Electronic Supplementary Information

Mononuclear Thorium Halide Clusters ThX_4 (X = F, Cl): Gas-Phase Hydrolysis Reactions

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Figure S1. B3LYP optimized structures for the reactants, intermediates (IM), transition states (TS) and the products shown in the energy profile of Figure 2. The bond lengths are in angstroms and the bond angles are in degrees.

Figure S2. B3LYP optimized structures for the reactants, intermediates (IM), transition states (TS) and the products shown in the energy profile of Figure 3. The bond lengths are in angstroms and the bond angles are in degrees.

Figure S3. B3LYP optimized structures for the reactants, intermediates (IM), transition states (TS) and the products shown in the energy profile of Figure 4. The bond lengths are in angstroms and the bond angles are in degrees.

Figure S4. B3LYP optimized structures for the reactants, intermediates (IM), transition states (TS) and the products shown in the energy profile of Figure 5. The bond lengths are in angstroms and the bond angles are in degrees.

Figure S5. B3LYP optimized structures for the reactants, intermediates (IM), transition states (TS) and the products shown in the energy profile of Figure 6. The bond lengths are in angstroms and the bond angles are in

degrees.

Figure S6. B3LYP optimized structures for the reactants, intermediates (IM), transition states (TS) and the products shown in the energy profile of Figure 7. The bond lengths are in angstroms and the bond angles are in degrees.

Figure S7. B3LYP optimized structures for the reactants, intermediates (IM), transition states (TS) and the products shown in the energy profile of Figure 8. The bond lengths are in angstroms and the bond angles are in degrees.

Figure S8. B3LYP optimized structures for the reactants, intermediates (IM), transition states (TS) and the products shown in the energy profile of Figure 9. The bond lengths are in angstroms and the bond angles are in degrees.

Figure S9. B3LYP optimized structures for the reactants, intermediates (IM), transition states (TS) and the products shown in the energy profile of Figure 10. The bond lengths are in angstroms and the bond angles are in degrees.

Table S1. Cartesian coordinates for all optimized structures at the B3LYP level.

Figure S1. B3LYP optimized structures for the reactants, intermediates (IM), transition states (TS) and the products shown in the energy profile of Figure 2. The bond lengths are in angstroms and the bond angles are in degrees.

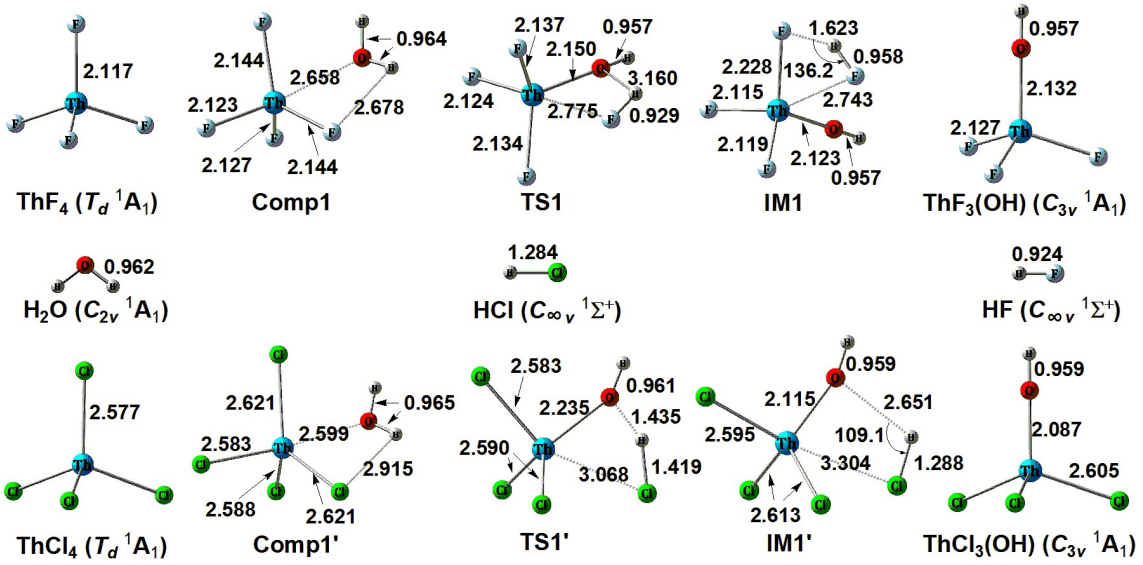

Figure S2. B3LYP optimized structures for the reactants, intermediates (IM), transition states (TS) and the products shown in the energy profile of Figure 3. The bond lengths are in angstroms and the bond angles are in degrees.

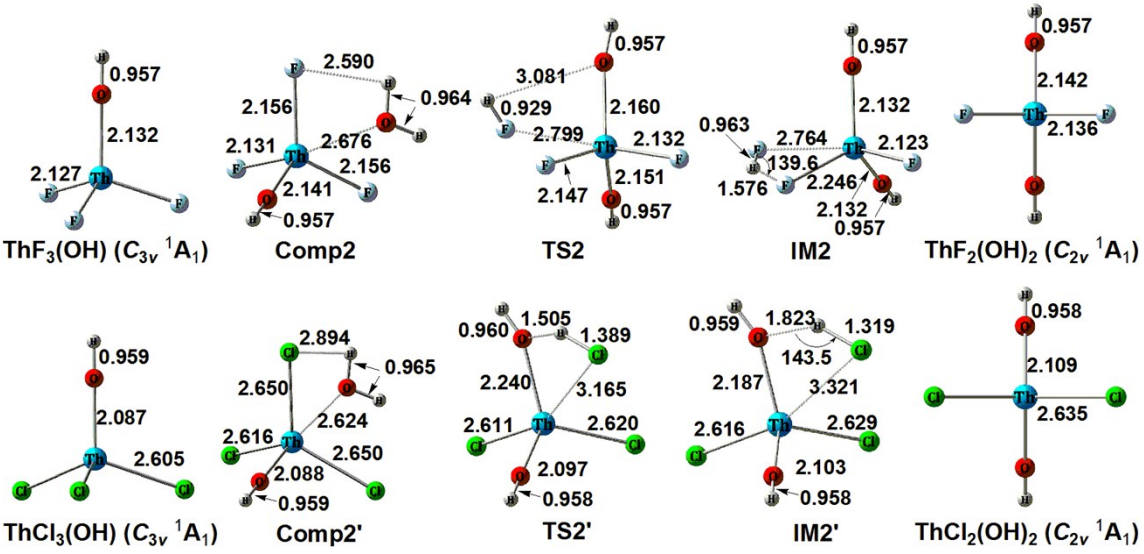

Figure S3. B3LYP optimized structures for the reactants, intermediates (IM), transition states (TS) and the products shown in the energy profile of Figure 4. The bond lengths are in angstroms and the bond angles are in degrees.

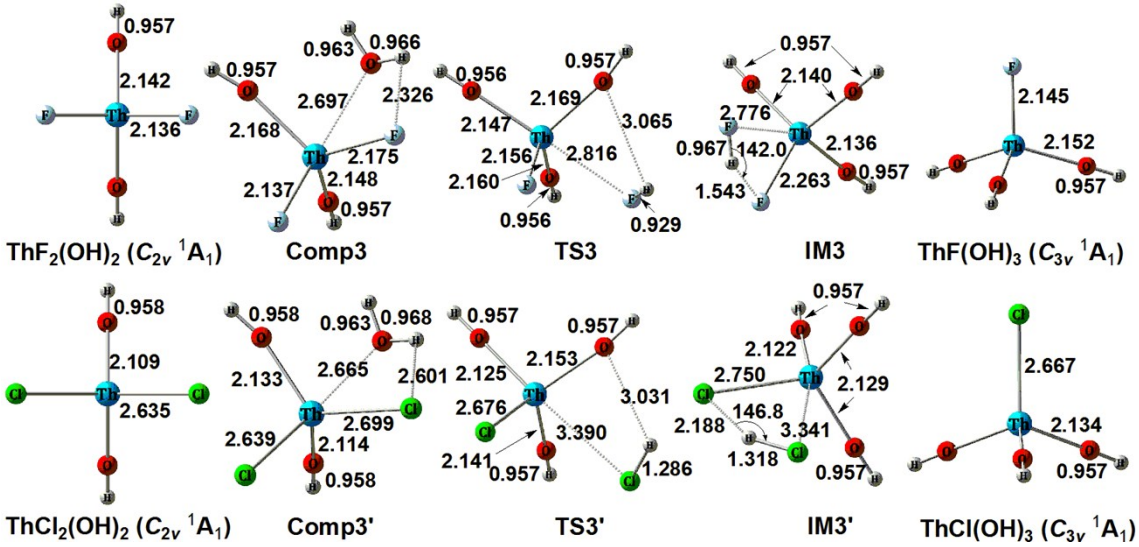

Figure S4. B3LYP optimized structures for the reactants, intermediates (IM), transition states (TS) and the products shown in the energy profile of Figure 5. The bond lengths are in angstroms and the bond angles are in degrees.

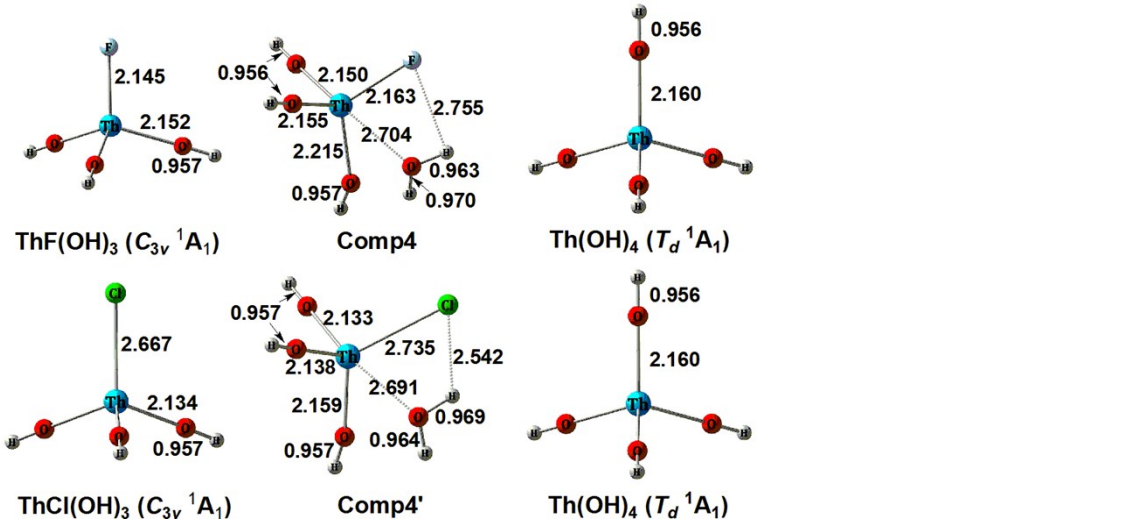

Figure S5. B3LYP optimized structures for the reactants, intermediates (IM), transition states (TS) and the products shown in the energy profile of Figure 6. The bond lengths are in angstroms and the bond angles are in degrees.

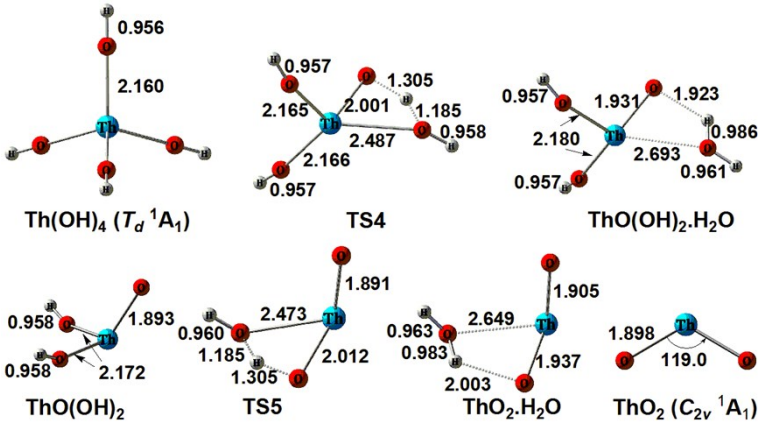

Figure S6. B3LYP optimized structures for the reactants, intermediates (IM), transition states (TS) and the products shown in the energy profile of Figure 7. The bond lengths are in angstroms and the bond angles are in degrees.

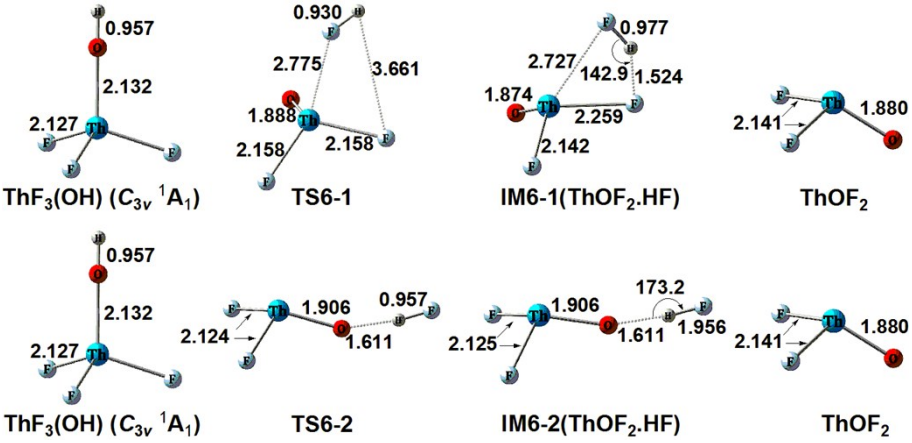

Figure S7. B3LYP optimized structures for the reactants, intermediates (IM), transition states (TS) and the products shown in the energy profile of Figure 8. The bond lengths are in angstroms and the bond angles are in degrees.

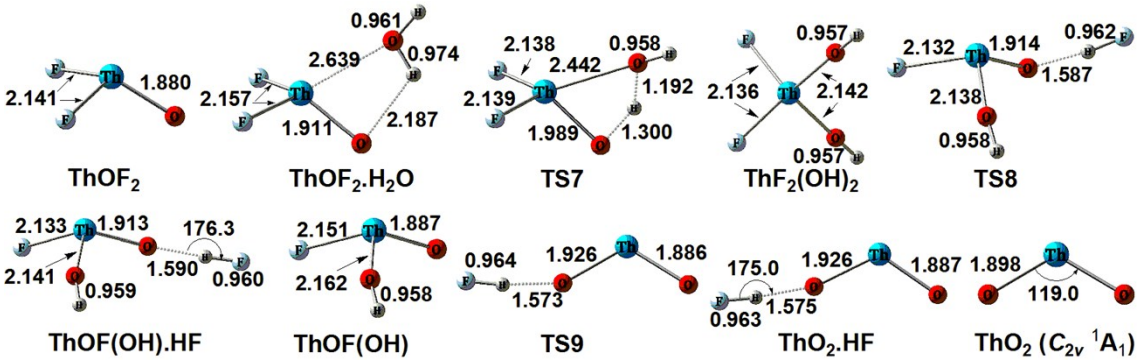

Figure S8. B3LYP optimized structures for the reactants, intermediates (IM), transition states (TS) and the products shown in the energy profile of Figure 9. The bond lengths are in angstroms and the bond angles are in degrees.

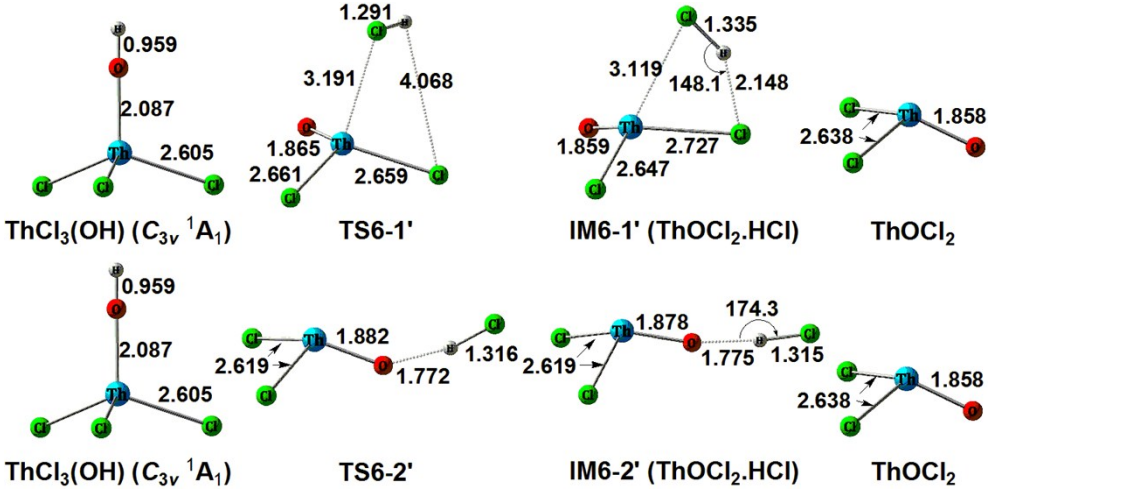

Figure S9. B3LYP optimized structures for the reactants, intermediates (IM), transition states (TS) and the products shown in the energy profile of Figure 10. The bond lengths are in angstroms and the bond angles are in degrees.

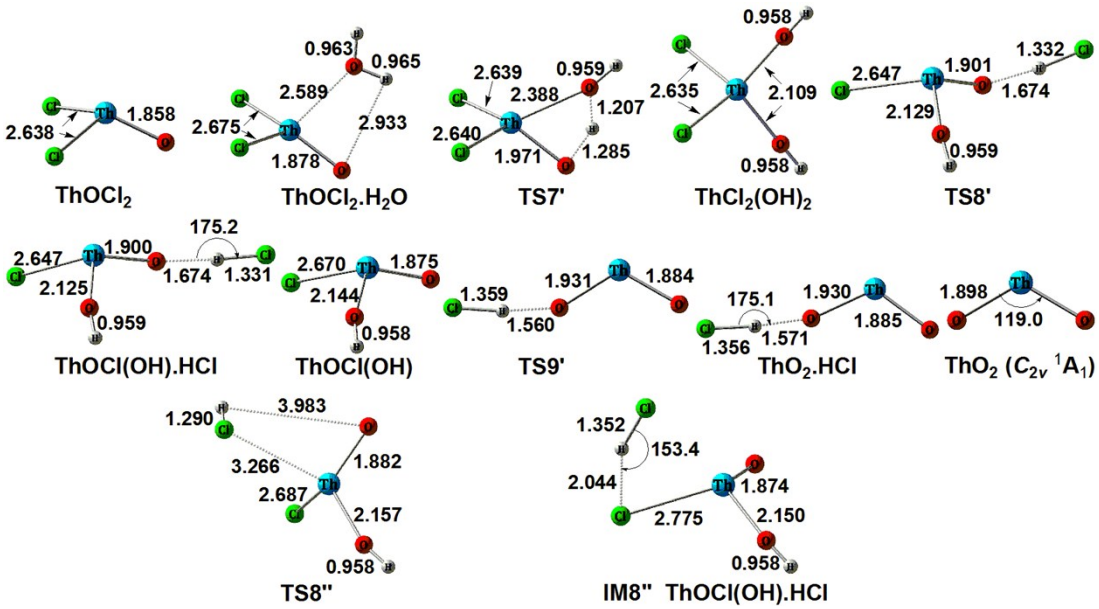

Table S1. Cartesian coordinates for all optimized structures at the B3LYP level.

[ThF4]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.000000	0.000000	0.000000
9	1.222309	1.222309	1.222309
9	-1.222309	-1.222309	1.222309
9	-1.222309	1.222309	-1.222309
9	1.222309	-1.222309	-1.222309

[comp1]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.005470	0.157676	0.000000
9	-2.109719	0.378534	0.000000
9	0.770200	2.138470	0.000000
9	0.770200	-0.615083	1.848379
9	0.770200	-0.615083	-1.848379
8	-0.293163	-2.483032	0.000000
1	0.022555	-2.954058	-0.779353

1	0.022555	-2.954058	0.779353

[TS1]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.172901	0.009137	0.000036
9	-0.411217	-0.116007	2.051411
9	-0.233838	1.854036	-0.992559
9	2.294418	-0.085907	0.053265
9	-2.596926	0.176205	-0.025416
8	-0.427399	-1.767857	-1.050056
1	-3.073429	-0.585903	0.208843
1	-0.540434	-2.548500	-1.591910

[im1]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.164696	0.000948	-0.006291
9	1.265253	-1.474625	0.854653
9	-0.161921	0.179606	-2.117645
9	-2.028744	-0.906800	0.412852
9	2.559616	0.284028	-0.160297
8	-0.258569	1.873796	0.989816
1	2.480782	-0.542261	0.318498
1	-0.297421	2.726720	1.423095

[$ThF_3(OH)$]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.000000	0.000000	0.007438
9	0.000000	2.004933	0.718795
9	1.736323	-1.002467	0.718795
9	-1.736323	-1.002467	0.718795
8	0.000000	0.000000	-2.124396
1	0.000000	0.000000	-3.081684

[comp2]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.001019	0.158934	0.000000
9	0.785835	-0.624477	1.848657
9	0.785835	2.140523	0.000000
8	-2.128136	0.382093	0.000000
1	0.201968	-2.910281	0.778774
8	-0.201552	-2.509855	0.000000
1	-3.075645	0.514479	0.000000
1	0.201968	-2.910281	-0.778774
9	0.785835	-0.624477	-1.848657

[TS2]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.173851	0.005012	0.005069
9	-2.288590	-0.258508	0.063718
9	0.489947	-0.756681	1.899029
8	0.064712	2.109934	-0.367973
1	0.603128	-1.852359	-2.355926
8	0.487287	-1.306655	-1.578649
1	0.218990	3.040230	-0.530082
1	3.026962	-0.643818	0.034872
9	2.618813	0.190593	0.033685

[im2]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.130422	0.101936	0.000000
9	0.920451	2.072167	0.000000
9	-2.078418	0.511237	0.000000
8	0.920451	-0.764009	1.780457
1	1.279594	-1.178834	-2.564740

8	0.920451	-0.764009	-1.780457
1	1.279594	-1.178834	2.564740
1	-2.316104	-1.047242	0.000000
9	-1.809617	-1.866201	0.000000

$[ThF_2(OH)_2]$

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
90	0.000000	0.000000	-0.007236
9	1.741568	0.000000	-1.244500
9	-1.741568	0.000000	-1.244500
8	0.000000	1.756668	1.218204
1	0.000000	-2.531002	1.780485
8	0.000000	-1.756668	1.218204
1	0.000000	2.531002	1.780485

[comp3]

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
90	0.156048	-0.003358	0.001969
9	2.177568	0.121992	-0.678500
8	-0.391762	2.083533	0.214749
1	-0.397369	3.034196	0.322252
1	0.385199	-1.561642	2.677679
1	-2.963878	0.765486	0.223230
8	0.304532	-1.080472	1.854903
8	-2.532579	-0.095210	0.194869
1	-2.787905	-0.519445	-0.634716
9	-0.768889	-1.086345	-1.641699

[TS3]

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
90	0.173115	0.007020	0.003043
9	-0.512053	-0.787649	1.886081

8	2.307062	-0.220697	0.065006
1	3.260109	-0.292428	0.096859
1	-0.284104	3.046627	-0.507787
1	-0.606737	-1.859387	-2.357547
8	-0.127415	2.116414	-0.349562
8	-0.504176	-1.312181	-1.579739
1	-3.003267	-0.678239	0.077148
9	-2.637959	0.174688	0.039678

[im3]

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

90	-0.131862	0.095437	0.000000
9	2.091702	0.515064	0.000000
8	-0.916635	2.081780	0.000000
1	-1.330768	2.944199	0.000000
1	-1.279742	-1.203983	2.565433
1	-1.279742	-1.203983	-2.565433
8	-0.916635	-0.795618	1.780002
8	-0.916635	-0.795618	-1.780002
1	2.321019	-1.010630	0.000000
9	1.845640	-1.852760	0.000000

[$ThF(OH)_3$]

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

90	0.000000	0.000000	0.004890
9	0.000000	0.000000	2.149602
8	0.000000	2.034064	-0.696395
1	0.000000	2.932753	-1.024346
1	-2.539839	-1.466377	-1.024346
1	2.539839	-1.466377	-1.024346
8	-1.761551	-1.017032	-0.696395
8	1.761551	-1.017032	-0.696395

[comp4]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.156561	-0.016073	-0.000871
8	-2.179084	0.657976	0.280621
1	-3.091077	0.909250	0.421843
1	0.757772	2.636882	-1.270716
1	2.635907	0.725398	-0.362569
8	0.822852	1.780234	-0.848425
8	2.540929	-0.193866	-0.066793
1	-0.392797	-2.448853	-1.925328
8	-0.313065	-1.705750	-1.328515
1	2.940476	-0.262240	0.807262
9	0.474126	-0.491406	2.012532

$[Th(OH)_4]$

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.000000	0.000000	0.000000
8	1.246933	1.246933	1.246933
1	1.799120	1.799120	1.799120
1	-1.799120	-1.799120	1.799120
1	-1.799120	1.799120	-1.799120
8	-1.246933	-1.246933	1.246933
8	-1.246933	1.246933	-1.246933
1	1.799120	-1.799120	-1.799120
8	1.246933	-1.246933	-1.246933

[TS4]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.096200	0.000626	-0.066517
8	1.213020	-0.039572	1.445931
8	-1.290089	1.807196	-0.009577
8	-1.367790	-1.751154	-0.032547
1	-1.738107	2.603903	0.275053
1	-1.820027	-2.554511	0.225642
8	2.317661	-0.071346	-0.662664

1	3.117062	0.373158	-0.948369
1	2.116645	-0.039886	0.505085

[$ThO(OH)_2.H_2O$]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.098862	-0.003073	-0.053702
8	0.996919	-0.181665	1.526352
8	-1.138306	1.913484	-0.069816
8	-1.547839	-1.626881	-0.186850
1	-1.549830	2.714026	0.255711
1	-2.098683	-2.363798	0.077377
8	2.527693	-0.134666	-0.634404
1	2.519298	-0.156473	0.351336
1	3.319007	0.320616	-0.933494

[$ThO(OH)_2$]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.000000	0.074958	-0.158097
8	0.000052	1.726136	0.767834
8	1.737624	-1.108385	0.386702
8	-1.737672	-1.108312	0.386710
1	-2.451021	-1.410829	0.949361
1	2.450963	-1.410919	0.949357

[TS5]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.215635	-0.094806	-0.146391
8	1.395871	0.958596	0.889115
8	-1.250040	-1.048378	0.849816
8	-2.026668	0.948158	-0.186827
1	-2.378172	1.703704	0.290497
1	-1.982252	-0.038185	0.467891

[$ThO_2.H_2O$]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.240959	-0.095130	-0.138101
8	1.071925	1.326225	0.819702
8	-0.922154	-1.266937	0.874452
8	-2.248886	0.804789	-0.220165
1	-2.538574	1.600161	0.238563
1	-2.354826	0.048926	0.398643

[ThO_2]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.000000	0.000000	0.145341
8	0.000000	1.635977	-0.817545
8	0.000000	-1.635977	-0.817545

[TS6-1]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.118542	-0.052083	0.003355
9	2.502078	-0.256759	-0.884995
9	0.432043	1.809813	0.944687
9	-1.898599	0.259299	-1.176001
8	-0.241050	-1.446493	1.269768
1	3.277496	-0.051782	-0.413349

[im6-1]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.183636	0.061568	-0.078537

9	-2.440169	-0.051219	-0.813272
9	-1.504324	-0.437118	1.337851
9	1.511887	-1.618111	-0.053061
8	0.974646	1.709430	0.335436
1	-2.430989	-0.258495	0.141138

[TS6-2]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.292176	0.000003	-0.159034
9	4.019639	0.000115	0.057166
9	-1.385803	1.686692	0.528004
9	-1.386809	-1.686041	0.527977
8	1.496961	-0.000858	0.498072
1	3.096926	-0.000307	0.310128

[im6-2]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.306444	-0.000037	-0.166017
9	-4.074639	-0.000199	0.121543
9	1.356621	-1.685280	0.590264
9	1.355432	1.686047	0.590016
8	-1.523084	-0.000242	0.367683
1	-3.132010	0.000174	0.283652

[$ThOF_2$]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.103426	0.123878	0.000000
9	-0.103426	-1.178119	1.699423
9	-0.103426	-1.178119	-1.699423
8	1.396254	1.257136	0.000000

[$ThOF_2.H_2O$]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.101471	-0.000001	-0.027408
9	1.328145	-1.765465	-0.202182
9	1.328052	1.765529	-0.202145
8	-0.935875	-0.000047	1.577206
8	-2.452111	0.000012	-0.693470
1	-2.677079	-0.000033	0.253799
1	-3.257192	-0.000156	-1.218051

[TS7]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.103596	0.000408	-0.051583
9	-1.280809	1.785839	-0.012884
9	-1.344830	-1.740314	-0.038213
8	1.227392	-0.032915	1.426447
8	2.246315	-0.058567	-0.714725
1	2.106706	-0.030255	0.468719
1	3.058076	0.315644	-1.060121

[TS8]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.270782	-0.027393	-0.171595
9	-1.745001	-1.366838	0.589256
9	3.836178	0.004984	0.018897
8	1.413216	-0.383985	0.664894
8	-0.959499	1.909230	0.415392
1	2.957564	-0.173883	0.367759
1	-1.037548	2.693961	0.960168

[ThOF(OH).HF]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.333905	-0.022902	-0.188828
9	-1.441260	-1.514376	0.858617
9	4.073240	0.013193	0.239276
8	1.538263	-0.231782	0.141693
8	-1.006171	1.860328	0.576854
1	3.119524	-0.099927	0.235518
1	-1.012653	2.643385	1.129602

[ThOF(OH)]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.025841	-0.066374	-0.153882
9	-1.438335	1.427099	0.478002
8	-0.344489	-1.703541	0.727628
8	1.915471	0.736860	0.355083
1	2.702886	0.863220	0.885688

[TS9]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.384843	-0.155606	0.000374
9	3.887716	0.086630	-0.065966
8	-1.819440	1.067093	-0.058168
8	1.405170	0.543922	0.125467
1	2.960569	0.336761	0.021621

[ThO_2.HF]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.410494	-0.157261	-0.000035
9	-3.986969	0.172251	-0.000386
8	1.701431	1.218625	-0.000147

8	-1.455440	0.321651	0.000939
1	-3.029670	0.281002	0.000265

[ThO_2]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.000000	0.000000	0.145341
8	0.000000	1.635977	-0.817545
8	0.000000	-1.635977	-0.817545

[$ThCl_4$]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.000000	0.000000	0.000000
17	1.487581	1.487581	1.487581
17	-1.487581	-1.487581	1.487581
17	1.487581	-1.487581	-1.487581
17	-1.487581	1.487581	-1.487581

[comp1']

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.050599	-0.000002	0.008835
17	0.015451	0.000215	2.596432
17	2.569306	0.000026	-0.563589
17	-0.648849	-2.302344	-1.028983
17	-0.648983	2.302156	-1.029301
8	-2.548488	-0.000070	0.024360
1	-3.021872	0.783838	-0.278836
1	-3.021862	-0.784025	-0.278729

[TS1']

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
90	-0.148186	0.000140	0.033449
17	0.001375	-2.187357	-1.345789
17	0.000219	2.189336	-1.343423
17	-2.603004	-0.001762	0.836934
17	2.895558	-0.000549	0.418943
8	0.715541	-0.000741	2.094804
1	2.044526	-0.000862	1.554020
1	0.567369	-0.000162	3.043813

[im1']

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.227804	0.000000	0.093208
17	0.312606	-2.214868	-1.184441
17	0.312660	2.214881	-1.184399
17	-2.816892	0.000029	0.270092
17	3.068680	-0.000003	0.322503
8	0.308243	-0.000058	2.139171
1	2.903317	-0.000141	1.599807
1	0.223206	-0.000075	3.094312

[$ThCl_3(OH)$]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.000000	0.000000	0.146322
17	0.000000	2.473470	-0.671079
17	-2.142088	-1.236735	-0.671079
17	2.142088	-1.236735	-0.671079
8	0.000000	0.000000	2.233018
1	0.000000	0.000000	3.191940

[comp2']

Atomic Number	Coordinates (Angstroms) X	Y	Z

90	-0.000014	0.070089	-0.186660
17	-2.310822	-1.213305	-0.003848
17	-0.000296	2.443469	0.912786
8	-0.000089	0.507688	-2.228544
1	-0.782337	-1.545424	2.431330
8	0.000210	-1.033481	2.193603
1	-0.000117	0.693261	-3.168985
1	0.782912	-1.545260	2.431175
17	2.311109	-1.212765	-0.003913

[TS2']

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.165222	-0.068258	0.097029
17	2.667649	-0.603719	-0.422997
17	-0.039513	2.516199	-0.283678
8	0.014473	-0.656096	2.103928
1	-0.660673	-2.011406	-2.180746
8	-0.761839	-1.386152	-1.459621
1	-0.098064	-0.919073	3.018739
1	-2.144597	-1.040061	-0.976621
17	-2.980353	-0.356494	-0.102056

[im2']

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.202754	-0.084550	0.074211
17	2.760029	-0.445309	-0.342439
17	-0.196127	2.502450	-0.171842
8	-0.089940	-0.814847	2.024348
1	-0.542452	-1.878251	-2.288361
8	-0.651604	-1.308355	-1.524403
1	-0.266757	-1.152925	2.903351
1	-2.367628	-0.998897	-0.991668
17	-3.101471	-0.373306	-0.091714

[$ThCl_2(OH)_2$]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.000000	0.000000	0.188693
17	2.186612	0.000000	-1.282485
17	-2.186612	0.000000	-1.282485
8	0.000000	1.715519	1.415761
1	0.000000	-2.486066	1.984984
8	0.000000	-1.715519	1.415761
1	0.000000	2.486066	1.984984

[comp3']

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.064648	-0.170188	0.035803
17	-2.525346	0.758451	-0.183074
8	0.004582	-1.482903	-1.644139
1	-0.218749	-2.041048	-2.389600
1	-0.177501	-1.632601	2.734155
1	2.775141	-1.373417	-0.863423
8	-0.114131	-1.178389	1.893601
8	2.512727	-0.831567	-0.111314
1	2.986736	0.010045	-0.176382
17	1.421070	2.082538	-0.030585

[TS3']

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.396889	-0.153600	-0.002227
17	-0.119904	2.471027	-0.060537
8	2.517842	-0.249014	0.076146
1	3.473463	-0.283097	0.110177
1	-0.268735	-1.747340	-2.572149
1	-0.337735	-1.561225	2.651056
8	-0.103456	-1.251598	-1.770393
8	-0.245356	-1.054626	1.844295

1	-3.057113	-0.123883	1.199630
17	-2.990812	-0.236825	-0.079971

[im3']

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.447430	-0.077307	0.000000
17	-1.181353	2.139042	-0.000056
8	2.370664	0.818402	-0.000020
1	3.263961	1.161719	-0.000048
1	0.451795	-1.812434	-2.552164
1	0.451586	-1.812092	2.552394
8	0.444609	-1.264338	-1.767521
8	0.444517	-1.264123	1.767662
1	-2.626182	0.495449	-0.000008
17	-2.812071	-0.809309	-0.000013

[$ThCl(OH)_3$]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.000000	0.000000	0.184435
17	0.000000	0.000000	-2.482344
8	-1.738283	-1.003598	0.910464
1	-2.513120	-1.451437	1.249840
1	-0.000421	2.902144	1.249840
1	2.513541	-1.450708	1.249840
8	0.000000	2.007196	0.910464
8	1.738283	-1.003598	0.910464

[comp4']

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.266293	0.031183	0.010670
8	-1.391244	1.788826	-0.431046
1	-1.890275	2.584770	-0.612709

1	-1.319372	-1.674801	-2.335296
1	1.456576	-2.587409	-0.592519
8	-0.847957	-1.284359	-1.599696
8	1.517997	-1.978220	0.151437
1	-1.400636	-0.816252	2.761369
8	-1.023680	-0.577464	1.915048
1	2.359329	-1.503789	0.069906
17	2.277639	1.035341	-0.031586

[$Th(OH)_4$]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.000000	0.000000	0.000000
8	1.246933	1.246933	1.246933
1	1.799120	1.799120	1.799120
1	-1.799120	-1.799120	1.799120
1	-1.799120	1.799120	-1.799120
8	-1.246933	-1.246933	1.246933
8	-1.246933	1.246933	-1.246933
1	1.799120	-1.799120	-1.799120
8	1.246933	-1.246933	-1.246933

[TS6-1']

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.180319	0.018361	-0.232217
17	-0.601441	2.387090	0.688214
17	2.352735	-0.975810	0.938930
17	-2.549877	-1.415385	0.586181
8	0.082529	-0.127364	-2.089349
1	-3.313083	-0.563804	-0.012225

[im6-1']

Atomic Number	Coordinates (Angstroms) X	Y	Z

90	-0.275048	-0.004210	0.280835
17	1.554555	1.769511	-0.691634
17	-2.319197	-0.363467	-1.362815
17	2.403058	-1.462506	-0.372611
8	-0.699236	0.187523	2.080355
1	2.495169	-0.161426	-0.657936

[TS6-2']

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.289006	-0.025828	-0.186010
17	-1.441716	2.281134	0.269616
17	4.245056	-0.109886	0.021461
17	-2.058729	-1.899446	0.279911
8	1.289075	-0.261973	0.811416
1	3.039571	-0.200363	0.542752

[im6-2']

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.387239	-0.000002	-0.285662
8	1.424127	-0.000036	0.210467
17	-1.658956	2.122415	0.573576
17	4.509867	-0.000012	0.248056
17	-1.659027	-2.122373	0.573585
1	3.196498	-0.000027	0.307136

[$ThOCl_2$]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.213450	0.248771	0.000000
17	0.457394	-1.124788	2.149488
17	0.457394	-1.124788	-2.149488
8	0.457394	1.981679	0.000000

[$ThOCl_2.H_2O$]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.000000	0.092377	0.139271
17	-2.273363	-1.234376	-0.337294
17	2.273377	-1.234353	-0.337297
8	-0.000008	1.295884	1.580390
8	-0.000019	2.222275	-1.332522
1	-0.000029	3.021611	-0.791065
1	-0.000032	2.487601	-2.258208

[TS7']

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.001583	0.097614	-0.011242
17	-2.308461	-1.177992	-0.075457
17	2.130081	-1.461989	-0.047048
8	0.070804	1.514365	1.356962
8	0.193052	2.325182	-0.851075
1	0.185850	2.311615	0.355747
1	0.593307	3.066425	-1.308448

[TS8']

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	-0.402605	0.196749	-0.197957
17	-2.319923	-1.552643	0.320263
17	4.229520	-0.404501	0.083838
8	1.262135	-0.391163	0.505657
8	-1.017111	2.047644	0.655150
1	2.930107	-0.450085	0.373535
1	-1.118976	2.762285	1.286445

[ThOCl(OH).HCl]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.462153	-0.228362	-0.229434
17	2.156683	1.696908	0.424729
17	-4.335988	0.412934	0.182340
8	-1.336714	0.272333	0.121443
8	1.014513	-1.916403	0.937160
1	-3.005007	0.388420	0.204085
1	1.037047	-2.550585	1.656034

[ThOCl(OH)]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.248780	-0.081657	-0.156655
17	-2.386756	0.155531	0.195471
8	0.964242	-1.514818	0.817527
8	1.116284	1.795246	0.410361
1	1.540460	2.461700	0.952807

[TS9']

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.687066	-0.154977	-0.000489
17	-3.965144	0.036509	0.027058
8	2.129599	1.056038	0.051498
8	-1.102027	0.563757	-0.098302
1	-2.649058	0.368886	-0.041576

[ThO_2.HCl]

Atomic Number	Coordinates (Angstroms) X	Y	Z
90	0.720663	-0.156135	-0.000027
17	-4.061558	0.083309	-0.000131

8	2.010732	1.218501	-0.000123
8	-1.147702	0.328558	0.000672
1	-2.717426	0.259406	0.000308

[ThO_2]

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

90	0.000000	0.000000	0.145341
8	0.000000	1.635977	-0.817545
8	0.000000	-1.635977	-0.817545

[TS8"]

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

90	0.293214	-0.230491	0.042069
17	0.447133	2.449992	-0.070817
17	-2.948545	-0.238827	-0.352456
8	0.350138	-0.836774	1.822645
8	1.740322	-1.153143	-1.264895
1	-3.109019	0.671311	0.547365
1	2.520059	-1.597602	-1.599923

[IM8"]

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

90	-0.467526	-0.094807	-0.058160
17	1.487846	1.873549	-0.043135
17	2.445251	-1.283413	0.200094
8	-1.394142	-0.288323	-1.675720
8	-1.702187	0.068661	1.694371
1	2.426801	0.065954	0.125401
1	-2.441500	0.191624	2.291503
