Electronic Supplementary Information for Dalton Transactions

Supplementary Information
for

The structure of the lanthanide aquo ions in solution as studied by ^{17}O NMR spectroscopy and DFT calculations

Kristina Djanashvili,* Carlos Platas-Iglesias and Joop A. Peters

1. Cartesian coordinates (Å) for the $Ln(H_2O)_8^{3+}$ and $Ln(H_2O)_9^{3+}$ systems obtained by DFT calculations

$Ce(H_2O)_8^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	58	-0.000352	0.000166	-0.002459
2	8	-1.079352	-1.845423	-1.368377
3	8	-1.869574	1.074147	-1.340060
4	8	1.048657	1.868119	-1.364916
5	8	1.843440	-1.064582	-1.379690
6	8	2.078466	0.557967	1.341134
7	8	0.579242	-2.060646	1.359633
8	8	-2.048098	-0.576698	1.375876
9	8	-0.548703	2.045147	1.390395
10	1	0.910803	2.838213	-1.251627
11	1	1.698559	1.766498	-2.099507
12	1	-2.840701	0.948506	-1.221572
13	1	-1.761883	1.746183	-2.053873
14	1	-1.756789	-1.724685	-2.074445
15	1	-0.948425	-2.818461	-1.274855
16	1	1.721387	-1.722447	-2.104571
17	1	2.816798	-0.943474	-1.276141
18	1	-2.432366	-0.031228	2.102061
19	1	-2.648805	-1.351204	1.265886
20	1	0.030628	-2.452781	2.079159
21	1	1.360015	-2.653594	1.253186
22	1	2.477181	-0.000818	2.049002
23	1	2.676768	1.334140	1.230466
24	1	-1.329808	2.641123	1.304728
25	1	0.014440	2.430170	2.102763

$Ce(H_2O)_9^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	58	0.000660	0.000736	0.001091
2	8	-1.852251	-1.782329	0.156033
3	8	1.837718	1.041012	1.470762
4	8	-1.850532	1.037240	1.460321
5	8	1.852951	0.746296	-1.624189
6	8	-1.835187	0.749575	-1.642582
7	8	1.845007	-1.788023	0.170955
8	1	-2.652698	1.253629	-1.428050
9	1	-1.968660	0.375962	-2.542707
10	1	-2.670245	0.592785	1.774608

11	1	-1.994409	2.001969	1.587180
12	1	-2.011376	-2.360087	0.935969
13	1	-2.661840	-1.838614	-0.400535
14	1	2.661833	-1.750342	0.718440
15	1	1.983165	-2.510518	-0.482073
16	1	1.979781	0.835892	2.422243
17	1	2.657955	1.485708	1.158094
18	1	1.996662	1.669874	-1.930432
19	1	2.669995	0.248625	-1.854685
20	8	0.001540	2.570525	-0.238270
21	8	0.006155	-1.492975	-2.097450
22	8	-0.006737	-1.083220	2.340304
23	1	-0.533414	-2.303519	-2.241218
24	1	0.547806	-1.370713	-2.909988
25	1	-0.547767	-0.811318	3.116284
26	1	0.521121	-1.862592	2.628252
27	1	0.527380	3.213705	0.289618
28	1	-0.532905	3.102072	-0.871362

$Pr(H_2O)_8^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	59	-0.000107	-0.000268	-0.003303
2	8	-1.118276	-1.798919	-1.357562
3	8	-1.813996	1.117356	-1.342140
4	8	1.102977	1.813983	-1.354888
5	8	1.802954	-1.112660	-1.360073
6	8	2.067162	0.494925	1.342486
7	8	0.504202	-2.055698	1.356456
8	8	-2.054078	-0.505136	1.359562
9	8	-0.488964	2.046097	1.375942
10	1	0.995157	2.788494	-1.246931
11	1	1.752889	1.686101	-2.085295
12	1	-2.788868	1.020467	-1.228130
13	1	-1.680533	1.781294	-2.058683
14	1	-1.785908	-1.654910	-2.068873
15	1	-1.019117	-2.775482	-1.261122
16	1	1.663815	-1.764053	-2.087285
17	1	2.778914	-1.019756	-1.251944
18	1	-2.421743	0.059067	2.079756
19	1	-2.676368	-1.262660	1.252197
20	1	-0.062991	-2.425935	2.073076
21	1	1.266897	-2.672954	1.257033
22	1	2.442450	-0.074325	2.054865
23	1	2.688371	1.253179	1.233803
24	1	-1.250181	2.666631	1.286434
25	1	0.087666	2.411056	2.087727

$Pr(H_2O)_9^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	59	-0.000031	-0.001238	0.000276
2	8	-1.842475	0.714999	-1.609600

3	8	1.854849	-1.753548	0.173469
4	8	-1.804652	-1.796935	0.157929
5	8	1.810465	1.054940	1.452871
6	8	-1.839392	1.008261	1.445466
7	8	1.827444	0.763838	-1.606853
8	1	-2.638290	0.551168	1.794716
9	1	-1.985596	1.972250	1.578999
10	1	-2.603855	-1.883347	-0.410561
11	1	-1.935372	-2.403275	0.921974
12	1	-1.978721	0.348084	-2.512547
13	1	-2.660313	1.212972	-1.381303
14	1	2.637448	0.267850	-1.865165
15	1	1.949149	1.687650	-1.923601
16	1	2.009495	-2.480451	-0.471775
17	1	2.661834	-1.701532	0.735269
18	1	1.944087	0.875869	2.411411
19	1	2.609498	1.539195	1.142706
20	8	0.005122	-1.062842	2.322830
21	8	-0.036107	2.547067	-0.247323
22	8	0.025326	-1.469165	-2.088669
23	1	-0.618367	3.070042	-0.844680
24	1	0.530419	3.193424	0.232167
25	1	-0.533133	-2.260882	-2.261146
26	1	0.601159	-1.352098	-2.877977
27	1	0.579036	-1.799368	2.632922
28	1	-0.571316	-0.817443	3.081376

$Nd(H_2O)_8^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	60	0.000091	-0.000265	-0.002972
2	8	-1.119265	-1.782403	-1.350234
3	8	-1.792531	1.120369	-1.339004
4	8	1.111119	1.788456	-1.349332
5	8	1.783244	-1.117906	-1.351246
6	8	2.052588	0.479178	1.342476
7	8	0.482213	-2.042681	1.353496
8	8	-2.043921	-0.484421	1.352090
9	8	-0.473928	2.038755	1.362021
10	1	1.041761	2.764049	-1.220533
11	1	1.715122	1.647352	-2.116812
12	1	-2.766973	1.070896	-1.194386
13	1	-1.650783	1.730811	-2.100551
14	1	-1.721291	-1.633855	-2.116868
15	1	-1.066925	-2.758594	-1.218932
16	1	1.634741	-1.716287	-2.120877
17	1	2.759309	-1.063666	-1.221032
18	1	-2.369827	0.048829	2.114433
19	1	-2.696504	-1.211700	1.218286
20	1	-0.056724	-2.370646	2.111272
21	1	1.213995	-2.691696	1.227441
22	1	2.384498	-0.058466	2.099068
23	1	2.706391	1.204741	1.204616
24	1	-1.202502	2.691833	1.238028
25	1	0.074119	2.367532	2.113035

$Nd(H_2O)_9^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	60	-0.001330	0.001368	-0.001611
2	8	1.752875	0.287898	-1.811318
3	8	-1.772094	1.360776	1.203432
4	8	1.798117	1.406271	1.116545
5	8	-1.771839	-1.705006	0.620946
6	8	1.790091	-1.688483	0.623698
7	8	-1.790632	0.342410	-1.767972
8	1	2.613411	-1.498892	1.130499
9	1	1.974357	-2.497822	0.095430
10	1	2.606534	1.764824	0.684308
11	1	2.001464	1.350429	2.077975
12	1	1.948338	1.155376	-2.234448
13	1	2.566265	-0.257554	-1.915806
14	1	-2.598345	0.898602	-1.674124
15	1	-1.997050	-0.327415	-2.458136
16	1	-1.977350	2.299628	0.988748
17	1	-2.576291	0.995311	1.639158
18	1	-1.953015	-1.982224	1.547048
19	1	-2.586716	-1.914641	0.109219
20	8	0.045682	-0.431467	2.505813
21	8	-0.021541	-1.944234	-1.636781
22	8	-0.011313	2.391972	-0.867316
23	1	0.482431	-2.006938	-2.480131
24	1	-0.520991	-2.787973	-1.542876
25	1	0.492509	3.149923	-0.491422
26	1	-0.535850	2.749267	-1.619028
27	1	-0.479371	0.035140	3.194937
28	1	0.542552	-1.145502	2.966985

$Sm(H_2O)_8^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	62	-0.000197	-0.000714	-0.003169
2	8	-0.498275	-2.008983	-1.331567
3	8	-2.017701	0.499503	-1.319586
4	8	0.489179	2.015175	-1.327571
5	8	2.012074	-0.499250	-1.325500
6	8	1.771495	1.078546	1.321727
7	8	1.076677	-1.763886	1.331837
8	8	-1.763654	-1.078979	1.332474
9	8	-1.067837	1.760084	1.340455
10	1	0.082537	2.907726	-1.227204
11	1	1.146899	2.087644	-2.057954
12	1	-2.916040	0.107919	-1.210949
13	1	-2.089316	1.178513	-2.030412
14	1	-1.160275	-2.072918	-2.059524
15	1	-0.093895	-2.903347	-1.238369
16	1	2.076982	-1.163500	-2.050826
17	1	2.910226	-0.105471	-1.222433

18	1	-2.286427	-0.646349	2.047415
19	1	-2.119868	-1.993254	1.234178
20	1	0.640837	-2.292763	2.040429
21	1	1.992343	-2.116836	1.237160
22	1	2.301486	0.645800	2.031222
23	1	2.123728	1.994236	1.223529
24	1	-1.985837	2.109782	1.256433
25	1	-0.626837	2.289418	2.045655

$Sm(H_2O)_9^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	62	0.003001	0.007459	-0.000305
2	8	1.724803	0.282473	-1.799959
3	8	-1.759388	1.335925	1.189505
4	8	1.776372	1.389581	1.109014
5	8	-1.744503	-1.684375	0.611176
6	8	1.768016	-1.659721	0.618976
7	8	-1.741981	0.351780	-1.764058
8	1	2.603390	-1.450513	1.097476
9	1	1.955703	-2.454569	0.069409
10	1	2.597778	1.720735	0.677850
11	1	1.987329	1.280786	2.064527
12	1	1.932541	1.150783	-2.213839
13	1	2.532165	-0.271718	-1.906889
14	1	-2.575164	0.866590	-1.658492
15	1	-1.932810	-0.345415	-2.433078
16	1	-1.962795	2.278601	0.993743
17	1	-2.569529	0.962813	1.607802
18	1	-1.931050	-1.920508	1.548887
19	1	-2.573745	-1.867532	0.111703
20	8	0.052743	-0.410220	2.483820
21	8	-0.013514	-1.934874	-1.608954
22	8	-0.003398	2.369624	-0.851226
23	1	0.464571	-1.983861	-2.467958
24	1	-0.521383	-2.772414	-1.515758
25	1	0.474655	3.142621	-0.474365
26	1	-0.554134	2.708992	-1.593023
27	1	-0.488257	0.052164	3.162997
28	1	0.519482	-1.144163	2.944787

$Eu(H_2O)_8^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	0.000278	-0.000446	-0.003776
2	8	-1.183821	-1.687791	-1.317723
3	8	-1.706999	1.178922	-1.303398

4	8	1.162756	1.699722	-1.325905
5	8	1.684704	-1.179061	-1.327128
6	8	2.035755	0.372192	1.304333
7	8	0.378987	-2.018228	1.324065
8	8	-2.014182	-0.376018	1.332604
9	8	-0.358678	2.011377	1.339256
10	1	1.113363	2.678233	-1.211403
11	1	1.791219	1.535097	-2.067528
12	1	-2.684476	1.142492	-1.177156
13	1	-1.538558	1.823901	-2.029894
14	1	-1.833706	-1.505308	-2.036491
15	1	-1.140653	-2.667877	-1.215388
16	1	1.500727	-1.817270	-2.055917
17	1	2.664447	-1.145785	-1.218922
18	1	-2.337073	0.208213	2.058193
19	1	-2.683887	-1.092027	1.223463
20	1	-0.206411	-2.345308	2.046781
21	1	1.100270	-2.682704	1.219322
22	1	2.374074	-0.216537	2.019284
23	1	2.706586	1.084854	1.182290
24	1	-1.074915	2.682813	1.242932
25	1	0.243286	2.336383	2.049504

$Eu(H_2O)_9^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	63	-0.004227	-0.005467	-0.006169
2	8	1.694238	0.284694	-1.809767
3	8	-1.756658	1.328205	1.156291
4	8	1.769164	1.351739	1.092791
5	8	-1.724014	-1.691060	0.616797
6	8	1.755629	-1.650129	0.627021
7	8	-1.739818	0.349262	-1.759613
8	1	2.591850	-1.426911	1.097627
9	1	1.944247	-2.457033	0.096010
10	1	2.578283	1.703648	0.654693
11	1	1.989228	1.253345	2.047189
12	1	1.898464	1.162285	-2.205147
13	1	2.508109	-0.260311	-1.916324
14	1	-2.555078	0.890400	-1.644525
15	1	-1.953278	-0.322112	-2.446883
16	1	-1.946544	2.269000	0.938312
17	1	-2.575681	0.967877	1.568248
18	1	-1.913616	-1.903208	1.559497
19	1	-2.543926	-1.905631	0.114423
20	8	0.027890	-0.414456	2.469033
21	8	-0.006486	-1.936250	-1.594320
22	8	0.005933	2.360177	-0.825439
23	1	0.468783	-1.977300	-2.455384
24	1	-0.501359	-2.781895	-1.502445
25	1	0.487917	3.111166	-0.410196
26	1	-0.540714	2.736832	-1.551900
27	1	-0.469142	0.082989	3.157199
28	1	0.531703	-1.118810	2.936751

$Gd(H_2O)_8^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	64	-0.000178	-0.007026	-0.000713
2	8	2.063382	-0.193111	1.286011
3	8	0.167144	2.022989	1.323195
4	8	-2.075271	0.193453	1.262628
5	8	-0.184508	-2.004189	1.364217
6	8	-1.571875	-1.325229	-1.305560
7	8	1.302675	-1.559624	-1.343912
8	8	1.592153	1.324369	-1.274915
9	8	-1.298166	1.580253	-1.313120
10	1	-2.792673	0.850975	1.102753
11	1	-2.385219	-0.389709	1.994163
12	1	0.827344	2.749038	1.225843
13	1	-0.446762	2.290876	2.046649
14	1	2.348811	0.387935	2.029296
15	1	2.779018	-0.859794	1.158585
16	1	0.459526	-2.276874	2.058975
17	1	-0.830545	-2.743506	1.269960
18	1	1.376991	1.971061	-1.987156
19	1	2.563452	1.388657	-1.116933
20	1	1.974124	-1.300164	-2.017794
21	1	1.352034	-2.540967	-1.257048
22	1	-1.347483	-1.928760	-2.051877
23	1	-2.549320	-1.374531	-1.184392
24	1	-1.342867	2.557162	-1.185750
25	1	-1.939298	1.356999	-2.027968

$Gd(H_2O)_9^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	64	-0.000529	-0.002103	-0.004245
2	8	1.695405	0.273912	-1.784751
3	8	-1.730895	1.320888	1.167177
4	8	1.747369	1.362436	1.092158
5	8	-1.732916	-1.663554	0.597733
6	8	1.746598	-1.646586	0.608221
7	8	-1.715589	0.352821	-1.758697
8	1	2.580523	-1.432304	1.087406
9	1	1.936316	-2.448621	0.070018
10	1	2.555753	1.721469	0.658882
11	1	1.961438	1.283262	2.049416
12	1	1.881799	1.151883	-2.188213
13	1	2.520635	-0.255996	-1.877589
14	1	-2.540930	0.879484	-1.648400
15	1	-1.920302	-0.339846	-2.426933
16	1	-1.936000	2.263365	0.971924
17	1	-2.533022	0.949788	1.602308
18	1	-1.917657	-1.899823	1.535084
19	1	-2.559454	-1.852538	0.095822
20	8	0.020809	-0.441860	2.453962

21	8	-0.030083	-1.918161	-1.592593
22	8	0.015854	2.341903	-0.851925
23	1	0.477299	-1.987723	-2.432463
24	1	-0.513474	-2.767825	-1.480993
25	1	0.453592	3.114258	-0.427869
26	1	-0.544304	2.697935	-1.578355
27	1	-0.449937	0.072099	3.148915
28	1	0.552599	-1.127519	2.917771

$Tb(H_2O)_8^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	65	0.000166	-0.000306	-0.002929
2	8	-0.594120	-1.951715	-1.299854
3	8	-1.964264	0.588816	-1.282160
4	8	0.570452	1.954923	-1.307875
5	8	1.945642	-0.587882	-1.312960
6	8	1.802426	0.975611	1.283078
7	8	0.983437	-1.784439	1.304833
8	8	-1.784120	-0.974346	1.307561
9	8	-0.960207	1.787866	1.312420
10	1	0.219484	2.868282	-1.185197
11	1	1.241303	2.003303	-2.028262
12	1	-2.871872	0.215087	-1.188440
13	1	-2.006565	1.270754	-1.992605
14	1	-1.301422	-1.999645	-1.984754
15	1	-0.227527	-2.862174	-1.203978
16	1	1.994210	-1.302869	-1.989807
17	1	2.860413	-0.236356	-1.202872
18	1	-2.276660	-0.528469	2.035723
19	1	-2.170364	-1.876508	1.211107
20	1	0.534386	-2.295857	2.017799
21	1	1.887530	-2.165284	1.205460
22	1	2.308379	0.525938	1.999534
23	1	2.177860	1.882787	1.192471
24	1	-1.867539	2.165457	1.231200
25	1	-0.506342	2.284748	2.032705

$Tb(H_2O)_9^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	65	0.000256	-0.000103	0.000150
2	8	-1.759827	0.718281	-1.556767
3	8	1.740779	-1.724547	0.173035
4	8	-1.771385	-1.699287	0.166053
5	8	1.768317	0.987502	1.392551
6	8	-1.763522	1.013321	1.382685
7	8	1.781406	0.689517	-1.542333

8	1	-2.567208	0.568699	1.735911
9	1	-1.853827	1.973355	1.576702
10	1	-2.562456	-1.789280	-0.412458
11	1	-1.865057	-2.356745	0.891511
12	1	-1.854543	0.419273	-2.488992
13	1	-2.554465	1.257740	-1.342181
14	1	2.571510	0.165984	-1.807217
15	1	1.885111	1.589054	-1.926611
16	1	1.825453	-2.507315	-0.416714
17	1	2.537926	-1.707814	0.750057
18	1	1.855730	0.880258	2.366404
19	1	2.566788	1.470267	1.080157
20	8	-0.012074	-1.012621	2.259074
21	8	0.020456	2.462460	-0.253235
22	8	-0.006048	-1.432961	-2.019449
23	1	-0.553448	2.992342	-0.851188
24	1	0.601939	3.096034	0.223954
25	1	-0.579461	-2.214923	-2.183648
26	1	0.581376	-1.337063	-2.802145
27	1	0.555367	-1.751803	2.573536
28	1	-0.592165	-0.754673	3.010288

$Dy(H_2O)_8^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	66	0.000587	-0.000581	-0.002447
2	8	0.998577	-1.766750	-1.293376
3	8	-1.771556	-1.007315	-1.280997
4	8	-1.010674	1.756241	-1.297905
5	8	1.764049	0.999573	-1.292789
6	8	0.537154	1.962896	1.282331
7	8	1.956717	-0.530344	1.293779
8	8	-0.530873	-1.951484	1.300601
9	8	-1.946511	0.540202	1.302190
10	1	-1.919835	2.120986	-1.184548
11	1	-0.582055	2.277421	-2.016149
12	1	-2.151059	-1.909524	-1.162679
13	1	-2.300158	-0.563334	-1.984324
14	1	0.558171	-2.280082	-2.010283
15	1	1.909333	-2.131364	-1.195001
16	1	2.288668	0.553444	-1.998000
17	1	2.144262	1.901934	-1.177763
18	1	-1.208918	-2.002456	2.014058
19	1	-0.149350	-2.855728	1.203421
20	1	2.014062	-1.222977	1.992676
21	1	2.862155	-0.155469	1.185349
22	1	1.214344	2.020539	1.995795
23	1	0.155229	2.865864	1.177585
24	1	-2.853006	0.163378	1.207409
25	1	-1.995621	1.231547	2.003278

$Dy(H_2O)_9^{3+}$

Center	Atomic	Coordinates (Angstroms)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	66	-0.000919	-0.001498	0.000452
2	8	1.728481	0.298594	-1.699308
3	8	-1.723870	1.312152	1.127876
4	8	1.751387	1.315034	1.080194
5	8	-1.741910	-1.607688	0.600351
6	8	1.760073	-1.606046	0.564593
7	8	-1.771302	0.292543	-1.657426
8	1	2.564876	-1.421015	1.099868
9	1	1.890393	-2.484732	0.141523
10	1	2.547355	1.700385	0.648718
11	1	1.884486	1.390082	2.052019
12	1	1.849474	1.110734	-2.239316
13	1	2.532937	-0.254620	-1.823279
14	1	-2.573767	0.856106	-1.573207
15	1	-1.899811	-0.281033	-2.446033
16	1	-1.851604	2.280674	1.014671
17	1	-2.522905	0.965486	1.585603
18	1	-1.851935	-2.016239	1.488058
19	1	-2.554236	-1.811106	0.083528
20	8	0.029360	-0.442146	2.426169
21	8	-0.019934	-1.883245	-1.592227
22	8	-0.011828	2.312807	-0.851969
23	1	0.547938	-1.977562	-2.389635
24	1	-0.586663	-2.685473	-1.544291
25	1	0.552272	3.053637	-0.535245
26	1	-0.591262	2.674440	-1.559267
27	1	-0.525350	-0.003371	3.109570
28	1	0.609163	-1.085854	2.891780

$Ho(H_2O)_8^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	67	0.000687	-0.000194	-0.002289
2	8	1.256094	-1.575719	-1.286696
3	8	-1.575144	-1.271367	-1.277202
4	8	-1.279068	1.568359	-1.280573
5	8	1.571025	1.261305	-1.289640
6	8	0.220261	2.008205	1.277563
7	8	2.006039	-0.210169	1.284102
8	8	-0.209813	-1.997669	1.293869
9	8	-1.991376	0.213424	1.304598
10	1	-2.240860	1.761619	-1.179915
11	1	-0.943138	2.157097	-1.995960
12	1	-1.786368	-2.228626	-1.171121
13	1	-2.194593	-0.912839	-1.954880
14	1	0.900061	-2.160193	-1.995996
15	1	2.218916	-1.772868	-1.206992
16	1	2.155975	0.903153	-1.997616
17	1	1.787920	2.218324	-1.192617
18	1	-0.877941	-2.155760	2.001202
19	1	0.317027	-2.826365	1.204259
20	1	2.181988	-0.903005	1.962727
21	1	2.838772	0.306963	1.177541
22	1	0.902572	2.176337	1.968794
23	1	-0.291226	2.844007	1.167922

24	1	-2.828896	-0.296926	1.201604
25	1	-2.170389	0.931110	1.956222

$Ho(H_2O)_9^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	67	-0.000175	0.000315	0.000041
2	8	1.729116	0.296474	-1.684330
3	8	-1.725994	1.302064	1.114864
4	8	1.748245	1.304934	1.068947
5	8	-1.741138	-1.588611	0.595542
6	8	1.756121	-1.589573	0.557153
7	8	-1.771780	0.287381	-1.642492
8	1	2.554591	-1.410004	1.103985
9	1	1.880110	-2.474006	0.146116
10	1	2.538028	1.701213	0.635544
11	1	1.873170	1.396606	2.040217
12	1	1.842204	1.095491	-2.246506
13	1	2.525908	-0.266784	-1.812521
14	1	-2.568854	0.857706	-1.554332
15	1	-1.897933	-0.266968	-2.445142
16	1	-1.847090	2.273779	1.023195
17	1	-2.518880	0.951778	1.580712
18	1	-1.849256	-2.022064	1.471753
19	1	-2.544651	-1.795360	0.066279
20	8	0.031316	-0.442565	2.417807
21	8	-0.016482	-1.879860	-1.582665
22	8	-0.010738	2.306550	-0.845746
23	1	0.559801	-1.984530	-2.372832
24	1	-0.589870	-2.677568	-1.537340
25	1	0.561706	3.041766	-0.530975
26	1	-0.592963	2.673907	-1.548332
27	1	-0.525418	-0.011620	3.104493
28	1	0.621803	-1.078777	2.880336

$Er(H_2O)_8^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	68	-0.001608	-0.001623	0.000869
2	8	0.528392	-1.953694	1.248091
3	8	1.951401	0.499574	1.271806
4	8	-0.501729	1.924252	1.306237
5	8	-1.939320	-0.536860	1.274485
6	8	-1.750767	1.027218	-1.244045
7	8	-1.018081	-1.704475	-1.302703
8	8	1.741514	-0.975924	-1.281535
9	8	1.001979	1.727253	-1.286053
10	1	-0.089076	2.815481	1.216494
11	1	-1.177978	1.991473	2.020182
12	1	2.846598	0.101601	1.156953

13	1	2.023799	1.180054	1.981105
14	1	1.211972	-2.024751	1.954259
15	1	0.110217	-2.842593	1.158185
16	1	-1.997662	-1.235608	1.967549
17	1	-2.841228	-0.151154	1.175228
18	1	2.265533	-0.514348	-1.977828
19	1	2.110671	-1.886249	-1.196737
20	1	-0.575120	-2.237333	-2.003719
21	1	-1.932366	-2.060498	-1.203797
22	1	-2.294318	0.597021	-1.944360
23	1	-2.108679	1.937569	-1.116994
24	1	1.912339	2.093078	-1.184796
25	1	0.537563	2.287870	-1.951056

$Er(H_2O)_9^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	68	-0.000093	-0.000940	-0.000066
2	8	1.715208	0.297177	-1.680754
3	8	-1.711784	1.298225	1.112999
4	8	1.734585	1.299461	1.070414
5	8	-1.727540	-1.585564	0.594408
6	8	1.743006	-1.588024	0.555192
7	8	-1.758953	0.288183	-1.637259
8	1	2.553462	-1.408974	1.083353
9	1	1.863912	-2.466589	0.130521
10	1	2.533844	1.684149	0.644774
11	1	1.857933	1.380511	2.042632
12	1	1.828625	1.100197	-2.235872
13	1	2.523420	-0.251603	-1.797961
14	1	-2.561037	0.850651	-1.546331
15	1	-1.886729	-0.269333	-2.437097
16	1	-1.835054	2.268309	1.010905
17	1	-2.513128	0.951069	1.565963
18	1	-1.834582	-2.005801	1.476812
19	1	-2.541289	-1.784001	0.078309
20	8	0.031147	-0.438807	2.407306
21	8	-0.014500	-1.873166	-1.575080
22	8	-0.011465	2.296708	-0.846289
23	1	0.546561	-1.968352	-2.377310
24	1	-0.569560	-2.682957	-1.516095
25	1	0.544223	3.040776	-0.522618
26	1	-0.581023	2.655337	-1.563562
27	1	-0.511220	0.006371	3.096522
28	1	0.602925	-1.091969	2.869956

$Tm(H_2O)_8^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	69	-0.000749	-0.002726	-0.004666
2	8	0.848593	-1.782960	-1.301396
3	8	-1.817738	-0.922464	-1.223972
4	8	-0.857716	1.761559	-1.323884

5	8	1.813023	0.886421	-1.247951
6	8	0.624483	1.851420	1.330430
7	8	1.922894	-0.655236	1.226744
8	8	-0.642122	-1.821814	1.356182
9	8	-1.900076	0.700550	1.228276
10	1	-1.757732	2.159443	-1.256217
11	1	-0.390921	2.227522	-2.056303
12	1	-2.282048	-1.769829	-1.026918
13	1	-2.345505	-0.458057	-1.915158
14	1	0.331061	-2.299934	-1.962366
15	1	1.727381	-2.221344	-1.211148
16	1	2.345345	0.396150	-1.917593
17	1	2.257836	1.755172	-1.106824
18	1	-1.330704	-1.782536	2.060781
19	1	-0.297232	-2.745610	1.338012
20	1	1.956915	-1.332960	1.941629
21	1	2.852149	-0.381921	1.042118
22	1	1.441743	1.877532	1.881188
23	1	0.361802	2.788765	1.169842
24	1	-2.833950	0.424431	1.074686
25	1	-1.915158	1.411479	1.910785

$Tm(H_2O)_9^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	69	0.004317	-0.000026	-0.005980
2	8	1.639536	0.270117	-1.758488
3	8	-1.680073	1.299353	1.129154
4	8	1.700234	1.328893	1.063027
5	8	-1.674693	-1.621079	0.592503
6	8	1.690877	-1.611709	0.590740
7	8	-1.672304	0.338178	-1.705075
8	1	2.522978	-1.406444	1.076570
9	1	1.874582	-2.410845	0.046694
10	1	2.523400	1.664891	0.638984
11	1	1.900496	1.219363	2.020507
12	1	1.814930	1.161652	-2.136413
13	1	2.477601	-0.240850	-1.841494
14	1	-2.511746	0.833436	-1.560580
15	1	-1.871648	-0.361503	-2.367623
16	1	-1.879240	2.238667	0.913361
17	1	-2.497826	0.927008	1.533182
18	1	-1.860175	-1.870127	1.526366
19	1	-2.501732	-1.797975	0.086928
20	8	0.046319	-0.403529	2.421303
21	8	-0.020696	-1.880817	-1.569398
22	8	0.030928	2.300847	-0.845480
23	1	0.480778	-1.934346	-2.414306
24	1	-0.493681	-2.736265	-1.458163
25	1	0.455242	3.069320	-0.401105
26	1	-0.537238	2.663753	-1.561876
27	1	-0.459094	0.091890	3.104451
28	1	0.518824	-1.130807	2.885981

$Yb(H_2O)_8^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	70	-0.000274	-0.000231	-0.003444
2	8	-1.729153	1.002197	-1.252501
3	8	0.978362	1.727759	-1.266338
4	8	1.741421	-0.989801	-1.245960
5	8	-0.984649	-1.703571	-1.290119
6	8	0.520707	-1.906143	1.274541
7	8	-1.925927	-0.547074	1.246351
8	8	-0.524214	1.887708	1.299618
9	8	1.930783	0.518924	1.246298
10	1	2.705470	-0.839003	-1.104074
11	1	1.654254	-1.608563	-2.007705
12	1	0.839747	2.696856	-1.148495
13	1	1.696771	1.616189	-1.931792
14	1	-1.617975	1.705554	-1.933670
15	1	-2.697831	0.878652	-1.116122
16	1	-1.676476	-1.574854	-1.980126
17	1	-0.834306	-2.674336	-1.205295
18	1	0.036753	2.267066	2.016127
19	1	-1.324463	2.459011	1.223560
20	1	-2.332408	0.004825	1.954801
21	1	-2.515985	-1.325118	1.108797
22	1	-0.063781	-2.313529	1.956033
23	1	1.298639	-2.501715	1.163636
24	1	2.492975	1.324845	1.165034
25	1	2.299177	-0.019699	1.985250

$Yb(H_2O)_9^{3+}$

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	70	0.000562	-0.000400	-0.002790
2	8	1.625010	0.277686	-1.752860
3	8	-1.679493	1.284377	1.134741
4	8	1.695839	1.317627	1.060372
5	8	-1.659426	-1.625649	0.586181
6	8	1.670969	-1.608310	0.598406
7	8	-1.659325	0.337917	-1.701321
8	1	2.508132	-1.400502	1.074517
9	1	1.852109	-2.400867	0.043739
10	1	2.518519	1.643879	0.627270
11	1	1.906235	1.209878	2.015577
12	1	1.806778	1.169722	-2.127134
13	1	2.459103	-0.238673	-1.842824
14	1	-2.503559	0.826301	-1.560785
15	1	-1.850968	-0.367692	-2.360294
16	1	-1.892476	2.212557	0.887420
17	1	-2.499651	0.905518	1.527909
18	1	-1.842847	-1.840007	1.529429
19	1	-2.495587	-1.792871	0.092436
20	8	0.020662	-0.411891	2.414799

21	8	-0.014041	-1.874633	-1.564948
22	8	0.004107	2.300502	-0.810757
23	1	0.473327	-1.917723	-2.418668
24	1	-0.491865	-2.728184	-1.459920
25	1	0.481710	3.056509	-0.400532
26	1	-0.507282	2.659756	-1.570554
27	1	-0.445398	0.112516	3.104041
28	1	0.539752	-1.106301	2.880321

2. listing of reference codes and literature references of crystal structures of $Ln(H_2O)_8^{3+}$ ions in a SAP coordination polyhedron data retrieved from the Cambridge Crystallographic Data Base (see also main text, Table 3.

Ln	Reference Code	Literature reference
Nd	YEGHIC	Zhao-Xi Wang, Xiao-Fei Shen, Jun Wang, Peng Zhang, Yi-Zhi Li, E. N. Nfor, You Song, S. Ohkoshi, K. Hashimoto, Xiao-Zeng You, *Angew. Chem., Int. Ed.,* 2006, **45,** 3287.
Eu	JEDLIO	S. J. Dalgarno, J. L. Atwood, C. L. Raston, *Cryst. Growth Des.*, 2006, **6**, 174.
Gd	SEYIF	M. Hatano, E. Takagi, M. Arinobe, K. Ishihara, *J. Organomet. Chem*., 2007, **692**, 569.
Tb	TAHDAI	S. J. Dalgarno, M. J. Hardie, M. Makha, C. L. Raston, *Chem.-Eur. J*., 2003, **9**, 2834.
	XUMKEV	J. L. Atwood, L. J. Barbour, S. Dalgarno, C. L. Raston, H. R. Webb *J. Chem.Soc., Dalton Trans*., 2002, **23**, 4351.
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