Supporting Materials for

Ion-Pairing in Polyoxometalate Chemistry: Impact of Fully Hydrated Alkali Metal Cations on Properties of the Keggin $[PW_{12}O_{40}]^{3-}$ Anion

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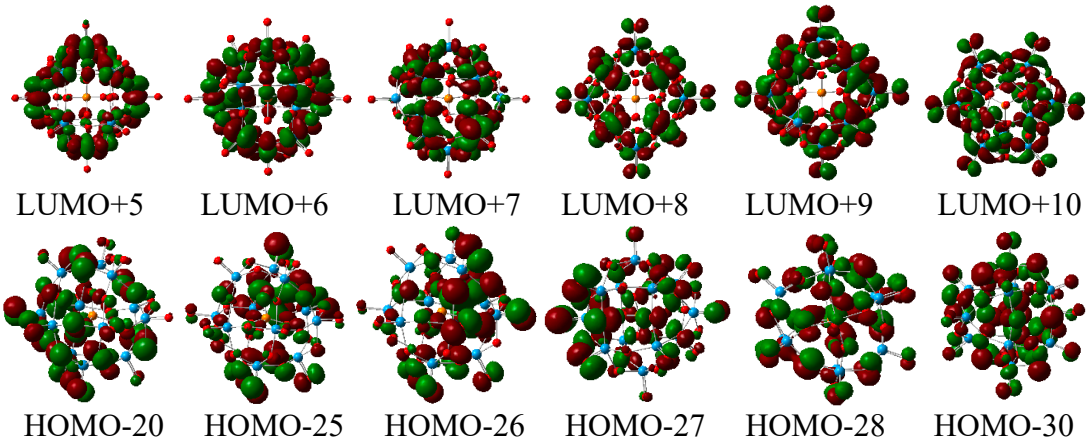


Figure S1. Representative molecular orbitals of $[PW_{12}O_{40}]^{3-}$.

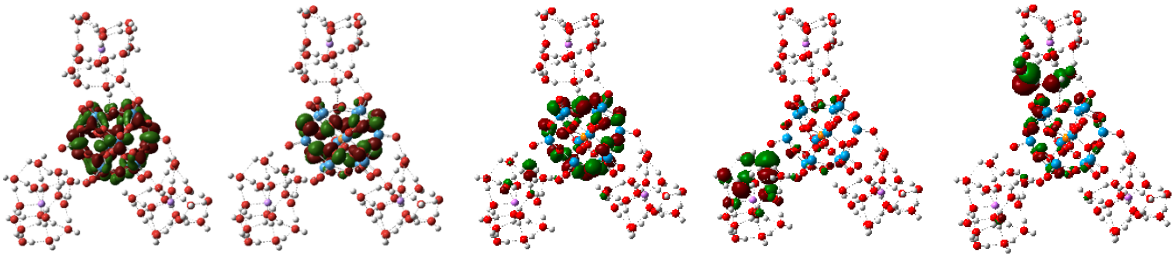


Figure S2-a. Representative molecular orbitals of the $[PW_{12}O_{40}]^{3-}[Li^{+}(H_2O)_n]_3$ complexes.

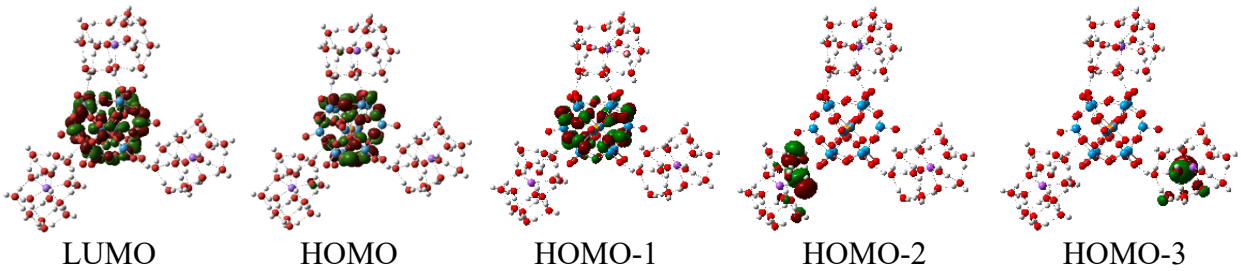
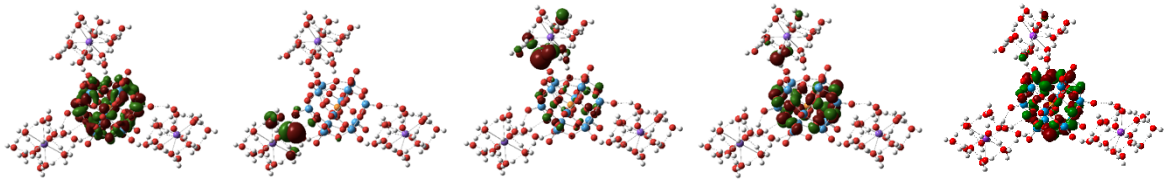
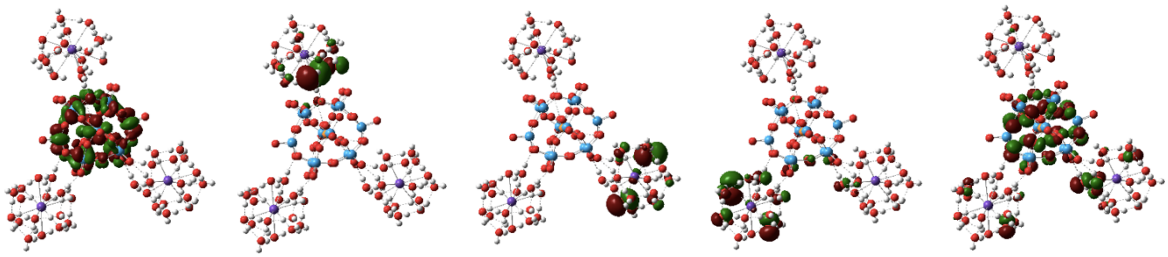


Figure S2-b. Representative molecular orbitals of the $[PW_{12}O_{40}]^{3-}[Na^{+}(H_2O)_n]_3$ complexes.



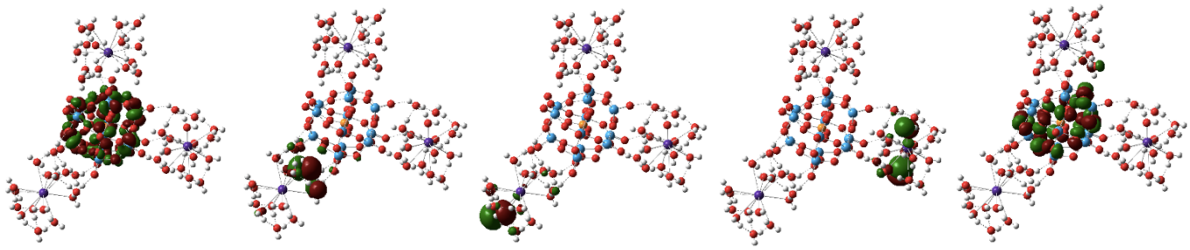
LUMO HOMO HOMO-1 HOMO-2 HOMO-3

Figure S2-c. Representative molecular orbitals of the $[PW_{12}O_{40}]^{3-}[K^{+}(H_2O)_n]_3$ complexes.



LUMO HOMO HOMO-1 HOMO-2 HOMO-6

Figure S2-d. Representative molecular orbitals of the $[PW_{12}O_{40}]^{3-}[Rb^{+}(H_2O)_n]_3$ complexes.



LUMO HOMO HOMO-1 HOMO-2 HOMO-7

Figure S2-e. Representative molecular orbitals of the $[PW_{12}O_{40}]^{3-}[Cs^{+}(H_2O)_n]_3$ complexes.

Table S4. Excited state energies (eV) of the excited singlets S_n, for n=18-96, of the POM anion $[PW_{12}O_{40}]^{3-}$ and $[PW_{12}O_{40}]^{3-}[M^{+}(H_2O)_{16}]_3$ complexes.

S_n	$[PW_{12}O_{40}]^{3-}$	M = Li	M = Na	M = K	M = Rb	M = Cs
18	3.391	2.976	2.987	2.851	2.877	2.423
19	3.391	2.990	3.006	2.897	2.896	2.460
20	3.545	3.024	3.015	2.968	2.926	2.769
21	3.545	3.049	3.030	2.980	2.934	2.794
22	3.546	3.061	3.034	3.012	2.941	2.796
23	3.594	3.081	3.036	3.013	2.954	2.817
24	3.594	3.132	3.038	3.038	2.955	2.831
25	3.595	3.134	3.050	3.051	2.980	2.831
26	3.602	3.188	3.058	3.056	2.982	2.860
27	3.602	3.192	3.062	3.060	2.987	2.868
28	3.603	3.203	3.087	3.072	2.991	2.897
29	3.625	3.211	3.096	3.083	2.999	2.906
30	3.626	3.215	3.144	3.096	3.012	2.919
31	3.627	3.223	3.151	3.128	3.037	2.942
32	3.634	3.234	3.152	3.136	3.039	2.954
33	3.634	3.262	3.159	3.140	3.045	2.955
34	3.635	3.264	3.177	3.180	3.070	2.986
35	3.654	3.265	3.186	3.182	3.096	2.991
36	3.655	3.275	3.274	3.185	3.167	3.030
37	3.655	3.282	3.276	3.203	3.185	3.049
38	3.658	3.283	3.283	3.226	3.214	3.054
39	3.658	3.287	3.285	3.227	3.218	3.072
40	3.659	3.298	3.291	3.253	3.225	3.087
41	3.667	3.306	3.299	3.260	3.226	3.107
42	3.667	3.310	3.310	3.260	3.229	3.140
43	3.668	3.315	3.316	3.269	3.237	3.140
44	3.671	3.320	3.319	3.272	3.240	3.144
45	3.671	3.325	3.323	3.290	3.241	3.147
46	3.671	3.329	3.328	3.297	3.247	3.157
47	3.672	3.340	3.335	3.300	3.248	3.160
48	3.672	3.342	3.336	3.303	3.253	3.168
49	3.673	3.344	3.343	3.305	3.265	3.174
50	3.684	3.345	3.345	3.309	3.268	3.177
51	3.687	3.360	3.356	3.314	3.271	3.177
52	3.689	3.363	3.358	3.319	3.272	3.180
53	3.719	3.367	3.364	3.321	3.276	3.183
54	3.719	3.372	3.367	3.323	3.278	3.186
55	3.743	3.375	3.370	3.331	3.280	3.189
56	3.744	3.376	3.372	3.333	3.282	3.189
57	3.745	3.378	3.374	3.335	3.293	3.192

58	3.745	3.386	3.379	3.337	3.293	3.197
59	3.746	3.386	3.385	3.343	3.295	3.204
60	3.747	3.391	3.389	3.351	3.297	3.206
61	3.753	3.397	3.390	3.354	3.300	3.208
62	3.754	3.400	3.390	3.356	3.302	3.212
63	3.755	3.410	3.393	3.360	3.304	3.214
64	3.785	3.411	3.393	3.363	3.305	3.217
65	3.785	3.421	3.398	3.368	3.308	3.221
66	3.786	3.432	3.400	3.373	3.313	3.221
67	3.835	3.432	3.402	3.377	3.317	3.225
68	3.867	3.436	3.404	3.378	3.318	3.225
69	3.877	3.444	3.410	3.379	3.321	3.227
70	3.877	3.446	3.412	3.383	3.324	3.234
71	3.878	3.449	3.413	3.387	3.326	3.242
72	3.879	3.454	3.416	3.390	3.328	3.244
73	3.879	3.455	3.426	3.400	3.332	3.246
74	3.885	3.475	3.436	3.401	3.333	3.248
75	3.885	3.482	3.441	3.401	3.336	3.252
76	3.885	3.484	3.447	3.403	3.338	3.254
77	3.897	3.485	3.449	3.407	3.339	3.257
78	3.897	3.495	3.450	3.410	3.343	3.258
79	3.898	3.511	3.454	3.417	3.349	3.260
80	3.899	3.514	3.463	3.420	3.351	3.261
81	3.945	3.516	3.468	3.421	3.356	3.265
82	3.946	3.520	3.472	3.426	3.356	3.277
83	3.946	3.526	3.475	3.426	3.357	3.278
84	3.950	3.529	3.477	3.426	3.358	3.279
85	3.950	3.534	3.481	3.434	3.359	3.280
86	3.955	3.538	3.486	3.435	3.363	3.283
87	3.955	3.542	3.492	3.438	3.369	3.292
88	3.955	3.546	3.500	3.446	3.375	3.295
89	3.962	3.552	3.504	3.451	3.375	3.296
90	3.982	3.554	3.507	3.457	3.380	3.300
91	3.982	3.555	3.511	3.458	3.384	3.300
92	3.983	3.559	3.514	3.458	3.385	3.300
93	3.983	3.560	3.516	3.460	3.397	3.306
94	3.984	3.567	3.518	3.466	3.402	3.309
95	3.984	3.569	3.524	3.469	3.404	3.313
96	3.988	3.574	3.526	3.472	3.404	3.313

Table S1. XYZ structure in Å and electronic energy in Hartree of $[PW_{12}O_{40}]^{3-}$.
E = -4167.33969532

Atom	X	Y	Z
O	0.916365	4.393266	2.803884
O	0.192752	0.108915	5.285171
O	4.443378	0.840037	2.749629
O	-2.027634	-0.092986	-3.422913
O	-2.412445	-2.360000	-2.110140
O	-0.162727	-1.973286	-3.452516
O	1.708319	-0.097323	-2.948041
O	-0.128891	1.752939	-2.917021
O	-2.894041	1.278811	-1.268264
O	-3.270060	-0.952732	0.024199
O	0.093658	0.173725	-5.286864
O	-0.980295	-3.264362	-0.010617
O	1.232734	-2.879356	-1.331917
O	2.110832	2.118009	-1.635484
O	-1.373437	3.503994	-1.288987
O	-2.870667	1.263301	1.340721
O	-2.372484	-2.387262	2.124398
O	1.260136	-2.902758	1.273937
O	3.475311	-1.379427	-1.364357
O	0.902036	3.876692	0.015061
O	-1.348204	3.489742	1.358277
O	-4.640651	-0.638598	-2.461747
O	-1.963097	-0.136936	3.459281
O	-0.097493	-2.015960	3.429542
O	3.498909	-1.397023	1.282752
O	3.884004	0.871016	-0.031208
O	2.141547	2.099608	1.621904
O	-0.074879	1.717886	2.942236
O	1.762126	-0.132291	2.911741
O	-0.647478	-0.622541	-1.265994
O	-0.254886	1.530351	0.012169
O	-0.624073	-0.639130	1.269626
O	-0.714192	-4.595733	-2.521680
O	1.529429	-0.267309	-0.015474
O	0.863667	4.425165	-2.767817
O	-3.866482	3.613335	0.056621
O	-4.592651	-0.671874	2.540177
O	-0.670402	-4.628568	2.477252
O	3.580023	-3.895768	-0.060183
O	4.390051	0.876974	-2.821410
P	0.000513	-0.000447	-0.000095
W	0.506133	3.109154	1.743879

W	-0.036396	-0.091173	3.597657
W	3.140333	0.455303	1.702814
W	-0.103007	-0.048409	-3.597804
W	-3.042688	-0.551933	-1.845213
W	-0.607277	-3.008193	-1.881465
W	0.474070	3.129314	-1.714312
W	-2.465612	2.624337	0.039732
W	-3.007213	-0.576357	1.894066
W	-0.570527	-3.032946	1.856597
W	2.604561	-2.485316	-0.039502
W	3.107723	0.476035	-1.755992

Table S2. XYZ geometries in Å and electronic energies in Hartree of $M^+(H_2O)_{16}$.
M = Li, E = -1230.52701352

Atom	X	Y	Z
Li	-0.178039	0.059748	-0.060928
O	0.867697	0.272986	-1.902650
H	1.548319	0.967884	-1.970650
H	1.237576	-0.525467	-2.314765
O	2.643875	2.331069	-1.398822
H	3.124953	3.018654	-1.868184
H	3.299994	1.837674	-0.847397
O	-0.694973	-2.066199	-0.813597
H	-0.718253	-2.620657	-0.010996
H	-1.601294	-2.104565	-1.174545
O	1.545719	-2.398937	-2.307660
H	1.587298	-3.067285	-2.998295
H	0.673437	-2.497940	-1.862774
O	4.070643	0.776905	0.288148
H	3.890911	-0.151959	0.053581
H	3.624949	0.906732	1.145050
O	-1.800156	0.750877	-1.410717
H	-1.092352	0.760745	-2.074376
H	-2.239179	1.629442	-1.460259
O	-3.335716	-1.504396	-1.403068
H	-2.960683	-0.605146	-1.535525
H	-3.926836	-1.670549	-2.143367
O	3.225365	-1.903603	-0.202046
H	3.776137	-2.642169	0.077142
H	2.774018	-2.197346	-1.023765
O	-1.564659	0.302617	1.648498
H	-1.135760	0.227462	2.508641
H	-1.840446	1.240972	1.592225
O	-0.879116	-3.000237	1.808569
H	-0.849669	-3.876082	2.205213
H	-1.826764	-2.723379	1.795909

O	0.628511	2.070053	0.504614
H	1.248680	2.409975	-0.168480
H	1.181780	1.923567	1.297336
O	-1.801343	3.048158	1.183542
H	-1.813444	3.695933	1.895605
H	-0.855881	2.927437	0.934257
O	-3.323236	-1.845066	1.428167
H	-2.893180	-0.975377	1.541112
H	-3.517762	-1.874222	0.474595
O	1.081257	-1.023421	1.308884
H	0.525700	-1.739513	1.668323
H	1.827523	-1.464436	0.850300
O	2.293932	1.076127	2.494846
H	1.847496	0.210333	2.375637
H	2.416068	1.206210	3.440168
O	-3.109807	3.157087	-1.234643
H	-2.837614	3.894588	-1.800308
H	-2.725557	3.347089	-0.355142

M = Na, E = -1223.18977965

Atom	X	Y	Z
Na	-0.151167	-0.060825	0.300497
O	1.298360	0.139825	2.095745
H	1.984262	-0.538475	2.215146
H	1.726219	1.000382	2.223003
O	2.938884	-2.100718	1.764108
H	3.515626	-2.680856	2.269521
H	3.484707	-1.717751	1.034444
O	-0.523937	2.379882	0.505726
H	-0.625663	2.694777	-0.412387
H	-1.393420	2.536149	0.918552
O	1.887355	2.853203	1.677193
H	2.028448	3.691298	2.127442
H	0.973990	2.876531	1.309993
O	4.062571	-0.896229	-0.382248
H	3.876396	0.060270	-0.333149
H	3.526661	-1.213551	-1.131767
O	-2.067648	-0.373057	1.739437
H	-1.782329	-0.609181	2.628323
H	-2.722227	-1.067222	1.484820
O	-3.156871	2.087190	1.339585
H	-2.909014	1.200868	1.684875
H	-3.785877	2.464381	1.961778
O	3.309267	1.843367	-0.425887
H	3.908185	2.467802	-0.847680
H	2.933282	2.311560	0.353422

O	-1.641025	-0.875828	-1.499951
H	-1.245932	-0.834287	-2.377541
H	-1.799664	-1.827308	-1.338813
O	-1.023067	2.570259	-2.239214
H	-1.135091	3.295750	-2.860688
H	-1.924279	2.200473	-2.067348
O	0.700363	-2.342806	0.099389
H	1.404374	-2.491563	0.758544
H	1.164080	-2.317327	-0.760768
O	-1.699084	-3.462789	-0.477555
H	-1.643638	-4.297919	-0.951806
H	-0.793308	-3.266310	-0.145872
O	-3.313385	1.365408	-1.408375
H	-2.913570	0.476858	-1.350016
H	-3.422579	1.657762	-0.484774
O	1.056457	0.782186	-1.661533
H	0.453454	1.427203	-2.074464
H	1.831700	1.289469	-1.346728
O	2.051750	-1.661220	-2.246077
H	1.642572	-0.770177	-2.311080
H	2.096613	-2.015996	-3.139090
O	-3.798599	-2.267111	0.835530
H	-4.275526	-2.773278	1.500662
H	-3.166760	-2.893751	0.431000

M = K, E = -1251.12888467

Atom	X	Y	Z
K	0.000000	0.000000	0.000000
O	2.766141	0.137746	0.554143
H	3.074735	-0.750847	0.325229
H	3.370375	0.762361	0.129364
O	2.224036	-2.512496	-0.142607
H	2.591202	-3.380002	-0.336981
H	1.986423	-2.117095	-1.008699
O	1.089530	2.550283	1.027476
H	0.537676	3.302366	1.265072
H	1.258109	2.074845	1.866664
O	3.351992	2.699021	-0.475890
H	3.887219	3.497035	-0.435883
H	2.591555	2.838782	0.132608
O	1.562782	-1.012998	-2.361799
H	1.866789	-0.092243	-2.478161
H	0.738483	-1.069924	-2.877477
O	0.840695	-1.640548	2.198539
H	1.258893	-2.160412	1.490511
H	-0.062492	-1.978084	2.335678

O	1.094981	0.880799	3.250629
H	1.237790	-0.037511	2.936199
H	1.535215	0.951965	4.102869
O	1.940217	1.779315	-2.622988
H	2.251371	2.097738	-3.476687
H	2.526046	2.200787	-1.953900
O	-2.766141	-0.137746	-0.554143
H	-3.074735	0.750847	-0.325229
H	-3.370375	-0.762361	-0.129364
O	-2.224036	2.512496	0.142607
H	-2.591202	3.380002	0.336981
H	-1.986423	2.117095	1.008699
O	-1.089530	-2.550283	-1.027476
H	-0.537676	-3.302366	-1.265072
H	-1.258109	-2.074845	-1.866664
O	-3.351992	-2.699021	0.475890
H	-3.887219	-3.497035	0.435883
H	-2.591555	-2.838782	-0.132608
O	-1.562782	1.012998	2.361799
H	-1.866789	0.092243	2.478161
H	-0.738483	1.069924	2.877477
O	-0.840695	1.640548	-2.198539
H	-1.258893	2.160412	-1.490511
H	0.062492	1.978084	-2.335678
O	-1.094981	-0.880799	-3.250629
H	-1.237790	0.037511	-2.936199
H	-1.535215	-0.951965	-4.102869
O	-1.940217	-1.779315	2.622988
H	-2.251371	-2.097738	3.476687
H	-2.526046	-2.200787	1.953900

M = Rb, E = -1246.83520609

Atom	X	Y	Z
Rb	0.000000	0.000000	0.000000
O	2.928851	0.113943	0.652665
H	3.206036	-0.767684	0.365273
H	3.487572	0.749257	0.182393
O	2.285087	-2.517078	-0.149241
H	2.626084	-3.401721	-0.312247
H	2.065195	-2.148022	-1.032402
O	1.216672	2.619280	1.112579
H	0.700451	3.381238	1.394476
H	1.335303	2.072251	1.916041
O	3.410716	2.637231	-0.485515
H	3.969490	3.417628	-0.547706
H	2.709260	2.841716	0.171835

O	1.670715	-1.134942	-2.452154
H	1.936612	-0.197061	-2.496820
H	0.803805	-1.148145	-2.896663
O	1.044181	-1.831937	2.345512
H	1.433606	-2.223635	1.543750
H	0.098686	-2.065004	2.349287
O	1.040908	0.787425	3.202928
H	1.235873	-0.134247	2.919559
H	1.437968	0.887107	4.073738
O	1.796172	1.701129	-2.481861
H	2.072331	2.021473	-3.347555
H	2.427585	2.110881	-1.845526
O	-2.928851	-0.113943	-0.652665
H	-3.206036	0.767684	-0.365273
H	-3.487572	-0.749257	-0.182393
O	-2.285087	2.517078	0.149241
H	-2.626084	3.401721	0.312247
H	-2.065195	2.148022	1.032402
O	-1.216672	-2.619280	-1.112579
H	-0.700451	-3.381238	-1.394476
H	-1.335303	-2.072251	-1.916041
O	-3.410716	-2.637231	0.485515
H	-3.969490	-3.417628	0.547706
H	-2.709260	-2.841716	-0.171835
O	-1.670715	1.134942	2.452154
H	-1.936612	0.197061	2.496820
H	-0.803805	1.148145	2.896663
O	-1.044181	1.831937	-2.345512
H	-1.433606	2.223635	-1.543750
H	-0.098686	2.065004	-2.349287
O	-1.040908	-0.787425	-3.202928
H	-1.235873	0.134247	-2.919559
H	-1.437968	-0.887107	-4.073738
O	-1.796172	-1.701129	2.481861
H	-2.072331	-2.021473	3.347555
H	-2.427585	-2.110881	1.845526

M = Cs, E = -1242.82678372

Atom	X	Y	Z
Cs	0.000000	0.000000	0.000000
O	3.256984	0.043261	0.653769
H	3.691604	-0.797065	0.441975
H	3.745908	0.727680	0.176295
O	3.509406	-2.663860	0.043550
H	4.086271	-3.417767	-0.108411
H	3.056886	-2.473332	-0.808908

O	1.658896	2.479171	1.528273
H	1.351350	3.220406	2.058042
H	1.753489	1.728913	2.155331
O	3.451853	2.570404	-0.525960
H	3.890534	3.412376	-0.677322
H	2.843553	2.702140	0.235812
O	2.058708	-1.737161	-2.064200
H	2.230721	-0.792782	-2.263529
H	2.031884	-2.179425	-2.918026
O	1.558205	-2.176971	1.962368
H	2.277281	-2.477950	1.370402
H	1.318192	-2.945932	2.487724
O	1.454534	0.305457	3.253892
H	1.667421	-0.554045	2.834958
H	1.976204	0.327054	4.061641
O	2.130102	1.008783	-2.383856
H	2.064692	1.415303	-3.252946
H	2.637963	1.639812	-1.831810
O	-3.256984	-0.043261	-0.653769
H	-3.691604	0.797065	-0.441975
H	-3.745908	-0.727680	-0.176295
O	-3.509406	2.663860	-0.043550
H	-4.086271	3.417767	0.108411
H	-3.056886	2.473332	0.808908
O	-1.658896	-2.479171	-1.528273
H	-1.351350	-3.220406	-2.058042
H	-1.753489	-1.728913	-2.155331
O	-3.451853	-2.570404	0.525960
H	-3.890534	-3.412376	0.677322
H	-2.843553	-2.702140	-0.235812
O	-2.058708	1.737161	2.064200
H	-2.230721	0.792782	2.263529
H	-2.031884	2.179425	2.918026
O	-1.558205	2.176971	-1.962368
H	-2.277281	2.477950	-1.370402
H	-1.318192	2.945932	-2.487724
O	-1.454534	-0.305457	-3.253892
H	-1.667421	0.554045	-2.834958
H	-1.976204	-0.327054	-4.061641
O	-2.130102	-1.008783	2.383856
H	-2.064692	-1.415303	3.252946
H	-2.637963	-1.639812	1.831810

Table S3. XYZ geometries in Å and electronic energies in Hartree of $[PW_{12}O_{40}]^{3-}[M^{+}(H_2O)_{16}]_3$. M = Li, E = -7858.97536612

Atom	X	Y	Z
O	-4.140484	1.973400	-2.714222
O	-1.056903	-1.266572	-4.986584
O	-4.479107	-2.889871	-1.747616
O	1.634255	1.544994	3.124694
O	3.252912	-0.185976	1.935414
O	1.414354	-1.036385	3.669329
O	-1.255659	-0.851210	3.367082
O	-1.043514	1.693392	2.844734
O	1.197468	2.736718	0.732409
O	2.781050	1.000271	-0.417102
O	0.022642	0.790732	5.332827
O	2.487204	-2.120763	0.236830
O	0.722513	-2.983299	1.941143
O	-3.128458	0.349344	1.975159
O	-1.374748	3.502612	0.869221
O	0.911446	2.189886	-1.798895
O	2.817499	-1.017501	-2.192119
O	0.446684	-3.502002	-0.609695
O	-1.938624	-3.223964	2.279367
O	-3.464954	2.141341	0.015497
O	-1.658438	2.971418	-1.715289
O	3.868135	2.580006	1.699055
O	0.936435	0.202425	-3.601665
O	0.710643	-2.376996	-3.056079
O	-2.203237	-3.750653	-0.293084
O	-3.819138	-1.991236	0.866414
O	-3.427818	-0.295984	-1.146786
O	-1.654320	0.543670	-2.874240
O	-1.835940	-1.999919	-2.325795
O	0.699355	-0.098946	1.327573
O	-1.100075	1.054238	-0.021343
O	0.452611	-0.600109	-1.151887
O	3.435639	-2.852372	2.830543
O	-1.292869	-1.425542	0.485755
O	-3.522597	3.091378	2.687383
O	0.317203	4.862393	-0.966180
O	3.362649	1.636508	-3.109361
O	2.912800	-3.833431	-2.007233
O	-0.477903	-5.451434	1.238295
O	-3.939137	-1.787091	3.686879
P	-0.308810	-0.267712	0.160162
W	-2.872302	1.459945	-1.684518
W	-0.581536	-0.963112	-3.372011

W	-3.130646	-2.197366	-0.935668
W	0.152951	0.431242	3.665473
W	2.535906	1.544266	1.414602
W	2.259154	-1.825797	2.129177
W	-2.498440	2.156919	1.684145
W	-0.127059	3.248631	-0.580055
W	2.159651	0.788381	-2.220153
W	1.860773	-2.569421	-1.526247
W	-0.683904	-3.774286	0.919684
W	-2.805943	-1.502113	2.437001
Li	-9.592898	0.917297	-0.518481
O	-8.229569	1.203624	-2.174046
H	-7.849840	2.091643	-2.315151
H	-7.500761	0.568608	-2.269930
O	-7.501471	3.853219	-2.012641
H	-7.134239	4.523645	-2.595717
H	-6.896044	3.777385	-1.231581
O	-9.159015	-1.247696	-0.672756
H	-9.193439	-1.603825	0.235656
H	-9.856247	-1.727456	-1.160435
O	-6.624244	-0.978502	-1.644368
H	-6.080754	-1.744854	-1.877971
H	-7.487974	-1.319154	-1.325532
O	-6.165364	3.397768	0.264053
H	-5.860569	2.471685	0.292032
H	-6.842505	3.462324	0.961775
O	-10.926238	0.669070	-2.303138
H	-10.106861	0.852026	-2.790154
H	-11.611355	1.272677	-2.667178
O	-11.527748	-1.957317	-1.904038
H	-11.456628	-1.032458	-2.231739
H	-11.749958	-2.503942	-2.663508
O	-5.874152	0.525071	0.542878
H	-5.020405	0.260649	0.915905
H	-5.988412	-0.028029	-0.261844
O	-11.363286	0.930431	0.752046
H	-11.163672	1.196611	1.657054
H	-11.920608	1.655556	0.400355
O	-9.719134	-1.703353	2.021397
H	-9.480017	-2.421754	2.614913
H	-10.654461	-1.858594	1.749469
O	-9.718445	3.170533	-0.451721
H	-9.114643	3.596522	-1.088282
H	-9.386674	3.444959	0.426193
O	-12.419992	3.208330	-0.473393
H	-12.840780	3.921385	0.017726

H	-11.462185	3.433894	-0.524732
O	-12.199236	-1.727804	0.863315
H	-12.121363	-0.755936	0.800941
H	-12.099146	-2.015429	-0.061115
O	-8.459830	0.762281	1.388306
H	-8.828159	-0.026026	1.826230
H	-7.508308	0.568285	1.243706
O	-8.425773	3.385034	1.992382
H	-8.494215	2.409796	2.084214
H	-8.578061	3.764395	2.863216
O	-12.991649	2.337357	-3.019191
H	-12.844911	3.005254	-3.695892
H	-12.948383	2.816432	-2.166721
Li	5.908070	6.957891	-0.627589
O	7.228900	6.435428	-2.134575
H	7.760408	7.115381	-2.583561
H	7.813890	5.675325	-1.989062
O	8.411172	8.830772	-2.916467
H	8.852532	9.239879	-3.666170
H	9.018751	8.909905	-2.140595
O	5.952320	4.730852	-0.003036
H	5.779826	4.767767	0.956379
H	5.175859	4.270489	-0.385631
O	8.460145	4.259474	-0.853064
H	8.739245	3.351351	-1.002308
H	7.546492	4.223432	-0.480650
O	9.721277	8.871253	-0.558318
H	9.783462	7.956979	-0.225298
H	9.089761	9.311326	0.039790
O	4.226920	6.570957	-1.929791
H	4.404595	6.896529	-2.818040
H	3.357564	6.943852	-1.661847
O	3.628943	3.984199	-1.257764
H	3.762857	4.830960	-1.732544
H	3.634740	3.299008	-1.941027
O	9.635922	6.258424	0.581360
H	10.315132	5.985935	1.206538
H	9.386897	5.450547	0.078910
O	4.334125	7.776545	0.736488
H	4.604134	8.157504	1.578130
H	3.880603	8.498689	0.260335
O	5.187691	5.490515	2.575753
H	5.196954	4.851352	3.294986
H	4.277110	5.448567	2.191394
O	6.111662	9.084357	-1.326223
H	6.774771	9.153829	-2.037550

H	6.519721	9.541854	-0.565705
O	3.414140	9.646009	-1.167499
H	3.263973	10.576965	-0.975735
H	4.357903	9.586278	-1.426572
O	2.775367	5.389903	1.271882
H	2.815700	6.227224	0.779324
H	2.774155	4.702120	0.588018
O	7.105490	7.155819	1.246143
H	6.588927	6.626473	1.879074
H	7.998459	6.756198	1.203426
O	7.519500	9.803682	0.977490
H	7.308015	8.921888	1.355944
H	7.426080	10.446201	1.687153
O	1.854145	7.267664	-0.819434
H	1.096793	6.705596	-1.039557
H	1.634720	8.173975	-1.066020
Li	5.698858	-6.006465	-0.591984
O	6.210523	-4.181980	-1.634544
H	5.953147	-3.331066	-1.237306
H	7.151865	-4.098979	-1.861163
O	5.368342	-2.099036	-0.007631
H	4.779143	-1.347291	0.122024
H	5.902566	-2.203720	0.816351
O	7.420419	-6.946685	-1.710934
H	7.756452	-7.659780	-1.135038
H	7.125284	-7.399098	-2.524771
O	8.953051	-4.718014	-1.834980
H	9.670054	-4.646940	-2.472289
H	8.583285	-5.626664	-1.917938
O	6.886521	-2.839615	2.100413
H	7.631317	-3.301624	1.672903
H	6.404791	-3.540508	2.576454
O	4.523625	-6.251071	-2.466356
H	4.743778	-5.320541	-2.625514
H	3.545986	-6.306674	-2.549424
O	5.927292	-8.226738	-3.651475
H	5.304994	-7.490529	-3.451353
H	5.941747	-8.333599	-4.607047
O	8.940038	-4.407685	0.884587
H	9.804006	-4.417496	1.309277
H	9.113499	-4.423217	-0.082502
O	4.521835	-7.736774	0.234111
H	4.730369	-7.941350	1.152534
H	3.592558	-7.429228	0.252344
O	7.699023	-8.980543	0.174881
H	8.398203	-9.617535	0.349778

H	6.991660	-9.461153	-0.318868
O	4.324215	-4.731602	0.556712
H	4.434147	-3.788515	0.330452
H	4.531459	-4.785258	1.510350
O	2.137816	-6.295596	0.107874
H	1.363936	-6.173822	0.677352
H	2.737298	-5.533160	0.270713
O	5.563505	-9.812654	-1.308272
H	5.007191	-9.146357	-0.859306
H	5.682859	-9.455976	-2.206547
O	7.044424	-6.405421	1.146292
H	7.363851	-7.318737	1.033457
H	7.838365	-5.831853	1.121646
O	5.548973	-5.177902	3.024968
H	6.116117	-5.847781	2.588913
H	5.293417	-5.529677	3.882773
O	1.760008	-6.606169	-2.594498
H	1.358572	-5.837208	-3.012624
H	1.708891	-6.423344	-1.632074

M = Na, E = -7836.94948216

Atom	X	Y	Z
O	0.805438	-4.547118	-2.918626
O	-0.555147	-0.285021	-5.090998
O	4.042565	-0.781439	-3.162104
O	-1.597747	-0.513260	3.826922
O	-2.325730	1.758278	2.673926
O	0.107647	1.510745	3.685370
O	2.021381	-0.192074	2.857831
O	0.345436	-2.183652	3.000748
O	-2.647800	-1.884533	1.750847
O	-3.340874	0.355482	0.609621
O	0.772169	-0.660186	5.384014
O	-1.260945	2.834053	0.438633
O	1.138682	2.626536	1.440962
O	2.423806	-2.337772	1.420085
O	-0.966832	-3.978054	1.486480
O	-2.949056	-1.786710	-0.838927
O	-2.850013	1.905196	-1.528300
O	0.806706	2.677326	-1.142941
O	3.458152	1.275362	1.122864
O	1.135754	-4.133095	-0.116778
O	-1.296744	-3.892550	-1.138540
O	-4.348390	-0.157073	3.227642
O	-2.460666	-0.255217	-2.993681
O	-0.747124	1.759039	-3.128587

O	3.135989	1.364264	-1.511334
O	3.854572	-0.895414	-0.343471
O	2.010324	-2.213121	-1.786627
O	-0.387812	-1.963486	-2.783957
O	1.301942	0.016760	-2.946245
O	-0.567063	0.190028	1.535073
O	-0.170363	-1.886168	0.136545
O	-0.884690	0.280754	-0.976955
O	-0.764118	4.107279	2.945476
O	1.443514	0.061416	-0.001066
O	1.528442	-4.764497	2.605429
O	-3.615431	-4.226153	0.480911
O	-4.976885	0.018976	-1.711026
O	-1.395227	4.292325	-2.000131
O	3.210981	3.817062	-0.093321
O	4.732615	-0.928757	2.355045
P	-0.045896	-0.340055	0.172720
W	0.456779	-3.350219	-1.748736
W	-0.571687	-0.149063	-3.386211
W	2.857440	-0.498370	-1.950406
W	0.329908	-0.407960	3.750849
W	-2.841104	-0.081936	2.415449
W	-0.619787	2.556798	2.236139
W	0.888136	-3.465734	1.679010
W	-2.284093	-3.157269	0.344162
W	-3.312298	0.040132	-1.286575
W	-1.089193	2.684377	-1.470164
W	2.350289	2.337681	-0.043190
W	3.291545	-0.617669	1.480426
Na	7.647009	-4.878690	-0.081004
O	6.507392	-6.607106	0.992742
H	5.562202	-6.448590	1.162568
H	6.577767	-7.485312	0.589209
O	3.954884	-5.512253	1.158520
H	3.144964	-5.524964	1.685881
H	3.691954	-5.636337	0.216075
O	9.282885	-6.628352	-0.719852
H	9.624853	-6.260478	-1.555137
H	10.041069	-6.607250	-0.106227
O	7.443635	-8.633784	-0.727569
H	7.761011	-9.541715	-0.727898
H	8.239141	-8.055223	-0.766107
O	3.701407	-5.762164	-1.536331
H	4.367920	-6.393273	-1.864035
H	3.970247	-4.902280	-1.907144
O	8.970528	-4.502343	1.904828

H	8.513754	-4.671706	2.735018
H	9.278780	-3.567496	1.950089
O	11.198654	-5.853191	1.138773
H	10.468196	-5.459892	1.664705
H	11.816465	-6.243029	1.764509
O	5.758672	-7.480039	-2.540883
H	5.572344	-8.009289	-3.322778
H	6.302630	-8.047539	-1.949692
O	8.538255	-2.816691	-1.013828
H	8.530044	-2.752437	-1.974282
H	8.088861	-2.016684	-0.695530
O	9.985952	-4.827629	-2.769143
H	10.578692	-4.942729	-3.518227
H	10.503289	-4.338002	-2.083370
O	5.718559	-3.476619	0.397312
H	5.013043	-3.978759	0.847841
H	5.353804	-3.265657	-0.485467
O	7.225170	-1.237118	0.842911
H	6.745191	-0.485269	1.206340
H	6.588808	-1.985108	0.891177
O	11.310675	-3.649397	-0.660528
H	10.620590	-3.089573	-0.268718
H	11.453148	-4.362652	-0.011786
O	7.166087	-5.109150	-2.428268
H	8.055916	-5.063374	-2.815993
H	6.789841	-5.980953	-2.662816
O	5.063318	-3.387889	-2.318880
H	5.892296	-3.838547	-2.583339
H	4.954728	-2.614016	-2.887853
O	9.804397	-1.949292	1.552581
H	10.215785	-1.445559	2.261950
H	8.927450	-1.537166	1.403894
Na	-9.318697	-2.095098	-0.133270
O	-11.233520	-3.098496	0.741675
H	-11.834950	-2.519610	1.241645
H	-11.770689	-3.529143	0.057862
O	-12.472090	-0.949376	2.033412
H	-13.134572	-0.820470	2.718181
H	-12.807473	-0.494456	1.221856
O	-9.336786	-3.798170	-1.906177
H	-8.919025	-3.291745	-2.628523
H	-8.716569	-4.525504	-1.718239
O	-12.037682	-4.111109	-1.777774
H	-12.398153	-4.930556	-2.129846
H	-11.069118	-4.132658	-1.954838
O	-13.039056	0.232943	-0.333421

H	-13.017104	-0.414408	-1.063371
H	-12.254822	0.795279	-0.473968
O	-7.913143	-3.588978	1.100949
H	-8.228975	-3.853419	1.970918
H	-7.055743	-3.128499	1.254459
O	-7.208754	-5.292834	-0.889751
H	-7.447184	-4.925533	-0.011145
H	-6.874174	-6.182311	-0.740064
O	-12.748731	-1.573874	-2.514320
H	-13.314820	-1.509575	-3.289700
H	-12.642587	-2.533911	-2.331365
O	-7.630881	-0.382557	-0.597277
H	-6.851687	-0.363626	-1.170076
H	-7.312922	0.012004	0.229983
O	-7.839791	-1.926329	-3.340272
H	-7.522227	-1.935849	-4.248258
H	-7.070568	-2.188584	-2.779138
O	-9.777460	-0.294663	1.515751
H	-10.629274	-0.473909	1.953400
H	-9.966784	0.453161	0.914367
O	-7.138934	0.037053	2.140719
H	-6.821091	0.563674	2.880158
H	-8.112692	-0.039395	2.221865
O	-5.881770	-2.924128	-1.708706
H	-5.679323	-2.486936	-0.865323
H	-6.180638	-3.817644	-1.456295
O	-10.125686	-0.811980	-2.038806
H	-9.386534	-0.995192	-2.644054
H	-10.952328	-1.057183	-2.493231
O	-10.487600	1.422471	-0.563809
H	-10.174820	0.763705	-1.224873
H	-10.142535	2.277477	-0.837579
O	-5.662046	-2.088195	1.158177
H	-4.898693	-2.352923	1.685969
H	-6.038020	-1.299428	1.603453
Na	2.360566	9.293193	-0.123461
O	1.506384	8.497833	1.935512
H	0.736895	8.979324	2.284257
H	1.283359	7.554145	1.964636
O	-0.592767	10.317856	2.313588
H	-1.106398	10.632646	3.063203
H	-1.227676	9.868020	1.704183
O	3.144625	7.003147	-0.374810
H	3.083530	6.866592	-1.337081
H	4.086779	6.871237	-0.167226
O	1.287791	5.776800	1.212958

H	1.430589	4.879399	1.537663
H	2.043904	5.986423	0.620132
O	-2.046383	9.051854	0.400908
H	-1.702742	8.157657	0.217592
H	-1.792148	9.583933	-0.375103
O	4.500761	9.755892	0.883287
H	4.466746	10.071987	1.791999
H	4.957212	10.457462	0.370789
O	5.842393	7.510507	0.095543
H	5.528268	8.285504	0.608358
H	6.620163	7.171437	0.548829
O	-0.871704	6.538782	-0.283092
H	-1.218808	5.824611	-0.840098
H	-0.191543	6.123511	0.292199
O	2.588901	10.457273	-2.201548
H	2.867903	10.177757	-3.078367
H	2.775052	11.407811	-2.149141
O	3.066669	7.578240	-3.123090
H	3.224527	7.035216	-3.901465
H	3.912973	8.053944	-2.946182
O	1.132833	11.307624	0.303772
H	0.623343	11.217514	1.129404
H	0.453834	11.253494	-0.399144
O	3.052994	12.872767	-0.880804
H	2.885294	13.816745	-0.954823
H	2.361141	12.510461	-0.286323
O	5.402208	8.840921	-2.377542
H	5.322102	9.753209	-2.049317
H	5.720947	8.334853	-1.607549
O	0.701232	8.350875	-1.652344
H	1.317019	8.037737	-2.334582
H	0.187408	7.581290	-1.333013
O	-0.776429	10.594950	-1.605750
H	-0.218856	9.832264	-1.884391
H	-1.066679	11.035793	-2.409942
O	5.428449	11.455696	-1.031641
H	6.240086	11.971878	-0.996540
H	4.692951	12.102409	-1.009436

M = K, E = -7920.78833242

Atom	X	Y	Z
O	-3.809523	2.122724	2.676655
O	-0.816945	-1.110252	5.065636
O	0.832578	3.470044	3.920433
O	0.092954	-0.936643	-3.880627
O	1.676103	-2.635076	-2.616650

O	2.548598	-0.210107	-3.228756
O	1.578070	2.128831	-2.270614
O	-0.840369	1.389522	-2.913335
O	-1.899287	-1.551625	-2.161073
O	-0.317451	-3.217613	-0.926006
O	1.109340	1.471644	-5.004451
O	2.711263	-2.360317	-0.130180
O	3.517778	0.048169	-0.744952
O	-0.478164	3.165426	-1.023944
O	-3.238384	0.744472	-1.847948
O	-2.378339	-2.211213	0.321686
O	0.930261	-3.646199	1.430330
O	3.059455	-0.567601	1.742700
O	3.153362	2.658816	-0.174240
O	-2.850654	2.547229	0.053179
O	-3.711886	0.116062	0.677890
O	-0.771140	-3.653401	-3.690562
O	-1.157052	-2.598589	2.684182
O	1.306628	-1.856364	3.342948
O	2.704531	2.016866	2.352849
O	1.092245	3.707415	1.106336
O	-1.033791	2.400534	2.030147
O	-1.894143	0.000740	2.662844
O	0.521822	0.710040	3.305324
O	0.733152	-0.531794	-1.375722
O	-1.254592	0.472673	-0.155776
O	0.283181	-1.153664	1.036683
O	4.460025	-2.122393	-2.354464
O	1.102812	1.173325	0.464398
O	-2.829430	3.412279	-2.658542
O	-4.631487	-1.675704	-1.323458
O	-1.576128	-4.875746	1.017380
O	3.558179	-3.303994	2.423070
O	5.202975	1.235299	1.190881
O	1.785906	4.849965	-1.390885
P	0.213740	-0.009580	-0.008969
W	-2.652915	1.423349	1.627524
W	-0.413668	-0.986233	3.408373
W	0.831826	2.436100	2.557131
W	0.910596	0.779309	-3.452575
W	-0.249663	-2.379686	-2.664084
W	2.968736	-1.464036	-1.816616
W	-2.040831	2.239355	-1.690224
W	-3.168306	-0.919299	-0.856413
W	-0.896917	-3.312157	0.893588
W	2.306566	-2.337795	1.762342

W	3.512057	1.087150	0.863011
W	1.410576	3.309355	-0.746772
K	-3.858365	7.609617	0.127356
O	-4.496103	4.906419	0.187324
H	-3.941638	4.111445	0.142121
H	-5.400378	4.602516	0.011505
O	-1.556389	5.276394	1.326894
H	-1.272880	4.353230	1.395796
H	-2.388244	5.347607	1.848007
O	-6.019673	7.005893	-1.677238
H	-6.462161	7.680364	-2.202364
H	-5.345877	6.607289	-2.272353
O	-7.267802	5.108897	-0.215780
H	-8.114005	4.727218	-0.466820
H	-7.030439	5.765005	-0.907832
O	-3.762949	5.855712	2.862278
H	-4.564786	5.715588	2.332409
H	-3.830836	6.778319	3.170043
O	-1.817395	6.238859	-1.293680
H	-1.599916	5.821850	-0.436844
H	-1.220307	6.997233	-1.422864
O	-3.840413	6.115443	-3.105954
H	-3.121409	5.968461	-2.451203
H	-3.897273	5.279745	-3.582694
O	-6.425187	6.715658	1.857120
H	-6.889285	6.624520	2.696158
H	-6.896655	6.120648	1.237325
O	-3.037702	10.287918	0.472994
H	-3.592879	10.834112	-0.099019
H	-2.123232	10.572364	0.325304
O	-5.335586	10.354739	-1.116658
H	-6.012833	10.799438	-1.635719
H	-4.784206	9.861605	-1.759493
O	-1.376139	8.047509	1.676153
H	-1.117094	7.126889	1.839461
H	-1.990705	8.305754	2.386438
O	-0.212453	10.081236	0.358725
H	0.624225	10.452220	0.654045
H	-0.428508	9.339362	0.967494
O	-3.493669	8.890833	-2.568855
H	-2.532738	8.973080	-2.412034
H	-3.601199	8.073426	-3.079203
O	-5.782069	9.439868	1.562982
H	-5.751747	9.786083	0.652552
H	-6.281851	8.604640	1.531672
O	-3.692788	8.657119	3.213084

H	-4.353968	9.123694	2.654535
H	-3.745436	9.069215	4.081136
O	-0.745678	8.745779	-1.955059
H	-0.087883	8.831691	-2.652437
H	-0.416904	9.289548	-1.204089
K	-6.815741	-5.987360	-0.174481
O	-8.950370	-7.768030	-0.459482
H	-8.577315	-8.612405	-0.745974
H	-9.650180	-7.973607	0.176481
O	-6.629828	-9.064329	-1.310929
H	-6.131030	-9.823613	-1.626820
H	-6.379889	-8.951438	-0.367598
O	-9.516553	-4.984894	0.457191
H	-9.687980	-4.059084	0.658426
H	-9.651902	-5.069480	-0.508764
O	-10.677141	-7.116069	1.659851
H	-11.542842	-7.055503	2.074302
H	-10.479782	-6.231859	1.278261
O	-6.272595	-8.537123	1.365960
H	-7.041122	-8.278889	1.910064
H	-5.510849	-8.101005	1.788502
O	-7.286213	-6.855891	-2.993881
H	-6.963606	-7.656753	-2.541893
H	-6.519106	-6.271794	-3.139767
O	-9.321729	-5.133632	-2.325864
H	-8.738897	-5.877659	-2.598345
H	-10.020808	-5.081503	-2.984741
O	-8.284680	-7.344778	2.966945
H	-8.374141	-7.687877	3.862154
H	-9.198783	-7.317040	2.604503
O	-4.770517	-4.215517	0.331526
H	-5.200821	-3.392245	0.607129
H	-4.082844	-3.948147	-0.294724
O	-7.011402	-2.704846	1.159820
H	-7.270116	-1.815386	1.417760
H	-7.277887	-2.804801	0.218143
O	-4.013092	-6.862935	-0.563405
H	-3.730783	-7.778518	-0.657061
H	-3.936691	-6.670999	0.393727
O	-3.081811	-4.685483	-1.943737
H	-2.277033	-4.701959	-2.477231
H	-3.156950	-5.558809	-1.503127
O	-7.462355	-3.210412	-1.488288
H	-6.667991	-3.473271	-1.988250
H	-8.187065	-3.716698	-1.897664
O	-6.597079	-5.129919	2.566967

H	-6.921037	-4.260009	2.274500
H	-7.358867	-5.671860	2.836592
O	-4.362736	-6.700601	2.229784
H	-4.987684	-5.965626	2.404229
H	-3.640043	-6.595958	2.855763
O	-5.564542	-4.624239	-3.068337
H	-5.536212	-4.261662	-3.960262
H	-4.630750	-4.600215	-2.752178
K	9.215999	-1.601445	0.036362
O	7.671343	-3.520904	-1.923650
H	8.512937	-3.921671	-1.644896
H	7.008149	-3.799632	-1.267229
O	10.042187	-4.509751	-0.571315
H	10.334215	-5.383901	-0.851012
H	9.567935	-4.641424	0.277729
O	6.492691	-1.008211	-0.161082
H	6.086836	-0.249312	0.284514
H	6.513575	-0.789406	-1.113671
O	5.690260	-3.558916	0.143576
H	4.776259	-3.767025	-0.084729
H	5.788234	-2.595041	-0.036879
O	8.854847	-4.042201	1.802433
H	7.983732	-3.815209	2.178815
H	9.503227	-3.686827	2.436850
O	10.344089	-1.947942	-2.468588
H	10.999880	-2.646166	-2.557523
H	10.802218	-1.131650	-2.735260
O	7.147192	-0.976679	-2.878832
H	7.425812	-1.897518	-2.679881
H	6.286186	-1.070158	-3.303611
O	6.454901	-2.909266	2.719363
H	5.867732	-3.117483	3.453670
H	5.953441	-3.172880	1.919566
O	10.800306	0.341367	1.259651
H	10.383464	1.208848	1.309090
H	11.640163	0.468924	0.789631
O	8.125190	1.457659	1.192055
H	7.193755	1.711031	1.254635
H	8.279447	1.299655	0.238352
O	12.003605	-2.684709	0.569291
H	11.531673	-3.429181	0.157982
H	11.677326	-2.619531	1.487432
O	12.958116	-0.307211	-0.408640
H	13.917055	-0.269750	-0.344665
H	12.700445	-1.219872	-0.148937
O	8.801178	0.836832	-1.455194

H	9.697838	0.921092	-1.830199
H	8.265716	0.392396	-2.133239
O	8.438232	-0.858767	2.789801
H	8.279937	-0.026570	2.301256
H	7.607549	-1.365287	2.786137
O	10.698307	-2.401864	3.059415
H	10.032816	-1.679620	3.064373
H	11.139072	-2.372888	3.914033
O	11.416028	0.641944	-2.476322
H	11.851242	1.229264	-3.101743
H	12.087674	0.408294	-1.799996

M = Rb, E = -7907.90903720

Atom	X	Y	Z
O	-4.151650	-3.027590	-2.374350
O	-0.540712	-5.444516	0.114439
O	-4.150417	-3.050906	2.638128
O	0.890146	3.344198	-1.166184
O	2.801403	2.049061	0.139998
O	0.918757	3.330147	1.467234
O	-1.721191	2.733734	1.478044
O	-1.742481	2.745952	-1.135071
O	0.593899	1.206260	-2.773587
O	2.477125	-0.045939	-1.506464
O	-0.851770	5.123179	0.174656
O	2.501280	-0.082331	1.765891
O	0.619081	1.171023	3.072288
O	-3.548646	1.379488	0.174983
O	-2.060141	1.152752	-3.281402
O	0.655715	-1.409844	-2.790387
O	2.926988	-2.158584	0.115145
O	0.695706	-1.441038	3.052975
O	-2.020613	1.108150	3.607493
O	-3.895634	-0.240032	-1.949506
O	-1.976823	-1.486431	-3.300835
O	3.156447	2.505769	-2.632013
O	1.109645	-3.550129	-1.194203
O	1.115915	-3.566311	1.435909
O	-1.941845	-1.537754	3.586826
O	-3.852328	-0.261446	2.271255
O	-3.431303	-1.853413	0.146468
O	-1.555493	-3.105085	-1.177572
O	-1.546676	-3.121525	1.440113
O	0.362408	1.140486	0.147573
O	-1.402367	-0.165756	-1.119769
O	0.430472	-1.396870	0.129463

O	3.185545	2.450689	2.904155
O	-1.384275	-0.182626	1.418969
O	-4.333151	2.527719	-2.334854
O	-0.319086	-0.100100	-5.140455
O	3.288232	-2.522205	-2.668644
O	3.325436	-2.583905	2.882944
O	-0.269340	-0.181248	5.429619
O	-4.311776	2.504736	2.686091
P	-0.501226	-0.150214	0.144297
W	-2.988359	-1.950928	-1.734895
W	-0.302298	-3.751390	0.124915
W	-2.977753	-1.970289	2.018483
W	-0.519987	3.445691	0.164371
W	1.981927	1.820737	-1.580319
W	1.998909	1.763002	1.880261
W	-3.111072	1.514940	-1.701666
W	-0.618195	-0.112647	-3.457271
W	2.075124	-1.911189	-1.620954
W	2.095417	-1.963352	1.853969
W	-0.584273	-0.174933	3.749560
W	-3.083844	1.498833	2.048234
Rb	-8.863685	0.081992	-0.593082
O	-6.768494	-0.053021	-2.630158
H	-5.819057	-0.165376	-2.473417
H	-6.939977	-0.417382	-3.511422
O	-6.028399	-0.284396	0.326540
H	-5.066295	-0.273661	0.433398
H	-6.221866	-1.126174	-0.149857
O	-9.750993	0.992710	-3.372823
H	-10.629642	1.300469	-3.617333
H	-9.236507	1.801915	-3.174846
O	-8.419044	-0.948797	-4.713228
H	-8.586678	-1.110936	-5.646260
H	-8.967236	-0.175350	-4.455472
O	-6.990113	-2.645938	-0.629941
H	-7.482670	-2.643668	-1.470613
H	-7.658406	-2.918719	0.028207
O	-6.754559	2.473831	-0.183286
H	-6.345459	1.597523	-0.081217
H	-7.283146	2.628035	0.623171
O	-8.402594	3.131649	-2.234817
H	-7.679418	2.907419	-1.600775
H	-8.120598	3.930818	-2.690798
O	-9.053220	-2.630416	-2.632562
H	-9.152666	-3.540003	-2.934540
H	-8.881568	-2.111400	-3.451218

O	-10.663426	-0.108189	1.736183
H	-11.513726	0.220945	1.418437
H	-10.461891	0.376757	2.551347
O	-12.124148	0.471457	-0.631987
H	-12.945096	0.616156	-1.111983
H	-11.652681	1.332548	-0.650197
O	-7.484463	-0.946108	2.682555
H	-6.861912	-0.687747	1.975610
H	-8.072866	-1.611478	2.279710
O	-9.006210	1.055289	3.664396
H	-8.845521	1.222666	4.597758
H	-8.384976	0.333768	3.394073
O	-10.555030	2.733670	-0.418572
H	-10.080324	2.877834	0.422157
H	-9.950422	3.074909	-1.101927
O	-11.021736	-2.199263	-0.603360
H	-11.489495	-1.348276	-0.673092
H	-10.573711	-2.341685	-1.456318
O	-9.062492	-2.861681	1.242087
H	-9.875239	-2.607989	0.750313
H	-9.272669	-3.690693	1.683971
O	-8.743790	2.977057	1.754381
H	-8.661444	3.852900	2.146463
H	-8.824644	2.355379	2.516502
Rb	6.184794	-6.048258	-0.350860
O	8.384485	-4.122516	-0.982385
H	9.055250	-4.313596	-0.308959
H	8.811806	-4.225612	-1.843881
O	9.382895	-5.270876	1.382474
H	10.155919	-5.253078	1.954347
H	9.426692	-6.119342	0.885822
O	5.799990	-3.984547	-2.684512
H	4.974918	-3.678916	-3.082053
H	5.864334	-3.457553	-1.856013
O	8.186474	-4.653163	-3.741285
H	8.356327	-4.387775	-4.649922
H	7.287507	-4.317809	-3.512059
O	9.302248	-7.450955	-0.257469
H	9.087702	-7.308297	-1.198176
H	8.810597	-8.257894	-0.014699
O	6.950772	-3.915473	1.937512
H	7.770943	-4.441165	1.897252
H	6.244452	-4.502145	2.253820
O	5.734984	-2.662574	-0.266941
H	6.246978	-3.042293	0.475235
H	4.819516	-2.585971	0.043876

O	8.225686	-7.242955	-2.889150
H	8.747249	-7.788978	-3.487560
H	8.222218	-6.347060	-3.303526
O	4.458782	-8.309809	0.732718
H	3.759495	-8.443915	0.078649
H	4.021497	-8.218252	1.591376
O	3.450796	-7.820143	-1.840930
H	2.808431	-7.941738	-2.546410
H	3.267905	-6.934633	-1.456068
O	6.905172	-7.511426	2.320237
H	7.739733	-7.403202	2.787767
H	7.027119	-8.302158	1.754620
O	4.410281	-7.512615	3.423206
H	4.273275	-7.682172	4.359771
H	5.373378	-7.605236	3.254011
O	3.247974	-5.413046	-0.541355
H	3.386552	-5.343905	0.423485
H	2.507818	-4.821865	-0.747653
O	6.072689	-8.854990	-1.941900
H	5.169839	-8.499725	-2.044882
H	6.664281	-8.309676	-2.489144
O	7.435682	-9.431918	0.366923
H	6.810105	-9.334343	-0.387176
H	7.551573	-10.377194	0.502752
O	4.339443	-5.137390	2.051816
H	3.952740	-4.372843	2.507941
H	4.218724	-5.901135	2.656183
Rb	5.536606	6.961861	-0.297242
O	7.903974	5.832578	-1.674275
H	8.215294	5.153222	-1.059599
H	7.789345	5.403716	-2.533913
O	7.836196	4.675308	0.892129
H	8.223405	4.064067	1.525935
H	6.974027	4.280796	0.631744
O	6.432332	8.173411	-2.997422
H	6.061042	8.973140	-3.383199
H	7.220300	8.467511	-2.497256
O	6.697256	5.756936	-4.233449
H	6.770829	5.723235	-5.191671
H	6.648783	6.707338	-3.989851
O	5.478829	3.777152	-0.197532
H	5.382391	4.035958	-1.132961
H	4.585388	3.926324	0.161391
O	8.342426	7.478975	1.094751
H	8.194479	6.518907	1.173451
H	7.771884	7.920572	1.749730

O	8.263048	9.099638	-1.116211
H	8.452350	8.452738	-0.399910
H	9.089275	9.562213	-1.286655
O	4.607785	4.949036	-2.644908
H	4.118998	4.158773	-2.924937
H	5.263821	5.134354	-3.351342
O	3.334659	8.266986	1.195915
H	3.003606	8.969656	0.620590
H	3.404911	8.642583	2.085127
O	3.412956	9.413106	-1.360786
H	3.099415	10.047338	-2.012440
H	4.282161	9.752148	-1.053359
O	4.825610	5.911442	2.570192
H	5.139426	5.102256	2.986505
H	4.062517	5.638777	2.016376
O	4.392947	8.284118	3.805228
H	4.272311	8.310699	4.758884
H	4.497910	7.337277	3.558358
O	5.802499	10.141124	-0.199734
H	5.908520	9.957043	0.752847
H	6.691979	9.995374	-0.570593
O	2.619558	6.676082	-1.568890
H	2.838314	7.625440	-1.597466
H	3.216354	6.234691	-2.199070
O	3.057170	5.077706	0.629613
H	2.766590	5.698491	-0.075669
H	2.264290	4.586672	0.894189
O	6.535194	9.237910	2.400521
H	7.037848	9.911766	2.870795
H	5.815406	8.974125	3.018854

M = Cs, E = -7895.90619142

Atom	X	Y	Z
O	-1.743806	-4.181599	-2.959115
O	-1.277865	0.431316	-4.822842
O	2.780757	-2.224312	-3.699733
O	-1.053242	-0.096983	4.146701
O	-0.799602	2.344437	3.155581
O	1.352405	0.930833	3.756276
O	2.126056	-1.372083	2.588160
O	-0.244468	-2.389287	2.980512
O	-2.866108	-0.658945	2.246819
O	-2.630868	1.744199	1.271838
O	1.174048	-1.449959	5.280507
O	0.334408	3.049306	0.799183
O	2.432444	1.601818	1.384198

O	1.269277	-3.313964	1.063074
O	-2.444976	-3.263374	1.673738
O	-3.482369	-0.191186	-0.252609
O	-1.774079	3.103862	-0.889015
O	1.868894	2.123554	-1.111693
O	3.828566	-0.586043	0.664156
O	-0.875444	-4.190592	-0.258450
O	-3.053388	-2.777617	-0.865832
O	-3.412852	1.510914	3.986242
O	-2.641814	1.136768	-2.433880
O	-0.231839	2.153504	-2.824638
O	3.211826	-0.101290	-1.860184
O	2.966108	-2.545302	-0.882780
O	0.540938	-2.751194	-2.020051
O	-1.590163	-1.347905	-2.612927
O	0.777949	-0.321820	-2.976467
O	-0.138512	0.261262	1.720936
O	-0.980631	-1.617026	0.238248
O	-0.718822	0.725765	-0.698053
O	1.712571	3.684400	3.202256
O	1.333589	-0.647323	-0.132897
O	-0.474001	-5.167919	2.383016
O	-4.999984	-2.168067	1.094266
O	-4.518171	2.443569	-0.750743
O	0.527584	4.585547	-1.592697
O	4.624406	1.896609	-0.438279
O	4.037106	-3.273501	1.637371
P	-0.128865	-0.321438	0.282363
W	-1.352194	-3.045596	-1.743081
W	-1.000563	0.405886	-3.136647
W	2.042544	-1.582891	-2.291263
W	0.671336	-0.874022	3.752325
W	-2.141859	0.973829	2.966738
W	1.003389	2.312676	2.455417
W	-0.572142	-3.659676	1.585477
W	-3.358199	-1.799235	0.792120
W	-3.008704	1.643312	-0.607310
W	0.130115	2.987670	-1.130483
W	3.181098	0.982573	-0.273984
W	2.824941	-2.216383	1.015241
Cs	5.815518	-5.406843	-0.307151
O	3.610892	-7.768192	-0.955415
H	2.778217	-7.395542	-1.270956
H	3.965630	-8.300701	-1.683682
O	1.883565	-5.510211	-0.977708
H	1.205898	-4.827353	-0.874650

H	2.529123	-5.137210	-1.613868
O	6.515418	-8.643298	0.127677
H	7.318797	-8.987219	0.528292
H	5.887567	-8.490495	0.868432
O	5.667874	-8.987585	-2.436006
H	5.905115	-9.833405	-2.827365
H	6.057370	-8.980902	-1.533429
O	3.797118	-4.740773	-2.880880
H	4.269642	-5.502152	-3.302282
H	3.331367	-4.285430	-3.594303
O	2.869620	-6.086082	1.582822
H	2.517332	-5.890895	0.688413
H	2.982423	-5.223634	1.999369
O	4.900770	-7.834773	2.194107
H	4.127729	-7.287960	1.932187
H	4.550459	-8.490177	2.804544
O	5.406881	-6.634299	-3.905554
H	6.245220	-6.133160	-3.914175
H	5.588001	-7.473109	-3.438582
O	8.464566	-3.489170	-0.805246
H	9.258187	-3.862881	-0.388468
H	8.350115	-2.617956	-0.408645
O	10.193672	-5.344406	0.374158
H	11.086082	-5.513481	0.689430
H	9.587346	-5.472045	1.138841
O	5.908240	-2.783602	-2.545804
H	5.089981	-3.293767	-2.685712
H	6.616325	-3.372165	-2.868928
O	6.426525	-1.633434	-0.099141
H	5.652681	-1.099992	0.135624
H	6.202230	-2.042555	-0.965945
O	8.100287	-5.538898	2.083588
H	7.713773	-4.646844	2.237750
H	8.128649	-5.963104	2.946613
O	8.685334	-6.425313	-1.670361
H	9.346196	-6.154411	-1.000406
H	8.900428	-7.334512	-1.899488
O	7.563142	-4.872724	-3.612820
H	8.139909	-5.320430	-2.954314
H	8.135122	-4.644177	-4.352305
O	6.856860	-3.096144	2.248628
H	5.941787	-3.202450	2.539882
H	6.764950	-2.601488	1.406082
Cs	4.426119	7.532553	-0.289749
O	2.300566	8.434310	2.086024
H	2.102497	9.351113	1.835203

H	1.513649	7.919295	1.864442
O	2.607844	11.024279	1.019418
H	2.264213	11.903711	1.204028
H	2.409838	10.842933	0.075194
O	3.766864	5.430928	2.097690
H	3.469203	4.787624	2.753809
H	4.199822	6.149982	2.607970
O	1.228739	6.040812	1.085507
H	0.747949	5.203624	1.047254
H	2.113965	5.809459	1.444707
O	2.092720	10.073300	-1.538032
H	1.603078	9.228646	-1.370086
H	1.474159	10.634215	-2.019090
O	5.037659	9.937208	1.848812
H	4.243275	10.460431	1.622546
H	5.738770	10.578071	1.998490
O	5.194366	7.530099	3.273614
H	5.011570	8.405849	2.875857
H	4.971069	7.634632	4.203733
O	1.034762	7.619187	-1.232008
H	1.358479	7.112527	-2.000895
H	1.049586	6.996121	-0.478908
O	5.778900	6.310763	-3.008211
H	6.252285	5.487077	-2.831775
H	6.439650	6.946032	-3.319760
O	6.289563	4.006281	-1.430519
H	6.138609	3.139773	-1.029891
H	6.663566	4.570989	-0.720680
O	3.998812	8.965002	-3.390682
H	3.369102	9.463606	-2.839229
H	3.594583	8.084014	-3.510415
O	6.722026	8.932263	-3.276656
H	7.113153	9.584013	-3.865609
H	5.746966	9.064065	-3.327082
O	7.190951	5.866774	0.397821
H	7.543313	6.688531	-0.000278
H	7.828557	5.609527	1.070587
O	3.573690	4.663164	-1.697482
H	4.511467	4.381861	-1.650027
H	3.049176	3.887878	-1.459975
O	2.517580	6.550143	-3.361904
H	2.943125	5.774356	-2.931597
H	2.112490	6.214192	-4.167646
O	7.615357	8.359754	-0.724079
H	8.225527	9.015483	-0.375057
H	7.412470	8.642336	-1.640532

Cs	-9.632865	-0.171603	-0.568692
O	-12.930145	-0.241948	-0.763802
H	-13.247839	0.577038	-0.352378
H	-13.226244	-0.216264	-1.684503
O	-12.916578	2.078915	0.799295
H	-13.483230	2.768471	1.156955
H	-12.298951	2.517665	0.172213
O	-11.409010	-2.735854	-1.836209
H	-11.192005	-3.649759	-2.041442
H	-11.606720	-2.719467	-0.875715
O	-12.654087	-0.916968	-3.467322
H	-13.026291	-1.271193	-4.280139
H	-12.245664	-1.675472	-2.994625
O	-11.077915	2.852809	-1.058172
H	-11.145586	2.410752	-1.930897
H	-10.866211	3.771547	-1.247870
O	-11.619792	-0.034389	2.073325
H	-12.127171	0.746382	1.774786
H	-11.511747	0.072834	3.022794
O	-11.503043	-2.593131	0.951820
H	-11.743783	-1.735722	1.357216
H	-11.994207	-3.256387	1.445352
O	-10.951684	1.254988	-3.297914
H	-10.676094	1.595580	-4.153974
H	-11.568305	0.516875	-3.490244
O	-6.448383	0.036560	-0.419985
H	-5.990794	-0.679152	-0.889153
H	-5.944834	0.151014	0.399468
O	-5.765178	-2.227703	-2.020014
H	-4.878011	-2.572653	-1.845535
H	-6.366667	-2.665678	-1.377891
O	-7.798261	2.278441	0.879220
H	-8.064573	3.182382	1.074467
H	-7.569580	2.284196	-0.075504
O	-5.922228	0.765722	2.241849
H	-5.315264	1.138714	2.893462
H	-6.499910	1.494816	1.933703
O	-7.739863	-2.945140	-0.250767
H	-7.607028	-2.440575	0.579860
H	-7.871466	-3.856039	0.029962
O	-7.518704	-0.239542	-3.104207
H	-6.820961	-0.888398	-2.904727
H	-7.645510	-0.291296	-4.056618
O	-7.188879	2.398536	-1.923713
H	-7.286320	1.496347	-2.283883
H	-6.260514	2.406478	-1.640892

O	-7.897339	-1.309225	2.038616
H	-8.039158	-1.754413	2.880004
H	-7.128218	-0.728243	2.189382