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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 3, The Structure, Thermodynamics and Reaction Mechanisms of 8- and 9-Coordinated Binary and Ternary Y – TTA - TBP Complexes Studied by Quantum Chemical Methods

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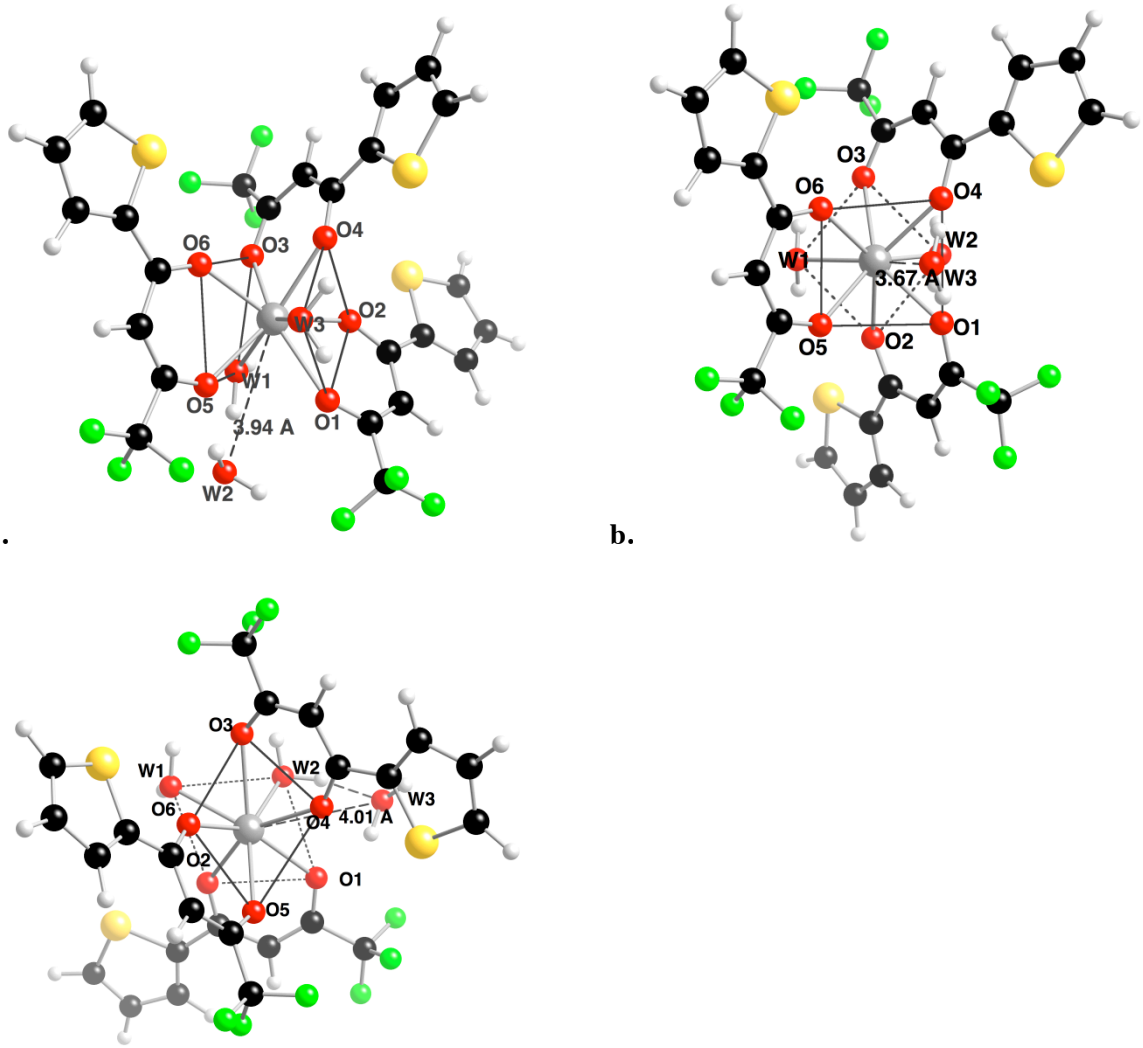
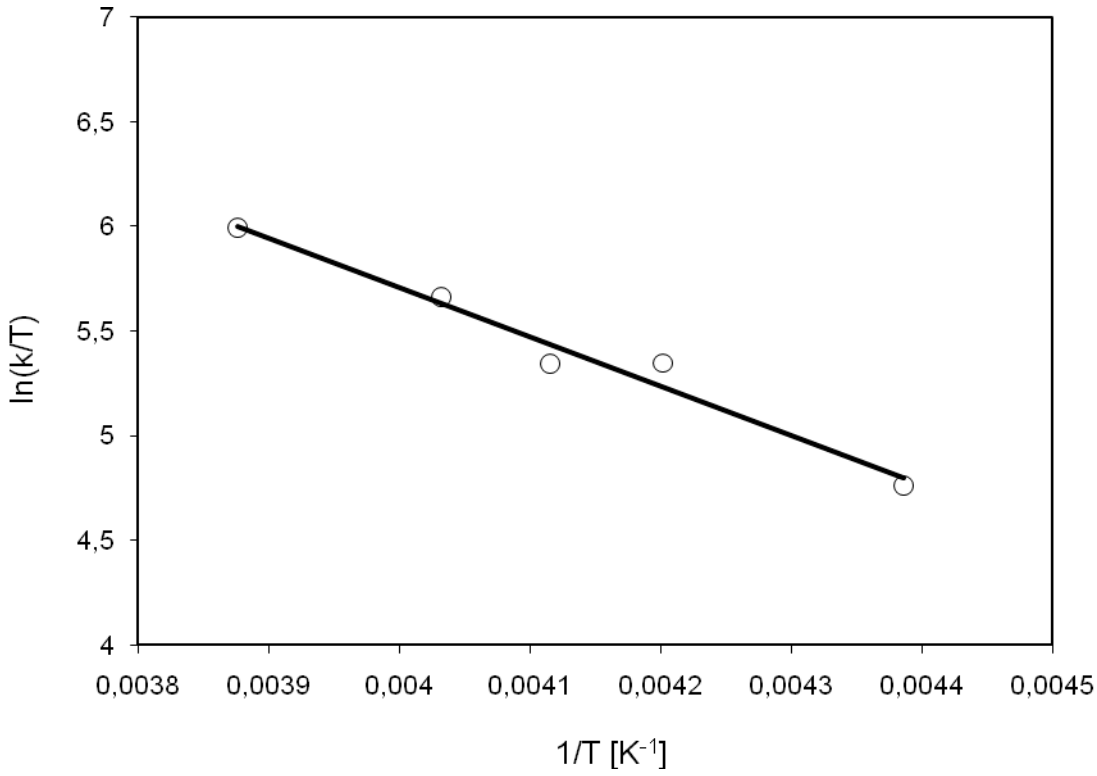
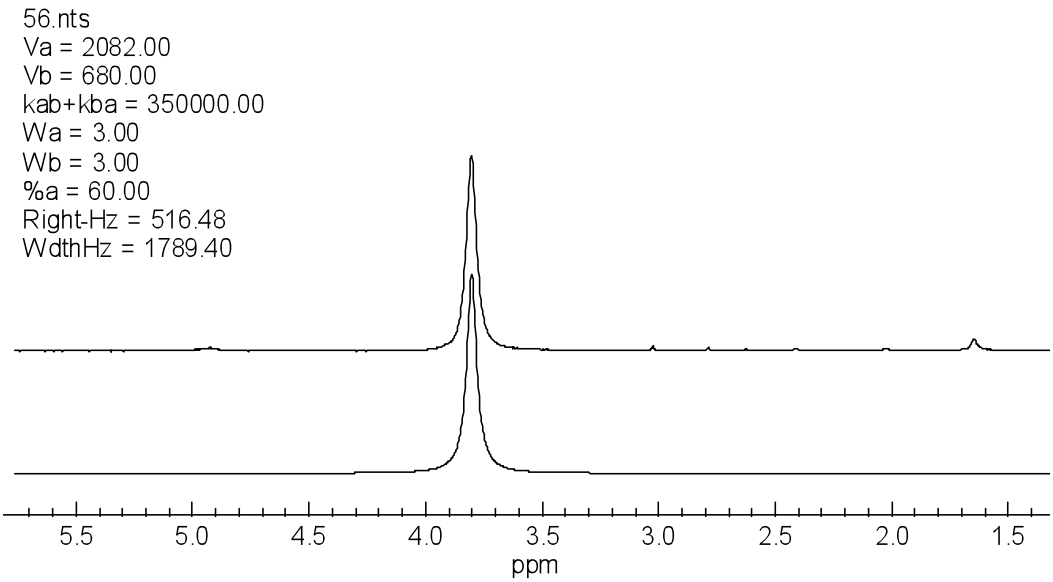


Figure S1. Square anti-prism views of isomers 1 (a), 2 (b), and 3 (c) of $[Y(TTA)_3(OH_2)_2],(H_2O)$.

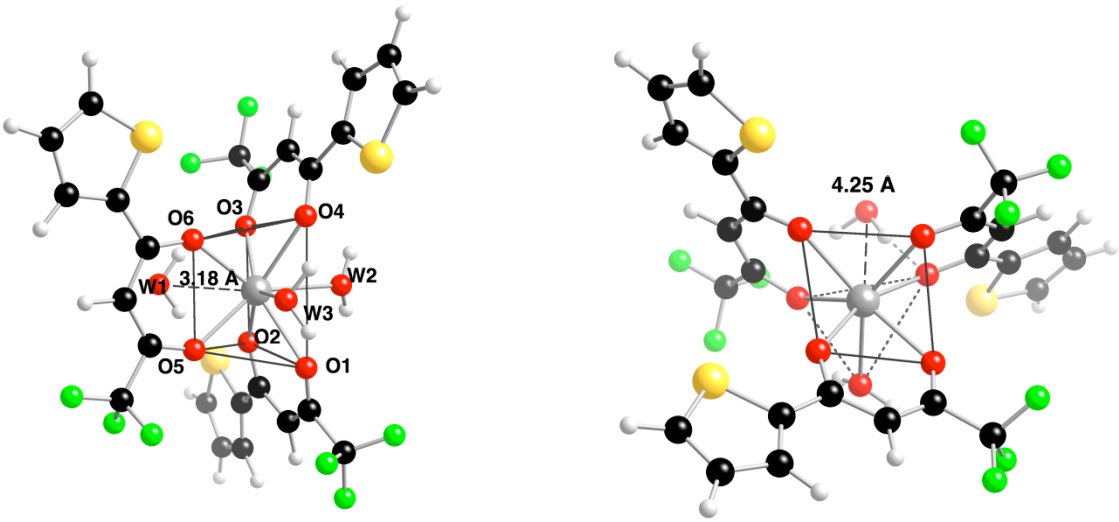


a.



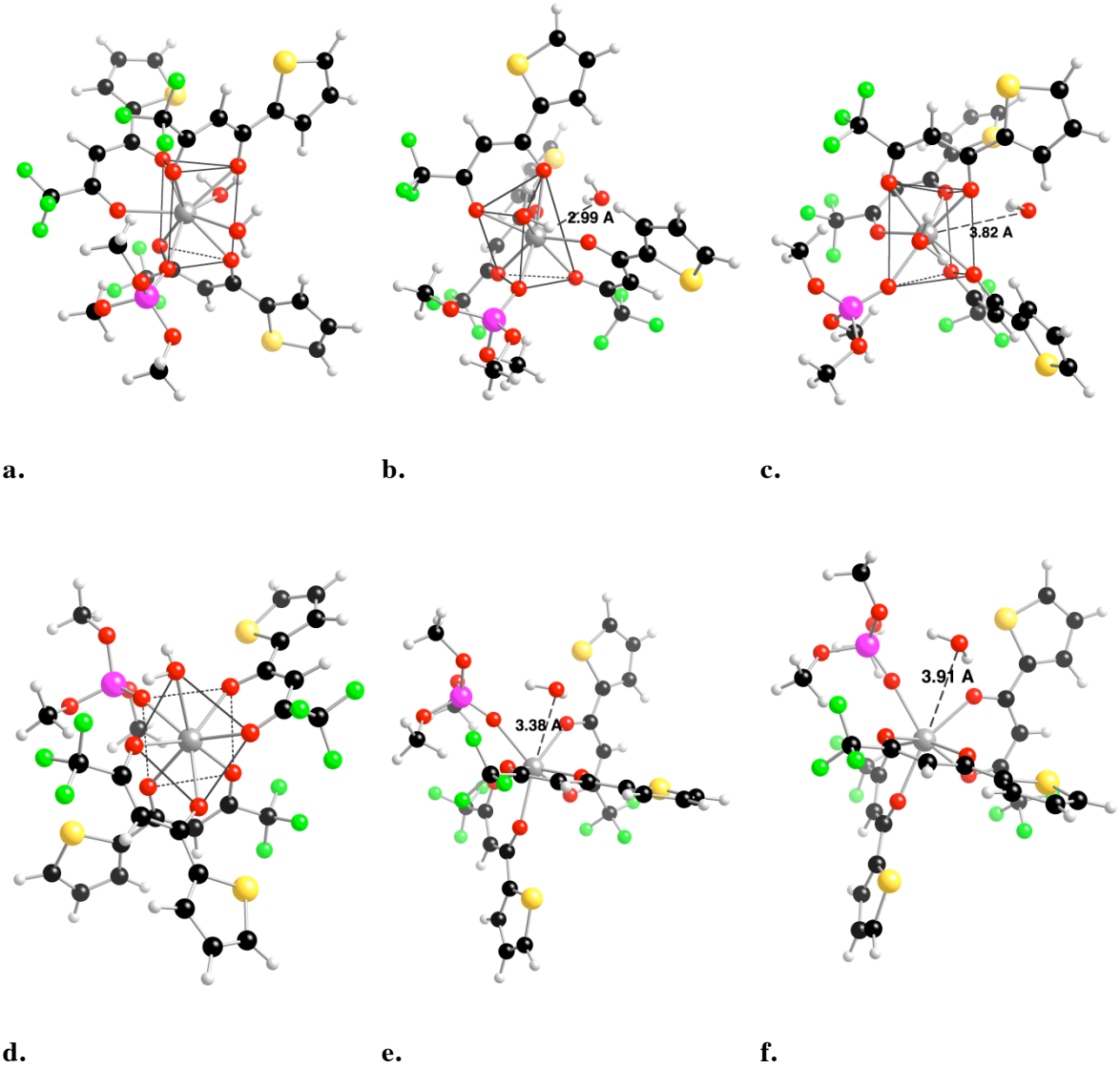
b.

Figure S2. a. Eyring plot of the temperature dependence of the rate constant for the exchange between the coordinated water in $Y(TTA)_3(H_2O)_2$ and free water based on the line shape analysis of the ^1H NMR water signal measured in $CDCl_3$ between 228 and 258 K. (Ref: Figure S3 in Part2). b. Comparison of experimental (top) and fitted (below) ^1H NMR spectra for the water peak in $Y(TTA)_3(OH_2)_2$ using the parameters given at the left side of the diagram.



a. **b.**

Figure S3. (a) The structure of the A-transition state $[Y(TTA)_3(OH_2)_2\ldots(H_2O)]$ where the distance Y – W1 for the entering ligand is 3.18 Å; (b) Structure of the D-transition state $[Y(TTA)_3(OH_2)\ldots(H_2O)]$ where the distance Y-W for the leaving ligand is 4.25 Å.



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

d. **e.** **f.**

Figure S4. Perspective views of the 7, 8, and 9 coordinated isomers in $Y(TTA)_3(TMP)(H_2O)_2$. **a.** $[Y(TTA)_3(TMP)(H_2O)],(H_2O)$; **b.** $[Y(TTA)_3(TMP)(H_2O)_2]^{\neq}$; **c.** $[Y(TTA)_3(TMP)(H_2O)_2]$; **d.** $[Y(TTA)_3(TMP)(H_2O)]$; **e.** $[Y(TTA)_3(TMP)(H_2O)]^{\neq}$; **f.** $[Y(TTA)_3(TMP)],(H_2O)$.

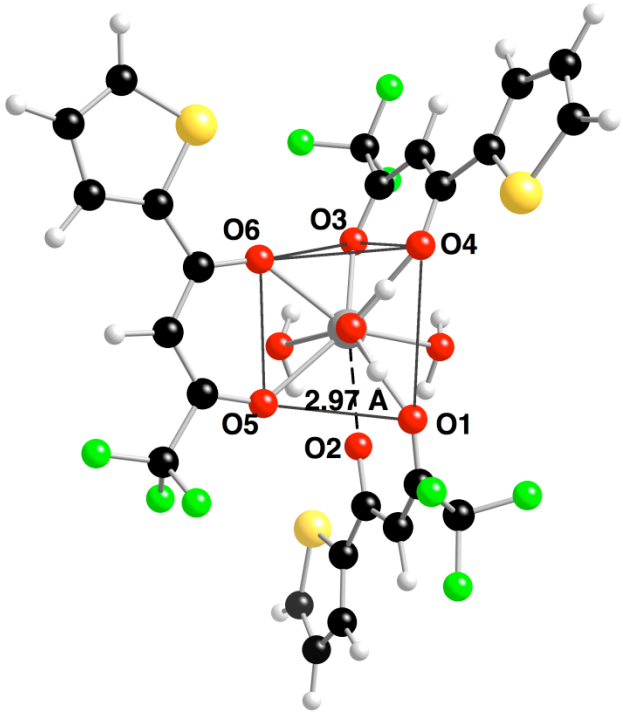


Figure S5. Perspective view of the ring-opening transition state in $[Y(TTA)_2(TTA\text{-open})(OH_2)_3]^{\neq}$.

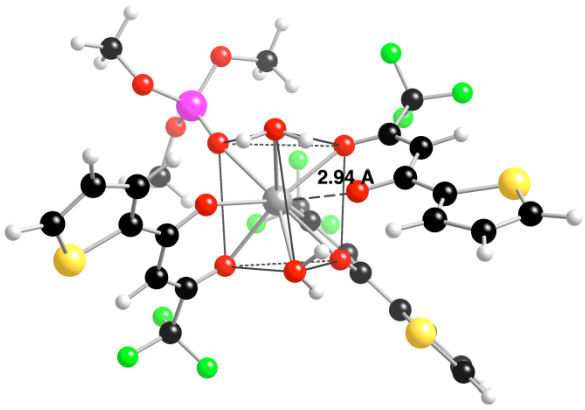


Figure S6. Perspective view of the ring-opening transition state in $[Y(TTA)_2(TTA\text{-}open)(TMP)(OH_2)_2]^{\neq}$.

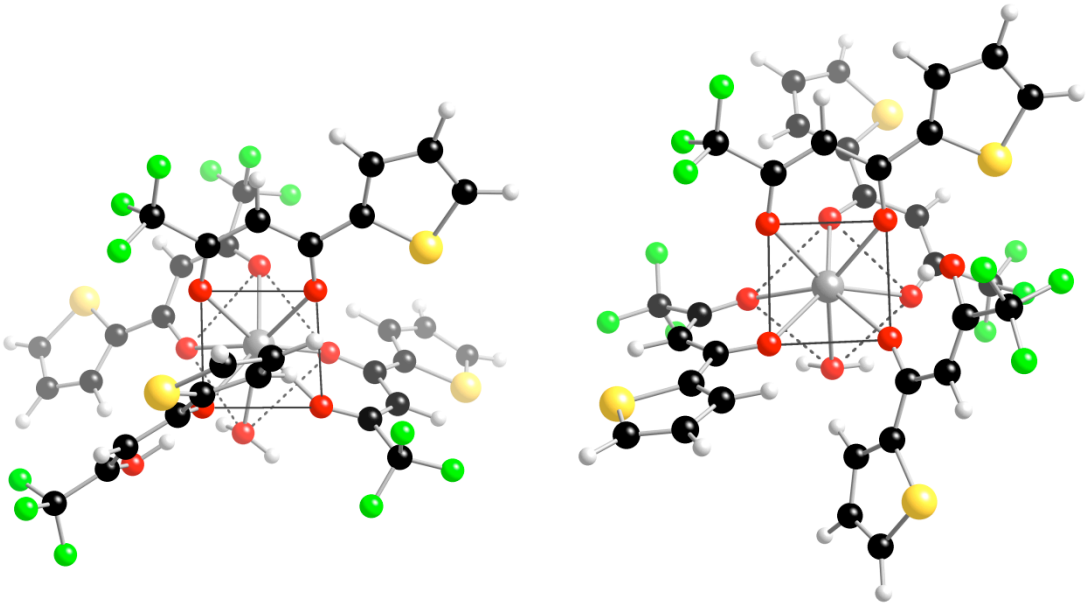


Figure S7. Perspective views of the triclinic isomers (Isomer I configuration of the TTA ligands) (a) $[Y(TTA)_3(HTTA)(OH_2), H_{in}]$, (b) $[Y(TTA)_3(HTTA\text{-flip})(OH_2), H_{in}]$.

$[La(TTA)_3(H_2O)_2],(H_2O)$, isomer 1 optimized with the QM/SPP in the chloroform CPCM solvent (Table 2)

Atom	X(Å)	Y(Å)	Z(Å)
La	-0.4753716	-0.1132728	0.1357599
O	0.8263603	1.4722801	1.5912245
C	1.7502755	1.4718697	2.4690434
C	2.2723248	2.7685365	2.9057975
S	1.6032642	4.2229415	2.1722171
C	2.6427553	5.2238846	3.1328013
H	2.5938549	6.3045084	3.0270924
C	3.4564563	4.4873974	3.9686454
H	4.1778614	4.9351890	4.6504124
C	3.2460132	3.0923886	3.8405777
H	3.7923041	2.3493683	4.4192757
C	2.2894977	0.2814555	3.0504535
H	3.0991970	0.3742379	3.7686793
C	1.8041389	-0.9895334	2.7851339
O	0.8590186	-1.3444931	1.9916545
C	2.4468006	-2.1765884	3.5431489
F	2.8811575	-3.1266647	2.6694426
F	1.5302411	-2.7737032	4.3591424
F	3.5078174	-1.8288754	4.3187518
O	-2.2582161	-1.5486388	1.3084830
H	-2.9564384	-1.2209954	1.8996726
H	-1.8877095	-2.4105685	1.6859933
O	1.6611439	0.2059523	-1.3682489
H	1.4529771	1.0462193	-1.8282262
H	2.0462433	-0.3974269	-2.0263914
O	-0.7896350	-3.5930067	2.0969492
H	-0.6094429	-4.1419123	1.3108703
H	-0.0242919	-2.9624547	2.1291119
O	-2.3695842	1.3829193	0.7179644
C	-2.7439702	2.5440422	0.3474134
C	-4.0318443	3.0141328	1.0706473
F	-3.8393846	3.0459160	2.4193714
F	-5.0585641	2.1503542	0.8329948
F	-4.4582650	4.2531955	0.6987230
C	-2.1707671	3.4046200	-0.5818132
H	-2.6636881	4.3576476	-0.7513496
C	-0.9830901	3.1244815	-1.3229004
O	-0.3057460	2.0464262	-1.2192419
C	-0.5002848	4.1362478	-2.2697845
S	0.9534629	3.7839702	-3.1987449
C	0.8631491	5.3201613	-3.9989031
H	1.6165511	5.5866466	-4.7352448
C	-0.2202329	6.0610941	-3.5779841
H	-0.4509397	7.0538125	-3.9614479
C	-0.9939155	5.3902774	-2.5975793
H	-1.8870315	5.8194148	-2.1467137
O	-0.0179765	-2.4356519	-0.7529172
C	-0.4209911	-3.1254780	-1.7474446
C	-1.3050758	-2.7773622	-2.7611580
C	-1.9470481	-1.5016566	-2.8348481
O	-1.7603316	-0.5634355	-1.9916180
C	0.1940729	-4.5465266	-1.7757860
F	-0.0867460	-5.2087810	-0.6067103
F	1.5492868	-4.4884164	-1.8788664
F	-0.2545946	-5.3329362	-2.7885816
H	-1.5235191	-3.5172380	-3.5262597
C	-2.8784379	-1.2446179	-3.9373280
S	-3.6589200	0.3321492	-4.0127647

C	-4.5142710	-0.1241014	-5.4504226
H	-5.1898115	0.5858000	-5.9205020
C	-4.2197829	-1.4108195	-5.8506911
H	-4.6573154	-1.8799964	-6.7306306
C	-3.2905368	-2.0479036	-4.9912684
H	-2.9373302	-3.0667151	-5.1422984

$[La(TTA)_3(H_2O)_2],(H_2O)$, isomer 3 optimized with the QM/SPP in the chloroform CPCM solvent (Table 2)

Atom	X(Å)	Y(Å)	Z(Å)
S	0.6875831	2.0405424	4.5858920
C	1.9832544	1.1363326	3.8082622
C	3.1327469	1.1587805	4.5850928
C	2.9805092	1.8900882	5.7894053
C	1.7161662	2.4233402	5.9286171
C	1.7065138	0.5080353	2.5135646
C	2.7436369	-0.2217859	1.8638625
C	2.5654247	-0.8643260	0.6407764
O	1.5229566	-0.9223520	-0.0849487
La	-0.7988687	0.0099560	0.0258416
O	0.5286798	0.6528208	2.0336860
O	0.0860858	1.7741849	-1.4905832
C	0.0456078	3.0409103	-1.6612587
C	-0.7497829	3.9273439	-0.8732263
C	-1.5937161	3.5101047	0.1512530
O	-1.8062600	2.3314324	0.5897880
C	0.8667710	3.5974193	-2.7382247
S	1.8545371	2.4880816	-3.6854120
C	2.4554536	3.7972319	-4.6497456
C	1.9325711	5.0154824	-4.2677188
C	1.0297290	4.9026683	-3.1821105
C	-2.4327390	4.5875460	0.8835005
F	-3.7666560	4.3341917	0.7283921
F	-2.2146335	5.8569827	0.4459918
F	-2.1790133	4.5738003	2.2206114
O	-1.3516628	-2.3501519	0.6495968
C	-1.1193302	-3.5130837	0.1751867
C	-1.3304896	-4.6577100	1.0630311
S	-1.8353125	-4.3413010	2.7208628
C	-1.8579660	-6.0387654	3.0727311
C	-1.4984627	-6.8051947	1.9837130
C	-1.1992085	-6.0217127	0.8421109
O	-0.8003424	-1.5173414	-2.0600121
C	-0.5692232	-2.7773333	-2.1407609
C	-0.1264973	-3.2265414	-3.5553781
F	1.0205148	-2.5953156	-3.9232834
O	-3.0453931	0.4069659	-1.3235755
O	-2.6315760	0.1471169	1.9036139
C	-0.6775135	-3.7544677	-1.1624002
F	0.0942719	-4.5634498	-3.6700705
F	-1.0769499	-2.8970179	-4.4799808
C	3.7701767	-1.6339304	0.0398055
F	4.0964841	-1.1400654	-1.1854279
F	4.8978054	-1.5772086	0.8062387
F	3.4667301	-2.9514187	-0.1236968
H	3.7170820	-0.2862922	2.3417465
H	4.0590987	0.6634859	4.2986398
H	3.7706520	2.0202569	6.5274024
H	1.3281966	3.0237225	6.7473106
H	3.1666028	3.5933685	-5.4460269
H	2.1898691	5.9564757	-4.7515571

H	0.5156234	5.7549180	-2.7406894
H	-0.7111787	4.9902561	-1.0948929
H	-0.4516299	-4.7773327	-1.4500182
H	-0.8982222	-6.4479322	-0.1134061
H	-1.4521739	-7.8928901	2.0056263
H	-2.1355225	-6.3763407	4.0678327
H	-3.5183378	1.2374271	-1.1439101
H	-2.9102131	0.3611514	-2.3213274
H	-3.4442366	-0.3776003	2.0001932
H	-2.8871884	1.0926358	1.9054588
H	-1.5990356	-0.6115748	-3.4615148
O	-2.2832707	0.0033885	-3.8316525
H	-1.7834370	0.7132374	-4.2707873

$[La(TTA)_3(H_2O)_3]$ optimized with the QM/SPP in the chloroform CPCM solvent (Table 2)

Atom	X(Å)	Y(Å)	Z(Å)
S	0.0803811	4.0824955	2.8413588
C	0.6791805	2.6317567	3.6401103
C	1.0884419	2.9180436	4.9341187
C	0.9260453	4.2819543	5.2851097
C	0.3935319	5.0328758	4.2584545
C	0.6724079	1.3744897	2.8828303
C	1.1542392	0.1914864	3.5182678
C	1.1953266	-1.0544233	2.8975461
O	0.8395630	-1.3788355	1.7207051
La	-0.1038473	-0.1446457	-0.2361336
O	0.2289411	1.4181548	1.6862096
O	0.5661622	1.9450812	-1.5791222
C	0.0772832	3.0849099	-1.8887358
C	-1.2633781	3.4878201	-1.6064912
C	-2.2164393	2.6701738	-1.0115802
O	-2.1067959	1.4649730	-0.6049441
C	0.9541613	4.0282275	-2.5895473
S	2.5745487	3.4935549	-3.0253602
C	2.9351914	5.0363492	-3.7300546
C	1.8731716	5.9108253	-3.6396674
C	0.7487098	5.3396159	-2.9932934
C	-3.6453972	3.2398377	-0.8255563
F	-4.5393718	2.5291676	-1.5770652
F	-3.7763988	4.5463894	-1.1796139
F	-4.0438112	3.1323787	0.4714671
O	-1.1861089	-2.4947644	-0.4756304
C	-0.8195009	-3.6662282	-0.8324271
C	-1.7475721	-4.7733917	-0.5770181
S	-3.3104341	-4.4019021	0.1447323
C	-3.7590458	-6.0772636	0.1304975
C	-2.7669911	-6.8760177	-0.3964911
C	-1.6260443	-6.1372922	-0.7987638
O	1.3802968	-1.7494631	-1.5614756
C	1.3799372	-3.0035720	-1.7948496
C	2.6448668	-3.4736822	-2.5572948
F	3.7740066	-3.0781397	-1.9057457
O	-1.3578074	-0.4420550	-2.6229952
O	-2.3100614	-0.5866445	1.1828976
C	0.4194649	-3.9574768	-1.4802134
F	2.7275214	-4.8213532	-2.7217306
F	2.6853591	-2.9139234	-3.8013648
C	1.7428941	-2.2538627	3.7136723
F	2.8246186	-2.8047691	3.0953694
F	2.1298389	-1.9332087	4.9816458
F	0.8012658	-3.2330196	3.8216250

H	1.5084743	0.2613788	4.5428727
H	1.4944753	2.1699988	5.6130806
H	1.1907384	4.6967270	6.2566753
H	0.1652798	6.0954865	4.2534052
H	3.9110193	5.2064074	-4.1769400
H	1.9022969	6.9288085	-4.0250908
H	-0.1813470	5.8799816	-2.8254579
H	-1.5709866	4.4874343	-1.9003886
H	0.6212330	-4.9867699	-1.7631351
H	-0.7400577	-6.5976177	-1.2326479
H	-2.8562743	-7.9572723	-0.4893627
H	-4.7317876	-6.3751862	0.5123527
H	-2.1348860	0.1420395	-2.6895457
H	-1.6820662	-1.3326264	-2.8456197
H	-2.6075717	-1.4693931	0.8849428
H	-2.9416920	0.0645748	0.8151788
O	2.5217945	0.4200333	-0.3703587
H	2.5130653	1.2059035	-0.9541363
H	2.8226149	-0.3232874	-0.9336093

$[La(TTA)_3(H_2O)_2]$ optimized with the QM/SPP in the chloroform CPCM solvent (Table 2)

Atom	X(Å)	Y(Å)	Z(Å)
S	0.7470744	2.5740084	-3.9296753
C	-0.4253917	3.4334577	-2.9358958
C	-0.6798073	4.6949505	-3.4563103
C	0.0537498	4.9717677	-4.6361490
C	0.8651740	3.9216604	-5.0133020
C	-0.9561903	2.7543605	-1.7519946
C	-1.8977428	3.4461958	-0.9276745
C	-2.4994186	2.8928064	0.1954145
C	-3.5323756	3.7514996	0.9654104
F	-3.7305570	4.9905953	0.4400621
O	-0.5494376	1.5652664	-1.5272048
La	-0.7419116	-0.2053811	0.2077873
O	-2.3352610	1.7349413	0.7101011
O	-1.1722260	-2.5980049	-0.5347024
C	-0.4929585	-3.5978970	-0.9647114
C	0.8935993	-3.5388827	-1.2834251
C	1.6564583	-2.3769499	-1.1929866
C	3.1453085	-2.4482288	-1.6213327
F	3.5420078	-3.6838990	-2.0367562
C	-1.2047205	-4.8660671	-1.1400778
S	-2.8994272	-4.9442169	-0.6648606
C	-2.9964553	-6.6059559	-1.1525188
C	-1.7982037	-7.0751877	-1.6473493
C	-0.7809747	-6.0884192	-1.6409096
O	1.3045108	-1.2184944	-0.8021472
O	-2.9287732	-0.6807165	-1.2502979
O	-2.7551105	-0.6541003	1.8993256
O	0.9159332	1.2769619	1.3443697
C	1.6986244	1.2675121	2.3528701
C	1.7271786	0.2201763	3.3253035
C	0.8808662	-0.8798797	3.2814025
C	0.9745420	-1.9223008	4.4217995
F	1.9046844	-1.6257803	5.3699974
O	-0.0109999	-1.1719816	2.4140857
F	3.3899708	-1.5840990	-2.6454224
F	3.9594231	-2.0919409	-0.5903887
C	2.6040551	2.4071195	2.5143394
C	3.5539200	2.6874852	3.4867051
C	4.2306664	3.9132706	3.2707174

C	3.7955234	4.5647405	2.1352686
S	2.5489317	3.6887427	1.3081159
F	-0.2265390	-2.0369137	5.0619523
F	1.2818521	-3.1535468	3.9286010
F	-3.1475906	3.9215545	2.2615154
F	-4.7471514	3.1280820	0.9898762
H	2.4260133	0.2955641	4.1536769
H	3.7596967	2.0310877	4.3306399
H	5.0090269	4.3034849	3.9247104
H	4.1388334	5.5151376	1.7350468
H	1.5307990	3.8632330	-5.8705081
H	-0.0111341	5.9076640	-5.1890496
H	-1.3740283	5.4014108	-3.0042090
H	-2.1770061	4.4593590	-1.2031491
H	1.3823934	-4.4424972	-1.6365011
H	0.2311251	-6.2710978	-1.9980767
H	-1.6557280	-8.0943855	-2.0032523
H	-3.9339244	-7.1439035	-1.0395519
H	-3.8183954	-0.3304197	-1.0719785
H	-2.9993130	-1.6560389	-1.2211208
H	-2.4257447	-0.9597181	2.7649731
H	-3.0947690	0.2554543	2.0324215

$[Eu(TTA)_3(H_2O)_2],(H_2O)$, isomer 1 optimized with the QM/SPP in the chloroform CPCM solvent (Table 2)

Atom	X(Å)	Y(Å)	Z(Å)
Eu	-0.3503848	0.0806951	0.1352888
O	0.6422775	1.4796808	1.7712236
C	1.5168695	1.4242777	2.6981893
C	1.9482273	2.6891059	3.2960808
S	1.2489818	4.1849881	2.6844958
C	2.1832529	5.1183340	3.8072049
H	2.0862896	6.2008172	3.8150892
C	2.9846342	4.3299910	4.6067620
H	3.6436923	4.7307113	5.3753606
C	2.8518212	2.9498468	4.3170898
H	3.4014591	2.1721957	4.8447529
C	2.0796946	0.2039934	3.1797798
H	2.8305145	0.2487324	3.9633059
C	1.6853238	-1.0462413	2.7243726
O	0.8310453	-1.3384540	1.8166285
C	2.3178242	-2.2878046	3.4021461
F	2.8134663	-3.1463639	2.4689151
F	1.3766885	-2.9715783	4.1147413
F	3.3330189	-1.9924515	4.2564524
O	-2.0519394	-1.3555423	1.2403861
H	-2.9609214	-1.3594283	0.8961921
H	-1.7532881	-2.3115784	1.3254218
O	2.0734130	0.2856118	-0.6559218
H	2.0839638	0.9913370	-1.3298328
H	2.2106369	-0.5537207	-1.1382628
O	-0.6900278	-3.6258492	1.5244705
H	-0.4650031	-4.1415412	0.7299583
H	0.0697027	-2.9990357	1.6438561
O	-2.1244862	1.6004763	0.6250030
C	-2.4985233	2.6973594	0.1082268
C	-3.7664250	3.2867121	0.7818714
F	-3.5423648	3.5219074	2.1034253
F	-4.8044698	2.4085098	0.6994651
F	-4.1907369	4.4589335	0.2315452
C	-1.9279575	3.4131742	-0.9446214

H	-2.4093634	4.3373724	-1.2515959
C	-0.7468096	3.0024173	-1.6287588
O	-0.0951554	1.9367107	-1.3543062
C	-0.2368132	3.8402526	-2.7181482
S	1.1848915	3.2877241	-3.5983147
C	1.1539508	4.6981956	-4.6075325
H	1.9069867	4.8204283	-5.3814383
C	0.1120885	5.5431231	-4.2894514
H	-0.0773306	6.4811505	-4.8089864
C	-0.6780603	5.0568912	-3.2178415
H	-1.5426021	5.5885096	-2.8238732
O	0.4513424	-1.8695926	-1.1045759
C	-0.0204768	-2.5894735	-2.0481959
C	-1.1933065	-2.4239304	-2.7707079
C	-2.0920497	-1.3384348	-2.5310792
O	-1.9070070	-0.4560187	-1.6297226
C	0.8677082	-3.8157565	-2.3701768
F	0.8817459	-4.6759162	-1.3030252
F	2.1551287	-3.4418598	-2.5955761
F	0.4593117	-4.5316082	-3.4502490
H	-1.4300591	-3.1442936	-3.5484843
C	-3.2981849	-1.2232247	-3.3546134
S	-4.4045304	0.1096920	-3.0382014
C	-5.4617548	-0.4252022	-4.3036530
H	-6.3719375	0.1310658	-4.5118875
C	-4.9945172	-1.5596240	-4.9339887
H	-5.5175666	-2.0476111	-5.7549510
C	-3.7655688	-2.0140056	-4.3952588
H	-3.2412065	-2.8950146	-4.7616894

$[Eu(TTA)_3(H_2O)_2],(H_2O)$, isomer 3 optimized with the QM/SPP in the chloroform CPCM solvent (Table 2)

Atom	X(Å)	Y(Å)	Z(Å)
S	0.5639781	2.0319937	4.4540790
C	1.8848352	1.2576520	3.5854726
C	3.0639771	1.3308714	4.3146979
C	2.9138782	2.0009505	5.5536126
C	1.6218092	2.4346791	5.7675426
C	1.6015928	0.6624135	2.2777363
C	2.6580433	0.0205431	1.5654091
C	2.4497657	-0.6069491	0.3360781
O	1.3694999	-0.7263429	-0.3164376
Eu	-0.8945728	0.0477064	-0.0160865
O	0.4049924	0.7396338	1.8394691
O	-0.0768529	1.5655512	-1.6526027
C	-0.1029260	2.8080220	-1.9539997
C	-0.7558599	3.8041256	-1.1705110
C	-1.5361408	3.4981336	-0.0584183
O	-1.7794678	2.3583230	0.4524492
C	0.5635283	3.2044752	-3.1968279
S	1.3481491	1.9482491	-4.1525615
C	1.8066868	3.1078322	-5.3588795
C	1.3924604	4.3840828	-5.0423298
C	0.6826879	4.4395436	-3.8166227
C	-2.2453312	4.6647262	0.6760404
F	-3.5963754	4.4668872	0.6897205
F	-2.0266238	5.8866089	0.1183340
F	-1.8400359	4.7365246	1.9733046
O	-1.1420611	-2.0598025	1.0796687
C	-0.9120635	-3.2816690	0.7946271
C	-0.9400443	-4.2446947	1.8984391

S	-1.2281694	-3.6362919	3.5260894
C	-1.1198099	-5.2390562	4.1785978
C	-0.8766127	-6.1867557	3.2062441
C	-0.7755200	-5.6227827	1.9105600
O	-0.9825674	-1.7085907	-1.7404187
C	-0.7241162	-2.9606482	-1.6575105
C	-0.5171470	-3.6426091	-3.0320491
F	0.3737711	-2.9476642	-3.7895689
O	-2.9665314	0.3844151	-1.4510897
O	-2.7733945	0.2598472	1.6594072
C	-0.6511663	-3.7594669	-0.5263257
F	-0.0661511	-4.9218891	-2.9504338
F	-1.6929234	-3.6735391	-3.7273014
C	3.6712928	-1.2562579	-0.3676369
F	3.8911826	-0.6777692	-1.5796327
F	4.8315108	-1.1534266	0.3418452
F	3.4534829	-2.5815534	-0.5858823
H	3.6556237	0.0069400	1.9949171
H	4.0094828	0.9163279	3.9688476
H	3.7246971	2.1596934	6.2629302
H	1.2288475	2.9720081	6.6266815
H	2.3665091	2.7802859	-6.2308609
H	1.5902637	5.2508599	-5.6710800
H	0.2706759	5.3593675	-3.4048018
H	-0.6853962	4.8428167	-1.4807702
H	-0.4288591	-4.8138606	-0.6630370
H	-0.5889101	-6.2122306	1.0144243
H	-0.7748000	-7.2500926	3.4176663
H	-1.2409426	-5.3918034	5.2478376
H	-3.3568117	1.2710371	-1.3625081
H	-2.7329480	0.2772773	-2.4234931
H	-3.6007069	-0.2498203	1.6771400
H	-3.0095023	1.2080591	1.5934517
H	-1.4292143	-0.8726647	-3.3119241
O	-1.9513947	-0.2253087	-3.8523853
H	-1.2920938	0.4138495	-4.1789558

$[Eu(TTA)_3(H_2O)_3]$ optimized with the QM/SPP in the chloroform CPCM solvent (Table 2)

Atom	X(Å)	Y(Å)	Z(Å)
S	0.4993521	4.0158985	2.7042628
C	1.3323817	2.5833873	3.2988177
C	2.0235180	2.8667045	4.4688056
C	1.8911345	4.2145903	4.8844386
C	1.0987270	4.9556001	4.0327623
C	1.2065449	1.3387127	2.5343217
C	1.8812651	0.1730521	3.0141324
C	1.8096548	-1.0630762	2.3744421
O	1.1636244	-1.3816806	1.3297018
Eu	-0.1571458	-0.1697060	-0.2278053
O	0.4907315	1.3649430	1.4808829
O	0.2589477	1.8501238	-1.6051736
C	-0.2359314	3.0167843	-1.7655996
C	-1.4793669	3.4397579	-1.2043640
C	-2.3234610	2.6017944	-0.4867369
O	-2.1644318	1.3717704	-0.1845511
C	0.5161389	3.9681578	-2.5899564
S	1.9886014	3.4103377	-3.3786923
C	2.2556999	4.9770670	-4.0720927
C	1.2706652	5.8759705	-3.7223418
C	0.2827506	5.3042574	-2.8822758
C	-3.6803678	3.1746882	-0.0060541

F	-4.7128319	2.5403194	-0.6375207
F	-3.8329606	4.5075119	-0.2297221
F	-3.8459580	2.9696101	1.3296541
O	-1.2842330	-2.4311866	-0.1637026
C	-1.0238836	-3.6082570	-0.5862748
C	-1.8579873	-4.7122795	-0.0997834
S	-3.1919736	-4.3395331	0.9875887
C	-3.6268282	-6.0153267	1.0905211
C	-2.7967581	-6.8152609	0.3346756
C	-1.7935438	-6.0769896	-0.3414903
O	0.8991386	-1.6883633	-1.8289742
C	0.8625671	-2.9406772	-2.0578100
C	1.9073351	-3.3965191	-3.1086468
F	3.1546188	-2.9740838	-2.7594256
O	-1.8201803	-0.4096637	-2.2414470
O	-1.8545711	-0.5618189	1.6535669
C	0.0178029	-3.9045614	-1.5178183
F	1.9726285	-4.7445913	-3.2775559
F	1.6272090	-2.8511757	-4.3270329
C	2.6244668	-2.2414008	2.9698935
F	3.5525064	-2.6820040	2.0772480
F	3.2878685	-1.9259936	4.1175059
F	1.8090051	-3.2929378	3.2561321
H	2.4826363	0.2500993	3.9153770
H	2.6099679	2.1283039	5.0129174
H	2.3606702	4.6260246	5.7766299
H	0.8306196	6.0059900	4.1103702
H	3.1232912	5.1415368	-4.7054117
H	1.2593299	6.9115175	-4.0588102
H	-0.5707038	5.8614774	-2.4997803
H	-1.8064828	4.4605749	-1.3807502
H	0.1503259	-4.9338449	-1.8389451
H	-1.0434237	-6.5376122	-0.9820292
H	-2.9051128	-7.8968048	0.2698027
H	-4.4727041	-6.3126215	1.7044793
H	-2.5846337	0.1223542	-1.9486299
H	-2.1671044	-1.3077662	-2.3853279
H	-2.1727131	-1.4415486	1.3596528
H	-2.5388261	0.0862504	1.3855230
O	2.3323767	0.3590641	-0.7924303
H	2.1267951	1.1391528	-1.3508619
H	2.4708657	-0.3773842	-1.4233489

$[Eu(TTA)_3(H_2O)_2]$ optimized with the QM/SPP in the chloroform CPCM solvent (Table 2)

Atom	X(Å)	Y(Å)	Z(Å)
S	2.0804706	2.5039855	-3.3846863
C	0.7758760	3.4534664	-2.6790750
C	0.8087490	4.7598883	-3.1475228
C	1.8653149	4.9996303	-4.0599073
C	2.6350796	3.8770604	-4.2852282
C	-0.1330942	2.7927620	-1.7412527
C	-1.1949026	3.5457866	-1.1563891
C	-2.1329196	2.9933077	-0.2899629
C	-3.2855032	3.9019323	0.2072718
F	-3.1952012	5.1951042	-0.2038703
O	0.0724566	1.5543781	-1.5004299
Eu	-0.6346506	-0.1487652	-0.0462288
O	-2.2096314	1.8018624	0.1555751
O	-1.2593108	-2.4117488	0.5959807
C	-0.9932360	-3.5741021	0.1371622
C	-0.4550247	-3.8181165	-1.1622925

C	-0.2034629	-2.8073080	-2.0895583
C	0.2773110	-3.2213557	-3.5054206
F	0.4710158	-4.5625545	-3.6516434
C	-1.2815349	-4.7230824	1.0022485
S	-1.9167415	-4.4116866	2.6149972
C	-1.9857685	-6.1115624	2.9550188
C	-1.5440316	-6.8738244	1.8946299
C	-1.1438828	-6.0864917	0.7859427
O	-0.3442886	-1.5529920	-1.9556090
O	-2.9449498	-0.4254135	-1.1501909
O	-2.0947129	-0.1998750	2.0210027
O	0.5037557	1.2143141	1.5588235
C	1.6222010	1.2327216	2.1732112
C	2.6354809	0.2421337	2.0033345
C	2.4777271	-0.8324668	1.1366517
C	3.6317441	-1.8606232	1.0236716
F	4.7100273	-1.5608094	1.8018591
O	1.4828047	-1.1159529	0.3931643
F	-0.6366860	-2.8449210	-4.4456913
F	1.4499659	-2.6108262	-3.8174026
C	1.8625892	2.3421402	3.1008937
C	2.9613874	2.6433820	3.8926329
C	2.7913394	3.8226326	4.6602185
C	1.5646137	4.4175053	4.4525271
S	0.5936668	3.5444357	3.3112320
F	3.2075905	-3.1018677	1.3905562
F	4.0761883	-1.9491276	-0.2589242
F	-3.3399227	3.9162825	1.5682993
F	-4.4882157	3.4240585	-0.2327241
H	3.5608229	0.3271752	2.5654582
H	3.8643088	2.0356245	3.9210689
H	3.5427406	4.2201872	5.3407939
H	1.1730172	5.3239060	4.9067359
H	3.5015033	3.7775798	-4.9338134
H	2.0545180	5.9612574	-4.5344762
H	0.0941809	5.5237106	-2.8452456
H	-1.2952659	4.5951397	-1.4190883
H	-0.2690631	-4.8450326	-1.4640348
H	-0.7673545	-6.5109302	-0.1432064
H	-1.5084068	-7.9620277	1.9133299
H	-2.3457672	-6.4508556	3.9226526
H	-3.5891955	0.2605357	-0.8999080
H	-3.4473398	-1.2301180	-1.3610055
H	-2.6588307	-0.9939208	2.0342533
H	-2.6845615	0.5740379	1.9292850

$[Y(TTA)_3(H_2O)_2],(H_2O)$, isomer 1 optimized with the QM/SPP in the chloroform CPCM solvent (Table 1, Table 2, Table 3)

Atom	X(Å)	Y(Å)	Z(Å)
Y	-0.3385234	-0.0348768	0.1297740
O	0.5472867	1.4753960	1.6682359
C	1.4579340	1.4874389	2.5608591
C	1.8195093	2.7815367	3.1401773
S	0.9957356	4.2206840	2.5476556
C	1.9055379	5.2248190	3.6285322
H	1.7341129	6.2980642	3.6350731
C	2.7898893	4.5003433	4.4008864
H	3.4487759	4.9518784	5.1409475
C	2.7413130	3.1121235	4.1241034
H	3.3631589	2.3781488	4.6339761
C	2.1225660	0.3114477	3.0265917

H	2.9053167	0.4128385	3.7727124
C	1.7807154	-0.9647286	2.6111014
O	0.8894110	-1.3229768	1.7591389
C	2.5429506	-2.1565209	3.2365890
F	3.1746240	-2.8809528	2.2697669
F	1.6791045	-3.0024467	3.8672696
F	3.4852165	-1.7931122	4.1458970
O	-1.9295008	-1.4157304	1.2484161
H	-2.8712782	-1.3912489	1.0104969
H	-1.6488056	-2.3751059	1.3896200
O	2.0067712	0.1368824	-0.6380320
H	2.0171943	0.8544266	-1.3013835
H	2.2446204	-0.6846117	-1.1082844
O	-0.6198396	-3.6626086	1.6524331
H	-0.4151031	-4.1865514	0.8568027
H	0.1426903	-3.0351077	1.7379597
O	-2.1288757	1.3691413	0.6171255
C	-2.4826248	2.4862771	0.1254970
C	-3.7814723	3.0388383	0.7664911
F	-3.6073950	3.2449233	2.1016751
F	-4.8037464	2.1493502	0.6283164
F	-4.2042145	4.2188759	0.2315936
C	-1.8733237	3.2458888	-0.8705209
H	-2.3473981	4.1807885	-1.1552443
C	-0.6691927	2.8733392	-1.5297104
O	-0.0139127	1.7992651	-1.2846537
C	-0.1231648	3.7639034	-2.5577049
S	1.3356961	3.2623759	-3.4077463
C	1.3311137	4.7167902	-4.3530981
H	2.1117885	4.8791946	-5.0913645
C	0.2708326	5.5388502	-4.0364953
H	0.0927555	6.4982038	-4.5199004
C	-0.5546114	4.9989418	-3.0183065
H	-1.4378588	5.5061601	-2.6338124
O	0.3141752	-1.9929860	-1.0192460
C	-0.1892838	-2.6979580	-1.9611979
C	-1.3266154	-2.4565587	-2.7141026
C	-2.1340873	-1.2904801	-2.5204635
O	-1.8945532	-0.4095147	-1.6323935
C	0.6194320	-3.9849710	-2.2421258
F	0.6025451	-4.8038269	-1.1402756
F	1.9235045	-3.6975161	-2.4984484
F	0.1536692	-4.7190818	-3.2849873
H	-1.6011438	-3.1710054	-3.4849852
C	-3.2988909	-1.0871387	-3.3849800
S	-4.2869504	0.3479621	-3.1314091
C	-5.3505160	-0.1180199	-4.4186988
H	-6.1994207	0.5135089	-4.6673164
C	-4.9712372	-1.3049459	-5.0105062
H	-5.5125222	-1.7625250	-5.8371772
C	-3.8055115	-1.8561338	-4.4236198
H	-3.3532490	-2.7895973	-4.7547445

$[Y(TTA)_3(H_2O)_2],(H_2O)$, isomer 2 optimized with the QM/SPP in the chloroform CPCM solvent (Table 1, Table 2, Table 3)

Atom	X(Å)	Y(Å)	Z(Å)
S	0.5031305	4.0002636	2.5942605
C	1.1950185	2.5315213	3.2758874
C	1.8888382	2.8117636	4.4445796
C	1.8676085	4.1850537	4.7923878
C	1.1585031	4.9490331	3.8890604

C	0.9711028	1.2665378	2.5752904
C	1.5139210	0.0666930	3.1171049
C	1.3625003	-1.1624880	2.4871200
O	0.7516211	-1.4267068	1.4005997
Y	-0.5055115	-0.1739336	-0.0859610
O	0.2867661	1.3088192	1.4939124
O	0.2276021	1.6093823	-1.4259226
C	-0.1859425	2.7864642	-1.7231013
C	-1.3969451	3.3566729	-1.2285843
C	-2.3026097	2.6749734	-0.4272636
O	-2.2490430	1.4723824	-0.0011460
C	0.6269097	3.5786332	-2.6461289
S	1.9807150	2.8064642	-3.4672191
C	2.3680895	4.2810410	-4.2886036
C	1.5129809	5.3102941	-3.9520126
C	0.5227429	4.9118950	-3.0225821
C	-3.5982832	3.4069386	-0.0018216
F	-4.6913549	2.7852849	-0.5383428
F	-3.6508051	4.7098231	-0.3866126
F	-3.7490911	3.3786019	1.3497834
O	-1.3512033	-2.4199913	-0.3479186
C	-0.8407527	-3.5170839	-0.7701048
C	-1.5874589	-4.7495017	-0.5134588
S	-3.1303313	-4.6337088	0.3290005
C	-3.3435753	-6.3531304	0.2518914
C	-2.2926278	-6.9801863	-0.3828978
C	-1.2963463	-6.0713940	-0.8180637
O	1.0011261	-1.2654728	-1.4952554
C	1.1696464	-2.4937425	-1.8059624
C	2.4256989	-2.7270789	-2.6813125
F	3.5207972	-2.1475558	-2.1152216
O	-2.0361146	-0.4228166	-2.0501525
O	-2.2383759	-0.6698764	1.5490327
C	0.3844960	-3.5953408	-1.4936816
F	2.7228578	-4.0386493	-2.8802136
F	2.2613890	-2.1595669	-3.9096274
C	1.9970089	-2.4116451	3.1450382
F	2.8783649	-3.0106314	2.2994440
F	2.6679789	-2.1414403	4.2998136
F	1.0392261	-3.3341666	3.4467582
O	2.9870106	0.7694797	-0.6632997
H	2.0784668	0.1110634	4.0438328
H	2.4001590	2.0526081	5.0341882
H	2.3560389	4.5981177	5.6736066
H	0.9832822	6.0214543	3.9099099
H	3.2076163	4.3034989	-4.9783088
H	1.5969165	6.3163185	-4.3599329
H	-0.2357958	5.5878891	-2.6317366
H	-1.6467754	4.3713240	-1.5249571
H	0.7168706	-4.5684186	-1.8438824
H	-0.3899888	-6.3815422	-1.3352963
H	-2.2397981	-8.0578228	-0.5294647
H	-4.2350727	-6.8025030	0.6809919
H	-2.7902466	0.1914306	-2.0972523
H	-2.4167150	-1.3202964	-2.0716261
H	-2.6221177	-1.5532221	1.3917830
H	-2.9513256	-0.0107511	1.4342465
H	2.7161355	-0.0850451	-1.0535248
H	2.2537887	1.3548163	-0.9390023

$[Y(TTA)_3(H_2O)_2],(H_2O)$, isomer 3 optimized with the QM/SPP in the chloroform CPCM solvent (Table 1, Table 2, Table 3)

Atom	X(Å)	Y(Å)	Z(Å)
S	0.7565964	2.8753606	3.9122925
C	2.0127534	1.8388615	3.2429632
C	3.2134981	2.0265622	3.9125796
C	3.1311935	2.9882526	4.9501823
C	1.8689582	3.5311383	5.0698241
C	1.6626682	0.9526775	2.1308873
C	2.6613013	0.1036957	1.5768824
C	2.3794463	-0.7821562	0.5410393
O	1.2724160	-0.9766575	-0.0529844
Y	-0.8643803	-0.0488487	0.1137072
O	0.4528586	0.9878727	1.7129287
O	-0.1032220	1.3640524	-1.5431618
C	-0.0619318	2.6186586	-1.7964965
C	-0.7902444	3.6000171	-1.0613698
C	-1.6651726	3.2747578	-0.0310237
O	-1.9258532	2.1269221	0.4600102
C	0.7697099	3.0445492	-2.9217185
S	1.6606826	1.8135287	-3.8125381
C	2.3225390	3.0155127	-4.8710222
C	1.8892127	4.2881825	-4.5600822
C	1.0064420	4.3055210	-3.4529912
C	-2.4966776	4.4133757	0.6088840
F	-3.8249472	4.2360700	0.3372094
F	-2.1615777	5.6565467	0.1704701
F	-2.3659858	4.4145078	1.9624503
O	-1.2552379	-2.1772912	0.9710517
C	-1.0077072	-3.3699905	0.5800776
C	-1.1068369	-4.4357529	1.5772937
S	-1.4850708	-3.9913609	3.2394740
C	-1.4213619	-5.6522948	3.7331978
C	-1.1258372	-6.4993981	2.6856238
C	-0.9473550	-5.8094792	1.4612784
O	-0.9366454	-1.5441713	-1.7822210
C	-0.6712649	-2.7976836	-1.8072324
C	-0.3411995	-3.3256919	-3.2244784
F	0.7454929	-2.6893283	-3.7364600
O	-3.1430711	0.0133161	-0.8279925
O	-2.2930768	0.0828974	2.0993864
C	-0.6621484	-3.7082208	-0.7609581
F	-0.0857551	-4.6607795	-3.2703985
F	-1.3816131	-3.0874307	-4.0774142
C	3.5268353	-1.6760106	0.0068784
F	3.7529072	-1.4360744	-1.3132970
F	4.7123002	-1.4890514	0.6558472
F	3.2097130	-2.9942451	0.1290222
H	3.6702793	0.1365978	1.9774878
H	4.1272524	1.4882343	3.6659892
H	3.9683516	3.2714787	5.5864344
H	1.5268907	4.2839354	5.7751434
H	2.9994746	2.7142403	-5.6661695
H	2.1958569	5.1768673	-5.1095390
H	0.5587277	5.2162889	-3.0585481
H	-0.6961682	4.6442640	-1.3455757
H	-0.4224074	-4.7424325	-0.9899673
H	-0.7114228	-6.3079194	0.5225935
H	-1.0407392	-7.5794896	2.7945026
H	-1.6048275	-5.9098901	4.7729890
H	-3.5491412	0.8659211	-0.5868959
H	-3.1412464	-0.0177288	-1.8358094

H	-2.9964250	-0.5753686	2.2350451
H	-2.7045646	0.9693241	2.1106330
H	-1.9088491	-0.7548105	-3.1577117
O	-2.7096256	-0.2449341	-3.4412950
H	-2.3655884	0.5382076	-3.9049752

$[Y(TTA)_3(H_2O)_2]$ optimized with the QM/SPP in the chloroform CPCM solvent (Table 1, Table 2, Table 3)

Atom	X(Å)	Y(Å)	Z(Å)
S	1.7613843	2.7611024	-3.4794505
C	0.4150064	3.5456774	-2.6590992
C	0.3052373	4.8728283	-3.0517639
C	1.2863446	5.2587367	-3.9974812
C	2.1416362	4.2261850	-4.3233998
C	-0.3750910	2.7545461	-1.7156141
C	-1.4672518	3.3779999	-1.0367180
C	-2.3066627	2.7033204	-0.1620399
C	-3.4991738	3.4750881	0.4502717
F	-3.5283435	4.7968168	0.1315611
O	-0.0458964	1.5298260	-1.5638795
Y	-0.5537893	-0.1874689	-0.1029286
O	-2.2635057	1.4804293	0.2109670
O	-1.3739054	-2.4600135	-0.1239143
C	-0.8765971	-3.5584803	-0.5611811
C	0.2289221	-3.6316764	-1.4552860
C	0.8744426	-2.5121671	-1.9703347
C	2.0120158	-2.7338578	-2.9987861
F	2.2904526	-4.0467263	-3.2359742
C	-1.5175013	-4.8026449	-0.1275250
S	-2.9139443	-4.6939498	0.9410482
C	-3.0596040	-6.4221168	0.9884920
C	-2.0932037	-7.0461096	0.2291401
C	-1.2185932	-6.1282286	-0.4049244
O	0.6564028	-1.2801906	-1.7331551
O	-2.4445507	-0.5131143	-1.7000442
O	-1.9730284	-0.6274823	1.8261697
O	0.5096860	1.3453420	1.2813254
C	1.3623729	1.3362231	2.2356653
C	2.0100483	0.1554154	2.7003296
C	1.7762209	-1.0872213	2.1224061
C	2.5433171	-2.3135664	2.6750467
F	3.3694130	-2.0180806	3.7184542
O	0.9951072	-1.3775887	1.1597315
F	1.6900666	-2.1707072	-4.1973463
F	3.1655018	-2.1501456	-2.5766945
C	1.6813640	2.6189074	2.8657105
C	2.5476510	2.9288463	3.9046819
C	2.5693846	4.3094412	4.2225802
C	1.7207170	5.0492722	3.4258144
S	0.8780176	4.0684171	2.2706385
F	1.6750696	-3.2682314	3.1116708
F	3.3109081	-2.8814934	1.7050659
F	-3.4891579	3.3889185	1.8089318
F	-4.6815510	2.9343595	0.0268667
H	2.7210842	0.2254477	3.5182964
H	3.1507513	2.1856310	4.4236820
H	3.1861354	4.7444931	5.0075577
H	1.5417175	6.1209866	3.4509923
H	2.9781284	4.2428551	-5.0171399
H	1.3626923	6.2577408	-4.4239855
H	-0.4585691	5.5495540	-2.6722084

H	-1.6702228	4.4271314	-1.2320463
H	0.5678382	-4.6105159	-1.7821973
H	-0.3914207	-6.4345213	-1.0430205
H	-2.0152341	-8.1278556	0.1318626
H	-3.8525733	-6.8776863	1.5754583
H	-3.1916762	0.0952703	-1.5545687
H	-2.8059298	-1.4160086	-1.6284792
H	-2.3707696	-1.5170303	1.7743925
H	-2.7009308	0.0248010	1.8291362

$[Y(TTA)_3(OH_2)_2\cdots(H_2O)_{W1}]^{\neq}$ optimized with the QM/SPP in the chloroform CPCM solvent (Table 3)

Atom	X(Å)	Y(Å)	Z(Å)
S	-1.3678672	4.0479273	2.1072476
C	-1.3325320	2.6233995	3.1419825
C	-1.8125753	2.9247301	4.4081873
C	-2.2041546	4.2793207	4.5514119
C	-2.0223221	5.0081229	3.3949057
C	-0.8324572	1.3674225	2.5772806
C	-0.8002398	0.2047579	3.3998456
C	-0.3597624	-1.0286041	2.9348796
O	0.0725944	-1.3355836	1.7769144
Y	0.4053407	-0.1276395	-0.1597538
O	-0.4472080	1.3896366	1.3583453
O	1.3659766	1.9511522	-0.9048721
C	0.9450614	2.9843834	-1.5271669
C	-0.3568187	3.0883528	-2.1073087
C	-1.3110961	2.0831225	-2.0411770
O	-1.2313824	0.9327555	-1.4887597
C	1.8645918	4.1158795	-1.6619996
S	3.4916665	3.9555899	-1.0079899
C	3.8947655	5.5629460	-1.5173539
C	2.8427852	6.1873887	-2.1535735
C	1.6905948	5.3670669	-2.2365028
C	-2.6699306	2.3203343	-2.7439608
F	-2.8077819	1.4796471	-3.8096731
F	-2.8368654	3.5873800	-3.2078329
F	-3.7018431	2.0617894	-1.8946251
O	-0.6130426	-2.0761342	-1.0323935
C	-0.2990856	-3.3160682	-1.1566391
C	-1.3427061	-4.2310979	-1.6206448
S	-2.8814707	-3.5592929	-2.1549275
C	-3.5005855	-5.1448283	-2.4825952
C	-2.5819632	-6.1333594	-2.1988188
C	-1.3569695	-5.6161000	-1.7108159
O	2.1098192	-1.8050004	-0.2547978
C	2.0740010	-3.0564677	-0.4816786
C	3.4461944	-3.7482272	-0.2843239
F	3.9361227	-3.5023567	0.9604594
O	1.2784972	-0.3355322	-2.5303037
O	-2.7034874	-0.6536564	0.2912997
C	0.9997928	-3.8372233	-0.8978578
F	3.4117724	-5.0984385	-0.4454545
F	4.3565934	-3.2602437	-1.1767827
C	-0.3725893	-2.2294272	3.9119859
F	0.8855212	-2.7240455	4.0842257
F	-0.8539979	-1.9246601	5.1504845
F	-1.1387167	-3.2430758	3.4239379
O	2.4678431	0.4683541	1.0231646
H	-1.1420265	0.2777029	4.4282348
H	-1.8826328	2.1933544	5.2116596

H	-2.6058946	4.7034422	5.4704410
H	-2.2380813	6.0595200	3.2239742
H	4.8889273	5.9543013	-1.3189203
H	2.8984828	7.2013754	-2.5463560
H	0.7602360	5.6896637	-2.7007641
H	-0.6193148	4.0029691	-2.6312209
H	1.1717332	-4.8983230	-1.0536708
H	-0.5162652	-6.2440177	-1.4207750
H	-2.7840386	-7.1946031	-2.3348809
H	-4.5091844	-5.2550680	-2.8717660
H	1.0063426	0.3461897	-3.1696049
H	1.1102039	-1.1852346	-2.9748946
H	-2.3732480	-1.4599600	-0.1536255
H	-2.6654446	0.0170655	-0.4212235
H	3.0816526	-0.2691441	0.8290305
H	2.8191885	1.2605542	0.5710038

$[Y(TTA)_3(OH_2)_2],(H_2O)$, successor W1 successor optimized with the QM/SPP in the chloroform CPCM solvent (Table 3)

Atom	X(Å)	Y(Å)	Z(Å)
S	-1.2555374	4.0483647	2.1383701
C	-1.2535041	2.6128739	3.1582766
C	-1.7286676	2.9112909	4.4272712
C	-2.0896593	4.2725457	4.5841303
C	-1.8894218	5.0091483	3.4354563
C	-0.7801655	1.3524480	2.5837769
C	-0.7674428	0.1810602	3.3944737
C	-0.3552130	-1.0512825	2.9039464
O	0.0652635	-1.3385106	1.7351208
Y	0.4966844	-0.1108434	-0.1705356
O	-0.3991238	1.3722399	1.3624698
O	1.3882042	1.9697208	-0.9261335
C	0.9191905	2.9958496	-1.5273021
C	-0.4083843	3.0757438	-2.0481981
C	-1.3504221	2.0623780	-1.9325352
O	-1.2386028	0.9145979	-1.3796215
C	1.8110053	4.1437106	-1.6995798
S	3.4673355	4.0114688	-1.1159960
C	3.8197276	5.6259754	-1.6401451
C	2.7306976	6.2322432	-2.2300317
C	1.5905913	5.3919876	-2.2645560
C	-2.7419428	2.2907700	-2.5727391
F	-2.9282599	1.4393226	-3.6215474
F	-2.9319984	3.5529737	-3.0415939
F	-3.7314135	2.0413456	-1.6725208
O	-0.6093121	-2.0202604	-1.0024007
C	-0.3160901	-3.2633315	-1.1378075
C	-1.3696526	-4.1622899	-1.6109430
S	-2.8799035	-3.4734016	-2.2013342
C	-3.5145804	-5.0527462	-2.5249659
C	-2.6239913	-6.0530483	-2.1951749
C	-1.4056946	-5.5488913	-1.6793670
O	2.1535471	-1.8067279	-0.2782588
C	2.0767437	-3.0605718	-0.4944004
C	3.4313818	-3.7888274	-0.3131285
F	3.9554049	-3.5339584	0.9158531
O	1.2950774	-0.3133422	-2.5514432
O	-3.1011330	-0.7443546	0.1358463
C	0.9764617	-3.8116449	-0.8903464
F	3.3542097	-5.1398628	-0.4472040
F	4.3364479	-3.3445791	-1.2341550

C	-0.3881051	-2.2730060	3.8533969
F	0.8621331	-2.7909525	4.0139458
F	-0.8646542	-1.9863174	5.0975338
F	-1.1700691	-3.2625895	3.3430438
O	2.5573712	0.4751130	1.0011874
H	-1.1053396	0.2450719	4.4246491
H	-1.8169383	2.1729996	5.2225946
H	-2.4834024	4.6960947	5.5068327
H	-2.0813798	6.0668397	3.2752857
H	4.8143419	6.0349288	-1.4838501
H	2.7517844	7.2472150	-2.6236413
H	0.6356442	5.6983349	-2.6881050
H	-0.7063458	3.9844768	-2.5633047
H	1.1218062	-4.8761667	-1.0496579
H	-0.5861955	-6.1863086	-1.3519066
H	-2.8414328	-7.1127871	-2.3185698
H	-4.5126223	-5.1518017	-2.9433633
H	1.0370627	0.3729984	-3.1915633
H	1.1372717	-1.1608445	-3.0038789
H	-2.5252399	-1.4789071	-0.1532509
H	-2.7921603	-0.0103865	-0.4338114
H	3.1852734	-0.2528115	0.8198819
H	2.9272341	1.2822679	0.5946773

$[Y(TTA)_3(OH_2)_2\cdots(H_2O)_{W2}]^{\neq}$ optimized with the QM/SPP in the chloroform CPCM solvent (Table 3)

Atom	X(Å)	Y(Å)	Z(Å)
S	-0.5231443	4.0279137	3.0200013
C	-0.0500681	2.5530836	3.8587164
C	0.0845510	2.7847534	5.2202353
C	-0.1867061	4.1254510	5.5897993
C	-0.5274706	4.9136743	4.5105586
C	0.1317349	1.3345838	3.0673217
C	0.5128158	0.1319362	3.7328386
C	0.7154741	-1.0801918	3.0821978
O	0.6154774	-1.3541860	1.8416763
Y	0.0393232	-0.0387088	0.0439288
O	-0.0672267	1.4272871	1.8072291
O	0.8387713	1.7488205	-1.2619339
C	0.3553937	2.7032700	-1.9638235
C	-1.0426052	2.9633713	-2.0869227
C	-2.0096725	2.1863784	-1.4687674
O	-1.8529194	1.1452219	-0.7427098
C	1.2998726	3.5703492	-2.6652405
S	3.0167539	3.1895441	-2.5743390
C	3.4091364	4.5610256	-3.5584172
C	2.2884445	5.2691500	-3.9394284
C	1.0908201	4.7075954	-3.4336171
C	-3.4962515	2.5597664	-1.6749769
F	-4.1382847	1.5761405	-2.3729239
F	-3.6827321	3.7212664	-2.3553303
F	-4.1353186	2.6827629	-0.4803685
O	-1.0393641	-2.0160922	-0.7851041
C	-0.6506711	-3.2103286	-1.0905166
C	-1.6772348	-4.2439656	-1.1734575
S	-3.3582045	-3.7838643	-0.9120747
C	-3.8779569	-5.4221705	-1.1367131
C	-2.8248863	-6.2729761	-1.4002279
C	-1.5760336	-5.6061896	-1.4217722
O	1.6774675	-1.3821460	-1.0156268
C	1.7293484	-2.6108003	-1.3462865

C	3.1440400	-3.0643161	-1.7854391
F	4.0719915	-2.7105847	-0.8542510
O	-0.8164368	-0.4954471	-3.2283898
O	-2.1320763	-0.5583346	1.2522225
C	0.6987187	-3.5446086	-1.3766806
F	3.2535375	-4.4058363	-1.9755844
F	3.4960801	-2.4586979	-2.9536745
C	1.1214205	-2.3076656	3.9346560
F	2.3196496	-2.8060176	3.5222519
F	1.2356961	-2.0416351	5.2660419
F	0.2046321	-3.3072816	3.8045874
O	2.4366442	0.6028797	0.5832183
H	0.6531603	0.1597893	4.8096074
H	0.3699850	2.0136725	5.9338710
H	-0.1339661	4.4983788	6.6115287
H	-0.7829613	5.9700376	4.5057957
H	4.4479196	4.7628461	-3.8057219
H	2.3280395	6.1618840	-4.5614752
H	0.1057297	5.1299414	-3.6244199
H	-1.3676472	3.8077970	-2.6878526
H	0.9363564	-4.5642540	-1.6657190
H	-0.6305307	-6.1127235	-1.6076891
H	-2.9479975	-7.3411817	-1.5710967
H	-4.9353230	-5.6625420	-1.0657124
H	-1.5870985	0.0487149	-3.4644942
H	-1.1727861	-1.1549237	-2.5999011
H	-2.3820284	-1.4242232	0.8729578
H	-2.6991953	0.0895797	0.7824164
H	2.8896619	-0.1157695	0.0940477
H	2.5400593	1.3893872	0.0100514

$[Y(TTA)_3(OH_2)_2],(H_2O)$, successor W2 successor optimized with the QM/SPP in the chloroform CPCM solvent (Table 3)

Atom	X(Å)	Y(Å)	Z(Å)
S	-0.5764389	4.1480534	2.9517369
C	-0.1282415	2.7119715	3.8679810
C	-0.0426093	3.0013059	5.2226613
C	-0.3313241	4.3547655	5.5255146
C	-0.6363674	5.0953235	4.4025142
C	0.0864962	1.4629267	3.1360232
C	0.4442024	0.2899996	3.8661911
C	0.6782327	-0.9490651	3.2805502
O	0.6316473	-1.2802242	2.0495845
Y	0.1177825	-0.0474700	0.1818492
O	-0.0627826	1.5015785	1.8659230
O	0.9060325	1.5647845	-1.3238210
C	0.4405218	2.5079219	-2.0559666
C	-0.9515177	2.8006715	-2.1655333
C	-1.9209075	2.0526426	-1.5186077
O	-1.7665194	1.0368553	-0.7542361
C	1.3984204	3.3106864	-2.8103080
S	3.1073163	2.8968877	-2.7060572
C	3.5225243	4.2028920	-3.7667029
C	2.4153237	4.9133014	-4.1820581
C	1.2089860	4.4078062	-3.6400552
C	-3.4051204	2.4300064	-1.7280577
F	-4.0661816	1.4136675	-2.3705232
F	-3.5904961	3.5530563	-2.4649866
F	-4.0320341	2.6139580	-0.5367606
O	-0.9018641	-1.9302985	-0.8280368
C	-0.5199162	-3.1151337	-1.1738855

C	-1.5559251	-4.1230282	-1.3694697
S	-3.2283877	-3.6971470	-1.0147151
C	-3.7599269	-5.2933566	-1.4272720
C	-2.7174170	-6.1057604	-1.8229928
C	-1.4667469	-5.4444616	-1.7879887
O	1.8243110	-1.3600932	-0.8013260
C	1.8828856	-2.5675609	-1.2095463
C	3.3198788	-3.0240884	-1.5587636
F	4.1630158	-2.7999490	-0.5139380
O	-2.1409999	-0.9654720	-3.3739730
O	-2.0836678	-0.5408441	1.3351973
C	0.8403737	-3.4694100	-1.3788423
F	3.4116797	-4.3418530	-1.8777502
F	3.7978007	-2.3150873	-2.6196402
C	1.0503456	-2.1350524	4.2038720
F	2.2663242	-2.6457249	3.8667983
F	1.1046911	-1.8095065	5.5254377
F	0.1420434	-3.1433159	4.0778217
O	2.4813575	0.6635796	0.7623591
H	0.5400229	0.3651772	4.9456054
H	0.2203629	2.2624908	5.9778407
H	-0.3161416	4.7706521	6.5317551
H	-0.8953381	6.1492479	4.3442951
H	4.5638479	4.3680688	-4.0300910
H	2.4706869	5.7681893	-4.8539884
H	0.2316373	4.8385085	-3.8511223
H	-1.2694198	3.6264735	-2.7952311
H	1.0780605	-4.4787446	-1.7016671
H	-0.5293777	-5.9232950	-2.0656324
H	-2.8501508	-7.1426063	-2.1273858
H	-4.8161877	-5.5396406	-1.3601506
H	-2.8467476	-0.3107660	-3.2355205
H	-1.8724327	-1.2156498	-2.4657960
H	-2.3679994	-1.4569515	1.1596587
H	-2.6523350	0.0159301	0.7613125
H	2.9393331	-0.0516578	0.2702685
H	2.6460912	1.4661937	0.2310482

$[Y(TTA)_3(OH_2)_2\cdots(H_2O)_{W3}]^{\neq}$ optimized with the QM/SPP in the chloroform CPCM solvent (Table 3)

Atom	X(Å)	Y(Å)	Z(Å)
S	0.5105931	4.0107753	2.6124281
C	1.2877740	2.5564246	3.2301770
C	2.0334214	2.8425879	4.3648723
C	1.9843515	4.2088566	4.7375273
C	1.2021239	4.9617672	3.8870154
C	1.0689171	1.2951698	2.5191807
C	1.6818341	0.1078876	3.0129199
C	1.5389173	-1.1220884	2.3827474
O	0.8806214	-1.4048833	1.3293411
Y	-0.4416635	-0.1655763	-0.0992929
O	0.3250721	1.3323703	1.4789546
O	0.1866054	1.6215180	-1.4932388
C	-0.2315422	2.8053515	-1.7564922
C	-1.4241977	3.3680217	-1.2148035
C	-2.3000426	2.6707561	-0.3930148
O	-2.2226005	1.4653708	0.0196817
C	0.5612279	3.6100778	-2.6858400
S	1.9181067	2.8540806	-3.5170482
C	2.2919667	4.3377184	-4.3297070
C	1.4275927	5.3561864	-3.9854103

C	0.4441126	4.9439199	-3.0540505
C	-3.5889187	3.3873791	0.0774773
F	-4.6912372	2.7634421	-0.4371111
F	-3.6616772	4.6944821	-0.2893865
F	-3.7027341	3.3411198	1.4320945
O	-1.3537523	-2.4238499	-0.2304811
C	-0.9037955	-3.5406075	-0.6685147
C	-1.6417650	-4.7532631	-0.3108832
S	-3.0949774	-4.5915696	0.6714149
C	-3.3407838	-6.3082047	0.6570882
C	-2.3649989	-6.9678032	-0.0594372
C	-1.4013837	-6.0867223	-0.6097000
O	0.8856060	-1.3411160	-1.6273842
C	1.0121198	-2.5795520	-1.9174161
C	2.1836275	-2.8510178	-2.8925152
F	3.3320449	-2.2794335	-2.4332214
O	-2.0943085	-0.4511379	-1.9677535
O	-2.0979120	-0.6355248	1.6267229
C	0.2471719	-3.6600328	-1.5015473
F	2.4420038	-4.1709351	-3.0897164
F	1.9243354	-2.3034584	-4.1135233
C	2.2493330	-2.3514256	2.9992673
F	3.1018967	-2.9194641	2.1039982
F	2.9745215	-2.0634405	4.1166750
F	1.3405139	-3.3059991	3.3493081
O	2.7197025	0.5942587	-0.6397539
H	2.2924094	0.1628823	3.9094638
H	2.6011673	2.0926574	4.9131724
H	2.5050894	4.6245942	5.5987487
H	0.9914658	6.0267749	3.9362914
H	3.1287995	4.3715293	-5.0221457
H	1.5001782	6.3648279	-4.3889193
H	-0.3199401	5.6106802	-2.6577000
H	-1.6851278	4.3865303	-1.4877067
H	0.5327947	-4.6476623	-1.8520674
H	-0.5534977	-6.4244951	-1.2031713
H	-2.3427806	-8.0491883	-0.1839582
H	-4.1938381	-6.7318560	1.1803073
H	-2.8522617	0.1583494	-1.9087606
H	-2.4717360	-1.3499590	-1.9412433
H	-2.4755359	-1.5192355	1.4503130
H	-2.8154286	0.0210820	1.5257027
H	2.5207295	-0.2076929	-1.1647048
H	2.1396029	1.2637793	-1.0549476

$[Y(TTA)_3(OH_2)_2],(H_2O)$, successor W3 successor optimized with the QM/SPP in the chloroform CPCM solvent (Table 3)

Atom	X(Å)	Y(Å)	Z(Å)
S	0.5031305	4.0002636	2.5942605
C	1.1950185	2.5315213	3.2758874
C	1.8888382	2.8117636	4.4445796
C	1.8676085	4.1850537	4.7923878
C	1.1585031	4.9490331	3.8890604
C	0.9711028	1.2665378	2.5752904
C	1.5139210	0.0666930	3.1171049
C	1.3625003	-1.1624880	2.4871200
O	0.7516211	-1.4267068	1.4005997
Y	-0.5055115	-0.1739336	-0.0859610
O	0.2867661	1.3088192	1.4939124
O	0.2276021	1.6093823	-1.4259226
C	-0.1859425	2.7864642	-1.7231013

C	-1.3969451	3.3566729	-1.2285843
C	-2.3026097	2.6749734	-0.4272636
O	-2.2490430	1.4723824	-0.0011460
C	0.6269097	3.5786332	-2.6461289
S	1.9807150	2.8064642	-3.4672191
C	2.3680895	4.2810410	-4.2886036
C	1.5129809	5.3102941	-3.9520126
C	0.5227429	4.9118950	-3.0225821
C	-3.5982832	3.4069386	-0.0018216
F	-4.6913549	2.7852849	-0.5383428
F	-3.6508051	4.7098231	-0.3866126
F	-3.7490911	3.3786019	1.3497834
O	-1.3512033	-2.4199913	-0.3479186
C	-0.8407527	-3.5170839	-0.7701048
C	-1.5874589	-4.7495017	-0.5134588
S	-3.1303313	-4.6337088	0.3290005
C	-3.3435753	-6.3531304	0.2518914
C	-2.2926278	-6.9801863	-0.3828978
C	-1.2963463	-6.0713940	-0.8180637
O	1.0011261	-1.2654728	-1.4952554
C	1.1696464	-2.4937425	-1.8059624
C	2.4256989	-2.7270789	-2.6813125
F	3.5207972	-2.1475558	-2.1152216
O	-2.0361146	-0.4228166	-2.0501525
O	-2.2383759	-0.6698764	1.5490327
C	0.3844960	-3.5953408	-1.4936816
F	2.7228578	-4.0386493	-2.8802136
F	2.2613890	-2.1595669	-3.9096274
C	1.9970089	-2.4116451	3.1450382
F	2.8783649	-3.0106314	2.2994440
F	2.6679789	-2.1414403	4.2998136
F	1.0392261	-3.3341666	3.4467582
O	2.9870106	0.7694797	-0.6632997
H	2.0784668	0.1110634	4.0438328
H	2.4001590	2.0526081	5.0341882
H	2.3560389	4.5981177	5.6736066
H	0.9832822	6.0214543	3.9099099
H	3.2076163	4.3034989	-4.9783088
H	1.5969165	6.3163185	-4.3599329
H	-0.2357958	5.5878891	-2.6317366
H	-1.6467754	4.3713240	-1.5249571
H	0.7168706	-4.5684186	-1.8438824
H	-0.3899888	-6.3815422	-1.3352963
H	-2.2397981	-8.0578228	-0.5294647
H	-4.2350727	-6.8025030	0.6809919
H	-2.7902466	0.1914306	-2.0972523
H	-2.4167150	-1.3202964	-2.0716261
H	-2.6221177	-1.5532221	1.3917830
H	-2.9513256	-0.0107511	1.4342465
H	2.7161355	-0.0850451	-1.0535248
H	2.2537887	1.3548163	-0.9390023

$[Y(TTA)_3(TMP)(H_2O)],(H_2O)$ optimized with the QM/SPP in the chloroform CPCM solvent (Table 4)

Atom	X(Å)	Y(Å)	Z(Å)
S	-1.0862187	4.2578593	1.6288906
C	-1.3270420	2.8667624	2.6806092
C	-1.9535981	3.2453683	3.8593739
C	-2.2392382	4.6322257	3.9221094
C	-1.8299471	5.3080942	2.7916319
C	-0.8711685	1.5526483	2.2171999

O	-0.2982417	1.4925819	1.0801016
Y	0.4204186	-0.1816855	-0.3959413
O	-1.8905542	-0.3324754	-0.6771355
C	-2.7243642	-1.2903218	-0.7673981
C	-4.1978272	-0.8206706	-0.6812488
F	-4.4900296	0.0296217	-1.7091650
C	-2.4741937	-2.6444403	-0.9575431
C	-1.1546798	-3.1542904	-1.1441288
O	-0.1042782	-2.4378386	-1.0728226
C	-0.9658312	-4.5784466	-1.4706926
C	0.2435282	-5.2090773	-1.7125014
C	0.1151458	-6.5894870	-2.0094369
C	-1.1946373	-7.0179336	-1.9948873
S	-2.2939719	-5.7295784	-1.6183293
F	-4.4276909	-0.1437248	0.4752429
F	-5.1037636	-1.8373879	-0.7374704
O	2.1914180	1.3862875	-0.3060687
C	2.2502307	2.6151668	-0.6155249
C	3.5389022	3.3119761	-0.1062133
F	3.6649763	3.1709453	1.2437767
O	-0.1934121	1.6294982	-1.8577480
C	0.1641673	2.8607341	-1.9339486
C	-0.7208440	3.7549149	-2.6926916
C	-2.0451633	3.5126889	-3.0205634
C	-2.6531556	4.5723303	-3.7397234
C	-1.7934745	5.6252139	-3.9653743
S	-0.2208269	5.3356916	-3.2910849
O	2.3823050	-1.4256404	-0.0125704
P	3.6595571	-2.1932997	0.2146833
O	3.6196065	-3.1732762	1.5056721
C	2.3901035	-3.9196706	1.7887420
O	0.0009089	-1.2182856	1.6665252
C	-0.6099113	-0.8452983	2.7235334
C	-0.8076270	-1.9865283	3.7507631
F	0.3969056	-2.3991213	4.2493137
O	1.2758334	-0.7015960	-2.6614755
C	1.3398308	3.3854941	-1.3375308
O	5.0008118	-1.3408337	0.4717008
C	5.0027329	-0.3281303	1.5303431
O	4.0191099	-3.0663406	-1.0939927
C	5.2327137	-3.8802440	-1.1280249
C	-1.0735560	0.4188108	3.0602956
F	-1.3899853	-3.0715689	3.1728616
F	-1.5791760	-1.6399832	4.8184870
F	4.6438996	2.7465750	-0.6709933
F	3.5917016	4.6457353	-0.3736790
H	-1.9846932	6.5546028	-4.4956073
H	-3.6886031	4.5659288	-4.0771023
H	-2.5587301	2.6025008	-2.7155343
H	-3.3215164	-3.3240322	-1.0189966
H	1.5504432	4.4458397	-1.4570429
H	-1.5838397	-8.0155373	-2.1815398
H	0.9538140	-7.2494938	-2.2269599
H	1.1875925	-4.6685368	-1.6735895
H	-1.5775835	0.5507389	4.0133325
H	-2.2014606	2.5472304	4.6574647
H	-2.7273899	5.1164972	4.7668169
H	-1.9221838	6.3691893	2.5739793
H	5.2654077	-4.5617406	-0.2680496
H	6.1178701	-3.2328472	-1.1367124
H	5.1741411	-4.4524047	-2.0587878
H	4.8816795	-0.8080095	2.5097851
H	4.2040071	0.4008297	1.3472087

H	5.9812481	0.1562188	1.4671681
H	2.2923322	-4.7556369	1.0838714
H	1.5207951	-3.2535823	1.7260928
H	2.5096636	-4.3027370	2.8063504
H	0.6231588	-0.4493158	-3.3793631
H	1.3245103	-1.6757519	-2.6829893
O	-0.6595013	0.3495134	-4.2139833
H	-1.4966856	-0.1351622	-4.3179132
H	-0.7782778	0.9300623	-3.4160657

$[Y(TTA)_3(TMP)(H_2O)\ldots(H_2O)]^{\neq}$ optimized with the QM/SPP in the chloroform CPCM solvent (Table 4)

Atom	X(Å)	Y(Å)	Z(Å)
S	1.5807677	4.8275064	-3.5906375
C	1.1427439	3.1402026	-3.3206099
C	0.7245899	2.5578328	-4.5073500
C	0.7529467	3.4420202	-5.6138987
C	1.1914659	4.7040014	-5.2755669
C	1.2307265	2.4867479	-2.0080561
C	1.8692511	3.1589474	-0.9320142
C	2.0365567	2.6058374	0.3387692
C	2.8252536	3.4333480	1.3888174
F	3.2339417	4.6516096	0.9376396
O	1.6394514	1.4858200	0.7814088
Y	0.2425346	-0.2148903	-0.0887834
O	-1.6813213	0.1666059	-2.3472423
O	-1.3945084	1.4814154	0.0592874
C	-2.0168174	2.1108200	0.9900703
C	-1.8647756	1.8306913	2.3719140
C	-1.0461357	0.8105886	2.8550903
C	-1.0172736	0.5849214	4.3904940
F	-1.7460491	1.4946195	5.0962354
C	-2.9339527	3.1784000	0.5801667
S	-3.0183919	3.6083830	-1.1258689
C	-4.2193264	4.8168982	-0.8006983
C	-4.5356366	4.8885936	0.5390902
C	-3.8069978	3.9593139	1.3231102
O	-1.6238125	-1.5916619	0.1912634
C	-2.0965057	-2.5725989	-0.4609580
C	-1.5602589	-3.2346714	-1.5628995
C	-0.3170162	-2.8851184	-2.1564165
C	0.1824349	-3.6667380	-3.2984947
C	1.2715891	-3.3585251	-4.0972686
C	1.5046443	-4.3007704	-5.1301495
C	0.5936032	-5.3345395	-5.1224824
S	-0.5688140	-5.1655148	-3.8464318
O	0.4134113	-1.9115204	-1.7618203
O	0.7436024	1.3006075	-1.9194382
O	1.3735959	-1.9340712	1.0379760
P	2.1880047	-2.6256561	2.1073627
O	2.8582133	-3.9512982	1.4776735
C	3.6928628	-4.8165810	2.3066596
O	-0.3066000	0.0042596	2.2149695
O	2.6162667	-0.6206423	-1.0846715
C	-3.4575079	-3.0671506	0.0940034
F	-3.9943064	-4.1067530	-0.6050625
F	-4.3759299	-2.0635098	0.0859304
F	-3.3276147	-3.4820103	1.3868237
F	2.0693470	3.6492824	2.4983777
F	3.9417236	2.7592369	1.7867692
O	1.3458523	-3.0426477	3.4262512

C	-0.0496924	-3.4601300	3.2761231
O	3.4503577	-1.8415452	2.7233306
C	3.2480059	-0.5591285	3.4044487
F	0.2565994	0.6412294	4.8682369
F	-1.5084955	-0.6477502	4.7048834
H	1.3054350	5.5751641	-5.9151412
H	0.4625128	3.1633278	-6.6255311
H	0.4201514	1.5146873	-4.5683997
H	-2.1286158	-4.0586094	-1.9888600
H	2.2881520	4.1463654	-1.1129931
H	0.5356055	-6.1912406	-5.7885323
H	2.3118584	-4.2235349	-5.8568639
H	1.8712943	-2.4646660	-3.9382467
H	-2.4193573	2.4281065	3.0894794
H	-3.9272215	3.8626041	2.4008012
H	-5.2683787	5.5847418	0.9444103
H	-4.6194523	5.4085365	-1.6196539
H	3.1535301	-5.1217875	3.2126275
H	4.6228699	-4.2994633	2.5722055
H	3.9105106	-5.6921222	1.6877699
H	2.6621870	-0.7123239	4.3181176
H	2.7449383	0.1503381	2.7358307
H	4.2523905	-0.2038479	3.6517933
H	-0.1011145	-4.4215845	2.7486286
H	-0.6150008	-2.6898367	2.7394870
H	-0.4295666	-3.5727509	4.2954608
H	2.6965944	0.0404753	-1.7970074
H	2.2987436	-1.4295318	-1.5451193
H	-2.1028021	0.7689095	-1.7001641
H	-0.8998243	0.6862351	-2.6358361

$[Y(TTA)_3(TMP)(H_2O)_2]$ optimized with the QM/SPP in the chloroform CPCM solvent (Table 4)

Atom	X(Å)	Y(Å)	Z(Å)
S	-0.4594183	5.0079847	-3.5803289
C	-0.7573943	3.3081415	-3.2153748
C	-1.8143885	2.8333880	-3.9761271
C	-2.3781694	3.8084823	-4.8360430
C	-1.7540029	5.0328175	-4.7338382
C	0.0320197	2.5430908	-2.2393047
C	1.2012147	3.1198010	-1.6770971
C	2.0387247	2.4532085	-0.7800552
C	3.3355298	3.1800789	-0.3311828
F	3.4627758	4.4416094	-0.8293927
O	1.9087891	1.3011764	-0.2685016
Y	0.1516515	-0.2998581	-0.2053016
O	-2.3792218	0.1032437	-0.8201155
O	-0.9445770	1.4674354	0.9528146
C	-0.8422199	2.0669209	2.0834228
C	0.0829830	1.6989005	3.0912889
C	0.9475155	0.6111163	2.9628641
C	1.8618660	0.2825706	4.1743856
F	1.7940196	1.1986451	5.1816155
C	-1.7504415	3.1924428	2.3270964
S	-2.8272828	3.6972374	1.0278681
C	-3.5083220	4.9427798	2.0254766
C	-2.9404480	4.9716690	3.2810746
C	-1.9433951	3.9784028	3.4531195
O	-1.1714371	-1.7017853	1.1301437
C	-1.9449257	-2.6749850	0.8758496
C	-2.1682951	-3.3342974	-0.3310298

C	-1.5142306	-2.9972472	-1.5486767
C	-1.7954453	-3.7894530	-2.7579122
C	-1.3880691	-3.4985546	-4.0494830
C	-1.8222699	-4.4457788	-5.0106515
C	-2.5629129	-5.4662049	-4.4551187
S	-2.7411077	-5.2784204	-2.7399733
O	-0.6870864	-2.0316889	-1.6723012
O	-0.3740074	1.3536260	-1.9729799
O	1.6984059	-2.0742963	-0.0140767
P	2.9514290	-2.8386974	0.3400171
O	3.0514875	-4.1497638	-0.5969477
C	4.1717695	-5.0735709	-0.4483967
O	1.0939836	-0.1861774	1.9901603
O	1.4333985	-0.6936622	-2.4307883
C	-2.7262092	-3.1643412	2.1238214
F	-3.5614463	-4.2135960	1.8789544
F	-3.4881904	-2.1600852	2.6386352
F	-1.8682286	-3.5606970	3.1061722
F	3.3914245	3.2771743	1.0238007
F	4.4368301	2.4806649	-0.7301075
O	3.0432062	-3.3015388	1.8901912
C	1.8140209	-3.6716592	2.5940906
O	4.3716913	-2.1200669	0.1000615
C	4.6761841	-0.8692542	0.8007863
F	3.1670667	0.2055739	3.7967110
F	1.5292530	-0.9254290	4.7140305
H	-1.9793331	5.9541215	-5.2643098
H	-3.2131762	3.6198612	-5.5089123
H	-2.1567129	1.8020289	-3.9146331
H	-2.8841318	-4.1534857	-0.3360244
H	1.4907761	4.1196734	-1.9927638
H	-3.0135735	-6.3228508	-4.9490685
H	-1.6011150	-4.3813291	-6.0749196
H	-0.7997639	-2.6141858	-4.2856807
H	0.1110268	2.2741116	4.0120548
H	-1.3889190	3.8419119	4.3800655
H	-3.2318630	5.6819600	4.0533951
H	-4.2870951	5.5856010	1.6240283
H	4.2569173	-5.4146484	0.5915049
H	5.1032479	-4.5909893	-0.7685550
H	3.9411658	-5.9202440	-1.1019650
H	4.7643182	-1.0592221	1.8767563
H	3.8968912	-0.1232521	0.6011752
H	5.6354987	-0.5373488	0.3935079
H	1.4102780	-4.6059572	2.1821263
H	1.0797353	-2.8618199	2.5165819
H	2.1104704	-3.8212101	3.6361829
H	1.0570913	-0.0024887	-3.0081077
H	0.8937289	-1.4938607	-2.6227177
H	-2.5169709	0.7257028	-0.0747688
H	-2.1103797	0.7006123	-1.5546604

$[Y(TTA)_3(TMP)(H_2O)]$ optimized with the QM/SPP in the chloroform CPCM solvent (Table 4)

Atom	X(Å)	Y(Å)	Z(Å)
S	0.1783428	2.4481945	-4.6734697
C	-0.2822152	3.3299388	-3.2209190
C	-0.0603741	4.6894239	-3.3838562
C	0.4694543	5.0241173	-4.6558953
C	0.6526460	3.9198958	-5.4608322
C	-0.7996191	2.5689457	-2.0768717

C	-1.1103839	3.2715144	-0.8754235
C	-1.6261702	2.6360804	0.2498046
O	-1.8636159	1.3992402	0.4246321
Y	-1.2985305	-0.5229036	-0.7556602
O	-0.9593832	1.3109870	-2.2289378
O	0.8550833	0.2654013	-0.2580583
C	2.0432814	0.0981377	-0.6748597
C	2.3937645	-0.7897269	-1.7442661
C	1.4590285	-1.5635018	-2.4095789
O	0.1923641	-1.6310005	-2.2241151
C	3.1078026	0.8566092	-0.0117650
S	2.6676841	1.9159286	1.3233760
C	4.3212091	2.3942958	1.5305696
C	5.1641105	1.7770125	0.6295208
C	4.4747280	0.9028743	-0.2473811
C	1.9491643	-2.4961846	-3.5400906
F	1.5595640	-3.7829077	-3.3091989
F	3.2992778	-2.5100308	-3.7027904
F	1.4066977	-2.1293040	-4.7395556
O	-3.3393045	-1.0159262	0.3092345
C	-3.6826240	-1.4527704	1.4570594
C	-5.1200734	-1.4918358	1.7551362
S	-6.2392354	-0.9183037	0.5223738
C	-7.5975924	-1.2601722	1.5472914
C	-7.2149554	-1.7823168	2.7645542
C	-5.8077080	-1.9139835	2.8827766
O	-0.7148569	-1.4906388	1.2662529
C	-1.3871593	-1.9039311	2.2631781
C	-0.4950633	-2.4579807	3.4021109
F	0.3291631	-1.4896155	3.8887516
O	-1.7643711	-3.0018013	-1.0944290
O	-2.8711023	-0.8110232	-2.5425790
C	-2.7657928	-1.9116202	2.4485915
F	-1.1970690	-2.9530804	4.4623973
F	0.2984571	-3.4677081	2.9459101
C	-2.0056500	3.5072208	1.4737072
F	-1.3799049	3.0711976	2.5981537
F	-1.6910128	4.8272771	1.3269421
F	-3.3479286	3.4432066	1.7089535
H	-0.9600395	4.3467602	-0.8397675
H	-0.2726292	5.4275947	-2.6119738
H	0.7085766	6.0398422	-4.9681882
H	1.0435275	3.8846516	-6.4745785
H	4.5797489	3.1045760	2.3119542
H	6.2396849	1.9462288	0.6010652
H	4.9689902	0.3255811	-1.0273105
H	3.4364852	-0.8743542	-2.0371656
H	-3.1571256	-2.2903690	3.3885923
H	-5.3163434	-2.3069991	3.7715473
H	-7.9205089	-2.0608140	3.5462965
H	-8.6040147	-1.0532255	1.1922575
H	-1.1436165	-3.1752185	-1.8323922
H	-2.6561604	-3.0899768	-1.4780945
P	-3.8406059	-0.5116746	-3.6628001
O	-4.7709899	-1.8056953	-3.9091550
O	-4.9104290	0.6711842	-3.4456697
O	-3.1386661	-0.0958488	-5.0634028
C	-1.9136717	-0.7871503	-5.4697774
C	-4.4550374	2.0324287	-3.1684072
C	-5.8113603	-1.7869549	-4.9356395
H	-1.5414427	-0.2355687	-6.3377778
H	-1.1785965	-0.7656224	-4.6567103
H	-2.1433654	-1.8223054	-5.7547014

H	-6.1902745	-2.8121524	-4.9847303
H	-6.6136283	-1.0991561	-4.6426338
H	-5.3913854	-1.4939752	-5.9065659
H	-5.3655833	2.6216206	-3.0273198
H	-3.8498726	2.0493315	-2.2538168
H	-3.8804898	2.4190279	-4.0190463

$[Y(TTA)_3(TMP)\ldots(H_2O)]^{\neq}$ optimized with the QM/SPP in the chloroform CPCM solvent (Table 4)

Atom	X(Å)	Y(Å)	Z(Å)
S	4.7106714	1.3013527	-0.8217964
C	3.5310491	2.4700969	-1.4068260
C	4.1617885	3.6176407	-1.8670225
C	5.5728391	3.5639826	-1.7533943
C	6.0146022	2.3764647	-1.2076226
C	2.1126815	2.1170160	-1.3403563
C	1.1411842	3.0542096	-1.8065393
C	-0.2166816	2.7726717	-1.8367854
O	-0.8239236	1.7137612	-1.4536272
Y	-0.1091198	-0.0919748	-0.1677599
O	1.8153376	0.9642636	-0.8802315
O	1.2121442	-1.1789387	1.3610466
C	2.0811408	-2.1158764	1.3378699
C	2.4525618	-2.8240771	0.1570761
C	1.8674079	-2.5888903	-1.0804807
O	0.9536469	-1.7532930	-1.3878280
C	2.7211955	-2.4644698	2.6070925
S	2.2676513	-1.5561187	4.0455099
C	3.3579965	-2.4891550	5.0181787
C	4.0318368	-3.4428811	4.2837479
C	3.6700878	-3.4295422	2.9139748
C	2.3367279	-3.4395714	-2.2846313
F	1.3039093	-4.1774643	-2.7853197
F	3.3416414	-4.3090883	-1.9890940
F	2.7823893	-2.6429682	-3.2965597
O	-1.8679993	-0.3558693	1.3684720
C	-2.2811926	0.2361513	2.4355738
C	-3.4807805	-0.2953289	3.0842728
S	-4.3959511	-1.5666387	2.2790296
C	-5.5388573	-1.6202622	3.5809346
C	-5.2369694	-0.7163441	4.5776456
C	-4.0709159	0.0366891	4.2960972
O	0.1086282	1.6356976	1.3821292
C	-0.5197310	1.9690509	2.4319492
C	0.0793889	3.2160159	3.1329535
F	0.0579933	4.2925507	2.3000855
O	-1.4233926	-3.0952771	0.6689066
C	-1.6480533	1.3754569	2.9964525
F	-0.5828709	3.5761128	4.2694059
F	1.3765881	2.9977595	3.4782096
C	-1.1630055	3.8324569	-2.4487760
F	-2.2275448	4.0676936	-1.6345860
F	-0.5664734	5.0320942	-2.6853980
F	-1.6647756	3.3938623	-3.6428692
H	1.4768547	4.0168535	-2.1814129
H	3.6261906	4.4735897	-2.2743847
H	6.2402740	4.3676763	-2.0606410
H	7.0383377	2.0704231	-1.0087052
H	3.4412265	-2.2796907	6.0813984
H	4.7600087	-4.1279867	4.7152946
H	4.0926995	-4.1099599	2.1765053

H	3.2160588	-3.5935704	0.2264112
H	-2.0687819	1.8184613	3.8942474
H	-3.6703516	0.7923639	4.9696232
H	-5.8335707	-0.6004511	5.4811304
H	-6.3718920	-2.3164057	3.5331591
H	-1.7234089	-3.0928726	-0.2576830
H	-1.8401006	-2.2881829	1.0412110
O	-1.8155554	-1.0142434	-1.5004755
P	-2.8131281	-1.2535479	-2.6155310
O	-3.2914818	-2.7900182	-2.5285348
O	-4.1894926	-0.4286756	-2.5641697
O	-2.2574571	-0.9322157	-4.0983889
C	-0.9075745	-1.3572717	-4.4834842
C	-4.1671558	1.0362037	-2.6327719
C	-4.2853762	-3.3168244	-3.4619139
H	-0.9572562	-2.3709842	-4.8992920
H	-0.5812627	-0.6505889	-5.2520603
H	-0.2271489	-1.3319996	-3.6229685
H	-4.3200346	-4.3935263	-3.2729034
H	-5.2631905	-2.8631815	-3.2614366
H	-3.9800987	-3.1265980	-4.4987935
H	-5.1565821	1.3580364	-2.2960093
H	-3.3859923	1.4382568	-1.9759311
H	-3.9956508	1.3488023	-3.6692996

$[Y(TTA)_3(TMP)],(H_2O)$ optimized with the QM/SPP in the chloroform CPCM solvent (Table 4)

Atom	X(Å)	Y(Å)	Z(Å)
S	4.8810034	0.8343758	-0.8442171
C	3.8409071	1.9301366	-1.7484078
C	4.5945394	2.8897367	-2.4100968
C	5.9881191	2.7513653	-2.1967260
C	6.2941115	1.6872299	-1.3738037
C	2.3946777	1.7154718	-1.6963802
C	1.5347453	2.6013670	-2.4135276
C	0.1570119	2.4377934	-2.4577578
O	-0.5603229	1.5457998	-1.8893099
Y	-0.0682381	-0.0043502	-0.2324752
O	1.9732973	0.7205376	-1.0145134
O	0.9464885	-0.9286711	1.6135980
C	1.7722511	-1.8772410	1.8504798
C	2.2071080	-2.8071300	0.8614503
C	1.7335523	-2.7864319	-0.4445990
O	0.8955841	-1.9849489	-0.9764598
C	2.2763974	-2.0008297	3.2179203
S	1.7394608	-0.8263596	4.4146911
C	2.6948711	-1.5919693	5.6416626
C	3.3864782	-2.6856776	5.1631548
C	3.1490354	-2.9185310	3.7862470
C	2.2391925	-3.8727642	-1.4236067
F	1.2047929	-4.6505085	-1.8567592
F	3.1694377	-4.7089955	-0.8867904
F	2.7999785	-3.3066000	-2.5283033
O	-1.9190980	0.1253683	1.2125618
C	-2.3008601	0.9203516	2.1506071
C	-3.5809970	0.6425363	2.8060536
S	-4.6822485	-0.5285404	2.0879626
C	-5.8427017	-0.2662932	3.3474962
C	-5.4083692	0.6589396	4.2735703
C	-4.1277532	1.1782427	3.9646469
O	0.2331690	1.9437232	0.9861692

C	-0.3837683	2.4751553	1.9602373
C	0.3054923	3.7583494	2.4909958
F	0.3992866	4.6967690	1.5094970
O	-2.2155173	-2.9211270	1.2630133
C	-1.5707806	2.0675165	2.5636427
F	-0.3479390	4.3381268	3.5380579
F	1.5704271	3.4855387	2.9111492
C	-0.6684852	3.4173155	-3.3248925
F	-1.6834457	3.9685960	-2.6054823
F	0.0601623	4.4435376	-3.8425830
F	-1.2386778	2.7604359	-4.3789780
H	1.9743799	3.4247674	-2.9690540
H	4.1587168	3.6708300	-3.0308879
H	6.7396496	3.4087924	-2.6311949
H	7.2754268	1.3541975	-1.0461491
H	2.6927451	-1.1898504	6.6513901
H	4.0412235	-3.2982591	5.7810716
H	3.6037234	-3.7366921	3.2300582
H	2.9194042	-3.5781769	1.1404892
H	-1.9764682	2.6808574	3.3627728
H	-3.6144983	1.9117801	4.5840242
H	-5.9911935	0.9531085	5.1450250
H	-6.7815223	-0.8133693	3.3321033
H	-2.4698469	-3.0715845	0.3331735
H	-2.2129301	-1.9452575	1.3443867
O	-1.7511695	-1.0551073	-1.4452427
P	-2.7848235	-1.6783749	-2.3543870
O	-3.2820444	-3.0568693	-1.6755857
O	-4.1437636	-0.8561749	-2.5856065
O	-2.2744664	-1.9597266	-3.8601148
C	-0.9400086	-2.5282727	-4.0842651
C	-4.0741926	0.4888408	-3.1682739
C	-4.3224794	-3.8758239	-2.2985807
H	-1.0090135	-3.6224403	-4.0619774
H	-0.6367170	-2.1888691	-5.0788535
H	-0.2332825	-2.1763330	-3.3226126
H	-4.3683414	-4.7908410	-1.7015848
H	-5.2823085	-3.3475890	-2.2636718
H	-4.0509742	-4.1143459	-3.3344749
H	-5.0426169	0.9494106	-2.9545626
H	-3.2655894	1.0658642	-2.7020130
H	-3.9193469	0.4091380	-4.2506401

$[Y(TTA)_3(HTTA)(OH_2), H_{in}],(H_2O)$ optimized with the QM/SPP in the chloroform CPCM solvent (Table 6)

Atom	X(Å)	Y(Å)	Z(Å)
S	-3.8722520	3.6326095	-0.8270672
C	-2.9116175	4.0794773	0.5789995
C	-3.3280221	5.2997424	1.0908018
C	-4.4039620	5.8726826	0.3672469
C	-4.8056924	5.0883535	-0.6934916
C	-1.8516110	3.1655176	1.0144878
C	-1.0695742	3.5034601	2.1567395
C	-0.0747294	2.6605419	2.6394819
O	0.3005693	1.5345750	2.1797452
Y	-0.2467295	0.2570899	0.3179427
O	-1.6894260	2.0927434	0.3397453
O	1.0581711	1.7195364	-0.9159765
C	0.9619830	2.3609110	-2.0184759
C	-0.0211406	2.0827766	-3.0119478
C	-0.9526293	1.0593102	-2.8755939

O	-1.1239535	0.2608374	-1.8982478
C	1.9394891	3.4238869	-2.2597760
S	3.1531170	3.7351043	-1.0225233
C	3.8421909	5.0095416	-1.9747894
C	3.1805616	5.1881718	-3.1721985
C	2.0995883	4.2869096	-3.3349429
C	-1.9199897	0.7892324	-4.0545247
F	-1.6754809	-0.4360195	-4.6043035
F	-1.8333404	1.7025648	-5.0608846
F	-3.2141634	0.7820481	-3.6307005
O	-0.4475731	-1.2632082	2.0968248
C	0.3660544	-1.7705444	2.9442020
C	-0.2226674	-2.4499524	4.1047817
S	-1.9583754	-2.2868363	4.3716973
C	-1.8755318	-3.2909321	5.7879317
C	-0.5908560	-3.7119343	6.0464675
C	0.3471076	-3.2338746	5.0934447
O	1.9475902	-0.4477333	0.7927218
C	2.4389156	-1.0918732	1.7709568
C	3.9873433	-1.1615494	1.7357990
F	4.5318805	0.0838025	1.7462287
O	-2.4269932	-0.7124333	0.2547618
C	1.7821274	-1.7216254	2.8263483
F	4.5329015	-1.8470164	2.7800731
F	4.4114747	-1.7757317	0.5928780
C	0.7048223	3.0917117	3.9059736
F	2.0363847	3.1960412	3.6440409
F	0.3023976	4.2917428	4.4144786
F	0.5613569	2.1700398	4.8986395
H	-1.2656283	4.4349386	2.6797097
H	-2.8737533	5.7705775	1.9611594
H	-4.8667451	6.8264025	0.6166498
H	-5.6007975	5.2828866	-1.4084835
H	4.7001775	5.5582448	-1.5951374
H	3.4626184	5.9411521	-3.9066431
H	1.4573352	4.2745063	-4.2141756
H	-0.0261136	2.6682028	-3.9269480
H	2.3853741	-2.1948195	3.5959477
H	1.4097417	-3.4679919	5.1314203
H	-0.3281567	-4.3437093	6.8936198
H	-2.7798882	-3.4953001	6.3545313
H	-2.8125731	-1.5322227	0.6901136
H	-2.8335131	-0.6056755	-0.6238540
O	0.2034211	-2.0831164	-0.8132772
C	0.5768091	-2.6769304	-1.8882850
C	1.5749725	-2.0819675	-2.7500422
S	1.8961333	-2.6935246	-4.3775707
C	3.1519968	-1.5285061	-4.6007875
C	3.3278958	-0.7243555	-3.4912708
C	2.4362032	-1.0341553	-2.4417497
C	0.0150281	-3.9750242	-2.2041520
C	-0.8594982	-4.5543391	-1.3302189
O	-1.2313133	-3.9973023	-0.1822653
C	-1.4883217	-5.9228017	-1.5643811
F	-1.1278858	-6.4466471	-2.7586378
F	-2.8448679	-5.8379511	-1.5359169
F	-1.1161272	-6.7984353	-0.5937230
H	-0.7081377	-3.0825358	-0.1850396
H	0.3035270	-4.5042402	-3.1082819
H	2.4338322	-0.5433594	-1.4684090
H	4.0826244	0.0581313	-3.4400594
H	3.6873547	-1.4983322	-5.5461956
O	-3.4508805	-2.9522072	1.3244479

H	-2.9031410	-3.6404361	0.8927947
H	-3.1990817	-2.9955513	2.2691595

[$Y(TTA)_3(HTTA)(OH_2)_2$, H_{in}] optimized with the QM/SPP in the chloroform CPCM solvent (Table 6)

Atom	X(Å)	Y(Å)	Z(Å)
S	-3.6823280	3.6695460	-1.6281466
C	-2.8251897	4.2561711	-0.2067371
C	-3.1250782	5.5895471	0.0322463
C	-4.0304227	6.1375864	-0.9105495
C	-4.4191560	5.2213216	-1.8652571
C	-1.9505470	3.3228038	0.5092900
C	-1.2628870	3.7807504	1.6750488
C	-0.5088887	2.9386007	2.4829133
O	-0.2664526	1.6943895	2.3366604
Y	-0.5996251	0.2298103	0.5394320
O	-1.8648083	2.1354709	0.0527994
O	0.9732710	1.6815810	-0.4192166
C	1.1284205	2.3106081	-1.5173995
C	0.3957842	2.0209631	-2.7086828
C	-0.5232182	0.9858207	-2.7796334
O	-0.8975050	0.1907335	-1.8520706
C	2.1388206	3.3709415	-1.5472760
S	3.0570823	3.6873486	-0.0788471
C	3.9412281	4.9530312	-0.8677519
C	3.5553088	5.1251326	-2.1811143
C	2.5315187	4.2253434	-2.5680992
C	-1.1865471	0.6833234	-4.1431413
F	-0.7836284	-0.5343175	-4.6125842
F	-0.9015850	1.5982280	-5.1090340
F	-2.5423995	0.6317749	-4.0255866
O	-0.9083679	-1.7228467	1.9355505
C	-0.1852795	-2.4183572	2.7411655
C	-0.8528552	-3.4904316	3.4839205
S	-2.5694975	-3.7663490	3.2004856
C	-2.5933049	-5.0527421	4.3635858
C	-1.3555159	-5.2618961	4.9332708
C	-0.3679092	-4.3753363	4.4358654
O	1.5053089	-0.3602172	1.4245954
C	1.9144682	-1.2006332	2.2796619
C	3.4273819	-1.0619735	2.5990615
F	3.7042572	0.1680507	3.1047330
O	-2.5203928	-1.0844558	-0.3651736
C	1.2004516	-2.1981313	2.9444071
F	3.8847324	-1.9786338	3.4998604
F	4.1747693	-1.2111619	1.4682756
C	0.1057260	3.5228828	3.7782171
F	1.4497582	3.3340812	3.8137402
F	-0.1166524	4.8583134	3.9394606
F	-0.4175569	2.8976181	4.8750130
H	-1.3732797	4.8188617	1.9750781
H	-2.7077687	6.1582576	0.8616316
H	-4.3843472	7.1672306	-0.8884772
H	-5.1012360	5.3692294	-2.6983909
H	4.6994841	5.5017621	-0.3151462
H	3.9926801	5.8721476	-2.8419188
H	2.0946809	4.2082580	-3.5653545
H	0.5946743	2.5994525	-3.6062225
H	1.7333285	-2.8306234	3.6483786
H	0.6679358	-4.3860872	4.7707961
H	-1.1644478	-6.0267960	5.6843920

H	-3.5212129	-5.5849277	4.5548801
H	-2.6803782	-2.0327864	-0.2135254
H	-2.3495137	-0.9627444	-1.3253494
O	0.4359874	-2.0923962	-0.6765384
C	1.0242222	-2.5886863	-1.7024903
C	2.1914180	-1.9334972	-2.2555395
S	2.9529846	-2.4630046	-3.7598368
C	4.1665659	-1.2410644	-3.6115764
C	4.0049318	-0.4747236	-2.4738046
C	2.8870852	-0.8642370	-1.7038007
C	0.5206371	-3.8196855	-2.2751808
C	-0.5592021	-4.4228404	-1.6898977
O	-1.1694442	-3.9566445	-0.6103395
C	-1.1737062	-5.7153847	-2.2165377
F	-0.5442957	-6.1577313	-3.3317392
F	-2.4858290	-5.5343428	-2.5232312
F	-1.1065755	-6.7004250	-1.2828091
H	-0.5976061	-3.0918738	-0.3865210
H	0.9902822	-4.2713502	-3.1447602
H	2.5902695	-0.4014254	-0.7627629
H	4.6775124	0.3381172	-2.2064150
H	4.9319078	-1.1556390	-4.3785497
O	-2.6458757	0.2513298	2.1312522
H	-2.5418248	-0.6708190	2.4489936
H	-2.3877521	0.8015694	2.8938676

$[Y(TTA)_3(HTTA\text{-}flip)(OH_2), H_{in}],(H_2O)$ optimized with the QM/SPP in the chloroform CPCM solvent (Table 6)

Atom	X(Å)	Y(Å)	Z(Å)
C	0.6407381	-2.2723446	-4.5856762
C	1.2523420	-2.4704425	-5.8148204
C	0.6784986	-3.5293376	-6.5623347
C	-0.3697190	-4.1364009	-5.9036715
C	0.9103586	-1.3002019	-3.5232294
C	1.9850201	-0.3835290	-3.6781368
C	2.2811489	0.5792139	-2.7152738
C	2.0996092	-1.9713507	1.3654131
C	1.3419385	-3.1793431	1.4328411
C	0.1045035	-3.3198449	0.8197008
C	3.4057472	-1.9114135	2.0176157
C	5.6204157	-1.1115503	2.8291434
C	5.3541207	-2.4093909	3.2167453
C	4.0958678	-2.8648470	2.7553018
C	-0.6346800	-4.6718089	0.9541524
C	-1.1049676	2.7301976	-1.8247395
C	-1.8042754	3.3531433	-2.9492793
C	-3.1849282	3.6823271	-5.0016307
C	-2.6709437	4.8657334	-4.5140772
C	-1.8873379	4.6797313	-3.3486612
C	0.2449467	3.1035562	0.2258344
C	0.8936367	4.1487435	1.1629276
C	-0.3663739	3.5627902	-0.9286882
C	3.4659749	1.5426135	-2.9832483
C	-1.9443392	0.0759758	2.6384797
C	-3.3850685	-0.1582720	2.6411308
C	-5.8048207	-0.4287437	3.1961827
C	-5.5461008	-0.6072476	1.8508197
C	-4.1760509	-0.4534440	1.5374788
C	-1.2847305	0.3661836	3.8991384
C	-0.0182289	0.8515147	4.0541563
C	0.5669062	1.0025015	5.4653238

F	-1.8387412	-4.5019793	1.5710748
F	0.0520496	-5.6063615	1.6657372
F	-0.8883776	-5.2076622	-0.2729890
F	2.1661760	3.8000589	1.4775169
F	0.9363250	5.4009113	0.6330328
F	0.1944407	4.2336892	2.3337023
F	4.4143477	1.4249819	-2.0156557
F	4.0858559	1.3261956	-4.1795006
F	3.0447887	2.8371672	-2.9817706
F	-0.2816665	0.5743268	6.4339004
F	0.8672874	2.3014334	5.7315722
F	1.7165574	0.2872561	5.5859887
H	2.5938927	-0.4270457	-4.5764481
H	2.0888616	-1.8712366	-6.1707741
H	1.0232718	-3.8350255	-7.5490197
H	-0.9823195	-4.9688201	-6.2396229
H	6.5051480	-0.5175913	3.0432996
H	6.0402078	-3.0105849	3.8113817
H	3.7083346	-3.8618049	2.9588175
H	1.7477860	-4.0266558	1.9778786
H	-0.3227410	4.6287117	-1.1318234
H	-1.3987354	5.4966481	-2.8203407
H	-2.8512000	5.8336666	-4.9791109
H	-3.8146883	3.5336496	-5.8748078
H	-8.2872453	-0.1961474	-0.7474383
H	-8.8988195	-1.4141908	-0.0462919
H	0.5406402	1.3958959	2.2173325
H	-1.8396697	0.1761716	4.8160530
H	-3.7517244	-0.5510143	0.5379665
H	-6.3233406	-0.8397186	1.1190285
H	-6.7591136	-0.4892346	3.7132831
H	-2.4366810	-1.0355869	-2.1193705
H	-2.1248755	-2.0228677	-0.9462353
O	1.7001275	0.7947171	-1.6073219
O	0.1461769	-1.3331851	-2.4940458
O	1.7005689	-0.9229996	0.7505763
O	-0.5415379	-2.4609832	0.1302492
O	-1.2104366	1.4646522	-1.6951858
O	0.3199450	1.8961027	0.6601804
O	-8.0658314	-1.0878903	-0.4281528
O	-1.3062299	0.0126950	1.5523411
O	0.8733577	1.2568081	3.1688231
O	-2.3333010	-1.0835470	-1.1517113
S	-0.6713845	-3.4235532	-4.3512927
S	4.3354097	-0.4219498	1.8948090
S	-2.7165533	2.3162906	-4.0423159
S	-4.3758925	-0.0649761	4.1017684
Y	-0.0996886	-0.1829669	-0.4770348

[$Y(TTA)_3(HTTA\text{-}flip)(OH_2)_2$, H_{in}] optimized with the QM/SPP in the chloroform CPCM solvent (Table 6)

Atom	X(Å)	Y(Å)	Z(Å)
C	1.4686525	-2.0949134	-4.3973462
C	1.3144499	-2.9000889	-5.5167595
C	2.1331351	-2.5084095	-6.6054302
C	2.9102286	-1.4070337	-6.3133523
C	0.8302041	-2.1499584	-3.0782211
C	-0.1050187	-3.1958884	-2.8099162
C	-0.7297342	-3.3361484	-1.5759343
C	-0.7060303	1.4375567	-2.3334773
C	0.5023434	2.1453771	-2.6169304

C	1.6565020	1.9802919	-1.8679883
C	-1.8862340	1.6883462	-3.1603514
C	-4.1954577	1.5942250	-4.0917434
C	-3.3813612	2.4654310	-4.7864968
C	-2.0686189	2.5191775	-4.2573877
C	2.8753800	2.8760425	-2.1840795
C	-0.0952485	-2.3913771	2.8834879
C	0.4243198	-3.3633746	3.8510682
C	1.9705418	-4.8372942	5.1509590
C	0.6522532	-4.9912184	5.5215882
C	-0.2253750	-4.1555299	4.7849953
C	-2.0462022	-1.1427801	2.0294840
C	-3.5441927	-0.7869639	2.2284035
C	-1.4738638	-2.0697044	2.9045312
C	-1.7063414	-4.5219543	-1.3781293
C	0.4809654	2.5051916	2.3687340
C	1.3555888	2.1919472	3.4976799
C	2.8710033	2.2399366	5.4819061
C	2.4992443	0.9591444	5.1294815
C	1.6409261	0.9294435	4.0042524
C	-0.0808643	3.8322667	2.2435245
C	-0.9887339	4.0912972	1.2539858
C	-1.6423213	5.4604098	1.0792488
F	3.1680343	3.6759263	-1.1150546
F	2.6961444	3.6937098	-3.2566223
F	3.9845492	2.1261005	-2.4310125
F	-4.2498421	-0.9763820	1.0853784
F	-4.1565797	-1.5191128	3.2044607
F	-3.6779869	0.5258944	2.5749537
F	-2.9393255	-4.0829222	-1.0124411
F	-1.8684654	-5.2917711	-2.4921065
F	-1.2621592	-5.3472960	-0.3860803
F	-1.2041589	6.3499846	2.0029453
F	-2.9923522	5.3704942	1.1957900
F	-1.3702651	5.9700070	-0.1496646
H	-0.3315857	-3.9157549	-3.5910608
H	0.6317385	-3.7473557	-5.5560555
H	2.1510283	-3.0165912	-7.5684321
H	3.6236645	-0.8996868	-6.9574455
H	-5.2407043	1.3619312	-4.2786871
H	-3.7171475	3.0446812	-5.6453505
H	-1.2817719	3.1483297	-4.6703563
H	0.5094801	2.8730572	-3.4231919
H	-2.1098483	-2.5355659	3.6516995
H	-1.3041878	-4.1446487	4.9311570
H	0.3259803	-5.6835582	6.2962707
H	2.8458367	-5.3444428	5.5477948
H	2.7089475	0.3255006	2.0424724
H	2.9515847	0.7091161	0.5425315
H	-0.9230969	2.3437704	0.5840928
H	0.1716809	4.6142904	2.9547324
H	1.1993931	0.0231859	3.5882368
H	2.8303087	0.0737048	5.6690047
H	3.5291042	2.5542934	6.2875241
H	2.2486166	-2.7289013	0.9516643
H	2.0531727	-3.3158025	-0.4760943
O	-0.6030552	-2.6154213	-0.5335629
O	1.1585968	-1.2569150	-2.2295119
O	-0.8298710	0.6038880	-1.3747533
O	1.8638877	1.1758137	-0.8964093
O	0.7560033	-1.8555163	2.0792783
O	-1.5060686	-0.5075208	1.0796571
O	2.7579767	-0.0486196	1.1421482

O	0.1866407	1.6014285	1.5238627
O	-1.4146956	3.2136319	0.3612508
O	2.3227270	-2.5090366	-0.0017580
S	2.6517418	-0.8271434	-4.6996933
S	-3.3709675	0.8239158	-2.7760218
S	2.1612049	-3.6603844	3.8892806
S	2.1644035	3.4349620	4.4489342
Y	0.5775001	-0.6657528	-0.0155870

[Y(TTA)$_3$(HTTA-flip)(OH$_2$), H$_{in}$] optimized with the QM/SPP in the chloroform CPCM solvent (Tables 5 and 6)

Atom	X(Å)	Y(Å)	Z(Å)
C	-0.5981628	-3.6625677	3.5551319
C	-0.5522738	-4.8938005	4.1933951
C	-0.9645349	-4.8379668	5.5480581
C	-1.3236978	-3.5652625	5.9397712
C	-0.2651698	-3.2830168	2.1800545
C	0.1907046	-4.2858690	1.2757306
C	0.5490245	-3.9872914	-0.0334738
C	0.4552711	1.1297999	2.6546156
C	-0.9098714	1.4115289	2.9694555
C	-1.9814052	1.0175739	2.1795853
C	1.4994553	1.5755476	3.5762019
C	3.7215083	1.9768376	4.6316445
C	2.6818256	2.4952217	5.3765120
C	1.4191927	2.2667006	4.7779018
C	-3.4053361	1.4218979	2.6313269
C	0.1171924	-0.9507196	-3.3983383
C	-0.5256745	-1.2484947	-4.6815398
C	-2.2396232	-1.8144621	-6.4121125
C	-0.9750654	-1.6742918	-6.9421547
C	-0.0026036	-1.3544556	-5.9616024
C	2.2566944	-0.4908422	-2.2187222
C	3.7913783	-0.3185841	-2.3518651
C	1.5314185	-0.7925866	-3.3672819
C	1.0544331	-5.1364180	-0.9398407
C	-0.7947462	2.8108221	-1.1473586
C	-2.1370835	2.8032991	-1.7085210
C	-4.4087052	3.3753275	-2.5711072
C	-4.0943633	2.0415227	-2.7401156
C	-2.8094727	1.7164573	-2.2501598
C	-0.1093668	4.0705325	-0.9477580
C	1.1753745	4.0945320	-0.4838794
C	1.9433839	5.3987485	-0.2818909
F	-3.9587831	2.3011675	1.7464919
F	-3.4514571	2.0084531	3.8586249
F	-4.2260090	0.3350186	2.6758690
F	4.4457197	-1.1761259	-1.5233042
F	4.2624310	-0.5416192	-3.6117686
F	4.1644195	0.9435950	-2.0036085
F	2.3150360	-4.8840131	-1.3855453
F	1.0834828	-6.3504726	-0.3203520
F	0.2583994	-5.2685964	-2.0383127
F	1.1924849	6.4821172	-0.5983397
F	3.0597448	5.4279531	-1.0551995
F	2.3380818	5.5314840	1.0107577
H	0.2781974	-5.3122531	1.6199207
H	-0.2308646	-5.8111883	3.7029041
H	-0.9959297	-5.7008512	6.2116408
H	-1.6746493	-3.2378048	6.9148919
H	4.7851284	2.0090454	4.8529306

H	2.8237301	3.0205184	6.3197397
H	0.4801576	2.5999506	5.2166767
H	-1.1268239	1.9623607	3.8802478
H	2.0819056	-0.9079875	-4.2965198
H	1.0506348	-1.2041936	-6.1921738
H	-0.7536724	-1.7983877	-8.0010761
H	-3.1636395	-2.0584207	-6.9292473
H	-2.6452013	-1.8490452	-1.3899709
H	-3.0721435	-1.2238000	-0.0065926
H	1.3133282	2.2286809	-0.3373248
H	-0.5972497	5.0095482	-1.1960663
H	-2.3473862	0.7315408	-2.3165264
H	-4.7709778	1.3281019	-3.2072545
H	-5.3268210	3.8911269	-2.8396393
O	0.5259811	-2.8584179	-0.6226772
O	-0.3976928	-2.0518246	1.8620002
O	0.8316868	0.5105700	1.6018705
O	-1.9780629	0.3544973	1.0873358
O	-0.6453044	-0.8502416	-2.3724093
O	1.8414062	-0.3165534	-1.0279418
O	-2.3968638	-1.7736459	-0.4507959
O	-0.2065995	1.7167562	-0.8608302
O	1.9063578	3.0360642	-0.1698894
S	-1.1631674	-2.4101841	4.6562471
S	3.1742095	1.2031845	3.1814461
S	-2.2604887	-1.5537369	-4.6972732
S	-3.1274996	4.2606376	-1.8201740
Y	-0.2136580	-0.7316259	-0.0462539

$[Y(TTA)_3(HTTA)(OH_2), H_{in}]$ optimized with the QM/SPP in the chloroform CPCM solvent (Tables 5 and 6)

Atom	X(Å)	Y(Å)	Z(Å)
S	-1.6686449	5.1428566	-0.9036749
C	-1.5753048	4.8948718	0.8370493
C	-1.9542972	6.0431129	1.5179786
C	-2.3154971	7.1101314	0.6584739
C	-2.2113537	6.7738184	-0.6751144
C	-1.1416470	3.5870582	1.3326714
C	-1.0605340	3.3693143	2.7379685
C	-0.6260065	2.1599554	3.2683086
O	-0.2685986	1.1074982	2.6474026
Y	-0.2573445	0.4512846	0.4154527
O	-0.8466708	2.6968310	0.4620845
O	1.1196540	1.3861163	-1.1921025
C	0.9505492	1.9366504	-2.3351923
C	-0.2691526	1.8953550	-3.0721777
C	-1.4233590	1.2659004	-2.6213762
O	-1.6295929	0.6589359	-1.5190322
C	2.0982414	2.6412638	-2.9088125
S	3.5715858	2.7534625	-1.9497379
C	4.3596324	3.6526683	-3.2049982
C	3.5421347	3.8555680	-4.2974631
C	2.2576540	3.2822692	-4.1295150
C	-2.6568193	1.2532744	-3.5577540
F	-2.9264394	-0.0177085	-3.9740764
F	-2.5102733	2.0173449	-4.6750109
F	-3.7649536	1.7030469	-2.9071731
O	-0.6249864	-1.5744957	1.6006317
C	0.0821374	-2.2568912	2.4185613
C	-0.5748387	-3.3714696	3.1063932
S	-2.2728310	-3.6836001	2.7594561

C	-2.2936256	-5.0153768	3.8699078
C	-1.0680115	-5.2122388	4.4699619
C	-0.0921989	-4.2799857	4.0372145
O	1.8331940	-0.1834906	1.1584893
C	2.1979166	-1.0084590	2.0615893
C	3.6839722	-0.8413872	2.4645890
F	3.9195038	0.4193470	2.9191126
O	-2.6285806	0.1095855	0.8782044
C	1.4583630	-1.9998967	2.6930804
F	4.0890887	-1.7016305	3.4408961
F	4.5033939	-1.0410669	1.3937866
C	-0.5374497	2.0188967	4.8077177
F	0.7361902	1.7356443	5.1951607
F	-0.9221478	3.1390671	5.4826721
F	-1.3273165	0.9986647	5.2447903
H	-1.3260314	4.1734336	3.4179774
H	-1.9725253	6.1168974	2.6041157
H	-2.6402139	8.0896626	1.0062156
H	-2.4234983	7.3945672	-1.5416642
H	5.3849797	3.9842743	-3.0638533
H	3.8555496	4.3984958	-5.1878502
H	1.4749670	3.3372255	-4.8843099
H	-0.3029259	2.3822939	-4.0426149
H	1.9626146	-2.6188323	3.4295769
H	0.9337535	-4.2768915	4.4013407
H	-0.8775580	-6.0002024	5.1969918
H	-3.2110935	-5.5799269	4.0129388
H	-2.8171567	-0.7400005	1.3184482
H	-3.1536806	0.1450445	0.0555761
O	0.0128163	-1.5774007	-1.1600109
C	0.6218296	-2.5344245	-1.7515472
C	2.0512649	-2.4700212	-1.9889381
S	2.9339020	-3.7988065	-2.7560059
C	4.4126646	-2.9088779	-2.6718250
C	4.2453504	-1.6659670	-2.0941956
C	2.9108762	-1.4145668	-1.7070913
C	-0.1344503	-3.6842192	-2.2091843
C	-1.4907032	-3.7191660	-2.0531148
O	-2.2138019	-2.7548708	-1.4995244
C	-2.3436216	-4.8939986	-2.5210238
F	-1.5897516	-5.8836526	-3.0577593
F	-3.2397297	-4.4970006	-3.4620431
F	-3.0474815	-5.4225336	-1.4859856
H	-1.5164818	-2.0453501	-1.2493720
H	0.3642779	-4.5190206	-2.6943825
H	2.5706220	-0.4957604	-1.2313864
H	5.0634745	-0.9623394	-1.9535172
H	5.3265226	-3.3581765	-3.0516811

[Y(TTA)$_3$(HTTA-flip)(OH$_2$), H$_{out}$] optimized with the QM/SPP in the chloroform CPCM solvent (Table 6)

Atom	X(Å)	Y(Å)	Z(Å)
C	-0.6689390	-3.7691219	3.5548795
C	-0.6505377	-5.0174071	4.1592998
C	-1.0943298	-4.9947745	5.5056068
C	-1.4495430	-3.7298612	5.9243447
C	-0.3009480	-3.3514345	2.1976517
C	0.1748219	-4.3308457	1.2776717
C	0.5698629	-3.9902372	-0.0110293
C	0.5455211	1.0867007	2.7586475
C	-0.8018135	1.3935003	3.1153612

C	-1.9076196	0.9783289	2.3812032
C	1.6316336	1.6016894	3.6013193
C	3.9099396	2.1479591	4.4672139
C	2.9053978	2.6289164	5.2785312
C	1.6112005	2.3207634	4.7859306
C	-3.3099740	1.4081544	2.8784837
C	0.0880698	-0.9572480	-3.3466777
C	-0.5587788	-1.2808457	-4.6251589
C	-2.2671331	-1.9356232	-6.3314072
C	-1.0266270	-1.7013073	-6.8836378
C	-0.0573706	-1.3310382	-5.9165284
C	2.2259947	-0.4217224	-2.1939049
C	3.7467399	-0.1639704	-2.3567802
C	1.4908391	-0.7168206	-3.3402859
C	1.1072433	-5.1098451	-0.9362427
C	-0.9055341	2.6784687	-1.1913081
C	-2.1529443	2.8072898	-1.9522766
C	-4.1948031	3.5593160	-3.1842854
C	-4.0512045	2.1864162	-3.1763157
C	-2.8977065	1.7619680	-2.4782571
C	-0.1322889	3.8973499	-0.9540231
C	1.0695901	3.9695148	-0.3278268
C	1.7859266	5.3141711	-0.1918002
F	-3.8884024	2.2724588	1.9934665
F	-3.3038405	2.0269618	4.0919635
F	-4.1401196	0.3335014	2.9825359
F	4.4677954	-0.9855222	-1.5475266
F	4.2064421	-0.3512193	-3.6273830
F	4.0583617	1.1173133	-2.0079938
F	2.3848948	-4.8458286	-1.3255849
F	1.1129701	-6.3449670	-0.3574449
F	0.3542389	-5.2050429	-2.0680300
F	0.9514871	6.3691097	-0.2792440
F	2.7419766	5.4555890	-1.1505775
F	2.4245408	5.3795004	1.0160190
H	0.2524253	-5.3672388	1.5932689
H	-0.3275441	-5.9242447	3.6504756
H	-1.1504081	-5.8755315	6.1436873
H	-1.8202189	-3.4257494	6.8997255
H	4.9844211	2.2391298	4.6025943
H	3.0910281	3.1846912	6.1965010
H	0.6931350	2.6159904	5.2914354
H	-0.9781113	1.9880303	4.0074510
H	2.0266801	-0.7758452	-4.2833723
H	0.9782259	-1.1057046	-6.1653576
H	-0.8191300	-1.7937609	-7.9486913
H	-3.1828647	-2.2356741	-6.8335713
H	-2.6199596	-1.7163381	-1.3338367
H	-3.0655479	-1.1735374	0.0829303
H	2.5319501	3.1736477	0.6423327
H	-0.5383266	4.8379044	-1.3221349
H	-2.5755647	0.7269796	-2.3744314
H	-4.7558564	1.5137993	-3.6622845
H	-4.9871492	4.1531505	-3.6322846
O	0.5611618	-2.8446777	-0.5648693
O	-0.4205260	-2.1130490	1.9130921
O	0.8838735	0.3986619	1.7415156
O	-1.9506859	0.2914237	1.3097289
O	-0.6601494	-0.9127527	-2.3094364
O	1.8347879	-0.3186223	-0.9908609
O	-2.3978818	-1.7129981	-0.3843915
O	-0.5385685	1.5525119	-0.7878980
O	1.7295081	2.9092062	0.1479478

S	-1.2473605	-2.5416702	4.6767322
S	3.2898620	1.2976969	3.0859357
S	-2.2683808	-1.7037370	-4.6115488
S	-2.9084329	4.3547564	-2.3439308
Y	-0.2021642	-0.7173808	0.0347744

[$Y(TTA)_3(HTTA)(OH_2)$, H_{out}] optimized with the QM/SPP in the chloroform CPCM solvent (Tables 5 and 6)

Atom	X(Å)	Y(Å)	Z(Å)
S	-2.0301614	4.9349730	-1.0342534
C	-1.8942886	4.7607546	0.7123286
C	-2.3241595	5.9123231	1.3557847
C	-2.7582369	6.9239756	0.4630513
C	-2.6583597	6.5419425	-0.8583348
C	-1.3769753	3.4983837	1.2484626
C	-1.2598201	3.3422026	2.6597815
C	-0.7490915	2.1785138	3.2231684
O	-0.3389806	1.1290816	2.6313649
Y	-0.2456613	0.3942180	0.4157727
O	-1.0489468	2.5929784	0.4081945
O	1.1666242	1.4293226	-1.0960862
C	1.0708495	1.9637436	-2.2539342
C	-0.0824210	1.8764609	-3.0858428
C	-1.2490429	1.2148529	-2.7135380
O	-1.5158952	0.6169477	-1.6238702
C	2.2406646	2.6996239	-2.7419480
S	3.6459399	2.8170134	-1.6870903
C	4.4988799	3.7523774	-2.8722736
C	3.7505068	3.9631854	-4.0115403
C	2.4675432	3.3656418	-3.9377959
C	-2.4065206	1.1501417	-3.7410602
F	-2.6164724	-0.1386683	-4.1439015
F	-2.1924059	1.8875845	-4.8657458
F	-3.5726677	1.5875197	-3.1918495
O	-0.5452824	-1.5785763	1.7649330
C	0.1900579	-2.1901328	2.6081621
C	-0.4211061	-3.2873190	3.3682713
S	-2.1213623	-3.6514575	3.0914352
C	-2.0769763	-4.9343667	4.2584771
C	-0.8297017	-5.0754298	4.8278582
C	0.1100569	-4.1412691	4.3230465
O	1.8652095	-0.1234561	1.2283189
C	2.2638362	-0.8997456	2.1587987
C	3.7547388	-0.6842356	2.5197943
F	3.9771006	0.6018797	2.9055628
O	-2.5779506	-0.2900916	0.6082769
C	1.5621172	-1.8787359	2.8498974
F	4.2023398	-1.4863704	3.5266281
F	4.5535616	-0.9208054	1.4390655
C	-0.6355185	2.0941984	4.7652445
F	0.6561653	1.8938812	5.1458588
F	-1.0728066	3.2143822	5.4087104
F	-1.3634508	1.0484068	5.2470137
H	-1.5625794	4.1537988	3.3149106
H	-2.3275606	6.0274616	2.4384921
H	-3.1301976	7.8973618	0.7794764
H	-2.9189626	7.1157258	-1.7438150
H	5.5075386	4.0965989	-2.6593167
H	4.1111115	4.5285229	-4.8696367
H	1.7333477	3.4241942	-4.7396653
H	-0.0536500	2.3480411	-4.0640568

H	2.0947693	-2.4451094	3.6084271
H	1.1463385	-4.0989488	4.6539476
H	-0.5979929	-5.8245532	5.5835190
H	-2.9767412	-5.5103363	4.4575476
H	-2.5129193	-1.2138026	0.9243394
H	-2.8481618	-0.3187762	-0.3335086
O	0.1146406	-1.5442037	-0.9607275
C	0.5599956	-2.4397624	-1.7125794
C	1.9589661	-2.4155679	-2.1368715
S	2.6607772	-3.6036722	-3.2437370
C	4.2053055	-2.8322697	-3.1513758
C	4.1891425	-1.7292401	-2.3207610
C	2.9205173	-1.4912224	-1.7467217
C	-0.2809859	-3.5382833	-2.1962355
C	-1.6093679	-3.6984350	-1.9866959
O	-2.3902110	-2.8766423	-1.2615112
C	-2.3232699	-4.9334626	-2.5408040
F	-1.6973416	-5.4769389	-3.6018089
F	-3.5947707	-4.5987688	-2.9253974
F	-2.4437325	-5.8959755	-1.5859405
H	-3.3313523	-3.1118751	-1.3945873
H	0.1951439	-4.3116663	-2.7971297
H	2.6961477	-0.6763863	-1.0587836
H	5.0684157	-1.1156827	-2.1334539
H	5.0390689	-3.2383692	-3.7181721

[$Y(TTA)_3(HTTA)(OH_2)$, H_{in}] – triclinic optimized with the QM/SPP in the chloroform CPCM solvent (Table 6)

Atom	X(Å)	Y(Å)	Z(Å)
C	1.6903640	1.5745104	13.0502271
C	2.5464703	1.1715569	12.0375743
S	2.0406280	1.8630414	10.4953438
C	0.7018174	2.6680869	11.2488884
C	0.6464829	2.4219393	12.6041844
C	3.7211907	0.3041166	12.1957603
O	3.9154852	-0.1870700	13.3582520
Y	5.5605363	-1.4294444	14.4318633
O	6.7987401	-3.5464530	14.0631536
O	7.1934191	-1.6081249	16.0923844
C	8.0396967	-0.7739739	16.5531644
C	8.7448779	-1.2725263	17.8381980
F	9.6687922	-0.4012678	18.3320424
C	8.3901410	0.4740929	16.0509123
C	7.8362487	1.0007973	14.8486019
O	6.9663980	0.3866583	14.1381148
C	8.2901575	2.3069202	14.3682862
C	9.2004924	3.2070176	14.9038973
C	9.3532172	4.3798554	14.1237007
C	8.5601275	4.3717785	12.9951221
S	7.6093558	2.9274153	12.8675693
O	4.0638993	-3.1906725	13.3982363
O	4.2922039	-2.6949580	15.9467030
C	3.7700331	-2.5178675	17.1065769
C	3.2076188	-3.7040833	17.7640402
S	2.3013269	-3.6331776	19.2766099
C	2.0777915	-5.3526878	19.2722189
C	2.6648608	-5.9474752	18.1762665
C	3.3034762	-5.0144622	17.3220712
O	4.7666813	0.0673983	16.0553064
C	4.1809913	-0.0818361	17.1700645
C	3.9845995	1.2501127	17.9399299

F	3.3619004	1.1019938	19.1429885
O	6.1135094	-1.4596260	12.1371055
C	5.6706489	-0.7994673	11.1418682
C	6.4976498	-1.0227372	9.8510984
F	6.0517265	-0.3113426	8.7794480
C	3.7039259	-1.2556317	17.7531209
F	3.2341708	2.1198571	17.2061206
F	5.1800785	1.8528124	18.1790038
C	4.5691301	0.0481168	11.0775384
F	7.8007870	-0.6769716	10.0467309
F	6.4822222	-2.3383150	9.4936345
F	9.3902002	-2.4512220	17.6087322
F	7.8389336	-1.4993738	18.8291530
H	0.0342839	3.2753123	10.6433127
H	-0.1203961	2.8408328	13.2538308
H	1.8373455	1.2589879	14.0812733
H	3.2435418	-1.1908678	18.7364210
H	4.3436645	0.5248142	10.1260306
H	1.5231574	-5.8212007	20.0808520
H	2.6376924	-7.0210368	17.9966648
H	3.8368258	-5.2793879	16.4108088
H	9.1361978	1.0551617	16.5851287
H	9.7406347	3.0314711	15.8327999
H	10.0203977	5.2009549	14.3816672
H	8.4791171	5.1365682	12.2271577
H	3.3572417	-3.3740846	14.0461311
H	3.6330304	-3.0653378	12.5352239
C	7.9272170	-4.1475888	14.1119006
C	9.1533725	-3.4406097	13.8024910
S	10.7483535	-4.1158751	14.1515628
C	11.5204757	-2.7315266	13.4640298
C	10.6132044	-1.8084680	12.9811675
C	9.2724110	-2.2069182	13.1723301
H	12.6057935	-2.6738539	13.4618786
H	10.9120669	-0.8787347	12.5007355
H	8.4059957	-1.6424127	12.8286904
C	7.9609538	-5.5584531	14.4313937
H	8.9076108	-6.0884247	14.4963819
C	6.7966621	-6.2507513	14.6072273
O	5.5769797	-5.7381999	14.5075983
C	6.7709255	-7.7425533	14.9262382
F	6.1163201	-8.4335114	13.9558257
F	8.0178580	-8.2590210	15.0337635
F	6.1220809	-7.9735141	16.0977210
H	5.7218240	-4.7522488	14.2776117

[Y(TTA)$_3$(HTTA-flip)(OH$_2$), H$_{in}$] – triclinic optimized with the QM/SPP in the chloroform CPCM solvent (Table 6)

Atom	X(Å)	Y(Å)	Z(Å)
C	3.3321843	3.1670350	13.9510963
C	3.6765708	2.5239563	12.7727081
S	3.6382682	3.6572137	11.4211038
C	3.1652044	4.9548564	12.4699810
C	3.0422548	4.5428251	13.7799439
C	4.0326996	1.1059696	12.6377621
O	4.0167625	0.4091758	13.7064870
Y	4.7173034	-1.6905849	14.3852229
O	6.2648145	-3.4921761	13.7743476
O	5.3945002	-0.5034681	16.2690747
C	6.2332870	0.4339133	16.4492093
C	6.1342936	1.0807810	17.8539746

F	7.0263588	2.0922173	18.0544152
C	7.1927649	0.9200532	15.5645790
C	7.4254581	0.3326881	14.2919623
O	6.7787642	-0.6935452	13.8577983
C	8.4482585	0.9106283	13.4220487
C	9.4001067	1.8891036	13.6798820
C	10.2066929	2.1952850	12.5578590
C	9.8655338	1.4559854	11.4433881
S	8.5575984	0.3644699	11.7526333
O	2.8879978	-3.1197760	13.4117935
O	4.6506486	-3.2538256	16.1123987
C	4.0157380	-3.3601839	17.2148245
C	4.5470380	-4.3214496	18.1908367
S	3.7758664	-4.6691204	19.7390137
C	5.0258272	-5.7965012	20.1566312
C	5.9800450	-5.8998825	19.1671062
C	5.7082765	-5.0648500	18.0553364
O	2.6358925	-1.3833853	15.4742338
C	2.2405087	-1.7366233	16.6342918
C	0.9000461	-1.0768324	17.0402611
F	0.4489458	-1.4531191	18.2685662
O	4.6440344	-1.7215900	12.0011540
C	4.5925949	-0.7790806	11.1417266
C	4.7962837	-1.2751353	9.6900662
F	4.7634437	-0.2839470	8.7579943
C	2.8347739	-2.6229709	17.5244778
F	-0.0773080	-1.3965472	16.1407232
F	1.0061797	0.2787494	17.0491084
C	4.3471255	0.5717734	11.3512790
F	5.9893486	-1.9144078	9.5547702
F	3.8220216	-2.1728060	9.3550648
F	6.3566952	0.1526384	18.8249638
F	4.8925734	1.5956620	18.0647454
H	3.0058677	5.9462843	12.0543641
H	2.7526596	5.2115771	14.5889559
H	3.2961985	2.6364348	14.9005102
H	2.3504131	-2.7854344	18.4849454
H	4.3369707	1.2332555	10.4877356
H	4.9802842	-6.3156806	21.1102545
H	6.8470229	-6.5543209	19.2432428
H	6.3332008	-4.9887841	17.1681299
H	7.7977249	1.7684118	15.8710425
H	9.5220281	2.3637783	14.6520438
H	11.0087760	2.9316819	12.5658686
H	10.3108429	1.4911794	10.4526071
H	2.0359344	-2.7577610	13.7208525
H	2.9301652	-2.9682168	12.4467614
C	6.7247180	-4.6738664	13.6923196
C	5.8531246	-5.8389838	13.7530540
S	6.4834802	-7.4886214	13.6052756
C	4.8997249	-8.1511804	13.7933200
C	3.9395939	-7.1727735	13.9604472
C	4.4767575	-5.8668579	13.9393511
H	4.7664041	-9.2295887	13.7669373
H	2.8824140	-7.3953422	14.0942600
H	3.8833448	-4.9614916	14.0460911
C	8.1507033	-4.8912032	13.5363937
H	8.5366175	-5.9060799	13.4782740
C	9.0524785	-3.8724718	13.4651736
O	8.8185520	-2.5695631	13.5069410
C	10.5502111	-4.1441967	13.3185170
F	11.0303919	-3.6011874	12.1695320
F	11.2433843	-3.5945526	14.3501318

F	10.8293955	-5.4702606	13.2952386
H	7.8356595	-2.3857128	13.5772730

[Y(TTA)$_3$(HTTA)(TMP), H$_{in}$] optimized with the QM/SPP in the chloroform CPCM solvent (Tables 5 and 6)

Atom	X(Å)	Y(Å)	Z(Å)
C	0.5641837	3.2624583	-4.8848551
C	0.2848915	2.2648003	-3.9623514
S	-0.7026477	1.0018057	-4.6889395
C	-0.7147318	1.8392638	-6.2077669
C	-0.0047725	3.0207375	-6.1606292
C	0.6661710	2.1214171	-2.5533225
O	0.2686976	1.0771158	-1.9403301
Y	0.1433862	0.3549333	0.3188936
O	2.2183587	-0.6110612	1.1267394
P	3.1060034	-1.0610681	2.2664999
O	4.1675026	0.0486776	2.7814236
C	3.7268261	1.4355921	2.9762396
O	-1.8731268	-0.4112790	-0.6557965
C	-2.9374065	0.1821243	-1.0158535
C	-3.2956545	1.5148968	-0.8274793
C	-2.4638668	2.4375834	-0.1322237
C	-2.9154543	3.8217412	0.0757251
C	-2.2359535	4.7996874	0.7828024
C	-2.9142526	6.0437491	0.8216590
C	-4.1137050	6.0191070	0.1432776
S	-4.4329712	4.4627604	-0.5551499
O	-1.3241827	2.1345988	0.3549557
O	0.1274080	1.1020380	2.5407834
C	-0.4726014	0.6930161	3.5841459
C	-1.1218519	-0.5185270	3.7965448
C	-1.1504521	-1.5545418	2.8162545
C	-1.7253399	-2.8624176	3.1729705
C	-1.9744139	-3.9190290	2.3136249
C	-2.5454673	-5.0481223	2.9540392
C	-2.7324587	-4.8588082	4.3058021
S	-2.2115696	-3.2845833	4.8169365
O	-0.7037870	-1.4188339	1.6301861
O	1.7473847	2.0838492	0.1946063
C	1.9503797	3.0169280	-0.6507726
C	1.4698621	3.1345219	-1.9487073
C	-3.9491838	-0.7497368	-1.7296542
F	-5.0629097	-0.1051816	-2.1828246
F	-4.3738215	-1.7336999	-0.8883049
F	-3.3781810	-1.3580149	-2.8044724
C	-0.4203795	1.7060260	4.7557544
F	0.8691350	1.9039022	5.1666029
F	-1.1261234	1.3142222	5.8549602
F	-0.9074487	2.9173871	4.3797669
C	2.9007670	4.1213409	-0.1265258
F	3.0530973	5.1710642	-0.9823131
F	2.4589550	4.6299981	1.0543516
F	4.1492157	3.6112387	0.1005416
O	4.0723167	-2.3201700	1.9625715
C	5.1113476	-2.2152695	0.9450935
O	2.2236687	-1.5800640	3.5077262
C	2.8658133	-2.0625337	4.7261638
H	-4.2615084	1.8482395	-1.2004673
H	-1.2773358	4.5953697	1.2556369
H	-2.5374118	6.9295443	1.3308232
H	-4.8330307	6.8226161	0.0092744

H	-1.5815661	-0.6954203	4.7662724
H	-1.7559977	-3.8593590	1.2493212
H	-2.8140257	-5.9699853	2.4402329
H	-3.1444975	-5.5497527	5.0364447
H	1.7574123	4.0034578	-2.5336506
H	-1.2497464	1.4116895	-7.0517057
H	0.1025774	3.6902816	-7.0128296
H	1.1592291	4.1441291	-4.6519513
H	5.8397992	-1.4438873	1.2246286
H	5.5948407	-3.1962112	0.9153699
H	4.6663596	-1.9880314	-0.0324327
H	3.5846765	-1.3248049	5.1052736
H	3.3669610	-3.0186724	4.5324720
H	2.0551399	-2.1996469	5.4476400
H	3.1650899	1.5139553	3.9144822
H	3.1075349	1.7626352	2.1320623
H	4.6464323	2.0252634	3.0360455
O	0.6580762	-1.6175728	-1.0730986
C	1.2902124	-2.2244568	-1.9935226
C	0.7845867	-3.4886133	-2.4900866
C	-0.3791404	-4.0154241	-2.0083530
O	-1.1707957	-3.4688704	-1.0974089
C	-0.9194763	-5.3601993	-2.4900516
F	-2.1453759	-5.2179646	-3.0548138
F	-1.0469908	-6.2277326	-1.4507630
F	-0.1044496	-5.9344372	-3.4083794
H	-0.7632748	-2.5772980	-0.8491212
H	1.3341306	-4.0444316	-3.2454770
C	2.5216352	-1.6771635	-2.5451028
C	3.2273785	-0.5626647	-2.1088905
C	4.3887691	-0.3004949	-2.8698228
C	4.5764751	-1.2114652	-3.8902375
S	3.3334530	-2.4111010	-3.9337860
H	5.3747765	-1.2438563	-4.6270356
H	5.0686621	0.5283085	-2.6808598
H	2.9130291	0.0301176	-1.2525731

[Y(TTA)$_3$(HTTA-flip)(TMP), H$_{in}$] optimized with the QM/SPP in the chloroform CPCM solvent (Tables 5 and 6)

Atom	X(Å)	Y(Å)	Z(Å)
C	1.4059723	-2.8094282	-5.0669873
C	1.3307479	-2.3931090	-3.7450467
C	2.9367687	-4.2715419	-4.1016693
C	2.3201006	-3.8729255	-5.2695121
C	0.5109735	-1.3577050	-3.1100321
C	-1.5495666	4.0056954	-1.1353911
C	-1.4228249	-2.5868812	1.8396503
C	-2.2753436	-3.2398673	0.9638164
C	-2.3841823	-2.8640404	-0.4108888
C	-3.2467817	-3.6442093	-1.3115500
C	-3.4409365	-3.4076345	-2.6619789
C	-4.3354539	-4.3202272	-3.2747686
C	-4.8281313	-5.2577484	-2.3924478
C	-3.1779755	1.1668474	1.4049475
C	-2.5433224	1.8463614	2.4394540
C	-1.1228729	1.9464765	2.5192467
C	-0.5118636	2.7564479	3.5858345
C	0.8269779	3.0917424	3.6907579
C	1.1228069	3.8964222	4.8200230
C	0.0097003	4.1761450	5.5828637
C	-1.3589121	0.2540732	-3.3686972

C	-0.4978547	-0.7175972	-3.8808768
C	-1.3061280	-3.1289694	3.2836106
C	-4.7266654	1.1564252	1.3715721
C	-2.3550299	0.9249289	-4.3512755
C	1.8715795	3.0951338	-3.7210150
C	2.1110723	5.4695013	-0.0041920
C	2.9340007	-0.1196849	1.2046398
C	4.1975808	0.1960370	0.5615722
C	4.3386989	0.1975809	-0.7939769
C	5.6724826	0.5324680	-1.4588992
C	2.8778826	-0.1710038	2.6567036
C	1.7937309	-0.5464890	3.4388933
C	2.0696955	-0.5187314	4.8240088
C	3.3608158	-0.1204861	5.1079444
F	-2.1799635	-4.1328067	3.5677980
F	-1.5232194	-2.1399911	4.1953462
F	-0.0507705	-3.6144798	3.5157068
F	-5.1887064	1.7705636	0.2459266
F	-5.3013423	1.7889496	2.4349255
F	-5.2037484	-0.1170974	1.3595375
F	-2.2469019	0.4840616	-5.6377472
F	-3.6410121	0.7106627	-3.9638197
F	-2.1644899	2.2761652	-4.3792749
F	5.5414694	1.5887292	-2.3050134
F	6.1283270	-0.5185724	-2.1911805
F	6.6306035	0.8483807	-0.5533880
H	-2.8467125	-4.0890316	1.3323027
H	-2.9359067	-2.5903850	-3.1733310
H	-4.6121820	-4.2916421	-4.3277729
H	-5.5265656	-6.0682026	-2.5844712
H	-3.1563709	2.3470051	3.1857520
H	1.5534814	2.7592598	2.9522437
H	2.1190221	4.2602016	5.0681105
H	-0.0564337	4.7580036	6.4986478
H	-0.6012092	-0.9912239	-4.9272860
H	3.6711047	-5.0613192	-3.9652400
H	2.5180224	-4.3306022	-6.2378380
H	0.8262859	-2.3580974	-5.8707367
H	0.9782972	3.5652645	-4.1510530
H	2.7554744	3.3596377	-4.3086751
H	1.7568164	2.0045757	-3.6860750
H	1.2670014	6.0966686	-0.3190348
H	2.9540489	5.5886004	-0.6959376
H	2.4161162	5.7365597	1.0121454
H	-1.5382866	4.1775117	-0.0510124
H	-1.8777205	2.9853810	-1.3684357
H	-2.2058058	4.7357999	-1.6186221
H	2.5547863	-0.3271323	-1.2364747
H	5.0719432	0.4276958	1.1654432
H	3.8338686	-0.0080067	6.0803730
H	1.3487591	-0.7819524	5.5959524
H	0.8425844	-0.8404247	2.9943343
O	0.7582046	-1.0835011	-1.8811584
O	0.7249222	1.9040880	-0.9085691
O	-0.2220710	4.2424284	-1.7053860
O	-0.6712779	-1.5764730	1.6164351
O	-1.7526739	-1.8872720	-0.9207905
O	-2.6530797	0.5451042	0.4274027
O	-0.3285241	1.3931696	1.6908930
O	-1.4637549	0.6887079	-2.1829923
O	2.1204270	3.6189200	-2.3805558
O	1.7130636	4.0664680	0.0640728
O	1.9082695	-0.3669906	0.4986652

O	3.4137771	-0.0830472	-1.7015529
P	1.0397528	3.3487622	-1.2129397
S	2.4139113	-3.3441820	-2.7338739
S	-4.1988265	-5.0353685	-0.7909050
S	-1.4258311	3.4578930	4.9222935
S	4.2700408	0.2252014	3.6780734
Y	-0.4839287	-0.0586810	-0.1571851

[Y(TTA)$_3$(HTTA)(TMP), H$_{out}$] optimized with the QM/SPP in the chloroform CPCM solvent (Tables 5 and 6)

Atom	X(Å)	Y(Å)	Z(Å)
C	1.1156349	4.1824199	-4.1212980
C	0.5204414	3.3555070	-3.1800797
S	-1.1895013	3.7347225	-3.0109770
C	-1.0652365	4.9871932	-4.2047358
C	0.2146741	5.1101519	-4.7029116
C	1.0802349	2.2738739	-2.3577175
O	0.2964901	1.6808238	-1.5507168
Y	0.4048342	-0.0702843	0.0671337
O	1.3670110	-2.2685225	0.1598607
P	2.1473767	-3.5212920	-0.1402318
O	3.7587612	-3.3600047	-0.0835288
C	4.3556680	-2.4295569	0.8781138
O	-1.8766534	0.5358100	-0.1275696
C	-2.4934909	1.6086089	0.1613191
C	-2.0288382	2.7363938	0.8303640
C	-0.7032053	2.8454416	1.3420479
C	-0.2977787	4.0684593	2.0553306
C	0.9632337	4.3330916	2.5626387
C	1.0655975	5.5975175	3.1958537
C	-0.1181364	6.3026899	3.1742139
S	-1.3820705	5.4233830	2.3729637
O	0.1812143	1.9360769	1.2333475
O	1.9548817	-0.0489391	1.8821877
C	1.8095034	-0.0446717	3.1363434
C	0.6819948	-0.3646310	3.8986616
C	-0.5401747	-0.8199412	3.3438513
C	-1.6319695	-1.2146383	4.2470188
C	-2.9793969	-1.2871716	3.9377096
C	-3.7936662	-1.6690162	5.0344760
C	-3.0683084	-1.8927527	6.1837550
S	-1.3700301	-1.6303757	5.9404300
O	-0.7655428	-0.8962077	2.0816617
O	2.5339721	0.1558097	-0.9091828
C	3.0582965	0.9288677	-1.7738770
C	2.4620606	1.9468530	-2.5071582
C	-3.9718886	1.6008051	-0.3027647
F	-4.6399315	2.7620440	-0.0502656
F	-4.6659350	0.6017504	0.3188491
F	-4.0641238	1.3725769	-1.6417267
C	3.0999981	0.3600638	3.9024861
F	4.0927722	-0.5528773	3.6917715
F	2.9349704	0.4601628	5.2520713
F	3.5654518	1.5622652	3.4685077
C	4.5646573	0.6528253	-2.0068102
F	5.1478304	1.4953061	-2.9071642
F	5.2669742	0.7634280	-0.8465030
F	4.7589896	-0.6165502	-2.4717169
O	1.9338373	-4.2194800	-1.5824637
C	2.3375952	-3.5002038	-2.7882459
O	1.7033006	-4.6908630	0.8812527

C	2.3288829	-6.0069283	0.8089116
H	-2.7181400	3.5649378	0.9774969
H	1.7765632	3.6165252	2.4659682
H	1.9769834	5.9799104	3.6531662
H	-0.3276791	7.2879641	3.5820643
H	0.7548154	-0.2756397	4.9801293
H	-3.3604079	-1.0420972	2.9489419
H	-4.8765594	-1.7715911	4.9838033
H	-3.4266664	-2.2054160	7.1608282
H	3.0699820	2.5096276	-3.2095995
H	-1.9467632	5.5651485	-4.4696085
H	0.4966024	5.8417716	-5.4588571
H	2.1704895	4.1269856	-4.3855659
H	3.4245312	-3.3543607	-2.7925898
H	2.0383786	-4.1391343	-3.6244628
H	1.8195935	-2.5341212	-2.8430188
H	3.4214682	-5.9205767	0.8710726
H	2.0393463	-6.5118942	-0.1208468
H	1.9480386	-6.5599344	1.6728959
H	4.2858260	-2.8466957	1.8908138
H	3.8537245	-1.4565755	0.8253347
H	5.4053341	-2.3417300	0.5825262
O	-0.2211135	-1.0828754	-2.0856887
C	-1.1807105	-1.5827296	-2.7241972
C	-2.3362510	-2.2137752	-2.0905111
C	-2.4447558	-2.4388753	-0.7568917
O	-1.4473701	-2.2193829	0.0956709
C	-3.6852998	-3.1161697	-0.1750500
F	-4.0576981	-2.5209281	0.9921110
F	-3.4269317	-4.4235012	0.1117505
F	-4.7431236	-3.0806505	-1.0152012
H	-1.6602175	-1.9510563	1.0432614
H	-3.1728808	-2.5145986	-2.7180469
C	-1.1436774	-1.5238381	-4.1874653
C	-0.1963741	-0.8541389	-4.9502201
C	-0.4108890	-0.9699315	-6.3421956
C	-1.5216274	-1.7308375	-6.6490888
S	-2.3255645	-2.3155477	-5.2328988
H	-1.9162806	-1.9842795	-7.6295112
H	0.2221284	-0.5108120	-7.0996023
H	0.6156340	-0.2933570	-4.4910031

[Y(TTA)$_3$(HTTA-flip)(TMP), H$_{out}$] optimized with the QM/SPP in the chloroform CPCM solvent (Tables 5 and 6)

Atom	X(Å)	Y(Å)	Z(Å)
C	-1.1992532	0.0757088	-5.9740736
C	-0.8156714	-0.2849335	-4.6907070
C	-0.2346229	-1.9953725	-6.4116628
C	-0.8695210	-0.8967735	-6.9520590
C	-0.9636369	0.4144541	-3.4076600
C	-2.0817224	4.0334787	1.9831974
C	0.7472200	-2.8666976	-0.6469089
C	-0.4791247	-3.5037133	-0.8281903
C	-1.7277249	-2.8351103	-0.6803250
C	-2.9817557	-3.5780366	-0.8994740
C	-4.2613660	-3.0595250	-0.7984012
C	-5.2811682	-4.0080671	-1.0668400
C	-4.7828822	-5.2553794	-1.3739295
C	-2.9047288	0.1224967	2.2110354
C	-2.2745915	-0.6908874	3.1512631
C	-0.9066628	-1.0801855	3.0568801

C	-0.3098373	-1.8836417	4.1401443
C	0.9046400	-2.5460332	4.0900281
C	1.2118666	-3.2595876	5.2770587
C	0.2326405	-3.1413676	6.2390298
C	-1.7109018	2.4425374	-2.2261803
C	-1.5903315	1.6978283	-3.3930749
C	2.0341473	-3.7191127	-0.7940576
C	-4.3930777	0.4867232	2.4542734
C	-2.3835055	3.8347787	-2.3224648
C	1.6059101	4.5741752	-0.1635812
C	1.3577746	4.5743076	4.1993176
C	3.0228353	0.9280718	-0.6641719
C	3.7657111	1.3568053	-1.8524252
C	3.2348602	1.9419732	-2.9537640
C	4.1249435	2.2913040	-4.1458665
C	3.7905549	0.4440209	0.4808990
C	3.2813729	0.0219468	1.7025618
C	4.2821248	-0.3596020	2.6237536
C	5.5596412	-0.2333988	2.1148135
F	1.8079811	-5.0004980	-1.2061997
F	2.6985492	-3.7996372	0.3965370
F	2.8929561	-3.1611442	-1.6906204
F	-4.5482861	1.8359178	2.5944598
F	-4.9317197	-0.0892684	3.5667704
F	-5.1644156	0.1067865	1.3979866
F	-2.8276103	4.1490029	-3.5738341
F	-3.4544199	3.9208188	-1.4879670
F	-1.5116334	4.8212341	-1.9563941
F	3.7645895	3.5114063	-4.6535003
F	3.9653387	1.3872131	-5.1514295
F	5.4349216	2.3415521	-3.8358707
H	-0.4757329	-4.5594009	-1.0912613
H	-4.4329049	-2.0174136	-0.5353608
H	-6.3468121	-3.7847096	-1.0358319
H	-5.3288283	-6.1626955	-1.6193348
H	-2.8578296	-1.0365953	4.0021667
H	1.5330603	-2.5168970	3.2017876
H	2.1189397	-3.8452597	5.4208917
H	0.2063250	-3.5717393	7.2368006
H	-1.9751647	2.1126950	-4.3204460
H	0.1262230	-2.8822073	-6.9266085
H	-1.0913263	-0.7937539	-8.0135622
H	-1.7062771	1.0109103	-6.2075137
H	0.8249435	5.3359975	-0.2733909
H	2.5802484	4.9891357	-0.4397280
H	1.3740544	3.6971146	-0.7808185
H	0.5426670	5.3077059	4.1440369
H	2.2778833	4.9951075	3.7751709
H	1.5230455	4.2773633	5.2396424
H	-2.2729691	3.7629193	3.0296588
H	-2.2803689	3.1834559	1.3205579
H	-2.6956760	4.8945960	1.7027525
H	1.7810267	2.7351919	-3.9324596
H	4.8428664	1.1994129	-1.8689473
H	6.5058280	-0.4568498	2.6013052
H	4.0804901	-0.7152172	3.6328102
H	2.2132013	-0.0138169	1.9138918
O	-0.5191876	-0.1659633	-2.3675157
O	0.1865895	2.0101005	1.4853410
O	-0.6952056	4.4803550	1.8286259
O	0.9850336	-1.6563901	-0.3559948
O	-1.8497072	-1.6100695	-0.3546245
O	-2.4343861	0.6399586	1.1527276

O	-0.1467395	-0.7945385	2.0765166
O	-1.3297867	2.1480120	-1.0473811
O	1.7311205	4.1884247	1.2405029
O	0.9957360	3.3479649	3.4965541
O	1.7729093	0.9883141	-0.6146487
O	1.9314824	2.2248966	-3.1114854
P	0.5107214	3.4052927	1.9563469
S	-0.0311008	-1.8602419	-4.6941814
S	-3.0469526	-5.2854937	-1.3388304
S	-1.0888621	-2.1528696	5.6989714
S	5.5582648	0.3596017	0.4912916
Y	-0.4342790	0.2122111	-0.0329090

$[Y(TTA)_3(HTTA\text{-}flip)(OH_2),H_{out}]^{\neq}$ optimized with the QM/SPP in the chloroform CPCM solvent (Table 9)

Atom	X(Å)	Y(Å)	Z(Å)
C	1.2476886	-2.3331889	-3.9850846
C	0.9404435	-3.0690921	-5.1204324
C	2.0675609	-3.3346638	-5.9376442
C	3.2312660	-2.8016139	-5.4240462
C	0.3963681	-1.8525263	-2.8937931
C	-0.9920123	-2.1623257	-2.9085415
C	-1.8464467	-1.7392613	-1.8948930
C	-0.4785122	2.4219510	-2.3689661
C	0.8763981	2.6298876	-2.7240716
C	1.9648051	2.1019194	-2.0220445
C	-1.5360090	2.8787098	-3.2560812
C	-3.7770417	3.4216841	-4.1957427
C	-2.7482192	3.7671837	-5.0508985
C	-1.4754957	3.4588777	-4.5188810
C	3.3846276	2.5549833	-2.4603851
C	-0.4454643	-2.8927265	1.8410984
C	-0.1683328	-4.3126495	2.0692121
C	0.8811570	-6.5737513	1.9690854
C	-0.2291468	-6.5416828	2.7866832
C	-0.8255970	-5.2573277	2.8440450
C	-1.8689174	-0.9387549	2.3681937
C	-3.0836115	-0.3954708	3.1618344
C	-1.5627206	-2.2921335	2.4851199
C	-3.3440039	-2.1265693	-1.9872883
C	1.4117502	1.1565717	3.2339021
C	2.1068636	0.8684595	4.4892530
C	3.0993054	0.8736380	6.7829698
C	3.3814143	-0.2825553	6.0827324
C	2.8215629	-0.2847634	4.7852192
C	0.5771852	2.3470232	3.1625404
C	0.0020838	2.7909397	2.0120911
C	-0.8439851	4.0641607	1.9816396
F	3.8787256	3.4653972	-1.5700044
F	3.4225416	3.1347992	-3.6900954
F	4.2492218	1.5073219	-2.4805973
F	-3.9743547	0.2104423	2.3346547
F	-3.7641916	-1.3557438	3.8506076
F	-2.6822936	0.5375340	4.0740318
F	-4.1371881	-1.0234168	-1.9572601
F	-3.6599551	-2.8154577	-3.1226389
F	-3.7038255	-2.9114066	-0.9333488
F	-1.0402435	4.5900861	3.2114166
F	-2.0620568	3.8180808	1.4312163
F	-0.2419429	5.0156311	1.2119575
H	-1.3999038	-2.7454006	-3.7289752

H	-0.0662622	-3.4075325	-5.3602993
H	2.0258825	-3.8968965	-6.8693627
H	4.2339183	-2.8537558	-5.8401709
H	-4.8456854	3.5432638	-4.3526854
H	-2.9077953	4.2235963	-6.0264565
H	-0.5422844	3.6496678	-5.0462305
H	1.0901471	3.2296385	-3.6049122
H	-2.1947335	-2.9089204	3.1174844
H	-1.7119164	-5.0346186	3.4359053
H	-0.6022761	-7.4113337	3.3255882
H	1.5240931	-7.4208008	1.7445779
H	2.9832479	-0.6526435	1.1683906
H	3.1865623	-0.2269207	-0.3147383
H	-0.3951007	2.3574217	-0.0563855
H	0.4078981	2.9262543	4.0674937
H	2.9159802	-1.1038242	4.0749570
H	3.9702147	-1.0993516	6.4965786
H	3.4037993	1.1435691	7.7907237
O	-1.5660551	-1.0642124	-0.8554673
O	0.9583650	-1.1656282	-1.9719558
O	-0.8557369	1.8471089	-1.2620369
O	1.9731228	1.3046674	-1.0378087
O	0.3590700	-2.2657429	1.0660298
O	-1.2684476	-0.0399596	1.6993749
O	2.7686535	-0.9117628	0.2486926
O	1.5615957	0.3569397	2.2682445
O	0.1854759	2.2063210	0.8423507
S	2.9678490	-1.9632042	-3.9289888
S	-3.2073786	2.7087110	-2.7255256
S	1.2169435	-5.0305411	1.2521280
S	2.1378136	1.9778952	5.8619200
Y	0.3936408	-0.2068052	0.0681862

$[Y(TTA)_3(HTTA\text{-}flip)(OH_2),H_{in}]$ Successor optimized with the QM/SPP in the chloroform CPCM solvent (Table 9)

Atom	X(Å)	Y(Å)	Z(Å)
C	0.7762233	-4.7681771	-0.2252269
C	0.3382336	-6.0196720	-0.6328952
C	1.3282573	-7.0274803	-0.5152221
C	2.5207657	-6.5458168	-0.0188075
C	0.0848611	-3.4757346	-0.1849569
C	-1.2761202	-3.4141934	-0.6058302
C	-2.0047162	-2.2308234	-0.6278385
C	0.1226937	0.3451556	-4.1326208
C	1.4899473	0.2158313	-3.8327965
C	2.0318852	-0.0569347	-2.5660478
C	-0.3406898	0.2847427	-5.5002246
C	-1.7425071	0.3931589	-7.5553314
C	-0.4484257	-0.0134820	-7.8187787
C	0.3476185	-0.0774617	-6.6541516
C	3.5780975	-0.2448152	-2.4971139
C	-0.7599816	-0.9414156	3.7261852
C	-0.5588388	-1.8812955	4.8311402
C	0.3093394	-3.7579288	6.2276486
C	-0.6878909	-3.0451894	6.8599132
C	-1.1812975	-1.9787819	6.0671528
C	-1.9500058	1.0241413	2.8477668
C	-3.0226928	2.1179260	3.0798445
C	-1.7423272	0.0797226	3.8498291
C	-3.4817359	-2.2878666	-1.0923801
C	1.3234666	3.0229586	1.0946463

C	2.1565849	3.8736035	1.9516996
C	3.3362288	5.7294562	3.1458484
C	3.6976325	4.4818234	3.6097494
C	3.0303743	3.4318437	2.9336477
C	0.4144221	3.6261136	0.1700902
C	-0.3116354	2.9151143	-0.7695616
C	-1.1349057	3.7177476	-1.8035459
F	4.0781753	0.3095279	-1.3559994
F	4.2463332	0.3106490	-3.5392548
F	3.8930458	-1.5702319	-2.4683145
F	-3.9609349	2.0952062	2.0967675
F	-3.6829676	1.9920628	4.2672386
F	-2.4563670	3.3573590	3.0694751
F	-3.6953682	-1.4515806	-2.1413230
F	-3.8833783	-3.5322765	-1.4835247
F	-4.3144001	-1.8984892	-0.0873637
F	-1.2343572	5.0411046	-1.5083325
F	-2.3946436	3.2308430	-1.9136411
F	-0.5566777	3.6277678	-3.0415834
H	-1.7668595	-4.3279113	-0.9283170
H	-0.6662935	-6.2104096	-1.0071611
H	1.1708187	-8.0706145	-0.7858571
H	3.4408800	-7.0919135	0.1723955
H	-2.5596354	0.5260517	-8.2599844
H	-0.0903729	-0.2601507	-8.8168716
H	1.3895957	-0.3932190	-6.6553196
H	2.1809327	0.2533911	-4.6711619
H	-2.3397549	0.1368911	4.7551019
H	-1.9700296	-1.3034816	6.3955090
H	-1.0519855	-3.2808353	7.8590219
H	0.8597020	-4.6176888	6.6013511
H	3.2545842	-0.4014959	0.7756291
H	2.5030120	-1.7619021	0.9647972
H	-0.5635943	0.8698123	-2.3331665
H	0.3248856	4.7102362	0.1609832
H	3.1652323	2.3726630	3.1450662
H	4.4185461	4.3319734	4.4121357
H	3.6873960	6.7031136	3.4779379
O	-1.6291943	-1.0579899	-0.3020303
O	0.7450821	-2.4623323	0.2285042
O	-0.8453024	0.5130905	-3.2492666
O	1.4355195	-0.2387362	-1.4761523
O	-0.0227733	-1.0928071	2.6898857
O	-1.3569193	1.1326697	1.7293070
O	2.5363511	-0.8314914	1.2748445
O	1.4753293	1.7635614	1.2154633
O	-0.3662409	1.6400815	-0.9313482
S	2.4503348	-4.8451114	0.3144857
S	-2.0120423	0.7039556	-5.8757980
S	0.6626531	-3.1363859	4.6471032
S	2.1677180	5.6358201	1.8688331
Y	0.2597687	-0.1235419	0.6145347

$[Y(TTA)_3(HTTA)(TMP), H_{out}]^{\neq}$ optimized with the QM/SPP in the chloroform CPCM solvent (Table 9)

Atom	X(Å)	Y(Å)	Z(Å)
C	0.2856758	2.9365824	-5.2173113
C	-0.1414248	2.2539502	-4.0878799
S	-1.8926232	2.0822030	-4.0895349
C	-2.0085912	2.9253809	-5.6010032
C	-0.7755129	3.3187089	-6.0767510

C	0.6141928	1.6880167	-2.9616962
O	-0.0458943	1.1195097	-2.0355177
Y	0.3895000	0.0501939	0.0535915
O	1.9341595	-1.6549689	0.7595679
P	3.0531142	-2.6599958	0.8371851
O	4.5458588	-2.0296795	0.8404407
C	4.7793553	-0.7394022	1.4942975
O	-1.9483443	-0.0299367	-0.3028436
C	-2.8237521	0.8883603	-0.3694033
C	-2.6951449	2.2457011	-0.0907929
C	-1.4783659	2.8337419	0.3595391
C	-1.4323809	4.2760453	0.6533811
C	-0.3220798	4.9826959	1.0838538
C	-0.5712021	6.3644712	1.2812082
C	-1.8735128	6.7174354	1.0013123
S	-2.8188745	5.3546826	0.4893926
O	-0.3971897	2.1857660	0.5421316
O	1.6895677	0.9792344	1.8461031
C	1.4512966	1.2992548	3.0419640
C	0.3931737	0.9090388	3.8718331
C	-0.6156546	-0.0010958	3.4774786
C	-1.6013913	-0.4605013	4.4643348
C	-2.8381141	-1.0264425	4.2026467
C	-3.5745778	-1.3439245	5.3719339
C	-2.9000197	-1.0240669	6.5296255
S	-1.3473928	-0.3211415	6.2036774
O	-0.7353187	-0.4416018	2.2735603
O	2.4445317	0.6672944	-0.8916696
C	2.8169408	1.2841534	-1.9417366
C	2.0378829	1.7987158	-2.9693700
C	-4.2187266	0.3706129	-0.8037227
F	-5.1424003	1.3573048	-0.9882753
F	-4.7311506	-0.4796391	0.1333424
F	-4.1423361	-0.3245318	-1.9710737
C	2.5234571	2.2474813	3.6514919
F	3.7562798	1.6657138	3.6248484
F	2.2800171	2.6001304	4.9457994
F	2.6110940	3.4015518	2.9348093
C	4.3533799	1.4497266	-2.0409259
F	4.7629057	2.1508407	-3.1367905
F	4.8480528	2.0937911	-0.9491657
F	4.9691183	0.2318813	-2.0991192
O	3.1601787	-3.7620805	-0.3409725
C	3.4335730	-3.3182409	-1.7058724
O	2.8692585	-3.5757392	2.1543844
C	3.8402504	-4.6193715	2.4660646
H	-3.5712552	2.8789994	-0.2119389
H	0.6359193	4.4922772	1.2453951
H	0.1790017	7.0787663	1.6173278
H	-2.3385892	7.6976127	1.0643598
H	0.3667408	1.3002834	4.8861986
H	-3.2025277	-1.1807302	3.1894480
H	-4.5687100	-1.7880589	5.3649584
H	-3.2172091	-1.1657886	7.5592689
H	2.5286903	2.3035662	-3.7963621
H	-2.9841822	3.0852671	-6.0525974
H	-0.6380302	3.8636592	-7.0096630
H	1.3314175	3.1602437	-5.4224203
H	4.4247091	-2.8515089	-1.7584615
H	3.4100414	-4.2241715	-2.3188412
H	2.6580414	-2.6153577	-2.0363262
H	4.8555292	-4.2039527	2.5066676
H	3.7863779	-5.4205177	1.7187184

H	3.5530226	-5.0016035	3.4502721
H	4.7616624	-0.8673508	2.5841223
H	4.0228777	-0.0118881	1.1780996
H	5.7768723	-0.4272389	1.1712435
O	0.2351728	-1.6719956	-1.6856003
C	-0.5046183	-2.6006880	-2.0994472
C	-1.4610269	-3.3127607	-1.2582552
C	-1.5919124	-3.1065012	0.0785500
O	-0.7829591	-2.3121452	0.7649299
C	-2.6276453	-3.8756558	0.8989157
F	-3.5309329	-3.0251510	1.4625368
F	-2.0254831	-4.5480367	1.9182889
F	-3.3172922	-4.7745972	0.1602606
H	-1.0898195	-1.8241906	1.6166954
H	-2.1163964	-4.0474958	-1.7207447
C	-0.3995296	-2.9903232	-3.5083625
C	0.3493498	-2.3379936	-4.4781165
C	0.2586807	-2.9356160	-5.7558500
C	-0.5585626	-4.0483644	-5.7672764
S	-1.2337792	-4.3795017	-4.2085764
H	-0.8038444	-4.6973147	-6.6038725
H	0.7702273	-2.5652371	-6.6426179
H	0.9314512	-1.4476605	-4.2481962

[Y(TTA)$_3$(HTTA)(TMP), H$_{out}$] successor optimized with the QM/SPP in the chloroform CPCM solvent (Table 9)

Atom	X(Å)	Y(Å)	Z(Å)
C	0.0967597	2.1023044	-5.7021358
C	-0.3244108	1.5696972	-4.4926036
S	-2.0609078	1.2851378	-4.5076927
C	-2.1790798	1.8848401	-6.1310239
C	-0.9576494	2.2821207	-6.6330420
C	0.4259089	1.2287372	-3.2765170
O	-0.2305524	0.7654970	-2.2925508
Y	0.2214347	0.0167094	-0.0843649
O	1.8377646	-1.3821888	1.0221702
P	2.9850051	-2.3433542	1.2054678
O	4.4598361	-1.6760592	1.1049612
C	4.6596886	-0.2932481	1.5390311
O	-2.1276647	0.0035426	-0.3260317
C	-2.9798483	0.9254557	-0.5125617
C	-2.7982246	2.3055447	-0.4747207
C	-1.5422002	2.9033533	-0.1710287
C	-1.4234180	4.3710475	-0.1263699
C	-0.2597387	5.0860262	0.1014563
C	-0.4441746	6.4918459	0.0778328
C	-1.7505160	6.8545568	-0.1682928
S	-2.7791350	5.4717833	-0.3764916
O	-0.4828729	2.2424823	0.0822602
O	1.5065022	1.3703126	1.6768819
C	1.3310282	1.8234428	2.8219592
C	0.3358927	1.4850268	3.7817074
C	-0.6257727	0.5080482	3.5748216
C	-1.5040661	0.0090212	4.6081597
C	-2.6998803	-0.6799397	4.4415903
C	-3.3277690	-1.0103606	5.6651999
C	-2.6151887	-0.5777703	6.7633943
S	-1.1557171	0.2431538	6.3200812
O	-0.7865974	0.0212641	2.3394312
O	2.2651599	0.5982086	-1.0511423
C	2.6223362	1.1038690	-2.1661249

C	1.8408365	1.4302947	-3.2649786
C	-4.4084232	0.3877246	-0.7823485
F	-5.3098670	1.3575148	-1.1130588
F	-4.8982837	-0.2460133	0.3244567
F	-4.4111457	-0.5191257	-1.7944574
C	2.4023980	2.8646884	3.2847713
F	3.5579568	2.2266766	3.6345986
F	2.0097886	3.6003354	4.3624500
F	2.7011015	3.7304628	2.2902138
C	4.1463756	1.3606880	-2.2566567
F	4.5437029	1.9175988	-3.4363704
F	4.5605740	2.1957534	-1.2640098
F	4.8445657	0.1960614	-2.1148953
O	3.1165047	-3.5876179	0.1852115
C	3.4137657	-3.3330084	-1.2237749
O	2.8414795	-3.0776154	2.6362780
C	3.8355784	-4.0558901	3.0636845
H	-3.6561883	2.9454428	-0.6692708
H	0.6903178	4.5843778	0.2752153
H	0.3541306	7.2157545	0.2350101
H	-2.1749351	7.8524377	-0.2398546
H	0.3638071	1.9812615	4.7487969
H	-3.1223005	-0.9154460	3.4658865
H	-4.2742785	-1.5423486	5.7397776
H	-2.8574050	-0.6996620	7.8156796
H	2.3249714	1.8478688	-4.1430475
H	-3.1473412	1.9105079	-6.6240778
H	-0.8239697	2.6885664	-7.6345872
H	1.1332465	2.3592110	-5.9151000
H	4.4038695	-2.8712371	-1.3197280
H	3.4060177	-4.3153560	-1.7050540
H	2.6402390	-2.6896574	-1.6615790
H	4.8446189	-3.6249911	3.0262074
H	3.7802406	-4.9510103	2.4321692
H	3.5744307	-4.3064089	4.0963691
H	4.6094220	-0.2335853	2.6337417
H	3.9073081	0.3581837	1.0794431
H	5.6635050	-0.0238770	1.1972530
O	0.2246870	-1.8664315	-1.4853569
C	-0.3706756	-2.9776290	-1.6576902
C	-1.1976262	-3.6097153	-0.6804046
C	-1.4105209	-3.0922732	0.5898085
O	-0.9557440	-2.0055663	1.0747515
C	-2.2820220	-3.9037926	1.5762465
F	-3.3731002	-3.1806736	1.9654734
F	-1.5803612	-4.1991026	2.7074930
F	-2.7418838	-5.0787588	1.0708970
H	-1.1377167	-0.9298288	2.2307176
H	-1.6749009	-4.5543403	-0.9319842
C	-0.1651524	-3.6374371	-2.9584588
C	0.4792102	-3.0897456	-4.0554396
C	0.5187885	-3.9522990	-5.1793965
C	-0.0948905	-5.1635966	-4.9434570
S	-0.7349666	-5.2640964	-3.3338781
H	-0.2097885	-6.0077100	-5.6182339
H	0.9782654	-3.6939879	-6.1322913
H	0.8963031	-2.0849913	-4.0279231

$Y(TTA)_2(TTA\text{-}uni)(OH_2)_3$ optimized with the QM/SPP in the chloroform CPCM solvent (Figure 6)

Atom	X(Å)	Y(Å)	Z(Å)

S	-0.1968894	5.0426563	0.7437435
C	-0.4899584	4.1154145	2.2116691
C	-0.7016229	4.9599683	3.2919580
C	-0.6291994	6.3337184	2.9514942
C	-0.3624096	6.5340501	1.6133449
C	-0.4737923	2.6532214	2.1265029
C	-0.7004050	1.8873740	3.3062096
C	-0.7206170	0.4975841	3.2847133
O	-0.5357242	-0.2800219	2.2932880
Y	0.0214521	0.0077153	0.0655764
O	-0.2600405	2.1342166	0.9770967
O	1.1564267	1.4602338	-1.4339287
C	0.7883556	2.3529609	-2.2706933
C	-0.5720678	2.6041221	-2.6259333
C	-1.6464977	1.8859435	-2.1191076
O	-1.6462847	0.9230461	-1.2795735
C	1.8387355	3.1471669	-2.9125562
S	3.5168908	2.7874412	-2.5177916
C	4.0739066	4.0431909	-3.5760681
C	3.0333545	4.7000121	-4.1979337
C	1.7647861	4.1919781	-3.8223627
C	-3.0672601	2.2442762	-2.6171553
F	-3.6561836	1.1619539	-3.2020948
F	-3.0937255	3.2552666	-3.5279034
F	-3.8615259	2.6187249	-1.5772291
O	-0.7346734	-3.5708493	-1.3930344
C	-0.0964994	-4.5629646	-0.8902213
C	-0.4781423	-5.9023124	-1.3470783
S	-1.7335451	-6.0255490	-2.5770982
C	-1.6228983	-7.7558235	-2.5648329
C	-0.6802596	-8.2144577	-1.6682134
C	-0.0305831	-7.1628282	-0.9761111
O	0.9517943	-2.0846253	0.5281208
C	1.3928989	-3.2659169	0.6560421
C	2.5787610	-3.3697288	1.6561467
F	3.4963333	-2.3736554	1.4044819
O	0.4571121	-1.2526548	-2.0022725
O	-1.8786447	-1.4989505	-0.0739839
C	0.9618545	-4.4496927	0.0621984
F	2.1591265	-3.1984364	2.9354178
F	3.2593495	-4.5428322	1.6032160
C	-1.0056249	-0.2570593	4.6063485
F	0.0458927	-1.0513936	4.9463723
F	-1.2430150	0.5678855	5.6656996
F	-2.0947728	-1.0633594	4.4759618
H	-0.8806013	2.3985255	4.2473729
H	-0.9040246	4.6030605	4.3004747
H	-0.7684954	7.1460849	3.6631709
H	-0.2551005	7.4777768	1.0850517
H	5.1406653	4.2219588	-3.6808645
H	3.1778821	5.5192415	-4.9005300
H	0.8260189	4.5855743	-4.2083599
H	-0.7814379	3.3868307	-3.3493382
H	1.4784365	-5.3610995	0.3523345
H	0.7391410	-7.3285089	-0.2241337
H	-0.4650648	-9.2705878	-1.5128973
H	-2.2627337	-8.3390739	-3.2218298
H	0.1653815	-0.9324254	-2.8726252
H	0.0843657	-2.1774426	-1.8822007
H	-1.5739085	-2.3602116	-0.4760001
H	-2.5372150	-1.1238971	-0.6884072
O	2.3171068	0.4024429	0.7780171
H	2.7804332	0.9336463	0.1027826

H	2.8542825	-0.3969546	0.9391112

$[Y(TTA)_2(TTA\text{-open})(TMP)(OH_2)_2]$ optimized with the QM/SPP in the chloroform CPCM solvent (Figure S6)

Atom	X(Å)	Y(Å)	Z(Å)
S	2.7492444	6.2820709	-2.4637640
C	2.1104775	4.7161653	-2.9708222
C	2.0306841	4.6581893	-4.3535880
C	2.4715844	5.8402893	-4.9985684
C	2.8902314	6.8080248	-4.1104777
C	1.7226681	3.6429010	-2.0387737
C	1.8959333	3.8572950	-0.6369064
C	1.5712478	2.9656386	0.3858207
C	1.8991353	3.4099856	1.8407176
F	2.4628975	4.6484562	1.9356648
O	1.0386005	1.8180827	0.3246764
Y	0.0003404	-0.2303659	-0.0756565
O	-0.9373983	1.1892619	-1.8442587
O	-1.9124852	0.9967171	0.5793175
C	-2.5414353	1.1943449	1.6780587
C	-2.0792497	0.7535800	2.9478637
C	-0.8667533	0.0959473	3.1349876
C	-0.4695636	-0.2826251	4.5849613
F	-1.3869665	0.0807836	5.5240516
C	-3.8063289	1.9302259	1.6021665
S	-4.4091717	2.4010996	0.0157397
C	-5.8003329	3.1556835	0.7261402
C	-5.8036455	3.0502890	2.1007314
C	-4.6726630	2.3554001	2.5984379
O	-1.5931916	-1.8752130	0.3766021
C	-2.1171429	-2.8387645	-0.2686787
C	-1.8343706	-3.2741827	-1.5586677
C	-0.8475484	-2.6500405	-2.3767565
C	-0.5956159	-3.1695853	-3.7301163
C	0.1939656	-2.5848512	-4.7066236
C	0.2337742	-3.3172752	-5.9194472
C	-0.5251257	-4.4666251	-5.8728427
S	-1.3056465	-4.6664099	-4.3367891
O	-0.1633982	-1.6391282	-2.0058437
O	1.2578205	2.5744856	-2.5662245
O	1.5892192	-1.8431241	0.5001935
P	2.7508393	-2.5992112	1.1034908
O	3.5965576	-3.3086062	-0.0697692
C	4.7702227	-4.1188001	0.2515867
O	0.0015337	-0.2535459	2.2746227
O	1.8516352	0.1040103	-1.6548091
C	-3.2151031	-3.5832101	0.5321409
F	-3.7256753	-4.6686424	-0.1148652
F	-4.2583785	-2.7536196	0.8079791
F	-2.7262363	-4.0246420	1.7252270
F	0.7729263	3.4271484	2.6035707
F	2.7677081	2.5348829	2.4216980
O	2.3085546	-3.7156095	2.1912722
C	1.0216688	-4.3975561	2.0528565
O	3.8662650	-1.7528540	1.8953744
C	3.4912490	-1.0292357	3.1150875
F	0.7103830	0.3051996	4.9333036

F	-0.2930474	-1.6291471	4.7014310
H	3.2738636	7.8026397	-4.3232731
H	2.4825921	5.9797153	-6.0786703
H	1.6600226	3.7738110	-4.8687089
H	-2.3975724	-4.1159557	-1.9555149
H	2.3343542	4.8045321	-0.3278292
H	-0.6721530	-5.2138668	-6.6484104
H	0.7982468	-3.0115593	-6.7991911
H	0.7151566	-1.6435733	-4.5439712
H	-2.6893061	0.9602608	3.8224585
H	-4.4996561	2.1774870	3.6586042
H	-6.5925088	3.4596631	2.7302640
H	-6.5384994	3.6307879	0.0852004
H	4.5109075	-4.9033830	0.9740157
H	5.5692531	-3.4809198	0.6482227
H	5.0801057	-4.5689916	-0.6962047
H	3.3503293	-1.7445409	3.9340698
H	2.5769959	-0.4462279	2.9495641
H	4.3342347	-0.3662879	3.3292969
H	1.0507909	-5.0911438	1.2026064
H	0.2178872	-3.6633248	1.9253317
H	0.8855347	-4.9538361	2.9849203
H	1.7633830	1.0222534	-2.0407356
H	1.6451250	-0.5297016	-2.3696755
H	-1.5968419	1.7042105	-1.3366624
H	-0.2344032	1.8353116	-2.1376988