0	-9.575130	-2.638217	1.098242
42	1	0	-12.384518	2.434163	0.576664
43	1	0	-13.908389	2.088422	-0.240903
44	1	0	-11.235135	2.069235	-1.674832
45	1	0	-12.748332	1.583017	-2.451959
46	1	0	14.403508	-2.339569	0.771755
47	1	0	12.736105	-2.698524	0.339802
48	1	0	13.798499	-1.910359	-0.834525
49	1	0	13.334170	-1.273554	2.835418
50	1	0	11.677852	-1.338565	2.208038
51	1	0	11.786900	2.516064	-2.346542
52	1	0	10.591243	1.230135	-2.089890
53	1	0	15.080148	-0.080390	1.590966

54	1	0	13.588124	1.951742	1.895510
55	1	0	12.904895	3.263803	-0.019224
56	1	0	11.050991	-1.816238	-0.557583
57	1	0	9.082337	-3.177877	-0.134211
58	1	0	7.621482	-3.106533	-1.116587
59	1	0	3.587242	-2.613960	-1.812656
60	1	0	2.093510	-2.655747	-0.881419
61	1	0	-1.288517	2.972476	0.443740
62	1	0	-2.871033	3.327581	-0.239364
63	1	0	-6.844061	3.334313	0.776518
64	1	0	-8.376811	3.293725	-0.089554
65	1	0	9.364638	0.671472	-0.015261
66	1	0	7.142262	0.468303	-0.076527
67	1	0	5.792488	-2.207503	-0.796655
68	1	0	4.776121	0.597212	-0.058100
69	1	0	2.558453	0.956331	0.027940
70	1	0	0.577960	-1.329798	-0.545631
71	1	0	0.246908	1.630422	0.199146
72	1	0	-1.722748	-0.672122	-0.344786
73	1	0	-3.935880	-0.346912	-0.200897
74	1	0	-6.290435	-0.277118	-0.086029
75	1	0	-4.989184	2.455739	0.493752
76	1	0	-8.494839	-0.557236	-0.020354
77	1	0	-10.252594	1.887419	0.493740
78	1	0	-13.025379	-1.105976	-1.812766
79	1	0	-12.214398	-2.963356	-0.227552
80	1	0	12.371995	0.205703	2.681162
81	1	0	9.183378	-2.698659	-1.822684
82	1	0	3.624728	-3.059716	-0.111894
83	1	0	10.549511	2.699991	-1.117015
84	1	0	-2.724041	2.914618	1.463829
85	1	0	-8.328780	2.904840	1.624370
86	1	0	-13.468033	1.211757	1.233261
87	1	0	-11.338901	0.510925	-2.486891
88	1	0	-9.493527	-1.141438	2.023069
89	1	0	14.964404	0.141016	-0.147789
90	1	0	15.069543	2.343600	1.039366
91	1	0	13.960596	2.394817	-1.101223
92	1	0	-12.616181	-2.802334	1.469834
93	6	0	-13.717738	-1.497070	0.151919
94	1	0	-14.110705	-0.952711	1.022993
95	1	0	-14.337702	-0.051458	-1.307569
96	8	0	-14.724105	-2.401725	-0.323864
97	1	0	-14.873988	-3.060179	0.364492

ZEA

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	14.198705	1.099335	0.182112
2	6	0	13.082446	1.839471	-0.545403
3	6	0	11.827212	1.014767	-0.754715
4	6	0	11.559828	-0.093605	-0.026060
5	6	0	12.549978	-0.657777	1.020911
6	6	0	13.624693	0.387659	1.388997
7	1	0	13.191182	1.148668	2.048416
8	6	0	13.227250	-1.933526	0.465549
9	6	0	11.806567	-1.026816	2.323006
10	6	0	10.937702	1.556503	-1.847312

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11	6	0	10.330288	-0.891121	-0.188649
12	6	0	9.063972	-0.423029	-0.220548
13	6	0	7.855508	-1.221757	-0.338422
14	6	0	7.997275	-2.715740	-0.483317
15	6	0	6.648920	-0.583356	-0.302773
16	6	0	5.338810	-1.161438	-0.372636
17	6	0	4.193539	-0.426965	-0.322336
18	6	0	2.845175	-0.935529	-0.367310
19	6	0	2.644255	-2.426190	-0.482990
20	6	0	1.806934	-0.042947	-0.298861
21	6	0	0.406228	-0.315846	-0.313453
22	6	0	-0.557819	0.648352	-0.238687
23	6	0	-1.956677	0.365400	-0.245971
24	6	0	-3.005290	1.245642	-0.178250
25	6	0	-2.824031	2.740183	-0.085551
26	6	0	-4.345481	0.714889	-0.196676
27	6	0	-5.505511	1.425570	-0.141521
28	6	0	-6.799741	0.809080	-0.165779
29	6	0	-8.026016	1.407956	-0.119846
30	6	0	-8.216917	2.900216	-0.026420
31	6	0	-9.206198	0.561282	-0.164278
32	6	0	-10.491990	0.971643	-0.115496
33	6	0	-11.677555	0.094230	-0.156629
34	6	0	-11.829429	-0.879809	-1.081253
35	6	0	-13.004093	-1.833066	-1.098294
36	6	0	-13.860297	-1.840675	0.157752
37	6	0	-14.033882	-0.416215	0.676334
38	6	0	-12.721855	0.353142	0.951415
39	6	0	-12.118785	-0.061985	2.314255
40	6	0	-13.096373	1.851825	1.026523
41	6	0	-10.892031	-1.116126	-2.240492
42	1	0	11.535966	1.804121	-2.731353
43	1	0	10.157894	0.860259	-2.149578
44	1	0	14.650783	0.367213	-0.502409
45	1	0	14.433025	-0.089620	1.952108
46	1	0	12.495638	-2.707781	0.221379
47	1	0	13.909370	-2.356966	1.209557
48	1	0	13.801244	-1.729972	-0.441131
49	1	0	11.252175	-0.170571	2.716175
50	1	0	12.522954	-1.343883	3.087401
51	1	0	11.094647	-1.841944	2.177112
52	1	0	10.473026	-1.969038	-0.215503
53	1	0	8.908086	0.648832	-0.119721
54	1	0	7.041042	-3.220537	-0.608495
55	1	0	8.617776	-2.968452	-1.349178
56	1	0	8.486307	-3.152438	0.394276
57	1	0	6.673096	0.501316	-0.199789
58	1	0	5.260729	-2.240057	-0.461010
59	1	0	4.289981	0.654752	-0.233661
60	1	0	1.594070	-2.711539	-0.500931
61	1	0	3.104812	-2.814003	-1.397541
62	1	0	3.112129	-2.951299	0.356163
63	1	0	2.075460	1.010231	-0.219540
64	1	0	0.077493	-1.349728	-0.385226
65	1	0	-0.233051	1.683687	-0.168474
66	1	0	-2.214807	-0.691182	-0.313255
67	1	0	-3.278344	3.134424	0.829370
68	1	0	-1.777542	3.039891	-0.086185
69	1	0	-3.310262	3.246784	-0.925689
70	1	0	-4.423087	-0.370044	-0.260827
71	1	0	-5.452750	2.507649	-0.077808
72	1	0	-6.791801	-0.278757	-0.230170

73	1	0	-8.776894	3.168015	0.875967
74	1	0	-7.275053	3.445618	0.000873
75	1	0	-8.792141	3.277347	-0.878381
76	1	0	-10.685168	2.033225	0.012981
77	1	0	-12.834771	0.119364	3.124364
78	1	0	-11.852683	-1.118289	2.316229
79	1	0	-11.217597	0.516072	2.533460
80	1	0	-12.279371	2.466946	1.408859
81	1	0	-13.942319	1.989186	1.707265
82	1	0	-13.390510	2.242731	0.047852
83	1	0	-14.647785	-0.416480	1.586997
84	1	0	-14.616889	0.129298	-0.076542
85	1	0	-9.012179	-0.507231	-0.227664
86	1	0	-11.468635	-1.305016	-3.153879
87	1	0	-10.276698	-2.009948	-2.080423
88	1	0	-10.220995	-0.279533	-2.427354
89	1	0	10.450131	2.490237	-1.539102
90	8	0	15.211754	1.991286	0.653210
91	1	0	15.592184	2.444770	-0.107907
92	8	0	-13.225653	-2.715808	1.099248
93	1	0	-13.724730	-2.684646	1.923839
94	1	0	-14.851188	-2.250413	-0.088520
95	1	0	12.839661	2.740259	0.036785
96	1	0	13.444102	2.205046	-1.516066
97	1	0	-12.640847	-2.853131	-1.269728
98	1	0	-13.637565	-1.599015	-1.965614

ZEA radical cation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	14.218403	1.070387	0.113996
2	6	0	13.069788	1.861792	-0.507116
3	6	0	11.782909	1.085042	-0.680369
4	6	0	11.541772	-0.072538	-0.005682
5	6	0	12.596847	-0.732841	0.917028
6	6	0	13.700762	0.276628	1.295146
7	1	0	13.315453	0.989878	2.032841
8	6	0	13.219452	-1.958219	0.206914
9	6	0	11.943724	-1.203987	2.235423
10	6	0	10.836257	1.716955	-1.670063
11	6	0	10.304004	-0.832252	-0.136361
12	6	0	9.029061	-0.354522	-0.200232
13	6	0	7.845201	-1.161474	-0.293072
14	6	0	7.976793	-2.658179	-0.399546
15	6	0	6.618822	-0.514680	-0.271901
16	6	0	5.340885	-1.102742	-0.329099
17	6	0	4.166825	-0.370909	-0.285432
18	6	0	2.858533	-0.901931	-0.326127
19	6	0	2.657214	-2.393115	-0.430936
20	6	0	1.787423	-0.002314	-0.262673
21	6	0	0.424314	-0.299496	-0.281645
22	6	0	-0.574723	0.669742	-0.207542
23	6	0	-1.934687	0.359707	-0.225185
24	6	0	-3.020343	1.242092	-0.152827
25	6	0	-2.844193	2.735618	-0.039532
26	6	0	-4.315844	0.684775	-0.187460
27	6	0	-5.510848	1.383648	-0.121082
28	6	0	-6.764885	0.750093	-0.168986

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29	6	0	-8.019852	1.341751	-0.104263
30	6	0	-8.214191	2.827314	0.049446
31	6	0	-9.161844	0.481507	-0.188951
32	6	0	-10.464596	0.879251	-0.088182
33	6	0	-11.650426	0.038873	-0.161055
34	6	0	-11.746827	-1.025927	-1.005587
35	6	0	-12.939945	-1.948686	-1.021506
36	6	0	-13.857793	-1.840549	0.183504
37	6	0	-14.081975	-0.369760	0.521561
38	6	0	-12.796673	0.446008	0.796676
39	6	0	-12.323549	0.236501	2.254848
40	6	0	-13.173060	1.935446	0.612030
41	6	0	-10.738373	-1.383835	-2.066914
42	1	0	11.393779	2.101261	-2.529016
43	1	0	10.074852	1.034185	-2.043205
44	1	0	14.638060	0.389494	-0.639726
45	1	0	14.532463	-0.248087	1.774033
46	1	0	12.468355	-2.711814	-0.045275
47	1	0	13.950860	-2.441716	0.860686
48	1	0	13.726620	-1.682151	-0.719665
49	1	0	11.425706	-0.382287	2.736975
50	1	0	12.710860	-1.579747	2.918179
51	1	0	11.222852	-2.010939	2.082741
52	1	0	10.423975	-1.911730	-0.103964
53	1	0	8.869327	0.716770	-0.129359
54	1	0	7.019224	-3.164471	-0.498157
55	1	0	8.584776	-2.935569	-1.264921
56	1	0	8.472876	-3.069157	0.485040
57	1	0	6.643436	0.570849	-0.194325
58	1	0	5.269376	-2.182010	-0.405158
59	1	0	4.254380	0.711103	-0.208566
60	1	0	1.608255	-2.679709	-0.450195
61	1	0	3.117837	-2.786890	-1.341432
62	1	0	3.118594	-2.910341	0.415160
63	1	0	2.049890	1.051536	-0.187419
64	1	0	0.104712	-1.334974	-0.355752
65	1	0	-0.260732	1.706867	-0.131777
66	1	0	-2.183584	-0.697244	-0.303376
67	1	0	-3.288686	3.112847	0.886045
68	1	0	-1.799972	3.040267	-0.044177
69	1	0	-3.335982	3.251957	-0.868760
70	1	0	-4.379103	-0.398287	-0.273034
71	1	0	-5.472565	2.463656	-0.030420
72	1	0	-6.747249	-0.333657	-0.269783
73	1	0	-8.757903	3.054445	0.971493
74	1	0	-7.276377	3.377483	0.083863
75	1	0	-8.803614	3.232707	-0.777399
76	1	0	-10.643493	1.924776	0.141876
77	1	0	-13.115279	0.515980	2.957521
78	1	0	-12.054336	-0.803913	2.432861
79	1	0	-11.452357	0.858163	2.480534
80	1	0	-12.401926	2.618175	0.976176
81	1	0	-14.079114	2.158125	1.182478
82	1	0	-13.374937	2.173765	-0.436076
83	1	0	-14.753528	-0.274756	1.383182
84	1	0	-14.618257	0.076287	-0.325008
85	1	0	-8.949601	-0.576133	-0.305746
86	1	0	-11.258532	-1.722716	-2.968676
87	1	0	-10.110340	-2.225085	-1.748932
88	1	0	-10.083765	-0.559133	-2.344225
89	1	0	10.324976	2.582272	-1.229569
90	8	0	15.244562	1.930690	0.601763

91	1	0	15.664198	2.371878	-0.145697
92	8	0	-13.242563	-2.582926	1.241303
93	1	0	-13.831730	-2.575361	2.004736
94	1	0	-14.823875	-2.301640	-0.064033
95	1	0	12.874850	2.728737	0.140900
96	1	0	13.375303	2.282092	-1.473130
97	1	0	-12.586434	-2.983160	-1.099515
98	1	0	-13.514748	-1.766029	-1.939848

ZEA radical anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	14.158583	1.216052	0.186731
2	6	0	12.983386	1.955167	-0.436725
3	6	0	11.767838	1.079939	-0.674673
4	6	0	11.559509	-0.085072	-0.008122
5	6	0	12.620189	-0.664676	0.964478
6	6	0	13.668343	0.398442	1.361170
7	1	0	13.231564	1.092877	2.088639
8	6	0	13.326743	-1.870719	0.300467
9	6	0	11.954925	-1.148422	2.271005
10	6	0	10.825779	1.636059	-1.714844
11	6	0	10.359559	-0.916138	-0.163035
12	6	0	9.065987	-0.485314	-0.220209
13	6	0	7.887511	-1.295078	-0.332838
14	6	0	8.050812	-2.789336	-0.459201
15	6	0	6.646185	-0.681611	-0.308441
16	6	0	5.360152	-1.259278	-0.372327
17	6	0	4.185594	-0.518766	-0.334376
18	6	0	2.863996	-1.004871	-0.374650
19	6	0	2.639551	-2.496250	-0.472781
20	6	0	1.794245	-0.098490	-0.317435
21	6	0	0.422757	-0.352147	-0.329160
22	6	0	-0.569473	0.632862	-0.263800
23	6	0	-1.939850	0.370845	-0.269135
24	6	0	-3.017619	1.266154	-0.207884
25	6	0	-2.809879	2.760505	-0.124807
26	6	0	-4.333820	0.761786	-0.222225
27	6	0	-5.519063	1.481834	-0.165791
28	6	0	-6.794347	0.874547	-0.189463
29	6	0	-8.048574	1.456580	-0.143648
30	6	0	-8.249715	2.948064	-0.047653
31	6	0	-9.207992	0.610656	-0.184485
32	6	0	-10.514131	0.994214	-0.113167
33	6	0	-11.678752	0.096089	-0.153248
34	6	0	-11.801475	-0.923331	-1.037528
35	6	0	-12.938150	-1.922455	-1.023784
36	6	0	-13.847270	-1.875721	0.194735
37	6	0	-14.050143	-0.430786	0.636841
38	6	0	-12.757558	0.367120	0.920713
39	6	0	-12.184179	0.007754	2.312017
40	6	0	-13.163945	1.859105	0.942826
41	6	0	-10.848349	-1.170929	-2.181449
42	1	0	11.392303	2.047455	-2.559458
43	1	0	10.138467	0.882763	-2.097935
44	1	0	14.607858	0.554322	-0.568121
45	1	0	14.519129	-0.081049	1.857945
46	1	0	12.614620	-2.656107	0.037036

47	1	0	14.061406	-2.310221	0.984335
48	1	0	13.846950	-1.581860	-0.615729
49	1	0	11.378180	-0.345113	2.737037
50	1	0	12.719160	-1.475282	2.985197
51	1	0	11.273205	-1.983182	2.101558
52	1	0	10.527307	-1.990490	-0.148898
53	1	0	8.885714	0.584896	-0.135637
54	1	0	7.100202	-3.300727	-0.607565
55	1	0	8.698096	-3.049394	-1.305625
56	1	0	8.518241	-3.222506	0.434854
57	1	0	6.660979	0.406623	-0.220684
58	1	0	5.281813	-2.340071	-0.445261
59	1	0	4.294202	0.564586	-0.259738
60	1	0	1.582917	-2.759973	-0.504296
61	1	0	3.105890	-2.911333	-1.374106
62	1	0	3.081977	-3.023636	0.380719
63	1	0	2.078264	0.953394	-0.250702
64	1	0	0.078953	-1.383542	-0.389801
65	1	0	-0.229192	1.665487	-0.203399
66	1	0	-2.215214	-0.683786	-0.328172
67	1	0	-3.241255	3.173696	0.794855
68	1	0	-1.756402	3.038411	-0.142545
69	1	0	-3.297267	3.277842	-0.959687
70	1	0	-4.427058	-0.323777	-0.283859
71	1	0	-5.460580	2.564452	-0.100430
72	1	0	-6.784547	-0.215248	-0.254282
73	1	0	-8.768801	3.224711	0.879309
74	1	0	-7.308860	3.497467	-0.068124
75	1	0	-8.867028	3.322840	-0.873333
76	1	0	-10.722589	2.048939	0.041884
77	1	0	-12.925463	0.196467	3.099178
78	1	0	-11.889750	-1.040379	2.353871
79	1	0	-11.301669	0.612957	2.530157
80	1	0	-12.362378	2.500168	1.312840
81	1	0	-14.023213	2.002123	1.607325
82	1	0	-13.448859	2.210712	-0.053429
83	1	0	-14.701055	-0.394056	1.522434
84	1	0	-14.608332	0.070806	-0.164178
85	1	0	-9.001609	-0.456035	-0.257691
86	1	0	-11.410180	-1.429595	-3.088925
87	1	0	-10.182143	-2.020851	-1.984904
88	1	0	-10.221744	-0.307165	-2.398695
89	1	0	10.217695	2.463315	-1.324424
90	8	0	15.164537	2.115805	0.672966
91	1	0	15.426195	2.684281	-0.060668
92	8	0	-13.258613	-2.703700	1.208450
93	1	0	-13.729408	-2.545254	2.034893
94	1	0	-14.826811	-2.302832	-0.072187
95	1	0	12.726380	2.798382	0.223256
96	1	0	13.295777	2.411939	-1.387414
97	1	0	-12.534787	-2.940003	-1.104724
98	1	0	-13.548801	-1.781579	-1.928638

LUT

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.791526	-0.945582	1.301804
2	6	0	13.892198	-0.008342	0.760302

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3	6	0	13.695774	1.499739	0.772598
4	6	0	12.563472	-0.797794	0.773708
5	6	0	11.528131	-0.165807	-0.186642
6	6	0	11.722698	1.038352	-0.772483
7	6	0	12.924719	1.909627	-0.474842
8	6	0	11.983239	-0.824196	2.206447
9	6	0	12.892576	-2.250185	0.359088
10	6	0	10.811969	1.644751	-1.812497
11	6	0	10.310229	-0.968465	-0.407807
12	6	0	9.041572	-0.511019	-0.332601
13	6	0	7.829027	-1.287512	-0.526569
14	6	0	6.627159	-0.655208	-0.383236
15	6	0	5.310843	-1.208566	-0.512114
16	6	0	4.176166	-0.474537	-0.347063
17	6	0	2.819485	-0.952293	-0.444847
18	6	0	2.591680	-2.410152	-0.758874
19	6	0	7.960881	-2.749227	-0.870638
20	6	0	1.798193	-0.059908	-0.245596
21	6	0	0.392227	-0.304285	-0.277179
22	6	0	-0.550333	0.661129	-0.068322
23	6	0	-1.955379	0.408932	-0.084770
24	6	0	-2.981483	1.295738	0.112114
25	6	0	-2.764516	2.764360	0.378848
26	6	0	-4.334071	0.797175	0.068291
27	6	0	-5.474608	1.517280	0.248214
28	6	0	-6.783264	0.929961	0.205144
29	6	0	-7.991694	1.537774	0.380389
30	6	0	-8.148649	3.011838	0.650142
31	6	0	-9.191879	0.714205	0.310870
32	6	0	-10.459100	1.134272	0.477651
33	6	0	-11.725753	0.305478	0.415135
34	6	0	-12.943949	-1.620851	1.261456
35	6	0	-13.479525	-0.912343	-1.049106
36	6	0	-12.211765	-0.001217	-1.071933
37	6	0	-12.553442	1.337957	-1.751556
38	6	0	-11.120021	-0.708394	-1.891628
39	1	0	-11.687135	2.004174	-1.785811
40	1	0	-12.884418	1.174675	-2.781407
41	1	0	-10.242836	-0.076522	-2.040192
42	1	0	-11.509308	-0.970625	-2.880192
43	1	0	13.729888	-2.623324	0.956397
44	1	0	12.056359	-2.933090	0.522549
45	1	0	13.182216	-2.309543	-0.694123
46	1	0	12.680328	-1.311484	2.895722
47	1	0	11.040334	-1.375236	2.236716
48	1	0	11.411667	2.078489	-2.621376
49	1	0	10.120020	0.925641	-2.247761
50	1	0	14.509825	-0.305789	1.613745
51	1	0	13.133241	1.795855	1.661988
52	1	0	10.461325	-2.027829	-0.595329
53	1	0	8.496653	-3.291458	-0.084097
54	1	0	6.998410	-3.239212	-1.006847
55	1	0	3.037430	-2.677280	-1.722643
56	1	0	1.536345	-2.672359	-0.804516
57	1	0	-1.712296	3.043011	0.377173
58	1	0	-3.266639	3.377598	-0.376513
59	1	0	-7.196865	3.539619	0.676479
60	1	0	-8.766895	3.487644	-0.118368
61	1	0	8.888955	0.536703	-0.082264
62	1	0	6.660897	0.405206	-0.134252
63	1	0	5.219472	-2.263757	-0.748130
64	1	0	4.289601	0.583315	-0.111934

65	1	0	2.086393	0.968816	-0.030804
66	1	0	0.042672	-1.314939	-0.473084
67	1	0	-0.202817	1.672948	0.125377
68	1	0	-2.238095	-0.626433	-0.273335
69	1	0	-4.437808	-0.270380	-0.123637
70	1	0	-6.800356	-0.142810	0.013820
71	1	0	-5.395788	2.582390	0.440385
72	1	0	-9.009059	-0.338269	0.109741
73	1	0	-10.622448	2.191731	0.668502
74	1	0	-13.243621	-1.895732	-1.464272
75	1	0	11.783601	0.181358	2.584271
76	1	0	8.533237	-2.885474	-1.794051
77	1	0	3.057374	-3.051871	-0.003838
78	1	0	10.220282	2.470291	-1.398167
79	1	0	-3.179845	3.052453	1.350193
80	1	0	-8.648577	3.185582	1.608943
81	1	0	-13.360186	1.859924	-1.226350
82	1	0	-10.800354	-1.638364	-1.412217
83	1	0	14.457827	-0.270222	-0.145989
84	8	0	14.929029	2.209284	0.897947
85	6	0	-14.050586	-1.179345	0.343764
86	8	0	-15.074924	-2.162415	0.188423
87	1	0	-14.500928	-0.248564	0.733117
88	1	0	-14.266839	-0.491128	-1.680781
89	1	0	12.610936	2.956909	-0.388762
90	1	0	15.490438	1.964531	0.151800
91	1	0	-15.507461	-2.284194	1.041131
92	1	0	13.609133	1.886180	-1.338957
93	1	0	-13.112139	-2.505363	1.872522
94	6	0	-10.680597	-1.332810	2.240005
95	1	0	-11.003162	-2.144089	2.896616
96	1	0	-9.783877	-1.671713	1.713196
97	1	0	-10.367170	-0.491214	2.864828
98	1	0	-12.511366	0.965092	0.809822

LUT radical cation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.774384	-0.975791	1.284008
2	6	0	13.965796	-0.108489	0.500083
3	6	0	13.778241	1.369281	0.807065
4	6	0	12.644183	-0.910821	0.517173
5	6	0	11.495898	-0.121640	-0.164966
6	6	0	11.640593	1.174993	-0.566363
7	6	0	12.881040	1.978709	-0.263261
8	6	0	12.245598	-1.225528	1.977529
9	6	0	12.916575	-2.243363	-0.218491
10	6	0	10.641651	1.942090	-1.394497
11	6	0	10.265508	-0.874201	-0.349798
12	6	0	8.982068	-0.406776	-0.296272
13	6	0	7.803896	-1.202696	-0.463914
14	6	0	6.574752	-0.567787	-0.328621
15	6	0	5.297420	-1.141578	-0.442558
16	6	0	4.127353	-0.413174	-0.290085
17	6	0	2.815631	-0.922661	-0.380770
18	6	0	2.593269	-2.387360	-0.664275
19	6	0	7.931961	-2.671169	-0.773713
20	6	0	1.756276	-0.022601	-0.199706

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21	6	0	0.389406	-0.297213	-0.232565
22	6	0	-0.589243	0.677409	-0.043066
23	6	0	-1.956622	0.398660	-0.062714
24	6	0	-3.016062	1.295437	0.116824
25	6	0	-2.800237	2.768694	0.353232
26	6	0	-4.329395	0.771999	0.077317
27	6	0	-5.498028	1.491144	0.241474
28	6	0	-6.776196	0.892795	0.207799
29	6	0	-8.001348	1.511763	0.369538
30	6	0	-8.150872	2.990658	0.602449
31	6	0	-9.181544	0.679904	0.316957
32	6	0	-10.454890	1.110115	0.465587
33	6	0	-11.717629	0.289548	0.417040
34	6	0	-12.930266	-1.643599	1.238910
35	6	0	-13.478314	-0.895542	-1.058404
36	6	0	-12.204742	0.005688	-1.081035
37	6	0	-12.538308	1.353890	-1.746654
38	6	0	-11.117989	-0.704690	-1.904034
39	1	0	-11.665507	2.011546	-1.798541
40	1	0	-12.888685	1.198762	-2.770551
41	1	0	-10.237306	-0.077925	-2.059389
42	1	0	-11.512335	-0.961398	-2.891171
43	1	0	13.826755	-2.699348	0.179767
44	1	0	12.118206	-2.977508	-0.088092
45	1	0	13.066119	-2.086064	-1.290136
46	1	0	13.023354	-1.818006	2.467539
47	1	0	11.315365	-1.798743	2.022335
48	1	0	11.172639	2.580117	-2.107659
49	1	0	9.958417	1.304419	-1.953501
50	1	0	14.669212	-0.547065	1.213621
51	1	0	13.308137	1.491867	1.786668
52	1	0	10.389051	-1.945021	-0.472767
53	1	0	8.470502	-3.191683	0.023866
54	1	0	6.970828	-3.166417	-0.891319
55	1	0	3.026780	-2.668663	-1.628300
56	1	0	1.540298	-2.657810	-0.693632
57	1	0	-1.750736	3.053194	0.328423
58	1	0	-3.315032	3.365180	-0.405049
59	1	0	-7.200410	3.519743	0.613111
60	1	0	-8.769982	3.445114	-0.176396
61	1	0	8.815517	0.640973	-0.069962
62	1	0	6.602459	0.497375	-0.106055
63	1	0	5.218449	-2.201299	-0.658147
64	1	0	4.226638	0.649675	-0.078604
65	1	0	2.034595	1.012404	-0.008986
66	1	0	0.051333	-1.313872	-0.410367
67	1	0	-0.252166	1.695327	0.130162
68	1	0	-2.232242	-0.640531	-0.232948
69	1	0	-4.422756	-0.298810	-0.092343
70	1	0	-6.793119	-0.182838	0.042249
71	1	0	-5.427671	2.560169	0.409793
72	1	0	-8.999385	-0.376308	0.146932
73	1	0	-10.612541	2.174505	0.617383
74	1	0	-13.253916	-1.871518	-1.495866
75	1	0	12.094834	-0.317378	2.565912
76	1	0	8.496683	-2.828346	-1.696696
77	1	0	3.067103	-3.010821	0.099080
78	1	0	10.043035	2.619926	-0.773553
79	1	0	-3.197217	3.070151	1.326937
80	1	0	-8.647211	3.185853	1.557508
81	1	0	-13.329439	1.884332	-1.207553
82	1	0	-10.803072	-1.638738	-1.429833

83	1	0	14.429421	-0.194585	-0.493153
84	8	0	15.010784	2.068311	0.928863
85	6	0	-14.042395	-1.189153	0.333302
86	8	0	-15.057079	-2.173240	0.158485
87	1	0	-14.493204	-0.267673	0.742744
88	1	0	-14.268004	-0.455555	-1.672893
89	1	0	12.592992	2.997627	0.021785
90	1	0	15.524632	1.931770	0.123054
91	1	0	-15.539558	-2.271999	0.986966
92	1	0	13.460743	2.098207	-1.192529
93	1	0	-13.099160	-2.533048	1.841391
94	6	0	-10.661318	-1.380734	2.213528
95	1	0	-10.994570	-2.184518	2.872672
96	1	0	-9.775618	-1.743903	1.682777
97	1	0	-10.328847	-0.547725	2.840799
98	1	0	-12.498032	0.949032	0.819422

LUT radical anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.773895	-0.966685	1.322595
2	6	0	13.910516	-0.003763	0.753012
3	6	0	13.683938	1.497992	0.810213
4	6	0	12.597675	-0.819815	0.763360
5	6	0	11.531500	-0.193781	-0.170288
6	6	0	11.714080	1.027031	-0.735980
7	6	0	12.891550	1.924429	-0.416387
8	6	0	12.041115	-0.894261	2.203637
9	6	0	12.958283	-2.253907	0.312285
10	6	0	10.800042	1.624327	-1.777741
11	6	0	10.325066	-1.006515	-0.370959
12	6	0	9.038291	-0.549477	-0.365761
13	6	0	7.843140	-1.322016	-0.535062
14	6	0	6.614117	-0.690154	-0.433788
15	6	0	5.316676	-1.233880	-0.536574
16	6	0	4.157095	-0.478785	-0.409194
17	6	0	2.826154	-0.932785	-0.481906
18	6	0	2.569225	-2.400654	-0.735932
19	6	0	7.974066	-2.800773	-0.802840
20	6	0	1.774791	-0.019140	-0.307515
21	6	0	0.399293	-0.249347	-0.313195
22	6	0	-0.575212	0.737087	-0.122480
23	6	0	-1.949317	0.493338	-0.116124
24	6	0	-3.011527	1.388998	0.070469
25	6	0	-2.781061	2.864587	0.299326
26	6	0	-4.335001	0.901349	0.053900
27	6	0	-5.506586	1.620434	0.235857
28	6	0	-6.790761	1.026910	0.208220
29	6	0	-8.032076	1.605308	0.383752
30	6	0	-8.216230	3.077686	0.648026
31	6	0	-9.205443	0.769678	0.321631
32	6	0	-10.495260	1.149779	0.495036
33	6	0	-11.733971	0.278383	0.425160
34	6	0	-12.903707	-1.680748	1.284948
35	6	0	-13.447950	-1.019766	-1.035337
36	6	0	-12.213835	-0.062289	-1.057628
37	6	0	-12.602021	1.259204	-1.745635
38	6	0	-11.094767	-0.730716	-1.872611

39	1	0	-11.761700	1.957620	-1.759352
40	1	0	-12.908982	1.082442	-2.781595
41	1	0	-10.239203	-0.068064	-2.008177
42	1	0	-11.467302	-1.005343	-2.865326
43	1	0	13.808295	-2.623829	0.895602
44	1	0	12.136672	-2.956751	0.459968
45	1	0	13.240381	-2.277775	-0.744434
46	1	0	12.757047	-1.384971	2.872689
47	1	0	11.107736	-1.460214	2.227452
48	1	0	11.396526	2.103393	-2.565583
49	1	0	10.152456	0.880410	-2.240094
50	1	0	14.549123	-0.312492	1.587847
51	1	0	13.129400	1.758887	1.715306
52	1	0	10.475839	-2.077644	-0.465845
53	1	0	8.446798	-3.323697	0.039002
54	1	0	7.011069	-3.278495	-0.980882
55	1	0	3.061655	-2.737037	-1.655553
56	1	0	1.508469	-2.628131	-0.836032
57	1	0	-1.727588	3.137169	0.241585
58	1	0	-3.315039	3.470586	-0.442017
59	1	0	-7.271508	3.620582	0.654520
60	1	0	-8.856832	3.544150	-0.111210
61	1	0	8.882292	0.512550	-0.182259
62	1	0	6.652395	0.383792	-0.240687
63	1	0	5.215557	-2.300479	-0.714809
64	1	0	4.288417	0.588617	-0.223623
65	1	0	2.079358	1.015039	-0.136654
66	1	0	0.037099	-1.264424	-0.468318
67	1	0	-0.217936	1.753567	0.034780
68	1	0	-2.241028	-0.546680	-0.274018
69	1	0	-4.444238	-0.170964	-0.117675
70	1	0	-6.794712	-0.049540	0.024546
71	1	0	-5.432641	2.689119	0.415000
72	1	0	-9.000514	-0.279783	0.115232
73	1	0	-10.694100	2.199180	0.696048
74	1	0	-13.171857	-2.001238	-1.430997
75	1	0	11.826297	0.098112	2.607968
76	1	0	8.602620	-2.993527	-1.680763
77	1	0	2.962228	-3.023247	0.076965
78	1	0	10.155312	2.411244	-1.364996
79	1	0	-3.146907	3.179618	1.284257
80	1	0	-8.703189	3.255214	1.615657
81	1	0	-13.438295	1.747034	-1.232496
82	1	0	-10.745650	-1.648824	-1.390560
83	1	0	14.466853	-0.226587	-0.169945
84	8	0	14.911094	2.227819	0.939418
85	6	0	-14.017596	-1.280545	0.358056
86	8	0	-15.023501	-2.290905	0.221133
87	1	0	-14.492896	-0.354906	0.730474
88	1	0	-14.244615	-0.638356	-1.681876
89	1	0	12.551161	2.960788	-0.292200
90	1	0	15.441943	2.037268	0.156124
91	1	0	-15.399414	-2.449381	1.094465
92	1	0	13.576914	1.952503	-1.282547
93	1	0	-13.046586	-2.566552	1.902068
94	6	0	-10.654781	-1.308649	2.267348
95	1	0	-10.947279	-2.129298	2.927919
96	1	0	-9.743725	-1.608722	1.742813
97	1	0	-10.375382	-0.448515	2.882339
98	1	0	-12.545225	0.912835	0.812158

3dhLUT

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.785101	-0.877960	-1.313774
2	6	0	-13.611445	1.186846	-1.004544
3	6	0	-12.333870	0.341676	-1.188232
4	6	0	-11.572462	0.296352	0.185706
5	6	0	-12.495795	-0.004027	1.370576
6	6	0	-13.826410	0.177991	1.303309
7	6	0	-11.449043	1.011064	-2.251373
8	6	0	-12.718437	-1.069111	-1.676423
9	6	0	-11.847948	-0.458447	2.649305
10	6	0	-10.374388	-0.621987	0.159243
11	6	0	-9.096724	-0.204975	0.185266
12	6	0	-7.904327	-1.041089	0.149874
13	6	0	-6.685762	-0.429994	0.170139
14	6	0	-5.385536	-1.037279	0.146441
15	6	0	-4.231170	-0.317113	0.153015
16	6	0	-2.887681	-0.841793	0.131558
17	6	0	-2.701211	-2.338323	0.113107
18	6	0	-8.086791	-2.535517	0.090404
19	6	0	-1.843499	0.045386	0.125924
20	6	0	-0.443780	-0.235070	0.103329
21	6	0	0.520627	0.730694	0.081652
22	6	0	1.920215	0.450146	0.054887
23	6	0	2.964013	1.336932	0.013648
24	6	0	2.776444	2.833281	-0.009164
25	6	0	4.307351	0.812015	-0.014423
26	6	0	5.460567	1.531241	-0.078808
27	6	0	6.760382	0.923579	-0.107380
28	6	0	7.977402	1.532722	-0.197480
29	6	0	8.153283	3.026262	-0.289483
30	6	0	9.168835	0.693289	-0.209832
31	6	0	10.440366	1.119455	-0.318384
32	6	0	11.704873	0.286027	-0.317281
33	6	0	12.938795	-1.552486	-1.319583
34	6	0	13.450592	-1.046907	1.051493
35	6	0	12.166899	-0.161490	1.141219
36	6	0	12.472880	1.105034	1.961664
37	6	0	11.070455	-0.965757	1.859088
38	1	0	11.593391	1.748091	2.052044
39	1	0	12.793836	0.840667	2.973550
40	1	0	10.179129	-0.366136	2.051242
41	1	0	11.443198	-1.321651	2.824422
42	1	0	-13.324459	-0.999116	-2.584070
43	1	0	-11.834727	-1.662355	-1.922301
44	1	0	-13.301087	-1.622604	-0.936036
45	1	0	-11.979744	1.074132	-3.205900
46	1	0	-10.526280	0.451070	-2.418221
47	1	0	-12.569403	-0.503668	3.466587
48	1	0	-11.389132	-1.445919	2.541217
49	1	0	-13.329957	2.221400	-0.761383
50	1	0	-10.588613	-1.686310	0.109088
51	1	0	-8.651653	-2.827000	-0.801558
52	1	0	-7.142118	-3.076011	0.069246
53	1	0	-3.166558	-2.802422	0.988800
54	1	0	-1.653720	-2.634031	0.105404
55	1	0	1.729591	3.129185	0.027640
56	1	0	3.280668	3.304306	0.840825

57	1	0	7.208082	3.565438	-0.258678
58	1	0	8.772917	3.400349	0.532189
59	1	0	-8.912176	0.868183	0.237445
60	1	0	-6.685984	0.659241	0.207752
61	1	0	-5.325818	-2.120388	0.121631
62	1	0	-4.314453	0.769106	0.174621
63	1	0	-2.104751	1.103289	0.136956
64	1	0	-0.118732	-1.272575	0.100339
65	1	0	0.195512	1.768261	0.081458
66	1	0	2.181633	-0.607665	0.064589
67	1	0	4.391366	-0.273912	0.014707
68	1	0	6.761863	-0.164894	-0.053496
69	1	0	5.399668	2.614099	-0.113125
70	1	0	8.975580	-0.372472	-0.121076
71	1	0	10.609542	2.190128	-0.397163
72	1	0	13.229169	-2.064471	1.384028
73	1	0	-11.174012	2.029678	-1.959360
74	1	0	-8.653399	-2.897417	0.955001
75	1	0	-3.172911	-2.781448	-0.770156
76	1	0	-11.037060	0.219153	2.937586
77	1	0	3.208312	3.268745	-0.916266
78	1	0	8.660292	3.305075	-1.219315
79	1	0	13.276126	1.693019	1.505403
80	1	0	10.777810	-1.846699	1.280127
81	1	0	-14.197214	1.229711	-1.926478
82	6	0	14.034308	-1.192254	-0.354391
83	8	0	15.058359	-2.184724	-0.274283
84	1	0	14.488086	-0.231647	-0.657321
85	1	0	14.228052	-0.666102	1.719865
86	1	0	15.504094	-2.227535	-1.127804
87	1	0	13.116763	-2.379117	-2.004368
88	6	0	10.686135	-1.184067	-2.295434
89	1	0	11.020932	-1.930738	-3.019050
90	1	0	9.786485	-1.575371	-1.811471
91	1	0	10.373056	-0.291439	-2.845135
92	1	0	12.496308	0.979213	-0.635581
93	6	0	-14.514883	0.700495	0.113732
94	8	0	-15.728379	0.783963	0.053559
95	1	0	-14.465664	-0.038474	2.155241
96	1	0	-11.191822	1.315082	0.360574

3dhLUT radical cation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.682317	-1.044850	1.289534
2	6	0	13.562821	0.803335	1.382623
3	6	0	12.267841	-0.030864	1.312803
4	6	0	11.543109	0.321022	-0.041075
5	6	0	12.485179	0.307467	-1.250900
6	6	0	13.814394	0.433503	-1.110114
7	6	0	11.368749	0.350319	2.499602
8	6	0	12.615870	-1.529780	1.407843
9	6	0	11.854859	0.219385	-2.614108
10	6	0	10.336115	-0.546497	-0.271135
11	6	0	9.058650	-0.114211	-0.212074
12	6	0	7.875897	-0.926316	-0.393606
13	6	0	6.647678	-0.302753	-0.291958
14	6	0	5.372504	-0.897678	-0.412053

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15	6	0	4.195080	-0.184269	-0.291303
16	6	0	2.888531	-0.718441	-0.381292
17	6	0	2.693679	-2.192824	-0.627689
18	6	0	8.035109	-2.395345	-0.676241
19	6	0	1.815064	0.168482	-0.232008
20	6	0	0.453116	-0.132036	-0.264690
21	6	0	-0.544891	0.829048	-0.105105
22	6	0	-1.904692	0.520800	-0.119274
23	6	0	-2.984593	1.401060	0.035970
24	6	0	-2.799078	2.884995	0.226757
25	6	0	-4.282708	0.846593	0.017207
26	6	0	-5.469130	1.544379	0.168786
27	6	0	-6.729680	0.915837	0.160531
28	6	0	-7.970332	1.512064	0.315549
29	6	0	-8.149973	2.992757	0.511288
30	6	0	-9.128397	0.652388	0.292108
31	6	0	-10.411291	1.059148	0.439690
32	6	0	-11.656667	0.214868	0.413811
33	6	0	-12.827901	-1.731030	1.260446
34	6	0	-13.425661	-0.990795	-1.031934
35	6	0	-12.147471	-0.096129	-1.079012
36	6	0	-12.476679	1.237780	-1.774323
37	6	0	-11.063237	-0.829494	-1.884901
38	1	0	-11.598415	1.884954	-1.856354
39	1	0	-12.843123	1.059057	-2.788621
40	1	0	-10.177588	-0.211880	-2.049575
41	1	0	-11.456113	-1.101389	-2.868441
42	1	0	13.216892	-1.715620	2.301499
43	1	0	11.719517	-2.149877	1.491745
44	1	0	13.192609	-1.882095	0.549580
45	1	0	11.881612	0.150985	3.444313
46	1	0	10.437187	-0.221357	2.504739
47	1	0	12.595595	0.350905	-3.403447
48	1	0	11.359598	-0.744276	-2.773410
49	1	0	13.308122	1.871810	1.418742
50	1	0	10.535018	-1.593107	-0.484594
51	1	0	8.586046	-2.888300	0.129971
52	1	0	7.086487	-2.915178	-0.790018
53	1	0	3.143626	-2.491442	-1.578834
54	1	0	1.646168	-2.482958	-0.661510
55	1	0	-1.756515	3.191333	0.181274
56	1	0	-3.334334	3.447444	-0.543092
57	1	0	-7.211655	3.542756	0.496601
58	1	0	-8.787764	3.412674	-0.271675
59	1	0	8.884410	0.939688	-0.002000
60	1	0	6.658320	0.766699	-0.090021
61	1	0	5.312710	-1.963365	-0.603001
62	1	0	4.274772	0.884913	-0.105689
63	1	0	2.074323	1.212704	-0.067394
64	1	0	0.134781	-1.159203	-0.416338
65	1	0	-0.228682	1.857661	0.041334
66	1	0	-2.158634	-0.528183	-0.260128
67	1	0	-4.352971	-0.230381	-0.120886
68	1	0	-6.723505	-0.163894	0.024305
69	1	0	-5.422048	2.618904	0.306621
70	1	0	-8.924345	-0.403054	0.145967
71	1	0	-10.589164	2.123402	0.567699
72	1	0	-13.217282	-1.963227	-1.484706
73	1	0	11.111610	1.414027	2.483870
74	1	0	8.607475	-2.553403	-1.595066
75	1	0	3.170195	-2.786819	0.157147
76	1	0	11.081448	0.985615	-2.738370

77	1	0	-3.191673	3.206714	1.195710
78	1	0	-8.639149	3.201933	1.466991
79	1	0	-13.255187	1.789865	-1.238624
80	1	0	-10.756904	-1.756762	-1.392459
81	1	0	14.125042	0.583295	2.293285
82	6	0	-13.959766	-1.295997	0.369932
83	8	0	-14.960037	-2.296701	0.210114
84	1	0	-14.419371	-0.382552	0.787301
85	1	0	-14.228253	-0.541083	-1.621969
86	1	0	-15.439152	-2.393548	1.040753
87	1	0	-12.976022	-2.619854	1.869081
88	6	0	-10.551542	-1.429018	2.206584
89	1	0	-10.866510	-2.230683	2.877048
90	1	0	-9.669582	-1.788001	1.666530
91	1	0	-10.219717	-0.587398	2.822698
92	1	0	-12.446957	0.864012	0.813602
93	6	0	14.484045	0.605847	0.191744
94	8	0	15.694528	0.634223	0.292148
95	1	0	14.470702	0.433286	-1.975939
96	1	0	11.186721	1.357569	0.057582

3dhLUT radical anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.790474	-0.883348	-1.267720
2	6	0	-13.602074	1.163140	-1.051504
3	6	0	-12.390034	0.217744	-1.182298
4	6	0	-11.550258	0.291248	0.143807
5	6	0	-12.428525	0.208119	1.395585
6	6	0	-13.751078	0.465243	1.370451
7	6	0	-11.526074	0.679817	-2.365419
8	6	0	-12.886597	-1.214239	-1.461513
9	6	0	-11.744729	-0.132275	2.690102
10	6	0	-10.394007	-0.679297	0.180148
11	6	0	-9.090872	-0.305463	0.135269
12	6	0	-7.925532	-1.147928	0.159762
13	6	0	-6.674378	-0.561584	0.114088
14	6	0	-5.396066	-1.162214	0.129133
15	6	0	-4.214638	-0.433703	0.083257
16	6	0	-2.895894	-0.928755	0.094275
17	6	0	-2.678823	-2.422644	0.160644
18	6	0	-8.127836	-2.639517	0.236812
19	6	0	-1.823056	-0.025684	0.043275
20	6	0	-0.451763	-0.280290	0.045311
21	6	0	0.537298	0.708409	-0.015398
22	6	0	1.909447	0.455366	-0.015599
23	6	0	2.979082	1.359645	-0.082516
24	6	0	2.758472	2.851935	-0.167864
25	6	0	4.300938	0.867621	-0.077624
26	6	0	5.476587	1.598873	-0.158039
27	6	0	6.761012	1.005698	-0.148442
28	6	0	8.004118	1.598974	-0.244919
29	6	0	8.188461	3.087640	-0.391180
30	6	0	9.179775	0.764658	-0.215327
31	6	0	10.470731	1.162073	-0.332155
32	6	0	11.714950	0.297068	-0.288807
33	6	0	12.925787	-1.589436	-1.248936
34	6	0	13.402010	-1.085042	1.124801

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35	6	0	12.159625	-0.139790	1.179524
36	6	0	12.519044	1.134721	1.964747
37	6	0	11.026625	-0.870722	1.918185
38	1	0	11.673387	1.825710	2.001733
39	1	0	12.799624	0.890885	2.994570
40	1	0	10.162095	-0.225373	2.078470
41	1	0	11.377712	-1.211354	2.898173
42	1	0	-13.524300	-1.225406	-2.351030
43	1	0	-12.050366	-1.891352	-1.646998
44	1	0	-13.471705	-1.620339	-0.632305
45	1	0	-12.096767	0.639203	-3.298922
46	1	0	-10.642234	0.049225	-2.477935
47	1	0	-12.416906	-0.007603	3.541674
48	1	0	-11.371623	-1.160224	2.685542
49	1	0	-13.242444	2.198396	-0.957871
50	1	0	-10.648863	-1.733582	0.252977
51	1	0	-8.721423	-3.008564	-0.609691
52	1	0	-7.186205	-3.187948	0.236996
53	1	0	-3.119118	-2.850832	1.069145
54	1	0	-1.623369	-2.693378	0.153170
55	1	0	1.703578	3.122261	-0.130695
56	1	0	3.258288	3.376343	0.655098
57	1	0	7.242014	3.627422	-0.381475
58	1	0	8.807755	3.496635	0.417218
59	1	0	-8.885583	0.765444	0.071500
60	1	0	-6.668589	0.529233	0.060807
61	1	0	-5.331775	-2.245270	0.180445
62	1	0	-4.315128	0.651994	0.033893
63	1	0	-2.104783	1.027857	-0.005569
64	1	0	-0.106864	-1.311969	0.095263
65	1	0	0.191659	1.739643	-0.068725
66	1	0	2.193038	-0.597309	0.040125
67	1	0	4.405209	-0.216529	-0.007623
68	1	0	6.763956	-0.082378	-0.055898
69	1	0	5.405734	2.679660	-0.238214
70	1	0	8.976088	-0.297208	-0.086469
71	1	0	10.665864	2.223948	-0.456572
72	1	0	13.123453	-2.093357	1.443886
73	1	0	-11.183767	1.711127	-2.230473
74	1	0	-8.672914	-2.926079	1.145750
75	1	0	-3.151723	-2.932511	-0.687192
76	1	0	-10.862503	0.498713	2.838743
77	1	0	3.168526	3.264744	-1.097598
78	1	0	8.698900	3.338717	-1.329975
79	1	0	13.365139	1.659840	1.507731
80	1	0	10.697474	-1.755482	1.365055
81	1	0	-14.237556	1.131622	-1.941377
82	6	0	14.011214	-1.246765	-0.266810
83	8	0	15.019927	-2.259181	-0.170633
84	1	0	14.490705	-0.296065	-0.562766
85	1	0	14.177771	-0.743927	1.817596
86	1	0	15.423602	-2.353371	-1.040885
87	1	0	13.092985	-2.430040	-1.920704
88	6	0	10.699185	-1.170150	-2.262383
89	1	0	11.017398	-1.941254	-2.969096
90	1	0	9.778616	-1.514422	-1.783425
91	1	0	10.425361	-0.273108	-2.824938
92	1	0	12.529430	0.963310	-0.610023
93	6	0	-14.469567	0.888087	0.163759
94	8	0	-15.678635	1.058527	0.151338
95	1	0	-14.354539	0.393123	2.272222
96	1	0	-11.112842	1.303033	0.170111

3hCAR

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.700869	2.369736	-0.758050
2	6	0	-11.490641	2.102598	0.701332
3	6	0	-11.594560	0.902912	1.278266
4	6	0	-11.867159	-0.362238	0.475952
5	6	0	-12.547359	-0.048458	-0.907054
6	6	0	-11.746969	1.081838	-1.583275
7	1	0	-10.714573	0.752695	-1.736171
8	6	0	-14.010741	0.372779	-0.665247
9	6	0	-12.554769	-1.282959	-1.822613
10	6	0	-11.438107	0.720619	2.765504
11	6	0	-10.624886	-1.227760	0.347306
12	6	0	-9.353178	-0.791416	0.368050
13	6	0	-8.155917	-1.612004	0.237097
14	6	0	-8.322930	-3.100247	0.068709
15	6	0	-6.942639	-0.990576	0.274538
16	6	0	-5.638471	-1.581141	0.173756
17	6	0	-4.488969	-0.854716	0.221090
18	6	0	-3.142826	-1.366095	0.135201
19	6	0	-2.948107	-2.853422	-0.023598
20	6	0	-2.102681	-0.476535	0.203191
21	6	0	-0.702256	-0.748026	0.145199
22	6	0	0.260860	0.216035	0.225057
23	6	0	1.660498	-0.060646	0.171007
24	6	0	2.705531	0.822558	0.244210
25	6	0	2.520722	2.311291	0.400193
26	6	0	4.048023	0.300606	0.170380
27	6	0	5.204461	1.014940	0.233435
28	6	0	6.501894	0.407084	0.149916
29	6	0	7.724067	1.008296	0.209783
30	6	0	7.915483	2.492377	0.387275
31	6	0	8.910409	0.170388	0.099523
32	6	0	10.191978	0.573810	0.143180
33	6	0	11.378173	-0.350317	0.009037
34	6	0	12.273812	-0.325428	1.251572
35	6	0	13.598319	-0.547152	1.178362
36	6	0	14.303656	-0.847416	-0.076723
37	6	0	13.421352	-1.038903	-1.297799
38	6	0	12.180573	-0.123494	-1.323065
39	6	0	11.307003	-0.507503	-2.527658
40	6	0	12.627244	1.343362	-1.479750
41	6	0	11.605287	-0.105508	2.580198
42	1	0	-11.167638	1.655212	3.261186
43	1	0	-12.371464	0.359351	3.214196
44	1	0	-12.163794	1.291437	-2.576996
45	1	0	-14.593545	-0.467722	-0.275409
46	1	0	-14.483437	0.691107	-1.599951
47	1	0	-14.097721	1.192217	0.050758
48	1	0	-11.545484	-1.586942	-2.107882
49	1	0	-13.109400	-1.070662	-2.741793
50	1	0	-13.040566	-2.136952	-1.338598
51	1	0	-10.817962	-2.289601	0.220736
52	1	0	-9.178686	0.274941	0.498268
53	1	0	-7.373246	-3.626991	-0.007580
54	1	0	-8.871946	-3.531066	0.912641

55	1	0	-8.899912	-3.331469	-0.833105
56	1	0	-6.952860	0.092011	0.396722
57	1	0	-5.571005	-2.657983	0.057738
58	1	0	-4.578965	0.224816	0.337049
59	1	0	-1.899199	-3.140696	-0.067799
60	1	0	-3.402604	-3.398916	0.809758
61	1	0	-3.426508	-3.215385	-0.939533
62	1	0	-2.368128	0.573951	0.318381
63	1	0	-0.374821	-1.778814	0.033686
64	1	0	-0.064507	1.247214	0.338068
65	1	0	1.921032	-1.112856	0.059090
66	1	0	2.986818	2.853235	-0.429212
67	1	0	1.473416	2.605912	0.433578
68	1	0	2.992626	2.671013	1.320492
69	1	0	4.129198	-0.779753	0.053819
70	1	0	5.148578	2.091963	0.352938
71	1	0	6.496324	-0.675517	0.024004
72	1	0	8.485902	2.917735	-0.445246
73	1	0	6.973801	3.035048	0.449036
74	1	0	8.480138	2.710078	1.300317
75	1	0	10.417421	1.628092	0.281048
76	1	0	11.868315	-0.392216	-3.459572
77	1	0	10.977799	-1.549758	-2.467598
78	1	0	10.415756	0.120241	-2.593845
79	1	0	11.771405	2.011311	-1.601749
80	1	0	13.251870	1.451974	-2.370874
81	1	0	13.211207	1.695675	-0.626064
82	1	0	13.097206	-2.089345	-1.297169
83	1	0	14.036202	-0.901065	-2.191016
84	1	0	8.717162	-0.894411	-0.032967
85	1	0	12.307020	-0.237178	3.405187
86	1	0	10.771723	-0.802698	2.716984
87	1	0	11.172140	0.896852	2.652817
88	1	0	-10.670132	-0.023785	2.996865
89	8	0	-10.638461	3.236106	-1.187134
90	1	0	-11.275637	2.983589	1.302497
91	1	0	14.218906	-0.532956	2.070496
92	1	0	-12.594003	-0.960369	1.046035
93	8	0	15.513483	-0.979980	-0.121541
94	1	0	10.978230	-1.375333	-0.044364
95	1	0	-10.830812	3.514859	-2.090050
96	1	0	-12.653688	2.913267	-0.871352

3hCAR radical cation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.507300	2.408514	0.863689
2	6	0	11.381911	2.157281	-0.608991
3	6	0	11.561979	0.975208	-1.202043
4	6	0	11.838302	-0.290493	-0.401966
5	6	0	12.465916	0.022282	1.012218
6	6	0	11.605953	1.114174	1.678295
7	1	0	10.586413	0.742049	1.820477
8	6	0	13.918750	0.496734	0.815236
9	6	0	12.489814	-1.227619	1.907009
10	6	0	11.502705	0.811041	-2.698302
11	6	0	10.617710	-1.175342	-0.302643
12	6	0	9.332894	-0.757345	-0.370368

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13	6	0	8.167235	-1.598220	-0.249886
14	6	0	8.339567	-3.079132	-0.049362
15	6	0	6.928209	-0.983527	-0.325825
16	6	0	5.663594	-1.594488	-0.222070
17	6	0	4.477301	-0.886132	-0.317173
18	6	0	3.178125	-1.427744	-0.212068
19	6	0	2.992408	-2.903506	0.034880
20	6	0	2.097145	-0.544588	-0.342991
21	6	0	0.737999	-0.845059	-0.261286
22	6	0	-0.263585	0.113032	-0.415730
23	6	0	-1.623738	-0.184412	-0.324283
24	6	0	-2.702418	0.695989	-0.472225
25	6	0	-2.517463	2.160068	-0.779694
26	6	0	-4.004961	0.164078	-0.324872
27	6	0	-5.187259	0.869295	-0.442503
28	6	0	-6.457096	0.274350	-0.271811
29	6	0	-7.690095	0.887932	-0.371047
30	6	0	-7.863019	2.345652	-0.700180
31	6	0	-8.865289	0.075967	-0.143324
32	6	0	-10.145876	0.498986	-0.197566
33	6	0	-11.344983	-0.368500	0.070904
34	6	0	-12.300716	-0.391308	-1.128158
35	6	0	-13.628204	-0.514708	-0.969743
36	6	0	-14.283356	-0.652484	0.343353
37	6	0	-13.348759	-0.819952	1.528076
38	6	0	-12.055952	0.014314	1.423621
39	6	0	-11.143218	-0.336746	2.609295
40	6	0	-12.405641	1.514596	1.486897
41	6	0	-11.685643	-0.341851	-2.500322
42	1	0	11.229412	1.743012	-3.196221
43	1	0	12.474143	0.492527	-3.093984
44	1	0	11.999843	1.333231	2.678134
45	1	0	14.541173	-0.312768	0.422528
46	1	0	14.352570	0.806897	1.770421
47	1	0	13.997018	1.337243	0.123665
48	1	0	11.485353	-1.562592	2.178434
49	1	0	13.023506	-1.015506	2.837337
50	1	0	13.006892	-2.061225	1.420527
51	1	0	10.821470	-2.231208	-0.148591
52	1	0	9.148324	0.303228	-0.521788
53	1	0	7.395885	-3.616880	0.010537
54	1	0	8.914461	-3.515678	-0.871010
55	1	0	8.894463	-3.284429	0.870792
56	1	0	6.929961	0.093860	-0.477986
57	1	0	5.612992	-2.665287	-0.058659
58	1	0	4.549618	0.186167	-0.486393
59	1	0	1.946441	-3.198879	0.072045
60	1	0	3.466964	-3.494194	-0.753575
61	1	0	3.449060	-3.201197	0.983054
62	1	0	2.349848	0.497682	-0.528662
63	1	0	0.425029	-1.866790	-0.067605
64	1	0	0.049700	1.133411	-0.615861
65	1	0	-1.876473	-1.221828	-0.112910
66	1	0	-2.980911	2.783229	-0.009887
67	1	0	-1.471673	2.451120	-0.844739
68	1	0	-2.986395	2.420033	-1.733142
69	1	0	-4.076404	-0.897475	-0.096834
70	1	0	-5.136526	1.927152	-0.675107
71	1	0	-6.457961	-0.787255	-0.031633
72	1	0	-8.407256	2.861492	0.096197
73	1	0	-6.919442	2.867584	-0.842837
74	1	0	-8.447825	2.469281	-1.616510

75	1	0	-10.353826	1.537567	-0.439687
76	1	0	-11.645418	-0.113913	3.554497
77	1	0	-10.885641	-1.400429	2.617365
78	1	0	-10.211876	0.234989	2.589506
79	1	0	-11.509541	2.137740	1.546984
80	1	0	-12.997553	1.720453	2.382266
81	1	0	-12.991968	1.846152	0.626805
82	1	0	-13.091449	-1.886775	1.586741
83	1	0	-13.901153	-0.579133	2.439504
84	1	0	-8.681530	-0.969966	0.096422
85	1	0	-12.435257	-0.495662	-3.277182
86	1	0	-10.913721	-1.111634	-2.611268
87	1	0	-11.192116	0.616579	-2.692686
88	1	0	10.779337	0.043194	-2.992893
89	8	0	10.366042	3.186201	1.254563
90	1	0	11.170373	3.041168	-1.206450
91	1	0	-14.293706	-0.539153	-1.828175
92	1	0	12.591405	-0.878748	-0.945860
93	8	0	-15.492706	-0.677754	0.458072
94	1	0	-10.981913	-1.400344	0.191944
95	1	0	10.530823	3.541488	2.135711
96	1	0	12.413098	3.014803	1.022896

3hCAR radical anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.701100	2.397829	-0.658483
2	6	0	-11.462663	2.091530	0.788675
3	6	0	-11.565727	0.876075	1.333508
4	6	0	-11.871334	-0.367624	0.508772
5	6	0	-12.565083	-0.003791	-0.855950
6	6	0	-11.754025	1.130283	-1.511828
7	1	0	-10.725660	0.789936	-1.666721
8	6	0	-14.019927	0.433844	-0.590142
9	6	0	-12.599545	-1.213172	-1.802470
10	6	0	-11.363265	0.655105	2.810042
11	6	0	-10.649489	-1.261869	0.364285
12	6	0	-9.358903	-0.850575	0.346259
13	6	0	-8.182842	-1.675338	0.211007
14	6	0	-8.367426	-3.164942	0.070654
15	6	0	-6.941238	-1.073472	0.219487
16	6	0	-5.656469	-1.659893	0.118744
17	6	0	-4.481655	-0.924547	0.142162
18	6	0	-3.159496	-1.411658	0.064560
19	6	0	-2.939251	-2.901413	-0.058223
20	6	0	-2.090231	-0.505953	0.106626
21	6	0	-0.718082	-0.755979	0.057775
22	6	0	0.271178	0.232958	0.112506
23	6	0	1.642273	-0.019265	0.073422
24	6	0	2.715347	0.883999	0.125991
25	6	0	2.497495	2.375393	0.234355
26	6	0	4.033961	0.391608	0.081893
27	6	0	5.215734	1.120169	0.133958
28	6	0	6.494000	0.522298	0.085746
29	6	0	7.745692	1.107857	0.140814
30	6	0	7.947355	2.595909	0.271254
31	6	0	8.910980	0.268176	0.077167
32	6	0	10.214729	0.640243	0.130321

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33	6	0	11.370258	-0.328811	0.053408
34	6	0	12.244129	-0.304763	1.310822
35	6	0	13.567010	-0.560041	1.278508
36	6	0	14.289787	-0.927163	0.056263
37	6	0	13.426299	-1.146204	-1.173285
38	6	0	12.215356	-0.195358	-1.264722
39	6	0	11.355004	-0.602470	-2.470650
40	6	0	12.712433	1.247859	-1.476649
41	6	0	11.554917	-0.027407	2.617411
42	1	0	-11.074857	1.576475	3.321352
43	1	0	-12.282371	0.281341	3.278854
44	1	0	-12.167672	1.365659	-2.502453
45	1	0	-14.610731	-0.409779	-0.218056
46	1	0	-14.499260	0.787102	-1.509803
47	1	0	-14.086343	1.232029	0.152024
48	1	0	-11.594865	-1.533803	-2.082851
49	1	0	-13.146060	-0.965901	-2.719177
50	1	0	-13.105471	-2.066988	-1.338335
51	1	0	-10.868062	-2.322030	0.266472
52	1	0	-9.167698	0.216817	0.455216
53	1	0	-7.420048	-3.696308	-0.015250
54	1	0	-8.902672	-3.585662	0.931650
55	1	0	-8.963965	-3.414324	-0.816428
56	1	0	-6.945195	0.013418	0.320826
57	1	0	-5.585769	-2.739556	0.023939
58	1	0	-4.585856	0.157837	0.234288
59	1	0	-1.883195	-3.166728	-0.097618
60	1	0	-3.379847	-3.441332	0.788459
61	1	0	-3.410145	-3.301502	-0.964246
62	1	0	-2.373494	0.544672	0.193283
63	1	0	-0.372743	-1.785369	-0.024762
64	1	0	-0.073557	1.262644	0.194296
65	1	0	1.923998	-1.070967	-0.005812
66	1	0	2.967243	2.908608	-0.600686
67	1	0	1.441795	2.645282	0.237480
68	1	0	2.940446	2.779044	1.152873
69	1	0	4.134942	-0.692181	0.001043
70	1	0	5.150863	2.201026	0.219837
71	1	0	6.488674	-0.566129	-0.004520
72	1	0	8.537244	2.996337	-0.563515
73	1	0	7.005278	3.143100	0.295311
74	1	0	8.495880	2.849982	1.187880
75	1	0	10.470179	1.690622	0.245143
76	1	0	11.929232	-0.521581	-3.399416
77	1	0	11.010238	-1.638043	-2.383045
78	1	0	10.472600	0.034093	-2.558076
79	1	0	11.876227	1.931982	-1.634319
80	1	0	13.353610	1.300154	-2.362205
81	1	0	13.293738	1.616480	-0.627568
82	1	0	13.065571	-2.184270	-1.127830
83	1	0	14.064596	-1.074654	-2.058802
84	1	0	8.705721	-0.799624	-0.027128
85	1	0	12.225294	-0.187535	3.464497
86	1	0	10.676010	-0.669783	2.733855
87	1	0	11.175378	0.997272	2.658521
88	1	0	-10.588969	-0.095648	2.990405
89	8	0	-10.655021	3.286512	-1.085331
90	1	0	-11.217541	2.952660	1.407526
91	1	0	14.167242	-0.529633	2.184848
92	1	0	-12.612860	-0.951359	1.077011
93	8	0	15.498918	-1.097329	0.040146
94	1	0	10.931543	-1.340210	0.031517

95	1	0	-10.806659	3.489016	-2.016014
96	1	0	-12.660271	2.937285	-0.746250

33CAR

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.762243	0.709370	1.418180
2	6	0	-13.477403	-1.113672	0.925263
3	6	0	-12.190387	-0.290352	1.138883
4	6	0	-11.402274	-0.249824	-0.220146
5	6	0	-12.297420	0.078620	-1.419112
6	6	0	-13.631566	-0.083972	-1.379238
7	6	0	-11.337468	-0.980187	2.215111
8	6	0	-12.561587	1.123678	1.628049
9	6	0	-11.617711	0.536671	-2.679828
10	6	0	-10.187250	0.644265	-0.162150
11	6	0	-8.917593	0.202958	-0.170384
12	6	0	-7.711050	1.016288	-0.098249
13	6	0	-6.503289	0.383881	-0.111857
14	6	0	-5.194053	0.968582	-0.050186
15	6	0	-4.050251	0.232057	-0.066355
16	6	0	-2.700508	0.737831	-0.006777
17	6	0	-2.496323	2.229470	0.083658
18	6	0	-7.867956	2.512253	-0.009907
19	6	0	-1.666818	-0.161187	-0.035759
20	6	0	-0.264825	0.103781	0.014850
21	6	0	0.692784	-0.868048	-0.025885
22	6	0	2.093297	-0.595990	0.029901
23	6	0	3.135246	-1.484926	-0.009744
24	6	0	2.946708	-2.976305	-0.130445
25	6	0	4.478257	-0.964976	0.069353
26	6	0	5.633968	-1.682561	0.038325
27	6	0	6.929796	-1.073292	0.133068
28	6	0	8.153855	-1.673935	0.097844
29	6	0	8.349582	-3.158972	-0.064443
30	6	0	9.335226	-0.831899	0.223037
31	6	0	10.617652	-1.235408	0.194907
32	6	0	11.834050	-0.334675	0.302513
33	6	0	12.382133	1.899013	1.313207
34	6	0	13.478528	1.191242	-0.850152
35	6	0	12.266537	0.268158	-1.088261
36	6	0	12.681979	-0.868510	-2.036109
37	6	0	11.140679	1.080982	-1.754074
38	1	0	11.841328	-1.528509	-2.264863
39	1	0	13.047228	-0.462782	-2.983945
40	1	0	10.286009	0.451338	-2.005007
41	1	0	11.508057	1.527352	-2.682631
42	1	0	-13.182954	1.058215	2.525568
43	1	0	-11.673158	1.702337	1.891052
44	1	0	-13.124052	1.689344	0.881329
45	1	0	-11.889489	-1.043485	3.157473
46	1	0	-10.410981	-0.434480	2.406835
47	1	0	-12.324508	0.614798	-3.507328
48	1	0	-11.133712	1.509109	-2.547797
49	1	0	-13.207843	-2.151615	0.683052
50	1	0	-10.381685	1.711766	-0.101602
51	1	0	-8.446811	2.794761	0.875867
52	1	0	-6.914728	3.035197	0.042685

53	1	0	-2.937912	2.738106	-0.779540
54	1	0	-1.445870	2.511267	0.124743
55	1	0	1.898977	-3.267347	-0.179085
56	1	0	3.436126	-3.361562	-1.030931
57	1	0	7.409459	-3.702402	-0.141206
58	1	0	8.932099	-3.382497	-0.964646
59	1	0	-8.752234	-0.872616	-0.234620
60	1	0	-6.521514	-0.703926	-0.175687
61	1	0	-5.118389	2.049137	0.012232
62	1	0	-4.147744	-0.851306	-0.129521
63	1	0	-1.939061	-1.213987	-0.105517
64	1	0	0.068429	1.135830	0.090565
65	1	0	0.362729	-1.901039	-0.103650
66	1	0	2.357243	0.457710	0.115739
67	1	0	4.560560	0.117311	0.164228
68	1	0	6.921561	0.010555	0.246661
69	1	0	5.578706	-2.761818	-0.059696
70	1	0	9.130584	0.229682	0.353743
71	1	0	10.833415	-2.290277	0.051840
72	1	0	13.818803	1.651385	-1.781299
73	1	0	-11.070109	-2.000186	1.920866
74	1	0	-8.409200	2.902721	-0.878292
75	1	0	-2.980817	2.638293	0.976295
76	1	0	-10.821096	-0.158250	-2.966995
77	1	0	3.392973	-3.498082	0.722436
78	1	0	8.904386	-3.577052	0.782118
79	1	0	13.484098	-1.477543	-1.606944
80	1	0	10.783740	1.896609	-1.120607
81	1	0	-14.082447	-1.151233	1.834899
82	6	0	13.205854	2.291918	0.159130
83	8	0	13.687169	3.405713	0.056880
84	1	0	14.319408	0.598963	-0.461554
85	1	0	12.340268	2.623703	2.122099
86	6	0	11.081044	0.324448	2.705139
87	1	0	11.293205	1.050330	3.491709
88	1	0	9.997768	0.240890	2.597216
89	1	0	11.425773	-0.659391	3.042865
90	1	0	12.666596	-0.992021	0.600516
91	6	0	-14.350731	-0.608017	-0.208583
92	8	0	-15.566089	-0.677250	-0.174564
93	1	0	-14.250924	0.151039	-2.240865
94	1	0	-11.038629	-1.274598	-0.395997

33CAR radical cation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.724040	0.720593	1.427572
2	6	0	-13.443455	-1.116749	0.903241
3	6	0	-12.140896	-0.321900	1.125993
4	6	0	-11.372936	-0.265322	-0.249492
5	6	0	-12.273852	0.122036	-1.428667
6	6	0	-13.607886	-0.017382	-1.371824
7	6	0	-11.286214	-1.056665	2.170774
8	6	0	-12.480197	1.086149	1.653901
9	6	0	-11.596896	0.599276	-2.684691
10	6	0	-10.155659	0.614002	-0.175213
11	6	0	-8.882289	0.164306	-0.186350
12	6	0	-7.693106	0.980740	-0.092588

13	6	0	-6.469790	0.337790	-0.114067
14	6	0	-5.191319	0.929964	-0.034329
15	6	0	-4.018915	0.197324	-0.062637
16	6	0	-2.710096	0.726069	0.014019
17	6	0	-2.505111	2.214062	0.141578
18	6	0	-7.839059	2.473253	0.024474
19	6	0	-1.642401	-0.179821	-0.035430
20	6	0	-0.279454	0.109766	0.026465
21	6	0	0.712686	-0.868563	-0.036439
22	6	0	2.074064	-0.573267	0.031440
23	6	0	3.149047	-1.470322	-0.025976
24	6	0	2.957425	-2.956908	-0.185282
25	6	0	4.451294	-0.931022	0.073520
26	6	0	5.634255	-1.647191	0.033502
27	6	0	6.900126	-1.035809	0.149446
28	6	0	8.138674	-1.650315	0.109027
29	6	0	8.318599	-3.131631	-0.080616
30	6	0	9.304008	-0.810433	0.256184
31	6	0	10.589958	-1.223495	0.208308
32	6	0	11.806920	-0.337424	0.325166
33	6	0	12.323972	1.915774	1.297912
34	6	0	13.436740	1.184254	-0.850830
35	6	0	12.239422	0.241103	-1.083823
36	6	0	12.678338	-0.909877	-2.003820
37	6	0	11.109404	1.029818	-1.771417
38	1	0	11.850201	-1.584954	-2.237618
39	1	0	13.051077	-0.516688	-2.953190
40	1	0	10.268057	0.387495	-2.037500
41	1	0	11.485101	1.475185	-2.696217
42	1	0	-13.106554	1.007692	2.545993
43	1	0	-11.581864	1.638245	1.942229
44	1	0	-13.027562	1.686656	0.923797
45	1	0	-11.830463	-1.139804	3.115244
46	1	0	-10.350693	-0.530211	2.376458
47	1	0	-12.312226	0.725745	-3.497878
48	1	0	-11.084265	1.555389	-2.534859
49	1	0	-13.197701	-2.151436	0.626423
50	1	0	-10.341843	1.681331	-0.094257
51	1	0	-8.416731	2.737490	0.915033
52	1	0	-6.886206	2.994031	0.086883
53	1	0	-2.932104	2.741214	-0.716329
54	1	0	-1.456365	2.494983	0.202751
55	1	0	1.911129	-3.244592	-0.257598
56	1	0	3.456617	-3.320298	-1.087905
57	1	0	7.376976	-3.669254	-0.166847
58	1	0	8.898217	-3.339363	-0.984952
59	1	0	-8.718962	-0.908574	-0.270776
60	1	0	-6.489827	-0.746960	-0.200227
61	1	0	-5.122906	2.008575	0.052793
62	1	0	-4.106393	-0.883536	-0.151724
63	1	0	-1.908329	-1.230670	-0.133541
64	1	0	0.045048	1.141104	0.128461
65	1	0	0.391076	-1.900478	-0.141990
66	1	0	2.333008	0.477983	0.143076
67	1	0	4.525915	0.147857	0.193063
68	1	0	6.897057	0.044225	0.283672
69	1	0	5.583542	-2.723198	-0.090958
70	1	0	9.106366	0.247425	0.412019
71	1	0	10.794095	-2.275310	0.030958
72	1	0	13.777453	1.625318	-1.790459
73	1	0	-11.037704	-2.071620	1.845375
74	1	0	-8.378748	2.878514	-0.836386

75	1	0	-2.997562	2.600998	1.037984
76	1	0	-10.829955	-0.112367	-3.010698
77	1	0	3.385617	-3.498799	0.662740
78	1	0	8.870697	-3.565773	0.757760
79	1	0	13.482336	-1.501180	-1.555452
80	1	0	10.730892	1.845552	-1.150929
81	1	0	-14.034685	-1.169041	1.820608
82	6	0	13.130540	2.305119	0.125933
83	8	0	13.566693	3.430872	-0.009094
84	1	0	14.281674	0.614730	-0.439806
85	1	0	12.282623	2.650023	2.097719
86	6	0	11.070911	0.334211	2.729784
87	1	0	11.273171	1.076846	3.502282
88	1	0	9.987560	0.220013	2.646095
89	1	0	11.453060	-0.631454	3.080312
90	1	0	12.632364	-0.999252	0.628114
91	6	0	-14.322420	-0.557226	-0.200977
92	8	0	-15.535681	-0.593014	-0.149849
93	1	0	-14.234540	0.251212	-2.217738
94	1	0	-11.025661	-1.289609	-0.453103

33CAR radical anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.726243	0.720526	1.437817
2	6	0	-13.428877	-1.204948	0.986604
3	6	0	-12.175354	-0.326684	1.182653
4	6	0	-11.395955	-0.249383	-0.179762
5	6	0	-12.321939	0.017365	-1.370049
6	6	0	-13.651259	-0.195204	-1.316053
7	6	0	-11.281619	-0.973175	2.251928
8	6	0	-12.601723	1.070943	1.672734
9	6	0	-11.678850	0.490335	-2.643774
10	6	0	-10.217292	0.693988	-0.144162
11	6	0	-8.922126	0.294480	-0.174917
12	6	0	-7.742547	1.118093	-0.133033
13	6	0	-6.501153	0.512119	-0.156865
14	6	0	-5.214715	1.096360	-0.121729
15	6	0	-4.041774	0.355051	-0.139703
16	6	0	-2.718424	0.839167	-0.103929
17	6	0	-2.490703	2.331714	-0.044124
18	6	0	-7.922483	2.612604	-0.056552
19	6	0	-1.652879	-0.072675	-0.121945
20	6	0	-0.280203	0.173775	-0.087548
21	6	0	0.704963	-0.820102	-0.105727
22	6	0	2.076736	-0.570371	-0.062966
23	6	0	3.146335	-1.477823	-0.072737
24	6	0	2.925936	-2.970904	-0.145735
25	6	0	4.465736	-0.987333	-0.008205
26	6	0	5.644403	-1.720649	-0.003005
27	6	0	6.923014	-1.125715	0.079238
28	6	0	8.171805	-1.719272	0.094125
29	6	0	8.369328	-3.210844	0.005651
30	6	0	9.338010	-0.884387	0.202591
31	6	0	10.637162	-1.274130	0.240697
32	6	0	11.835286	-0.348692	0.349705
33	6	0	12.345728	1.913393	1.333663
34	6	0	13.511498	1.170468	-0.778719

35	6	0	12.310908	0.236930	-1.033171
36	6	0	12.758808	-0.914262	-1.947509
37	6	0	11.198264	1.027013	-1.745567
38	1	0	11.929261	-1.590972	-2.164629
39	1	0	13.133512	-0.527366	-2.900531
40	1	0	10.349099	0.385414	-1.982752
41	1	0	11.579599	1.443865	-2.683224
42	1	0	-13.199977	0.984075	2.585091
43	1	0	-11.731637	1.687998	1.905636
44	1	0	-13.204832	1.604629	0.933670
45	1	0	-11.812663	-1.043550	3.206737
46	1	0	-10.370825	-0.392820	2.410888
47	1	0	-12.392418	0.504139	-3.470291
48	1	0	-11.255486	1.491942	-2.529919
49	1	0	-13.115180	-2.230431	0.742434
50	1	0	-10.450613	1.754195	-0.089182
51	1	0	-8.487022	2.903636	0.838783
52	1	0	-6.972811	3.146017	-0.029065
53	1	0	-2.933381	2.837761	-0.910280
54	1	0	-1.433434	2.593865	-0.021674
55	1	0	1.870539	-3.236272	-0.199693
56	1	0	3.416160	-3.403993	-1.025665
57	1	0	7.426682	-3.751800	-0.071607
58	1	0	8.976044	-3.484258	-0.867272
59	1	0	-8.735004	-0.779842	-0.234674
60	1	0	-6.510255	-0.578720	-0.206956
61	1	0	-5.138498	2.178748	-0.075469
62	1	0	-4.151497	-0.729904	-0.183798
63	1	0	-1.940876	-1.124638	-0.166699
64	1	0	0.069044	1.204016	-0.041052
65	1	0	0.357301	-1.850905	-0.153088
66	1	0	2.360716	0.482317	-0.011427
67	1	0	4.568055	0.097769	0.047071
68	1	0	6.919629	-0.035550	0.142228
69	1	0	5.578031	-2.803253	-0.059716
70	1	0	9.128436	0.184307	0.269247
71	1	0	10.872650	-2.331910	0.167608
72	1	0	13.876019	1.622019	-1.705823
73	1	0	-10.984105	-1.986639	1.963027
74	1	0	-8.487181	2.994384	-0.916890
75	1	0	-2.954564	2.771162	0.846961
76	1	0	-10.836523	-0.155109	-2.913934
77	1	0	3.346018	-3.479947	0.729955
78	1	0	8.899565	-3.598440	0.885103
79	1	0	13.562481	-1.500405	-1.488661
80	1	0	10.830508	1.861099	-1.142927
81	1	0	-14.023729	-1.268734	1.902374
82	6	0	13.216324	2.282733	0.212066
83	8	0	13.724139	3.388896	0.117269
84	1	0	14.344398	0.584742	-0.361967
85	1	0	12.263918	2.656570	2.123111
86	6	0	10.983953	0.366502	2.697936
87	1	0	11.160910	1.107421	3.480371
88	1	0	9.908573	0.281970	2.531693
89	1	0	11.303036	-0.615189	3.065238
90	1	0	12.671704	-0.982476	0.690441
91	6	0	-14.335024	-0.742688	-0.139555
92	8	0	-15.548506	-0.868652	-0.091287
93	1	0	-14.288311	0.010127	-2.173080
94	1	0	-10.989396	-1.258942	-0.355751

OXO

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-15.958984	-0.884003	0.349652
2	6	0	-14.560954	-0.416240	0.644744
3	6	0	-16.619286	-1.931261	0.858203
4	6	0	-11.873289	1.245562	-0.740005
5	6	0	-12.235969	0.004067	-0.351160
6	6	0	-13.645705	-0.481447	-0.605565
7	6	0	-16.066703	-2.885919	1.886564
8	6	0	-18.030624	-2.241593	0.422232
9	6	0	-11.330670	-0.957404	0.373964
10	6	0	-10.600776	1.938282	-0.607366
11	6	0	-9.355103	1.403933	-0.581175
12	6	0	-8.112669	2.140654	-0.456514
13	6	0	-6.939215	1.439054	-0.484442
14	6	0	-5.602330	1.941124	-0.381053
15	6	0	-4.500840	1.140232	-0.421217
16	6	0	-3.126912	1.562308	-0.324212
17	6	0	-2.835411	3.033377	-0.160389
18	6	0	-8.175815	3.638976	-0.302115
19	6	0	-2.145216	0.606040	-0.385255
20	6	0	-0.732536	0.786368	-0.310707
21	6	0	0.168634	-0.238195	-0.380305
22	6	0	1.580083	-0.050225	-0.299282
23	6	0	2.570046	-0.998255	-0.352460
24	6	0	2.295492	-2.471675	-0.522408
25	6	0	3.936830	-0.561351	-0.235275
26	6	0	5.050335	-1.346974	-0.255218
27	6	0	6.373002	-0.816818	-0.119360
28	6	0	7.563484	-1.489959	-0.114552
29	6	0	7.673469	-2.984871	-0.272252
30	6	0	8.775990	-0.717129	0.059537
31	6	0	10.042014	-1.199750	0.051930
32	6	0	11.279415	-0.433455	0.200203
33	6	0	11.411724	0.607864	1.079003
34	6	0	12.683700	1.346808	1.185899
35	6	0	13.548422	0.143752	-0.804760
36	6	0	12.453147	-0.934877	-0.673696
37	6	0	10.336960	1.100776	2.016769
38	6	0	13.039062	-2.222139	-0.041833
39	6	0	11.973384	-1.262008	-2.104741
40	1	0	10.795610	1.510910	2.917126
41	1	0	9.754042	1.917209	1.577148
42	1	0	12.293179	-3.019219	0.012401
43	1	0	13.869862	-2.594068	-0.648678
44	1	0	11.289047	-2.111687	-2.137254
45	1	0	12.834467	-1.509698	-2.732575
46	1	0	-18.100375	-3.247959	-0.008041
47	1	0	-18.721615	-2.221565	1.273655
48	1	0	-18.395338	-1.531593	-0.322824
49	1	0	-16.079874	-3.914241	1.506416
50	1	0	-16.688345	-2.885070	2.789778
51	1	0	-10.804633	-1.616208	-0.328572
52	1	0	-10.572545	-0.445227	0.969537
53	1	0	-16.483764	-0.279210	-0.391353
54	1	0	-14.591464	0.626784	0.984142
55	1	0	-13.620817	-1.518957	-0.961682
56	1	0	-10.688723	3.022512	-0.574748

57	1	0	-8.763363	3.917983	0.578421
58	1	0	-7.192856	4.094889	-0.197751
59	1	0	-3.232241	3.607585	-1.003798
60	1	0	-1.770777	3.248507	-0.091638
61	1	0	1.233982	-2.695171	-0.611385
62	1	0	2.788296	-2.861469	-1.419014
63	1	0	6.703391	-3.471016	-0.359870
64	1	0	8.250689	-3.245819	-1.165989
65	1	0	-9.245594	0.329602	-0.696060
66	1	0	-7.020357	0.358453	-0.599349
67	1	0	-5.464047	3.011256	-0.266035
68	1	0	-4.660356	0.068870	-0.538347
69	1	0	-2.477318	-0.424771	-0.505033
70	1	0	-0.340500	1.793296	-0.190530
71	1	0	-0.219833	-1.246375	-0.500505
72	1	0	1.903970	0.982842	-0.175620
73	1	0	4.081731	0.511748	-0.114534
74	1	0	6.426427	0.264978	-0.000195
75	1	0	4.933531	-2.419161	-0.373763
76	1	0	8.629859	0.352688	0.171924
77	1	0	10.176748	-2.258215	-0.152929
78	1	0	13.198929	0.947501	-1.462057
79	1	0	-15.044945	-2.658151	2.189274
80	1	0	-8.662026	4.102702	-1.166907
81	1	0	-3.308586	3.427834	0.744550
82	1	0	-11.901562	-1.610807	1.039440
83	1	0	2.681071	-3.044000	0.327738
84	1	0	8.190125	-3.434556	0.581899
85	1	0	13.410244	-2.052913	0.970818
86	1	0	11.465328	-0.406625	-2.557110
87	1	0	9.641971	0.307764	2.293820
88	1	0	-14.114030	-0.986738	1.461935
89	1	0	-14.102789	0.108360	-1.406423
90	6	0	13.924855	0.768518	0.524755
91	1	0	14.303252	-0.009301	1.210383
92	1	0	14.437797	-0.283690	-1.278065
93	8	0	14.908143	1.762938	0.353375
94	1	0	14.676960	2.468102	0.979338
95	8	0	12.787876	2.391605	1.816412
96	1	0	-12.656236	1.851882	-1.196233

OXO radical cation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-15.729713	-1.007383	0.786219
2	6	0	-14.257143	-0.708578	0.823303
3	6	0	-16.341410	-2.193406	0.893289
4	6	0	-11.895553	1.468292	-0.497359
5	6	0	-12.276282	0.157293	-0.526896
6	6	0	-13.741054	-0.181745	-0.548323
7	6	0	-15.641816	-3.514493	1.088764
8	6	0	-17.845605	-2.292028	0.833280
9	6	0	-11.323901	-1.006244	-0.509477
10	6	0	-10.598016	2.073954	-0.443993
11	6	0	-9.344634	1.508970	-0.420384
12	6	0	-8.125291	2.246399	-0.368981
13	6	0	-6.933788	1.522233	-0.364206
14	6	0	-5.627604	2.028514	-0.321870

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15	6	0	-4.501049	1.216179	-0.329408
16	6	0	-3.163927	1.656810	-0.290353
17	6	0	-2.856382	3.132424	-0.229506
18	6	0	-8.155974	3.752164	-0.324231
19	6	0	-2.157728	0.679820	-0.312503
20	6	0	-0.777711	0.877210	-0.282164
21	6	0	0.143058	-0.168793	-0.310961
22	6	0	1.524660	0.030778	-0.272165
23	6	0	2.530531	-0.940582	-0.292148
24	6	0	2.233274	-2.415929	-0.378258
25	6	0	3.872267	-0.494440	-0.220705
26	6	0	4.997711	-1.294531	-0.216177
27	6	0	6.306305	-0.771033	-0.120057
28	6	0	7.496649	-1.472387	-0.095679
29	6	0	7.573393	-2.972026	-0.195790
30	6	0	8.711875	-0.709816	0.042261
31	6	0	9.970563	-1.219803	0.055239
32	6	0	11.219780	-0.469748	0.181935
33	6	0	11.361650	0.575689	1.050427
34	6	0	12.652273	1.308373	1.138008
35	6	0	13.488048	0.062848	-0.835902
36	6	0	12.381182	-1.001421	-0.689630
37	6	0	10.304215	1.097273	1.989777
38	6	0	12.950247	-2.288996	-0.043298
39	6	0	11.885918	-1.338020	-2.113090
40	1	0	10.774808	1.478907	2.896193
41	1	0	9.765310	1.945843	1.554827
42	1	0	12.196101	-3.077873	0.022846
43	1	0	13.772101	-2.679139	-0.649561
44	1	0	11.183352	-2.174360	-2.129691
45	1	0	12.736006	-1.617246	-2.741276
46	1	0	-18.165789	-2.943875	0.012259
47	1	0	-18.248030	-2.732967	1.752492
48	1	0	-18.316775	-1.317404	0.693499
49	1	0	-15.904059	-4.211616	0.284881
50	1	0	-15.966641	-3.987786	2.022238
51	1	0	-10.648674	-0.978839	-1.371400
52	1	0	-10.698800	-1.008223	0.389726
53	1	0	-16.360678	-0.129613	0.645742
54	1	0	-14.060161	0.063814	1.576467
55	1	0	-13.927631	-0.954888	-1.302646
56	1	0	-10.636922	3.159883	-0.423777
57	1	0	-8.720335	4.105760	0.543023
58	1	0	-7.164538	4.195293	-0.267502
59	1	0	-3.257050	3.652237	-1.104430
60	1	0	-1.789739	3.340953	-0.191705
61	1	0	1.169514	-2.630589	-0.451157
62	1	0	2.714131	-2.860440	-1.254131
63	1	0	6.596955	-3.444023	-0.281551
64	1	0	8.158029	-3.273087	-1.070484
65	1	0	-9.239991	0.431994	-0.443612
66	1	0	-7.026907	0.438247	-0.399897
67	1	0	-5.484242	3.102497	-0.283606
68	1	0	-4.662702	0.140860	-0.370912
69	1	0	-2.495173	-0.354174	-0.359111
70	1	0	-0.382062	1.887435	-0.233196
71	1	0	-0.251100	-1.179657	-0.362250
72	1	0	1.858175	1.065391	-0.214484
73	1	0	4.024715	0.581118	-0.156535
74	1	0	6.379256	0.312626	-0.048469
75	1	0	4.869950	-2.369536	-0.281017
76	1	0	8.587168	0.365754	0.111813

77	1	0	10.087190	-2.288164	-0.104222
78	1	0	13.149222	0.862420	-1.503499
79	1	0	-14.554817	-3.437436	1.119122
80	1	0	-8.644565	4.159692	-1.213851
81	1	0	-3.306968	3.590563	0.655353
82	1	0	-11.856959	-1.956789	-0.543434
83	1	0	2.612849	-2.943032	0.501868
84	1	0	8.068762	-3.397626	0.681630
85	1	0	13.329571	-2.114144	0.965123
86	1	0	11.397541	-0.478199	-2.578704
87	1	0	9.574157	0.334595	2.258877
88	1	0	-13.677070	-1.583799	1.123543
89	1	0	-14.330626	0.693082	-0.835586
90	6	0	13.880208	0.701340	0.485185
91	1	0	14.243758	-0.074202	1.182036
92	1	0	14.371139	-0.381195	-1.303749
93	8	0	14.879404	1.669510	0.286660
94	1	0	14.698761	2.386273	0.914345
95	8	0	12.749765	2.365913	1.738361
96	1	0	-12.708231	2.190314	-0.517642

OXO radical anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-15.945033	-1.106075	0.022341
2	6	0	-14.587870	-0.633865	0.463418
3	6	0	-16.571880	-2.254312	0.305519
4	6	0	-11.890838	1.321373	-0.545167
5	6	0	-12.232549	0.029831	-0.328558
6	6	0	-13.606428	-0.464936	-0.725878
7	6	0	-16.016722	-3.346613	1.185189
8	6	0	-17.941680	-2.549372	-0.256619
9	6	0	-11.328455	-0.986650	0.321067
10	6	0	-10.653576	2.036656	-0.293451
11	6	0	-9.384513	1.535506	-0.242470
12	6	0	-8.176324	2.278023	-0.015978
13	6	0	-6.967759	1.610805	-0.066194
14	6	0	-5.657451	2.117861	0.102410
15	6	0	-4.523369	1.330224	0.011957
16	6	0	-3.178319	1.742016	0.150699
17	6	0	-2.885121	3.194290	0.446031
18	6	0	-8.276670	3.758626	0.254699
19	6	0	-2.159487	0.795868	-0.000733
20	6	0	-0.775049	0.973718	0.067624
21	6	0	0.157827	-0.050986	-0.112396
22	6	0	1.539958	0.123814	-0.060571
23	6	0	2.558507	-0.827716	-0.236550
24	6	0	2.249175	-2.280747	-0.519143
25	6	0	3.898359	-0.418264	-0.153578
26	6	0	5.036126	-1.211095	-0.308651
27	6	0	6.339805	-0.710740	-0.220295
28	6	0	7.557635	-1.382954	-0.366497
29	6	0	7.621482	-2.861975	-0.666088
30	6	0	8.756555	-0.648218	-0.223921
31	6	0	10.044591	-1.161019	-0.276778
32	6	0	11.291954	-0.483299	-0.112904
33	6	0	11.482148	0.891011	-0.268351
34	6	0	12.713899	1.532802	0.126103

35	6	0	13.835389	-0.663568	0.200519
36	6	0	12.486095	-1.411424	0.252411
37	6	0	10.466750	1.821562	-0.888035
38	6	0	12.268937	-1.993425	1.669625
39	6	0	12.603098	-2.586049	-0.747110
40	1	0	10.992131	2.660198	-1.346807
41	1	0	9.861594	1.317284	-1.644188
42	1	0	11.328952	-2.546299	1.727044
43	1	0	13.083130	-2.677748	1.932400
44	1	0	11.788682	-3.307918	-0.661025
45	1	0	13.535623	-3.129981	-0.562527
46	1	0	-17.934604	-3.464672	-0.861512
47	1	0	-18.673267	-2.715173	0.544151
48	1	0	-18.309958	-1.735121	-0.884418
49	1	0	-15.963614	-4.295817	0.638387
50	1	0	-16.673004	-3.524379	2.046026
51	1	0	-10.724442	-1.529737	-0.418063
52	1	0	-10.633693	-0.525091	1.026093
53	1	0	-16.466838	-0.408069	-0.634677
54	1	0	-14.686767	0.341613	0.956090
55	1	0	-13.521101	-1.432556	-1.238774
56	1	0	-10.774981	3.113652	-0.194770
57	1	0	-8.923455	3.962639	1.115790
58	1	0	-7.307490	4.211624	0.459721
59	1	0	-3.225243	3.844446	-0.368616
60	1	0	-1.822707	3.384974	0.592034
61	1	0	1.179360	-2.479246	-0.569432
62	1	0	2.685339	-2.602036	-1.471519
63	1	0	6.637372	-3.291996	-0.849558
64	1	0	8.234398	-3.062890	-1.551541
65	1	0	-9.243487	0.474494	-0.431319
66	1	0	-7.026068	0.540588	-0.271449
67	1	0	-5.533431	3.177724	0.303008
68	1	0	-4.678450	0.271071	-0.198308
69	1	0	-2.492918	-0.222004	-0.209130
70	1	0	-0.378701	1.967831	0.265009
71	1	0	-0.241573	-1.044022	-0.310523
72	1	0	1.880730	1.140746	0.139030
73	1	0	4.066750	0.639734	0.050701
74	1	0	6.418448	0.356726	-0.008821
75	1	0	4.896277	-2.269021	-0.509938
76	1	0	8.628101	0.406776	-0.011484
77	1	0	10.111000	-2.237752	-0.382478
78	1	0	14.143189	-0.515919	-0.841115
79	1	0	-15.020052	-3.130273	1.568595
80	1	0	-8.713296	4.292515	-0.598286
81	1	0	-3.402783	3.527129	1.352586
82	1	0	-11.906174	-1.743120	0.861767
83	1	0	2.665652	-2.933877	0.255832
84	1	0	8.071825	-3.422274	0.162617
85	1	0	12.230002	-1.209638	2.429745
86	1	0	12.626006	-2.223146	-1.778044
87	1	0	9.778684	2.256558	-0.152268
88	1	0	-14.154625	-1.304996	1.208484
89	1	0	-14.052918	0.224240	-1.450677
90	6	0	13.769084	0.702566	0.852379
91	1	0	13.454665	0.604641	1.904394
92	1	0	14.613704	-1.271376	0.675172
93	8	0	15.018360	1.362938	0.802568
94	1	0	14.787720	2.269781	0.530560
95	8	0	12.976129	2.729432	-0.071031
96	1	0	-12.679292	1.950707	-0.962720

ECH

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-13.591518	1.636959	0.740393
2	6	0	-12.540052	2.191112	-0.198779
3	6	0	-11.419489	1.296463	-0.597030
4	6	0	-11.336747	0.007980	-0.147952
5	6	0	-12.467289	-0.656829	0.669084
6	6	0	-13.780244	0.140525	0.533644
7	1	0	-14.189272	-0.028072	-0.469841
8	6	0	-12.028761	-0.730452	2.150650
9	6	0	-12.758850	-2.092320	0.176706
10	6	0	-10.420676	1.957066	-1.515061
11	6	0	-10.159305	-0.834558	-0.382889
12	6	0	-8.868225	-0.438145	-0.281856
13	6	0	-7.697891	-1.270059	-0.475892
14	6	0	-7.894373	-2.711041	-0.872200
15	6	0	-6.468831	-0.700386	-0.290430
16	6	0	-5.178755	-1.306782	-0.427208
17	6	0	-4.016804	-0.627949	-0.214246
18	6	0	-2.679617	-1.150727	-0.329013
19	6	0	-2.501596	-2.595854	-0.722517
20	6	0	-1.629229	-0.306314	-0.075282
21	6	0	-0.232116	-0.590474	-0.128067
22	6	0	0.735753	0.333598	0.145578
23	6	0	2.134257	0.056223	0.092794
24	6	0	3.178104	0.907634	0.349413
25	6	0	2.986708	2.349635	0.748571
26	6	0	4.521748	0.399140	0.231771
27	6	0	5.674172	1.091322	0.447809
28	6	0	6.976726	0.509656	0.307357
29	6	0	8.192114	1.103347	0.496751
30	6	0	8.355102	2.545187	0.905078
31	6	0	9.387962	0.303975	0.291491
32	6	0	10.665666	0.725708	0.409855
33	6	0	11.869551	-0.096731	0.185485
34	6	0	12.026414	-1.321584	0.739462
35	6	0	13.214727	-2.211601	0.443373
36	6	0	14.033272	-1.769854	-0.765628
37	6	0	14.256411	-0.263264	-0.699514
38	6	0	12.938560	0.542759	-0.732773
39	6	0	12.395027	0.608443	-2.178098
40	6	0	13.273455	1.981181	-0.276733
41	6	0	11.082031	-1.933912	1.745894
42	1	0	-10.949537	2.609699	-2.210855
43	1	0	-9.728979	2.606508	-0.967206
44	1	0	-13.275874	1.856181	1.767946
45	1	0	-14.517921	-0.257303	1.238795
46	1	0	-11.102355	-1.300129	2.254798
47	1	0	-12.797314	-1.223952	2.753945
48	1	0	-11.850137	0.260225	2.574678
49	1	0	-12.925916	-2.121890	-0.903882
50	1	0	-13.666661	-2.463677	0.661014
51	1	0	-11.959828	-2.795294	0.419786
52	1	0	-10.353422	-1.881392	-0.590202
53	1	0	-8.665725	0.592264	-0.002549
54	1	0	-6.954074	-3.240479	-1.015288

55	1	0	-8.462948	-3.254817	-0.110049
56	1	0	-8.460827	-2.788991	-1.805858
57	1	0	-6.458117	0.350387	-0.002193
58	1	0	-5.129500	-2.351887	-0.714359
59	1	0	-4.091908	0.420473	0.072486
60	1	0	-1.455968	-2.894700	-0.767340
61	1	0	-3.001984	-3.260709	-0.010945
62	1	0	-2.941370	-2.792614	-1.705857
63	1	0	-1.884488	0.716201	0.201791
64	1	0	0.088255	-1.592798	-0.401020
65	1	0	0.412460	1.335099	0.418425
66	1	0	2.396023	-0.963700	-0.187483
67	1	0	3.479005	3.021338	0.037976
68	1	0	1.938676	2.638849	0.798030
69	1	0	3.428044	2.546538	1.731051
70	1	0	4.608267	-0.646709	-0.060990
71	1	0	5.608562	2.134119	0.740553
72	1	0	6.986733	-0.538805	0.010526
73	1	0	8.918839	3.104746	0.151063
74	1	0	7.403548	3.054876	1.045270
75	1	0	8.914279	2.627171	1.842747
76	1	0	10.837640	1.773225	0.641357
77	1	0	13.110395	1.111125	-2.837460
78	1	0	12.202422	-0.387007	-2.585399
79	1	0	11.454346	1.162937	-2.219286
80	1	0	12.452010	2.680085	-0.448297
81	1	0	14.132730	2.355803	-0.841340
82	1	0	13.534271	2.013686	0.785194
83	1	0	14.900005	0.074883	-1.519332
84	1	0	14.792814	-0.029877	0.229359
85	1	0	9.214126	-0.728862	-0.002968
86	1	0	11.656613	-2.400128	2.555017
87	1	0	10.482232	-2.736518	1.299068
88	1	0	10.395686	-1.212640	2.186412
89	1	0	-9.830319	1.231766	-2.073574
90	8	0	-12.594507	3.346287	-0.588360
91	1	0	14.990677	-2.300432	-0.791500
92	1	0	13.508044	-2.036623	-1.689060
93	1	0	-14.514911	2.197287	0.577178
94	1	0	12.857719	-3.241226	0.309896
95	1	0	13.856627	-2.249009	1.336714

ECH radical cation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-13.627825	1.616263	0.719800
2	6	0	-12.561492	2.187017	-0.186888
3	6	0	-11.413044	1.301171	-0.565613
4	6	0	-11.334246	0.011773	-0.117662
5	6	0	-12.480746	-0.670708	0.663047
6	6	0	-13.795373	0.119062	0.495661
7	1	0	-14.176514	-0.046655	-0.518842
8	6	0	-12.081108	-0.750319	2.155371
9	6	0	-12.746676	-2.103627	0.149195
10	6	0	-10.406628	1.981358	-1.456802
11	6	0	-10.148644	-0.816294	-0.334747
12	6	0	-8.854583	-0.405634	-0.249848
13	6	0	-7.697484	-1.240225	-0.438166

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14	6	0	-7.882080	-2.687477	-0.809327
15	6	0	-6.455156	-0.655730	-0.266582
16	6	0	-5.190784	-1.267378	-0.402537
17	6	0	-4.004061	-0.586486	-0.207178
18	6	0	-2.703066	-1.129143	-0.325332
19	6	0	-2.524429	-2.579932	-0.694456
20	6	0	-1.621266	-0.273232	-0.091107
21	6	0	-0.260845	-0.580921	-0.151269
22	6	0	0.743290	0.352725	0.099363
23	6	0	2.102373	0.045015	0.041660
24	6	0	3.186028	0.902992	0.276314
25	6	0	3.003269	2.356136	0.636911
26	6	0	4.482583	0.360493	0.167692
27	6	0	5.672419	1.045679	0.365795
28	6	0	6.932762	0.439136	0.245040
29	6	0	8.178773	1.033429	0.418086
30	6	0	8.343074	2.489199	0.768980
31	6	0	9.334789	0.208582	0.250000
32	6	0	10.630610	0.641174	0.331459
33	6	0	11.845263	-0.134569	0.156905
34	6	0	11.951381	-1.443765	0.534600
35	6	0	13.178061	-2.272631	0.244743
36	6	0	14.127966	-1.651730	-0.772292
37	6	0	14.335116	-0.183135	-0.422517
38	6	0	13.029038	0.641306	-0.479270
39	6	0	12.681382	0.973962	-1.948152
40	6	0	13.298200	1.963168	0.276297
41	6	0	10.917443	-2.199777	1.329374
42	1	0	-10.931976	2.634011	-2.154604
43	1	0	-9.741169	2.638891	-0.886383
44	1	0	-13.339773	1.831805	1.756069
45	1	0	-14.547764	-0.288812	1.177603
46	1	0	-11.159520	-1.323579	2.286090
47	1	0	-12.865828	-1.245454	2.734538
48	1	0	-11.913702	0.237632	2.589846
49	1	0	-12.878602	-2.127251	-0.936284
50	1	0	-13.668073	-2.482585	0.598979
51	1	0	-11.956054	-2.808141	0.416610
52	1	0	-10.331646	-1.869829	-0.515545
53	1	0	-8.654326	0.628688	0.010947
54	1	0	-6.940982	-3.216314	-0.943352
55	1	0	-8.446987	-3.217909	-0.036770
56	1	0	-8.447776	-2.782457	-1.740467
57	1	0	-6.447337	0.398458	0.004295
58	1	0	-5.146677	-2.316410	-0.673515
59	1	0	-4.070909	0.465682	0.062366
60	1	0	-1.480611	-2.883928	-0.725054
61	1	0	-3.030960	-3.231339	0.023161
62	1	0	-2.952828	-2.788001	-1.679284
63	1	0	-1.870094	0.754439	0.167680
64	1	0	0.049047	-1.590641	-0.404487
65	1	0	0.432909	1.362453	0.351627
66	1	0	2.352280	-0.983284	-0.213768
67	1	0	3.514327	3.004795	-0.079856
68	1	0	1.958948	2.658998	0.656375
69	1	0	3.422015	2.570066	1.624572
70	1	0	4.552516	-0.693238	-0.094859
71	1	0	5.622091	2.096557	0.627943
72	1	0	6.932982	-0.618111	-0.013996
73	1	0	8.908464	3.014238	-0.006712
74	1	0	7.394530	3.008642	0.883724
75	1	0	8.897118	2.606786	1.704112

76	1	0	10.777228	1.706826	0.471972
77	1	0	13.481343	1.561513	-2.408048
78	1	0	12.538539	0.072280	-2.548440
79	1	0	11.759611	1.558508	-2.018412
80	1	0	12.521853	2.715857	0.120331
81	1	0	14.232705	2.402310	-0.082877
82	1	0	13.403539	1.796491	1.351803
83	1	0	15.070665	0.279580	-1.087735
84	1	0	14.754648	-0.120039	0.589376
85	1	0	9.142969	-0.829330	-0.000106
86	1	0	11.418644	-2.867982	2.036429
87	1	0	10.310724	-2.846677	0.683649
88	1	0	10.242368	-1.556483	1.891901
89	1	0	-9.793958	1.274951	-2.014992
90	8	0	-12.600448	3.340253	-0.572175
91	1	0	15.081725	-2.186703	-0.773031
92	1	0	13.715962	-1.753122	-1.781730
93	1	0	-14.552856	2.167553	0.539225
94	1	0	12.850094	-3.269037	-0.078640
95	1	0	13.704977	-2.448271	1.194701

ECH radical anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-13.711073	1.471500	0.744442
2	6	0	-12.595688	2.152928	-0.029922
3	6	0	-11.456516	1.336298	-0.444220
4	6	0	-11.358991	-0.017117	-0.143513
5	6	0	-12.578455	-0.793123	0.423111
6	6	0	-13.875766	0.029861	0.289935
7	1	0	-14.185177	0.029627	-0.762657
8	6	0	-12.318823	-1.129708	1.909730
9	6	0	-12.819176	-2.115442	-0.341901
10	6	0	-10.405596	2.101733	-1.211768
11	6	0	-10.168710	-0.806291	-0.297198
12	6	0	-8.850166	-0.387483	-0.295751
13	6	0	-7.706445	-1.216427	-0.407762
14	6	0	-7.886752	-2.699792	-0.627302
15	6	0	-6.442423	-0.634214	-0.295887
16	6	0	-5.179521	-1.239032	-0.352564
17	6	0	-3.984463	-0.534248	-0.213684
18	6	0	-2.679739	-1.052304	-0.254896
19	6	0	-2.485074	-2.534763	-0.479895
20	6	0	-1.590765	-0.181436	-0.085243
21	6	0	-0.226241	-0.468050	-0.096350
22	6	0	0.782153	0.480336	0.096523
23	6	0	2.149053	0.190121	0.080835
24	6	0	3.235820	1.049557	0.273428
25	6	0	3.052314	2.523077	0.551251
26	6	0	4.547430	0.525730	0.211186
27	6	0	5.735379	1.212133	0.389341
28	6	0	7.009063	0.599380	0.296351
29	6	0	8.259806	1.158148	0.461402
30	6	0	8.464186	2.613805	0.798998
31	6	0	9.420865	0.322849	0.298633
32	6	0	10.723625	0.703228	0.391583
33	6	0	11.895637	-0.165266	0.193910
34	6	0	11.997065	-1.407402	0.728383

35	6	0	13.138574	-2.354145	0.420073
36	6	0	13.992066	-1.924885	-0.769105
37	6	0	14.291567	-0.434586	-0.656836
38	6	0	13.016246	0.437117	-0.689877
39	6	0	12.507933	0.569579	-2.143368
40	6	0	13.419123	1.843797	-0.190890
41	6	0	11.018151	-1.986122	1.721208
42	1	0	-10.890564	2.899833	-1.775835
43	1	0	-9.675789	2.597174	-0.559274
44	1	0	-13.477888	1.523031	1.815661
45	1	0	-14.676531	-0.470800	0.847986
46	1	0	-11.410133	-1.725595	2.019335
47	1	0	-13.154498	-1.700859	2.330354
48	1	0	-12.186915	-0.228149	2.512870
49	1	0	-12.860538	-1.946058	-1.421339
50	1	0	-13.778030	-2.545399	-0.032764
51	1	0	-12.054741	-2.869538	-0.146822
52	1	0	-10.318220	-1.879299	-0.331075
53	1	0	-8.644103	0.666953	-0.146798
54	1	0	-6.941690	-3.211910	-0.805566
55	1	0	-8.359065	-3.181356	0.238346
56	1	0	-8.533265	-2.899388	-1.488987
57	1	0	-6.437641	0.445325	-0.137029
58	1	0	-5.123509	-2.312518	-0.506965
59	1	0	-4.069769	0.541240	-0.053234
60	1	0	-1.435253	-2.825533	-0.473299
61	1	0	-2.990124	-3.123455	0.294178
62	1	0	-2.905821	-2.850446	-1.441354
63	1	0	-1.851992	0.865093	0.078833
64	1	0	0.095851	-1.494402	-0.263729
65	1	0	0.462136	1.505850	0.270870
66	1	0	2.405720	-0.854107	-0.105537
67	1	0	3.572928	3.136094	-0.193394
68	1	0	2.005276	2.823333	0.543542
69	1	0	3.463743	2.798796	1.529467
70	1	0	4.625095	-0.541497	-0.001859
71	1	0	5.687640	2.274097	0.610251
72	1	0	6.993673	-0.465570	0.057808
73	1	0	9.025361	3.132392	0.011559
74	1	0	7.523983	3.147383	0.932895
75	1	0	9.042459	2.731633	1.723159
76	1	0	10.929048	1.754994	0.567852
77	1	0	13.259054	1.057092	-2.775321
78	1	0	12.277953	-0.404634	-2.582188
79	1	0	11.593078	1.164652	-2.182956
80	1	0	12.635062	2.586088	-0.351065
81	1	0	14.305351	2.189424	-0.733694
82	1	0	13.663635	1.832105	0.875388
83	1	0	14.967829	-0.106745	-1.455349
84	1	0	14.821082	-0.255946	0.288432
85	1	0	9.213767	-0.716457	0.048350
86	1	0	11.563234	-2.505707	2.520006
87	1	0	10.362286	-2.737912	1.263276
88	1	0	10.381239	-1.228603	2.175685
89	1	0	-9.851432	1.455171	-1.894307
90	8	0	-12.667300	3.360772	-0.263079
91	1	0	14.920843	-2.505528	-0.804430
92	1	0	13.460306	-2.134742	-1.703741
93	1	0	-14.622526	2.056897	0.597095
94	1	0	12.729564	-3.360104	0.251808
95	1	0	13.772381	-2.454228	1.315851

3hECH

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-14.403058	-1.724669	-0.727496
2	6	0	-13.607047	-2.127025	0.509766
3	6	0	-12.412615	-1.239035	0.786458
4	6	0	-12.234247	-0.039278	0.185900
5	6	0	-13.285636	0.576722	-0.768236
6	6	0	-14.612147	-0.214667	-0.721828
7	1	0	-15.158255	0.059016	0.190208
8	6	0	-12.725323	0.584519	-2.208489
9	6	0	-13.610928	2.033946	-0.368403
10	6	0	-11.487726	-1.821143	1.828278
11	6	0	-11.021872	0.776099	0.388694
12	6	0	-9.748666	0.332919	0.304227
13	6	0	-8.544961	1.127321	0.480416
14	6	0	-8.693574	2.589049	0.817869
15	6	0	-7.335291	0.512121	0.325940
16	6	0	-6.027310	1.087226	0.439241
17	6	0	-4.881329	0.374180	0.259544
18	6	0	-3.533308	0.877126	0.346530
19	6	0	-3.329248	2.337135	0.666284
20	6	0	-2.497100	0.004660	0.133048
21	6	0	-1.096548	0.274595	0.160991
22	6	0	-0.136830	-0.670694	-0.065077
23	6	0	1.262228	-0.392874	-0.043149
24	6	0	2.304787	-1.257927	-0.256977
25	6	0	2.114255	-2.723496	-0.558625
26	6	0	3.645895	-0.737101	-0.192841
27	6	0	4.800941	-1.434872	-0.382087
28	6	0	6.095822	-0.829113	-0.303833
29	6	0	7.318706	-1.416537	-0.476161
30	6	0	7.501007	-2.880501	-0.785975
31	6	0	8.495612	-0.580812	-0.355688
32	6	0	9.782567	-0.992703	-0.455790
33	6	0	10.972707	-0.153419	-0.298509
34	6	0	11.056333	1.110504	-0.816429
35	6	0	12.192248	1.985436	-0.480971
36	6	0	13.463805	1.404018	0.135574
37	6	0	13.460609	-0.110618	0.191588
38	6	0	12.108006	-0.752191	0.560712
39	6	0	11.767875	-0.507259	2.050837
40	6	0	12.263110	-2.273471	0.344456
41	6	0	10.015345	1.770620	-1.688080
42	1	0	-12.077615	-2.251353	2.646244
43	1	0	-10.889098	-2.645334	1.420886
44	1	0	-13.866424	-2.031319	-1.631828
45	1	0	-15.241534	0.098152	-1.562457
46	1	0	-11.777919	1.126657	-2.258658
47	1	0	-13.427537	1.071404	-2.893350
48	1	0	-12.540134	-0.427046	-2.577790
49	1	0	-13.881847	2.107915	0.688892
50	1	0	-14.460794	2.395714	-0.955193
51	1	0	-12.781130	2.718499	-0.557012
52	1	0	-11.181653	1.835439	0.569298
53	1	0	-9.585293	-0.714644	0.060180
54	1	0	-7.737081	3.093540	0.942338
55	1	0	-9.244016	3.118707	0.033061

56	1	0	-9.259629	2.722404	1.745399
57	1	0	-7.355495	-0.549503	0.081027
58	1	0	-5.951633	2.143293	0.676780
59	1	0	-4.977513	-0.684800	0.022279
60	1	0	-2.278856	2.620164	0.698370
61	1	0	-3.817803	2.973213	-0.078825
62	1	0	-3.766922	2.590126	1.637430
63	1	0	-2.767818	-1.027266	-0.088483
64	1	0	-0.764580	1.288253	0.371298
65	1	0	-0.465881	-1.685305	-0.274845
66	1	0	1.526456	0.642910	0.168353
67	1	0	2.623237	-3.345951	0.184466
68	1	0	1.066878	-3.019401	-0.568177
69	1	0	2.537484	-2.982027	-1.534869
70	1	0	3.730949	0.326312	0.028442
71	1	0	4.741421	-2.495138	-0.604185
72	1	0	6.095453	0.237165	-0.079484
73	1	0	8.080424	-3.379165	-0.001558
74	1	0	6.555655	-3.412050	-0.878783
75	1	0	8.050069	-3.020051	-1.722830
76	1	0	9.965219	-2.051980	-0.598717
77	1	0	12.523603	-0.975456	2.689152
78	1	0	11.753203	0.555834	2.286430
79	1	0	10.795880	-0.939523	2.303400
80	1	0	11.428384	-2.842191	0.758541
81	1	0	13.167178	-2.618090	0.853635
82	1	0	12.364080	-2.529939	-0.714548
83	1	0	14.233788	-0.438002	0.893661
84	1	0	13.755695	-0.479822	-0.797361
85	1	0	8.302721	0.464519	-0.132192
86	1	0	10.503756	2.425076	-2.412066
87	1	0	9.346482	2.415174	-1.108274
88	1	0	9.403775	1.041708	-2.219189
89	1	0	-10.801055	-1.089470	2.250886
90	8	0	13.628365	1.949346	1.446881
91	8	0	12.148014	3.197466	-0.652948
92	1	0	13.505232	2.904404	1.359507
93	1	0	14.293779	1.745890	-0.500340
94	1	0	-13.259946	-3.164979	0.422543
95	1	0	-14.261863	-2.121847	1.394468
96	1	0	-15.365074	-2.247076	-0.747860

3hECH radical cation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-14.474966	-1.652247	-0.653823
2	6	0	-13.536866	-2.212081	0.408199
3	6	0	-12.308272	-1.371791	0.652887
4	6	0	-12.193071	-0.090387	0.190551
5	6	0	-13.372481	0.651687	-0.492603
6	6	0	-14.681220	-0.164976	-0.394798
7	1	0	-15.106904	-0.040420	0.608779
8	6	0	-13.021127	0.902555	-1.976533
9	6	0	-13.639787	2.013153	0.190126
10	6	0	-11.282388	-2.078992	1.500848
11	6	0	-10.972909	0.686267	0.311379
12	6	0	-9.679986	0.238652	0.266287
13	6	0	-8.518687	1.066182	0.369268

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14	6	0	-8.673034	2.546204	0.604254
15	6	0	-7.276594	0.452006	0.241587
16	6	0	-6.012419	1.058422	0.306976
17	6	0	-4.827682	0.351950	0.157466
18	6	0	-3.527518	0.893519	0.212840
19	6	0	-3.334333	2.369607	0.455899
20	6	0	-2.450535	0.013209	0.037473
21	6	0	-1.089350	0.316090	0.058922
22	6	0	-0.093195	-0.639963	-0.131571
23	6	0	1.269678	-0.337687	-0.109162
24	6	0	2.343115	-1.214930	-0.297039
25	6	0	2.151651	-2.686321	-0.564252
26	6	0	3.649195	-0.674308	-0.233357
27	6	0	4.828088	-1.374292	-0.404699
28	6	0	6.099033	-0.765338	-0.324172
29	6	0	7.333510	-1.367904	-0.485243
30	6	0	7.501869	-2.833385	-0.785791
31	6	0	8.500413	-0.534504	-0.355070
32	6	0	9.788551	-0.960402	-0.443543
33	6	0	10.985497	-0.137143	-0.270143
34	6	0	11.069143	1.134962	-0.765459
35	6	0	12.216761	2.014318	-0.421478
36	6	0	13.377374	1.460206	0.399149
37	6	0	13.455252	-0.049188	0.327300
38	6	0	12.121257	-0.795056	0.541375
39	6	0	11.718777	-0.797914	2.036518
40	6	0	12.362001	-2.257163	0.097016
41	6	0	10.050567	1.802369	-1.654353
42	1	0	-11.790354	-2.696106	2.248405
43	1	0	-10.676322	-2.770996	0.902908
44	1	0	-14.052898	-1.815499	-1.651016
45	1	0	-15.411498	0.258387	-1.091235
46	1	0	-12.096047	1.477278	-2.077114
47	1	0	-13.817120	1.469260	-2.468368
48	1	0	-12.883745	-0.031279	-2.526989
49	1	0	-13.750093	1.904229	1.272523
50	1	0	-14.571157	2.436180	-0.195785
51	1	0	-12.860039	2.753942	-0.001864
52	1	0	-11.110561	1.760759	0.369106
53	1	0	-9.495853	-0.816910	0.098042
54	1	0	-7.721046	3.065701	0.685753
55	1	0	-9.228479	3.013554	-0.214388
56	1	0	-9.232608	2.740684	1.523055
57	1	0	-7.284293	-0.622757	0.069323
58	1	0	-5.954155	2.126877	0.482012
59	1	0	-4.905721	-0.719042	-0.018810
60	1	0	-2.288315	2.667140	0.445484
61	1	0	-3.846021	2.962292	-0.307435
62	1	0	-3.746294	2.663532	1.425613
63	1	0	-2.708372	-1.030223	-0.135158
64	1	0	-0.770756	1.340060	0.230700
65	1	0	-0.411733	-1.663580	-0.306005
66	1	0	1.527684	0.703937	0.073511
67	1	0	2.668159	-3.290393	0.186812
68	1	0	1.106279	-2.986458	-0.556292
69	1	0	2.562029	-2.962199	-1.540051
70	1	0	3.726511	0.392333	-0.032173
71	1	0	4.772840	-2.437422	-0.610930
72	1	0	6.102980	0.301802	-0.109960
73	1	0	8.072823	-3.328993	0.005167
74	1	0	6.555024	-3.360241	-0.881563
75	1	0	8.054578	-2.979662	-1.718105

76	1	0	9.960291	-2.021697	-0.584328
77	1	0	12.495927	-1.287373	2.630472
78	1	0	11.598846	0.214306	2.418734
79	1	0	10.785317	-1.347338	2.189256
80	1	0	11.564211	-2.933405	0.411396
81	1	0	13.281899	-2.624727	0.558568
82	1	0	12.482244	-2.342203	-0.987096
83	1	0	14.194303	-0.404201	1.051374
84	1	0	13.839971	-0.305778	-0.666678
85	1	0	8.312497	0.511068	-0.133453
86	1	0	10.562618	2.437745	-2.377950
87	1	0	9.397350	2.473267	-1.085986
88	1	0	9.426628	1.086068	-2.186980
89	1	0	-10.606340	-1.403324	2.022884
90	8	0	13.205698	1.877746	1.756724
91	8	0	12.213434	3.197415	-0.719537
92	1	0	13.208365	2.843449	1.764829
93	1	0	14.295507	1.902361	-0.008289
94	1	0	-13.210892	-3.228283	0.151221
95	1	0	-14.072098	-2.325030	1.363010
96	1	0	-15.430111	-2.184271	-0.631838

3hECH radical anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	14.362204	-2.100024	0.252995
2	6	0	13.513122	-2.148371	-1.013598
3	6	0	12.388242	-1.134964	-1.036587
4	6	0	12.297521	-0.104072	-0.160854
5	6	0	13.414169	0.193501	0.869669
6	6	0	14.679846	-0.647087	0.587451
7	1	0	15.219542	-0.203636	-0.259715
8	6	0	12.892237	-0.104886	2.293538
9	6	0	13.836471	1.679262	0.813517
10	6	0	11.414328	-1.380389	-2.163848
11	6	0	11.137766	0.802385	-0.109428
12	6	0	9.832653	0.423483	-0.135623
13	6	0	8.676186	1.281312	-0.083356
14	6	0	8.890127	2.772729	-0.023459
15	6	0	7.423734	0.705832	-0.089765
16	6	0	6.150066	1.327991	-0.055131
17	6	0	4.963502	0.619797	-0.068485
18	6	0	3.648771	1.143367	-0.045934
19	6	0	3.461592	2.641421	-0.004797
20	6	0	2.566843	0.259360	-0.063521
21	6	0	1.196854	0.539931	-0.052864
22	6	0	0.197336	-0.435547	-0.071518
23	6	0	-1.170581	-0.164724	-0.065169
24	6	0	-2.249593	-1.064063	-0.079427
25	6	0	-2.037083	-2.560937	-0.101721
26	6	0	-3.560004	-0.560962	-0.072719
27	6	0	-4.747022	-1.294837	-0.081132
28	6	0	-6.016315	-0.706892	-0.073966
29	6	0	-7.274291	-1.319656	-0.078437
30	6	0	-7.429957	-2.822126	-0.095123
31	6	0	-8.426108	-0.502509	-0.058070
32	6	0	-9.741872	-0.940947	0.017810
33	6	0	-10.938176	-0.168384	0.058087

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34	6	0	-11.066756	1.139386	-0.421493
35	6	0	-12.312254	1.853696	-0.291221
36	6	0	-13.339853	1.422752	0.758829
37	6	0	-13.041788	0.084598	1.414989
38	6	0	-12.222225	-0.892000	0.546217
39	6	0	-13.048536	-1.352815	-0.677508
40	6	0	-11.942236	-2.128827	1.423720
41	6	0	-10.024988	1.839449	-1.261144
42	1	0	11.962834	-1.648980	-3.075976
43	1	0	10.745009	-2.224510	-1.953470
44	1	0	13.820246	-2.568899	1.081711
45	1	0	15.352541	-0.579247	1.450769
46	1	0	11.983719	0.463834	2.503310
47	1	0	13.642676	0.162895	3.046108
48	1	0	12.647896	-1.162430	2.421736
49	1	0	14.090832	1.981958	-0.206578
50	1	0	14.720969	1.837046	1.439713
51	1	0	13.058318	2.349865	1.182573
52	1	0	11.355403	1.859663	0.011891
53	1	0	9.617652	-0.642863	-0.183044
54	1	0	7.953431	3.328822	-0.015548
55	1	0	9.447957	3.060009	0.876464
56	1	0	9.475818	3.126554	-0.880128
57	1	0	7.403133	-0.384563	-0.130066
58	1	0	6.103650	2.412146	-0.019185
59	1	0	5.042348	-0.467801	-0.101426
60	1	0	2.411988	2.932685	0.001494
61	1	0	3.926175	3.076366	0.887783
62	1	0	3.929126	3.124971	-0.870328
63	1	0	2.828447	-0.799737	-0.090417
64	1	0	0.869492	1.577580	-0.029491
65	1	0	0.529434	-1.472087	-0.092630
66	1	0	-1.443507	0.891359	-0.046673
67	1	0	-2.494164	-3.013969	-0.988481
68	1	0	-0.982987	-2.835643	-0.104377
69	1	0	-2.496014	-3.040294	0.770126
70	1	0	-3.659094	0.525016	-0.058956
71	1	0	-4.675702	-2.378391	-0.090705
72	1	0	-6.028394	0.384023	-0.061140
73	1	0	-8.073175	-3.146268	-0.920442
74	1	0	-6.476980	-3.338618	-0.204927
75	1	0	-7.894400	-3.188078	0.828655
76	1	0	-9.871872	-2.011541	0.122292
77	1	0	-13.936729	-1.904385	-0.350265
78	1	0	-13.389666	-0.509782	-1.277561
79	1	0	-12.454588	-2.012423	-1.317753
80	1	0	-11.538382	-2.968969	0.853845
81	1	0	-12.879447	-2.472614	1.873400
82	1	0	-11.242766	-1.904751	2.233236
83	1	0	-13.992462	-0.376442	1.703831
84	1	0	-12.482653	0.262805	2.340314
85	1	0	-8.237870	0.565200	-0.048578
86	1	0	-10.527481	2.560322	-1.907270
87	1	0	-9.458349	1.137019	-1.877217
88	1	0	-9.300066	2.403597	-0.661099
89	1	0	10.791207	-0.513916	-2.379941
90	8	0	-14.632633	1.409988	0.149726
91	8	0	-12.632618	2.845351	-0.967747
92	1	0	-14.594166	2.141276	-0.487169
93	1	0	-13.325192	2.214091	1.526571
94	1	0	13.088279	-3.152588	-1.149270
95	1	0	14.152712	-1.991946	-1.896876

96	1	0	15.283677	-2.677839	0.119496

CAN

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	14.149257	1.380741	0.021394
2	6	0	12.969284	1.891585	-0.781415
3	6	0	11.707490	1.099837	-0.769013
4	6	0	11.578996	-0.030433	-0.010568
5	6	0	12.735397	-0.579974	0.856130
6	6	0	13.712533	0.554928	1.222780
7	1	0	13.219933	1.214501	1.946808
8	6	0	13.468638	-1.694761	0.073377
9	6	0	12.210185	-1.169473	2.183043
10	6	0	10.653884	1.630583	-1.709628
11	6	0	10.373385	-0.862418	-0.012508
12	6	0	9.087908	-0.437644	-0.021604
13	6	0	7.907593	-1.279347	-0.002711
14	6	0	8.087249	-2.775661	-0.014168
15	6	0	6.685567	-0.667075	0.016571
16	6	0	5.387731	-1.272778	0.020369
17	6	0	4.234797	-0.547362	0.031874
18	6	0	2.890577	-1.065864	0.025654
19	6	0	2.695151	-2.561157	0.005870
20	6	0	1.851074	-0.171556	0.034591
21	6	0	0.450872	-0.443817	0.021174
22	6	0	-0.507818	0.528943	0.033375
23	6	0	-1.907925	0.256613	0.012455
24	6	0	-2.947653	1.150601	0.025883
25	6	0	-2.752926	2.645369	0.073202
26	6	0	-4.291465	0.632234	-0.008435
27	6	0	-5.444777	1.357058	0.004644
28	6	0	-6.741943	0.751682	-0.041211
29	6	0	-7.964486	1.363076	-0.024898
30	6	0	-8.146409	2.856800	0.059859
31	6	0	-9.143862	0.523428	-0.095711
32	6	0	-10.430467	0.941904	-0.045873
33	6	0	-11.613256	0.074576	-0.089452
34	6	0	-11.714432	-0.981399	-0.951023
35	6	0	-12.837993	-1.953747	-0.863364
36	6	0	-13.868081	-1.751545	0.228809
37	6	0	-14.046092	-0.274352	0.552370
38	6	0	-12.723301	0.423804	0.927054
39	6	0	-12.259066	-0.014673	2.335828
40	6	0	-13.007297	1.942393	0.960123
41	6	0	-10.736174	-1.291185	-2.057240
42	1	0	11.136164	2.129982	-2.549615
43	1	0	9.998640	0.842127	-2.079734
44	1	0	14.771724	0.786028	-0.658849
45	1	0	14.582990	0.130762	1.735367
46	1	0	12.795179	-2.519422	-0.174359
47	1	0	14.283977	-2.108329	0.675180
48	1	0	13.890750	-1.327749	-0.864326
49	1	0	11.610125	-0.439227	2.732202
50	1	0	13.053644	-1.455578	2.818818
51	1	0	11.596643	-2.060701	2.038024
52	1	0	10.551644	-1.931694	0.063270
53	1	0	8.896268	0.630978	-0.013390

54	1	0	7.140916	-3.313529	-0.025641
55	1	0	8.658436	-3.096712	-0.891231
56	1	0	8.643108	-3.111662	0.867733
57	1	0	6.687158	0.422471	0.024533
58	1	0	5.324745	-2.355886	0.009300
59	1	0	4.323511	0.538399	0.043087
60	1	0	1.646010	-2.850942	0.009159
61	1	0	3.155247	-3.005006	-0.882943
62	1	0	3.166484	-3.029276	0.876105
63	1	0	2.118948	0.884454	0.051259
64	1	0	0.119309	-1.478927	-0.002406
65	1	0	-0.176393	1.564053	0.058301
66	1	0	-2.175472	-0.799119	-0.019903
67	1	0	-3.224248	3.073999	0.963639
68	1	0	-1.703896	2.935150	0.088773
69	1	0	-3.213413	3.128229	-0.794754
70	1	0	-4.379570	-0.452831	-0.050259
71	1	0	-5.382739	2.439348	0.049247
72	1	0	-6.742677	-0.336383	-0.098441
73	1	0	-8.695403	3.135332	0.965878
74	1	0	-7.201083	3.396448	0.074598
75	1	0	-8.726237	3.231241	-0.789794
76	1	0	-10.616449	2.000067	0.103660
77	1	0	-13.010607	0.250303	3.086102
78	1	0	-12.087567	-1.091931	2.394404
79	1	0	-11.323204	0.478644	2.608626
80	1	0	-12.194540	2.516794	1.408972
81	1	0	-13.900396	2.130372	1.563062
82	1	0	-13.195935	2.338995	-0.041643
83	1	0	-14.767065	-0.141381	1.366111
84	1	0	-14.472143	0.229682	-0.323482
85	1	0	-8.952433	-0.543605	-0.171017
86	1	0	-11.282297	-1.655032	-2.928563
87	1	0	-10.048821	-2.098067	-1.780183
88	1	0	-10.140957	-0.423130	-2.337422
89	1	0	10.024973	2.388302	-1.229003
90	8	0	13.070600	2.906557	-1.450914
91	8	0	-12.909960	-2.904307	-1.624813
92	1	0	-14.799505	-2.218786	-0.098807
93	1	0	14.755717	2.241919	0.311280
94	1	0	-13.537192	-2.311267	1.112459

CAN radical cation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	14.137683	1.372047	-0.034201
2	6	0	12.945469	1.900923	-0.798834
3	6	0	11.670540	1.107596	-0.770070
4	6	0	11.558563	-0.022649	-0.007970
5	6	0	12.729206	-0.582614	0.832766
6	6	0	13.718651	0.549325	1.177098
7	1	0	13.247477	1.212225	1.911957
8	6	0	13.436960	-1.702300	0.034291
9	6	0	12.224327	-1.166140	2.170633
10	6	0	10.608800	1.653357	-1.688788
11	6	0	10.354034	-0.846305	0.003238
12	6	0	9.061932	-0.417387	-0.007600
13	6	0	7.900914	-1.264203	0.013291

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14	6	0	8.071786	-2.759343	0.002778
15	6	0	6.661551	-0.643948	0.035243
16	6	0	5.393906	-1.257633	0.038584
17	6	0	4.213387	-0.534748	0.052959
18	6	0	2.907917	-1.073706	0.045021
19	6	0	2.709013	-2.567858	0.021261
20	6	0	1.837058	-0.170471	0.055873
21	6	0	0.473605	-0.464228	0.039880
22	6	0	-0.516272	0.517739	0.052153
23	6	0	-1.879813	0.224649	0.029689
24	6	0	-2.950030	1.128551	0.041695
25	6	0	-2.750426	2.622062	0.089156
26	6	0	-4.255858	0.591261	0.007094
27	6	0	-5.435498	1.315530	0.017951
28	6	0	-6.703876	0.704905	-0.028403
29	6	0	-7.942295	1.327369	-0.015446
30	6	0	-8.111294	2.820531	0.068838
31	6	0	-9.104444	0.485462	-0.088616
32	6	0	-10.396300	0.913351	-0.034868
33	6	0	-11.587880	0.070035	-0.086416
34	6	0	-11.673615	-1.015743	-0.914171
35	6	0	-12.831308	-1.966066	-0.830510
36	6	0	-13.894840	-1.697241	0.209055
37	6	0	-14.052921	-0.202799	0.458688
38	6	0	-12.734107	0.487805	0.863576
39	6	0	-12.340415	0.103083	2.309099
40	6	0	-12.987980	2.011411	0.812840
41	6	0	-10.670709	-1.392601	-1.972462
42	1	0	11.082895	2.150427	-2.534286
43	1	0	9.932810	0.881175	-2.054529
44	1	0	14.731055	0.769476	-0.733031
45	1	0	14.596850	0.120490	1.669811
46	1	0	12.755417	-2.525066	-0.198719
47	1	0	14.260446	-2.120733	0.619840
48	1	0	13.843592	-1.340273	-0.911862
49	1	0	11.643874	-0.430695	2.733980
50	1	0	13.076801	-1.459829	2.789035
51	1	0	11.603846	-2.055897	2.040572
52	1	0	10.528355	-1.915254	0.087349
53	1	0	8.869778	0.649919	-0.000416
54	1	0	7.125890	-3.296498	0.001625
55	1	0	8.633715	-3.081702	-0.878254
56	1	0	8.633821	-3.091564	0.880796
57	1	0	6.664144	0.444365	0.044696
58	1	0	5.337078	-2.340429	0.024668
59	1	0	4.294450	0.550231	0.067681
60	1	0	1.660630	-2.857040	0.034087
61	1	0	3.156274	-3.007268	-0.874944
62	1	0	3.185217	-3.039202	0.885548
63	1	0	2.101271	0.885261	0.076534
64	1	0	0.147986	-1.500102	0.014877
65	1	0	-0.190473	1.553487	0.079328
66	1	0	-2.144508	-0.830708	-0.001632
67	1	0	-3.214870	3.049890	0.982210
68	1	0	-1.701790	2.910300	0.101650
69	1	0	-3.209206	3.105434	-0.777924
70	1	0	-4.337778	-0.493054	-0.032080
71	1	0	-5.377591	2.397452	0.061795
72	1	0	-6.708015	-0.382095	-0.082698
73	1	0	-8.660567	3.098457	0.973547
74	1	0	-7.164794	3.356363	0.087709
75	1	0	-8.685570	3.196956	-0.782073

76	1	0	-10.569650	1.971493	0.127281
77	1	0	-13.122682	0.406203	3.010725
78	1	0	-12.184578	-0.972087	2.422320
79	1	0	-11.413936	0.599286	2.610188
80	1	0	-12.193098	2.594679	1.283136
81	1	0	-13.907841	2.241398	1.356497
82	1	0	-13.116940	2.367064	-0.213326
83	1	0	-14.804596	-0.021439	1.232908
84	1	0	-14.431314	0.270653	-0.454870
85	1	0	-8.913862	-0.580220	-0.162537
86	1	0	-11.199721	-1.789872	-2.839196
87	1	0	-10.013511	-2.202198	-1.635862
88	1	0	-10.050076	-0.553254	-2.282495
89	1	0	10.007871	2.422931	-1.191139
90	8	0	13.012704	2.926990	-1.447932
91	8	0	-12.876558	-2.940822	-1.556290
92	1	0	-14.823010	-2.160035	-0.132087
93	1	0	14.765816	2.221661	0.241241
94	1	0	-13.609060	-2.224155	1.127756

CAN radical anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	14.264802	1.305631	0.317544
2	6	0	13.060810	2.018341	-0.276533
3	6	0	11.778643	1.306770	-0.342988
4	6	0	11.626652	-0.000739	0.094490
5	6	0	12.844750	-0.792326	0.642448
6	6	0	13.874094	0.176887	1.256187
7	1	0	13.440484	0.604479	2.168311
8	6	0	13.482494	-1.598019	-0.512902
9	6	0	12.452805	-1.776875	1.767233
10	6	0	10.681820	2.092303	-1.019254
11	6	0	10.411287	-0.767585	0.006580
12	6	0	9.098651	-0.348796	-0.048604
13	6	0	7.954580	-1.192268	-0.108559
14	6	0	8.142643	-2.688374	-0.181604
15	6	0	6.693387	-0.604347	-0.092438
16	6	0	5.429215	-1.217106	-0.127202
17	6	0	4.235218	-0.504714	-0.112905
18	6	0	2.930017	-1.030236	-0.138610
19	6	0	2.742872	-2.529303	-0.181111
20	6	0	1.840385	-0.147545	-0.125807
21	6	0	0.476290	-0.437408	-0.145757
22	6	0	-0.533784	0.528690	-0.134509
23	6	0	-1.897732	0.237980	-0.152579
24	6	0	-2.988137	1.119762	-0.146831
25	6	0	-2.802447	2.619387	-0.122407
26	6	0	-4.292722	0.592418	-0.162774
27	6	0	-5.487844	1.303082	-0.157707
28	6	0	-6.750823	0.687085	-0.170819
29	6	0	-8.013028	1.273025	-0.167867
30	6	0	-8.205002	2.770259	-0.155288
31	6	0	-9.155993	0.426955	-0.166279
32	6	0	-10.470405	0.834752	-0.092062
33	6	0	-11.658625	0.020406	-0.038733
34	6	0	-11.757145	-1.260515	-0.557265
35	6	0	-12.893918	-2.140232	-0.265314

36	6	0	-13.996673	-1.602094	0.628873
37	6	0	-14.163560	-0.103123	0.435146
38	6	0	-12.860816	0.683160	0.684348
39	6	0	-12.563741	0.747724	2.200670
40	6	0	-13.113095	2.121280	0.175058
41	6	0	-10.719628	-1.889085	-1.455985
42	1	0	11.128854	2.902554	-1.594049
43	1	0	10.082284	1.462955	-1.681629
44	1	0	14.868738	0.930223	-0.518473
45	1	0	14.759636	-0.389253	1.570652
46	1	0	12.765781	-2.306125	-0.937347
47	1	0	14.345797	-2.171146	-0.155587
48	1	0	13.816148	-0.949491	-1.325512
49	1	0	11.870220	-1.278677	2.546336
50	1	0	13.358646	-2.181683	2.231282
51	1	0	11.869921	-2.627308	1.410135
52	1	0	10.553400	-1.841927	0.051298
53	1	0	8.885484	0.711727	0.009540
54	1	0	7.198866	-3.222047	-0.285618
55	1	0	8.771515	-2.969947	-1.033601
56	1	0	8.637990	-3.074877	0.717362
57	1	0	6.682876	0.485561	-0.044749
58	1	0	5.377535	-2.300874	-0.164901
59	1	0	4.315139	0.582395	-0.078630
60	1	0	1.693588	-2.821366	-0.183873
61	1	0	3.203850	-2.962410	-1.075975
62	1	0	3.213145	-3.013038	0.682245
63	1	0	2.097677	0.912243	-0.097316
64	1	0	0.156966	-1.477489	-0.172408
65	1	0	-0.214800	1.568934	-0.109955
66	1	0	-2.154240	-0.822170	-0.173635
67	1	0	-3.257839	3.062335	0.770521
68	1	0	-1.753465	2.912510	-0.130672
69	1	0	-3.279095	3.092675	-0.988047
70	1	0	-4.371265	-0.495203	-0.179358
71	1	0	-5.438290	2.387466	-0.138995
72	1	0	-6.738586	-0.403769	-0.181858
73	1	0	-8.688205	3.105280	0.770845
74	1	0	-7.263935	3.311755	-0.243202
75	1	0	-8.847290	3.095895	-0.980895
76	1	0	-10.627893	1.900331	0.026734
77	1	0	-13.386532	1.234944	2.735872
78	1	0	-12.422414	-0.247100	2.629769
79	1	0	-11.650362	1.314636	2.393701
80	1	0	-12.346132	2.829761	0.492724
81	1	0	-14.066577	2.486047	0.571605
82	1	0	-13.172170	2.151824	-0.916428
83	1	0	-14.951583	0.292023	1.087462
84	1	0	-14.492463	0.081669	-0.594907
85	1	0	-8.944400	-0.636774	-0.178211
86	1	0	-11.214864	-2.580290	-2.139284
87	1	0	-9.986851	-2.489267	-0.902871
88	1	0	-10.169401	-1.140972	-2.028858
89	1	0	9.994305	2.558347	-0.303202
90	8	0	13.207888	3.158270	-0.715763
91	8	0	-12.963974	-3.289843	-0.696379
92	1	0	-14.911422	-2.153130	0.395656
93	1	0	14.880745	2.058695	0.816752
94	1	0	-13.748619	-1.839578	1.671079

ADO

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	13.776004	1.160833	-0.089314
2	6	0	12.553938	1.706830	-0.810660
3	6	0	11.322215	0.894799	-0.837813
4	6	0	11.188717	-0.197669	-0.025041
5	6	0	12.323896	-0.684233	0.905956
6	6	0	13.343273	0.442468	1.174614
7	1	0	12.903182	1.188362	1.845792
8	6	0	13.025963	-1.900667	0.253332
9	6	0	11.760727	-1.117259	2.277415
10	6	0	10.290792	1.380352	-1.826653
11	6	0	9.987084	-1.033271	-0.006560
12	6	0	8.702121	-0.609363	-0.064115
13	6	0	7.520094	-1.446417	-0.018704
14	6	0	7.694470	-2.942198	0.037709
15	6	0	6.300643	-0.828406	-0.033806
16	6	0	4.999413	-1.425688	-0.012783
17	6	0	3.852613	-0.690219	-0.022790
18	6	0	2.503607	-1.195268	-0.013166
19	6	0	2.292597	-2.688378	0.000270
20	6	0	1.474125	-0.289304	-0.017726
21	6	0	0.070828	-0.545109	-0.017693
22	6	0	-0.874819	0.440461	-0.012895
23	6	0	-2.278605	0.187417	-0.019879
24	6	0	-3.305186	1.096540	-0.006843
25	6	0	-3.088748	2.588630	0.025950
26	6	0	-4.656565	0.597225	-0.026817
27	6	0	-5.799160	1.338645	-0.010133
28	6	0	-7.105050	0.751470	-0.043487
29	6	0	-8.318691	1.380091	-0.022517
30	6	0	-8.479833	2.876365	0.057014
31	6	0	-9.509748	0.556171	-0.084551
32	6	0	-10.790466	0.991680	-0.032474
33	6	0	-11.984017	0.138883	-0.071668
34	6	0	-12.099548	-0.916804	-0.931659
35	6	0	-13.234641	-1.875633	-0.839930
36	6	0	-14.259536	-1.659642	0.254460
37	6	0	-14.419472	-0.179861	0.575771
38	6	0	-13.087700	0.503310	0.946446
39	6	0	-12.625923	0.062295	2.355195
40	6	0	-13.353204	2.025314	0.976680
41	6	0	-11.127910	-1.239938	-2.039862
42	1	0	10.788861	1.849018	-2.676187
43	1	0	9.653672	0.570815	-2.182735
44	1	0	14.247079	0.444589	-0.784839
45	1	0	14.220489	0.037605	1.688722
46	1	0	12.332008	-2.731116	0.100696
47	1	0	13.829744	-2.262991	0.900925
48	1	0	13.459923	-1.655700	-0.718031
49	1	0	11.178272	-0.314905	2.737160
50	1	0	12.585587	-1.361424	2.953342
51	1	0	11.119984	-1.998620	2.211641
52	1	0	10.164351	-2.095467	0.137647
53	1	0	8.511649	0.458214	-0.115870
54	1	0	6.746432	-3.477141	0.027076
55	1	0	8.284771	-3.302251	-0.810998
56	1	0	8.227788	-3.242264	0.946218
57	1	0	6.307874	0.260588	-0.068850

58	1	0	4.928549	-2.508138	0.009468
59	1	0	3.951552	0.394553	-0.041418
60	1	0	1.240401	-2.966946	0.002728
61	1	0	2.753975	-3.157480	-0.874741
62	1	0	2.752804	-3.141153	0.884538
63	1	0	1.754027	0.763702	-0.023124
64	1	0	-0.273607	-1.576230	-0.023020
65	1	0	-0.529238	1.471201	-0.004718
66	1	0	-2.561293	-0.864646	-0.039291
67	1	0	-3.549459	3.031705	0.914819
68	1	0	-2.035682	2.863655	0.034215
69	1	0	-3.546659	3.070191	-0.844049
70	1	0	-4.760470	-0.486692	-0.060353
71	1	0	-5.721549	2.420250	0.026780
72	1	0	-7.121532	-0.336696	-0.095423
73	1	0	-9.022364	3.165429	0.963583
74	1	0	-7.527321	3.403375	0.067143
75	1	0	-9.057189	3.255398	-0.792275
76	1	0	-10.963002	2.052618	0.113618
77	1	0	-13.372839	0.337703	3.106313
78	1	0	-12.467149	-1.016803	2.415670
79	1	0	-11.683781	0.545061	2.625261
80	1	0	-12.531857	2.591047	1.420986
81	1	0	-14.241748	2.225617	1.582358
82	1	0	-13.540807	2.421622	-0.025406
83	1	0	-15.137121	-0.037004	1.390752
84	1	0	-14.841374	0.327614	-0.300083
85	1	0	-9.332938	-0.513601	-0.156513
86	1	0	-11.680712	-1.598378	-2.909196
87	1	0	-10.449724	-2.054748	-1.763425
88	1	0	-10.522934	-0.379591	-2.322850
89	1	0	9.643189	2.150989	-1.395068
90	8	0	12.640657	2.789270	-1.376234
91	8	0	14.685019	2.195676	0.206603
92	1	0	14.461276	2.920789	-0.398828
93	8	0	-13.319535	-2.826224	-1.599882
94	1	0	-15.197151	-2.116592	-0.069951
95	1	0	-13.932864	-2.221632	1.138256

ADO radical cation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-13.775527	-1.134363	-0.121121
2	6	0	-12.555000	-1.700470	-0.821878
3	6	0	-11.305091	-0.893199	-0.843324
4	6	0	-11.174789	0.195427	-0.027309
5	6	0	-12.312952	0.700115	0.890303
6	6	0	-13.344794	-0.417411	1.147094
7	1	0	-12.922031	-1.167049	1.824877
8	6	0	-12.992619	1.923963	0.228245
9	6	0	-11.754374	1.126158	2.265895
10	6	0	-10.276799	-1.396518	-1.823462
11	6	0	-9.966965	1.017421	-0.005968
12	6	0	-8.680493	0.579390	-0.053209
13	6	0	-7.509599	1.415081	-0.012337
14	6	0	-7.668044	2.910811	0.028209
15	6	0	-6.277878	0.782602	-0.015374
16	6	0	-5.002716	1.383423	0.003538

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17	6	0	-3.830977	0.648022	0.003264
18	6	0	-2.518764	1.172847	0.010974
19	6	0	-2.303701	2.664708	0.015161
20	6	0	-1.458625	0.257596	0.013199
21	6	0	-0.091717	0.536262	0.011982
22	6	0	0.886892	-0.457064	0.018834
23	6	0	2.253423	-0.178584	0.011011
24	6	0	3.314036	-1.094420	0.021026
25	6	0	3.097976	-2.586035	0.051607
26	6	0	4.624926	-0.570433	0.000241
27	6	0	5.797592	-1.307110	0.010416
28	6	0	7.071264	-0.708638	-0.024278
29	6	0	8.304312	-1.343381	-0.013246
30	6	0	8.458550	-2.838718	0.058086
31	6	0	9.473448	-0.511662	-0.077094
32	6	0	10.761831	-0.952262	-0.027616
33	6	0	11.961517	-0.121363	-0.073536
34	6	0	12.054296	0.976048	-0.885596
35	6	0	13.222760	1.913010	-0.793613
36	6	0	14.288488	1.617438	0.236229
37	6	0	14.432827	0.117561	0.460452
38	6	0	13.109561	-0.566597	0.861903
39	6	0	12.728768	-0.202933	2.316305
40	6	0	13.347701	-2.091617	0.783305
41	6	0	11.050717	1.379502	-1.933140
42	1	0	-10.777348	-1.841374	-2.683781
43	1	0	-9.607151	-0.608845	-2.166955
44	1	0	-14.222824	-0.411401	-0.826042
45	1	0	-14.223904	-0.003928	1.649061
46	1	0	-12.290290	2.749169	0.082690
47	1	0	-13.797332	2.295509	0.868107
48	1	0	-13.421391	1.684768	-0.746600
49	1	0	-11.190653	0.315898	2.735188
50	1	0	-12.579793	1.386272	2.933740
51	1	0	-11.101546	2.000217	2.205466
52	1	0	-10.135222	2.082649	0.124644
53	1	0	-8.497423	-0.489206	-0.090690
54	1	0	-6.718004	3.440653	0.022975
55	1	0	-8.246970	3.265463	-0.829011
56	1	0	-8.207690	3.219108	0.928903
57	1	0	-6.290887	-0.305453	-0.037565
58	1	0	-4.935031	2.465635	0.016253
59	1	0	-3.923542	-0.436091	-0.004986
60	1	0	-1.252201	2.942526	0.022125
61	1	0	-2.755910	3.127014	-0.866803
62	1	0	-2.765578	3.123151	0.894163
63	1	0	-1.734615	-0.795305	0.015107
64	1	0	0.245600	1.568659	0.004499
65	1	0	0.549487	-1.489370	0.029817
66	1	0	2.529763	0.874104	-0.005884
67	1	0	3.557498	-3.029003	0.939748
68	1	0	2.046233	-2.862797	0.061338
69	1	0	3.551305	-3.064619	-0.820992
70	1	0	4.718393	0.513266	-0.027670
71	1	0	5.728591	-2.388774	0.043273
72	1	0	7.086319	0.378698	-0.068353
73	1	0	9.006153	-3.129521	0.959702
74	1	0	7.506905	-3.365439	0.073876
75	1	0	9.028048	-3.213585	-0.796705
76	1	0	10.924675	-2.013387	0.125512
77	1	0	13.512069	-0.526147	3.007702
78	1	0	12.584703	0.871627	2.449233

79	1	0	11.799088	-0.694834	2.614695
80	1	0	12.551432	-2.674967	1.251148
81	1	0	14.269942	-2.339551	1.314812
82	1	0	13.464172	-2.431251	-0.249730
83	1	0	15.187083	-0.083960	1.227090
84	1	0	14.801282	-0.344522	-0.462938
85	1	0	9.292554	0.556276	-0.140579
86	1	0	11.580097	1.785913	-2.795372
87	1	0	10.402903	2.189905	-1.580599
88	1	0	10.420816	0.551314	-2.254185
89	1	0	-9.668123	-2.196396	-1.388217
90	8	0	-12.622859	-2.787272	-1.370700
91	8	0	-14.704049	-2.145506	0.177970
92	1	0	-14.525987	-2.877223	-0.432756
93	8	0	13.274140	2.897767	-1.505174
94	1	0	15.219495	2.076647	-0.101936
95	1	0	14.012220	2.132007	1.164783

ADO radical anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-13.916511	-1.070862	-0.065228
2	6	0	-12.654000	-1.871893	-0.363163
3	6	0	-11.371600	-1.193724	-0.376790
4	6	0	-11.232988	0.123299	0.052526
5	6	0	-12.466390	0.925981	0.556031
6	6	0	-13.618651	-0.012390	0.972595
7	1	0	-13.357867	-0.526182	1.904804
8	6	0	-12.938946	1.884435	-0.564033
9	6	0	-12.129270	1.766306	1.809260
10	6	0	-10.241109	-2.025974	-0.931442
11	6	0	-10.015966	0.882092	0.028431
12	6	0	-8.696741	0.472973	-0.041848
13	6	0	-7.561083	1.323774	-0.055408
14	6	0	-7.752117	2.821287	-0.055235
15	6	0	-6.295703	0.738498	-0.065472
16	6	0	-5.034048	1.351812	-0.076024
17	6	0	-3.840780	0.635103	-0.085752
18	6	0	-2.534352	1.154331	-0.096274
19	6	0	-2.337367	2.652721	-0.098391
20	6	0	-1.450386	0.263695	-0.104842
21	6	0	-0.084358	0.542905	-0.115878
22	6	0	0.915256	-0.433775	-0.123786
23	6	0	2.282862	-0.158668	-0.134658
24	6	0	3.360749	-1.054500	-0.143165
25	6	0	3.156193	-2.551695	-0.141535
26	6	0	4.673167	-0.543816	-0.152760
27	6	0	5.856677	-1.271217	-0.160517
28	6	0	7.129846	-0.673499	-0.167875
29	6	0	8.381042	-1.279199	-0.176442
30	6	0	8.550963	-2.778973	-0.184005
31	6	0	9.538547	-0.450300	-0.168866
32	6	0	10.844883	-0.879868	-0.107193
33	6	0	12.045944	-0.081607	-0.049458
34	6	0	12.161342	1.196339	-0.567924
35	6	0	13.312395	2.060335	-0.276624
36	6	0	14.406390	1.507347	0.618718
37	6	0	14.550862	0.005488	0.428514

38	6	0	13.236172	-0.760711	0.677286
39	6	0	12.934309	-0.817102	2.193026
40	6	0	13.467180	-2.203815	0.172157
41	6	0	11.133039	1.840001	-1.466421
42	1	0	-10.653573	-2.897366	-1.439003
43	1	0	-9.627692	-1.457724	-1.636180
44	1	0	-14.218546	-0.593984	-1.013323
45	1	0	-14.519585	0.576439	1.178631
46	1	0	-12.154910	2.598070	-0.829067
47	1	0	-13.813201	2.456756	-0.235306
48	1	0	-13.209793	1.346961	-1.475058
49	1	0	-11.674319	1.148091	2.587219
50	1	0	-13.049566	2.196882	2.217722
51	1	0	-11.449583	2.594136	1.601980
52	1	0	-10.156461	1.952412	0.132333
53	1	0	-8.473616	-0.585788	-0.040340
54	1	0	-6.808842	3.360920	-0.129616
55	1	0	-8.378918	3.143944	-0.893916
56	1	0	-8.249890	3.161835	0.860631
57	1	0	-6.283717	-0.352381	-0.064214
58	1	0	-4.980490	2.436202	-0.075245
59	1	0	-3.925679	-0.452076	-0.084923
60	1	0	-1.286161	2.937844	-0.105792
61	1	0	-2.805950	3.113711	-0.974971
62	1	0	-2.793821	3.114690	0.784030
63	1	0	-1.715594	-0.794425	-0.102574
64	1	0	0.244464	1.580353	-0.118592
65	1	0	0.584671	-1.470568	-0.121028
66	1	0	2.552458	0.898383	-0.136722
67	1	0	3.616587	-3.014725	0.738433
68	1	0	2.103711	-2.831787	-0.141276
69	1	0	3.616380	-3.016428	-1.020617
70	1	0	4.766312	0.542719	-0.153536
71	1	0	5.791606	-2.354857	-0.157876
72	1	0	7.134174	0.417382	-0.164260
73	1	0	9.038577	-3.131769	0.733053
74	1	0	7.601501	-3.305997	-0.268631
75	1	0	9.180278	-3.103583	-1.019917
76	1	0	10.987648	-1.949175	-0.004539
77	1	0	13.748178	-1.315761	2.731131
78	1	0	12.807171	0.180603	2.619874
79	1	0	12.011951	-1.369611	2.385247
80	1	0	12.689527	-2.899687	0.491690
81	1	0	14.414748	-2.581429	0.570554
82	1	0	13.526858	-2.238762	-0.919170
83	1	0	15.331749	-0.399512	1.083149
84	1	0	14.878819	-0.186770	-0.600449
85	1	0	9.344190	0.616896	-0.166075
86	1	0	11.638685	2.518957	-2.154329
87	1	0	10.413907	2.456236	-0.913265
88	1	0	10.567040	1.099918	-2.034099
89	1	0	-9.572892	-2.404351	-0.149174
90	8	0	-12.804053	-3.073374	-0.621544
91	8	0	-14.950037	-1.934988	0.365114
92	1	0	-14.663884	-2.812741	0.057474
93	8	0	13.397871	3.207267	-0.709749
94	1	0	15.329446	2.044110	0.385224
95	1	0	14.160978	1.750937	1.660112

ASTA

Standard orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	14.173867	0.990640	0.273661
2	6	0	13.019809	1.652765	-0.462121
3	6	0	11.766651	0.896264	-0.648114
4	6	0	11.545524	-0.268734	0.033861
5	6	0	12.603774	-0.894627	0.972504
6	6	0	13.636544	0.159667	1.422883
7	1	0	13.174291	0.846202	2.140705
8	6	0	13.308770	-2.058950	0.233443
9	6	0	11.944784	-1.451204	2.253653
10	6	0	10.813930	1.522846	-1.636840
11	6	0	10.317621	-1.053841	-0.101107
12	6	0	9.051003	-0.581266	-0.182195
13	6	0	7.845549	-1.382549	-0.254526
14	6	0	7.978379	-2.882705	-0.315383
15	6	0	6.643121	-0.731725	-0.256289
16	6	0	5.329081	-1.298887	-0.299465
17	6	0	4.195480	-0.543478	-0.284548
18	6	0	2.839492	-1.029599	-0.308058
19	6	0	2.609650	-2.519335	-0.357714
20	6	0	1.820624	-0.112059	-0.279031
21	6	0	0.415204	-0.355620	-0.282897
22	6	0	-0.525381	0.634140	-0.247331
23	6	0	-1.929510	0.382734	-0.244071
24	6	0	-2.956765	1.290424	-0.208231
25	6	0	-2.742544	2.782521	-0.168639
26	6	0	-4.306637	0.787235	-0.207866
27	6	0	-5.452478	1.523156	-0.171868
28	6	0	-6.753996	0.925835	-0.174579
29	6	0	-7.972994	1.543761	-0.139776
30	6	0	-8.147495	3.039467	-0.084118
31	6	0	-9.155280	0.706099	-0.160879
32	6	0	-10.439968	1.129050	-0.092377
33	6	0	-11.625281	0.266855	-0.082259
34	6	0	-11.743138	-0.824517	-0.898797
35	6	0	-12.855230	-1.776556	-0.728059
36	6	0	-14.060411	-1.411901	0.137160
37	6	0	-14.072405	0.045154	0.551100
38	6	0	-12.704165	0.625119	0.962286
39	6	0	-12.255431	0.068332	2.335358
40	6	0	-12.892266	2.152729	1.098147
41	6	0	-10.763848	-1.221041	-1.977015
42	1	0	11.377864	2.062115	-2.398705
43	1	0	10.176262	0.780752	-2.117712
44	1	0	14.671038	0.335585	-0.462623
45	1	0	14.465050	-0.328656	1.945275
46	1	0	12.600276	-2.840838	-0.051669
47	1	0	14.057298	-2.519189	0.885028
48	1	0	13.811756	-1.726317	-0.676484
49	1	0	11.351781	-0.685277	2.759746
50	1	0	12.720492	-1.786586	2.948428
51	1	0	11.291572	-2.303239	2.056847
52	1	0	10.451237	-2.130745	-0.050058
53	1	0	8.893956	0.492436	-0.145914
54	1	0	7.018944	-3.386968	-0.415008
55	1	0	8.598384	-3.187718	-1.164419
56	1	0	8.460691	-3.273207	0.587264
57	1	0	6.677365	0.356364	-0.211473
58	1	0	5.236769	-2.379163	-0.337395

59	1	0	4.311006	0.539093	-0.245722
60	1	0	1.554263	-2.784576	-0.374624
61	1	0	3.071279	-2.957513	-1.248447
62	1	0	3.057733	-3.014208	0.510023
63	1	0	2.111502	0.937407	-0.244974
64	1	0	0.063423	-1.383786	-0.312423
65	1	0	-0.176767	1.663468	-0.217993
66	1	0	-2.212191	-0.669135	-0.272013
67	1	0	-3.189488	3.219102	0.730390
68	1	0	-1.689822	3.059108	-0.176606
69	1	0	-3.215294	3.268865	-1.028027
70	1	0	-4.407039	-0.297093	-0.238558
71	1	0	-5.380976	2.605355	-0.140009
72	1	0	-6.761824	-0.163093	-0.209778
73	1	0	-8.673752	3.340022	0.828208
74	1	0	-7.200041	3.575271	-0.104318
75	1	0	-8.745906	3.397376	-0.928030
76	1	0	-10.621762	2.190714	0.033508
77	1	0	-12.974938	0.355415	3.108399
78	1	0	-12.200257	-1.019144	2.325289
79	1	0	-11.278251	0.470294	2.616143
80	1	0	-12.039005	2.639380	1.574623
81	1	0	-13.764317	2.352274	1.726766
82	1	0	-13.067260	2.632310	0.130247
83	1	0	-14.792585	0.175887	1.364829
84	1	0	-14.448646	0.625737	-0.299104
85	1	0	-8.966527	-0.362645	-0.206368
86	1	0	-11.303355	-1.657654	-2.819305
87	1	0	-10.071099	-1.996588	-1.634107
88	1	0	-10.175559	-0.374003	-2.327899
89	1	0	10.163847	2.265464	-1.161865
90	8	0	13.177342	2.782746	-0.906372
91	8	0	15.089476	1.955985	0.737316
92	1	0	14.929839	2.747641	0.198692
93	8	0	-14.065312	-2.255353	1.292412
94	8	0	-12.832173	-2.892429	-1.231867
95	1	0	-13.966587	-3.161095	0.969492
96	1	0	-14.951111	-1.629990	-0.469603

ASTA radical cation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	14.162358	1.039436	0.016159
2	6	0	12.961505	1.685011	-0.648312
3	6	0	11.694100	0.910633	-0.740180
4	6	0	11.531657	-0.234320	-0.011729
5	6	0	12.650400	-0.833192	0.873452
6	6	0	13.704419	0.238132	1.222510
7	1	0	13.291813	0.943273	1.952281
8	6	0	13.309050	-2.018101	0.124758
9	6	0	12.071199	-1.350282	2.208764
10	6	0	10.686348	1.511361	-1.686412
11	6	0	10.307699	-1.029877	-0.060691
12	6	0	9.028962	-0.567580	-0.095539
13	6	0	7.846476	-1.387215	-0.114644
14	6	0	7.984632	-2.885058	-0.156396
15	6	0	6.622585	-0.739325	-0.093687
16	6	0	5.341261	-1.326320	-0.107888

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17	6	0	4.175698	-0.581270	-0.081579
18	6	0	2.860034	-1.096901	-0.094194
19	6	0	2.634975	-2.586643	-0.140795
20	6	0	1.805495	-0.175450	-0.062633
21	6	0	0.437191	-0.446697	-0.071062
22	6	0	-0.536771	0.550640	-0.036362
23	6	0	-1.904508	0.277860	-0.049548
24	6	0	-2.961283	1.197452	-0.018598
25	6	0	-2.739207	2.687129	0.043506
26	6	0	-4.274638	0.679146	-0.050236
27	6	0	-5.443545	1.420749	-0.028753
28	6	0	-6.720859	0.829506	-0.075806
29	6	0	-7.949188	1.471758	-0.059913
30	6	0	-8.094887	2.966717	0.031612
31	6	0	-9.124732	0.648336	-0.138703
32	6	0	-10.408434	1.099020	-0.089884
33	6	0	-11.616250	0.278459	-0.144903
34	6	0	-11.721611	-0.797837	-0.983243
35	6	0	-12.890839	-1.714065	-0.902581
36	6	0	-14.060196	-1.378721	0.018294
37	6	0	-14.092222	0.087396	0.393572
38	6	0	-12.740558	0.691600	0.829068
39	6	0	-12.350678	0.220166	2.251502
40	6	0	-12.933783	2.225776	0.858429
41	6	0	-10.713836	-1.205722	-2.026785
42	1	0	11.204783	2.014626	-2.502761
43	1	0	10.005749	0.767870	-2.100131
44	1	0	14.600397	0.362540	-0.738618
45	1	0	14.569775	-0.231957	1.697756
46	1	0	12.590301	-2.814343	-0.087032
47	1	0	14.100513	-2.454224	0.739830
48	1	0	13.750466	-1.715094	-0.826321
49	1	0	11.526766	-0.564204	2.738253
50	1	0	12.885140	-1.684573	2.857528
51	1	0	11.395636	-2.199005	2.077346
52	1	0	10.454363	-2.104161	0.003064
53	1	0	8.862433	0.503956	-0.068952
54	1	0	7.028076	-3.400880	-0.202144
55	1	0	8.568130	-3.198509	-1.026490
56	1	0	8.510271	-3.251062	0.730818
57	1	0	6.648741	0.348246	-0.062297
58	1	0	5.263029	-2.407341	-0.140319
59	1	0	4.276546	0.501609	-0.048367
60	1	0	1.581726	-2.857677	-0.138765
61	1	0	3.080071	-3.020834	-1.040530
62	1	0	3.097473	-3.078512	0.719535
63	1	0	2.087627	0.875247	-0.028171
64	1	0	0.094654	-1.476732	-0.106838
65	1	0	-0.194982	1.580867	0.000824
66	1	0	-2.184976	-0.773045	-0.090694
67	1	0	-3.199367	3.113442	0.939379
68	1	0	-1.686374	2.959259	0.061498
69	1	0	-3.188251	3.185452	-0.820250
70	1	0	-4.372542	-0.403439	-0.098239
71	1	0	-5.369473	2.501341	0.022428
72	1	0	-6.742030	-0.256979	-0.135078
73	1	0	-8.643922	3.247858	0.935391
74	1	0	-7.140397	3.487815	0.057639
75	1	0	-8.659500	3.356697	-0.819692
76	1	0	-10.565024	2.159546	0.072297
77	1	0	-13.117671	0.526547	2.968304
78	1	0	-12.264777	-0.863779	2.303686

79	1	0	-11.402514	0.666951	2.564739
80	1	0	-12.115301	2.747036	1.359849
81	1	0	-13.842472	2.461241	1.417717
82	1	0	-13.049673	2.645034	-0.145540
83	1	0	-14.832771	0.235539	1.184712
84	1	0	-14.452111	0.639827	-0.482193
85	1	0	-8.951546	-0.420304	-0.211537
86	1	0	-11.235140	-1.595525	-2.901875
87	1	0	-10.080359	-2.026639	-1.673802
88	1	0	-10.070470	-0.382165	-2.332643
89	1	0	10.087762	2.285270	-1.193745
90	8	0	13.058169	2.808328	-1.112641
91	8	0	15.110389	2.003255	0.399008
92	1	0	14.955458	2.783403	-0.155426
93	8	0	-13.947746	-2.182347	1.195647
94	8	0	-12.899372	-2.771364	-1.510251
95	1	0	-13.978720	-3.107223	0.919159
96	1	0	-14.976964	-1.645512	-0.523105

ASTA radical anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	14.325238	1.024580	0.073699
2	6	0	13.076807	1.845585	-0.229105
3	6	0	11.791274	1.176050	-0.318552
4	6	0	11.632728	-0.156265	0.046667
5	6	0	12.846172	-0.992840	0.541476
6	6	0	13.988085	-0.085115	1.044538
7	1	0	13.698868	0.380181	1.993563
8	6	0	13.347431	-1.888990	-0.617137
9	6	0	12.468114	-1.900439	1.734901
10	6	0	10.684187	2.039663	-0.872188
11	6	0	10.408441	-0.901278	-0.041612
12	6	0	9.096372	-0.473145	-0.101421
13	6	0	7.950582	-1.310482	-0.164101
14	6	0	8.127246	-2.808064	-0.236250
15	6	0	6.692451	-0.712916	-0.148707
16	6	0	5.424903	-1.315796	-0.180614
17	6	0	4.237404	-0.591923	-0.161370
18	6	0	2.927594	-1.104858	-0.179805
19	6	0	2.724194	-2.601705	-0.221659
20	6	0	1.848352	-0.209774	-0.158296
21	6	0	0.481139	-0.484603	-0.166140
22	6	0	-0.515961	0.494271	-0.146686
23	6	0	-1.883424	0.220516	-0.152808
24	6	0	-2.961354	1.117288	-0.140816
25	6	0	-2.755590	2.614272	-0.119791
26	6	0	-4.272223	0.606416	-0.151039
27	6	0	-5.457748	1.333533	-0.148208
28	6	0	-6.727406	0.734290	-0.161203
29	6	0	-7.983038	1.337447	-0.168699
30	6	0	-8.153381	2.837411	-0.164065
31	6	0	-9.132933	0.503631	-0.179549
32	6	0	-10.444249	0.938427	-0.137406
33	6	0	-11.669280	0.188996	-0.128825
34	6	0	-11.801291	-1.133981	-0.536409
35	6	0	-13.037202	-1.866458	-0.337873
36	6	0	-14.347988	-1.126454	-0.085853

37	6	0	-14.206491	0.380981	-0.108989
38	6	0	-12.892148	0.924557	0.484378
39	6	0	-12.863339	0.719528	2.018537
40	6	0	-12.892901	2.444252	0.206285
41	6	0	-10.688834	-1.962175	-1.132316
42	1	0	11.118257	2.919260	-1.346616
43	1	0	10.077271	1.499589	-1.603893
44	1	0	14.658945	0.594857	-0.886312
45	1	0	14.879036	-0.689448	1.248571
46	1	0	12.567013	-2.578815	-0.947958
47	1	0	14.206309	-2.487568	-0.294802
48	1	0	13.651317	-1.302024	-1.486212
49	1	0	11.993920	-1.323525	2.532862
50	1	0	13.373521	-2.359786	2.145054
51	1	0	11.790249	-2.710340	1.461796
52	1	0	10.537197	-1.977030	0.003029
53	1	0	8.885540	0.586908	-0.045175
54	1	0	7.179878	-3.333976	-0.346652
55	1	0	8.758866	-3.094449	-1.084344
56	1	0	8.613130	-3.198775	0.665848
57	1	0	6.690115	0.376936	-0.101327
58	1	0	5.363799	-2.399056	-0.217340
59	1	0	4.328079	0.494205	-0.126921
60	1	0	1.671884	-2.882428	-0.228001
61	1	0	3.183325	-3.040083	-1.114681
62	1	0	3.186128	-3.089594	0.643733
63	1	0	2.117582	0.846958	-0.131716
64	1	0	0.149379	-1.520751	-0.188953
65	1	0	-0.183703	1.530314	-0.126490
66	1	0	-2.153879	-0.836073	-0.170674
67	1	0	-3.218064	3.066376	0.764514
68	1	0	-1.702890	2.893445	-0.113152
69	1	0	-3.212773	3.090117	-0.994418
70	1	0	-4.365193	-0.479961	-0.164079
71	1	0	-5.393467	2.417138	-0.136086
72	1	0	-6.729488	-0.356535	-0.167056
73	1	0	-8.660901	3.179748	0.745685
74	1	0	-7.202313	3.365147	-0.221589
75	1	0	-8.763602	3.171744	-1.010127
76	1	0	-10.565672	2.008914	-0.035758
77	1	0	-13.683419	1.271946	2.490173
78	1	0	-12.981358	-0.330127	2.284787
79	1	0	-11.921025	1.082995	2.437690
80	1	0	-12.131435	2.980953	0.775494
81	1	0	-13.860310	2.861204	0.502350
82	1	0	-12.746254	2.665584	-0.854826
83	1	0	-15.063082	0.823991	0.410536
84	1	0	-14.268331	0.707123	-1.153717
85	1	0	-8.927552	-0.558967	-0.177395
86	1	0	-11.116144	-2.810890	-1.666861
87	1	0	-10.022520	-2.385636	-0.371320
88	1	0	-10.073334	-1.377522	-1.819968
89	1	0	10.006135	2.406477	-0.092879
90	8	0	13.238170	3.056428	-0.425067
91	8	0	15.345342	1.860332	0.583757
92	1	0	15.077658	2.753839	0.307036
93	8	0	-14.899657	-1.567410	1.160058
94	8	0	-13.108130	-3.101278	-0.366175
95	1	0	-14.748707	-2.523600	1.171806
96	1	0	-15.025384	-1.440161	-0.895740

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DHIR

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-14.028637	1.350854	0.279322
2	6	0	-12.964438	1.670353	1.111170
3	6	0	-11.767450	0.964189	1.057920
4	6	0	-11.631644	-0.089298	0.120845
5	6	0	-12.723053	-0.406805	-0.728880
6	6	0	-13.936717	0.293406	-0.637344
7	6	0	-10.686198	1.346042	2.043961
8	6	0	-10.412525	-0.917030	0.044806
9	6	0	-9.133672	-0.481953	0.060367
10	6	0	-7.942538	-1.312389	0.015890
11	6	0	-8.113142	-2.809620	-0.022610
12	6	0	-6.723693	-0.696003	0.012762
13	6	0	-5.422848	-1.297450	-0.015578
14	6	0	-4.269210	-0.573975	-0.016859
15	6	0	-2.925305	-1.094959	-0.032377
16	6	0	-2.734534	-2.591223	-0.046236
17	6	0	-1.881608	-0.206001	-0.031193
18	6	0	-0.481899	-0.483643	-0.035437
19	6	0	0.482006	0.483801	-0.035539
20	6	0	1.881717	0.206168	-0.031148
21	6	0	2.925404	1.095136	-0.032509
22	6	0	2.734617	2.591395	-0.046780
23	6	0	4.269318	0.574177	-0.016803
24	6	0	5.422939	1.297676	-0.015707
25	6	0	6.723803	0.696271	0.012829
26	6	0	7.942624	1.312698	0.015731
27	6	0	8.113186	2.809919	-0.023292
28	6	0	9.133799	0.482321	0.060432
29	6	0	10.412629	0.917409	0.044589
30	6	0	11.631700	0.089558	0.120887
31	6	0	11.767677	-0.962887	1.059115
32	6	0	12.964543	-1.669230	1.112755
33	6	0	14.028475	-1.350938	0.280099
34	6	0	13.936313	-0.294655	-0.637855
35	6	0	12.722803	0.405785	-0.729677
36	6	0	10.686717	-1.343413	2.046000
37	1	0	-11.123563	1.843157	2.912486
38	1	0	-10.123778	0.479065	2.393527
39	1	0	-13.098923	2.479602	1.821248
40	1	0	-10.581855	-1.987259	-0.041866
41	1	0	-8.950414	0.588929	0.092488
42	1	0	-7.163801	-3.342113	-0.040904
43	1	0	-8.673749	-3.164400	0.848361
44	1	0	-8.678050	-3.117908	-0.908941
45	1	0	-6.728715	0.393488	0.038514
46	1	0	-5.358836	-2.380586	-0.032371
47	1	0	-4.355589	0.512100	-0.001892
48	1	0	-1.686180	-2.883954	-0.056595
49	1	0	-3.195692	-3.053650	0.832608
50	1	0	-3.208148	-3.038571	-0.926274
51	1	0	-2.145051	0.851413	-0.023500
52	1	0	-0.154776	-1.520604	-0.036038
53	1	0	0.154881	1.520760	-0.036432
54	1	0	2.145170	-0.851242	-0.023170
55	1	0	3.208105	3.038487	-0.927018
56	1	0	1.686260	2.884114	-0.057072

57	1	0	3.195894	3.054085	0.831861
58	1	0	4.355716	-0.511892	-0.001533
59	1	0	5.358902	2.380806	-0.032826
60	1	0	6.728859	-0.393211	0.038933
61	1	0	8.677929	3.117933	-0.909825
62	1	0	7.163831	3.342386	-0.041592
63	1	0	8.673942	3.164997	0.847461
64	1	0	10.581991	1.987608	-0.042404
65	1	0	13.099135	-2.477633	1.823778
66	1	0	8.950602	-0.588565	0.093013
67	1	0	11.124358	-1.839267	2.915108
68	1	0	9.961576	-2.040624	1.613349
69	1	0	10.124304	-0.476008	2.394494
70	1	0	-9.961107	2.042576	1.610142
71	1	0	11.521892	1.630853	-2.052497
72	6	0	12.565691	1.495349	-1.772463
73	1	0	12.937996	2.464435	-1.417394
74	1	0	13.107028	1.259794	-2.689826
75	6	0	15.153386	0.038648	-1.473779
76	1	0	15.067459	1.000677	-1.973770
77	1	0	16.056206	0.105199	-0.854272
78	1	0	15.345928	-0.710971	-2.252588
79	8	0	15.162326	-2.106389	0.420751
80	1	0	15.817227	-1.847986	-0.236035
81	8	0	-15.162554	2.106296	0.419546
82	1	0	-15.817504	1.847336	-0.236969
83	6	0	-15.154236	-0.041279	-1.472087
84	1	0	-16.056819	-0.106127	-0.852067
85	1	0	-15.346824	0.706670	-2.252487
86	1	0	-15.068919	-1.004476	-1.969928
87	6	0	-12.565743	-1.497652	-1.770291
88	1	0	-11.522347	-1.630042	-2.053420
89	1	0	-12.933386	-2.467411	-1.412188
90	1	0	-13.110875	-1.265752	-2.686287

DHIR radical cation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-14.100005	-1.320645	-0.078806
2	6	0	-12.991700	-1.892209	-0.697445
3	6	0	-11.759117	-1.262658	-0.698823
4	6	0	-11.628526	-0.005406	-0.038000
5	6	0	-12.777852	0.577659	0.589155
6	6	0	-14.021135	-0.061119	0.547386
7	6	0	-10.642977	-1.939051	-1.459493
8	6	0	-10.396528	0.757839	-0.018159
9	6	0	-9.100300	0.322971	-0.082075
10	6	0	-7.949295	1.173377	-0.076606
11	6	0	-8.125153	2.669888	-0.067229
12	6	0	-6.699248	0.567233	-0.079573
13	6	0	-5.440153	1.192660	-0.076180
14	6	0	-4.247678	0.487293	-0.075664
15	6	0	-2.951194	1.044866	-0.074366
16	6	0	-2.777842	2.543452	-0.073802
17	6	0	-1.863436	0.163340	-0.073916
18	6	0	-0.504507	0.480598	-0.073598
19	6	0	0.504483	-0.480461	-0.073586
20	6	0	1.863412	-0.163206	-0.073974

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21	6	0	2.951165	-1.044739	-0.074397
22	6	0	2.777801	-2.543321	-0.073734
23	6	0	4.247653	-0.487176	-0.075749
24	6	0	5.440123	-1.192553	-0.076231
25	6	0	6.699222	-0.567138	-0.079653
26	6	0	7.949260	-1.173305	-0.076622
27	6	0	8.125087	-2.669818	-0.067195
28	6	0	9.100280	-0.322920	-0.082107
29	6	0	10.396501	-0.757811	-0.018126
30	6	0	11.628526	0.005379	-0.037949
31	6	0	11.759149	1.262684	-0.698663
32	6	0	12.991779	1.892147	-0.697338
33	6	0	14.100075	1.320458	-0.078811
34	6	0	14.021158	0.060930	0.547379
35	6	0	12.777856	-0.577808	0.589123
36	6	0	10.643003	1.939241	-1.459176
37	1	0	-11.053717	-2.677280	-2.149546
38	1	0	-10.048879	-1.231491	-2.040984
39	1	0	-13.128991	-2.844908	-1.196526
40	1	0	-10.530174	1.828770	0.086459
41	1	0	-8.894957	-0.739894	-0.097365
42	1	0	-7.180180	3.208216	-0.085795
43	1	0	-8.707945	3.001417	-0.930955
44	1	0	-8.665086	2.993642	0.827814
45	1	0	-6.690297	-0.521423	-0.084646
46	1	0	-5.395568	2.276169	-0.074622
47	1	0	-4.312308	-0.599165	-0.076225
48	1	0	-1.733958	2.849173	-0.072776
49	1	0	-3.246267	2.992227	-0.954491
50	1	0	-3.247787	2.991737	0.806333
51	1	0	-2.108210	-0.897571	-0.074106
52	1	0	-0.198186	1.522869	-0.073591
53	1	0	0.198162	-1.522732	-0.073499
54	1	0	2.108193	0.897704	-0.074244
55	1	0	3.247754	-2.991557	0.806423
56	1	0	1.733914	-2.849035	-0.072675
57	1	0	3.246211	-2.992156	-0.954401
58	1	0	4.312291	0.599281	-0.076376
59	1	0	5.395533	-2.276062	-0.074623
60	1	0	6.690289	0.521517	-0.084793
61	1	0	8.665104	-2.993555	0.827802
62	1	0	7.180099	-3.208127	-0.085640
63	1	0	8.707782	-3.001389	-0.930971
64	1	0	10.530100	-1.828742	0.086525
65	1	0	13.129114	2.844860	-1.196377
66	1	0	8.894954	0.739943	-0.097472
67	1	0	11.053730	2.677754	-2.148931
68	1	0	9.957526	2.474379	-0.793867
69	1	0	10.049019	1.231834	-2.040980
70	1	0	-9.957602	-2.474484	-0.794311
71	1	0	11.710494	-1.898687	1.937283
72	6	0	12.626416	-1.883248	1.345404
73	1	0	12.596141	-2.747254	0.671011
74	1	0	13.443122	-2.051688	2.043024
75	6	0	15.292762	-0.516313	1.131707
76	1	0	15.227907	-1.585499	1.315416
77	1	0	16.136072	-0.393400	0.442468
78	1	0	15.569566	-0.040480	2.080298
79	8	0	15.247779	2.039757	-0.134383
80	1	0	15.957118	1.600290	0.348025
81	8	0	-15.247641	-2.040059	-0.134303
82	1	0	-15.956922	-1.600774	0.348354

83	6	0	-15.292681	0.516178	1.131791
84	1	0	-16.136295	0.392306	0.443103
85	1	0	-15.568848	0.041174	2.080981
86	1	0	-15.228121	1.585584	1.314361
87	6	0	-12.626522	1.883042	1.345556
88	1	0	-11.710488	1.898601	1.937258
89	1	0	-12.596560	2.747141	0.671265
90	1	0	-13.443128	2.051203	2.043367

DHIR radical anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	14.002135	-1.427440	0.209993
2	6	0	12.917902	-1.767889	1.005409
3	6	0	11.741871	-1.023632	0.989045
4	6	0	11.633587	0.089669	0.115527
5	6	0	12.752066	0.424566	-0.696383
6	6	0	13.951528	-0.305542	-0.627379
7	6	0	10.646187	-1.425781	1.949807
8	6	0	10.437686	0.945025	0.061111
9	6	0	9.135335	0.540946	0.079649
10	6	0	7.968563	1.375264	0.042026
11	6	0	8.154500	2.871419	0.010327
12	6	0	6.719400	0.778865	0.033888
13	6	0	5.439601	1.374343	0.006374
14	6	0	4.259286	0.643034	0.003481
15	6	0	2.940522	1.139276	-0.011954
16	6	0	2.724518	2.634807	-0.025618
17	6	0	1.866967	0.236307	-0.011116
18	6	0	0.495976	0.493912	-0.014171
19	6	0	-0.495730	-0.493683	-0.014196
20	6	0	-1.866722	-0.236058	-0.009278
21	6	0	-2.940288	-1.138984	-0.009939
22	6	0	-2.724400	-2.634514	-0.025007
23	6	0	-4.259057	-0.642694	0.005966
24	6	0	-5.439381	-1.373950	0.007604
25	6	0	-6.719188	-0.778442	0.035530
26	6	0	-7.968378	-1.374772	0.042474
27	6	0	-8.154356	-2.870877	0.008897
28	6	0	-9.135105	-0.540376	0.080544
29	6	0	-10.437455	-0.944455	0.060739
30	6	0	-11.633591	-0.089616	0.115453
31	6	0	-11.742486	1.023418	0.989232
32	6	0	-12.918722	1.767369	1.005390
33	6	0	-14.002635	1.426832	0.209589
34	6	0	-13.951532	0.304974	-0.627882
35	6	0	-12.751854	-0.424725	-0.696748
36	6	0	-10.647223	1.425556	1.950457
37	1	0	11.063604	-1.985037	2.791246
38	1	0	10.113815	-0.556815	2.339996
39	1	0	13.019129	-2.625692	1.663147
40	1	0	10.631651	2.010333	-0.030653
41	1	0	8.934182	-0.528084	0.100746
42	1	0	7.206698	3.408907	0.018713
43	1	0	8.737965	3.221197	0.870880
44	1	0	8.701739	3.189293	-0.886548
45	1	0	6.719679	-0.312786	0.053995
46	1	0	5.372139	2.458230	-0.010161

47	1	0	4.359831	-0.443534	0.017057
48	1	0	1.669310	2.905664	-0.044471
49	1	0	3.167870	3.110471	0.857286
50	1	0	3.195175	3.097760	-0.901015
51	1	0	2.146856	-0.818759	-0.005217
52	1	0	0.153598	1.527587	-0.014625
53	1	0	-0.153368	-1.527359	-0.016504
54	1	0	-2.146564	0.819014	-0.002215
55	1	0	-3.187765	-3.095661	-0.905296
56	1	0	-1.669118	-2.905539	-0.035381
57	1	0	-3.175234	-3.111837	0.853142
58	1	0	-4.359529	0.443868	0.020607
59	1	0	-5.371971	-2.457810	-0.010620
60	1	0	-6.719363	0.313184	0.056990
61	1	0	-8.700495	-3.187772	-0.888999
62	1	0	-7.206589	-3.408412	0.017875
63	1	0	-8.738885	-3.221565	0.868349
64	1	0	-10.631090	-2.009675	-0.032660
65	1	0	-13.020309	2.625034	1.663254
66	1	0	-8.933754	0.528582	0.102840
67	1	0	-11.065056	1.984111	2.792152
68	1	0	-9.896131	2.069307	1.480771
69	1	0	-10.114508	0.556591	2.340176
70	1	0	9.894917	-2.068915	1.479582
71	1	0	-11.608681	-1.642058	-2.060553
72	6	0	-12.627023	-1.574285	-1.676029
73	1	0	-12.856846	-2.543552	-1.214222
74	1	0	-13.290369	-1.459889	-2.534479
75	6	0	-15.189402	-0.074448	-1.414774
76	1	0	-15.194196	-1.127113	-1.692917
77	1	0	-16.100723	0.078726	-0.824443
78	1	0	-15.300204	0.503164	-2.342510
79	8	0	-15.123801	2.223966	0.316736
80	1	0	-15.749166	1.991397	-0.376446
81	8	0	15.123090	-2.224880	0.317411
82	1	0	15.748877	-1.992133	-0.375335
83	6	0	15.189481	0.073429	-1.414332
84	1	0	16.100806	-0.079654	-0.823971
85	1	0	15.300140	-0.504607	-2.341818
86	1	0	15.194428	1.125974	-1.692907
87	6	0	12.627993	1.574355	-1.675470
88	1	0	11.609107	1.644625	-2.057984
89	1	0	12.861273	2.543062	-1.214178
90	1	0	13.289355	1.458275	-2.535253

TOR

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-17.737672	0.500711	0.142971
2	6	0	-16.877972	1.727125	-0.004886
3	6	0	-9.891663	-1.000957	0.138678
4	6	0	-8.595892	-0.584979	0.073108
5	6	0	7.253437	0.541500	-0.294113
6	6	0	8.465946	1.164857	-0.375415
7	6	0	5.947654	1.125241	-0.387841

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8	6	0	-7.419809	-1.415410	0.135296
9	6	0	11.477317	-1.747800	-1.729796
10	6	0	12.401688	-1.147087	-0.697669
11	6	0	-12.867712	-1.807438	0.261542
12	6	0	-12.339526	-0.402097	0.116299
13	6	0	4.797840	0.402989	-0.283536
14	6	0	-11.005622	-0.104157	0.066921
15	6	0	-14.644357	0.580742	0.062299
16	6	0	-13.292333	0.682725	0.025509
17	6	0	-17.642436	3.018733	-0.121317
18	6	0	-15.527669	1.719254	-0.035511
19	6	0	-7.598983	-2.905357	0.291692
20	6	0	-6.191478	-0.813343	0.048556
21	6	0	-4.899578	-1.423070	0.084917
22	6	0	-2.400802	-1.240973	0.012096
23	6	0	-1.351936	-0.364214	-0.108740
24	6	0	-3.739058	-0.713069	-0.016725
25	6	0	-2.216141	-2.729535	0.174203
26	6	0	0.045367	-0.647716	-0.100528
27	6	0	1.011313	0.309386	-0.235093
28	6	0	13.176108	0.627814	0.953903
29	6	0	12.160682	0.010169	-0.037922
30	6	0	2.410400	0.032606	-0.217831
31	6	0	3.452228	0.915123	-0.347182
32	6	0	8.620582	2.646756	-0.606205
33	6	0	9.666809	0.360970	-0.222911
34	6	0	10.939519	0.812962	-0.232832
35	6	0	3.256423	2.397287	-0.549042
36	6	0	14.214918	-0.423875	1.401137
37	6	0	14.779440	-1.235112	0.241223
38	6	0	13.649861	-1.977124	-0.469919
39	6	0	12.457146	1.132005	2.223764
40	1	0	-18.416193	0.397686	-0.712598
41	1	0	-17.169143	-0.424895	0.226610
42	1	0	-18.274102	3.187214	0.760016
43	1	0	-16.980909	3.880431	-0.229854
44	1	0	-15.028656	2.681807	-0.147284
45	1	0	-15.093182	-0.401610	0.170958
46	1	0	-12.863172	1.678598	-0.082629
47	1	0	-10.746130	0.948818	-0.040734
48	1	0	-10.093036	-2.061391	0.250381
49	1	0	-8.415113	0.483675	-0.038856
50	1	0	-6.189803	0.270701	-0.062856
51	1	0	-4.842506	-2.500779	0.198260
52	1	0	-3.819716	0.367475	-0.131105
53	1	0	-13.461830	-1.911436	1.175675
54	1	0	-13.524586	-2.067375	-0.575050
55	1	0	-8.181749	-3.319644	-0.537529
56	1	0	-6.653048	-3.442976	0.325630
57	1	0	-1.169253	-3.027655	0.175054
58	1	0	-2.658587	-3.080198	1.112344
59	1	0	-1.611222	0.687824	-0.224880
60	1	0	0.369810	-1.678318	0.021018
61	1	0	0.684577	1.338967	-0.358730
62	1	0	2.675817	-1.015329	-0.080322
63	1	0	3.733418	2.968949	0.253757
64	1	0	3.711005	2.727940	-1.488679
65	1	0	4.889146	-0.671908	-0.130191
66	1	0	5.876398	2.197019	-0.541562
67	1	0	7.268992	-0.535540	-0.128526
68	1	0	9.141243	3.123470	0.231298
69	1	0	9.217530	2.843893	-1.502585

70	1	0	9.499378	-0.701008	-0.057530
71	1	0	11.095946	1.885605	-0.325881
72	1	0	12.053421	-2.095335	-2.594379
73	1	0	10.720038	-1.050976	-2.084320
74	1	0	14.001940	-2.366160	-1.432768
75	1	0	15.293046	-0.577205	-0.467910
76	1	0	15.016868	0.079357	1.953422
77	1	0	13.191377	1.480911	2.957124
78	1	0	11.870771	0.334870	2.688943
79	1	0	-18.375943	0.579770	1.031450
80	1	0	-18.320240	3.002523	-0.984095
81	1	0	-12.076570	-2.554223	0.299158
82	1	0	-8.143420	-3.141077	1.212008
83	1	0	-2.711076	-3.276218	-0.635111
84	1	0	2.207190	2.685445	-0.575660
85	1	0	7.666881	3.156775	-0.729730
86	1	0	10.957567	-2.630913	-1.336317
87	1	0	13.369129	-2.869988	0.109981
88	1	0	15.532159	-1.945224	0.599479
89	1	0	13.736290	-1.109956	2.111324
90	6	0	13.893703	1.824278	0.286649
91	1	0	14.590800	2.293078	0.989052
92	1	0	14.457496	1.518015	-0.596963
93	1	0	13.186682	2.595471	-0.029621
94	1	0	11.777825	1.961544	2.016835

TOR radical cation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-17.679598	0.524717	0.176347
2	6	0	-16.834135	1.751342	-0.013621
3	6	0	-9.881640	-0.967081	0.145098
4	6	0	-8.559535	-0.567051	0.065910
5	6	0	7.211654	0.469085	-0.299521
6	6	0	8.435254	1.111482	-0.360796
7	6	0	5.929235	1.051552	-0.389037
8	6	0	-7.427269	-1.410010	0.141765
9	6	0	11.419982	-1.837752	-1.576461
10	6	0	12.370598	-1.161809	-0.618930
11	6	0	-12.840748	-1.760990	0.309517
12	6	0	-12.315625	-0.360506	0.123426
13	6	0	4.759570	0.323353	-0.296539
14	6	0	-10.961263	-0.067738	0.057393
15	6	0	-14.604041	0.628337	0.061407
16	6	0	-13.240771	0.723800	0.011062
17	6	0	-17.603397	3.033222	-0.157855
18	6	0	-15.476252	1.757331	-0.058316
19	6	0	-7.610613	-2.896070	0.326622
20	6	0	-6.166178	-0.815842	0.039262
21	6	0	-4.916326	-1.442233	0.082947
22	6	0	-2.426090	-1.293315	0.001882
23	6	0	-1.343013	-0.413874	-0.128817
24	6	0	-3.720552	-0.742211	-0.032209
25	6	0	-2.244232	-2.781104	0.177204
26	6	0	0.018507	-0.719712	-0.116811
27	6	0	1.013274	0.244827	-0.254096
28	6	0	13.180350	0.726478	0.897114
29	6	0	12.130997	0.027914	-0.003601

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30	6	0	2.379691	-0.047305	-0.235190
31	6	0	3.445754	0.847242	-0.359797
32	6	0	8.569004	2.598822	-0.559442
33	6	0	9.621886	0.311261	-0.218020
34	6	0	10.896402	0.787278	-0.182974
35	6	0	3.241321	2.329212	-0.552241
36	6	0	14.259469	-0.280104	1.352685
37	6	0	14.793235	-1.138188	0.213000
38	6	0	13.653218	-1.938708	-0.412795
39	6	0	12.514208	1.289367	2.172014
40	1	0	-18.365692	0.400497	-0.669067
41	1	0	-17.110091	-0.397555	0.281010
42	1	0	-18.228765	3.214687	0.724190
43	1	0	-16.951571	3.896916	-0.295880
44	1	0	-14.986507	2.719257	-0.200277
45	1	0	-15.053018	-0.349564	0.199394
46	1	0	-12.808676	1.713482	-0.125685
47	1	0	-10.699054	0.980212	-0.077857
48	1	0	-10.092554	-2.022142	0.280907
49	1	0	-8.367787	0.495841	-0.068646
50	1	0	-6.155885	0.265121	-0.090833
51	1	0	-4.871887	-2.518029	0.211504
52	1	0	-3.789713	0.336557	-0.159912
53	1	0	-13.414439	-1.841936	1.237704
54	1	0	-13.512325	-2.037337	-0.508316
55	1	0	-8.197808	-3.322954	-0.491499
56	1	0	-6.667834	-3.437444	0.363741
57	1	0	-1.199245	-3.083153	0.163414
58	1	0	-2.667484	-3.119047	1.127712
59	1	0	-1.595619	0.638024	-0.252902
60	1	0	0.335707	-1.751227	0.006688
61	1	0	0.690585	1.274725	-0.378442
62	1	0	2.644921	-1.094962	-0.103633
63	1	0	3.709408	2.896960	0.257064
64	1	0	3.694784	2.667234	-1.488479
65	1	0	4.849323	-0.752066	-0.155217
66	1	0	5.856675	2.124389	-0.530009
67	1	0	7.235923	-0.609800	-0.155864
68	1	0	9.071497	3.062628	0.294955
69	1	0	9.172645	2.821141	-1.443744
70	1	0	9.460708	-0.753843	-0.083042
71	1	0	11.022337	1.866331	-0.218930
72	1	0	11.976530	-2.279488	-2.408076
73	1	0	10.671111	-1.166149	-1.993101
74	1	0	13.969718	-2.367357	-1.370025
75	1	0	15.265539	-0.509857	-0.548811
76	1	0	15.071316	0.270324	1.839764
77	1	0	13.277532	1.690973	2.844870
78	1	0	11.969427	0.510785	2.712954
79	1	0	-18.309937	0.631399	1.066391
80	1	0	-18.289367	2.982869	-1.011601
81	1	0	-12.052232	-2.509363	0.348354
82	1	0	-8.145842	-3.112258	1.255810
83	1	0	-2.750904	-3.334970	-0.618319
84	1	0	2.191668	2.612809	-0.580801
85	1	0	7.611464	3.099873	-0.683395
86	1	0	10.891113	-2.667665	-1.090789
87	1	0	13.416728	-2.807977	0.220321
88	1	0	15.572265	-1.815825	0.574730
89	1	0	13.829129	-0.935804	2.119803
90	6	0	13.838492	1.893194	0.124936
91	1	0	14.555841	2.415359	0.765195

92	1	0	14.368554	1.546722	-0.764250
93	1	0	13.103592	2.633526	-0.202949
94	1	0	11.813265	2.099851	1.958753

TOR radical anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-17.758447	0.672239	0.134226
2	6	0	-16.830516	1.852560	0.022792
3	6	0	-9.921767	-1.103771	0.147293
4	6	0	-8.600692	-0.698871	0.081009
5	6	0	7.243639	0.616812	-0.327814
6	6	0	8.482812	1.220673	-0.396237
7	6	0	5.956700	1.201088	-0.414001
8	6	0	-7.445093	-1.513641	0.126904
9	6	0	11.429835	-1.771791	-1.662034
10	6	0	12.370401	-1.173613	-0.643135
11	6	0	-12.926456	-1.854744	0.263521
12	6	0	-12.367006	-0.459226	0.135042
13	6	0	4.782629	0.473579	-0.323300
14	6	0	-11.010547	-0.201429	0.088653
15	6	0	-14.649174	0.589030	0.092280
16	6	0	-13.284738	0.638728	0.059314
17	6	0	-17.520923	3.187427	-0.074339
18	6	0	-15.480102	1.762958	0.007616
19	6	0	-7.612689	-3.008569	0.265946
20	6	0	-6.188062	-0.912476	0.041565
21	6	0	-4.916900	-1.502652	0.062376
22	6	0	-2.418716	-1.274703	-0.025421
23	6	0	-1.343029	-0.378515	-0.138734
24	6	0	-3.731608	-0.775385	-0.037155
25	6	0	-2.200943	-2.764739	0.110230
26	6	0	0.026303	-0.641148	-0.142425
27	6	0	1.017792	0.336713	-0.265663
28	6	0	13.195696	0.624923	0.951147
29	6	0	12.153501	0.010813	-0.018492
30	6	0	2.390114	0.074770	-0.259145
31	6	0	3.460204	0.969004	-0.374882
32	6	0	8.654628	2.703914	-0.609748
33	6	0	9.661938	0.409546	-0.242963
34	6	0	10.953327	0.837071	-0.222049
35	6	0	3.246346	2.454479	-0.548551
36	6	0	14.213293	-0.436549	1.424022
37	6	0	14.746362	-1.302086	0.288969
38	6	0	13.589530	-2.037497	-0.383720
39	6	0	12.504834	1.184309	2.213173
40	1	0	-18.442731	0.625645	-0.723813
41	1	0	-17.234920	-0.282244	0.187796
42	1	0	-18.157220	3.379164	0.801250
43	1	0	-16.807826	4.011657	-0.152519
44	1	0	-14.931381	2.702335	-0.080466
45	1	0	-15.136002	-0.377250	0.187915
46	1	0	-12.828061	1.625275	-0.035679
47	1	0	-10.733067	0.849826	-0.007353
48	1	0	-10.131430	-2.164491	0.248283
49	1	0	-8.422617	0.372869	-0.019634
50	1	0	-6.196679	0.174553	-0.055881
51	1	0	-4.846307	-2.582126	0.160162

52	1	0	-3.832420	0.306407	-0.134913
53	1	0	-13.518052	-1.965664	1.180572
54	1	0	-13.595821	-2.093683	-0.571661
55	1	0	-8.202854	-3.422372	-0.560172
56	1	0	-6.659604	-3.536348	0.279706
57	1	0	-1.146697	-3.038343	0.085571
58	1	0	-2.615005	-3.144007	1.051502
59	1	0	-1.621319	0.672044	-0.236476
60	1	0	0.366782	-1.670494	-0.042097
61	1	0	0.677825	1.365516	-0.369411
62	1	0	2.668121	-0.974382	-0.143994
63	1	0	3.709682	3.022368	0.266870
64	1	0	3.698431	2.815866	-1.479712
65	1	0	4.883385	-0.604815	-0.190750
66	1	0	5.885472	2.276358	-0.547142
67	1	0	7.251581	-0.464314	-0.177310
68	1	0	9.141204	3.181271	0.250430
69	1	0	9.288624	2.909775	-1.480432
70	1	0	9.477478	-0.653055	-0.094511
71	1	0	11.127373	1.909279	-0.281906
72	1	0	11.997582	-2.201040	-2.496429
73	1	0	10.728928	-1.041784	-2.064416
74	1	0	13.926535	-2.476807	-1.331311
75	1	0	15.266998	-0.680699	-0.448073
76	1	0	15.033233	0.064302	1.953550
77	1	0	13.256521	1.532833	2.930541
78	1	0	11.900524	0.416234	2.703359
79	1	0	-18.394333	0.750670	1.026666
80	1	0	-18.185768	3.237230	-0.948253
81	1	0	-12.147487	-2.616145	0.283913
82	1	0	-8.142319	-3.266794	1.190634
83	1	0	-2.698371	-3.314090	-0.697045
84	1	0	2.191608	2.725679	-0.574203
85	1	0	7.705778	3.214545	-0.770064
86	1	0	10.837938	-2.595475	-1.240847
87	1	0	13.290719	-2.898875	0.235508
88	1	0	15.486641	-2.017626	0.665214
89	1	0	13.723898	-1.086713	2.160529
90	6	0	13.939495	1.783179	0.245809
91	1	0	14.654631	2.255056	0.929245
92	1	0	14.487561	1.436256	-0.633205
93	1	0	13.247432	2.559613	-0.089028
94	1	0	11.843981	2.022530	1.987021

LYC

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.510429	-0.885407	0.523626
2	6	0	10.328863	-1.644211	0.186670
3	6	0	9.071479	-1.143256	0.279893
4	6	0	7.840109	-1.832638	-0.036713
5	6	0	6.658346	-1.160119	0.113799
6	6	0	5.330532	-1.632412	-0.137188
7	6	0	4.219750	-0.863074	0.040596
8	6	0	2.853842	-1.256871	-0.190949
9	6	0	1.862050	-0.336792	0.036041
10	6	0	0.453863	-0.494729	-0.126835
11	6	0	-0.453838	0.494494	0.126814

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12	6	0	-1.862026	0.336561	-0.036062
13	6	0	-2.853809	1.256653	0.190910
14	6	0	-4.219722	0.862869	-0.040627
15	6	0	-5.330490	1.632237	0.137120
16	6	0	-6.658313	1.159962	-0.113849
17	6	0	-7.840058	1.832525	0.036615
18	6	0	-9.071449	1.143164	-0.279952
19	6	0	-10.328815	1.644177	-0.186781
20	6	0	7.922842	-3.259550	-0.518195
21	6	0	2.580904	-2.660157	-0.672897
22	6	0	-2.580854	2.659947	0.672823
23	6	0	-7.922746	3.259471	0.518005
24	6	0	-11.510410	0.885396	-0.523681
25	6	0	-12.800645	1.285352	-0.467806
26	6	0	-13.241589	2.658670	-0.032442
27	6	0	12.800683	-1.285296	0.467697
28	6	0	13.241692	-2.658548	0.032188
29	1	0	-11.322373	-0.133037	-0.863867
30	1	0	-10.462166	2.663699	0.161166
31	1	0	-8.960741	0.115828	-0.626191
32	1	0	-13.776520	2.623861	0.923630
33	1	0	-12.415384	3.359435	0.084169
34	1	0	-8.516581	3.330099	1.435353
35	1	0	-6.945842	3.691530	0.727449
36	1	0	-6.725277	0.131394	-0.467772
37	1	0	-5.206653	2.651763	0.487547
38	1	0	-4.365159	-0.158410	-0.391346
39	1	0	-2.965115	3.399990	-0.036729
40	1	0	-3.076650	2.850145	1.630442
41	1	0	-2.181980	-0.645345	-0.384139
42	1	0	-0.071579	1.451860	0.472550
43	1	0	0.071605	-1.452093	-0.472578
44	1	0	2.181999	0.645112	0.384129
45	1	0	3.076695	-2.850322	-1.630525
46	1	0	2.965182	-3.400212	0.036633
47	1	0	4.365170	0.158195	0.391350
48	1	0	5.206715	-2.651923	-0.487663
49	1	0	6.725284	-0.131568	0.467778
50	1	0	8.516665	-3.330099	-1.435557
51	1	0	6.945951	-3.691633	-0.727650
52	1	0	8.960735	-0.115951	0.626212
53	1	0	10.462254	-2.663697	-0.161365
54	1	0	11.322348	0.132983	0.863913
55	1	0	12.415528	-3.359364	-0.084409
56	1	0	13.776539	-2.623626	-0.923926
57	1	0	-8.411415	3.896990	-0.226226
58	1	0	-13.939257	3.088057	-0.760816
59	1	0	-1.519781	2.860242	0.809663
60	1	0	1.519833	-2.860466	-0.809733
61	1	0	8.411545	-3.897099	0.225989
62	1	0	13.939452	-3.087942	0.760470
63	6	0	-13.906888	0.330252	-0.850387
64	1	0	-14.551289	0.801339	-1.605954
65	1	0	-13.482590	-0.561687	-1.320415
66	6	0	-14.796886	-0.116915	0.338244
67	1	0	-14.163050	-0.581117	1.097302
68	1	0	-15.237187	0.770948	0.808672
69	6	0	13.906880	-0.330184	0.850379
70	1	0	13.482533	0.561697	1.320473
71	1	0	14.551285	-0.801307	1.605919
72	6	0	14.796883	0.117125	-0.338196
73	1	0	14.163040	0.581351	-1.097233

74	1	0	15.237247	-0.770676	-0.808682
75	6	0	-15.907117	-1.031419	-0.098252
76	1	0	-16.623007	-0.569810	-0.779984
77	6	0	-16.113380	-2.313553	0.225580
78	6	0	15.907051	1.031658	0.098401
79	1	0	16.622957	0.570032	0.780104
80	6	0	16.113241	2.313833	-0.225315
81	6	0	-15.235767	-3.124176	1.145878
82	1	0	-14.367036	-2.578127	1.512507
83	1	0	-15.803470	-3.470737	2.017774
84	1	0	-14.872647	-4.025754	0.638711
85	6	0	-17.296835	-3.070051	-0.327139
86	1	0	-17.907807	-2.450749	-0.987108
87	1	0	-16.973763	-3.951410	-0.894198
88	1	0	-17.941400	-3.441272	0.478889
89	6	0	17.296640	3.070354	0.327493
90	1	0	16.973505	3.951645	0.894621
91	1	0	17.907636	2.451032	0.987420
92	1	0	17.941199	3.441683	-0.478492
93	6	0	15.235595	3.124484	-1.145556
94	1	0	15.803296	3.471170	-2.017404
95	1	0	14.366911	2.578409	-1.512261
96	1	0	14.872399	4.025987	-0.638312

LYC radical cation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.510429	-0.885407	0.523626
2	6	0	10.328863	-1.644211	0.186670
3	6	0	9.071479	-1.143256	0.279893
4	6	0	7.840109	-1.832638	-0.036713
5	6	0	6.658346	-1.160119	0.113799
6	6	0	5.330532	-1.632412	-0.137188
7	6	0	4.219750	-0.863074	0.040596
8	6	0	2.853842	-1.256871	-0.190949
9	6	0	1.862050	-0.336792	0.036041
10	6	0	0.453863	-0.494729	-0.126835
11	6	0	-0.453838	0.494494	0.126814
12	6	0	-1.862026	0.336561	-0.036062
13	6	0	-2.853809	1.256653	0.190910
14	6	0	-4.219722	0.862869	-0.040627
15	6	0	-5.330490	1.632237	0.137120
16	6	0	-6.658313	1.159962	-0.113849
17	6	0	-7.840058	1.832525	0.036615
18	6	0	-9.071449	1.143164	-0.279952
19	6	0	-10.328815	1.644177	-0.186781
20	6	0	7.922842	-3.259550	-0.518195
21	6	0	2.580904	-2.660157	-0.672897
22	6	0	-2.580854	2.659947	0.672823
23	6	0	-7.922746	3.259471	0.518005
24	6	0	-11.510410	0.885396	-0.523681
25	6	0	-12.800645	1.285352	-0.467806
26	6	0	-13.241589	2.658670	-0.032442
27	6	0	12.800683	-1.285296	0.467697
28	6	0	13.241692	-2.658548	0.032188
29	1	0	-11.322373	-0.133037	-0.863867
30	1	0	-10.462166	2.663699	0.161166
31	1	0	-8.960741	0.115828	-0.626191

32	1	0	-13.776520	2.623861	0.923630
33	1	0	-12.415384	3.359435	0.084169
34	1	0	-8.516581	3.330099	1.435353
35	1	0	-6.945842	3.691530	0.727449
36	1	0	-6.725277	0.131394	-0.467772
37	1	0	-5.206653	2.651763	0.487547
38	1	0	-4.365159	-0.158410	-0.391346
39	1	0	-2.965115	3.399990	-0.036729
40	1	0	-3.076650	2.850145	1.630442
41	1	0	-2.181980	-0.645345	-0.384139
42	1	0	-0.071579	1.451860	0.472550
43	1	0	0.071605	-1.452093	-0.472578
44	1	0	2.181999	0.645112	0.384129
45	1	0	3.076695	-2.850322	-1.630525
46	1	0	2.965182	-3.400212	0.036633
47	1	0	4.365170	0.158195	0.391350
48	1	0	5.206715	-2.651923	-0.487663
49	1	0	6.725284	-0.131568	0.467778
50	1	0	8.516665	-3.330099	-1.435557
51	1	0	6.945951	-3.691633	-0.727650
52	1	0	8.960735	-0.115951	0.626212
53	1	0	10.462254	-2.663697	-0.161365
54	1	0	11.322348	0.132983	0.863913
55	1	0	12.415528	-3.359364	-0.084409
56	1	0	13.776539	-2.623626	-0.923926
57	1	0	-8.411415	3.896990	-0.226226
58	1	0	-13.939257	3.088057	-0.760816
59	1	0	-1.519781	2.860242	0.809663
60	1	0	1.519833	-2.860466	-0.809733
61	1	0	8.411545	-3.897099	0.225989
62	1	0	13.939452	-3.087942	0.760470
63	6	0	-13.906888	0.330252	-0.850387
64	1	0	-14.551289	0.801339	-1.605954
65	1	0	-13.482590	-0.561687	-1.320415
66	6	0	-14.796886	-0.116915	0.338244
67	1	0	-14.163050	-0.581117	1.097302
68	1	0	-15.237187	0.770948	0.808672
69	6	0	13.906880	-0.330184	0.850379
70	1	0	13.482533	0.561697	1.320473
71	1	0	14.551285	-0.801307	1.605919
72	6	0	14.796883	0.117125	-0.338196
73	1	0	14.163040	0.581351	-1.097233
74	1	0	15.237247	-0.770676	-0.808682
75	6	0	-15.907117	-1.031419	-0.098252
76	1	0	-16.623007	-0.569810	-0.779984
77	6	0	-16.113380	-2.313553	0.225580
78	6	0	15.907051	1.031658	0.098401
79	1	0	16.622957	0.570032	0.780104
80	6	0	16.113241	2.313833	-0.225315
81	6	0	-15.235767	-3.124176	1.145878
82	1	0	-14.367036	-2.578127	1.512507
83	1	0	-15.803470	-3.470737	2.017774
84	1	0	-14.872647	-4.025754	0.638711
85	6	0	-17.296835	-3.070051	-0.327139
86	1	0	-17.907807	-2.450749	-0.987108
87	1	0	-16.973763	-3.951410	-0.894198
88	1	0	-17.941400	-3.441272	0.478889
89	6	0	17.296640	3.070354	0.327493
90	1	0	16.973505	3.951645	0.894621
91	1	0	17.907636	2.451032	0.987420
92	1	0	17.941199	3.441683	-0.478492
93	6	0	15.235595	3.124484	-1.145556

94	1	0	15.803296	3.471170	-2.017404
95	1	0	14.366911	2.578409	-1.512261
96	1	0	14.872399	4.025987	-0.638312

LYC radical anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.503128	0.906079	-0.526713
2	6	0	10.350103	1.690716	-0.177833
3	6	0	9.067715	1.215252	-0.258612
4	6	0	7.859721	1.904480	0.063149
5	6	0	6.647608	1.245102	-0.080428
6	6	0	5.340934	1.708981	0.171955
7	6	0	4.204884	0.930368	-0.013422
8	6	0	2.864844	1.300436	0.210880
9	6	0	1.845423	0.365722	-0.025946
10	6	0	0.466650	0.504363	0.132623
11	6	0	-0.466571	-0.503811	-0.134783
12	6	0	-1.845340	-0.365195	0.023841
13	6	0	-2.864758	-1.299908	-0.213004
14	6	0	-4.204785	-0.929924	0.011516
15	6	0	-5.340824	-1.708557	-0.173836
16	6	0	-6.647480	-1.244819	0.078905
17	6	0	-7.859578	-1.904235	-0.064611
18	6	0	-9.067545	-1.215221	0.257711
19	6	0	-10.349910	-1.690780	0.177126
20	6	0	7.953205	3.330083	0.549560
21	6	0	2.565290	2.697021	0.705006
22	6	0	-2.565213	-2.696420	-0.707343
23	6	0	-7.953072	-3.329683	-0.551476
24	6	0	-11.502909	-0.906413	0.526703
25	6	0	-12.810237	-1.267496	0.510363
26	6	0	-13.283919	-2.644103	0.112765
27	6	0	12.810486	1.267041	-0.510084
28	6	0	13.284135	2.643793	-0.112943
29	1	0	-11.283031	0.114670	0.844567
30	1	0	-10.510977	-2.704914	-0.177068
31	1	0	-8.943937	-0.188412	0.606627
32	1	0	-13.613773	-2.689325	-0.934020
33	1	0	-12.507503	-3.401693	0.234220
34	1	0	-8.542090	-3.399345	-1.474339
35	1	0	-6.975547	-3.765354	-0.755738
36	1	0	-6.712324	-0.216143	0.438780
37	1	0	-5.212111	-2.724935	-0.534436
38	1	0	-4.365413	0.087992	0.370310
39	1	0	-2.960501	-3.454891	-0.021751
40	1	0	-3.028294	-2.883527	-1.683543
41	1	0	-2.182012	0.609768	0.380966
42	1	0	-0.069119	-1.452813	-0.491054
43	1	0	0.069199	1.453372	0.488873
44	1	0	2.182098	-0.609275	-0.382974
45	1	0	3.028184	2.884210	1.681280
46	1	0	2.960767	3.455388	0.019409
47	1	0	4.365519	-0.087618	-0.372013
48	1	0	5.212217	2.725438	0.532330
49	1	0	6.712460	0.216320	-0.439997
50	1	0	8.541870	3.399994	1.472630
51	1	0	6.975655	3.765953	0.753276

52	1	0	8.944112	0.188323	-0.607178
53	1	0	10.511171	2.704968	0.176024
54	1	0	11.283253	-0.115123	-0.844198
55	1	0	12.507956	3.401456	-0.235474
56	1	0	13.613161	2.689594	0.934077
57	1	0	-8.450438	-3.971990	0.185705
58	1	0	-14.141634	-2.955142	0.721849
59	1	0	-1.496978	-2.882009	-0.814045
60	1	0	1.497045	2.882693	0.811461
61	1	0	8.450944	3.972067	-0.187651
62	1	0	14.142384	2.954300	-0.721541
63	6	0	-13.886367	-0.276181	0.880828
64	1	0	-14.531472	-0.699460	1.666569
65	1	0	-13.433976	0.624354	1.308413
66	6	0	-14.792276	0.147710	-0.305457
67	1	0	-14.164073	0.586492	-1.084207
68	1	0	-15.238989	-0.752998	-0.746093
69	6	0	13.886650	0.275436	-0.879660
70	1	0	13.434322	-0.625270	-1.306954
71	1	0	14.532094	0.698249	-1.665375
72	6	0	14.792066	-0.147945	0.307183
73	1	0	14.163501	-0.586186	1.085946
74	1	0	15.238776	0.752933	0.747480
75	6	0	-15.895558	1.076471	0.116004
76	1	0	-16.598807	0.638484	0.826828
77	6	0	-16.108325	2.349379	-0.239312
78	6	0	15.895338	-1.077130	-0.113362
79	1	0	16.598820	-0.639715	-0.824310
80	6	0	16.107870	-2.349820	0.242874
81	6	0	-15.246924	3.132398	-1.198254
82	1	0	-14.388698	2.571071	-1.565811
83	1	0	-15.829712	3.459224	-2.068579
84	1	0	-14.867883	4.045126	-0.722852
85	6	0	-17.278662	3.124715	0.316563
86	1	0	-17.877608	2.524031	1.004725
87	1	0	-16.942593	4.019575	0.855203
88	1	0	-17.939639	3.478052	-0.485081
89	6	0	17.278245	-3.125673	-0.312199
90	1	0	16.942196	-4.020854	-0.850316
91	1	0	17.877428	-2.525527	-1.000625
92	1	0	17.938988	-3.478551	0.489840
93	6	0	15.246162	-3.132087	1.202152
94	1	0	15.828725	-3.458410	2.072817
95	1	0	14.387934	-2.570406	1.569166
96	1	0	14.867100	-4.045082	0.727280

BDOR

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-14.118500	-1.655729	0.257010
2	6	0	-13.722430	-0.890941	1.491396
3	6	0	-12.626998	-0.128091	1.478850
4	6	0	-11.785808	-0.163575	0.197310
5	6	0	-12.683023	0.025436	-1.103355
6	6	0	-14.047805	-0.711719	-0.943857
7	1	0	-14.855110	0.011505	-0.798700
8	6	0	-11.919544	-0.562760	-2.302942
9	6	0	-12.962324	1.515893	-1.367561

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10	6	0	-12.181763	0.678612	2.667532
11	6	0	-10.595785	0.756728	0.229631
12	6	0	-9.319501	0.345611	0.129510
13	6	0	-8.126624	1.181756	0.160713
14	6	0	-8.305437	2.671368	0.299704
15	6	0	-6.909564	0.574197	0.067496
16	6	0	-5.608876	1.180306	0.081618
17	6	0	-4.456412	0.462299	-0.006308
18	6	0	-3.111788	0.983966	0.005024
19	6	0	-2.919414	2.475444	0.118530
20	6	0	-2.070740	0.097103	-0.086041
21	6	0	-0.670618	0.373086	-0.087507
22	6	0	0.289481	-0.593188	-0.184284
23	6	0	1.689597	-0.319117	-0.180514
24	6	0	2.729006	-1.208584	-0.275247
25	6	0	2.532865	-2.698161	-0.409156
26	6	0	4.073395	-0.692352	-0.244733
27	6	0	5.224417	-1.416241	-0.332762
28	6	0	6.524719	-0.819140	-0.285471
29	6	0	7.742915	-1.434560	-0.373587
30	6	0	7.910859	-2.922127	-0.550880
31	6	0	8.928956	-0.607220	-0.292457
32	6	0	10.210885	-1.046671	-0.326063
33	6	0	11.414901	-0.223367	-0.199856
34	6	0	11.528768	1.014241	-0.774045
35	6	0	12.674872	1.884351	-0.461471
36	6	0	13.928431	1.309786	0.196162
37	6	0	13.899009	-0.200671	0.313627
38	6	0	12.532470	-0.804862	0.694587
39	6	0	12.182632	-0.496659	2.170553
40	6	0	12.667017	-2.335894	0.539191
41	6	0	10.511622	1.653477	-1.688178
42	1	0	-12.860924	0.537603	3.511234
43	1	0	-11.173585	0.398486	2.990286
44	1	0	-13.423604	-2.499109	0.098249
45	1	0	-14.289347	-1.269573	-1.853124
46	1	0	-10.932150	-0.107441	-2.414024
47	1	0	-12.472149	-0.395465	-3.232276
48	1	0	-11.779437	-1.643260	-2.194922
49	1	0	-13.415922	1.997365	-0.495725
50	1	0	-13.662247	1.626041	-2.201155
51	1	0	-12.054779	2.065111	-1.630807
52	1	0	-10.802336	1.815943	0.353200
53	1	0	-9.136295	-0.722985	0.016363
54	1	0	-7.361093	3.213049	0.298949
55	1	0	-8.914673	3.070782	-0.517806
56	1	0	-8.825601	2.918780	1.231170
57	1	0	-6.911895	-0.511516	-0.026394
58	1	0	-5.546924	2.260170	0.168732
59	1	0	-4.542631	-0.620470	-0.091324
60	1	0	-1.871397	2.769205	0.107774
61	1	0	-3.414246	2.997588	-0.706756
62	1	0	-3.358344	2.857835	1.045811
63	1	0	-2.336057	-0.956685	-0.165875
64	1	0	-0.340865	1.405901	-0.005922
65	1	0	-0.040766	-1.625612	-0.267032
66	1	0	1.957280	0.733219	-0.089638
67	1	0	3.018758	-3.233265	0.413210
68	1	0	1.483720	-2.987870	-0.411010
69	1	0	2.977072	-3.070465	-1.338110
70	1	0	4.164441	0.388227	-0.139560
71	1	0	5.157117	-2.493596	-0.440924

72	1	0	6.533715	0.263467	-0.162573
73	1	0	8.462517	-3.358907	0.288447
74	1	0	6.960494	-3.447728	-0.624217
75	1	0	8.481440	-3.148282	-1.457466
76	1	0	10.373781	-2.116873	-0.383317
77	1	0	12.925987	-0.949329	2.834118
78	1	0	12.180009	0.575048	2.364007
79	1	0	11.202488	-0.905574	2.430507
80	1	0	11.824882	-2.877590	0.974020
81	1	0	13.565712	-2.671848	1.063393
82	1	0	12.765922	-2.635414	-0.508576
83	1	0	14.659791	-0.512473	1.036005
84	1	0	14.196959	-0.614164	-0.656732
85	1	0	8.747112	0.454748	-0.157315
86	1	0	11.021134	2.274637	-2.426644
87	1	0	9.840299	2.327313	-1.145497
88	1	0	9.900832	0.912362	-2.203292
89	1	0	-12.146794	1.750504	2.443892
90	8	0	-15.455020	-2.154602	0.314801
91	1	0	-15.501318	-2.811956	1.018175
92	8	0	14.085042	1.905603	1.486236
93	8	0	12.652364	3.088547	-0.685281
94	1	0	13.979014	2.858198	1.358891
95	1	0	14.772082	1.611913	-0.441870
96	1	0	-14.374710	-0.949717	2.360463
97	1	0	-11.389633	-1.186372	0.122631

BDOR radical cation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-14.198410	-1.481602	0.256285
2	6	0	-13.785165	-0.680892	1.462534
3	6	0	-12.642064	0.006906	1.458047
4	6	0	-11.751253	-0.160883	0.219495
5	6	0	-12.572140	-0.017182	-1.145076
6	6	0	-13.999786	-0.615822	-0.988567
7	1	0	-14.738808	0.185736	-0.909846
8	6	0	-11.808695	-0.782771	-2.240278
9	6	0	-12.704883	1.459199	-1.560024
10	6	0	-12.186469	0.841908	2.624391
11	6	0	-10.542034	0.720920	0.240770
12	6	0	-9.266888	0.277863	0.161536
13	6	0	-8.082112	1.102592	0.175678
14	6	0	-8.231264	2.596165	0.275075
15	6	0	-6.855272	0.467708	0.100738
16	6	0	-5.580250	1.069493	0.100893
17	6	0	-4.404552	0.343939	0.029282
18	6	0	-3.097944	0.881751	0.027273
19	6	0	-2.897200	2.373930	0.103998
20	6	0	-2.027312	-0.019042	-0.045553
21	6	0	-0.664769	0.278213	-0.056484
22	6	0	0.328948	-0.697473	-0.130629
23	6	0	1.690450	-0.395271	-0.138897
24	6	0	2.766656	-1.289630	-0.210240
25	6	0	2.576649	-2.782880	-0.293087
26	6	0	4.068450	-0.742199	-0.202257
27	6	0	5.253098	-1.455700	-0.267642
28	6	0	6.517239	-0.834831	-0.250817

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29	6	0	7.759516	-1.446449	-0.313773
30	6	0	7.937786	-2.937308	-0.417691
31	6	0	8.916597	-0.594908	-0.277076
32	6	0	10.210211	-1.020733	-0.286849
33	6	0	11.400762	-0.178151	-0.206092
34	6	0	11.475512	1.037888	-0.830124
35	6	0	12.615701	1.959066	-0.575464
36	6	0	13.752188	1.515114	0.339670
37	6	0	13.865975	0.007898	0.401801
38	6	0	12.545359	-0.748867	0.658479
39	6	0	12.132982	-0.654188	2.148009
40	6	0	12.820315	-2.233342	0.318632
41	6	0	10.458564	1.600406	-1.789791
42	1	0	-12.896966	0.774975	3.450105
43	1	0	-11.207516	0.520483	2.997498
44	1	0	-13.576988	-2.390859	0.177228
45	1	0	-14.263714	-1.198251	-1.875298
46	1	0	-10.780801	-0.424085	-2.346114
47	1	0	-12.301793	-0.660404	-3.208352
48	1	0	-11.770742	-1.855409	-2.025992
49	1	0	-13.148018	2.063505	-0.762809
50	1	0	-13.359360	1.544607	-2.431460
51	1	0	-11.742947	1.900999	-1.835785
52	1	0	-10.722799	1.787916	0.327675
53	1	0	-9.101787	-0.795223	0.084231
54	1	0	-7.280406	3.124303	0.263691
55	1	0	-8.831457	2.981556	-0.553975
56	1	0	-8.749211	2.871988	1.198286
57	1	0	-6.871887	-0.618606	0.036409
58	1	0	-5.515497	2.150250	0.160732
59	1	0	-4.488669	-0.739318	-0.028528
60	1	0	-1.849261	2.663646	0.079350
61	1	0	-3.392074	2.877980	-0.730792
62	1	0	-3.324319	2.778433	1.026045
63	1	0	-2.290836	-1.073785	-0.098436
64	1	0	-0.341673	1.313866	-0.004520
65	1	0	0.008181	-1.733774	-0.183192
66	1	0	1.948673	0.660697	-0.083096
67	1	0	3.061898	-3.285919	0.548097
68	1	0	1.530040	-3.078665	-0.285212
69	1	0	3.019966	-3.182956	-1.209398
70	1	0	4.143029	0.341514	-0.138855
71	1	0	5.202587	-2.536834	-0.333418
72	1	0	6.514250	0.251221	-0.179929
73	1	0	8.495762	-3.322384	0.441093
74	1	0	6.994599	-3.477493	-0.460735
75	1	0	8.507521	-3.200122	-1.313328
76	1	0	10.386241	-2.090412	-0.278470
77	1	0	12.918089	-1.079740	2.779456
78	1	0	11.984536	0.379678	2.454940
79	1	0	11.212896	-1.215120	2.336671
80	1	0	12.037883	-2.904723	0.678717
81	1	0	13.746827	-2.545985	0.806519
82	1	0	12.945532	-2.390941	-0.756614
83	1	0	14.598867	-0.266397	1.165990
84	1	0	14.275911	-0.323392	-0.559585
85	1	0	8.719652	0.468994	-0.199579
86	1	0	10.971969	2.162590	-2.570598
87	1	0	9.796561	2.321556	-1.297904
88	1	0	9.844251	0.828432	-2.250851
89	1	0	-12.090552	1.901481	2.361924
90	8	0	-15.573878	-1.848907	0.279657

91	1	0	-15.710101	-2.499704	0.977428
92	8	0	13.506615	2.042629	1.646758
93	8	0	12.615824	3.094690	-1.020133
94	1	0	13.510603	3.005732	1.577823
95	1	0	14.676633	1.945413	-0.065113
96	1	0	-14.466409	-0.649915	2.309766
97	1	0	-11.393838	-1.199435	0.230788

BDOR radical anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	14.104547	-1.814495	-0.208476
2	6	0	13.867537	-0.786036	-1.280875
3	6	0	12.813957	0.030239	-1.196179
4	6	0	11.846071	-0.208497	-0.030155
5	6	0	12.620395	-0.371879	1.350898
6	6	0	13.964529	-1.138465	1.154426
7	1	0	14.810082	-0.448538	1.230926
8	6	0	11.715831	-1.161595	2.313106
9	6	0	12.930684	1.000940	1.973125
10	6	0	12.526060	1.091741	-2.221509
11	6	0	10.705155	0.772643	0.034793
12	6	0	9.402562	0.423822	-0.051603
13	6	0	8.248663	1.294124	0.004726
14	6	0	8.481098	2.773398	0.177137
15	6	0	6.994953	0.738671	-0.095597
16	6	0	5.724073	1.372516	-0.059881
17	6	0	4.535100	0.679903	-0.168388
18	6	0	3.221675	1.210015	-0.135560
19	6	0	3.041808	2.699856	0.032724
20	6	0	2.137348	0.338411	-0.253669
21	6	0	0.767315	0.622443	-0.230918
22	6	0	-0.232546	-0.343415	-0.361413
23	6	0	-1.601232	-0.076965	-0.326162
24	6	0	-2.677248	-0.971741	-0.448479
25	6	0	-2.458670	-2.452140	-0.667327
26	6	0	-3.989792	-0.481727	-0.362935
27	6	0	-5.172883	-1.216112	-0.458555
28	6	0	-6.445785	-0.648997	-0.339260
29	6	0	-7.698386	-1.269432	-0.412187
30	6	0	-7.837927	-2.750635	-0.675880
31	6	0	-8.855871	-0.485532	-0.213948
32	6	0	-10.163652	-0.952820	-0.164906
33	6	0	-11.364841	-0.224125	0.066923
34	6	0	-11.526376	1.149969	-0.142266
35	6	0	-12.769873	1.803369	0.179999
36	6	0	-13.740765	1.158691	1.173617
37	6	0	-13.403784	-0.278476	1.537210
38	6	0	-12.622489	-1.049731	0.453490
39	6	0	-13.502101	-1.261378	-0.800874
40	6	0	-12.296903	-2.435146	1.047410
41	6	0	-10.529099	2.018485	-0.870893
42	1	0	13.265896	1.070572	-3.025679
43	1	0	11.531830	0.963206	-2.660594

44	1	0	13.358750	-2.624717	-0.290761
45	1	0	14.099157	-1.885442	1.942824
46	1	0	10.740658	-0.681853	2.424637
47	1	0	12.173606	-1.234493	3.304862
48	1	0	11.547387	-2.182081	1.953051
49	1	0	13.496843	1.633254	1.281868
50	1	0	13.538000	0.877560	2.875589
51	1	0	12.020293	1.533006	2.257542
52	1	0	10.966879	1.820504	0.152467
53	1	0	9.176364	-0.636600	-0.177193
54	1	0	7.552096	3.341603	0.205410
55	1	0	9.024596	2.986793	1.105873
56	1	0	9.089026	3.179954	-0.640376
57	1	0	6.963882	-0.345642	-0.216530
58	1	0	5.685937	2.450673	0.062362
59	1	0	4.607640	-0.402017	-0.289067
60	1	0	1.994974	3.000317	0.010313
61	1	0	3.462364	3.048051	0.983544
62	1	0	3.556345	3.254198	-0.760675
63	1	0	2.394900	-0.714788	-0.377519
64	1	0	0.442359	1.652828	-0.100580
65	1	0	0.099845	-1.371309	-0.495499
66	1	0	-1.876709	0.968378	-0.179840
67	1	0	-2.921311	-2.787328	-1.602265
68	1	0	-1.403500	-2.718029	-0.715114
69	1	0	-2.908170	-3.043810	0.137838
70	1	0	-4.094124	0.591324	-0.198500
71	1	0	-5.094929	-2.286424	-0.624650
72	1	0	-6.466662	0.426028	-0.154257
73	1	0	-8.535862	-2.944301	-1.497322
74	1	0	-6.889605	-3.216299	-0.942481
75	1	0	-8.227723	-3.282054	0.201063
76	1	0	-10.277476	-2.026728	-0.248380
77	1	0	-14.372884	-1.879804	-0.556521
78	1	0	-13.872256	-0.317289	-1.199195
79	1	0	-12.935533	-1.767408	-1.588796
80	1	0	-11.909104	-3.133841	0.302138
81	1	0	-13.211831	-2.879252	1.452699
82	1	0	-11.566909	-2.369623	1.858354
83	1	0	-14.336689	-0.801782	1.773349
84	1	0	-12.800611	-0.279475	2.451980
85	1	0	-8.676589	0.567211	-0.026905
86	1	0	-11.065468	2.845129	-1.338502
87	1	0	-9.986479	1.461481	-1.638739
88	1	0	-9.780945	2.464197	-0.203252
89	1	0	12.536090	2.094767	-1.781441
90	8	0	15.416302	-2.384705	-0.263719
91	1	0	15.497329	-2.856785	-1.100161
92	8	0	-15.062841	1.247445	0.638032
93	8	0	-13.131185	2.902064	-0.274450
94	1	0	-15.059275	2.089810	0.155944
95	1	0	-13.690620	1.783513	2.080802
96	1	0	14.597361	-0.709194	-2.085242
97	1	0	11.397730	-1.195252	-0.218438

ahLUT

Standard orientation:

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

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1	6	0	-14.678684	-1.379420	0.126401
2	6	0	-14.096631	-0.913092	1.380388
3	6	0	-12.850705	-0.414724	1.434966
4	6	0	-12.000164	-0.421741	0.156424
5	6	0	-12.865326	-0.217412	-1.141098
6	6	0	-14.105944	-1.088257	-1.047482
7	6	0	-12.042924	-0.619554	-2.377382
8	6	0	-13.334187	1.248043	-1.301984
9	6	0	-12.219680	0.016411	2.728203
10	6	0	-10.825504	0.519040	0.224772
11	6	0	-9.540212	0.133855	0.140229
12	6	0	-8.363248	0.990461	0.198318
13	6	0	-8.570511	2.474773	0.355444
14	6	0	-7.134204	0.406684	0.111230
15	6	0	-5.844260	1.035229	0.142591
16	6	0	-4.678797	0.337883	0.058784
17	6	0	-3.343179	0.881913	0.078878
18	6	0	-3.177647	2.376500	0.196732
19	6	0	-2.286112	0.014207	-0.008531
20	6	0	-0.890511	0.314545	-0.010357
21	6	0	0.087008	-0.634996	-0.093677
22	6	0	1.482858	-0.337007	-0.097871
23	6	0	2.538096	-1.209211	-0.166571
24	6	0	2.367778	-2.705768	-0.249304
25	6	0	3.874930	-0.669468	-0.159365
26	6	0	5.038243	-1.374920	-0.212218
27	6	0	6.330368	-0.753809	-0.206873
28	6	0	7.557851	-1.350501	-0.252638
29	6	0	7.752237	-2.844101	-0.309663
30	6	0	8.736054	-0.500330	-0.250423
31	6	0	10.022759	-0.910394	-0.278635
32	6	0	11.207534	-0.032241	-0.281662
33	6	0	11.315854	1.032596	-1.107662
34	6	0	12.494712	1.979510	-1.073923
35	6	0	13.373953	1.877093	0.170240
36	6	0	13.598190	0.413986	0.513925
37	6	0	12.311608	-0.419436	0.727424
38	6	0	11.777888	-0.232405	2.166671
39	6	0	12.716533	-1.902831	0.550847
40	6	0	10.330112	1.384979	-2.195413
41	1	0	-12.898348	-0.141903	3.569292
42	1	0	-11.295084	-0.537779	2.925790
43	1	0	-14.565006	-1.402968	-1.982037
44	1	0	-11.146572	-0.003681	-2.476957
45	1	0	-12.635691	-0.499016	-3.289504
46	1	0	-11.729060	-1.666163	-2.322708
47	1	0	-13.873433	1.593019	-0.416444
48	1	0	-14.010117	1.335355	-2.157179
49	1	0	-12.492151	1.922679	-1.481059
50	1	0	-11.057969	1.572421	0.357819
51	1	0	-9.336060	-0.929812	0.016661
52	1	0	-7.635464	3.031903	0.379525
53	1	0	-9.172452	2.876608	-0.466464
54	1	0	-9.110812	2.699718	1.281257
55	1	0	-7.116020	-0.677815	0.004709
56	1	0	-5.801749	2.115421	0.237212
57	1	0	-4.746047	-0.745827	-0.032680
58	1	0	-2.134596	2.687765	0.193436
59	1	0	-3.676721	2.892885	-0.629789
60	1	0	-3.628291	2.748940	1.122623
61	1	0	-2.532640	-1.044407	-0.086764
62	1	0	-0.579401	1.354102	0.058560

63	1	0	-0.225186	-1.674411	-0.160015
64	1	0	1.731740	0.722209	-0.037590
65	1	0	2.857063	-3.203099	0.594567
66	1	0	1.323683	-3.013421	-0.247358
67	1	0	2.825713	-3.102676	-1.161210
68	1	0	3.946365	0.416501	-0.106364
69	1	0	4.989894	-2.457825	-0.262688
70	1	0	6.319628	0.335084	-0.163895
71	1	0	8.331755	-3.196578	0.550186
72	1	0	6.811839	-3.392621	-0.315586
73	1	0	8.309498	-3.134133	-1.206461
74	1	0	10.219312	-1.978372	-0.251936
75	1	0	12.534471	-0.542247	2.895491
76	1	0	11.532082	0.810363	2.359437
77	1	0	10.884725	-0.840482	2.332891
78	1	0	11.930016	-2.591367	0.866645
79	1	0	13.595110	-2.121214	1.165722
80	1	0	12.972435	-2.129740	-0.488672
81	1	0	14.228293	0.340849	1.405766
82	1	0	14.172741	-0.021499	-0.312271
83	1	0	8.539752	0.568830	-0.209212
84	1	0	10.868278	1.670248	-3.107422
85	1	0	9.718013	2.253445	-1.920743
86	1	0	9.653624	0.568270	-2.440936
87	1	0	-11.939164	1.075367	2.717125
88	8	0	12.788710	2.524800	1.304555
89	1	0	12.630576	3.447998	1.077362
90	1	0	14.347486	2.344509	-0.041157
91	1	0	-14.688579	-0.998773	2.288325
92	1	0	-11.595366	-1.445025	0.083942
93	1	0	12.127905	3.011435	-1.178959
94	1	0	13.114795	1.814322	-1.967741
95	1	0	-15.601286	-1.952339	0.162614

ahLUT radical cation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-14.683168	-1.362604	0.166326
2	6	0	-14.126236	-0.809832	1.395411
3	6	0	-12.876057	-0.323296	1.447816
4	6	0	-11.998086	-0.446272	0.193285
5	6	0	-12.830582	-0.310123	-1.140009
6	6	0	-14.079533	-1.163110	-1.011229
7	6	0	-11.988273	-0.801641	-2.329678
8	6	0	-13.279803	1.146548	-1.400106
9	6	0	-12.270090	0.200986	2.719094
10	6	0	-10.822878	0.483838	0.216853
11	6	0	-9.532614	0.088550	0.152930
12	6	0	-8.374667	0.952913	0.166493
13	6	0	-8.575627	2.441853	0.248170
14	6	0	-7.129067	0.359690	0.107544
15	6	0	-5.870297	1.000722	0.108688
16	6	0	-4.675723	0.309338	0.056988
17	6	0	-3.381487	0.881615	0.054606
18	6	0	-3.222955	2.380115	0.105532
19	6	0	-2.287900	0.010643	0.005848
20	6	0	-0.931809	0.342136	-0.006016
21	6	0	0.085707	-0.609212	-0.052219

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22	6	0	1.440238	-0.277293	-0.067030
23	6	0	2.536735	-1.149437	-0.110323
24	6	0	2.376619	-2.649040	-0.142152
25	6	0	3.825291	-0.577693	-0.125341
26	6	0	5.025130	-1.272426	-0.167496
27	6	0	6.276376	-0.635444	-0.189657
28	6	0	7.531028	-1.234005	-0.231725
29	6	0	7.719161	-2.728318	-0.246506
30	6	0	8.674920	-0.375226	-0.263360
31	6	0	9.976003	-0.796473	-0.261709
32	6	0	11.179297	0.017716	-0.282505
33	6	0	11.262570	1.198232	-0.960284
34	6	0	12.486809	2.078349	-0.901659
35	6	0	13.444234	1.768421	0.246555
36	6	0	13.657817	0.266432	0.322475
37	6	0	12.369677	-0.570682	0.514927
38	6	0	11.991339	-0.636757	2.013050
39	6	0	12.702647	-2.001578	0.026603
40	6	0	10.209005	1.741990	-1.890835
41	1	0	-12.965872	0.104042	3.554458
42	1	0	-11.352615	-0.340123	2.979099
43	1	0	-14.515006	-1.546079	-1.930790
44	1	0	-11.089796	-0.194984	-2.466171
45	1	0	-12.567426	-0.746024	-3.255703
46	1	0	-11.678703	-1.842312	-2.196833
47	1	0	-13.827600	1.554122	-0.547552
48	1	0	-13.943530	1.183362	-2.267457
49	1	0	-12.430303	1.801984	-1.615637
50	1	0	-11.048582	1.544059	0.290924
51	1	0	-9.328986	-0.978891	0.088219
52	1	0	-7.642265	3.000669	0.241828
53	1	0	-9.178797	2.798765	-0.591649
54	1	0	-9.112979	2.710329	1.162517
55	1	0	-7.109366	-0.727436	0.056302
56	1	0	-5.838469	2.083801	0.153032
57	1	0	-4.728889	-0.776803	0.016210
58	1	0	-2.182813	2.697653	0.090048
59	1	0	-3.720198	2.854857	-0.745059
60	1	0	-3.674270	2.789842	1.013730
61	1	0	-2.522667	-1.051835	-0.025954
62	1	0	-0.635546	1.386837	0.021997
63	1	0	-0.210535	-1.653848	-0.078068
64	1	0	1.675115	0.785458	-0.042987
65	1	0	2.871597	-3.113886	0.715216
66	1	0	1.335925	-2.964373	-0.122514
67	1	0	2.826672	-3.072027	-1.044796
68	1	0	3.879877	0.508959	-0.103485
69	1	0	4.990193	-2.355942	-0.187063
70	1	0	6.260035	0.452893	-0.175283
71	1	0	8.299147	-3.054741	0.621849
72	1	0	6.779402	-3.275649	-0.231144
73	1	0	8.269386	-3.044881	-1.136685
74	1	0	10.141071	-1.864015	-0.161140
75	1	0	12.809162	-1.078446	2.590174
76	1	0	11.796450	0.356996	2.411997
77	1	0	11.104796	-1.258844	2.169496
78	1	0	11.940572	-2.734947	0.300143
79	1	0	13.634632	-2.336473	0.490105
80	1	0	12.839678	-2.037870	-1.057966
81	1	0	14.357506	0.035879	1.130195
82	1	0	14.146088	-0.035006	-0.611245
83	1	0	8.469301	0.689664	-0.249503

84	1	0	10.689378	2.218992	-2.751100
85	1	0	9.615151	2.526550	-1.405231
86	1	0	9.523431	0.983581	-2.265336
87	1	0	-11.992681	1.258545	2.642875
88	8	0	12.933411	2.221286	1.502704
89	1	0	12.941411	3.184917	1.510250
90	1	0	14.409230	2.255064	0.049786
91	1	0	-14.740666	-0.820323	2.291658
92	1	0	-11.609966	-1.477552	0.197829
93	1	0	12.161230	3.126214	-0.844440
94	1	0	13.023450	2.004880	-1.859046
95	1	0	-15.611156	-1.923612	0.222136

ahLUT radical anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-14.647039	-1.481066	0.161865
2	6	0	-14.089058	-0.959861	1.405337
3	6	0	-12.861192	-0.414904	1.448850
4	6	0	-11.997332	-0.415316	0.178411
5	6	0	-12.865884	-0.294907	-1.128228
6	6	0	-14.076341	-1.205546	-1.017228
7	6	0	-12.018848	-0.705615	-2.344423
8	6	0	-13.385182	1.146187	-1.342425
9	6	0	-12.254009	0.069930	2.733653
10	6	0	-10.852216	0.565444	0.224990
11	6	0	-9.547028	0.211891	0.149448
12	6	0	-8.391646	1.073625	0.181155
13	6	0	-8.616441	2.559551	0.296982
14	6	0	-7.134217	0.509727	0.108229
15	6	0	-5.863539	1.132861	0.117471
16	6	0	-4.672077	0.426712	0.048688
17	6	0	-3.360375	0.945495	0.047379
18	6	0	-3.170070	2.442582	0.119880
19	6	0	-2.273132	0.062549	-0.017098
20	6	0	-0.905898	0.341255	-0.031049
21	6	0	0.100004	-0.630476	-0.088827
22	6	0	1.467077	-0.354597	-0.104006
23	6	0	2.552989	-1.242515	-0.149624
24	6	0	2.356301	-2.740466	-0.186418
25	6	0	3.864631	-0.729306	-0.160697
26	6	0	5.055375	-1.444125	-0.195350
27	6	0	6.326226	-0.830619	-0.210537
28	6	0	7.584701	-1.407969	-0.241094
29	6	0	7.792975	-2.901615	-0.253150
30	6	0	8.738159	-0.556239	-0.261361
31	6	0	10.048981	-0.935952	-0.252803
32	6	0	11.208233	-0.034591	-0.278751
33	6	0	11.276380	1.061086	-1.075550
34	6	0	12.414586	2.055033	-1.027093
35	6	0	13.340681	1.932620	0.179252
36	6	0	13.616544	0.464457	0.456878
37	6	0	12.361964	-0.415770	0.679077
38	6	0	11.877769	-0.303220	2.142965
39	6	0	12.812013	-1.876461	0.433312
40	6	0	10.268558	1.401004	-2.146476
41	1	0	-12.932788	-0.087105	3.576208
42	1	0	-11.311806	-0.447086	2.946038

43	1	0	-14.518352	-1.566370	-1.944244
44	1	0	-11.136531	-0.070251	-2.440420
45	1	0	-12.601848	-0.623124	-3.268134
46	1	0	-11.678432	-1.741988	-2.257725
47	1	0	-13.952470	1.495610	-0.475836
48	1	0	-14.047409	1.185344	-2.212971
49	1	0	-12.561005	1.841772	-1.520546
50	1	0	-11.114935	1.614870	0.333407
51	1	0	-9.326812	-0.853329	0.053298
52	1	0	-7.683792	3.123118	0.297569
53	1	0	-9.228564	2.938915	-0.531410
54	1	0	-9.152727	2.814039	1.220435
55	1	0	-7.110456	-0.579479	0.033299
56	1	0	-5.817605	2.216079	0.182629
57	1	0	-4.753487	-0.660148	-0.009739
58	1	0	-2.120160	2.733034	0.093550
59	1	0	-3.669772	2.949658	-0.714166
60	1	0	-3.599818	2.856093	1.040345
61	1	0	-2.536417	-0.996026	-0.060974
62	1	0	-0.578824	1.379236	0.007035
63	1	0	-0.228339	-1.668291	-0.122087
64	1	0	1.733318	0.703656	-0.074425
65	1	0	2.838717	-3.227452	0.669386
66	1	0	1.304778	-3.025642	-0.170321
67	1	0	2.800047	-3.179508	-1.087922
68	1	0	3.951120	0.358407	-0.138937
69	1	0	5.002775	-2.528912	-0.211604
70	1	0	6.311305	0.261103	-0.198617
71	1	0	8.340569	-3.237985	0.636796
72	1	0	6.853440	-3.452886	-0.282539
73	1	0	8.386405	-3.216231	-1.120475
74	1	0	10.264689	-1.996370	-0.162532
75	1	0	12.667284	-0.624039	2.832929
76	1	0	11.614072	0.724449	2.386484
77	1	0	11.003689	-0.937224	2.308112
78	1	0	12.057702	-2.601099	0.744571
79	1	0	13.718430	-2.088035	1.011122
80	1	0	13.038157	-2.053456	-0.622791
81	1	0	14.281488	0.373812	1.322733
82	1	0	14.174544	0.080859	-0.406339
83	1	0	8.524562	0.511459	-0.261182
84	1	0	10.785623	1.755603	-3.048491
85	1	0	9.594791	2.214113	-1.844367
86	1	0	9.647414	0.549174	-2.419671
87	1	0	-12.001626	1.134372	2.688954
88	8	0	12.788865	2.526031	1.361098
89	1	0	12.429199	3.387826	1.123121
90	1	0	14.293388	2.436745	-0.049643
91	1	0	-14.681722	-1.045022	2.313772
92	1	0	-11.554585	-1.425675	0.142346
93	1	0	12.007732	3.079114	-1.069427
94	1	0	13.017843	1.966902	-1.944982
95	1	0	-15.549454	-2.086109	0.209787