The Prediction of the pK_as of Aqueous Metal Ion +2 Complexes

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Supporting Information Total energies in a.u. at the B3LYP/DZVP2 level. Complete author lists for references 68, 71, 83. Cartesian Coordinates (x, y, z) in Angstroms. The pK_as of Metal/H_2O complexes at the B3LYP/DZVP level.

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Table SI1. The pK_as of Metal/H_2O Complexes at the B3LYP/DZVP level (Same references as in the paper repeated here with new numbers).

Metal ion/H_2O complex	COSMO	CPCM-COSMO-RS Radii	IEF-PCM UA0	IEF-PCM UFF	IPCM	IEF-PCM-Pauling	CSC-PCM Pauling	Exp pK_a
$[Be(H_2O)_4]^{2+}$	-5.1[a] -3.3[b] 3.8[f]	-3.0[a] -1.5[b]	-2.6[a] -1.1[b]	-8.8[a] -6.7[b]	0.3[a] 1.6[b]	-3.2[a] -1.7[b]	-1.9[a] -0.2[b]	5.4[c,d,e]
$[Be(H_2O)_4(H_2O)_8]^{2+}$	5.4[a] 4.4[b]	6.3[a] 5.0[b]	9.5[a] 8.0[b]	2.2[a] 2.2[b]	i	7.9[a] 5.7[b]	6.3[a] 5.6[b]	5.4[c,d,e]
$[Mg(H_2O)_6]^{2+}$	11.4 11.2[h]	12.7	14.7	7.7	15.6	12.8	13.4	11.4[c,g] 11.2[d,e]
$[Ca(H_2O)_7]^{2+}$	12.0	13.6	14.3	8.5	18.1	15.1	13.7	12.9[c] 12.7[d,e] 12.8[g]
$[Ca(H_2O)_8]^{2+}$	8.4	9.6	15.8	3.4	5.0	8.5	6.9	12.9[c] 12.7[d,e] 12.8[g]
$[Sr(H_2O)_7]^{2+}$	15.5	17.0	16.2	10.0	i	17.1	16.3	13.3[c,g] 13.2[d,e]
$[Sr(H_2O)_8]^{2+}$	12.5	14.1	14.6	7.1	i	11.6	13.3	13.3[c,g] 13.2[d,e]
[6]$[Mn(H_2O)_6]^{2+}$	8.1	9.4	12.3	i	16.0	9.3	10.8	10.6[c,e]

								11.0[g]
$^{5}[Fe(H_2O)_6]^{2+}$	5.7	6.7	9.4	1.9	8.1	6.4	11.4	9.3[c] 9.5[g]
$^{4}[Co(H_2O)_6]^{2+}$	2.8	3.7	6.7	-0.4	3.4	3.2	4.1	9.7[c,d,e]
$^{3}[Ni(H_2O)_6]^{2+}$	6.9	8.9	11.8	4.5	10.5	9.0	8.9	9.86[c]
$^{2}[Cu(H_2O)_6]^{2+}$	-1.7	-0.8	2.6	-7.4	5.9	-9.0	-3.7	8[c,g]
$[Zn(H_2O)_6]^{2+}$	5.0 8.4[h]	6.3	11.6	-4.1	14.8	-0.5	0.9	9.0[c,d,e]
$[Cd(H_2O)_6]^{2+}$	9.7	11.1	8.1	-3.8	24.6	-0.6	8.5	10.0[c] 10.1[d,e]
$[Hg(H_2O)_6]^{2+}$	3.2	4.3	-4.0	-14.3	i	-10.8	0.8	3.4[c,d,e]

[a] 6-311G** basis set for Be. [b] DZVP2 basis set on Be. [c] Reference 1. [d] Reference 2. [e] References 3 and 4. [f] Reference 5. [g] Reference 6. [h] Reference 7. [i] Solvation calculations did not converge.

Table SI2. Charge on Central Metal, Selected Bond Lengths (r, Å) for Metal +3 Complexes (Values in parentheses represent the number of M-OH_2 bond with specified lengths.)

Molecule	Mulliken Atomic Charge M^{2+}	Sym 2+ complex	Calc. r(M-OH_2)	Calc. r(M-OH)
$[Al(H_2O)_6]^{3+}$	0.67	C_i	1.95	
$[Al\ (H_2O)_5OH]^{2+}$	0.52	C_1	2.00 1.99(x2) 1.98(x2)	1.73
$[Al(H_2O)_6(H_2O)_{12}]^{3+}$	0.59	C_i	1.95(x2) 1.93(x2) 1.92(x2) 1.92[a]	
$[Al(H_2O)_5OH(H_2O)_{12}]^{2+}$	0.53	C_1	2.00 1.96 1.98 1.94 1.93 1.96[a]	1.82 1.78[a]

[a] Yang, W.; Qian, Z.; Miao, Q. Wang, Y.; Bi, S. Density Functional Theory Study of the Aluminium(III) Hydrolysis in Aqueous Solution. *Phys. Chem. Chem. Phys.*, **2009**, *11*, 2396–2401.

COORDINATES

$[Be(H_2O)_4]^{2+}$ S_4 B3LYP/6-311G** -320.0643787 A.u.s

BE	0.000000	0.000000	0.000000
O	-1.382284	0.000000	1.007393
O	0.000000	1.382284	-1.007393
O	0.000000	-1.382284	-1.007393
O	1.382284	0.000000	1.007393
H	-1.517876	-0.536200	1.810944
H	-2.172128	0.558997	0.881756
H	2.172128	-0.558997	0.881756
H	1.517876	0.536200	1.810944
H	-0.558997	-2.172128	-0.881756
H	0.536200	-1.517876	-1.810944
H	-0.536200	1.517876	-1.810944
H	0.558997	2.172128	-0.881756

$[Be(H_2O)_3OH]^{+}$ C_1 B3LYP/6-311G** -319.856853 A.u.s

BE	0.049231	0.025282	0.179427
O	-0.769596	1.452539	-0.462705
O	0.951361	0.261733	1.377815
O	1.119598	-0.516727	-1.114075
O	-1.227070	-1.203473	0.162585
H	-1.706071	1.517667	-0.707681
H	-0.507673	2.272293	-0.009396
H	-1.120977	-1.985489	-0.404592
H	-1.513914	-1.516669	1.037175
H	1.227215	-0.058409	-1.962564
H	2.000999	-0.607889	-0.705290
H	0.829159	0.324791	2.325682

$[Be(H_2O)_4]^{2+}$ S_4 B3LYP/6-311G** -320.1161325 A.u.s

BE	0.000000	0.000000	0.000000
O	-1.335305	0.000000	0.971898
O	0.000000	1.335305	-0.971898
O	0.000000	-1.335305	-0.971898
O	1.335305	0.000000	0.971898
H	-1.468020	-0.536006	1.776479
H	-2.124830	0.559397	0.844647
H	2.124830	-0.559397	0.844647
H	1.468020	0.536006	1.776479
H	-0.559397	-2.124830	-0.844647
H	0.536006	-1.468020	-1.776479

H	-0.536006	1.468020	-1.776479
H	0.559397	2.124830	-0.844647

$[Be(H_2O)_3OH]^+$ C_1 B3LYP/6-311G** -319.9165174 A.u.s

BE	-0.045717	-0.021810	0.175488
O	1.042822	-1.262831	-0.295772
O	-0.803014	-0.182798	1.413958
O	-1.208693	0.057407	-1.082687
O	0.902153	1.398374	-0.066132
H	1.979699	-1.102089	-0.493961
H	0.976262	-2.072452	0.238491
H	0.700065	1.986510	-0.813166
H	0.963139	1.953213	0.730442
H	-1.233039	-0.569615	-1.823234
H	-2.079853	0.041107	-0.643375
H	-0.589552	-0.230651	2.347921

$[Be(H_2O)_4(H_2O)_8]^{2+}$ B3LYP/6-311G** -932.0629192 A.u.s

BE	0.000000	0.000000	0.000000
O	-0.470832	1.250839	0.946429
H	-1.319039	1.200708	1.484079
H	-0.288265	2.194556	0.735062
O	1.250839	0.470832	-0.946429
H	1.200708	1.319039	-1.484079
H	2.194556	0.288265	-0.735062
O	-1.250839	-0.470832	-0.946429
H	-2.194556	-0.288265	-0.735062
H	-1.200708	-1.319039	-1.484079
O	0.470832	-1.250839	0.946429
H	0.288265	-2.194556	0.735062
H	1.319039	-1.200708	1.484079
O	2.796201	-1.129694	2.089989
H	3.496683	-0.767173	1.517802
H	3.131683	-1.188367	2.996209
O	0.000000	-3.957705	0.293333
H	0.793453	-4.517843	0.257267
H	-0.625067	-4.441851	0.858828
O	1.129694	2.796201	-2.089989
H	1.188367	3.131683	-2.996209
H	0.767173	3.496683	-1.517802
O	0.000000	3.957705	0.293333
H	0.625067	4.441851	0.858828
H	-0.793453	4.517843	0.257267
O	-1.129694	-2.796201	-2.089989

H	-0.767173	-3.496683	-1.517802
H	-1.188367	-3.131683	-2.996209
O	3.957705	0.000000	-0.293333
H	4.441851	-0.625067	-0.858828
H	4.517843	0.793453	-0.257267
O	-3.957705	0.000000	-0.293333
H	-4.517843	-0.793453	-0.257267
H	-4.441851	0.625067	-0.858828
O	-2.796201	1.129694	2.089989
H	-3.496683	0.767173	1.517802
H	-3.131683	1.188367	2.996209

$[Be(H_2O)_3OH(H_2O)_8]^+$ B3LYP/6-311G** -931.771496 A.u.s

BE	0.274734	0.198039	-0.423847
O	-0.273302	1.726122	-0.792390
H	-1.262852	1.848766	-0.575816
H	0.215189	2.393705	-0.268070
O	1.684135	0.001503	-1.290080
H	2.371657	0.724022	-1.167907
H	2.153010	-0.856860	-1.221938
O	-0.797670	-0.912863	-1.093947
H	-1.415750	-0.623172	-1.792378
H	-1.369217	-1.422323	-0.460448
O	0.385318	0.063142	1.138380
H	0.892890	-0.712398	1.453803
O	1.837779	-2.320790	1.664505
H	2.443230	-2.518304	0.927826
H	2.225647	-2.709044	2.460754
O	-2.084496	0.123927	2.078460
H	-2.184983	0.274910	3.029235
H	-1.097032	0.114446	1.861868
O	3.409259	1.866737	-0.662205
H	3.787091	2.563299	-1.217180
H	2.951541	2.298916	0.093457
O	1.515527	2.509622	1.233392
H	1.179313	1.603075	1.476018
H	1.509415	3.060835	2.028571
O	-2.740389	-1.924251	0.471821
H	-2.650114	-1.305040	1.242385
H	-2.855264	-2.818374	0.824852
O	3.181462	-2.395072	-0.933949
H	2.989317	-3.150941	-1.511397
H	4.136553	-2.240702	-1.011349
O	-3.507451	-0.379227	-1.795515
H	-3.692032	-1.072632	-1.132785

H	-4.181365	-0.454413	-2.487078
O	-2.760755	1.836030	-0.127249
H	-3.266461	1.258257	-0.732412
H	-2.774061	1.392782	0.745580

$[Be(H_2O)_4(H_2O)_8]^{2+}$ B3LYP/DGDZVP2 -932.0100107 A.u.s

BE	0.000000	0.000000	0.000000
O	1.416557	0.000000	0.917182
H	1.806102	0.838622	1.306509
H	2.089081	-0.716589	0.946262
O	0.000000	-1.416557	-0.917182
H	0.838622	-1.806102	-1.306509
H	-0.716589	-2.089081	-0.946262
O	0.000000	1.416557	-0.917182
H	0.716589	2.089081	-0.946262
H	-0.838622	1.806102	-1.306509
O	-1.416557	0.000000	0.917182
H	-2.089081	0.716589	0.946262
H	-1.806102	-0.838622	1.306509
O	-2.415004	-2.270691	1.682895
H	-2.504359	-2.923895	0.965421
H	-2.769223	-2.651183	2.499216
O	-3.418331	1.983560	0.917545
H	-4.327214	1.647966	0.993831
H	-3.356462	2.698889	1.572527
O	2.270691	-2.415004	-1.682895
H	2.651183	-2.769223	-2.499216
H	2.923895	-2.504359	-0.965421
O	3.418331	-1.983560	0.917545
H	3.356462	-2.698889	1.572527
H	4.327214	-1.647966	0.993831
O	-2.270691	2.415004	-1.682895
H	-2.923895	2.504359	-0.965421
H	-2.651183	2.769223	-2.499216
O	-1.983560	-3.418331	-0.917545
H	-2.698889	-3.356462	-1.572527
H	-1.647966	-4.327214	-0.993831
O	1.983560	3.418331	-0.917545
H	1.647966	4.327214	-0.993831
H	2.698889	3.356462	-1.572527
O	2.415004	2.270691	1.682895
H	2.504359	2.923895	0.965421
H	2.769223	2.651183	2.499216

$[Be(H_2O)_3OH(H_2O)_8]^+$ B3LYP/DGDZVP2 -931.7092284 A.u.s

BE	0.287585	0.011513	-0.242073
O	-0.079786	1.687076	-0.190802
H	-1.049190	1.843828	0.107361
H	0.494970	2.258561	0.356496
O	1.824387	-0.078880	-1.013720
H	2.433046	0.708094	-0.975976
H	2.367377	-0.891937	-0.942694
O	-0.871642	-0.613676	-1.408434
H	-1.398817	0.004323	-1.947696
H	-1.541652	-1.229738	-1.017701
O	0.098678	-0.728640	1.156165
H	0.584107	-1.552623	1.336920
O	1.610016	-3.156632	1.352635
H	2.373850	-3.116503	0.752405
H	1.844681	-3.758958	2.071352
O	-2.308450	-0.558046	1.924280
H	-2.474872	-0.729834	2.861536
H	-1.292029	-0.668628	1.739411
O	3.419220	2.030267	-0.722759
H	3.818514	2.557585	-1.428883
H	3.044573	2.652188	-0.069442
O	1.785857	3.306018	1.264347
H	1.958221	3.007681	2.171813
H	1.587108	4.253513	1.330349
O	-3.076041	-1.781388	-0.310529
H	-2.944304	-1.481257	0.631642
H	-3.370821	-2.702754	-0.288777
O	3.395811	-2.435478	-0.863774
H	3.283499	-3.023742	-1.627467
H	4.353011	-2.314148	-0.762742
O	-3.483187	0.559694	-1.796362
H	-3.735589	-0.305229	-1.412739
H	-4.163331	0.798448	-2.442465
O	-2.519989	1.878835	0.554144
H	-3.064294	1.640523	-0.223152
H	-2.617401	1.131352	1.187206

$[Mg(H_2O)_6]^{2+}$ T_h -658.4957477 A.u.s

MG	-0.000851	0.000589	-0.001436
O	1.433821	0.070971	-1.548510
H	2.327713	-0.309624	-1.521012
H	1.331905	0.479158	-2.424651
H	-1.302889	-0.441612	2.440819

O	-1.430302	-0.072447	1.550827
H	-2.341878	0.262958	1.516367
H	0.357829	2.341857	1.496031
O	0.700568	1.852926	0.729156
H	1.430127	2.382039	0.365208
H	-1.415826	-2.391724	-0.351231
O	-0.701485	-1.852497	-0.730235
H	-0.375596	-2.331344	-1.510710
O	-1.389162	1.009815	-1.230266
H	-1.518997	1.971125	-1.291074
H	-2.017859	0.604470	-1.850803
H	2.035522	-0.601530	1.828130
O	1.386873	-1.008996	1.229894
H	1.497658	-1.971023	1.313229

$[Mg(H_2O)_5OH]^+$ C_1 -658.2275469 A.u.s

MG	0.016004	-0.027303	-0.021652
O	-1.569558	-1.147282	0.885491
H	-2.122939	-1.197843	1.675806
H	-2.109926	-0.785432	0.130421
H	2.182673	0.857372	-1.538915
O	1.691263	1.078668	-0.733309
H	1.506726	2.032317	-0.753911
H	-1.793771	0.401393	-2.080613
O	-1.533693	0.324413	-1.157675
H	2.130314	-0.030280	1.727146
O	1.293044	-0.500275	1.593374
H	1.058874	-0.932592	2.427686
O	-0.607527	1.965124	0.539251
H	-1.318155	1.784823	-0.138672
H	-0.993315	2.423689	1.297927
H	0.081613	-1.994892	-1.776466
O	0.731623	-1.689520	-1.122996
H	1.144639	-2.479947	-0.743673

$[Ca(H_2O)_7]^{2+}$ C_2 -571.751252 A.u.s

CA	0.000170	0.045273	-0.000095
O	2.136449	-0.520910	1.123208
H	2.974778	-0.825836	0.739124
H	2.290164	-0.480986	2.081649
O	-0.005601	-2.410028	0.001729
H	-0.700082	-2.994153	-0.342692
H	0.685775	-2.997066	0.347440
O	-0.878601	-0.331057	2.224285

H	-1.365988	0.308885	2.768195
H	-0.916536	-1.171708	2.708507
O	0.876980	-0.339828	-2.223747
H	1.367390	0.296372	-2.769325
H	0.910742	-1.181858	-2.705876
O	1.439310	2.021198	-0.319829
H	1.250897	2.876214	-0.739366
H	2.348196	2.088386	0.014962
O	-1.429514	2.028621	0.316115
H	-2.338241	2.099612	-0.018318
H	-1.236446	2.883743	0.733314
O	-2.139264	-0.512991	-1.121633
H	-2.978932	-0.813067	-0.736658
H	-2.293191	-0.474033	-2.080081

$[Ca(H_2O)_6OH]^+$ C_1 -571.4725065A.u.s

CA	0.145315	-0.007036	-0.029063
O	-1.097248	-1.429784	-1.586963
H	-1.856404	-1.089920	-1.030217
H	-1.391767	-1.478959	-2.506295
O	1.492916	-1.948408	-0.502149
H	2.298986	-2.371238	-0.173887
H	0.996337	-2.612170	-1.007490
O	1.156702	1.300285	-1.786590
H	0.640064	2.113423	-1.911631
H	1.727983	1.192358	-2.560001
O	-0.483147	-0.805651	2.193239
H	-1.395612	-0.643387	1.816337
H	-0.514957	-1.605198	2.735471
O	-2.167652	-0.060586	0.349146
H	-3.120082	-0.082074	0.504448
O	-0.953874	2.192368	-0.129000
H	-1.043345	3.015540	0.370037
H	-1.743185	1.611316	0.078252
O	1.841811	0.763495	1.504500
H	2.579022	1.390443	1.497279
H	1.600592	0.606843	2.431508

$[Ca(H_2O)_8]^{2+}$ C_4 -648.2339707 A.u.s

CA	-0.000105	0.000194	-0.001476
O	1.283515	-1.654385	-1.364748
H	2.188497	-1.982733	-1.245980
H	0.908338	-2.160848	-2.102364
O	2.073677	-0.267009	1.365151

H	2.946809	0.138505	1.246473
H	2.165782	-0.894694	2.099213
O	1.656540	1.284122	-1.361723
H	1.985667	2.188830	-1.242994
H	2.163673	0.907978	-2.098391
O	0.264503	2.072947	1.367041
H	-0.140662	2.946121	1.247409
H	0.891146	2.165323	2.101963
O	-1.281882	1.657768	-1.362434
H	-0.904568	2.165195	-2.098306
H	-2.187179	1.986016	-1.245786
O	-2.074768	0.263098	1.364348
H	-2.168710	0.889365	2.099393
H	-2.947712	-0.141898	1.242523
O	-1.655939	-1.280983	-1.365151
H	-2.162457	-0.904338	-2.101986
H	-1.983478	-2.186588	-1.248880
O	-0.265573	-2.075813	1.362389
H	-0.893127	-2.169178	2.096410
H	0.139500	-2.948899	1.241844

$[Ca(H_2O)_7OH]^+$ C_1 -647.9632251 A.u.s

CA	0.610554	-0.210051	-0.107990
O	-0.125141	-2.477289	-0.190581
O	-1.099447	0.357536	-1.449627
O	-2.573706	-1.416271	-0.247406
O	-1.422268	2.536126	-0.071965
O	1.211849	2.108872	0.032025
O	-1.150072	0.232201	1.560760
O	1.491821	-0.546356	2.141125
O	2.586477	-0.431266	-1.487993
H	0.744614	-0.377459	2.740480
H	2.247209	-0.814983	2.682113
H	3.050543	0.351756	-1.823067
H	2.934789	-1.187305	-1.984320
H	1.796940	2.637212	0.591875
H	0.343262	2.586533	-0.025724
H	-1.465488	1.142184	1.378462
H	-1.898506	-0.349033	1.309400
H	-2.210163	-0.713534	-0.879837
H	-3.468841	-1.659498	-0.522012
H	0.101958	-3.352224	0.151019
H	-1.113590	-2.420821	-0.257076
H	-1.117599	0.403042	-2.415487
H	-2.036768	3.244901	-0.308327

H	-1.475549	1.801822	-0.768400

$[Sr(H_2O)_7]^{2+}$ C_2 -565.6452038 A.u.s

SR	0.000000	0.000000	0.044292
O	1.078511	-1.146753	2.148887
H	1.223864	-2.102435	2.240731
H	1.360326	-0.763263	2.995195
O	0.000000	2.576492	-0.523460
H	0.772777	3.164001	-0.485654
H	-0.732481	3.141737	-0.818860
O	0.000000	0.000000	-2.576124
H	-0.027453	0.771325	-3.164977
H	0.027453	-0.771325	-3.164977
O	-1.078511	1.146753	2.148887
H	-1.223864	2.102435	2.240731
H	-1.360326	0.763263	2.995195
O	-2.546900	-0.248069	-0.409431
H	-2.985200	-0.447202	-1.252594
H	-3.266517	-0.082357	0.221140
O	2.546900	0.248069	-0.409431
H	2.985200	0.447202	-1.252594
H	3.266517	0.082357	0.221140
O	0.000000	-2.576492	-0.523460
H	-0.772777	-3.164001	-0.485654
H	0.732481	-3.141737	-0.818860

$[Sr(H_2O)_6OH]^{+}$ C_3 -565.3610415 A.u.s

SR	0.000539	-0.001466	-0.293416
O	-0.010997	0.004063	2.209095
H	-0.016510	0.004717	3.175202
O	-0.532087	2.255755	-1.402985
H	-0.188971	2.912034	-0.771299
H	-1.026630	2.732767	-2.084197
H	2.894731	-0.469536	-2.065477
O	2.229655	-0.664206	-1.390238
H	2.625095	-1.287132	-0.755415
O	-2.308410	-0.191317	0.965733
H	-3.108284	0.296393	1.205396
H	-1.668031	-0.136893	1.737398
O	-1.681684	-1.602939	-1.395593
H	-1.843774	-2.276710	-2.070808
H	-2.424872	-1.627543	-0.767462
O	0.977608	2.093152	0.976606
H	1.797281	2.542609	1.224034

H	0.698042	1.510789	1.745499
O	1.323820	-1.889813	0.986232
H	1.308330	-2.824402	1.234012
H	0.949871	-1.358938	1.752144

$[Sr(H_2O)_8]2+$ S_8 -642.1297857 A.u.s

SR	0.000000	0.000000	0.000000
O	0.000000	2.214973	1.461791
H	-0.609123	2.380133	2.198900
H	0.506679	3.035008	1.352235
O	1.566223	1.566223	-1.461791
H	1.252293	2.113723	-2.198900
H	2.504351	1.787798	-1.352235
O	2.214973	0.000000	1.461791
H	3.035008	-0.506679	1.352235
H	2.380133	0.609123	2.198900
O	1.566223	-1.566223	-1.461791
H	1.787798	-2.504351	-1.352235
H	2.113723	-1.252293	-2.198900
O	-1.566223	-1.566223	-1.461791
H	-2.504351	-1.787798	-1.352235
H	-1.252293	-2.113723	-2.198900
O	0.000000	-2.214973	1.461791
H	-0.506679	-3.035008	1.352235
H	0.609123	-2.380133	2.198900
O	-2.214973	0.000000	1.461791
H	-2.380133	-0.609123	2.198900
H	-3.035008	0.506679	1.352235
O	-1.566223	1.566223	-1.461791
H	-2.113723	1.252293	-2.198900
H	-1.787798	2.504351	-1.352235

$[Sr(H_2O)_7OH]+$ C_1 -641.843735 A.u.s

SR	-0.423761	-0.186382	0.094006
O	2.781183	0.676746	-0.424237
H	3.692484	0.950661	-0.592755
O	-0.271715	-1.280071	2.414956
H	0.532334	-0.833242	2.740637
H	-0.548359	-1.928321	3.076928
O	-1.242021	2.371086	0.015475
H	-1.338328	3.167361	0.556728
H	-0.533525	2.546172	-0.643763
O	1.703662	-1.594637	-0.549463
H	2.169295	-2.314574	-0.101558

H	2.349501	-0.786969	-0.578284
O	-0.692626	-1.927388	-1.781089
H	-1.190908	-2.316864	-2.512132
H	0.240611	-2.204361	-1.860506
O	1.415006	0.784158	1.684165
H	1.506227	1.578762	2.227531
H	2.156795	0.823551	0.959413
O	0.734333	1.457603	-1.565476
H	0.779566	1.512413	-2.530123
H	1.717856	1.261854	-1.205771
O	-2.982867	0.123922	-0.128940
H	-3.828615	-0.339658	-0.208061
H	-3.161645	1.074377	-0.223639

$[Mn(H_2O)_6]^{2+}$ T_h -562.7091595 A.u.s

MN	0.000000	0.000000	0.000000
O	0.000000	0.000000	2.216537
O	0.000000	2.216537	0.000000
O	0.000000	0.000000	-2.216537
O	0.000000	-2.216537	0.000000
O	-2.216537	0.000000	0.000000
O	2.216537	0.000000	0.000000
H	-2.798316	-0.778514	0.000000
H	-2.798316	0.778514	0.000000
H	0.000000	2.798316	-0.778514
H	0.000000	2.798316	0.778514
H	-0.778514	0.000000	2.798316
H	0.778514	0.000000	2.798316
H	0.000000	-2.798316	-0.778514
H	0.000000	-2.798316	0.778514
H	-0.778514	0.000000	-2.798316
H	0.778514	0.000000	-2.798316
H	2.798316	0.778514	0.000000
H	2.798316	-0.778514	0.000000

$[Mn(H_2O)_5OH]^{+}$ C_1 -562.4428741 A.u.s

MN	0.057130	-0.076700	-0.072003
O	-0.491223	-2.026257	0.950503
H	-1.175966	-2.154395	0.255401
H	-0.793020	-2.443890	1.769252
O	-1.933053	1.174989	0.444401
H	-2.582765	1.278735	1.154432
H	-2.287606	0.527202	-0.217604
O	0.441287	2.098016	-0.573250

H	-0.438789	2.507674	-0.484750
H	0.858148	2.461785	-1.369314
O	1.896463	-0.754959	-1.155294
H	2.768862	-0.862491	-0.745708
H	1.826728	-1.427344	-1.851210
O	-1.424314	-0.801985	-1.158162
H	-1.550364	-0.941829	-2.104266
O	1.372538	0.494007	1.635126
H	1.577777	1.435705	1.748788
H	1.475148	0.065858	2.498458

$^{5}[Fe(H_2O)_6]^{2+}$ C_i -582.2400449 A.u.s

FE	0.000000	0.000000	0.000000
O	1.566518	-0.864063	-1.227103
H	2.526138	-0.772868	-1.102421
H	1.435328	-1.424676	-2.010157
O	0.000535	1.776642	-1.258352
H	-0.423068	2.628611	-1.060416
H	0.424991	1.871300	-2.127490
O	-1.566518	0.864063	1.227103
H	-1.435328	1.424676	2.010157
H	-2.526138	0.772868	1.102421
O	-0.000535	-1.776642	1.258352
H	-0.424991	-1.871300	2.127490
H	0.423068	-2.628611	1.060416
O	1.516124	0.871885	1.235977
H	1.944863	0.457015	2.003732
H	1.940433	1.736903	1.105267
O	-1.516124	-0.871885	-1.235977
H	-1.944863	-0.457015	-2.003732
H	-1.940433	-1.736903	-1.105267

$^{5}[Fe(H_2O)_5OH]^{+}$ C_1 -581.9825473 A.u.s

FE	0.041347	-0.083229	-0.141660
O	-2.165679	-0.569397	0.717193
H	-2.130746	-1.226311	-0.017155
H	-2.593409	-0.987284	1.478261
O	-1.275456	1.695781	-0.529921
H	-1.396409	2.120588	-1.392567
H	-2.137215	1.315667	-0.274596
O	1.985389	0.619117	-1.073268
H	2.173273	0.518091	-2.019244
H	2.385113	1.458811	-0.797486
O	1.418402	-1.412879	1.038057

H	2.306629	-1.481198	0.652617
H	1.080376	-2.321346	1.092150
O	0.596869	1.255159	1.474493
H	0.028022	2.020743	1.652891
H	0.909547	0.901489	2.321878
O	-0.706120	-1.394702	-1.236651
H	-0.527437	-1.699916	-2.132803

$^4[Co(H_2O)_6]^{2+}$ C_i -604.142278 A.u.s

CO	0.000000	0.000000	0.000000
O	1.524208	0.879190	1.245463
H	2.485180	0.796704	1.129182
H	1.380263	1.434069	2.029786
O	-1.524208	-0.879190	-1.245463
H	-1.380263	-1.434069	-2.029786
H	-2.485180	-0.796704	-1.129182
O	-1.514085	0.873763	1.237883
H	-1.921913	1.747760	1.120178
H	-1.921958	0.469601	2.021674
O	1.514085	-0.873763	-1.237883
H	1.921958	-0.469601	-2.021674
H	1.921913	-1.747760	-1.120178
O	-0.000293	-1.688874	1.196562
H	0.555755	-1.834434	1.980970
H	-0.556354	-2.477068	1.073222
O	0.000293	1.688874	-1.196562
H	-0.555755	1.834434	-1.980970
H	0.556354	2.477068	-1.073222

$^4[Co(H_2O)_5OH]^{+}$ C_1 -603.8914134 A.u.s

CO	0.027319	-0.059337	-0.089942
O	-2.049937	-0.595184	0.829549
O	-1.297646	1.601543	-0.568679
O	1.837497	0.542299	-1.177361
O	1.447999	-1.366266	0.965149
O	-0.771293	-1.279404	-1.264478
O	0.688779	1.304557	1.440057
H	-0.311337	-1.946199	-1.789597
H	-1.454826	1.774666	-1.510409
H	-2.136323	1.249009	-0.215606
H	-2.049082	-1.242644	0.082304
H	-2.423614	-1.023813	1.612665
H	2.305027	-1.419574	0.511824
H	1.170103	-2.279910	1.136785

H	1.847591	0.424565	-2.140413
H	2.242403	1.404919	-0.993873
H	0.114081	2.041218	1.700976
H	1.115162	0.959499	2.239876

$^{3}[Ni(H_2O)_6]^{2+}$ S_6 -629.2451035 A.u.s

NI	0.000277	0.000506	-0.000247
O	1.809968	-0.118629	1.031646
O	0.744001	-1.301383	-1.449897
O	-1.809969	0.118095	-1.031500
O	-0.745484	1.298373	1.451903
O	0.725860	1.628082	-1.083889
O	-0.725759	-1.627293	1.083290
H	0.647021	2.563369	-0.833170
H	1.201587	1.587512	-1.929944
H	0.272201	-1.607115	-2.242029
H	1.631663	-1.695911	-1.462611
H	2.578544	0.462640	0.908769
H	2.032470	-0.761843	1.724687
H	-1.630591	1.698705	1.460522
H	-0.269560	1.613950	2.237651
H	-2.034212	0.758964	-1.726150
H	-2.577983	-0.463207	-0.905306
H	-0.647065	-2.562520	0.832329
H	-1.200773	-1.586657	1.929738

$^{3}[Ni(H_2O)_5OH]^{+}$ C_1 -628.9876323 A.u.s

NI	0.006431	-0.013796	0.003440
O	1.483345	-0.262441	1.502903
O	0.958284	-1.570881	-1.046109
O	-1.556724	0.149437	-1.148467
O	-0.924162	1.802526	0.651638
O	1.420733	1.316237	-0.833805
O	-1.377056	-1.412689	0.822787
H	1.069273	2.220293	-0.892494
H	1.793445	1.092630	-1.701454
H	0.331900	-2.100564	-1.565983
H	1.476404	-2.196270	-0.514273
H	-1.604163	1.590342	-0.042876
H	-1.373353	2.052512	1.472308
H	-1.546714	0.199050	-2.112829
H	-1.984490	-1.142125	0.086948
H	-1.878008	-1.399436	1.651413
H	2.183097	0.410397	1.508549

H	1.317203	-0.518047	2.422811

$[Cu(H_2O)_6]^{2+}$ C_i -655.5799058 A.u.s

CU	0.000000	0.000000	0.000000
O	-0.373071	-0.174385	-1.965686
O	-2.254930	0.116055	0.286776
O	0.373071	0.174385	1.965686
O	2.254930	-0.116055	-0.286776
O	0.101071	2.047321	-0.179294
O	-0.101071	-2.047321	0.179294
H	0.914021	2.558057	-0.333147
H	-0.656296	2.656756	-0.196927
H	-2.789533	0.236263	1.088996
H	-2.888405	0.073828	-0.449028
H	-0.231421	0.542333	-2.607394
H	-0.313677	-1.023433	-2.436279
H	2.888405	-0.073828	0.449028
H	2.789533	-0.236263	-1.088996
H	0.313677	1.023433	2.436279
H	0.231421	-0.542333	2.607394
H	-0.914021	-2.558057	0.333147
H	0.656296	-2.656756	0.196927

$[Cu(H_2O)_5OH]^{+}$ C_1 -655.3359779 A.u.s

CU	0.100300	0.114401	-0.014737
O	-0.285488	-1.229880	-1.464896
O	-1.346383	1.490509	-0.773034
O	0.201906	1.383491	1.341325
O	1.079086	-1.126047	1.433109
O	2.198768	0.130804	-0.949934
O	-2.185478	-0.947571	0.459127
H	2.884116	-0.179580	-0.334890
H	2.633148	0.771124	-1.542891
H	-1.142577	2.119878	-0.045323
H	-1.312163	1.969859	-1.619576
H	0.428084	-1.788691	-1.824665
H	-1.049288	-1.786782	-1.222038
H	0.928004	-0.464023	2.138014
H	0.784461	-1.993422	1.762658
H	0.998124	1.934327	1.319912
H	-2.742911	-0.206584	0.163437
H	-2.617008	-1.304175	1.267150

$[Zn(H_2O)_6]^{2+}$ T_h -685.4213799 A.u.s

ZN	0.000000	0.000000	0.000000
O	0.000000	0.000000	2.123007
O	0.000000	2.123007	0.000000
O	0.000000	0.000000	-2.123007
O	0.000000	-2.123007	0.000000
O	-2.123007	0.000000	0.000000
O	2.123007	0.000000	0.000000
H	-2.698126	-0.783411	0.000000
H	-2.698126	0.783411	0.000000
H	0.000000	2.698126	-0.783411
H	0.000000	2.698126	0.783411
H	-0.783411	0.000000	2.698126
H	0.783411	0.000000	2.698126
H	0.000000	-2.698126	-0.783411
H	0.000000	-2.698126	0.783411
H	-0.783411	0.000000	-2.698126
H	0.783411	0.000000	-2.698126
H	2.698126	0.783411	0.000000
H	2.698126	-0.783411	0.000000

$[Zn(H_2O)_5OH]^+$ C_s -685.1757911 A.u.s

ZN	0.123305	-0.517324	0.000000
O	-0.018152	-1.356292	1.822949
O	-0.018152	-1.356292	-1.822949
H	-0.048255	-0.552509	2.404431
H	-0.669092	-2.004928	2.132252
O	1.347218	0.919898	0.000000
H	-0.048255	-0.552509	-2.404431
H	-0.669092	-2.004928	-2.132252
H	2.292346	0.709486	0.000000
O	-0.018152	1.275045	2.332539
H	0.094951	1.884815	3.076634
H	0.689933	1.464429	1.666120
O	-0.018152	1.275045	-2.332539
H	0.094951	1.884815	-3.076634
H	0.689933	1.464429	-1.666120
O	-1.638041	0.600929	0.000000
H	-1.609568	1.179975	-0.786368
H	-1.609568	1.179975	0.786368

$[Cd(H_2O)_6]^{2+}$ T_h -626.0449483 A.u.s

CD	0.000000	0.000000	0.000000
O	0.000000	0.000000	2.323373

O	0.000000	2.323373	0.000000
O	0.000000	0.000000	-2.323373
O	0.000000	-2.323373	0.000000
O	-2.323373	0.000000	0.000000
O	2.323373	0.000000	0.000000
H	-2.902640	-0.780223	0.000000
H	-2.902640	0.780223	0.000000
H	0.000000	2.902640	-0.780223
H	0.000000	2.902640	0.780223
H	-0.780223	0.000000	2.902640
H	0.780223	0.000000	2.902640
H	0.000000	-2.902640	-0.780223
H	0.000000	-2.902640	0.780223
H	-0.780223	0.000000	-2.902640
H	0.780223	0.000000	-2.902640
H	2.902640	0.780223	0.000000
H	2.902640	-0.780223	0.000000

$[Cd(H_2O)_5OH]^+$ C_s -625.7832881 A.u.s

CD	0.123231	-0.567869	0.000000
O	-0.048732	-1.197893	2.129284
O	-0.048732	-1.197893	-2.129284
H	-0.087638	-0.309202	2.568328
H	-0.686331	-1.794007	2.551034
O	1.354760	1.144312	0.000000
H	-0.087638	-0.309202	-2.568328
H	-0.686331	-1.794007	-2.551034
H	2.315626	1.020965	0.000000
O	-0.048732	1.493353	2.275973
H	0.069899	2.159675	2.969017
H	0.650438	1.639787	1.582494
O	-0.048732	1.493353	-2.275973
H	0.069899	2.159675	-2.969017
H	0.650438	1.639787	-1.582494
O	-1.758450	0.780987	0.000000
H	-1.667247	1.357235	-0.783445
H	-1.667247	1.357235	0.783445

$[Hg(H_2O)_6]^{2+}$ T_h -611.7035469 A.u.s

HG	0.000000	0.000000	0.000000
O	0.000000	0.000000	2.391324
O	0.000000	2.391324	0.000000
H	0.782673	0.000000	2.967039
H	-0.782673	0.000000	2.967039

O	2.391324	0.000000	0.000000
O	0.000000	0.000000	-2.391324
O	0.000000	-2.391324	0.000000
O	-2.391324	0.000000	0.000000
H	0.000000	2.967039	0.782673
H	0.000000	2.967039	-0.782673
H	2.967039	-0.782673	0.000000
H	2.967039	0.782673	0.000000
H	0.782673	0.000000	-2.967039
H	-0.782673	0.000000	-2.967039
H	0.000000	-2.967039	-0.782673
H	0.000000	-2.967039	0.782673
H	-2.967039	-0.782673	0.000000
H	-2.967039	0.782673	0.000000

$[Hg(H_2O)_5OH]^+$ C_s -611.4600836 A.u.s

HG	0.192415	-0.439009	0.000000
O	-0.216432	-1.103622	2.161806
O	-0.216432	-1.103622	-2.161806
H	-0.286685	-0.201513	2.568614
H	-1.005050	-1.615575	2.403904
O	1.268384	1.401559	0.000000
H	-0.286685	-0.201513	-2.568614
H	-1.005050	-1.615575	-2.403904
H	2.231001	1.272806	0.000000
O	-0.216432	1.610831	2.345837
H	-0.136185	2.238824	3.079454
H	0.483623	1.831607	1.685505
O	-0.216432	1.610831	-2.345837
H	-0.136185	2.238824	-3.079454
H	0.483623	1.831607	-1.685505
O	-1.910145	0.885568	0.000000
H	-1.837836	1.464433	-0.781142
H	-1.837836	1.464433	0.781142

$[Al(H_2O)_6]^{3+}$ C_i -700.1213431 A.u.s

AL	0.000000	0.000000	0.000000
O	-1.653020	-0.188432	-1.019906
O	0.450149	-1.858145	-0.388781
O	-0.450149	1.858145	0.388781
O	0.934168	0.562589	-1.618079
O	1.653020	0.188432	1.019906
O	-0.934168	-0.562589	1.618079
H	1.254469	-2.338802	-0.099164

H	-0.081609	-2.494474	-0.912333
H	-1.773355	-0.013645	-1.977386
H	-2.525399	-0.476937	-0.677082
H	1.393816	-0.019053	-2.260055
H	1.034411	1.479607	-1.951029
H	0.081609	2.494474	0.912333
H	-1.254469	2.338802	0.099164
H	2.525399	0.476937	0.677082
H	1.773355	0.013645	1.977386
H	-1.034411	-1.479607	1.951029
H	-1.393816	0.019053	2.260055

$[Al(H_2O)_5OH]^{2+}$ C_1 -700.0510911 A.u.s

AL	-0.049246	0.007135	-0.110749
O	1.889898	-0.063027	-0.580841
O	0.656790	-0.028543	1.748743
O	-0.897400	0.048809	-1.622940
O	0.172132	1.977908	-0.083593
O	-1.853499	0.016817	0.706336
O	0.034534	-1.980997	-0.104641
H	0.181800	-0.186199	2.584214
H	1.611769	-0.040844	1.945654
H	2.323629	0.688841	-1.026270
H	2.277659	-0.876621	-0.954831
H	0.343043	2.634981	0.613995
H	-0.289498	2.423592	-0.820457
H	-0.647561	-0.014269	-2.550782
H	-2.289520	0.521086	1.414510
H	-2.466916	-0.005301	-0.059986
H	0.054121	-2.626579	0.624362
H	-0.477958	-2.379169	-0.835191

$[Al(H_2O)_6(H_2O)_{12}]^{3+}$ C_i -1617.7897327 A.u.s

AL	0.000000	0.000000	0.000000
O	-1.523589	-0.259748	-1.184599
O	0.519632	-1.831571	-0.313336
O	-0.519632	1.831571	0.313336
O	1.053168	0.552930	-1.507157
O	1.523589	0.259748	1.184599
O	-1.053168	-0.552930	1.507157
H	1.098984	-2.405740	0.260603
H	0.134439	-2.398062	-1.042049
H	-1.719563	0.269145	-2.012751
H	-2.233661	-0.937477	-1.091058

H	1.152795	-0.129591	-2.256338
H	0.891584	1.417108	-1.972721
H	-0.134439	2.398062	1.042049
H	-1.098984	2.405740	-0.260603
H	2.233661	0.937477	1.091058
H	1.719563	-0.269145	2.012751
H	-0.891584	-1.417108	1.972721
H	-1.152795	0.129591	2.256338
O	-1.784593	3.407727	-1.441976
O	0.590266	3.149679	2.335115
O	0.354046	2.709676	-3.001829
O	0.971943	-1.065010	-3.503120
O	3.195822	2.428999	1.554963
O	2.058020	-1.360611	3.219284
O	-0.354046	-2.709676	3.001829
O	-0.971943	1.065010	3.503120
O	-3.195822	-2.428999	-1.554963
O	-2.058020	1.360611	-3.219284
O	-0.590266	-3.149679	-2.335115
O	1.784593	-3.407727	1.441976
H	-1.002894	3.658554	-1.982888
H	-2.279854	4.225143	-1.259354
H	1.565986	3.070173	2.225611
H	0.425994	4.075723	2.584125
H	-0.418466	1.860971	3.368879
H	-1.682682	1.327514	4.109931
H	0.305860	-2.234299	3.551485
H	-0.963406	-3.143298	3.624567
H	2.279854	-4.225143	1.259354
H	1.002894	-3.658554	1.982888
H	-0.425994	-4.075723	-2.584125
H	-1.565986	-3.070173	-2.225611
H	-3.610549	-2.969008	-0.858108
H	-3.903256	-2.334130	-2.218902
H	-2.669586	1.211810	-3.960686
H	-2.392071	2.146277	-2.729859
H	2.392071	-2.146277	2.729859
H	2.669586	-1.211810	3.960686
H	3.903256	2.334130	2.218902
H	3.610549	2.969008	0.858108
H	0.963406	3.143298	-3.624567
H	-0.305860	2.234299	-3.551485
H	1.682682	-1.327514	-4.109931
H	0.418466	-1.860971	-3.368879

$[Al(H_2O)_5OH(H_2O)_{12}]^{2+}$ C_1 -1617.5795648 A.u.s

AL	-0.115552	0.116815	-0.308505
O	1.364083	-0.049393	-1.347593
O	-0.056594	-1.775651	0.146457
O	-0.305629	2.000565	-0.684911
O	0.921943	0.615549	1.320875
O	-1.699450	0.233971	0.877491
O	-1.406742	-0.212414	-1.741488
H	-0.766251	-2.354761	0.509659
H	0.801348	-2.295021	0.102701
H	1.138164	-0.253200	-2.266664
H	1.323363	-0.165822	1.838704
H	1.719167	1.196678	1.128001
H	-0.985682	2.605147	-0.302667
H	0.475577	2.540685	-1.035628
H	-1.679050	0.741601	1.722562
H	-2.579423	-0.215193	0.773126
H	-1.874828	-1.076684	-1.840394
H	-2.124102	0.490344	-1.777270
O	1.814231	3.300332	-1.372160
O	-2.315126	3.327484	0.510347
O	3.074127	2.109076	0.741515
O	2.175887	-1.297865	2.486618
O	-1.176324	2.046640	2.741173
O	-3.908022	-1.279891	0.648606
O	-3.064906	-2.399280	-1.712780
O	-3.397346	1.499262	-1.463078
O	4.258066	-2.248209	-0.975281
O	3.876075	0.470971	-1.143099
O	2.236565	-3.053025	0.417299
O	-2.208589	-3.384982	0.674403
H	2.396860	3.188795	-0.589672
H	1.918129	4.214108	-1.676249
H	-2.079480	3.094642	1.434956
H	-2.488781	4.282838	0.512687
H	-3.216041	2.159447	-0.762886
H	-3.830704	1.995957	-2.174824
H	-3.747282	-1.937201	-1.178279
H	-3.511090	-2.729639	-2.510218
H	-2.203328	-4.295357	1.012274
H	-2.455594	-3.439462	-0.278152
H	2.282357	-4.022293	0.436377
H	3.041293	-2.761591	-0.137359
H	5.162876	-2.540294	-0.789109
H	4.299128	-1.265526	-1.046716

H	4.210650	0.916941	-1.938612
H	2.885289	0.296097	-1.315221
H	-3.546137	-2.117776	1.018049
H	-4.762809	-1.122358	1.081424
H	-1.256409	2.132751	3.705121
H	-0.240242	1.820932	2.559920
H	3.709046	2.379010	1.424242
H	3.574228	1.511381	0.105756
H	2.148754	-1.650591	3.387584
H	2.305171	-2.068297	1.882184

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