Supporting Information for: Structure and Dynamics of Binary and Ternary Lanthanide(III) and Actinide(III) - Tris[4,4,4-trifluoro-1-(2-thienyl)-1,3-butanedione] (TTA) – Tributylphosphate (TBP) Complexes. Part 1, The Structure and Bonding of Y, Eu, U, Am and Cm Complexes as Studied by Quantum Chemical Methods and X-Ray crystallography

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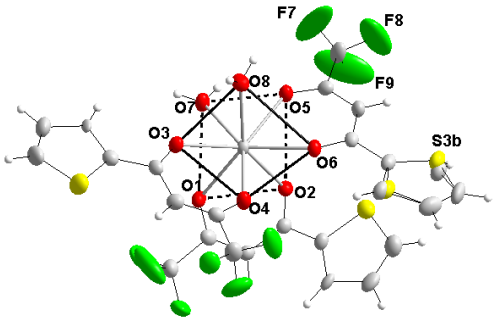
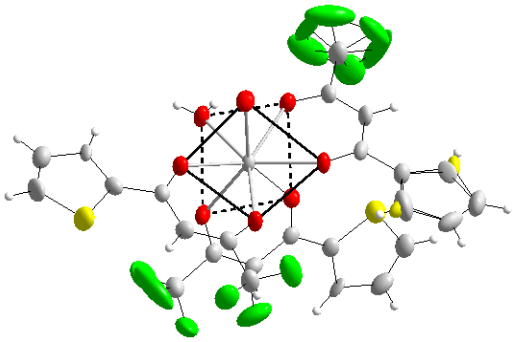


a.



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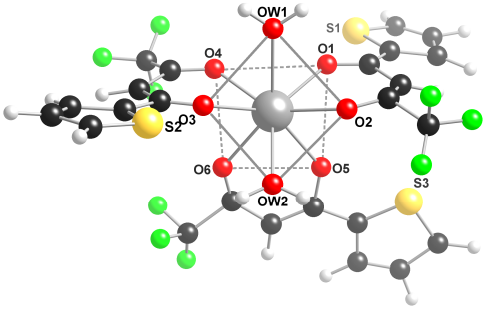
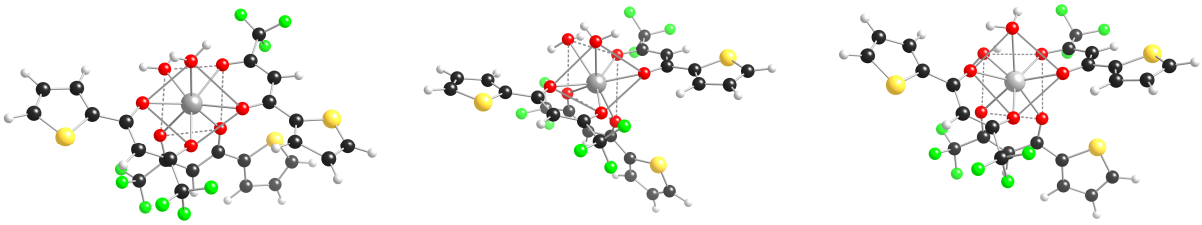


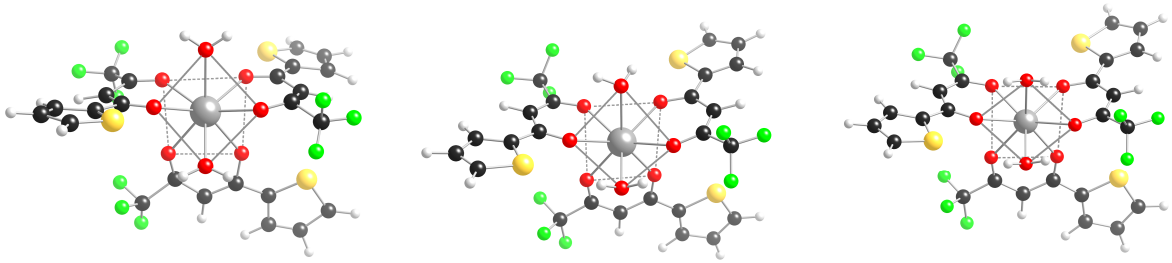
c.

Figure S1. (a) The triclinic (Isomer I) X-ray structure of $Eu(TTA)_3(OH_2)_2$. The disorder in the thienyl ring seems to be related to two possible orientations related by a 180° rotation, where the occupation of the site S3b is 0.7. The large thermal anisotropy in the $–CF_3$ group (F7, F8, F9) is possibly related to this rotational disorder. The disorder might be related to the absence of strong packing interactions between the complexes. (b) The triclinic structure of $Y(TTA)_3(OH_2)_2$ displays the same type of disorder as in the Eu complex. However, here there is a complete rotational disorder in the $–CF_3$ group in the TTA ligand containing the disordered thienyl group. In both structures (a) and (b) we noted that the C – C distances in the disordered thienyl group deviated significantly form those in the other two thienyl groups. This is presumable due to the overlap of S and a C atom. (c) The monoclinic structure of $Eu(TTA)_3(OH_2)_2$ plotted using the coordinates from the X-ray structure of White.[25]



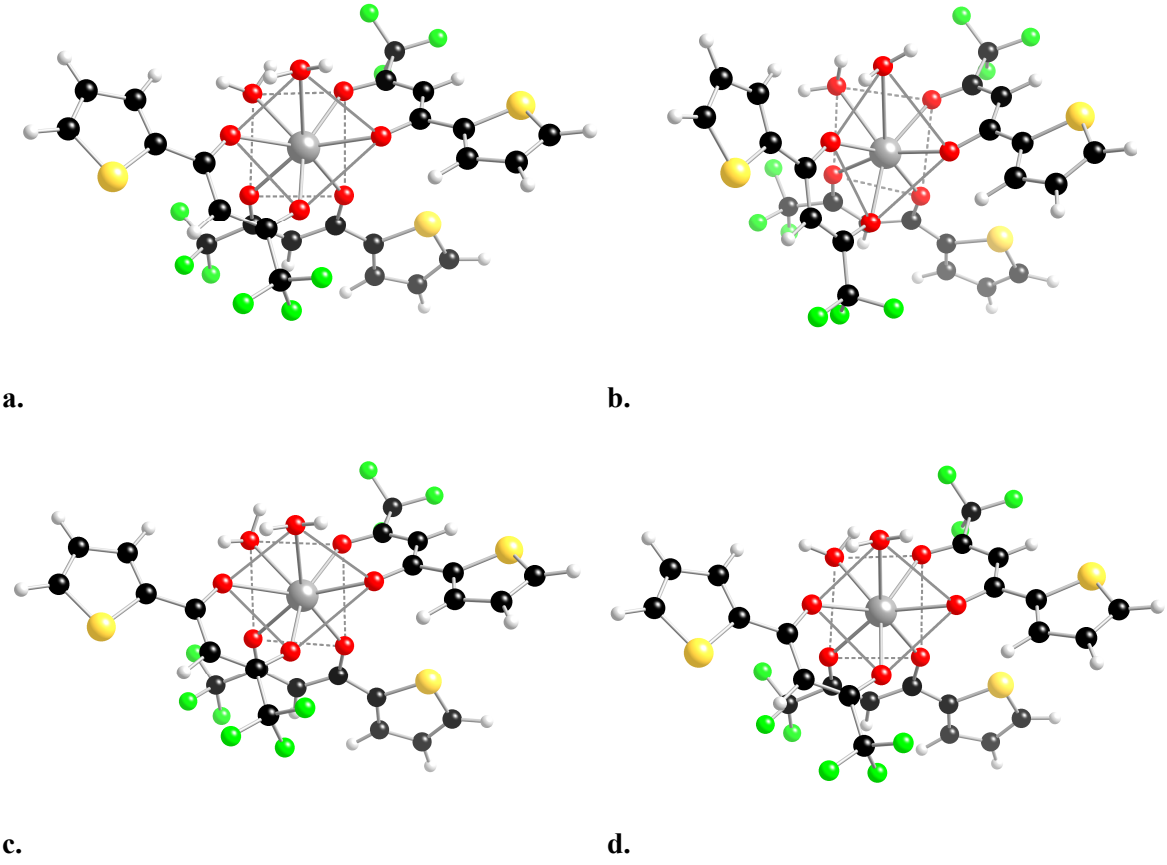
a. **b.** **c.**

Figures S2. Comparison of the X-ray structure of Isomer I, of $Y(TTA)_3(OH_2)_2$ with: (a) the corresponding QM/SPP structures in gas-phase and CCl_4 (b) the structure in the CPCM model of $CHCl_3$ and (c) water. The latter almost superposes the X-Ray structure, with the exception of the disordered thienyl group.



a. **b.** **c.**

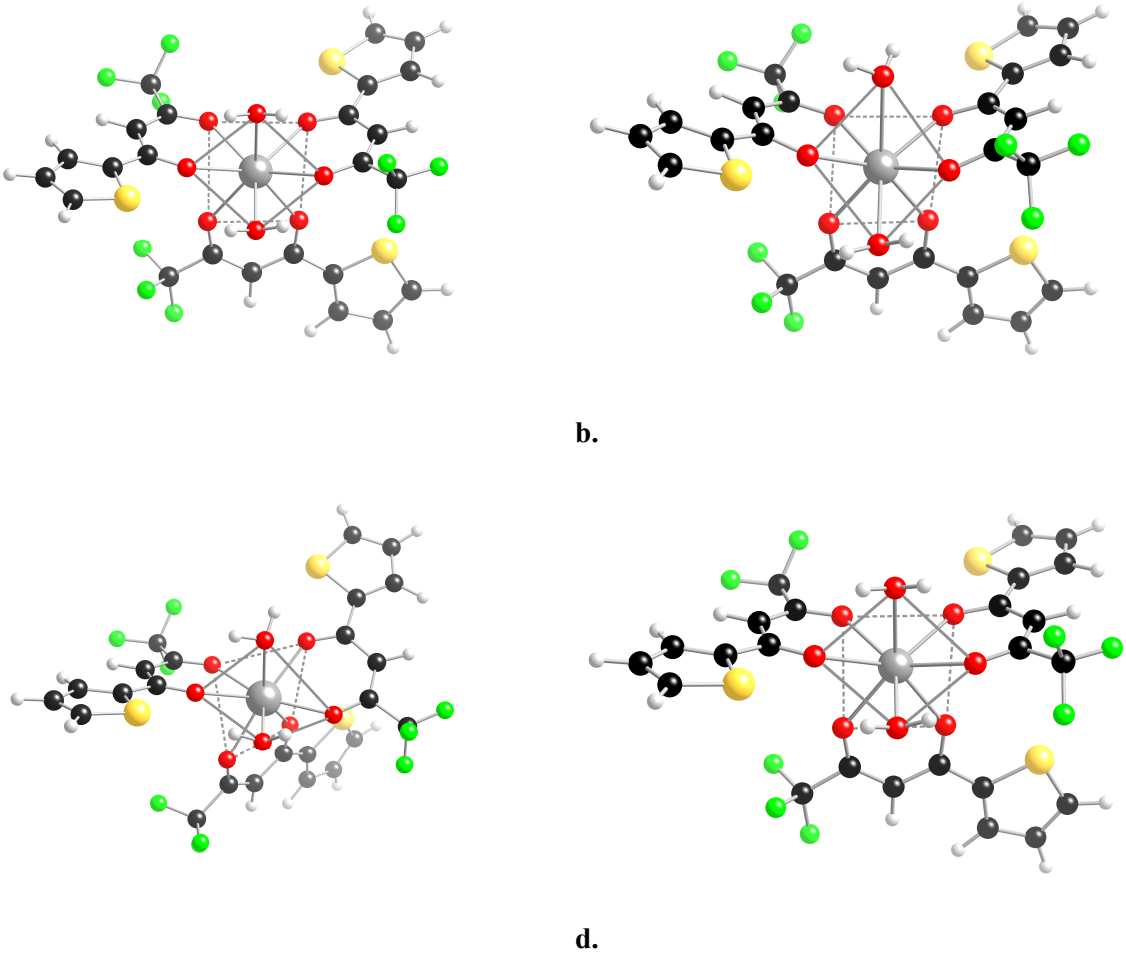
Figure S3. (a) The X-ray structure of $Eu(TTA)_3(OH_2)_2$, Isomer II from White[25]. (b) The QM/LPP structure optimized in gas phase. (c) The structure in the CPCM model of $CHCl_3$. The differences between the structures in Isomer II are much smaller than in Isomer I.



a. **b.**

c. **d.**

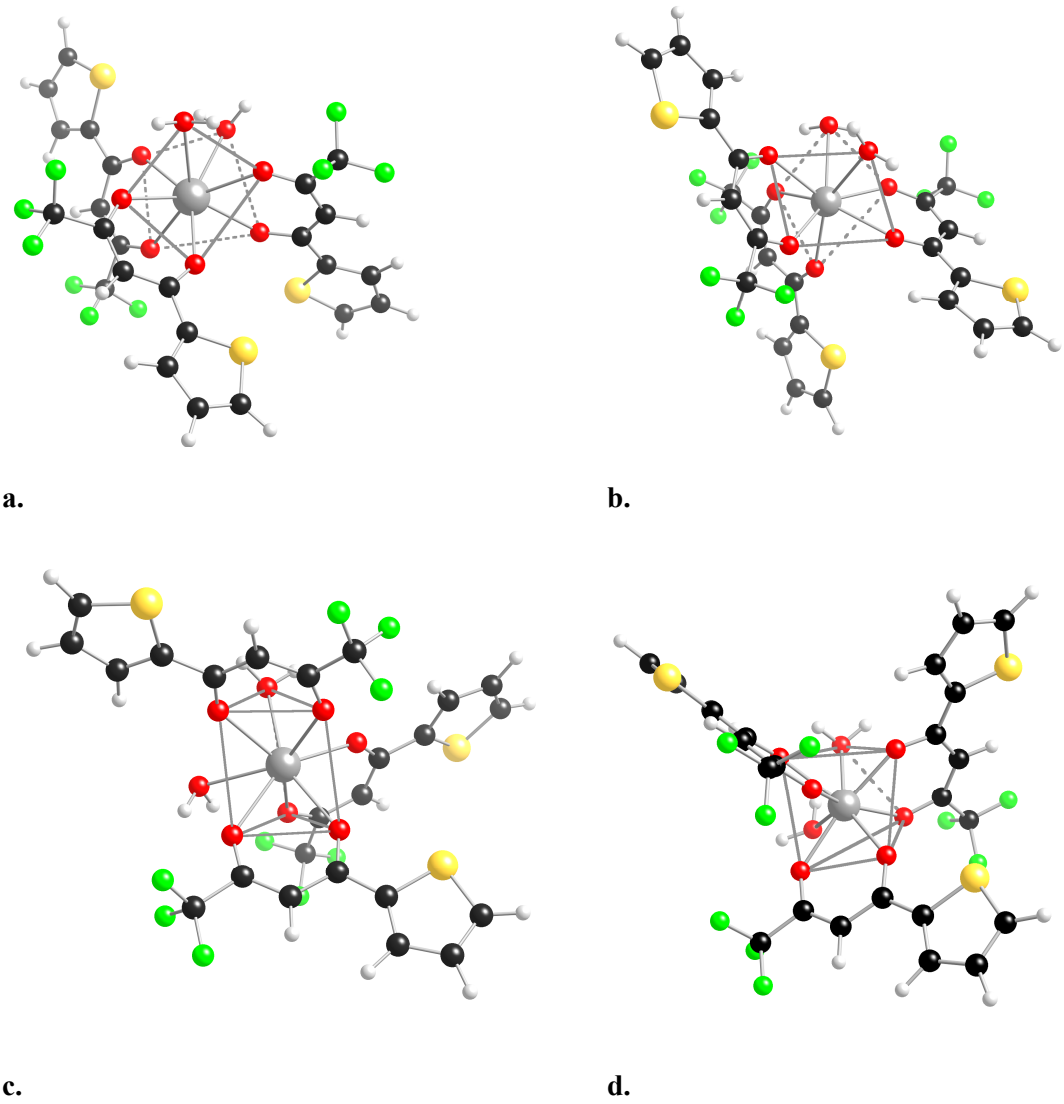
Figure S4. Perspective views of the QM/SPP structures of Isomer I in $CHCl_3$ for Eu (a), U (b), Am (c), Cm (d), illustrating that Eu and Cm structures are very similar to the X-Ray one (see Fig. S1 a). In the U and Am structures the TTA ligand at the backside is rotated, resulting in a structure similar to the one in gas-phase for yttrium (see Fig. S2 b).



a. **b.**

c. **d.**

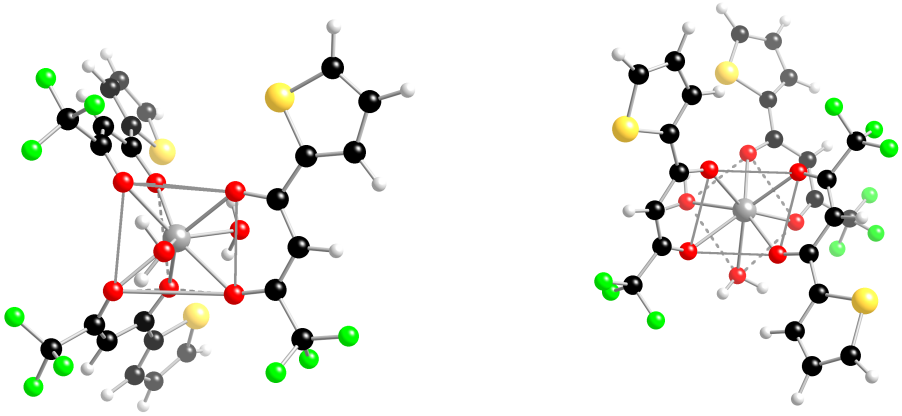
Figure S5. Perspective views of QM/SPP structures of Isomer II for Eu (a), U (b), Am (c), Cm (d) optimized in the CPCM model of $CHCl_3$. The actinide structures are very similar but deviate significantly from that of Eu.



a. **b.**

c. **d.**

Figure S6. The structure of $U(TTA)_3(OH_2)_2$, calculated using the LPP potential and the chloroform CPCM solvent. Structure a. has been obtained using the isomer II as the starting structure for the geometry refinement and has been the ligand configuration found in Isomer II. Structure b. has been obtained using isomer I as the starting structure. The geometry has changed significantly and the square anti-prism geometry is strongly distorted. c. Is the same structure as b., but now viewed from a different angle, demonstrating that the geometry is close to bicapped trigonal prismatic. Figure d. shows the U(III) structure calculated using the SPP and Isomer I as the starting structure. It differs significantly from the corresponding LPP one (c) and is shown in a direction that demonstrates that it also can be described as a distorted bicapped trigonal prism.



a. **b.**

Figure S7. The QM/SPP structure of two $Y(TTA)_3(OH_2)_2$ isomers with different TTA configurations from those in Isomers I and II, optimized in the CPCM model of $CHCl_3$. Structure (a) is closest to a bicapped trigonal prism geometry. The Y - O_{TTA} bond distances differ by less than 0.01 Å from those in Isomer I and its electronic MP2 energies is 7 kJ/mol higher. The geometry of structure (b) is closest to a square anti-prism where the TTA ligands are all located along edges in the square faces, two in the upper one and the third in the lower one. The Y - O_{TTA} bond distances differ by less than 0.01 Å from those in Isomer I and its electronic MP2 energies is 8 kJ/mol higher.

Table S1. Comparison of some interatomic distances in the triclinic (Isomer I) Y and Eu structures obtained from X-Ray and QM (DFT/BP86) calculations with the def2-TZVP basis sets. NPA charges were computed at the DFT level: q(M) is the net charge of the metal, n(p), n(d), n(f) are the population of the valence orbitals, ρ(M) is the spin density of the metal.

	$Y(TTA)_3(OH_2)_2$			$Eu(TTA)_3(OH_2)_2$			$U(TTA)_3(OH_2)_2$		$Am(TTA)_3(OH_2)_2$		$Cm(TTA)_3(OH_2)_2$	
		QM/SPP			QM/LPP	QM/SPP	QM/LPP	QM/SPP	QM/LPP	QM/SPP	QM/LPP	QM/SPP
	X-Ray	GP	$CHCl_3$	X-Ray	$CHCl_3$	$CHCl_3$	$CHCl_3$	$CHCl_3$	$CHCl_3$	$CHCl_3$	$CHCl_3$	$CHCl_3$
Dist in Å	tricl	tricl	tricl	tricl	tricl	tricl	tricl	tricl	tricl	tricl	tricl	tricl
M-O1	2.340	2.327	2.339	2.389	2.377	2.388	2.523	2.283	2.462	2.386	2.424	2.387
M-O2	2.313	2.279	2.315	2.369	2.445	2.466	2.510	2.341	2.466	2.587	2.487	2.453
M-O3	2.335	2.321	2.352	2.380	2.369	2.335	2.495	2.270	2.440	2.349	2.415	2.381
M-O4	2.270	2.288	2.308	2.330	2.421	2.403	2.552	2.303	2.491	2.397	2.472	2.439
M-O5	2.355	2.383	2.359	2.405	2.397	2.354	2.502	2.237	2.457	2.368	2.447	2.404
M-O6	2.379	2.336	2.310	2.419	2.366	2.334	2.474	2.247	2.428	2.346	2.416	2.373
$M\text{-}O7_{wat}$	2.349	2.608	2.505	2.408	2.586	3.865	2.665	2.854	2.607	2.658	2.627	2.618
$M\text{-}O8_{wat}$	2.373	2.501	2.498	2.424	2.506	2.476	2.688	2.590	2.628	2.558	2.548	2.532
M-S1	5.044	5.015	5.057	5.098	5.105	5.070	5.187	4.992	5.153	5.079	5.149	5.110
M-S2	6.139	6.184	6.216	6.199	6.284	6.260	6.399	6.237	6.348	6.408	6.328	6.289
M-S3	6.069	6.201	6.175	6.086	6.265	6.237	6.391	6.148	6.335	6.232	6.316	6.273
q(M)	-	1.35	1.35	-	1.26	1.52	2.23	1.29	2.19	1.36	1.59	**1.41**
n(p)	-	0.42	0.42	-	6.35	6.24	5.98	6.34	5.99	6.35	6.28	6.36
n(d)	-	0.99	0.98	-	1.02	0.74	0.60	1.03	0.72	0.79	0.90	0.80
n(f)	-	-	-	-	6.20	6.32	3.02	3.10	6.02	6.29	7.02	7.21
ρ(M)	-	-	-	-	-	6.24	-	2.12	-	6.01	-	6.91

Table S2. Comparison of some interatomic distances in the monoclinic (ISOMER II) Y and Eu structures obtained from X-Ray and QM (DFT/BP86) calculations with the def2-TZVP basis sets. NPA charges were computed at the DFT level: q(M) is the net charge of the metal, n(p), n(d), n(f) are the population of the valence orbitals, ρ(M) is the spin density of the metal. The X-ray data are from White[25] that does not report any uncertainty in the bond distances due to uncertainties in the data collection. Based on his discussion we estimate the uncertainty in the M – O distances to at least 0.02 Å.

	$Y(TTA)_3(OH_2)_2$		$Eu(TTA)_3(OH_2)_2$				$U(TTA)_3(OH_2)_2$		$Am(TTA)_3(OH_2)_2$		$Cm(TTA)_3(OH_2)_2$	
	QM/SPP			QM/LPP		QM/SPP	QM/LPP	QM/SPP	QM/LPP	QM/SPP	QM/LPP	QM/SPP
	GP	$CHCl_3$	X-Ray	GP	$CHCl_3$	$CHCl_3$	$CHCl_3$	$CHCl_3$	$CHCl_3$	$CHCl_3$	$CHCl_3$	$CHCl_3$
	mono	mono	mono	mono	mono	dist. mono	dist. mono	mono	dist. mono	dist. mono	mono	mono
M-O1	2.328	2.300	2.50	2.350	2.363	2.347	2.483	2.313	2.432	2.377	2.419	2.374
M-O2	2.370	2.398	2.38	2.474	2.459	2.509	2.550	2.338	2.496	2.400	2.504	2.472
M-O3	2.402	2.407	2.39	2.493	2.457	2.431	2.538	2.278	2.484	2.567	2.495	2.469
M-O4	2.303	2.301	2.38	2.344	2.360	2.387	2.488	2.278	2.436	2.348	2.405	2.366
M-O5	2.289	2.316	2.47	2.362	2.376	2.392	2.487	2.273	2.437	2.348	2.421	2.383
M-O6	2.307	2.311	2.38	2.362	2.377	2.367	2.515	2.314	2.464	2.386	2.432	2.388
$M\text{-}O_{wat}$	2.557	2.505	2.51	2.609	2.571	2.588	2.678	2.660	2.625	2.661	2.612	2.601
$M\text{-}O_{wat}$	2.453	2.441	2.55	2.520	2.506	2.545	2.675	2.582	2.618	2.557	2.547	2.529
M-S1	5.052	5.034	5.25	5.064	5.087	5.050	5.198	5.060	5.157	5.108	5.139	5.097
M-S2	5.168	5.180	5.13	5.254	5.219	5.175	5.272	5.041	5.225	5.346	5.247	5.228
M-S3	5.032	5.069	5.15	5.098	5.116	5.132	5.203	5.011	5.162	5.082	5.152	5.122
q(M)	1.34	1.34	-	1.26	1.26	1.40	2.24	1.25	2.11	1.36	1.59	1.40
n(p)	6.43	6.43	-	6.34	6.35	6.29	5.98	6.37	5.98	6.36	6.28	6.37
n(d)	0.98	0.98	-	1.03	1.03	0.81	0.60	1.08	0.71	0.79	0.90	0.80
n(f)	-	-	-	6.19	6.19	6.32	3.03	3.11	6.02	6.29	7.02	7.21
ρ(M)	-	-	-	-	-	6.25	-	2.20	-	6.01	-	6.91

Table S3 Average M - O_{TTA} distances in Å in the X-ray structures and corresponding QM values obtained using the LPP and SPP potentials in the QM calculations, with the def-TZVP basis sets. Δ denotes the difference in the average distance in the various structures obtained using the two core potentials.

Metal ion	X-ray	LPP	SPP	Δ(LPP –SPP)
Isomer II				
Y	-	-	2.379	-
Eu	2.44	2.425	2.432	-0.010
U	-	2.551	2.377	0.173
Am	-	2.498	2.453	0.044
Cm	-	2.479	2.447	0.032
Isomer I				
Y	2.332	2.379	-	-
Eu	2.382	2.432	2.446	-0.014
U	-	2.550	2.392	0.158
Am	-	2.497	2.454	0.043
Cm	-	2.478	2.447	0.031

Table S4 Relative electronic and Gibbs energies in kJ/mol between isomers I and II, *E*(IsomII) - *E*(IsomI), computed at the MP2 level from structures optimized with the LPP and SPP pseudopotentials, in the gas-phase, or solvent models of carbon tetrachloride, chloroform and water, using the def-TZVP basis sets.

Complex	ECP	Gas-phase		CCl_4	$CHCl_3$	Water
		ΔE	ΔG^o	ΔE	ΔE	ΔE
$Y(TTA)_3(OH_2)_2$	SPP	-0.5	-0.3	-4.7	-3.9	-6.4
$Eu(TTA)_3(OH_2)_2$	LPP	-2.2	-1.6	-	-7.5	-
	SPP	-	-	-	-9.3	-
$U(TTA)_3(OH_2)_2$	LPP	-6.7	-3.4	-	-14.7	-
	SPP	-	-	-	-21.0	-
$Am(TTA)_3(OH_2)_2$	LPP	-5.5	-0.7	-	-13.0	-
	SPP	-	-	-	-13.5	-
$Cm(TTA)_3(OH_2)_2$	LPP	-5.3	-0.2	-	-7.6	-
	SPP	-	-	-	-7.6	-

Table S5. Relative energies in kJ/mol of various $Y(TTA)_3(OH_2)_2$ isomers (computed at the MP2 level with the COSMO solvent model for CH_3Cl with the def2-TZVP basis sets) calculated relative to the energy of Isomer I.

Complex	ΔE(kJ/mol)
$Y(TTA)_3$ – Isomer I	0.0
$Y(TTA)_3$ – Isomer I / flip1	4.8
$Y(TTA)_3$ – Isomer I / flip2	8.4
$Y(TTA)_3$ – Isomer I / flip3	-4.0
$Y(TTA)_3$ –Isomer II	-3.2
$Y(TTA)_3$ – Isomer II / flip1	-8.9
$Y(TTA)_3$ – Isomer II / flip2	-2.4
$Y(TTA)_3$ – Isomer II / flip3	1.9

Table S6. Cartesian coordinates in Angstroms of the QM structures reported in Fig. 2 and S1-S4.

Isomer II / flip2 $Y(TTA)_3(OH_2)_2$ optimized with the QM/SPP in the chloroform CPCM solvent (Fig. 2)

Atom	X(Å)	Y(Å)	Z(Å)
S	-1.6727971	3.0416971	-3.3413608
C	-1.4782582	3.9048101	-1.8419509
C	-1.6452092	5.2710265	-2.0361343
C	-1.9252681	5.6074370	-3.3801169
C	-1.9703801	4.4954596	-4.1997113
C	-1.1774053	3.1375953	-0.6339583
C	-1.0353182	3.8294861	0.6060343
C	-0.8045294	3.1910891	1.8161543
C	-0.7560669	4.0511590	3.0986509
F	-0.8490657	5.3864334	2.8764154
O	-1.0757502	1.8711744	-0.7607106
Y	-0.2959872	0.1301982	0.5063467
O	-0.6500753	1.9442769	2.0482790
O	-0.8312264	-2.0356948	1.4013000
C	-1.2682562	-3.1227701	0.8854650
C	-1.7622462	-3.2316275	-0.4437456
C	-1.8410287	-2.1566218	-1.3256534
C	-2.4519155	-2.4094876	-2.7259878
F	-2.7884056	-3.7076412	-2.9543547
C	-1.2722901	-4.3148969	1.7386323
S	-0.6803626	-4.1686517	3.3692870
C	-0.9810283	-5.8269748	3.6905179
C	-1.5147492	-6.4779230	2.5959615
C	-1.6811874	-5.6176161	1.4851518
O	-1.4912094	-0.9490617	-1.1492339
O	-2.5945200	0.1672256	1.4939614
O	0.7840158	-0.2876270	2.6532309
O	1.5981616	1.4502229	0.2753007
C	2.7902445	1.2338263	-0.1083579
C	3.3345819	0.0576032	-0.6132202
C	2.5568247	-1.1220430	-0.7778048
C	3.1848087	-2.3175118	-1.3431199
O	1.3203101	-1.2034700	-0.4611138
F	-3.5808200	-1.6694719	-2.8945205
F	-1.5826166	-2.0452022	-3.7036605
C	3.7073892	2.4730405	0.0187112
F	0.3975533	3.8368540	3.7841526
F	-1.7820629	3.7122894	3.9334791
H	4.3808716	0.0487028	-0.9025450
H	-2.1653632	4.4619831	-5.2684982
H	-2.0875484	6.6236211	-3.7358659
H	-1.5661218	6.0054094	-1.2364940
H	-1.1443863	4.9098140	0.6123277
H	-2.1177422	-4.1984714	-0.7865076
H	-2.0874286	-5.9434915	0.5292826
H	-1.7759262	-7.5349779	2.5951820
H	-0.7495671	-6.2397701	4.6688153
H	-2.5934513	0.8384043	2.2026302

H	-2.8865862	-0.6648842	1.9071196
H	0.3879699	-1.0943357	3.0357775
H	0.5640874	0.4543288	3.2497723
C	4.4851453	-2.5393770	-1.7796467
C	4.6891626	-3.8517286	-2.2650837
C	3.5430088	-4.6200976	-2.1951479
S	2.2171185	-3.7508153	-1.5410276
H	5.2650903	-1.7804284	-1.7513786
H	5.6377789	-4.2205501	-2.6520155
H	3.4140066	-5.6556946	-2.4989262
F	3.7680795	2.8956194	1.3096976
F	3.2253669	3.5069625	-0.7202112
F	4.9861639	2.2523304	-0.3892123

Isomer I, of $Y(TTA)_3(OH_2)_2$ optimized with the QM/SPP in gas phase (Fig. S2b)

Atom	X(Å)	Y(Å)	Z(Å)
C	-1.9517644	2.0412756	-4.4248655
C	-1.1337365	1.7016205	-3.3543932
S	0.4142061	2.4824891	-3.4896449
C	-0.0423198	3.2453582	-4.9541795
C	-1.3297476	2.9221568	-5.3372016
C	-1.3750719	0.8331154	-2.2025742
C	-2.6218763	0.1568185	-2.0872361
C	-2.9139867	-0.6971896	-1.0311867
O	-2.1712394	-1.0110856	-0.0439877
Y	-0.0506396	-0.3349689	0.6332583
O	1.2378841	-0.7597705	2.7343112
O	0.0093261	-2.6504270	0.7832130
C	0.8377061	-3.5727172	0.4803710
C	2.0671725	-3.3405702	-0.1961143
C	2.4679222	-2.0744721	-0.6102182
O	1.8572487	-0.9694592	-0.4592476
C	0.4647517	-4.9457851	0.8524728
S	1.5127151	-6.3185575	0.6283123
C	0.3482422	-7.3949055	1.2794261
C	-0.8059668	-6.7385257	1.6556407
C	-0.7375282	-5.3475566	1.4141206
C	3.8135093	-1.9338973	-1.3616441
F	4.6461854	-1.0933848	-0.6917789
F	3.6196675	-1.4139273	-2.5985187
F	4.4727878	-3.1123514	-1.5156971
O	-1.3613246	1.3732415	1.6549096
C	-1.1903591	2.6317601	1.7917206
C	-0.0314530	3.3619554	1.5660606
C	1.2078057	2.7462593	1.2197428
C	2.4163771	3.5669988	1.0736099
S	2.4750983	5.2755857	1.4069191
C	4.1332387	5.3626354	0.9809165
C	4.6325777	4.1346073	0.5948099
C	3.6571222	3.1138501	0.6486715
O	1.3465628	1.4911589	1.0473105
O	-0.4303623	0.7254266	-1.3475233

O	-1.5268921	-1.0520450	2.6601138
C	-2.4541882	3.3742888	2.2812491
F	-3.4670938	3.2357307	1.3908499
F	-2.8775567	2.8496493	3.4637034
F	-2.2612353	4.7032799	2.4751124
C	-4.2909995	-1.3991835	-1.0063576
F	-4.9227347	-1.1695052	0.1743216
F	-4.1402343	-2.7443805	-1.1280153
F	-5.1251599	-0.9943454	-1.9973475
H	4.6568467	6.3130490	1.0369392
H	5.6638145	3.9806743	0.2821425
H	3.8215911	2.0728864	0.3774450
H	2.7135457	-4.1843273	-0.4243211
H	-0.0669145	4.4394436	1.7075513
H	0.5727776	-8.4553321	1.3533770
H	-1.6678965	-7.2445468	2.0868695
H	-1.5362948	-4.6400039	1.6231686
H	-3.3767810	0.3038625	-2.8529829
H	-2.9670702	1.6679617	-4.5444868
H	-1.8039131	3.3051186	-6.2391521
H	0.6601892	3.8957384	-5.4681779
H	0.5459473	-0.9959212	3.3820783
H	1.6609965	0.0612266	3.0415435
H	-2.0061076	-0.1933452	2.6428576
H	-2.1002248	-1.6741882	2.1723734

Isomer I, of $Y(TTA)_3(OH_2)_2$ optimized with the QM/SPP in the chloroform CPCM solvent (Fig. S2c)

Atom	X(Å)	Y(Å)	Z(Å)
C	-4.4159090	2.2372773	-1.7855377
C	-3.1352822	2.0831811	-1.2682224
S	-2.1671560	3.4928053	-1.5920336
C	-3.4661182	4.2630972	-2.4040175
C	-4.6042206	3.4798995	-2.4330698
C	-2.5247526	0.9705006	-0.5400642
C	-3.3102090	-0.1887854	-0.2614761
C	-2.8163190	-1.2599574	0.4669126
O	-1.6427538	-1.4198022	0.9459869
Y	0.3536156	-0.2175790	0.7425679
O	2.5871632	-0.3638340	1.8525383
O	1.2212724	-2.3994883	0.8855769
C	1.3103736	-3.4050096	0.1015509
C	1.0121272	-3.3453783	-1.2879694
C	0.6312633	-2.1693961	-1.9266753
O	0.4447213	-1.0182308	-1.4204207
C	1.7596559	-4.6710607	0.6941306
S	2.0724737	-6.1096071	-0.2380774
C	2.5015648	-7.0013291	1.1616963
C	2.4111829	-6.2361757	2.3078897
C	1.9910752	-4.9127352	2.0413051
C	0.4033639	-2.2063999	-3.4566572
F	1.2479473	-1.3453640	-4.0858822

F	-0.8633077	-1.8229243	-3.7638760
F	0.5964692	-3.4324366	-4.0102687
O	0.3149456	1.5960649	2.2499362
C	0.6522758	2.8187695	2.0978146
C	1.3391026	3.4036735	1.0442274
C	1.8242257	2.6719574	-0.0843592
C	2.6074386	3.3701544	-1.1119370
S	3.0405336	5.0557907	-1.0197072
C	3.8694236	4.9902404	-2.5190473
C	3.8227552	3.7282237	-3.0788115
C	3.1067066	2.8087349	-2.2789326
O	1.6307927	1.4274293	-0.2577549
O	-1.3111042	1.1040052	-0.1736359
O	-0.0959375	-0.8986508	3.1106908
C	0.2324776	3.7112746	3.2864293
F	-1.1146247	3.6701991	3.4679979
F	0.8028917	3.2656266	4.4417281
F	0.5787889	5.0162134	3.1483351
C	-3.7650011	-2.4354947	0.7878340
F	-3.8655353	-2.6115658	2.1361095
F	-3.2891443	-3.5980474	0.2694900
F	-5.0261966	-2.2707314	0.3124345
H	4.3483742	5.8838892	-2.9105015
H	4.2879545	3.4802428	-4.0314299
H	2.9425453	1.7624540	-2.5285855
H	1.1106428	-4.2472768	-1.8872952
H	1.5395320	4.4711868	1.0989223
H	2.7989721	-8.0424637	1.0680693
H	2.6378780	-6.6198299	3.3012765
H	1.8435015	-4.1463258	2.7996014
H	-4.3419223	-0.2215443	-0.5979094
H	-5.1926087	1.4791424	-1.7016951
H	-5.5361001	3.7904178	-2.9028746
H	-3.3292528	5.2571132	-2.8218986
H	2.6240700	-1.3076100	2.1052057
H	2.7348995	0.1454006	2.6687852
H	-0.3211348	-0.0500401	3.5417233
H	-0.9295187	-1.4055847	3.0515898

Isomer II, of $Eu(TTA)_3(OH_2)_2$ optimized with the QM/LPP in gas phase (Fig. S3b)

Atom	X(Å)	Y(Å)	Z(Å)
S	2.2780234	2.9796532	-3.1861531
C	0.7941514	3.6800154	-2.6093480
C	0.6719030	4.9967537	-3.0369556
C	1.7667887	5.4270089	-3.8184532
C	2.7136300	4.4335513	-3.9797802
C	-0.0899970	2.8472422	-1.7931502
C	-1.3194057	3.4026001	-1.3201450
C	-2.2569301	2.6966616	-0.5807423
C	-3.5788899	3.4039937	-0.2070293
F	-3.6239702	4.7132111	-0.5566778
O	0.2898555	1.6540641	-1.5593915

Eu	-0.3464230	-0.1446342	-0.1870487
O	-2.2079897	1.4843833	-0.1726457
O	-1.3066943	-2.4398898	-0.3482052
C	-0.7842908	-3.5597006	-0.7035940
C	0.4280860	-3.6832778	-1.4281081
C	1.2018956	-2.6034336	-1.8566720
C	2.4501820	-2.9014749	-2.7266973
F	2.7060438	-4.2301649	-2.8688935
C	-1.5238559	-4.7765154	-0.3525531
S	-3.0388353	-4.6053870	0.4860825
C	-3.2675977	-6.3044208	0.5442924
C	-2.2273646	-6.9867703	-0.0522832
C	-1.2357923	-6.1174712	-0.5632882
O	1.0172648	-1.3654519	-1.6516228
O	-2.0720444	-0.4985224	-2.1116904
O	-2.1328714	-0.5823077	1.5356000
O	0.4950591	1.3867495	1.4024509
C	1.1772236	1.3522667	2.4841510
C	1.7410160	0.1648084	3.0252072
C	1.6018007	-1.0779641	2.4144870
C	2.2558619	-2.3079598	3.0894247
F	2.9252282	-2.0049220	4.2343200
O	0.9876593	-1.3589569	1.3368015
F	2.2838576	-2.3884277	-3.9731579
F	3.5545283	-2.3318804	-2.1917907
C	1.3774982	2.6221481	3.1868902
C	2.0610844	2.9168121	4.3592659
C	2.0102728	4.2874117	4.7002243
C	1.2877753	5.0264318	3.7843578
S	0.6707331	4.0598804	2.5103041
F	1.3120093	-3.2310775	3.4087985
F	3.1397103	-2.9011193	2.2503267
F	-3.8054359	3.3319169	1.1286712
F	-4.6270984	2.7853383	-0.8253247
H	2.3076724	0.2221680	3.9490694
H	2.5818761	2.1674157	4.9522810
H	2.4836993	4.7169945	5.5814004
H	1.0892943	6.0945923	3.7999369
H	3.6481939	4.4901612	-4.5313219
H	1.8598613	6.4232577	-4.2472390
H	-0.1798662	5.6292731	-2.7941051
H	-1.5522434	4.4323034	-1.5733551
H	0.7673291	-4.6786250	-1.6971211
H	-0.3341938	-6.4630653	-1.0651774
H	-2.1805342	-8.0724111	-0.1173206
H	-4.1550736	-6.7175369	1.0152869
H	-2.8190579	0.0955404	-1.9126116
H	-2.3707426	-1.4080092	-1.9171337
H	-2.4999005	-1.4639510	1.3327437
H	-2.8093968	0.0913802	1.3198817

Isomer II, of $Eu(TTA)_3(OH_2)_2$ optimized with the QM/LPP in the chloroform CPCM solvent (Fig. S3c)

Atom	X(Å)	Y(Å)	Z(Å)
S	2.2658487	2.8223603	-3.2160040
C	0.8258128	3.5893759	-2.6086708
C	0.7594238	4.9125058	-3.0294343
C	1.8603627	5.2932981	-3.8301316
C	2.7571716	4.2578558	-4.0137930
C	-0.0836386	2.7980400	-1.7792694
C	-1.2694223	3.4152750	-1.2773163
C	-2.2227140	2.7520912	-0.5160812
C	-3.4891574	3.5321667	-0.0954379
F	-3.4856864	4.8398411	-0.4589430
O	0.2366396	1.5821119	-1.5615030
Eu	-0.4700208	-0.1760330	-0.1489622
O	-2.2300460	1.5406244	-0.1134128
O	-1.2911400	-2.4867801	-0.3000566
C	-0.7655895	-3.5824331	-0.7014471
C	0.4351792	-3.6620663	-1.4625834
C	1.1684472	-2.5528407	-1.8726919
C	2.4154428	-2.7928827	-2.7579247
F	2.6893624	-4.1059323	-2.9816150
C	-1.4704779	-4.8239360	-0.3691988
S	-2.9547522	-4.7143363	0.5342973
C	-3.1508452	-6.4189088	0.5320472
C	-2.1229543	-7.0578456	-0.1326188
C	-1.1667427	-6.1503696	-0.6463019
O	0.9572843	-1.3203348	-1.6391087
O	-2.1730415	-0.4993194	-2.0470727
O	-2.2514851	-0.6019169	1.5609673
O	0.4041608	1.3780752	1.4219259
C	1.1099868	1.3661102	2.4873565
C	1.6952181	0.1876838	3.0323741
C	1.5535960	-1.0594256	2.4334321
C	2.2378860	-2.2755261	3.1014538
F	2.9249942	-1.9663824	4.2339829
O	0.9195869	-1.3613057	1.3728515
F	2.2543715	-2.2060788	-3.9752809
F	3.5210671	-2.2450610	-2.1911842
C	1.3197778	2.6449785	3.1691713
C	2.0276371	2.9542317	4.3241716
C	1.9800816	4.3293572	4.6504069
C	1.2365389	5.0577251	3.7417899
S	0.5950208	4.0749908	2.4911827
F	1.3162714	-3.2176195	3.4397289
F	3.1172593	-2.8629087	2.2482938
F	-3.6583509	3.4910738	1.2528344
F	-4.5995173	2.9658047	-0.6515312
H	2.2817443	0.2622697	3.9429747
H	2.5633749	2.2139631	4.9158644
H	2.4709587	4.7701782	5.5166339

H	1.0351219	6.1258097	3.7476426
H	3.6840976	4.2705685	-4.5813084
H	1.9928626	6.2862838	-4.2567199
H	-0.0558580	5.5853836	-2.7694973
H	-1.4508694	4.4578612	-1.5206797
H	0.7882736	-4.6428375	-1.7666116
H	-0.2817641	-6.4602848	-1.1991578
H	-2.0612189	-8.1391793	-0.2443280
H	-4.0127236	-6.8657619	1.0204967
H	-2.9269625	0.1142137	-1.9774485
H	-2.5523572	-1.3970138	-2.0233881
H	-2.6603655	-1.4797270	1.4442774
H	-2.9525890	0.0635989	1.4160254

Isomer I, of $Eu(TTA)_3(OH_2)_2$ optimized with the QM/SPP in the chloroform CPCM solvent (Fig. S4a)

Atom	X(Å)	Y(Å)	Z(Å)
C	2.3986617	-1.8590630	3.1362538
C	2.4867098	-2.3489212	1.8398761
S	3.5762516	-3.7083054	1.7795266
C	3.8945024	-3.6064963	3.4600892
C	3.1978779	-2.5729559	4.0567630
C	1.7773402	-1.8263180	0.6687351
O	1.0204299	-0.8168382	0.8485829
Eu	-0.5947230	0.4162482	-0.3402015
O	-0.3498610	1.8660900	1.4740250
C	0.5033961	2.7500687	1.7966366
C	0.2853024	3.3124637	3.2232061
F	1.2181773	4.2233725	3.6026235
O	-1.3555015	1.0588626	-2.6074182
O	1.0644144	1.3803168	-3.6957795
O	1.1656799	2.0261694	-0.9630800
C	1.8558935	2.8810348	-0.2964696
C	1.5566096	3.2595445	1.0441372
O	-2.7959294	1.3319571	-0.2084152
C	-3.9363593	0.8368171	0.0566764
C	-4.2586262	-0.4766853	0.3853283
C	-3.2850306	-1.5112126	0.4589395
O	-2.0371881	-1.3276068	0.2290732
O	0.5194196	-1.0285391	-1.9044875
C	1.3451501	-1.9876007	-1.7645544
C	1.9693162	-2.4390214	-0.6068357
C	3.0109372	3.5094496	-0.9501600
C	3.3851158	3.4443885	-2.2874095
C	4.5616111	4.1713618	-2.5764805
C	5.0915737	4.7865348	-1.4594839
S	4.1535490	4.4864897	-0.0601679
F	0.3085363	2.3082726	4.1387650
F	-0.9282993	3.9147780	3.3152423
C	-5.0817113	1.8755273	-0.0199999
F	-6.3083355	1.3615423	0.2523885
F	-5.1421482	2.4216898	-1.2651599

F	-4.8665047	2.8914782	0.8544601
C	-3.7042872	-2.8646374	0.8148118
S	-2.5005634	-4.1207901	0.8793036
C	-3.6712168	-5.2919754	1.3210105
C	-4.9404081	-4.7535058	1.4195378
C	-4.9600987	-3.3703728	1.1317723
C	1.6588347	-2.7107370	-3.0953259
F	2.0890587	-1.8087335	-4.0294621
F	2.6151464	-3.6654228	-2.9974237
F	0.5449866	-3.3003980	-3.5986373
H	2.8184734	2.9056701	-3.0440718
H	5.0058604	4.2438823	-3.5676536
H	5.9874108	5.3977741	-1.3880584
H	2.1746358	4.0230879	1.5098477
H	-5.2972295	-0.7185294	0.5882304
H	-3.3686981	-6.3227328	1.4864640
H	-5.8206553	-5.3351221	1.6882855
H	-5.8635511	-2.7636780	1.1558946
H	2.6538955	-3.2802147	-0.6885516
H	4.5776798	-4.3136540	3.9231923
H	3.2637761	-2.3437433	5.1189750
H	-0.5789924	1.2325965	-3.2185418
H	-1.9611064	1.8167956	-2.6783475
H	1.3178769	0.4457467	-3.8192596
H	1.3088231	1.5823385	-2.7556748
H	1.7674497	-1.0098301	3.3895867

Isomer I, of $U(TTA)_3(OH_2)_2$ optimized with the QM/SPP in the chloroform CPCM solvent (Fig. S4b)

Atom	X(Å)	Y(Å)	Z(Å)
C	3.6200195	-1.3633445	2.5910100
C	3.4116583	-2.1754313	1.4792194
S	4.5272940	-3.5203555	1.4996442
C	5.2430415	-2.9860501	2.9683554
C	4.6570275	-1.8253061	3.4327639
C	2.4259272	-1.9766631	0.4345197
O	1.6694775	-0.9159957	0.5394458
U	0.0095915	0.1071954	-0.5560208
O	-0.3957328	1.1981066	1.3932242
C	-0.1665770	2.3627686	1.9062272
C	-0.7194101	2.5205408	3.3250667
F	-0.4952396	3.7528817	3.8519046
O	-0.1589253	0.7218465	-3.0661116
O	2.3787028	0.4151850	-2.1174875
O	0.9815738	2.2308709	-0.7086210
C	1.0699495	3.3157913	0.0051196
C	0.5058909	3.4133983	1.3035302
O	-2.0682059	0.8682835	-1.1188617
C	-3.2800237	0.5385281	-0.7933902
C	-3.6682341	-0.5423442	-0.0210342
C	-2.7384247	-1.4554998	0.5446179
O	-1.4557708	-1.3277914	0.3609594

O	0.4958433	-1.7718103	-1.7951114
C	1.3269697	-2.7509425	-1.6417527
C	2.2770255	-2.8940251	-0.6373358
C	1.7891718	4.4348496	-0.5841659
C	2.3199847	4.5053057	-1.8690692
C	2.9611633	5.7348319	-2.1442738
C	2.9224156	6.6048784	-1.0731798
S	2.1024086	5.9238588	0.2738553
F	-0.1558309	1.6138866	4.1719275
F	-2.0624723	2.3076033	3.3566019
C	-4.3336192	1.4918526	-1.3592495
F	-5.6049292	1.1434729	-1.0358166
F	-4.2652790	1.5449341	-2.7203768
F	-4.1375045	2.7628096	-0.9092173
C	-3.1870470	-2.5707017	1.3515218
S	-2.0034762	-3.6570235	2.0311841
C	-3.2236569	-4.6079718	2.7766764
C	-4.4917760	-4.1214238	2.5216419
C	-4.4744866	-2.9638483	1.7123929
C	1.1981017	-3.8288808	-2.7206153
F	1.4279487	-3.3084077	-3.9609743
F	2.0645942	-4.8626528	-2.5571150
F	-0.0566626	-4.3546340	-2.7435466
H	2.2259228	3.6897216	-2.5831179
H	3.4330216	5.9798140	-3.0945393
H	3.3312074	7.6092662	-1.0036930
H	0.6097268	4.3441852	1.8565738
H	-4.7283775	-0.6942477	0.1593633
H	-2.9460658	-5.4780874	3.3655166
H	-5.3996490	-4.5843794	2.9052323
H	-5.3724259	-2.4327809	1.4014836
H	2.9122860	-3.7769192	-0.6588206
H	6.0559373	-3.5562223	3.4096852
H	4.9666701	-1.3279406	4.3506335
H	0.7704403	0.8326390	-3.3533700
H	-0.6257022	1.5516304	-3.2700791
H	3.0747983	-0.2658904	-2.1061689
H	2.7518498	1.1993980	-1.6729314
H	3.0251921	-0.4709261	2.7732908

Isomer I, of $Am(TTA)_3(OH_2)_2$ optimized with the QM/SPP in the chloroform CPCM solvent (Fig. S4c)

Atom	X(Å)	Y(Å)	Z(Å)
C	3.1021806	-3.1702098	2.2394261
C	2.5605098	-3.6635270	1.0599937
S	2.9183037	-5.3614273	0.8951754
C	3.7740195	-5.3898117	2.3807341
C	3.7908183	-4.1502994	2.9899957
C	1.7881666	-2.8972670	0.0766995
O	1.6503009	-1.6457061	0.3048083
Am	0.2870655	0.1095321	-0.5138308
O	0.7100073	1.1382579	1.5545654

C	0.8824039	2.3199492	2.0061468
C	0.8361542	2.3885727	3.5491143
F	1.0105400	3.6393323	4.0488769
O	0.1239076	1.0512198	-2.8869955
O	2.7901730	0.3704757	-1.3682349
O	1.1272804	2.5284900	-0.8811362
C	1.2260825	3.5508103	-0.1237189
C	1.1063143	3.4922351	1.2979785
O	-1.7115716	1.4097606	-0.5986650
C	-2.9027923	1.2245938	-0.1903880
C	-3.4456634	0.1035933	0.4294810
C	-2.6789496	-1.0589182	0.7160290
O	-1.4373791	-1.1781426	0.4194363
O	0.1973011	-1.6641575	-2.1239756
C	0.5221134	-2.8936213	-2.0546282
C	1.2484444	-3.5512794	-1.0664794
C	1.5029479	4.8456510	-0.7621003
C	1.6868409	5.0794291	-2.1182022
C	1.9364242	6.4364121	-2.4255923
C	1.9418768	7.2386468	-1.3014692
S	1.6447283	6.3391316	0.1265081
F	1.8077112	1.6023801	4.0896091
F	-0.3546400	1.9311622	4.0160684
C	-3.8229674	2.4422586	-0.4406369
F	-5.1070209	2.2524314	-0.0356336
F	-3.8632316	2.7505434	-1.7641536
F	-3.3559573	3.5392677	0.2128908
C	-3.3157240	-2.1919457	1.3850654
S	-2.3579123	-3.6061492	1.7217019
C	-3.6921685	-4.4025685	2.4468988
C	-4.8342548	-3.6248427	2.4370060
C	-4.6202184	-2.3650370	1.8323511
C	0.0264836	-3.7158018	-3.2672157
F	0.5491519	-3.2212007	-4.4229889
F	0.3559897	-5.0326608	-3.2118042
F	-1.3257418	-3.6446219	-3.3766382
H	1.6425986	4.2832805	-2.8584781
H	2.1046305	6.8164832	-3.4318493
H	2.1025884	8.3117676	-1.2401761
H	1.2207868	4.4111941	1.8682578
H	-4.4947029	0.1233735	0.7084204
H	-3.5714114	-5.4065800	2.8452769
H	-5.7875056	-3.9514764	2.8494974
H	-5.3957057	-1.6082421	1.7278967
H	1.4211969	-4.6182234	-1.1870749
H	4.2204502	-6.3177288	2.7284223
H	4.2808195	-3.9605759	3.9435582
H	0.6925550	0.5986289	-3.5352348
H	0.5319670	1.9265391	-2.7122461
H	3.4062163	-0.1450291	-0.8167722
H	3.0176795	1.3080961	-1.2225537
H	2.9850609	-2.1296514	2.5353237

Isomer I, of $Cm(TTA)_3(OH_2)_2$ optimized with the QM/SPP in the chloroform CPCM solvent (Fig. S4d)

Atom	X(Å)	Y(Å)	Z(Å)
C	2.6636524	-2.9814272	2.7765330
C	2.3458443	-3.5296205	1.5415630
S	2.7835456	-5.2163530	1.5002991
C	3.3763763	-5.1678203	3.1085043
C	3.2479584	-3.9111119	3.6669914
C	1.7245104	-2.8194713	0.4149581
O	1.5204249	-1.5704323	0.5689939
Cm	0.3194817	0.1617237	-0.5865254
O	0.5167489	1.0659374	1.6069283
C	0.6095481	2.2570442	2.0473010
C	0.3507482	2.3602390	3.5694851
F	0.4081923	3.6284467	4.0538849
O	0.0870520	0.6995510	-3.0493092
O	2.8222786	0.2589419	-1.3495582
O	1.2625180	2.4182230	-0.7825914
C	1.2661060	3.4496570	-0.0282872
C	0.9249147	3.4212650	1.3546042
O	-1.6549503	1.4978581	-0.7063653
C	-2.8754406	1.3147936	-0.3971814
C	-3.4749370	0.1783804	0.1351411
C	-2.7486178	-1.0133774	0.4168716
O	-1.4934487	-1.1463260	0.2089094
O	0.4862315	-1.7512103	-2.0907986
C	0.8432095	-2.9598012	-1.9053056
C	1.4031699	-3.5407952	-0.7735783
C	1.6767577	4.7207836	-0.6409463
C	2.0320860	4.9174366	-1.9683537
C	2.3802703	6.2554558	-2.2634230
C	2.2896363	7.0789358	-1.1583639
S	1.7820475	6.2226956	0.2370673
F	1.2683863	1.6270620	4.2583759
F	-0.8745561	1.8661402	3.8836318
C	-3.7629051	2.5514770	-0.6725227
F	-5.0752663	2.3666334	-0.3680748
F	-3.7039276	2.9015314	-1.9859590
F	-3.3331761	3.6220503	0.0467340
C	-3.4595984	-2.1658495	0.9722297
S	-2.5562445	-3.6162392	1.3038807
C	-3.9572017	-4.4211396	1.8784706
C	-5.0812131	-3.6194084	1.8230593
C	-4.7978768	-2.3340246	1.3066720
C	0.6064252	-3.8552349	-3.1439701
F	1.2812452	-3.3649778	-4.2214317
F	0.9996867	-5.1445939	-2.9803885
F	-0.7117540	-3.8772078	-3.4767100
H	2.0332447	4.1051446	-2.6921443
H	2.6846093	6.6080382	-3.2475320
H	2.4935730	8.1444852	-1.0935046
H	0.9534113	4.3519533	1.9165801
H	-4.5412574	0.2036586	0.3379581

H	-3.8858442	-5.4473475	2.2294314
H	-6.0695132	-3.9465118	2.1422272
H	-5.5494012	-1.5560512	1.1840798
H	1.6260725	-4.6047297	-0.8102140
H	3.7885311	-6.0668467	3.5592060
H	3.5626307	-3.6738752	4.6819420
H	0.4393515	-0.0686964	-3.5386755
H	0.4519743	1.5004791	-3.4627039
H	3.4279332	-0.2548845	-0.7856304
H	3.0492140	1.1980355	-1.2041044
H	2.4627455	-1.9379873	3.0109850

Isomer II, of $Eu(TTA)_3(OH_2)_2$ optimized with the QM/SPP in the chloroform CPCM solvent (Fig. S5a)

Atom	X(Å)	Y(Å)	Z(Å)
S	2.0590672	2.4930875	-3.3861606
C	0.7727779	3.4337620	-2.6852677
C	0.8040547	4.7398238	-3.1595887
C	1.8559596	4.9688991	-4.0757890
C	2.6177331	3.8364348	-4.2928393
C	-0.1327177	2.7776814	-1.7411028
C	-1.1920418	3.5329158	-1.1576923
C	-2.1269725	2.9894637	-0.2821189
C	-3.2727943	3.9043578	0.2133295
F	-3.1750017	5.1943654	-0.1966357
O	0.0765106	1.5427854	-1.4947043
Eu	-0.6396974	-0.1479453	-0.0332448
O	-2.2046014	1.8031100	0.1709697
O	-1.2753806	-2.4088555	0.5930641
C	-0.9991136	-3.5645158	0.1274444
C	-0.4569360	-3.7979702	-1.1708076
C	-0.2036588	-2.7832954	-2.0935778
C	0.2814986	-3.1917128	-3.5076115
F	0.4808553	-4.5285855	-3.6578526
C	-1.2804475	-4.7197300	0.9860538
S	-1.9245899	-4.4274286	2.5765766
C	-1.9819163	-6.1068171	2.9236691
C	-1.5238660	-6.8717315	1.8690403
C	-1.1238562	-6.0821291	0.7654954
O	-0.3462167	-1.5314839	-1.9559669
O	-2.9556858	-0.4221862	-1.1559833
O	-2.0922276	-0.1887238	2.0556845
O	0.4939404	1.2146818	1.5724385
C	1.6149991	1.2327903	2.1782820
C	2.6261334	0.2423156	2.0059200
C	2.4655303	-0.8373829	1.1462455
C	3.6180782	-1.8647317	1.0355680
F	4.6991455	-1.5597184	1.8024049
O	1.4696888	-1.1253276	0.4090265
F	-0.6303264	-2.8162830	-4.4469219
F	1.4504063	-2.5758398	-3.8137102
C	1.8609351	2.3442563	3.1017675

C	2.9648079	2.6448215	3.8896287
C	2.7954559	3.8250876	4.6505369
C	1.5645451	4.4145901	4.4367914
S	0.6118575	3.5378583	3.3117070
F	3.1958398	-3.1004026	1.4148706
F	4.0528273	-1.9639015	-0.2471887
F	-3.3283920	3.9185546	1.5718863
F	-4.4757374	3.4343668	-0.2272977
H	3.5535195	0.3303508	2.5632360
H	3.8662568	2.0351762	3.9177267
H	3.5454949	4.2282146	5.3291783
H	1.1716512	5.3227069	4.8865686
H	3.4814870	3.7276530	-4.9435976
H	2.0493465	5.9252604	-4.5590229
H	0.0920662	5.5059206	-2.8576001
H	-1.2920564	4.5801256	-1.4269817
H	-0.2676144	-4.8225965	-1.4764434
H	-0.7341996	-6.4994905	-0.1612724
H	-1.4776345	-7.9593777	1.8913830
H	-2.3467327	-6.4481748	3.8888509
H	-3.5991858	0.2453450	-0.8581341
H	-3.4498061	-1.2470073	-1.2992157
H	-2.6811520	-0.9644917	2.0645350
H	-2.6617735	0.5992385	1.9540982

Isomer II, of $U(TTA)_3(OH_2)_2$ optimized with the QM/SPP in the chloroform CPCM solvent (Fig. S5b)

Atom	X(Å)	Y(Å)	Z(Å)
S	3.4618908	2.9614230	-1.1278265
C	1.9171768	3.4592681	-1.7674677
C	2.0194715	4.7097468	-2.3723834
C	3.3256614	5.2461318	-2.3154720
C	4.2137138	4.4073179	-1.6696189
C	0.7762103	2.5760641	-1.6027709
C	-0.4965395	2.9504819	-2.1246670
C	-1.6354571	2.1747050	-2.0039575
C	-2.9404897	2.6516764	-2.6496448
F	-2.8407784	3.8614467	-3.2565372
O	0.9809265	1.4571270	-0.9853870
U	-0.2764554	-0.3224690	-0.2096231
O	-1.7628391	1.0403332	-1.3937231
O	-0.6933348	-2.4525102	-0.9021995
C	-0.0181555	-3.5629572	-1.0531009
C	1.3842837	-3.6284922	-0.8386943
C	2.1640323	-2.5398159	-0.4746956
C	3.6645573	-2.7254154	-0.2477760
F	4.0781507	-4.0121754	-0.3910153
C	-0.7629222	-4.7391788	-1.4494505
S	-2.4844754	-4.5990301	-1.7086030
C	-2.6212833	-6.2677227	-2.1018948
C	-1.4019233	-6.9136576	-2.0406711
C	-0.3453398	-6.0504264	-1.6720592

O	1.7716407	-1.3142392	-0.3089605
O	0.2940050	-0.5749726	-2.7957064
O	-2.7628984	-0.7131515	0.3640581
O	-0.5236585	1.2067611	1.4534232
C	-0.6155356	1.2853438	2.7470977
C	-0.5450911	0.1309531	3.5715643
C	-0.3765447	-1.1406470	3.0477010
C	-0.3287797	-2.3470807	3.9927741
F	-0.4500853	-2.0106819	5.3041328
O	-0.2572515	-1.4642766	1.8035330
F	4.3894556	-1.9747026	-1.1283073
F	4.0291634	-2.3226522	0.9999019
C	-0.8007354	2.6018831	3.3257818
C	-0.9323175	2.9919761	4.6567144
C	-1.1051092	4.3859831	4.8095743
C	-1.1050167	5.0544883	3.6003276
S	-0.8941321	3.9877311	2.2709980
F	-1.3319707	-3.2261296	3.7113935
F	0.8409437	-3.0291920	3.8604106
F	-3.9371443	2.7482444	-1.7238451
F	-3.3700688	1.7643240	-3.5924241
H	-0.6313561	0.2442470	4.6481705
H	-0.9046764	2.2934636	5.4911929
H	-1.2253816	4.8844937	5.7701933
H	-1.2179412	6.1209567	3.4246630
H	5.2723928	4.5682086	-1.4842883
H	3.6075893	6.2122649	-2.7313226
H	1.1789992	5.2208591	-2.8386370
H	-0.5770226	3.8910987	-2.6620706
H	1.8784832	-4.5883044	-0.9609722
H	0.6884912	-6.3751681	-1.5681873
H	-1.2756094	-7.9739698	-2.2546053
H	-3.5907975	-6.6855722	-2.3588088
H	1.1894581	-0.2380927	-2.9805264
H	0.2855245	-1.4900348	-3.1292814
H	-3.0908314	-1.6276352	0.2911879
H	-3.2822723	-0.1786480	-0.2676113

Isomer II, of $Am(TTA)_3(OH_2)_2$ optimized with the QM/SPP in the chloroform CPCM solvent (Fig. S5c)

Atom	X(Å)	Y(Å)	Z(Å)
S	-3.2811360	2.9509841	-2.2571269
C	-2.6508394	3.6888684	-0.8114224
C	-3.0228940	5.0261139	-0.7414513
C	-3.8069303	5.4398759	-1.8428517
C	-4.0271144	4.4162272	-2.7443562
C	-1.8516579	2.8684301	0.0977655
C	-1.3174470	3.4582297	1.2776983
C	-0.5655875	2.7538351	2.2124723
C	-0.0836604	3.5042828	3.4760628
F	-0.4463322	4.8133813	3.5129857
O	-1.6868328	1.6376048	-0.2188651

Am	-0.2664928	-0.1377815	0.4741004
O	-0.2064235	1.5318593	2.1965678
O	-1.0627023	-2.5688279	0.6835253
C	-1.1486967	-3.5459310	-0.1364796
C	-1.0190319	-3.4076688	-1.5505033
C	-0.8058812	-2.1911472	-2.1837530
C	-0.7422616	-2.1662185	-3.7274791
F	-0.8863749	-3.3890017	-4.3024894
C	-1.4186498	-4.8761332	0.4154711
S	-1.6131809	-5.0363125	2.1383139
C	-1.8701858	-6.7278235	2.0111805
C	-1.8106985	-7.1644813	0.7025747
C	-1.5545924	-6.1110360	-0.2060882
O	-0.6563944	-1.0368386	-1.6590891
O	-2.7422496	-0.4940697	1.3807674
O	-0.0242038	-1.1886066	2.7919976
O	1.4183573	1.2602825	-0.3737151
C	2.6602649	1.1947803	-0.6840027
C	3.4580358	0.0342786	-0.4885536
C	2.9480452	-1.1433572	0.0489439
C	3.9007629	-2.3521964	0.2016453
F	5.1771836	-2.0984958	-0.1926863
O	1.7652231	-1.3890826	0.4488842
F	-1.7222266	-1.3685947	-4.2327235
F	0.4450582	-1.6605100	-4.1523110
C	3.2646576	2.3906035	-1.2691466
C	4.5615389	2.6297338	-1.7078402
C	4.7406672	3.9367333	-2.2161433
C	3.5797739	4.6841205	-2.1618182
S	2.2701100	3.8016762	-1.4933901
F	3.9569922	-2.7602538	1.4971678
F	3.4582460	-3.4076022	-0.5327279
F	1.2705387	3.4606483	3.5755688
F	-0.5870932	2.9190160	4.5978943
H	4.5052503	0.0622251	-0.7735637
H	5.3560693	1.8868445	-1.6646191
H	5.6829619	4.3173962	-2.6069317
H	3.4317254	5.7120562	-2.4823602
H	-4.5899931	4.4534877	-3.6733869
H	-4.1959408	6.4485584	-1.9723791
H	-2.7398399	5.6859375	0.0767874
H	-1.5193794	4.5074815	1.4707729
H	-1.1165883	-4.2938418	-2.1702529
H	-1.4688893	-6.2542941	-1.2817255
H	-1.9460327	-8.2046260	0.4104849
H	-2.0519853	-7.3163220	2.9065405
H	-3.3932531	0.0247353	0.8747583
H	-2.9394555	-1.4311923	1.1924089
H	-0.4212309	-2.0726054	2.6534641
H	-0.5550320	-0.7461272	3.4783743

Isomer II, of $Cm(TTA)_3(OH_2)_2$ optimized with the QM/SPP in the chloroform CPCM solvent (Fig. S5d)

Atom	X(Å)	Y(Å)	Z(Å)
S	-2.9046281	2.8962095	-2.6132848
C	-2.4606067	3.6425628	-1.1043901
C	-2.8726101	4.9697858	-1.0731518
C	-3.5361957	5.3700495	-2.2553494
C	-3.6253198	4.3453273	-3.1784230
C	-1.7499238	2.8338185	-0.1134064
C	-1.3816079	3.4354891	1.1280759
C	-0.7395812	2.7604236	2.1577849
C	-0.4571268	3.5313399	3.4676430
F	-0.8085877	4.8418025	3.4310312
O	-1.5099425	1.6180026	-0.4200320
Cm	-0.1807388	-0.1599832	0.4224178
O	-0.3502254	1.5452870	2.2044592
O	-0.4853849	-2.4814735	1.2061052
C	-0.7876616	-3.5709853	0.6065955
C	-1.3354118	-3.6378977	-0.7064786
C	-1.6276678	-2.5236610	-1.4861176
C	-2.2875076	-2.7549383	-2.8668190
F	-2.4480502	-4.0661259	-3.1891203
C	-0.5726967	-4.8199871	1.3427113
S	0.0717066	-4.7252154	2.9575350
C	0.0433497	-6.4319196	3.1318282
C	-0.4394521	-7.0605813	2.0011917
C	-0.7908425	-6.1434130	0.9828706
O	-1.4469431	-1.2903548	-1.2259298
O	-2.3247171	-0.4980998	1.8551835
O	1.3022374	-0.5959042	2.4237464
O	1.4772021	1.3933157	-0.2967582
C	2.6098183	1.3786294	-0.8911861
C	3.2315521	0.1933381	-1.3762993
C	2.6455590	-1.0620548	-1.2542717
C	3.4075172	-2.2850830	-1.8173917
F	4.6018810	-1.9732178	-2.3887359
O	1.5290640	-1.3678218	-0.7266939
F	-3.5204977	-2.1803969	-2.9069924
F	-1.5481418	-2.1884305	-3.8549719
C	3.2874830	2.6634085	-1.0739617
C	4.5023851	2.9728145	-1.6734313
C	4.7983627	4.3551075	-1.6419361
C	3.8072301	5.0889011	-1.0188307
S	2.5155770	4.1025212	-0.4712030
F	3.6616398	-3.1867232	-0.8305491
F	2.6671602	-2.9221572	-2.7618127
F	0.8638527	3.4791041	3.7849277
F	-1.1369425	2.9641631	4.5062204
H	4.1974143	0.2683553	-1.8664667
H	5.1574271	2.2276834	-2.1215188
H	5.7016768	4.7971922	-2.0593197
H	3.7744266	6.1629870	-0.8555438

H	-4.0812468	4.3733069	-4.1647050
H	-3.9341090	6.3691363	-2.4258132
H	-2.7020009	5.6321178	-0.2262664
H	-1.6348533	4.4791584	1.2886521
H	-1.5678310	-4.6159444	-1.1169323
H	-1.1884931	-6.4443100	0.0152859
H	-0.5355810	-8.1413413	1.9102392
H	0.3837152	-6.8876392	4.0578850
H	-2.3735705	0.1030228	2.6203758
H	-2.3082340	-1.4013409	2.2226443
H	1.1572602	-1.4708383	2.8283149
H	1.0550124	0.0743506	3.0913265

Structure of $U(TTA)_3(OH_2)_2$ with the QM/LPP in the chloroform CPCM solvent obtained using isomer II as the starting structure (Fig. S6a)

Atom	X(Å)	Y(Å)	Z(Å)
S	2.7395545	2.6501357	-2.8805089
C	1.2106048	3.4538735	-2.6644227
C	1.2474405	4.7325579	-3.2079713
C	2.4965821	5.0501064	-3.7893223
C	3.4021549	4.0115678	-3.6846867
C	0.1386528	2.7289880	-1.9784295
C	-1.1177468	3.3831766	-1.7878562
C	-2.2205926	2.7938914	-1.1823289
C	-3.5222900	3.6228790	-1.0812331
F	-3.4303135	4.8742197	-1.5998355
O	0.3909566	1.5395495	-1.5945877
U	-0.6895864	-0.2818777	-0.2989954
O	-2.3378511	1.6249795	-0.6850277
O	-0.6284948	-2.6620847	-1.1782631
C	0.1933858	-3.6435175	-1.1838732
C	1.5392553	-3.5576401	-0.7275274
C	2.1210133	-2.3862635	-0.2493198
C	3.6116900	-2.4339440	0.1685842
F	4.1888575	-3.6564742	0.0228823
C	-0.2952745	-4.9232060	-1.7033275
S	-1.9586076	-5.0288192	-2.2076587
C	-1.7779685	-6.6757554	-2.6523842
C	-0.4970183	-7.1389870	-2.4239795
C	0.3475496	-6.1413317	-1.8834103
O	1.5993250	-1.2360022	-0.1021795
O	-1.6303153	-0.6962285	-2.7715825
O	-3.2877118	-0.8763074	-0.0734925
O	0.0519022	1.1409486	1.6014127
C	0.1478107	1.0821014	2.8720416
C	-0.3707157	0.0097038	3.6602833
C	-1.0522186	-1.0741813	3.1228514
C	-1.6045192	-2.1439553	4.0933102
F	-1.3650276	-1.8825662	5.4042383
O	-1.3136936	-1.3308625	1.9002337
F	4.3421867	-1.5566142	-0.5704556

F	3.7546369	-2.0774381	1.4722792
C	0.8218263	2.1923818	3.5479937
C	1.0802897	2.4191918	4.8944816
C	1.7690577	3.6315463	5.1284462
C	2.0300633	4.3195052	3.9588751
S	1.4413560	3.4960189	2.5748729
F	-2.9551717	-2.2629428	3.9501976
F	-1.0676021	-3.3633203	3.8229575
F	-3.9088174	3.7543003	0.2164025
F	-4.5387317	2.9929895	-1.7361821
H	-0.2469117	0.0503557	4.7383449
H	0.7841596	1.7336779	5.6865861
H	2.0633930	3.9879465	6.1142922
H	2.5415540	5.2717436	3.8448874
H	4.4284909	3.9823508	-4.0412112
H	2.7255449	6.0017130	-4.2664268
H	0.4021241	5.4182613	-3.1887506
H	-1.2264526	4.4009210	-2.1509695
H	2.1569708	-4.4495991	-0.7716823
H	1.3944175	-6.3096626	-1.6370568
H	-0.1800496	-8.1584735	-2.6379157
H	-2.6256077	-7.2236351	-3.0555999
H	-2.4609964	-0.3138432	-3.1035597
H	-1.7483503	-1.6666561	-2.7883756
H	-3.4224834	-1.2193062	0.8305155
H	-3.6816864	0.0199133	-0.0865801

Structure of $U(TTA)_3(OH_2)_2$ with the QM/LPP in the chloroform CPCM solvent obtained using isomer I as the starting structure (Fig. S6b and S6c)

Atom	X(Å)	Y(Å)	Z(Å)
C	3.8285834	-3.2950687	0.2232741
C	2.7486704	-3.7649912	-0.5114286
S	2.9736789	-5.4478371	-0.9051745
C	4.4844083	-5.5009583	-0.0962067
C	4.8142674	-4.2803504	0.4600658
C	1.5707925	-2.9816253	-0.9100954
O	1.5745664	-1.7444384	-0.6054571
U	0.0055021	0.2039042	-0.5986598
O	1.6365801	1.1179084	1.0537231
C	2.1353944	2.2619718	1.3003851
C	3.1170024	2.2498567	2.4976372
F	3.6573544	3.4641209	2.7835240
O	-1.4634441	0.8222337	-2.7629565
O	1.8136445	0.4130421	-2.5444780
O	0.3927448	2.6515482	-0.9952242
C	1.0488338	3.6134223	-0.4778591
C	1.9148234	3.4711148	0.6474752
O	-2.3231518	1.0400421	-0.1074055
C	-3.1753776	0.8286560	0.8188238
C	-3.0757859	-0.0122568	1.9196725
C	-1.9347320	-0.8282333	2.1858550

O	-0.8943096	-0.8570023	1.4471686
O	-0.9600102	-1.7487026	-1.9274529
C	-0.6299714	-2.9717598	-2.0701535
C	0.5093628	-3.6256979	-1.6157191
C	0.8903219	4.9356204	-1.1022470
C	0.0798737	5.2328084	-2.1889269
C	0.1301038	6.5940722	-2.5682097
C	0.9799801	7.3334297	-1.7691011
S	1.7163613	6.3701340	-0.5565774
F	4.1531652	1.3999749	2.2559704
F	2.4958074	1.8129518	3.6244150
C	-4.4725157	1.6518462	0.6436390
F	-5.4248151	1.3920524	1.5761014
F	-5.0298561	1.4127411	-0.5753742
F	-4.2050883	2.9847227	0.7043981
C	-1.9427495	-1.6910072	3.3679234
S	-0.5392526	-2.6711465	3.6835741
C	-1.2516647	-3.3288432	5.0975317
C	-2.5170175	-2.8244132	5.3303824
C	-2.9111361	-1.8908446	4.3446981
C	-1.6731441	-3.7919305	-2.8655487
F	-1.8780502	-3.2391308	-4.0930801
F	-1.3251163	-5.0892441	-3.0646566
F	-2.8722962	-3.7923180	-2.2236012
H	-0.5254103	4.4721022	-2.6778858
H	-0.4349348	7.0221955	-3.3946218
H	1.2101700	8.3938813	-1.8299871
H	2.4363247	4.3506158	1.0183055
H	-3.9162325	-0.0549595	2.6059637
H	-0.7037005	-4.0559436	5.6912429
H	-3.1344221	-3.1168972	6.1781948
H	-3.8733792	-1.3818076	4.3494978
H	0.6013486	-4.6876243	-1.8325375
H	5.0515055	-6.4278329	-0.0721401
H	5.7327654	-4.1077659	1.0186652
H	-1.7417189	-0.0828221	-3.0158889
H	-2.2465073	1.2161169	-2.3274884
H	2.6063984	-0.1459420	-2.4604963
H	2.1245712	1.2800638	-2.8587521
H	3.8781376	-2.2668084	0.5759296

Structure of $U(TTA)_3(OH_2)_2$ with the QM/SPP in the chloroform CPCM solvent obtained using isomer I as the starting structure (Fig. S6d)

Atom	X(Å)	Y(Å)	Z(Å)
C	3.6200195	-1.3633445	2.5910100
C	3.4116583	-2.1754313	1.4792194
S	4.5272940	-3.5203555	1.4996442
C	5.2430415	-2.9860501	2.9683554
C	4.6570275	-1.8253061	3.4327639
C	2.4259272	-1.9766631	0.4345197
O	1.6694775	-0.9159957	0.5394458

U	0.0095915	0.1071954	-0.5560208
O	-0.3957328	1.1981066	1.3932242
C	-0.1665770	2.3627686	1.9062272
C	-0.7194101	2.5205408	3.3250667
F	-0.4952396	3.7528817	3.8519046
O	-0.1589253	0.7218465	-3.0661116
O	2.3787028	0.4151850	-2.1174875
O	0.9815738	2.2308709	-0.7086210
C	1.0699495	3.3157913	0.0051196
C	0.5058909	3.4133983	1.3035302
O	-2.0682059	0.8682835	-1.1188617
C	-3.2800237	0.5385281	-0.7933902
C	-3.6682341	-0.5423442	-0.0210342
C	-2.7384247	-1.4554998	0.5446179
O	-1.4557708	-1.3277914	0.3609594
O	0.4958433	-1.7718103	-1.7951114
C	1.3269697	-2.7509425	-1.6417527
C	2.2770255	-2.8940251	-0.6373358
C	1.7891718	4.4348496	-0.5841659
C	2.3199847	4.5053057	-1.8690692
C	2.9611633	5.7348319	-2.1442738
C	2.9224156	6.6048784	-1.0731798
S	2.1024086	5.9238588	0.2738553
F	-0.1558309	1.6138866	4.1719275
F	-2.0624723	2.3076033	3.3566019
C	-4.3336192	1.4918526	-1.3592495
F	-5.6049292	1.1434729	-1.0358166
F	-4.2652790	1.5449341	-2.7203768
F	-4.1375045	2.7628096	-0.9092173
C	-3.1870470	-2.5707017	1.3515218
S	-2.0034762	-3.6570235	2.0311841
C	-3.2236569	-4.6079718	2.7766764
C	-4.4917760	-4.1214238	2.5216419
C	-4.4744866	-2.9638483	1.7123929
C	1.1981017	-3.8288808	-2.7206153
F	1.4279487	-3.3084077	-3.9609743
F	2.0645942	-4.8626528	-2.5571150
F	-0.0566626	-4.3546340	-2.7435466
H	2.2259228	3.6897216	-2.5831179
H	3.4330216	5.9798140	-3.0945393
H	3.3312074	7.6092662	-1.0036930
H	0.6097268	4.3441852	1.8565738
H	-4.7283775	-0.6942477	0.1593633
H	-2.9460658	-5.4780874	3.3655166
H	-5.3996490	-4.5843794	2.9052323
H	-5.3724259	-2.4327809	1.4014836
H	2.9122860	-3.7769192	-0.6588206
H	6.0559373	-3.5562223	3.4096852
H	4.9666701	-1.3279406	4.3506335
H	0.7704403	0.8326390	-3.3533700
H	-0.6257022	1.5516304	-3.2700791
H	3.0747983	-0.2658904	-2.1061689
H	2.7518498	1.1993980	-1.6729314

H	3.0251921	-0.4709261	2.7732908

Structure of another isomer of $Y(TTA)_3(OH_2)_2$ with the QM/SPP in the chloroform CPCM solvent (Fig. S7a)

Atom	X(Å)	Y(Å)	Z(Å)
Y	0.007642	-0.261945	0.400221
O	-0.480641	1.781652	1.465905
C	-0.716433	2.968511	1.066585
C	-0.978904	3.960868	2.222103
F	-1.172869	5.239947	1.810656
F	-2.082298	3.592199	2.926128
F	0.066423	3.970998	3.091045
C	-0.768434	3.441669	-0.237808
H	-0.992876	4.491335	-0.399936
C	-0.534078	2.602754	-1.362438
O	-0.263711	1.353738	-1.270015
C	-0.598756	3.177612	-2.704984
S	-0.355728	2.128522	-4.072832
C	-0.554347	3.427198	-5.174829
H	-0.483613	3.244946	-6.243926
C	-0.802010	4.623988	-4.530760
H	-0.958845	5.565834	-5.053919
C	-0.827688	4.482590	-3.124338
H	-1.004841	5.310603	-2.440279
O	-2.001465	-0.874364	1.405111
C	-3.021131	-1.559260	1.059615
C	-4.091759	-1.653759	2.170132
F	-3.547394	-2.134893	3.319745
F	-4.597725	-0.423008	2.450509
F	-5.139106	-2.457058	1.854166
C	-3.265195	-2.191288	-0.150811
H	-4.196547	-2.735607	-0.271627
C	-2.339462	-2.157924	-1.232109
O	-1.222134	-1.535106	-1.182551
C	-2.668773	-2.865381	-2.468305
S	-1.552074	-2.790486	-3.800900
C	-2.556508	-3.781443	-4.774468
H	-2.249240	-4.034652	-5.785661
C	-3.709078	-4.160630	-4.114112
H	-4.476248	-4.790974	-4.560658
C	-3.773848	-3.639575	-2.801665
H	-4.601868	-3.828678	-2.120962
O	0.964395	-2.289401	0.873599
C	2.159091	-2.588635	1.197488
C	2.351626	-4.103945	1.440714
F	2.045483	-4.810889	0.319296
F	3.616265	-4.450384	1.797753
F	1.523883	-4.540398	2.427236
C	3.262784	-1.755990	1.347383
H	4.206652	-2.213321	1.628261
C	3.228759	-0.344371	1.151565

O	2.179670	0.310853	0.829832
C	4.462954	0.422919	1.324632
S	4.403723	2.147387	1.091208
C	6.075915	2.305684	1.436423
H	6.542512	3.287084	1.413748
C	6.668323	1.090543	1.721982
H	7.723170	0.978976	1.967686
C	5.749579	0.017720	1.658324
H	6.021665	-1.018635	1.850352
O	0.198723	-0.340952	2.932172
H	0.031965	0.613729	3.082638
H	-0.647987	-0.766150	3.174083
O	1.312179	-0.873206	-1.694055
H	1.293606	-0.044597	-2.211691
H	0.585781	-1.410529	-2.078041

Structure of another isomer of $Y(TTA)_3(OH_2)_2$ with the QM/SPP in the chloroform CPCM solvent (Fig. S7b)

Atom	X(Å)	Y(Å)	Z(Å)
Y	-0.430979	-3.243195	-3.710691
O	0.933740	-1.660702	-2.702192
C	1.962191	-1.732717	-1.963111
C	2.519016	-0.347547	-1.554268
F	1.583185	0.362774	-0.869303
F	2.852099	0.380819	-2.651847
F	3.625677	-0.412667	-0.766473
C	2.615026	-2.870989	-1.495448
H	3.489740	-2.742136	-0.862708
C	2.174109	-4.185584	-1.807394
O	1.150187	-4.434879	-2.531040
C	2.907007	-5.344291	-1.279874
S	4.360426	-5.212153	-0.327882
C	4.490657	-6.914888	-0.173816
H	5.317195	-7.344472	0.385567
C	3.463540	-7.571106	-0.822799
H	3.365050	-8.655085	-0.841417
C	2.565198	-6.678265	-1.451319
H	1.682961	-6.977432	-2.012971
O	1.181742	-3.001733	-5.383813
C	1.522069	-2.005330	-6.099887
C	2.830026	-2.244852	-6.889265
F	2.704278	-3.328698	-7.703567
F	3.862636	-2.499401	-6.042464
F	3.202529	-1.198541	-7.671387
C	0.872184	-0.786538	-6.258423
H	1.322979	-0.047199	-6.913168
C	-0.379699	-0.487877	-5.649821
O	-1.000888	-1.287760	-4.869378
C	-1.023566	0.794010	-5.943257
S	-2.537472	1.157528	-5.164085
C	-2.638690	2.679359	-5.948778

H	-3.487819	3.330426	-5.759474
C	-1.557385	2.912954	-6.775702
H	-1.433573	3.822863	-7.360399
C	-0.637327	1.838911	-6.772986
H	0.277842	1.830071	-7.362055
O	-1.675219	-5.107291	-2.849829
C	-2.481469	-5.223073	-1.870684
C	-2.965830	-6.674772	-1.649457
F	-3.626132	-7.128154	-2.752023
F	-1.911963	-7.509418	-1.446195
F	-3.804339	-6.822323	-0.592648
C	-2.966515	-4.230401	-1.026825
H	-3.656293	-4.518350	-0.237091
C	-2.604670	-2.857571	-1.163956
O	-1.792316	-2.429134	-2.047387
C	-3.180799	-1.857775	-0.257137
S	-4.346295	-2.231297	0.983383
C	-4.425880	-0.594625	1.487651
H	-5.080826	-0.314193	2.308087
C	-3.593771	0.216694	0.740949
H	-3.499056	1.288298	0.907407
C	-2.887128	-0.501169	-0.250531
H	-2.174496	-0.068026	-0.949422
O	-0.193037	-5.313346	-5.029972
H	-0.445952	-6.020025	-4.404033
H	0.732544	-5.472233	-5.288181
O	-2.526574	-3.425986	-5.043926
H	-3.283350	-3.940103	-4.713879
H	-2.844922	-2.517886	-5.204523