Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting information

Small molecules activation with divalent samarium triflate: a synergistic effort to cleave O_2

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Contents

I. Experimental Procedures

General methods and starting material

All reactions were performed using standard Schlenk-line techniques or in an argon filled glovebox (MBraun). All glassware was dried at 120°C for at least 12 h prior to use. $Sm(OTf)_2(dme)_2$ was prepared according published procedure.[1] THF, pyridine, pyridine-d_5 , thf-d_8 and pentane were dried over sodium and transferred under reduced pressure in a cold flask. All solvents were degassed prior to use. CO_2 and N_2O were purchased from Air Liquide as Alphagaz N48. Air and O_2 were dried on a column of potassium hydroxide. NMR spectra were recorded in 5 mm tube adapted with a J.Young valve on Bruker 300 MHz Avance III spectrometers. Chemical shifts are expressed relative to TMS in ppm. Elemental analyses were obtained from Mikroanalytisches Labor Pascher.

Synthesis of $[Sm_4(\mu_3\text{-}O)(\mu_2\text{-}OTf)_6(\mu_3\text{-}OTf)_2(thf)_6(dme)_2]$ (1)

153.2 mg (257 µmol, 4 eq.) of $Sm(OTf)_2(dme)_2$ was dissolved in 7 mL of thf; the dark purple solution that was obtained was transferred in a J. Young tapered flask, which was then sealed and connected to a vacuum line. The solution was degassed by three freeze-pump-thaws and an atmosphere of 0.2 Bar of N_2O was added in the flask. The mixture was let still overnight until a complete discoloration was observed. The obtained cloudy solution was filtered and slow evaporation of the solvents yielded 124.7 mg (54.3 µmol, 85 %) of the product as a white micro-crystalline solid. Crystals suitable for XRD can be obtained by slow diffution of pentane in a THF solution of the product.

^{19}F NMR (282 MHz, THF, 298 K) -79.43 (s, OTf)

Elemental analysis Calculated for $C_{32}H_{52}F_{24}O_{34}S_8Sm_4$: C, 16.75; H, 2.27; Found: C, 16.88; H, 2.11.

Reactivity of 1 with CO_2 in a thf/pyridine mixture.

39.5 mg (17 µmol) of 1 was dissolved in a mixture of 1 mL of thf and 0.2 mL of pyridine, transferred in a J. Young valved NMR tube, which was then closed and connected to a vacuum line. The solution was then degassed by three freeze-pump-thaws, before 0.2 Bar of CO_2 were added. The obtained mixture was then let to react for 72 h. It was then brought back in the glovebox, transferred in a tube where the clear solution was layered with pentane yielding X-Ray quality crystals of $[Sm_4(\mu_3\text{-}CO_3\text{-}\kappa_4O,O',O'')_2(\mu_2\text{-}OTf)_6(OTf)_2Sm(thf)_{10}]$ (**2-py**).

In situ synthesis of $[Sm_4(\mu_3\text{-}CO_3\text{-}\kappa_4O,O',O'')_2(\mu_2\text{-}OTf)_6(OTf)_2Sm(py)_{10}]$ (2-thf) from $Sm(OTf)_2(dme)_2$.

2 can be obtained directly from $Sm(OTf)_2(dme)_2$ by in situ addition CO_2 on the degassed suspension obtained by reacting $Sm(OTf)_2(dme)_2$ with N_2O without isolating the **1** intermediate. 303.0 mg (0.51 mmol) of $Sm(OTf)_2(dme)_2$ was dissolved in thf; the dark purple solution was transferred in a J. Young tapered flask, which was then tighly closed and connected to a vacuum line. After it was degassed by three freeze-pump-thaws, an atmosphere of 0.2 Bar of N_2O was added in the flask. The mixture was then vigorously stirred for 72 h until a complete discoloration was observed. The clear solution was then degassed by freeze-pump-thaws and an atmosphere of 0.2 Bar of CO_2 was added in the flask. The obtained suspension was stirred for 72 h at room temperature. After filtration, the final product, **2-thf**, obtained in good yield (268.9 mg, 80 %) by slow diffusion of pentane into a thf solution of the raw product.

^{19}F NMR (282 MHz, THF, 298 K) -79.20 (s, OTf), -80.19 (s, OTf)

Elemental analysis Calculated for $C_{50}H_{80}F_{24}O_{40}S_8Sm_4 – 1.5(C_4H_8O)$: C, 20.92; H, 2.69; Found: C: 20.80; H: 2.73.

Reactivity of $Sm(OTf)_2(dme)_2$ with O_2

38.8 mg (69.7 µmol) of $Sm(OTf)_2(dme)_2$ were dissolved in 0.5 mL of thf-d 8 . The obtained dark purple solution was transferred in a J. Yound tapered NMR tube, which was sealed and connected to a vacuum line. The solution was degassed by three freeze-pump-thaws before one atmosphere of dry O_2 was added. The atmosphere was let to diffuse in the solution for ca. 5 min before the excess of O_2 was removed by degassing by one freeze-pump-thaw. The progression of the diffusion can be observed by a complete discoloration of the solution.

^{19}F NMR (282 MHz, THF, 298 K) -79.48 (s, OTf), -80.90 (s, OTf), -80.41 (s, OTf)

If the excess of O_2 is not removed quickly, an intractable solid start crashed out and only $Sm(OTf)_3$ can be recrystallised from the supernatant.

^{19}F NMR (282 MHz, THF, 298 K) -79.30 (s, OTf), -80.10 (s, OTf).

II. ^{19}F NMR spectroscopy

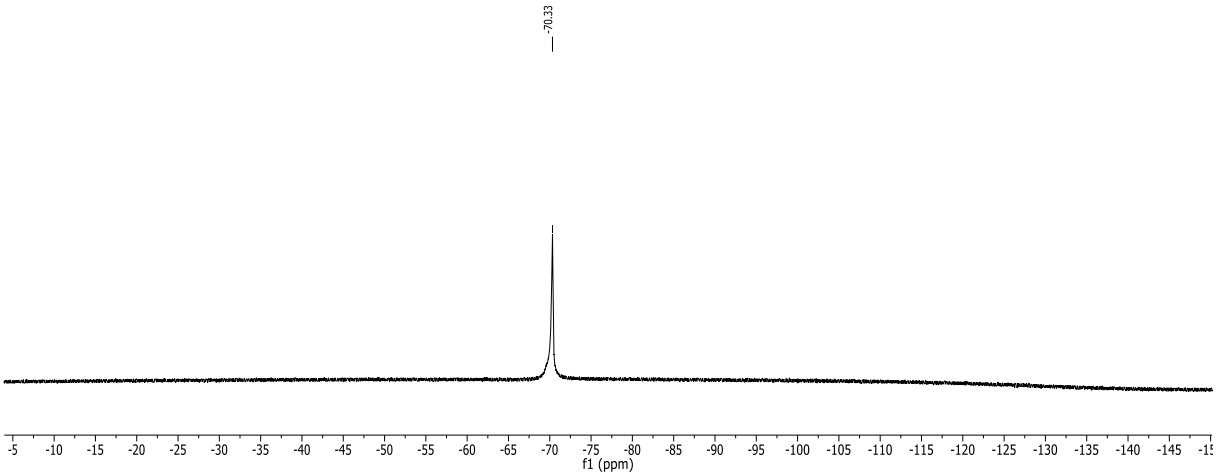


Figure S1: ^{19}F NMR of $Sm(OTf)_2(dme)_2$ in thf.

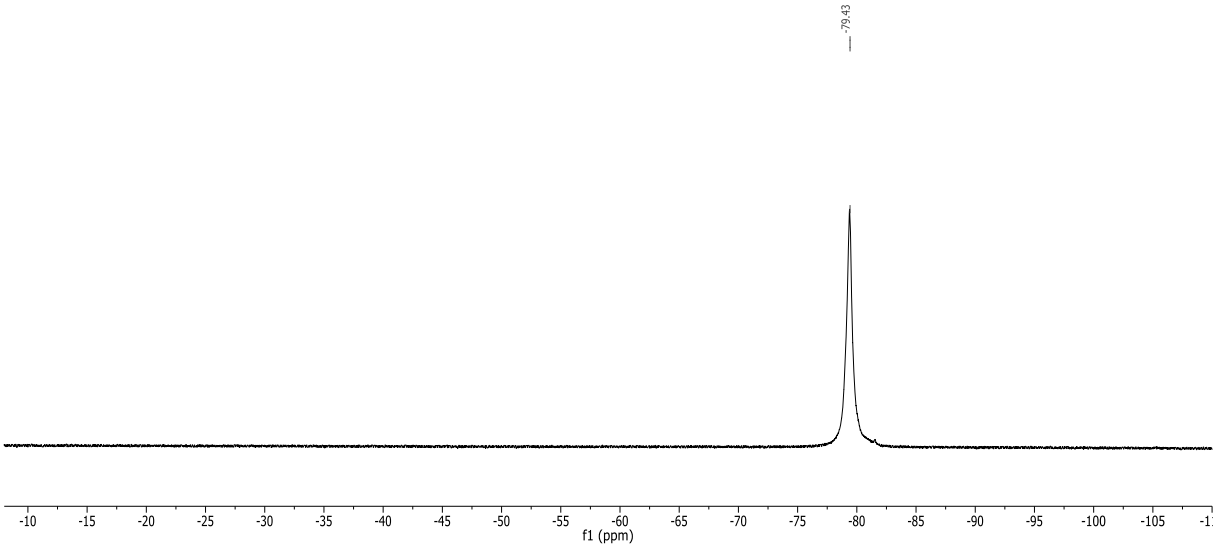


Figure S2: ^{19}F NMR of **1** in thf.

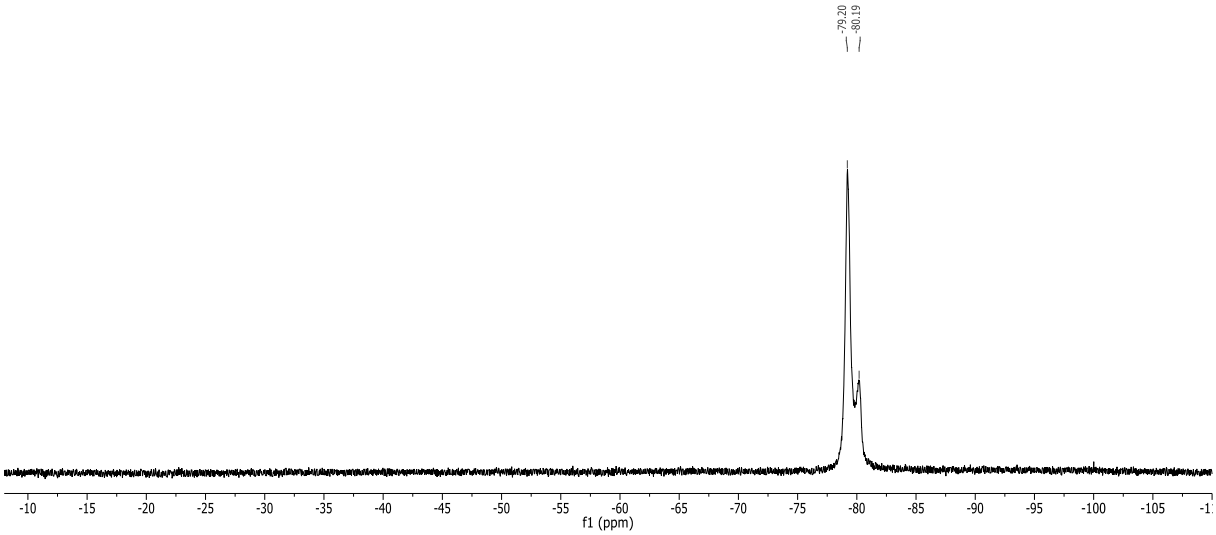


Figure S3: ^{19}F NMR of **2-thf** in thf.

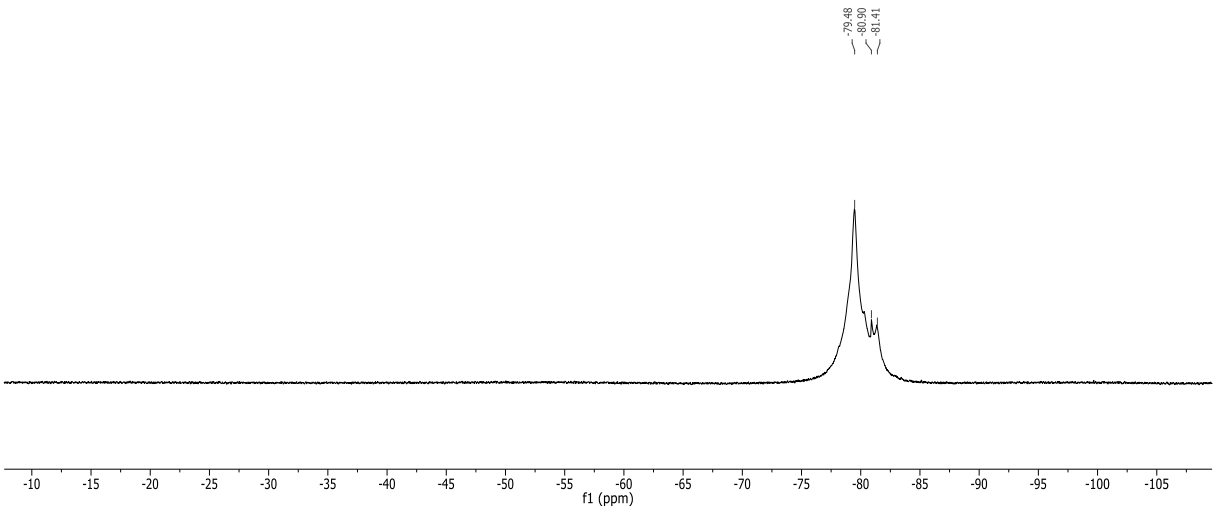


Figure S4: ^{19}F NMR of the crude mixture obtained from the 5 min reaction of $Sm(OTf)_2(dme)_2$ in thf with dry O_2.

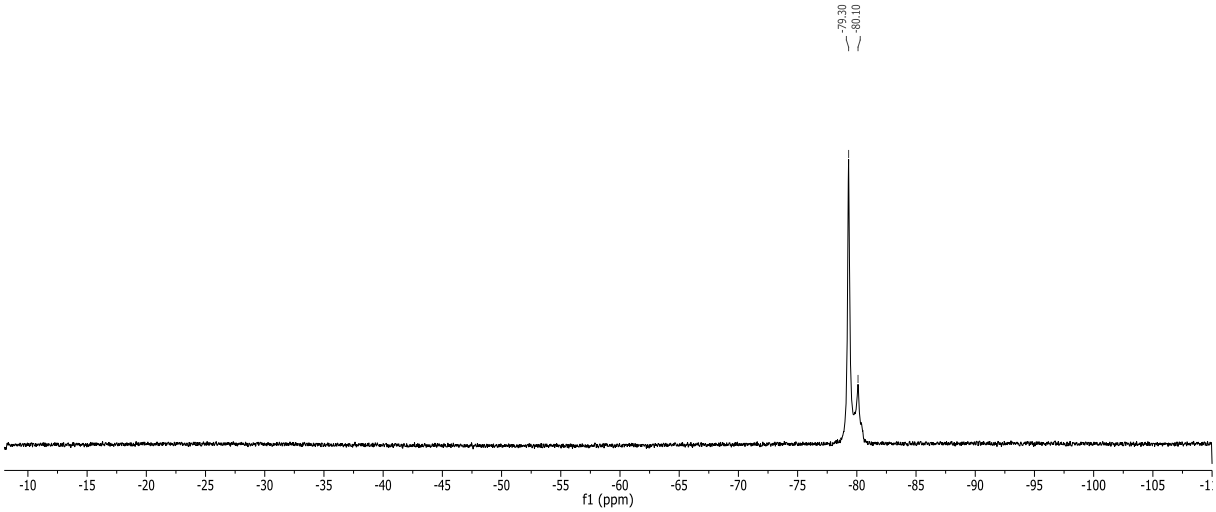


Figure S5: ^{19}F NMR of recrystallized crystals of $Sm(OTf)_3$.

III. Theorerical calculations

Computational Details

Calculations have been carried out with the Gaussian 09 program[2] at the DFT level of theory using the hybrid functional B3PW91[3,4]. Samarium atoms were treated with two large-core Stuttgart Dresden relativistic effective core potential (RECP) adapted to the samarium +3 and +2 oxidation states. These RECP were used in combination with their corresponding adapted basis set augmented by a f polarization function (α=1.000).[5] The change of oxidation state was treated by using small-core RECP. The Stuttgart Dresden RECP was employed for sulfur atoms in combination with its optimized basis set. Carbon, oxygen and fluorine atoms were described with a 6-31G(d,p) double-ζ- quality basis set. Electronic energies and enthalpies were computed at T = 298 K in the gas phase. Geometry optimizations were performed without any symmetry constraints and the nature of the extrema was verified by analytical frequency calculations. Intrinsic reaction coordinate (IRC) were carried out to verify the connections of the optimized transition states. Natural bond orbital (NBO) analysis[6] was used to analyze electron density.

Electronic energies (atomic units) and optimized geometries

Electronic energies (atomic units) and optimized geometries

O_2

E:	-150.194750		
O	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.210000

$Sm^{II}(OTf)_2$

E(large core):	-1175.190161		
E(small core):	-1804.502483		
C	-0.790419	-1.392003	-7.382674
F	-1.300070	-1.556571	-8.584641
F	-0.197091	-0.222801	-7.274069
S	-2.250684	-1.463596	-6.081501
O	-1.500751	-1.450550	-4.662974
Sm	-2.150984	-3.777781	-3.974563
O	-3.179724	-5.004080	-2.043423
S	-2.085508	-6.175401	-1.963031
C	-3.080166	-7.770662	-2.507756
F	-3.632132	-7.511156	-3.684037
F	0.050709	-2.373164	-7.092218
O	-3.212808	-0.311829	-6.378339
O	-2.822738	-2.956776	-6.237965
O	-1.095449	-5.907391	-3.199376
O	-1.445798	-6.449223	-0.600942
F	-2.235244	-8.774850	-2.601981
F	-4.004667	-8.010678	-1.603021

$(OTf)_2Sm^{III}-O_2-Sm^{III}(OTf)_2$

E(large core):	-2512.583197		
E(small core):	-3759.312265		

Sm	-1.927384	-4.630033	-4.982360
O	-2.398140	-6.204009	-6.555945
O	-1.016204	-5.644541	-6.799113
Sm	-1.880505	-6.440356	-8.751305
O	0.226145	-6.768008	-9.894301
S	0.164252	-8.379452	-9.980231
O	0.383452	-9.036911	-11.337376
O	-2.998576	-2.688135	-5.877585
S	-1.787510	-1.631989	-5.659754
C	-1.165566	-1.221173	-7.488167
F	-0.672535	-2.332193	-7.996524
S	-2.551451	-5.860181	-2.235456
C	-2.770005	-7.816395	-2.236484
F	-3.984736	-8.079686	-1.812943
O	-3.581187	-5.337128	-3.364084
O	-0.641679	-2.580583	-5.032412
O	-1.120484	-5.621265	-2.959208
O	-2.108113	-0.323487	-4.947463
O	-2.722775	-5.346132	-0.811154
O	-2.649773	-4.428859	-9.791920
S	-4.118355	-4.945930	-10.244995
C	-5.361837	-3.942513	-9.085194
F	-5.136659	-4.322800	-7.843954
O	-4.123296	-6.451331	-9.661771
O	-1.220605	-8.697036	-9.199873
O	-4.527096	-4.735320	-11.697844
F	-2.594704	-8.229679	-3.475428
F	-1.859955	-8.317939	-1.433346
F	-2.203262	-0.799884	-8.172739
F	-0.243593	-0.292631	-7.387405
C	1.564208	-8.995154	-8.740951
F	2.724079	-8.637705	-9.242072
F	1.343655	-8.411442	-7.580127
F	1.462330	-10.300960	-8.644635
F	-5.107884	-2.665207	-9.248769
F	-6.581772	-4.245074	-9.462779

Isomer of complex 1

E(large core): -4875.045550

C	-4.232808	-3.597254	-9.733972
F	-5.112183	-4.016043	-10.615426
F	-4.719682	-3.661790	-8.509549
S	-2.682223	-4.806704	-9.846136
O	-1.957374	-4.719167	-8.394342
Sm	-2.420652	-7.125857	-7.726849
O	-0.146924	-6.866212	-8.858520
S	0.012173	-8.416380	-9.330097
O	0.125622	-8.639921	-10.833344
F	-3.815191	-2.383469	-10.015947
O	-1.884800	-4.411124	-11.082144
O	-3.339870	-6.268755	-9.791292
O	-1.213515	-9.103931	-8.554835
O	-3.913848	-6.164727	-6.203306
O	-1.109033	-6.127566	-6.248933
Sm	-2.438003	-4.968031	-5.018329
O	-2.024647	-5.123499	-2.559033
S	-3.040292	-6.243371	-2.080988
O	-4.082276	-5.920105	-1.019168
C	1.646281	-9.175230	-8.493669
F	1.788209	-10.365763	-9.034988
F	2.649181	-8.391032	-8.784443
F	1.432232	-9.265407	-7.201549
O	-2.871812	-2.548180	-5.139846
S	-1.379973	-2.019617	-5.424551
O	-0.689877	-1.223952	-4.322378
O	-3.615563	-6.769241	-3.524423
O	-0.669334	-3.421333	-5.854620
C	-1.462442	-0.853379	-7.027771
F	-0.248104	-0.431526	-7.253087
F	-1.940544	-1.559364	-8.024185
F	-2.271697	0.132210	-6.708179
C	-1.960863	-7.782049	-1.475198
F	-1.410767	-7.452650	-0.333313
F	-2.787836	-8.795964	-1.343628
F	-1.057205	-8.019773	-2.401175
Sm	-5.211089	-7.501709	-5.137001
O	-4.825601	-9.892651	-4.742334
S	-4.054509	-10.337617	-6.072925
O	-4.625879	-11.465129	-6.917376
C	-2.224140	-10.836440	-5.473041
F	-2.360696	-11.519914	-4.362377
F	-1.676127	-11.543977	-6.422772
F	-1.568635	-9.708854	-5.259269
O	-3.884375	-8.882291	-6.798427
O	-7.322632	-7.300853	-6.241479
S	-8.113768	-6.493610	-5.080882
F	-9.202512	-4.844676	-6.886553
F	-7.236199	-4.228352	-6.198676

C	-8.415033	-4.705026	-5.845810
F	-8.968712	-3.964373	-4.914899
O	-6.945405	-6.273337	-3.986517
O	-9.446856	-7.057597	-4.604487
Sm	0.548291	-4.951867	-7.419852
O	0.625622	-3.017427	-8.869063
S	2.047590	-3.308809	-9.582476
O	3.100989	-2.204285	-9.507980
C	1.620662	-3.565324	-11.487730
F	0.825686	-2.581950	-11.855177
F	2.761318	-3.521406	-12.145283
F	1.037927	-4.733931	-11.630066
O	2.412237	-4.769176	-9.031094
O	2.122587	-6.583033	-6.480819
S	3.014939	-5.543740	-5.643889
F	3.044965	-7.286449	-3.606796
F	1.371686	-5.904976	-3.549316
C	2.671483	-6.032097	-3.780677
F	3.360847	-5.223486	-3.005715
O	2.206872	-4.169973	-5.823711
O	4.528841	-5.559118	-5.830115

Complex 1

E(large core): -4875.113100

E(small core): -7368.474650

C	8.228112	13.595133	3.806686
F	9.488840	13.237929	3.783525
S	7.622983	13.455652	5.680959
O	6.758925	14.736905	5.955229
Sm	5.616666	15.206970	8.174107
O	3.887088	14.694189	6.532447
S	3.496020	13.399574	5.705538
C	1.545941	13.405281	5.782261
F	1.174933	13.552198	7.037225
Sm	8.850626	13.803318	8.954042
O	10.580966	14.315876	10.595047
S	10.972865	15.610435	11.421616
C	12.922903	15.604734	11.342880
F	13.292595	15.457110	10.087608
O	10.594571	15.239547	7.908121
S	10.555015	16.325816	6.751967
O	9.935485	15.961144	5.399066
Sm	8.718632	17.577348	9.348169
O	7.689161	16.901577	11.420122
S	6.844786	15.554419	11.447356
O	5.542667	15.691336	10.571568
O	6.675123	13.212716	8.412049
Sm	5.749055	11.432576	7.780109
O	3.852070	12.066859	6.533051
O	7.791981	15.797493	8.716319
O	8.924949	13.318078	6.556934

O	7.709471	14.273507	11.173188
O	9.187706	11.435661	9.271644
S	8.937382	9.999198	8.645113
C	9.089201	8.829544	10.206418
F	8.198377	9.224730	11.090459
O	10.025225	17.708753	7.383538
C	12.442400	16.705287	6.438862
F	12.515573	17.547076	5.428448
O	10.615972	16.943369	10.594710
O	7.085637	19.177387	8.862645
S	5.529667	19.010919	8.485127
C	5.376300	20.181001	6.924278
F	6.266382	19.786187	6.039325
O	10.566735	15.633342	12.898064
O	5.278205	17.574683	7.858509
O	6.778166	12.108816	5.708128
F	7.483262	12.770259	3.109789
F	8.056650	14.834120	3.428026
C	6.239907	15.414731	13.321635
F	4.979360	15.772600	13.345115
F	6.410756	14.175552	13.699938
F	6.985315	16.239018	14.018668
O	9.916372	9.538979	7.564729
O	7.381847	9.832331	8.265809
O	4.440983	11.302073	9.743516
S	3.911650	12.684978	10.375696
C	2.024266	12.305854	10.689051
F	1.951113	11.463431	11.698930
O	4.531556	13.048773	11.728679
O	3.903580	13.376567	4.229514
O	4.552044	19.471115	9.566741
F	4.152733	20.060924	6.457007
F	5.614230	21.412071	7.324103
F	1.123581	12.254743	5.296996
F	1.122711	14.410936	5.044637
F	1.429492	13.444749	10.979501
F	1.517855	11.774541	9.594460
F	10.312359	8.949571	10.674758
F	8.851454	7.598395	9.806722
F	13.345755	16.755542	11.827052
F	13.346897	14.599489	12.080621
F	13.037619	15.566392	6.149338
F	12.948314	17.237487	7.533259
O	3.872060	13.771780	9.220062

Complex 2

E(large core): -5252.175619

C	18.718372	8.611650	1.754038
F	17.931183	7.908521	0.977776
S	17.755365	9.002735	3.410920
O	18.620348	9.907111	4.294657

O	16.401102	9.670390	2.872297
Sm	14.276589	9.851532	3.804512
O	14.488250	7.495648	3.884978
S	14.760396	6.123643	3.034462
O	15.270565	6.299423	1.608378
C	15.500156	10.502418	6.433967
O	15.735655	10.963331	7.584964
Sm	15.631773	9.138623	9.010968
O	13.339161	9.072300	8.131327
S	12.889519	8.291984	6.839505
O	12.700834	9.203040	5.565110
O	15.573958	9.167240	6.265435
Sm	16.068525	6.889813	5.851966
O	18.374731	6.970180	6.727186
S	18.822328	7.759422	8.010882
O	19.013282	6.847700	9.291411
O	15.132074	11.200158	5.441423
O	13.800929	11.569770	2.196152
S	12.363530	11.044980	1.680718
C	11.099020	12.364305	2.397582
F	11.320963	13.506175	1.787132
O	15.954356	5.066496	7.272312
C	16.180778	5.532928	8.424080
O	16.513857	4.845521	9.430938
Sm	17.472560	6.200902	11.032680
O	17.214328	8.556763	10.956843
S	16.925442	9.912689	11.825910
O	16.426471	9.721734	13.253752
O	17.435072	7.558723	3.998558
O	15.578235	5.255734	4.080962
O	13.725067	6.976335	6.612545
F	19.798648	7.936178	2.085721
F	19.030068	9.767060	1.208422
C	12.964797	5.309895	2.953131
F	12.573517	5.075863	4.183809
F	12.177702	6.172066	2.351319
F	13.082066	4.198879	2.262945
O	16.134900	6.876667	8.568634
O	14.277638	8.397325	10.858654
S	13.994283	6.956899	11.467486
O	13.138205	6.019500	10.611540
O	16.075613	10.769483	10.792729
O	17.979321	9.068357	8.243463
C	13.041725	7.350783	13.128939
F	13.823129	8.076276	13.891061
O	15.369503	6.324510	12.006829
F	11.945903	8.002640	12.802052
F	12.756083	6.195874	13.692063
C	18.700257	10.775032	11.891123
F	19.073463	11.010900	10.654898
F	19.517068	9.943424	12.492814

F	18.553497	11.888330	12.572745
C	20.640000	8.374073	7.637333
F	21.321919	7.327746	7.236300
F	20.565215	9.293809	6.711847
F	21.113601	8.855387	8.765224
C	11.077037	7.681356	7.225576
F	10.387308	8.735433	7.596402
F	11.152729	6.789132	8.178823
F	10.603595	7.165145	6.112888
O	18.476408	4.383256	12.219486
S	19.424712	5.217192	13.230480
C	18.611827	4.937829	14.996786
F	18.768254	3.672758	15.315352
O	20.897758	4.827888	13.312066
O	19.053505	6.731098	12.841756
F	19.230203	5.726333	15.847973
F	17.334871	5.251690	14.898644
O	12.136532	10.919827	0.177517
O	12.151555	9.739670	2.597773
F	9.881166	11.925648	2.166188
F	11.329682	12.463666	3.693428

Transition state 1

E(large core): -5063.601774

Sm	-3.505692	-1.501612	-5.283774
Sm	-6.678593	-2.872466	-6.993256
Sm	-6.606875	-0.436484	-3.912578
Sm	-4.232895	1.201545	-1.592555
O	-4.339013	0.125443	-3.665295
C	-2.587083	1.278105	-4.207605
O	-2.662960	2.164708	-3.431079
O	-6.010888	-4.874573	-5.956950
S	-4.652995	-5.037917	-5.107747
C	-3.944485	-6.711087	-5.816173
F	-2.691132	-6.814924	-5.422720
O	-9.114009	-3.124335	-7.207598
S	-9.634017	-2.278652	-5.946595
C	-10.471256	-3.602332	-4.749426
F	-10.865195	-2.961803	-3.673831
O	-5.616153	-1.799190	-5.474312
O	-4.770548	-3.190716	-8.351226
S	-3.407983	-2.443384	-8.755106
C	-2.348467	-3.908925	-9.493859
F	-3.086132	-4.514594	-10.402834
O	-6.565161	-0.712853	-8.036324
S	-5.857050	0.466634	-7.235303
C	-5.959139	1.991875	-8.452196
F	-5.105606	2.888922	-8.022588
O	-6.347149	0.205712	-1.370410
S	-7.926370	0.077853	-1.016166
C	-7.915287	-1.259251	0.427958

F	-7.571852	-2.421221	-0.084083
O	-5.510265	-2.315439	-2.507884
S	-4.034457	-2.287189	-1.979057
O	-3.696046	-1.095299	-0.997500
O	-8.229247	-1.932106	-5.215326
O	-8.507437	-0.657984	-2.296010
O	-6.688743	0.888295	-5.969654
O	-2.937061	-2.432790	-3.112643
O	-4.325563	0.240797	-6.970364
O	-3.579790	-3.968701	-5.560052
O	-2.095713	0.609633	-5.056693
O	-2.581986	-2.038301	-7.455066
O	-5.395434	3.089525	-2.303494
S	-6.532082	3.208223	-3.434197
O	-7.334723	1.839849	-3.496719
O	-4.298866	1.522956	0.863401
S	-2.814994	2.110410	1.014816
C	-1.816367	0.762137	2.034942
F	-1.847955	-0.373468	1.367565
O	-2.237361	1.992660	-0.490590
O	-4.866369	-5.235849	-3.601605
O	-8.625519	1.320437	-0.474899
C	-3.818505	-3.893974	-0.841873
F	-4.976585	-4.499763	-0.787758
F	-2.889273	-4.640321	-1.382591
F	-3.451036	-3.462569	0.345215
O	-10.615063	-1.137987	-6.189496
O	-3.543002	-1.375901	-9.843286
C	-7.820907	4.450673	-2.632006
F	-8.967938	4.275267	-3.252037
O	-6.044322	3.805699	-4.757650
F	-7.918596	4.181583	-1.352874
F	-7.354359	5.665742	-2.832379
O	-2.632259	3.444344	1.735937
F	-2.402152	0.636897	3.207632
F	-0.581458	1.198882	2.165865
F	-4.024604	-6.678245	-7.131175
F	-4.675848	-7.689951	-5.324628
F	-11.486442	-4.128685	-5.396831
F	-9.560431	-4.508237	-4.464988
F	-1.270936	-3.381355	-10.035902
F	-2.030780	-4.734081	-8.518241
F	-5.642902	1.557359	-9.648580
F	-7.193866	2.433897	-8.409978
F	-7.046098	-0.860112	1.330030
F	-9.134214	-1.298928	0.923102

Adduct

E(large core):	-5063.622063		
Sm	1.662457	-0.266475	-0.566047
Sm	-1.061661	-1.827430	-2.853545

Sm	-1.707307	0.384541	0.320182
Sm	0.606404	2.001643	2.810360
O	0.382778	0.961331	0.906242
C	3.710874	2.743591	-0.580678
O	3.888553	3.884713	-0.509537
O	-0.341051	-3.830207	-1.868421
S	0.877100	-3.897488	-0.815393
C	1.844684	-5.470292	-1.435725
F	3.002528	-5.504426	-0.805653
O	-3.412328	-2.229894	-3.449299
S	-4.204511	-1.608514	-2.203247
C	-5.039125	-3.147852	-1.304695
F	-5.533824	-2.710513	-0.167734
O	-0.354573	-0.797387	-1.127500
O	0.957704	-1.940989	-4.059259
S	2.252547	-0.993720	-4.159098
C	3.610282	-2.246350	-4.787296
F	3.144889	-2.834175	-5.871335
O	-0.928571	0.410046	-3.737150
S	-0.581882	1.608629	-2.751469
C	-0.676050	3.205602	-3.894107
F	0.174043	4.079553	-3.419520
O	-1.535972	1.545323	3.671586
S	-3.099757	1.294628	3.436214
C	-3.511974	0.044512	4.878119
F	-2.810562	-1.056357	4.694720
O	-0.900131	-1.412526	1.941346
S	0.549725	-1.442035	2.547692
O	0.825252	-0.288785	3.597470
O	-2.990085	-1.218167	-1.207734
O	-3.328981	0.410987	2.131731
O	-1.717730	1.776024	-1.674075
O	1.734183	-1.556735	1.510567
O	0.881105	1.575951	-2.183489
O	1.898693	-2.719244	-1.074704
O	3.559861	1.581828	-0.690040
O	2.782941	-0.591107	-2.720542
O	-0.120644	4.057511	1.914173
S	-1.295391	4.056716	0.818332
O	-2.104005	2.693316	0.980636
O	2.317707	2.727587	4.417494
S	3.610069	2.617078	3.472606
C	4.658085	1.118057	4.189936
F	3.841051	0.113337	4.426963
O	2.990629	2.051821	2.096788
O	0.434135	-4.184534	0.625828
O	-4.004001	2.516039	3.614115
C	0.633394	-3.078583	3.644807
F	-0.372901	-3.844434	3.313300
F	1.791185	-3.648053	3.412893
F	0.539427	-2.689192	4.898665

O	-5.271610	-0.551779	-2.469841
O	2.156663	0.135066	-5.190438
C	-2.553595	5.395092	1.502134
F	-3.705008	5.193687	0.899842
O	-0.862878	4.490468	-0.585584
F	-2.654622	5.243299	2.801261
F	-2.058664	6.577349	1.196460
O	4.547648	3.819783	3.382544
F	5.239569	1.529762	5.295216
F	5.550956	0.793553	3.275384
F	2.020964	-5.371512	-2.737830
F	1.116808	-6.527633	-1.138593
F	-5.983055	-3.606365	-2.095205
F	-4.099995	-4.046936	-1.104462
F	4.694751	-1.548824	-5.059643
F	3.845496	-3.128057	-3.837495
F	-0.350815	2.824446	-5.106244
F	-1.911870	3.640799	-3.841522
F	-3.186396	0.624973	6.015613
F	-4.804164	-0.207663	4.830740

Product

E(large core): -5063.650546

Sm	2.044679	-0.575007	-1.608868
Sm	-1.306834	-1.845557	-2.874176
Sm	-1.136035	0.632348	0.114180
Sm	1.213325	2.347612	2.847130
O	1.103321	1.344132	0.448890
C	2.381015	1.742146	0.292879
O	2.857388	2.482281	1.201985
O	-0.606047	-3.849646	-1.875876
S	0.796699	-4.046467	-1.110961
C	1.373172	-5.783983	-1.784573
F	2.638094	-5.942268	-1.453231
O	-3.758905	-2.093220	-2.961229
S	-4.209608	-1.166128	-1.735071
C	-4.999196	-2.403198	-0.409359
F	-5.438086	-1.678100	0.589367
O	-0.112035	-0.745656	-1.453595
O	0.488062	-2.226252	-4.351184
S	1.841780	-1.620529	-4.965798
C	2.710141	-3.210412	-5.709431
F	1.818285	-3.838826	-6.448026
O	-1.288133	0.289620	-3.970962
S	-0.422895	1.441149	-3.290725
C	-0.549694	2.946600	-4.528639
F	0.331586	3.835591	-4.145286
O	-0.881047	1.242084	2.647498
S	-2.429253	0.976085	3.040341
C	-2.326702	-0.516092	4.351975
F	-2.507834	-1.642424	3.698606

O	-0.087505	-1.185070	1.526432
S	1.429791	-1.179376	1.938729
O	1.831231	-0.011582	2.926847
O	-2.754865	-0.796424	-1.105549
O	-3.008120	0.329759	1.706493
O	-1.074066	1.954521	-1.955140
O	2.417637	-1.312190	0.718420
O	1.112291	1.103755	-3.212296
O	1.886868	-3.053688	-1.683733
O	3.029924	1.309813	-0.704977
O	2.827125	-1.201335	-3.781798
O	-0.001428	4.106761	1.950704
S	-0.989692	4.246801	0.691421
O	-1.823476	2.904349	0.507120
O	0.867925	2.154740	5.270751
S	1.961933	3.241282	5.725616
C	3.373968	2.189027	6.588164
F	3.774749	1.271788	5.727454
O	2.604462	3.680274	4.315024
O	0.669198	-4.163252	0.412274
O	-3.184456	2.123978	3.700817
C	1.723698	-2.794303	3.052671
F	0.580794	-3.424465	3.150228
F	2.646397	-3.514878	2.468668
F	2.129192	-2.364363	4.226913
O	-5.175767	-0.018114	-1.994975
O	1.659745	-0.612598	-6.100657
C	-2.335453	5.498164	1.361624
F	-3.316901	5.521971	0.484119
O	-0.342550	4.841140	-0.561398
F	-2.748968	5.071275	2.531196
F	-1.756713	6.676358	1.456634
O	1.533261	4.336926	6.698076
F	2.860960	1.630829	7.664792
F	4.356094	3.006525	6.898726
F	1.223214	-5.793360	-3.093801
F	0.616972	-6.699845	-1.216832
F	-5.975990	-3.039878	-1.013796
F	-4.046887	-3.227817	-0.031891
F	3.722515	-2.795275	-6.439006
F	3.119694	-3.968183	-4.715166
F	-0.286656	2.485647	-5.727592
F	-1.776026	3.406139	-4.445017
F	-1.143338	-0.478302	4.921347
F	-3.286669	-0.311143	5.224952

IV. Crystal structures

Single crystals were mounted on a Kapton loop using a Paratone N oil. An APEX II CCD BRUKER detector and a graphite Mo-Kα monochromator were used for the data acquisition. All measurements were done at 150 K and a refinement method was used for solving the structure. The structure resolution was accomplished using the SHELXS-97 and SHELXT-2014 program.[7] and the refinement was done with the SHELXL-2018 program. The structure solution and the refinement were achieved with the PLATON software.[8] Finally, pictures of the compound structure were obtained using the MERCURY software. During the refinement steps, all atoms- except hydrogens- were refined anisotropically. The position of the hydrogens was determined using residual electronic densities which are calculated by a Fourier difference. Finally, in order to obtain a complete refinement, a weighting step followed by multiples loops of refinement was done.

Table S1: Selected Crystal Data Collection Parameters for **1**, **2-py**, **2-thf** and **3**.

Compound	**1**	**2-py**	**2-thf**	**3**
Molecular formula	'C_{32} H_{52} F_{24} O_{34} S_8 Sm_4, C_4 H_8 O'	'C_{60} H_{50} F_{24} N_{10} O_{30} S_8 Sm_4, C_4 H_8 O'	'C_{50} H_{80} F_{24} O_{40} S_8 Sm_4'	'C_{56} H_{96} F_{24} O_{36} S_8 Sm_4, $_2(C_4$ H_8 O)'
Molecular weight	2366.72	2777.08	2635.02	2803.41
Crystal habit	colorless block	colorless block	colorless block	red block
Crystal dimensions (mm)	0.100x0.100 x0.080	0.180x0.160x0.060	0.180x0.160 x0.080	0.220x0.140 x0.100
Crystal system	monoclinic	monoclinic	triclinic	triclinic
Space group	P 2_1/n	P 2_1/n	P -1	P-1
a(Å)	14.473	12.2749(5)	12.5403(4)	13.0196(8)
b(Å)	14.473(3)	12.8852(6)	12.7821(4)	14.5677(8)
c(Å)	17.246(3)	29.6815(12)	15.8869(5)	15.4211(9)
α(°)	90	90	72.254(2)	95.673(2)
β (°)	90	93.453(1)	84.907(2)	114.423(2)
γ (°)	90	90	65.760(1)	101.168(2)
V($Å^3$)	3612.4(10)	4686.0(3)	2209.59(12)	2559.7(3)
Z	2	2	1	1
d(g-cm^{-3})	2.176	1.968	1.980	1.819
F(000)	2296	2704	1292	1392
μ(cm^{-1})	3.581	2.777	2.942	2.545
Absorption corrections	multi-scan;	multi-scan;	multi-scan;	multi-scan;
Diffractometer	Kappa APEX II	Kappa APEX II	Kappa APEX II	Kappa APEX II
X-ray source	MoKα	MoKα	MoKα	MoKα
λ(Å)	0.71073	0.71069	0.71069	0.71069
Monochromator	graphite	graphite	graphite	graphite
T (K)	150.0(1)	150.0(1)	150.0(1)	150.0(1)
Scan mode	phi and omega scans	phi and omega scans	phi and omega scans	phi and omega scans
Maximum θ	26.370	25.756	27.876	29.751
HKL ranges	-16 17; -9 18; -21 13	-14 15; -15 15; -36 22	-16 16; -16 16; -20 20	-18 18 ; -20 20 ; -21 21
Reflections measured	7487	26457	70815	86507
Unique data	4340	8858	10503	14501
Rint	0.0615	0.0438	0.0355	0.0570
Reflections used	2481	7499	9476	11012
Criterion	I > 2σI)	I > 2σI)	I > 2σI)	I > 2σI)
Refinement type	Fsqd	Fsqd	Fsqd	Fsqd

Compound	**1**	**2-py**	**2-thf**	**3**
Parameters refined	498	641	688	724
Reflections / parameter	4	11	13	15
wR2	0.1007	0.1258	0.0676	0.0736
R1	0.0503	0.0485	0.0201	0.0294
Weights a, b	0.0000; 0.0000	0.0491 ; 37.778	0.0515; 0.4658	0.0233 ; 3.7649
GoF	0.816	1.078	0.981	1.064
difference peak / hole (e $Å^{-3}$)	1.260(0.144) / -0.647(0.144)	1.815(0.156) / -1.216(0.156)	0.938(0.080) / -0.611(0.080)	1.305(0.114) / -0.690(0.114)

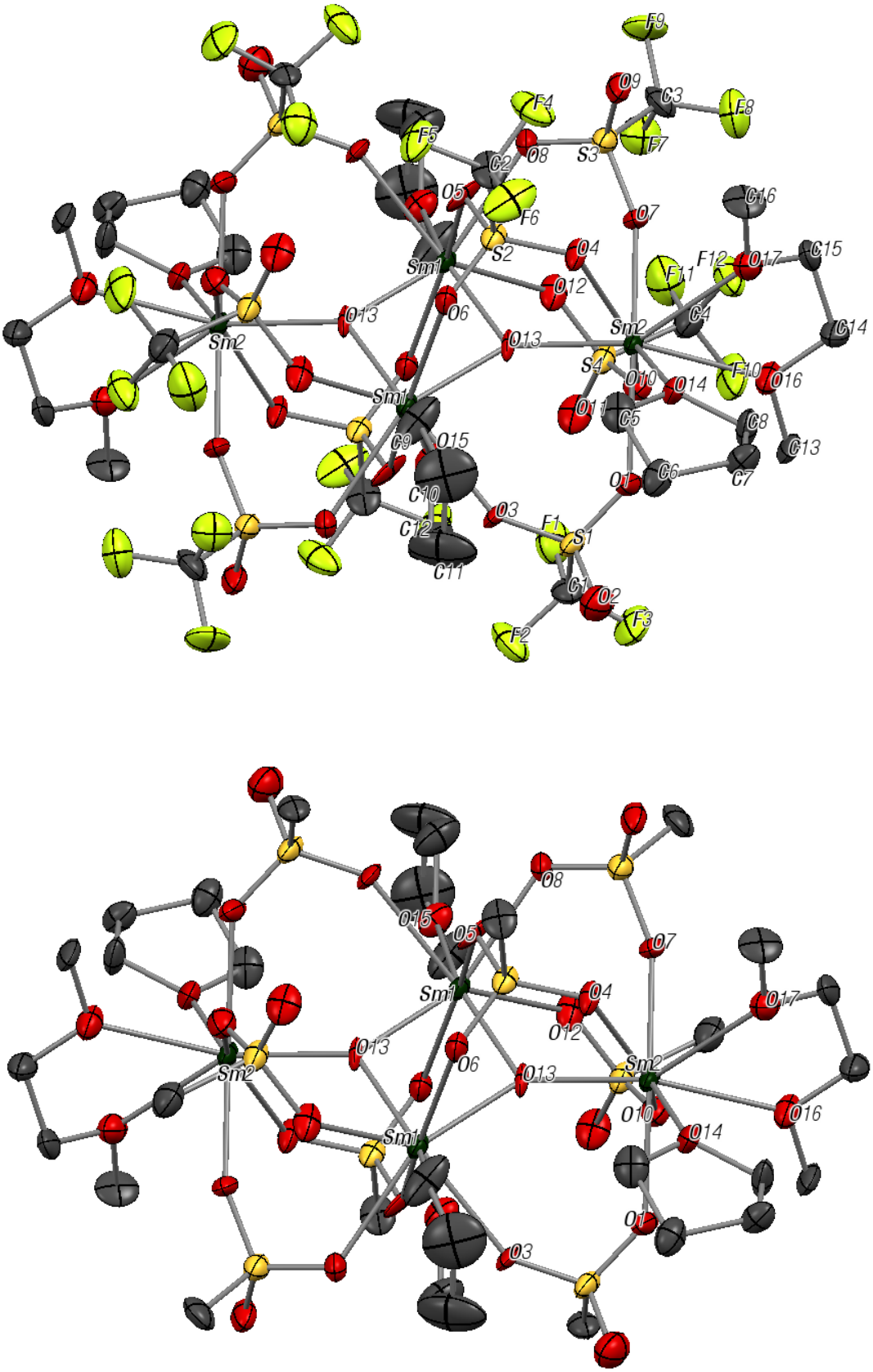


Figure S6: ORTEP of cluster **1**. Top, complete structure where only H atoms are removed for clarity. Bottom, H and CF_3 groups from the triflate anions are removed for clarity. Carbon atoms are shown in grey, oxygen atoms in red, fluoride in green, sulfur in yellow and samarium in green.

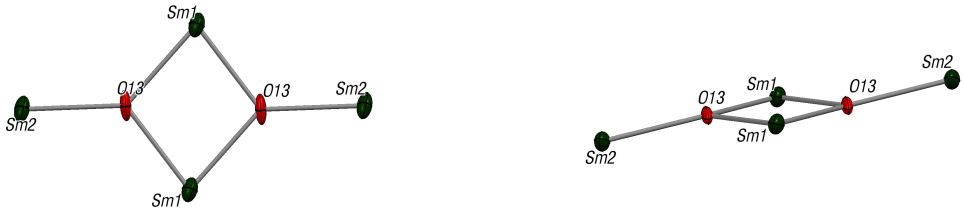


Figure S7: ORTEP of the $[Sm_2(\mu_3\text{-}O)]_2$ core of **1**.

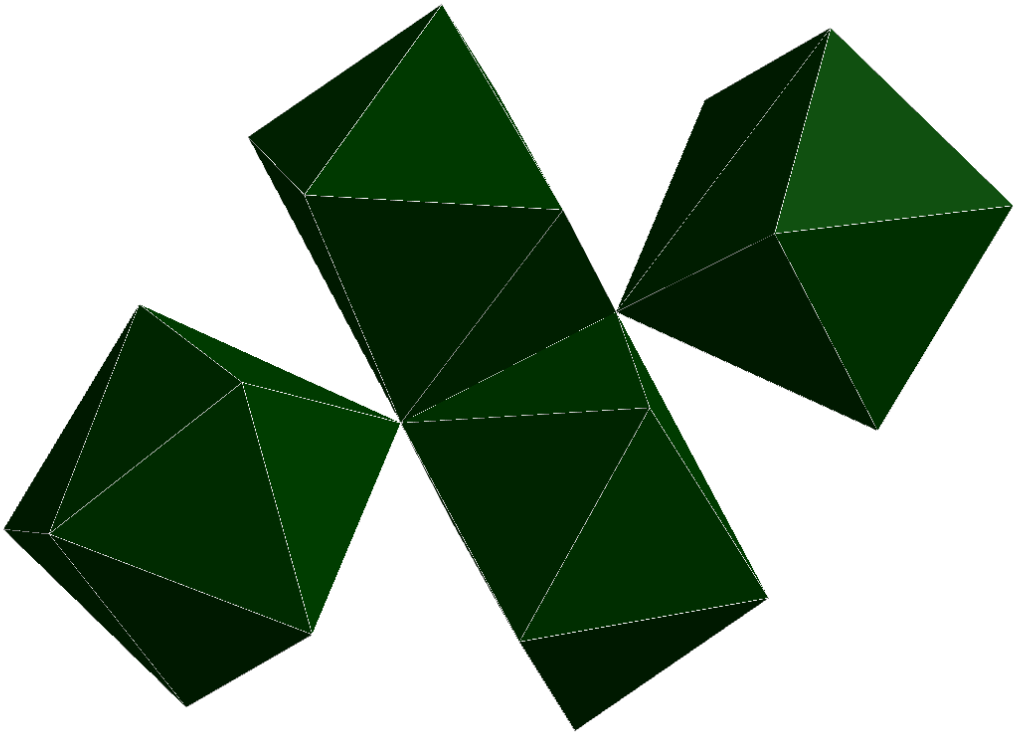


Figure S8: Polyhedral representation of cluster **1**.

Table S2: Bond lengths (Å) and angles (deg) in **1**.

Sm(1)-O(13)#3	2.250(8)	Sm(1)-O(13)	2.271(7)
Sm(1)-O(3)	2.444(7)	Sm(1)-O(6)	2.471(7)
Sm(1)-O(8)	2.480(7)	Sm(1)-O(12)	2.490(8)
Sm(1)-O(15)	2.594(8)	Sm(1)-O(5)	2.596(7)
Sm(1)-Sm(1)#3	3.497(1)	Sm(1)-Sm(2)#3	3.940(1)
Sm(2)-O(13)	2.207(7)	Sm(2)-O(7)#3	2.400(8)
Sm(2)-O(1)	2.447(7)	Sm(2)-O(10)#3	2.458(7)
Sm(2)-O(4)#3	2.484(7)	Sm(2)-O(14)	2.49(1)
Sm(2)-O(16)	2.52(1)	Sm(2)-O(17)	2.563(8)
S(1)-O(1)	1.42(1)	S(1)-O(3)	1.434(8)
S(1)-O(2)	1.45(1)	S(1)-C(1)	1.80(1)
S(2)-O(6)#3	1.435(8)	S(2)-O(5)	1.444(8)
S(2)-O(4)	1.449(8)	S(2)-C(2)	1.80(1)
S(3)-O(9)	1.412(7)	S(3)-O(8)	1.444(8)
S(3)-O(7)	1.476(8)	S(3)-C(3)	1.82(1)
S(4)-O(11)	1.415(7)	S(4)-O(10)	1.42(1)
S(4)-O(12)	1.458(8)	S(4)-C(4)	1.86(1)
F(1)-C(1)	1.32(2)	F(2)-C(1)	1.32(1)
F(3)-C(1)	1.31(1)	F(4)-C(2)	1.32(1)
F(5)-C(2)	1.35(1)	F(6)-C(2)	1.30(1)
F(7)-C(3)	1.35(1)	F(8)-C(3)	1.31(1)
F(9)-C(3)	1.32(1)	F(10)-C(4)	1.28(1)

F(11)-C(4)	1.35(2)	F(12)-C(4)	1.33(1)
O(14)-C(8)	1.44(1)	O(14)-C(5)	1.47(2)
O(15)-C(12)	1.41(2)	O(15)-C(9)	1.44(1)
O(16)-C(14)	1.41(1)	O(16)-C(13)	1.42(1)
O(17)-C(15)	1.45(2)	O(17)-C(16)	1.45(1)
C(5)-C(6)	1.49(2)	C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900	C(6)-C(7)	1.52(2)
C(6)-H(6A)	0.9900	C(6)-H(6B)	0.9900
C(7)-C(8)	1.46(2)	C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900	C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900	C(9)-C(10)	1.51(2)
C(9)-H(9A)	0.9900	C(9)-H(9B)	0.9900
C(10)-C(11)	1.42(2)	C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900	C(11)-C(12)	1.44(2)
C(11)-H(11A)	0.9900	C(11)-H(11B)	0.9900
C(12)-H(12A)	0.9900	C(12)-H(12B)	0.9900
C(13)-H(13A)	0.9800	C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800	C(14)-C(15)	1.48(1)
C(14)-H(14A)	0.9900	C(14)-H(14B)	0.9900
C(15)-H(15A)	0.9900	C(15)-H(15B)	0.9900
C(16)-H(16A)	0.9800	C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800	O(18)-C(20)	1.4200
O(18)-C(17)	1.4200	C(17)-C(18)	1.4200
C(17)-H(17A)	0.9900	C(17)-H(17B)	0.9900
C(18)-C(19)	1.4200	C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900	C(19)-C(20)	1.4200
C(19)-H(19A)	0.9900	C(19)-H(19B)	0.9900
C(20)-H(20A)	0.9900	C(20)-H(20B)	0.9900

O(13)#3-Sm(1)-O(13)	78.7(3)	O(13)#3-Sm(1)-O(3)	140.1(2)
O(13)-Sm(1)-O(3)	81.5(3)	O(13)#3-Sm(1)-O(6)	91.7(2)
O(13)-Sm(1)-O(6)	74.5(2)	O(3)-Sm(1)-O(6)	115.8(2)
O(13)#3-Sm(1)-O(8)	106.6(3)	O(13)-Sm(1)-O(8)	145.8(2)
O(3)-Sm(1)-O(8)	73.2(3)	O(6)-Sm(1)-O(8)	137.4(3)
O(13)#3-Sm(1)-O(12)	83.3(3)	O(13)-Sm(1)-O(12)	139.2(2)
O(3)-Sm(1)-O(12)	131.9(3)	O(6)-Sm(1)-O(12)	69.8(2)
O(8)-Sm(1)-O(12)	74.5(2)	O(13)#3-Sm(1)-O(15)	149.7(3)
O(13)-Sm(1)-O(15)	116.7(3)	O(3)-Sm(1)-O(15)	70.1(3)
O(6)-Sm(1)-O(15)	69.9(3)	O(8)-Sm(1)-O(15)	75.8(3)
O(12)-Sm(1)-O(15)	68.1(3)	O(13)#3-Sm(1)-O(5)	72.0(2)
O(13)-Sm(1)-O(5)	83.7(3)	O(3)-Sm(1)-O(5)	71.7(2)
O(6)-Sm(1)-O(5)	155.1(3)	O(8)-Sm(1)-O(5)	66.9(3)
O(12)-Sm(1)-O(5)	124.6(3)	O(15)-Sm(1)-O(5)	132.5(3)
O(13)#3-Sm(1)-Sm(1)#3	39.5(2)	O(13)-Sm(1)-Sm(1)#3	39.1(2)
O(3)-Sm(1)-Sm(1)#3	113.4(2)	O(6)-Sm(1)-Sm(1)#3	81.1(2)
O(8)-Sm(1)-Sm(1)#3	136.2(2)	O(12)-Sm(1)-Sm(1)#3	114.6(2)
O(15)-Sm(1)-Sm(1)#3	148.0(2)	O(5)-Sm(1)-Sm(1)#3	74.3(2)
O(13)#3-Sm(1)-Sm(2)#3	27.6(2)	O(13)-Sm(1)-Sm(2)#3	105.7(2)
O(3)-Sm(1)-Sm(2)#3	140.0(2)	O(6)-Sm(1)-Sm(2)#3	103.9(2)
O(8)-Sm(1)-Sm(2)#3	81.2(2)	O(12)-Sm(1)-Sm(2)#3	65.8(2)
O(15)-Sm(1)-Sm(2)#3	132.4(2)	O(5)-Sm(1)-Sm(2)#3	70.2(2)
Sm(1)#3-Sm(1)-Sm(2)#3	66.79(2)	O(13)-Sm(2)-O(7)#3	87.2(3)
O(13)-Sm(2)-O(1)	87.2(3)	O(7)#3-Sm(2)-O(1)	154.5(3)
O(13)-Sm(2)-O(10)#3	81.3(3)	O(7)#3-Sm(2)-O(10)#3	80.3(3)
O(1)-Sm(2)-O(10)#3	74.3(3)	O(13)-Sm(2)-O(4)#3	74.9(2)
O(7)#3-Sm(2)-O(4)#3	77.1(3)	O(1)-Sm(2)-O(4)#3	125.1(3)
O(10)#3-Sm(2)-O(4)#3	147.7(3)	O(13)-Sm(2)-O(14)	115.3(3)
O(7)#3-Sm(2)-O(14)	134.7(2)	O(1)-Sm(2)-O(14)	69.5(2)
O(10)#3-Sm(2)-O(14)	138.7(3)	O(4)#3-Sm(2)-O(14)	72.5(3)
O(13)-Sm(2)-O(16)	148.2(2)	O(7)#3-Sm(2)-O(16)	93.8(3)
O(1)-Sm(2)-O(16)	78.3(3)	O(10)#3-Sm(2)-O(16)	67.6(3)
O(4)#3-Sm(2)-O(16)	136.3(2)	O(14)-Sm(2)-O(16)	86.0(3)

O(13)-Sm(2)-O(17)	146.6(2)	O(7)#3-Sm(2)-O(17)	72.3(3)
O(1)-Sm(2)-O(17)	122.2(3)	O(10)#3-Sm(2)-O(17)	119.3(3)
O(4)#3-Sm(2)-O(17)	74.9(3)	O(14)-Sm(2)-O(17)	67.9(3)
O(16)-Sm(2)-O(17)	61.7(2)	O(13)-Sm(2)-Sm(1)#3	28.2(2)
O(7)#3-Sm(2)-Sm(1)#3	59.5(2)	O(1)-Sm(2)-Sm(1)#3	110.1(2)
O(10)#3-Sm(2)-Sm(1)#3	73.1(2)	O(4)#3-Sm(2)-Sm(1)#3	75.7(2)
O(14)-Sm(2)-Sm(1)#3	138.1(2)	O(16)-Sm(2)-Sm(1)#3	135.7(2)
O(17)-Sm(2)-Sm(1)#3	127.8(2)	O(1)-S(1)-O(3)	114.8(5)
O(1)-S(1)-O(2)	113.1(5)	O(3)-S(1)-O(2)	114.3(6)
O(1)-S(1)-C(1)	104.1(6)	O(3)-S(1)-C(1)	104.1(5)
O(2)-S(1)-C(1)	104.9(6)	O(6)#3-S(2)-O(5)	114.5(5)
O(6)#3-S(2)-O(4)	113.7(5)	O(5)-S(2)-O(4)	116.0(6)
O(6)#3-S(2)-C(2)	103.4(6)	O(5)-S(2)-C(2)	106.0(6)
O(4)-S(2)-C(2)	101.0(5)	O(9)-S(3)-O(8)	116.4(5)
O(9)-S(3)-O(7)	115.1(5)	O(8)-S(3)-O(7)	111.2(5)
O(9)-S(3)-C(3)	104.7(5)	O(8)-S(3)-C(3)	102.7(6)
O(7)-S(3)-C(3)	105.0(6)	O(11)-S(4)-O(10)	118.9(6)
O(11)-S(4)-O(12)	115.1(5)	O(10)-S(4)-O(12)	111.6(5)
O(11)-S(4)-C(4)	101.0(6)	O(10)-S(4)-C(4)	102.2(6)
O(12)-S(4)-C(4)	105.7(6)	S(1)-O(1)-Sm(2)	138.0(5)
S(1)-O(3)-Sm(1)	147.9(5)	S(2)-O(4)-Sm(2)#3	122.3(4)
S(2)-O(5)-Sm(1)	122.5(4)	S(2)#3-O(6)-Sm(1)	121.8(4)
S(3)-O(7)-Sm(2)#3	151.6(5)	S(3)-O(8)-Sm(1)	122.5(5)
S(4)-O(10)-Sm(2)#3	134.4(5)	S(4)-O(12)-Sm(1)	135.5(6)
Sm(2)-O(13)-Sm(1)#3	124.2(3)	Sm(2)-O(13)-Sm(1)	133.2(4)
Sm(1)#3-O(13)-Sm(1)	101.3(3)	C(8)-O(14)-C(5)	109(1)
C(8)-O(14)-Sm(2)	124.1(7)	C(5)-O(14)-Sm(2)	123.4(7)
C(12)-O(15)-C(9)	106(1)	C(12)-O(15)-Sm(1)	123.0(7)
C(9)-O(15)-Sm(1)	126.2(7)	C(14)-O(16)-C(13)	112(1)
C(14)-O(16)-Sm(2)	123.3(6)	C(13)-O(16)-Sm(2)	124.8(6)
C(15)-O(17)-C(16)	112(1)	C(15)-O(17)-Sm(2)	112.4(6)
C(16)-O(17)-Sm(2)	127.1(7)	F(3)-C(1)-F(2)	110(1)
F(3)-C(1)-F(1)	106(1)	F(2)-C(1)-F(1)	107(1)
F(3)-C(1)-S(1)	112(1)	F(2)-C(1)-S(1)	111(1)
F(1)-C(1)-S(1)	112.4(8)	F(6)-C(2)-F(4)	109(1)
F(6)-C(2)-F(5)	107(1)	F(4)-C(2)-F(5)	106(1)
F(6)-C(2)-S(2)	113(1)	F(4)-C(2)-S(2)	110(1)
F(5)-C(2)-S(2)	111.8(8)	F(8)-C(3)-F(9)	111(1)
F(8)-C(3)-F(7)	108(1)	F(9)-C(3)-F(7)	105(1)
F(8)-C(3)-S(3)	110(1)	F(9)-C(3)-S(3)	110(1)
F(7)-C(3)-S(3)	112.7(8)	F(10)-C(4)-F(12)	109(1)
F(10)-C(4)-F(11)	109(1)	F(12)-C(4)-F(11)	111(1)
F(10)-C(4)-S(4)	110(1)	F(12)-C(4)-S(4)	108(1)
F(11)-C(4)-S(4)	110(1)	O(14)-C(5)-C(6)	104(1)
O(14)-C(5)-H(5A)	111.0	C(6)-C(5)-H(5A)	111.0
O(14)-C(5)-H(5B)	111.0	C(6)-C(5)-H(5B)	111.0
H(5A)-C(5)-H(5B)	109.0	C(5)-C(6)-C(7)	104(1)
C(5)-C(6)-H(6A)	111.0	C(7)-C(6)-H(6A)	111.0
C(5)-C(6)-H(6B)	111.0	C(7)-C(6)-H(6B)	111.0
H(6A)-C(6)-H(6B)	109.0	C(8)-C(7)-C(6)	102(1)
C(8)-C(7)-H(7A)	111.5	C(6)-C(7)-H(7A)	111.5
C(8)-C(7)-H(7B)	111.5	C(6)-C(7)-H(7B)	111.5
H(7A)-C(7)-H(7B)	109.3	O(14)-C(8)-C(7)	108(1)
O(14)-C(8)-H(8A)	110.1	C(7)-C(8)-H(8A)	110.1
O(14)-C(8)-H(8B)	110.1	C(7)-C(8)-H(8B)	110.1
H(8A)-C(8)-H(8B)	108.5	O(15)-C(9)-C(10)	106(1)
O(15)-C(9)-H(9A)	110.5	C(10)-C(9)-H(9A)	110.5
O(15)-C(9)-H(9B)	110.5	C(10)-C(9)-H(9B)	110.5
H(9A)-C(9)-H(9B)	108.7	C(11)-C(10)-C(9)	103(1)
C(11)-C(10)-H(10A)	111.2	C(9)-C(10)-H(10A)	111.2
C(11)-C(10)-H(10B)	111.2	C(9)-C(10)-H(10B)	111.2
H(10A)-C(10)-H(10B)	109.1	C(10)-C(11)-C(12)	111(2)
C(10)-C(11)-H(11A)	109.5	C(12)-C(11)-H(11A)	109.5

C(10)-C(11)-H(11B)	109.5	C(12)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	108.0	O(15)-C(12)-C(11)	107(1)
O(15)-C(12)-H(12A)	110.3	C(11)-C(12)-H(12A)	110.3
O(15)-C(12)-H(12B)	110.3	C(11)-C(12)-H(12B)	110.3
H(12A)-C(12)-H(12B)	108.6	O(16)-C(13)-H(13A)	109.5
O(16)-C(13)-H(13B)	109.5	H(13A)-C(13)-H(13B)	109.5
O(16)-C(13)-H(13C)	109.5	H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5	O(16)-C(14)-C(15)	109(1)
O(16)-C(14)-H(14A)	110.0	C(15)-C(14)-H(14A)	110.0
O(16)-C(14)-H(14B)	110.0	C(15)-C(14)-H(14B)	110.0
H(14A)-C(14)-H(14B)	108.3	O(17)-C(15)-C(14)	107(1)
O(17)-C(15)-H(15A)	110.3	C(14)-C(15)-H(15A)	110.3
O(17)-C(15)-H(15B)	110.3	C(14)-C(15)-H(15B)	110.3
H(15A)-C(15)-H(15B)	108.5	O(17)-C(16)-H(16A)	109.5
O(17)-C(16)-H(16B)	109.5	H(16A)-C(16)-H(16B)	109.5
O(17)-C(16)-H(16C)	109.5	H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5	C(20)-O(18)-C(17)	108.0
C(18)-C(17)-O(18)	108.0	C(18)-C(17)-H(17A)	110.1
O(18)-C(17)-H(17A)	110.1	C(18)-C(17)-H(17B)	110.1
O(18)-C(17)-H(17B)	110.1	H(17A)-C(17)-H(17B)	108.4
C(19)-C(18)-C(17)	108.0	C(19)-C(18)-H(18A)	110.1
C(17)-C(18)-H(18A)	110.1	C(19)-C(18)-H(18B)	110.1
C(17)-C(18)-H(18B)	110.1	H(18A)-C(18)-H(18B)	108.4
C(18)-C(19)-C(20)	108.0	C(18)-C(19)-H(19A)	110.1
C(20)-C(19)-H(19A)	110.1	C(18)-C(19)-H(19B)	110.1
C(20)-C(19)-H(19B)	110.1	H(19A)-C(19)-H(19B)	108.4
O(18)-C(20)-C(19)	108.0	O(18)-C(20)-H(20A)	110.1
C(19)-C(20)-H(20A)	110.1	O(18)-C(20)-H(20B)	110.1
C(19)-C(20)-H(20B)	110.1	H(20A)-C(20)-H(20B)	108.4

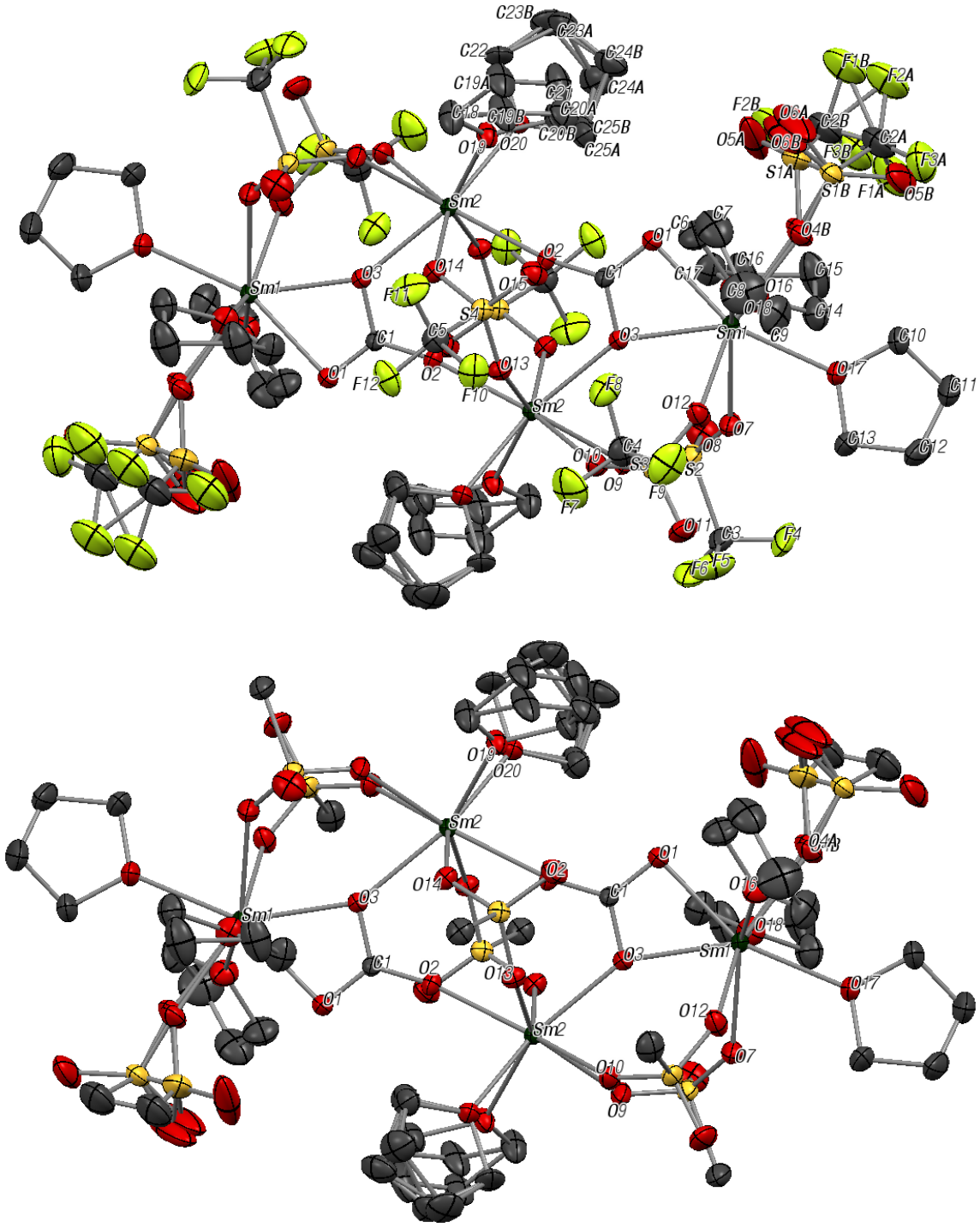


Figure S9: ORTEP of cluster **2-thf**. Top, complete structure where only hydrogen atoms are removed for clarity. Bottom, hydrogen atoms and CF_3 groups are removed for clarity. Carbon atoms are shown in grey, oxygen atoms in red, fluoride in green, sulfur in yellow and samarium in green.

Figure S10: ORTEP of the $[Sm_2(\mu_3\text{-}\eta_2(O,O'):\eta^1(O):\eta^1(O')\text{-}CO_3)]_2$ core of **2-thf**.

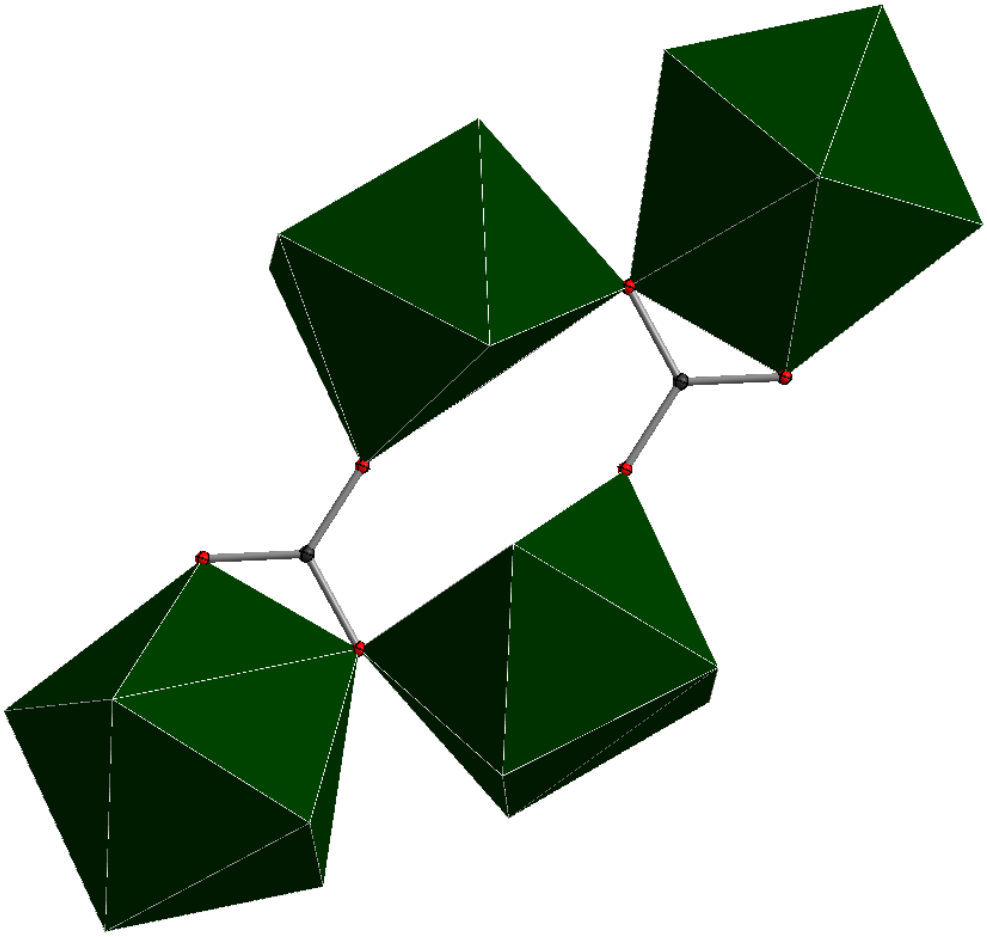


Figure S11: Polyhedral representation of cluster **2-thf**.

Table S3: Bond lengths (Å) and angles (deg) in **2-thf**.

Sm(1)-O(4B)	2.33(1)	Sm(1)-O(1)	2.379(2)
Sm(1)-O(3)	2.392(2)	Sm(1)-O(12)	2.410(2)
Sm(1)-O(18)	2.416(2)	Sm(1)-O(4A)	2.424(4)
Sm(1)-O(17)	2.434(2)	Sm(1)-O(16)	2.434(2)
Sm(1)-O(7)	2.469(2)	Sm(1)-C(1)	2.805(2)
Sm(2)-O(2)#2	2.295(2)	Sm(2)-O(3)	2.362(2)
Sm(2)-O(9)	2.421(2)	Sm(2)-O(20)	2.430(2)
Sm(2)-O(10)	2.462(2)	Sm(2)-O(13)	2.471(2)
Sm(2)-O(14)	2.472(2)	Sm(2)-O(19)	2.501(2)
S(2)-O(8)	1.420(2)	S(2)-O(9)	1.450(2)
S(2)-O(7)	1.454(2)	S(2)-C(3)	1.825(3)
S(3)-O(11)	1.414(2)	S(3)-O(10)	1.450(2)
S(3)-O(12)	1.451(2)	S(3)-C(4)	1.821(3)
S(4)-O(15)	1.425(2)	S(4)-O(13)	1.454(2)
S(4)-O(14)#2	1.457(2)	S(4)-C(5)	1.826(2)

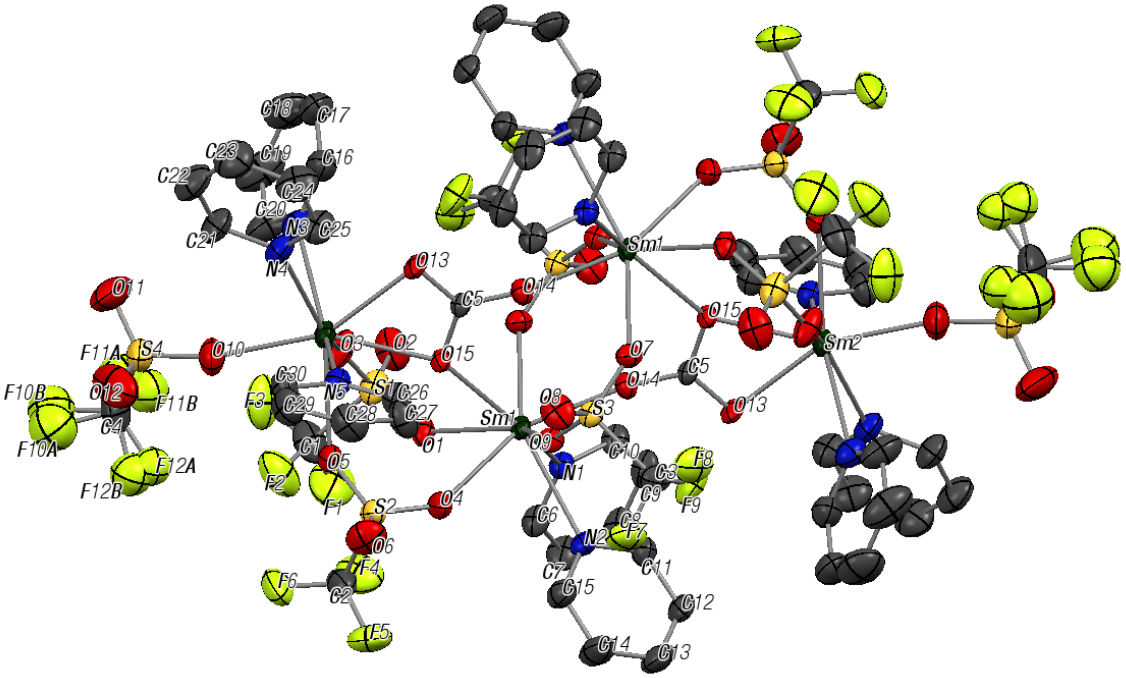
F(4)-C(3)	1.319(3)	F(5)-C(3)	1.300(4)
F(6)-C(3)	1.328(3)	F(7)-C(4)	1.330(3)
F(8)-C(4)	1.320(3)	F(9)-C(4)	1.325(3)
F(10)-C(5)	1.315(3)	F(11)-C(5)	1.321(3)
F(12)-C(5)	1.330(3)	O(1)-C(1)	1.267(3)
O(2)-C(1)	1.263(2)	O(3)-C(1)	1.315(3)
O(16)-C(9)	1.436(3)	O(16)-C(6)	1.464(4)
O(17)-C(10)	1.453(3)	O(17)-C(13)	1.465(3)
O(18)-C(14)	1.448(3)	O(18)-C(17)	1.455(3)
C(6)-C(7)	1.494(4)	C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900	C(7)-C(8)	1.485(6)
C(7)-H(7A)	0.9900	C(7)-H(7B)	0.9900
C(8)-C(9)	1.503(5)	C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900	C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900	C(10)-C(11)	1.484(5)
C(10)-H(10A)	0.9900	C(10)-H(10B)	0.9900
C(11)-C(12)	1.497(6)	C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900	C(12)-C(13)	1.503(4)
C(12)-H(12A)	0.9900	C(12)-H(12B)	0.9900
C(13)-H(13A)	0.9900	C(13)-H(13B)	0.9900
C(14)-C(15)	1.504(4)	C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900	C(15)-C(16)	1.527(4)
C(15)-H(15A)	0.9900	C(15)-H(15B)	0.9900
C(16)-C(17)	1.493(4)	C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900	C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900	O(19)-C(21)	1.455(3)
O(19)-C(18)	1.462(3)	C(18)-C(19B)	1.51(1)
C(18)-C(19A)	1.548(7)	C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900	C(18)-H(18C)	0.9900
C(18)-H(18D)	0.9900	C(19A)-C(20A)	1.521(8)
C(19A)-H(19A)	0.9900	C(19A)-H(19B)	0.9900
C(20A)-C(21)	1.526(7)	C(20A)-H(20A)	0.9900
C(20A)-H(20B)	0.9900	C(19B)-C(20B)	1.500(4)
C(19B)-H(19C)	0.9900	C(19B)-H(19D)	0.9900
C(20B)-C(21)	1.50(1)	C(20B)-H(20C)	0.9900
C(20B)-H(20D)	0.9900	C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900	C(21)-H(21C)	0.9900
C(21)-H(21D)	0.9900	O(20)-C(25A)	1.44(4)
O(20)-C(22)	1.449(3)	O(20)-C(25B)	1.47(3)
C(22)-C(23B)	1.49(1)	C(22)-C(23A)	1.54(1)
C(22)-H(22A)	0.9900	C(22)-H(22B)	0.9900
C(22)-H(22C)	0.9900	C(22)-H(22D)	0.9900
C(23A)-C(24A)	1.54(2)	C(23A)-H(23A)	0.9900
C(23A)-H(23B)	0.9900	C(24A)-C(25A)	1.53(3)
C(24A)-H(24A)	0.9900	C(24A)-H(24B)	0.9900
C(25A)-H(25A)	0.9900	C(25A)-H(25B)	0.9900
C(23B)-C(24B)	1.58(1)	C(23B)-H(23C)	0.9900
C(23B)-H(23D)	0.9900	C(24B)-C(25B)	1.48(2)
C(24B)-H(24C)	0.9900	C(24B)-H(24D)	0.9900
C(25B)-H(25C)	0.9900	C(25B)-H(25D)	0.9900
S(1A)-O(4A)	1.449(4)	S(1A)-O(6A)	1.452(4)
S(1A)-O(5A)	1.458(4)	S(1A)-C(2A)	1.812(6)
C(2A)-F(3A)	1.307(7)	C(2A)-F(2A)	1.312(6)
C(2A)-F(1A)	1.351(7)	S(1B)-O(5B)	1.442(4)
S(1B)-O(4B)	1.449(4)	S(1B)-O(6B)	1.450(4)
S(1B)-C(2B)	1.820(4)	C(2B)-F(3B)	1.18(2)
C(2B)-F(2B)	1.19(2)	C(2B)-F(1B)	1.36(1)
F(3B)-F(2B)	1.76(2)		

O(4B)-Sm(1)-O(1)	80.9(6)	O(4B)-Sm(1)-O(3)	134.6(6)
O(1)-Sm(1)-O(3)	54.57(5)	O(4B)-Sm(1)-O(12)	137.7(7)
O(1)-Sm(1)-O(12)	114.05(6)	O(3)-Sm(1)-O(12)	76.70(5)

O(4B)-Sm(1)-O(18)	75(1)	O(1)-Sm(1)-O(18)	84.93(6)
O(3)-Sm(1)-O(18)	90.63(6)	O(12)-Sm(1)-O(18)	141.85(6)
O(1)-Sm(1)-O(4A)	78.2(2)	O(3)-Sm(1)-O(4A)	130.8(2)
O(12)-Sm(1)-O(4A)	143.2(2)	O(18)-Sm(1)-O(4A)	70.4(3)
O(4B)-Sm(1)-O(17)	76.6(6)	O(1)-Sm(1)-O(17)	156.82(6)
O(3)-Sm(1)-O(17)	148.52(5)	O(12)-Sm(1)-O(17)	80.25(6)
O(18)-Sm(1)-O(17)	94.49(6)	O(4A)-Sm(1)-O(17)	79.8(2)
O(4B)-Sm(1)-O(16)	72(1)	O(1)-Sm(1)-O(16)	82.00(6)
O(3)-Sm(1)-O(16)	106.75(6)	O(12)-Sm(1)-O(16)	71.88(6)
O(18)-Sm(1)-O(16)	145.88(6)	O(4A)-Sm(1)-O(16)	76.1(3)
O(17)-Sm(1)-O(16)	85.77(6)	O(4B)-Sm(1)-O(7)	134(1)
O(1)-Sm(1)-O(7)	124.28(5)	O(3)-Sm(1)-O(7)	76.21(5)
O(12)-Sm(1)-O(7)	72.15(6)	O(18)-Sm(1)-O(7)	69.90(6)
O(4A)-Sm(1)-O(7)	131.3(3)	O(17)-Sm(1)-O(7)	76.50(5)
O(16)-Sm(1)-O(7)	142.01(6)	O(4B)-Sm(1)-C(1)	107.3(6)
O(1)-Sm(1)-C(1)	26.70(6)	O(3)-Sm(1)-C(1)	27.89(6)
O(12)-Sm(1)-C(1)	95.72(6)	O(18)-Sm(1)-C(1)	88.04(6)
O(4A)-Sm(1)-C(1)	104.2(2)	O(17)-Sm(1)-C(1)	175.84(6)
O(16)-Sm(1)-C(1)	94.00(6)	O(7)-Sm(1)-C(1)	101.33(5)
O(2)#2-Sm(2)-O(3)	113.68(5)	O(2)#2-Sm(2)-O(9)	146.32(6)
O(3)-Sm(2)-O(9)	75.69(5)	O(2)#2-Sm(2)-O(20)	82.38(5)
O(3)-Sm(2)-O(20)	144.62(5)	O(9)-Sm(2)-O(20)	108.99(6)
O(2)#2-Sm(2)-O(10)	141.29(6)	O(3)-Sm(2)-O(10)	74.28(5)
O(9)-Sm(2)-O(10)	71.76(6)	O(20)-Sm(2)-O(10)	74.28(5)
O(2)#2-Sm(2)-O(13)	74.31(5)	O(3)-Sm(2)-O(13)	79.16(5)
O(9)-Sm(2)-O(13)	138.68(5)	O(20)-Sm(2)-O(13)	75.25(5)
O(10)-Sm(2)-O(13)	70.16(5)	O(2)#2-Sm(2)-O(14)	75.40(5)
O(3)-Sm(2)-O(14)	74.63(5)	O(9)-Sm(2)-O(14)	76.49(6)
O(20)-Sm(2)-O(14)	140.71(5)	O(10)-Sm(2)-O(14)	139.89(5)
O(13)-Sm(2)-O(14)	126.95(5)	O(2)#2-Sm(2)-O(19)	84.41(5)
O(3)-Sm(2)-O(19)	138.37(5)	O(9)-Sm(2)-O(19)	70.45(5)
O(20)-Sm(2)-O(19)	71.39(5)	O(10)-Sm(2)-O(19)	115.52(5)
O(13)-Sm(2)-O(19)	142.38(5)	O(14)-Sm(2)-O(19)	74.51(5)
O(8)-S(2)-O(9)	115.2(1)	O(8)-S(2)-O(7)	115.9(1)
O(9)-S(2)-O(7)	112.6(1)	O(8)-S(2)-C(3)	105.4(1)
O(9)-S(2)-C(3)	103.1(1)	O(7)-S(2)-C(3)	102.6(1)
O(11)-S(3)-O(10)	115.5(1)	O(11)-S(3)-O(12)	115.4(1)
O(10)-S(3)-O(12)	113.3(1)	O(11)-S(3)-C(4)	104.9(1)
O(10)-S(3)-C(4)	103.9(1)	O(12)-S(3)-C(4)	101.6(1)
O(15)-S(4)-O(13)	116.2(1)	O(15)-S(4)-O(14)#2	115.5(1)
O(13)-S(4)-O(14)#2	113.0(1)	O(15)-S(4)-C(5)	104.0(1)
O(13)-S(4)-C(5)	102.6(1)	O(14)#2-S(4)-C(5)	103.0(1)
C(1)-O(1)-Sm(1)	95.8(1)	C(1)-O(2)-Sm(2)#2	169.7(2)
C(1)-O(3)-Sm(2)	117.1(1)	C(1)-O(3)-Sm(1)	93.8(1)
Sm(2)-O(3)-Sm(1)	148.88(7)	S(2)-O(7)-Sm(1)	140.0(1)
S(2)-O(9)-Sm(2)	145.9(1)	S(3)-O(10)-Sm(2)	151.6(1)
S(3)-O(12)-Sm(1)	146.6(1)	S(4)-O(13)-Sm(2)	141.2(1)
S(4)#2-O(14)-Sm(2)	129.2(1)	C(9)-O(16)-C(6)	109.4(2)
C(9)-O(16)-Sm(1)	126.2(2)	C(6)-O(16)-Sm(1)	124.3(2)
C(10)-O(17)-C(13)	108.6(2)	C(10)-O(17)-Sm(1)	128.4(2)
C(13)-O(17)-Sm(1)	123.0(1)	C(14)-O(18)-C(17)	109.7(2)
C(14)-O(18)-Sm(1)	124.0(2)	C(17)-O(18)-Sm(1)	126.1(2)
O(2)-C(1)-O(1)	125.1(2)	O(2)-C(1)-O(3)	119.1(2)
O(1)-C(1)-O(3)	115.8(2)	O(2)-C(1)-Sm(1)	176.8(2)
O(1)-C(1)-Sm(1)	57.5(1)	O(3)-C(1)-Sm(1)	58.3(1)
F(5)-C(3)-F(4)	108.6(2)	F(5)-C(3)-F(6)	109.3(2)
F(4)-C(3)-F(6)	107.8(2)	F(5)-C(3)-S(2)	112.0(2)
F(4)-C(3)-S(2)	109.4(2)	F(6)-C(3)-S(2)	109.5(2)
F(8)-C(4)-F(9)	107.8(2)	F(8)-C(4)-F(7)	107.8(2)
F(9)-C(4)-F(7)	108.4(2)	F(8)-C(4)-S(3)	111.8(2)
F(9)-C(4)-S(3)	110.5(2)	F(7)-C(4)-S(3)	110.5(2)
F(10)-C(5)-F(11)	108.3(2)	F(10)-C(5)-F(12)	107.9(2)
F(11)-C(5)-F(12)	107.5(2)	F(10)-C(5)-S(4)	110.4(2)

F(11)-C(5)-S(4)	110.7(2)	F(12)-C(5)-S(4)	111.9(2)
O(16)-C(6)-C(7)	106.4(3)	O(16)-C(6)-H(6A)	110.5
C(7)-C(6)-H(6A)	110.5	O(16)-C(6)-H(6B)	110.5
C(7)-C(6)-H(6B)	110.5	H(6A)-C(6)-H(6B)	108.6
C(8)-C(7)-C(6)	104.5(3)	C(8)-C(7)-H(7A)	110.8
C(6)-C(7)-H(7A)	110.8	C(8)-C(7)-H(7B)	110.8
C(6)-C(7)-H(7B)	110.8	H(7A)-C(7)-H(7B)	108.9
C(7)-C(8)-C(9)	104.6(3)	C(7)-C(8)-H(8A)	110.8
C(9)-C(8)-H(8A)	110.8	C(7)-C(8)-H(8B)	110.8
C(9)-C(8)-H(8B)	110.8	H(8A)-C(8)-H(8B)	108.9
O(16)-C(9)-C(8)	104.7(3)	O(16)-C(9)-H(9A)	110.8
C(8)-C(9)-H(9A)	110.8	O(16)-C(9)-H(9B)	110.8
C(8)-C(9)-H(9B)	110.8	H(9A)-C(9)-H(9B)	108.9
O(17)-C(10)-C(11)	105.5(2)	O(17)-C(10)-H(10A)	110.7
C(11)-C(10)-H(10A)	110.7	O(17)-C(10)-H(10B)	110.7
C(11)-C(10)-H(10B)	110.7	H(10A)-C(10)-H(10B)	108.8
C(10)-C(11)-C(12)	102.8(3)	C(10)-C(11)-H(11A)	111.2
C(12)-C(11)-H(11A)	111.2	C(10)-C(11)-H(11B)	111.2
C(12)-C(11)-H(11B)	111.2	H(11A)-C(11)-H(11B)	109.1
C(11)-C(12)-C(13)	105.1(3)	C(11)-C(12)-H(12A)	110.7
C(13)-C(12)-H(12A)	110.7	C(11)-C(12)-H(12B)	110.7
C(13)-C(12)-H(12B)	110.7	H(12A)-C(12)-H(12B)	108.8
O(17)-C(13)-C(12)	105.5(2)	O(17)-C(13)-H(13A)	110.6
C(12)-C(13)-H(13A)	110.6	O(17)-C(13)-H(13B)	110.6
C(12)-C(13)-H(13B)	110.6	H(13A)-C(13)-H(13B)	108.8
O(18)-C(14)-C(15)	104.9(2)	O(18)-C(14)-H(14A)	110.8
C(15)-C(14)-H(14A)	110.8	O(18)-C(14)-H(14B)	110.8
C(15)-C(14)-H(14B)	110.8	H(14A)-C(14)-H(14B)	108.8
C(14)-C(15)-C(16)	102.4(2)	C(14)-C(15)-H(15A)	111.3
C(16)-C(15)-H(15A)	111.3	C(14)-C(15)-H(15B)	111.3
C(16)-C(15)-H(15B)	111.3	H(15A)-C(15)-H(15B)	109.2
C(17)-C(16)-C(15)	102.9(3)	C(17)-C(16)-H(16A)	111.2
C(15)-C(16)-H(16A)	111.2	C(17)-C(16)-H(16B)	111.2
C(15)-C(16)-H(16B)	111.2	H(16A)-C(16)-H(16B)	109.1
O(18)-C(17)-C(16)	105.9(2)	O(18)-C(17)-H(17A)	110.6
C(16)-C(17)-H(17A)	110.6	O(18)-C(17)-H(17B)	110.6
C(16)-C(17)-H(17B)	110.6	H(17A)-C(17)-H(17B)	108.7
C(21)-O(19)-C(18)	108.6(2)	C(21)-O(19)-Sm(2)	122.6(1)
C(18)-O(19)-Sm(2)	126.8(1)	O(19)-C(18)-C(19B)	104.4(5)
O(19)-C(18)-C(19A)	105.3(3)	O(19)-C(18)-H(18A)	110.7
C(19A)-C(18)-H(18A)	110.7	O(19)-C(18)-H(18B)	110.7
C(19A)-C(18)-H(18B)	110.7	H(18A)-C(18)-H(18B)	108.8
O(19)-C(18)-H(18C)	110.9	C(19B)-C(18)-H(18C)	110.9
O(19)-C(18)-H(18D)	110.9	C(19B)-C(18)-H(18D)	110.9
H(18C)-C(18)-H(18D)	108.9	C(20A)-C(19A)-C(18)	101.2(5)
C(20A)-C(19A)-H(19A)	111.5	C(18)-C(19A)-H(19A)	111.5
C(20A)-C(19A)-H(19B)	111.5	C(18)-C(19A)-H(19B)	111.5
H(19A)-C(19A)-H(19B)	109.4	C(19A)-C(20A)-C(21)	100.8(5)
C(19A)-C(20A)-H(20A)	111.6	C(21)-C(20A)-H(20A)	111.6
C(19A)-C(20A)-H(20B)	111.6	C(21)-C(20A)-H(20B)	111.6
H(20A)-C(20A)-H(20B)	109.4	C(20B)-C(19B)-C(18)	101(1)
C(20B)-C(19B)-H(19C)	111.5	C(18)-C(19B)-H(19C)	111.5
C(20B)-C(19B)-H(19D)	111.5	C(18)-C(19B)-H(19D)	111.5
H(19C)-C(19B)-H(19D)	109.3	C(21)-C(20B)-C(19B)	103(1)
C(21)-C(20B)-H(20C)	111.1	C(19B)-C(20B)-H(20C)	111.1
C(21)-C(20B)-H(20D)	111.1	C(19B)-C(20B)-H(20D)	111.1
H(20C)-C(20B)-H(20D)	109.1	O(19)-C(21)-C(20B)	105.5(5)
O(19)-C(21)-C(20A)	105.2(3)	O(19)-C(21)-H(21A)	110.7
C(20A)-C(21)-H(21A)	110.7	O(19)-C(21)-H(21B)	110.7
C(20A)-C(21)-H(21B)	110.7	H(21A)-C(21)-H(21B)	108.8
O(19)-C(21)-H(21C)	110.6	C(20B)-C(21)-H(21C)	110.6
O(19)-C(21)-H(21D)	110.6	C(20B)-C(21)-H(21D)	110.6
H(21C)-C(21)-H(21D)	108.8	C(25A)-O(20)-C(22)	113(1)

C(22)-O(20)-C(25B)	106(1)	C(25A)-O(20)-Sm(2)	123(1)
C(22)-O(20)-Sm(2)	124.4(2)	C(25B)-O(20)-Sm(2)	129(1)
O(20)-C(22)-C(23B)	108.5(4)	O(20)-C(22)-C(23A)	101.8(5)
O(20)-C(22)-H(22A)	111.4	C(23A)-C(22)-H(22A)	111.4
O(20)-C(22)-H(22B)	111.4	C(23A)-C(22)-H(22B)	111.4
H(22A)-C(22)-H(22B)	109.3	O(20)-C(22)-H(22C)	110.0
C(23B)-C(22)-H(22C)	110.0	O(20)-C(22)-H(22D)	110.0
C(23B)-C(22)-H(22D)	110.0	H(22C)-C(22)-H(22D)	108.4
C(24A)-C(23A)-C(22)	103(1)	C(24A)-C(23A)-H(23A)	111.2
C(22)-C(23A)-H(23A)	111.2	C(24A)-C(23A)-H(23B)	111.2
C(22)-C(23A)-H(23B)	111.2	H(23A)-C(23A)-H(23B)	109.1
C(25A)-C(24A)-C(23A)	99(2)	C(25A)-C(24A)-H(24A)	112.0
C(23A)-C(24A)-H(24A)	112.0	C(25A)-C(24A)-H(24B)	112.0
C(23A)-C(24A)-H(24B)	112.0	H(24A)-C(24A)-H(24B)	109.7
O(20)-C(25A)-C(24A)	103(2)	O(20)-C(25A)-H(25A)	111.3
C(24A)-C(25A)-H(25A)	111.3	O(20)-C(25A)-H(25B)	111.3
C(24A)-C(25A)-H(25B)	111.3	H(25A)-C(25A)-H(25B)	109.2
C(22)-C(23B)-C(24B)	100.2(6)	C(22)-C(23B)-H(23C)	111.7
C(24B)-C(23B)-H(23C)	111.7	C(22)-C(23B)-H(23D)	111.7
C(24B)-C(23B)-H(23D)	111.7	H(23C)-C(23B)-H(23D)	109.5
C(25B)-C(24B)-C(23B)	100(1)	C(25B)-C(24B)-H(24C)	111.9
C(23B)-C(24B)-H(24C)	111.9	C(25B)-C(24B)-H(24D)	111.9
C(23B)-C(24B)-H(24D)	111.9	H(24C)-C(24B)-H(24D)	109.6
O(20)-C(25B)-C(24B)	106(2)	O(20)-C(25B)-H(25C)	110.5
C(24B)-C(25B)-H(25C)	110.5	O(20)-C(25B)-H(25D)	110.5
C(24B)-C(25B)-H(25D)	110.5	H(25C)-C(25B)-H(25D)	108.7
O(4A)-S(1A)-O(6A)	113.5(7)	O(4A)-S(1A)-O(5A)	113.4(4)
O(6A)-S(1A)-O(5A)	118.7(5)	O(4A)-S(1A)-C(2A)	100.7(5)
O(6A)-S(1A)-C(2A)	101.5(4)	O(5A)-S(1A)-C(2A)	106.2(3)
F(3A)-C(2A)-F(2A)	110.3(5)	F(3A)-C(2A)-F(1A)	105.6(5)
F(2A)-C(2A)-F(1A)	106.3(5)	F(3A)-C(2A)-S(1A)	111.6(4)
F(2A)-C(2A)-S(1A)	111.3(4)	F(1A)-C(2A)-S(1A)	111.5(4)
S(1A)-O(4A)-Sm(1)	142.6(6)	O(5B)-S(1B)-O(4B)	114(1)
O(5B)-S(1B)-O(6B)	127(1)	O(4B)-S(1B)-O(6B)	105(2)
O(5B)-S(1B)-C(2B)	106.0(6)	O(4B)-S(1B)-C(2B)	107(1)
O(6B)-S(1B)-C(2B)	96(2)	F(3B)-C(2B)-F(2B)	96(1)
F(3B)-C(2B)-F(1B)	113(1)	F(2B)-C(2B)-F(1B)	110(1)
F(3B)-C(2B)-S(1B)	116(1)	F(2B)-C(2B)-S(1B)	115(1)
F(1B)-C(2B)-S(1B)	107.1(8)	S(1B)-O(4B)-Sm(1)	168(2)
C(2B)-F(3B)-F(2B)	42.3(8)	C(2B)-F(2B)-F(3B)	42.1(8)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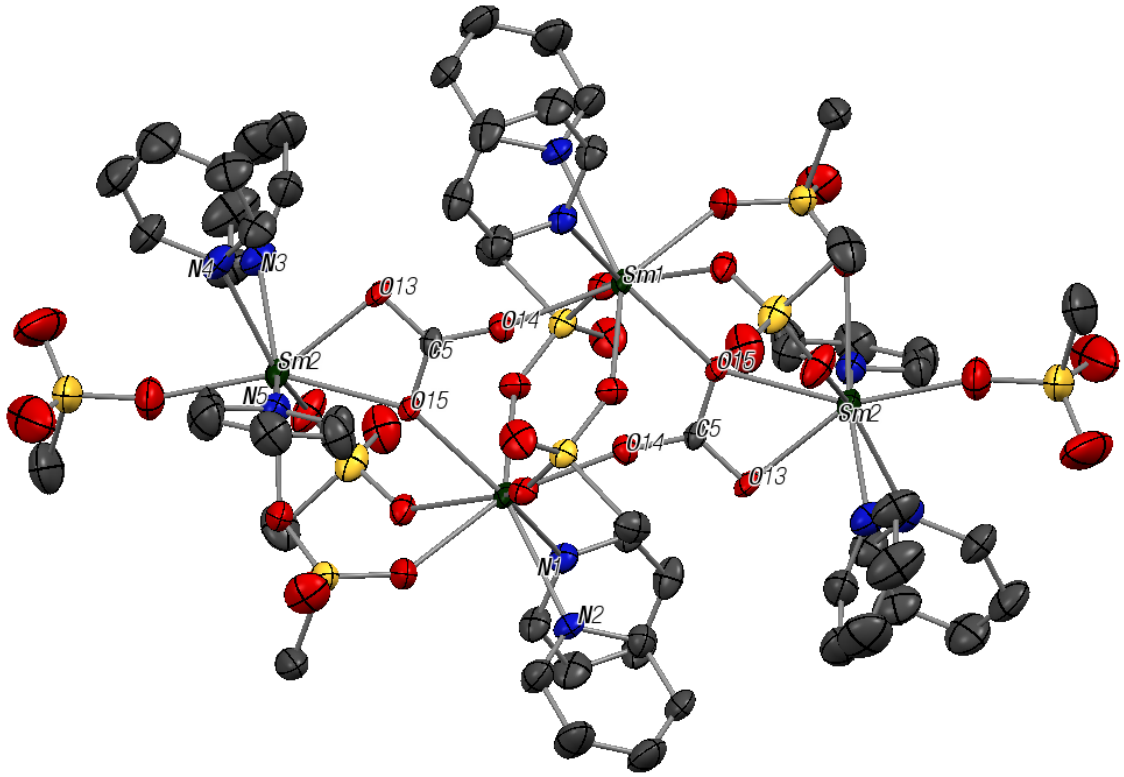
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Sm2
O15
N5
O15
Sm2
O14
C5
O13
N1
N2

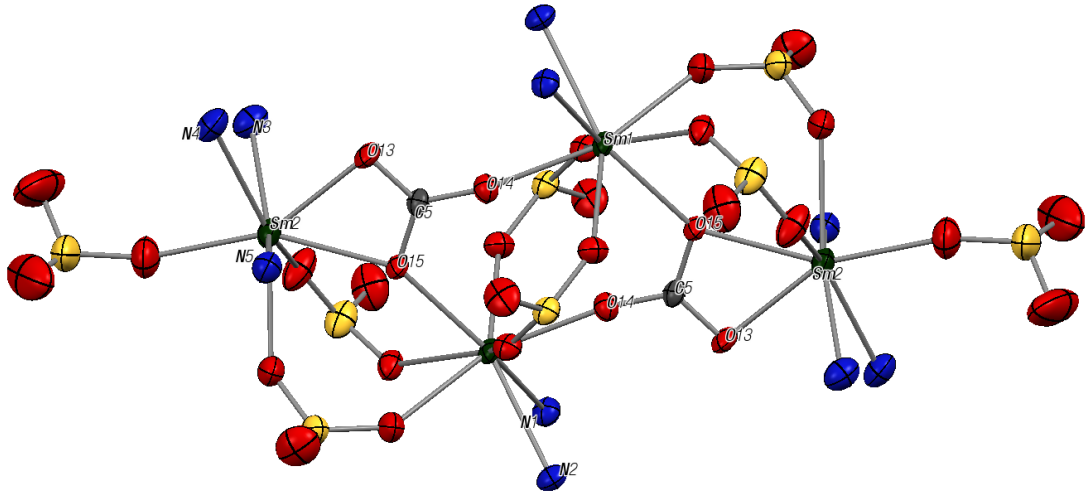


Figure S12: ORTEP of cluster **2-py**. Top, complete structure where only hydrogen atoms are removed for clarity. Middle, hydrogen atoms and CF_3 groups are removed for clarity. Bottom, hydrogen, carbon (excepted from the carbonate C) and fluorine atoms are removed for clarity. Carbon atoms are shown in grey, nitrogen atoms in blue, oxygen atoms in red, fluoride in green, sulfur in yellow and samarium in green.

Figure S13: ORTEP of the $[Sm_2(\mu_3\text{-}\eta_2(O,O'):\eta_1(O):\eta_1(O')\text{-}CO_3)]_2$ core of **2-py**.

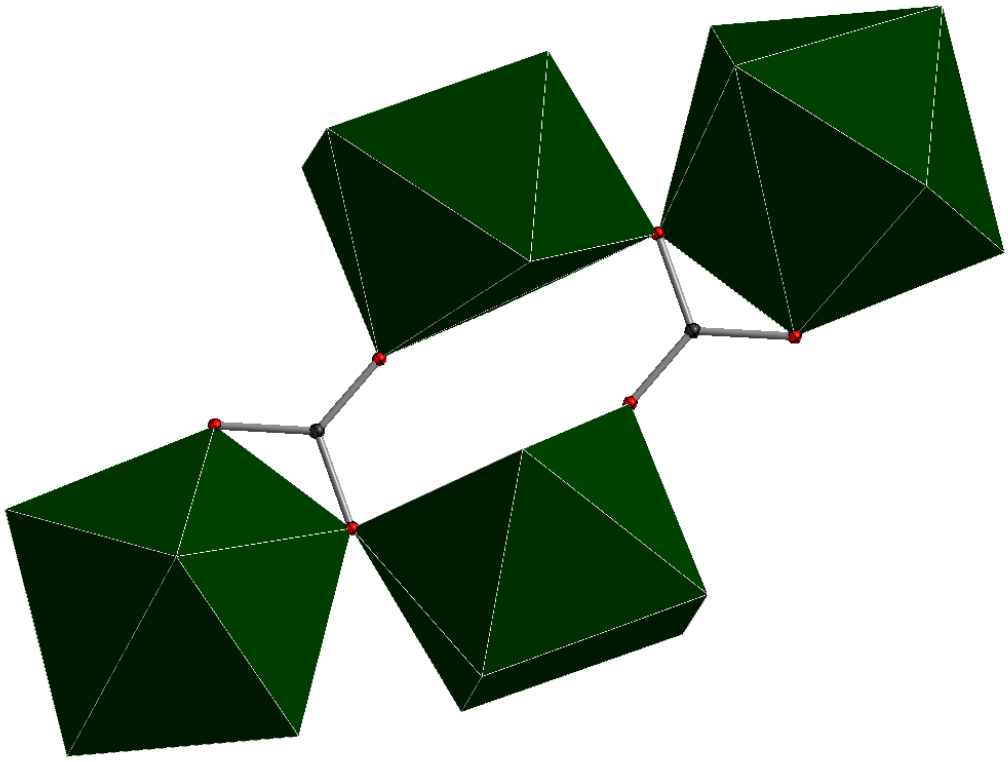


Figure S14: Polyhedral representation of cluster **2-py**.

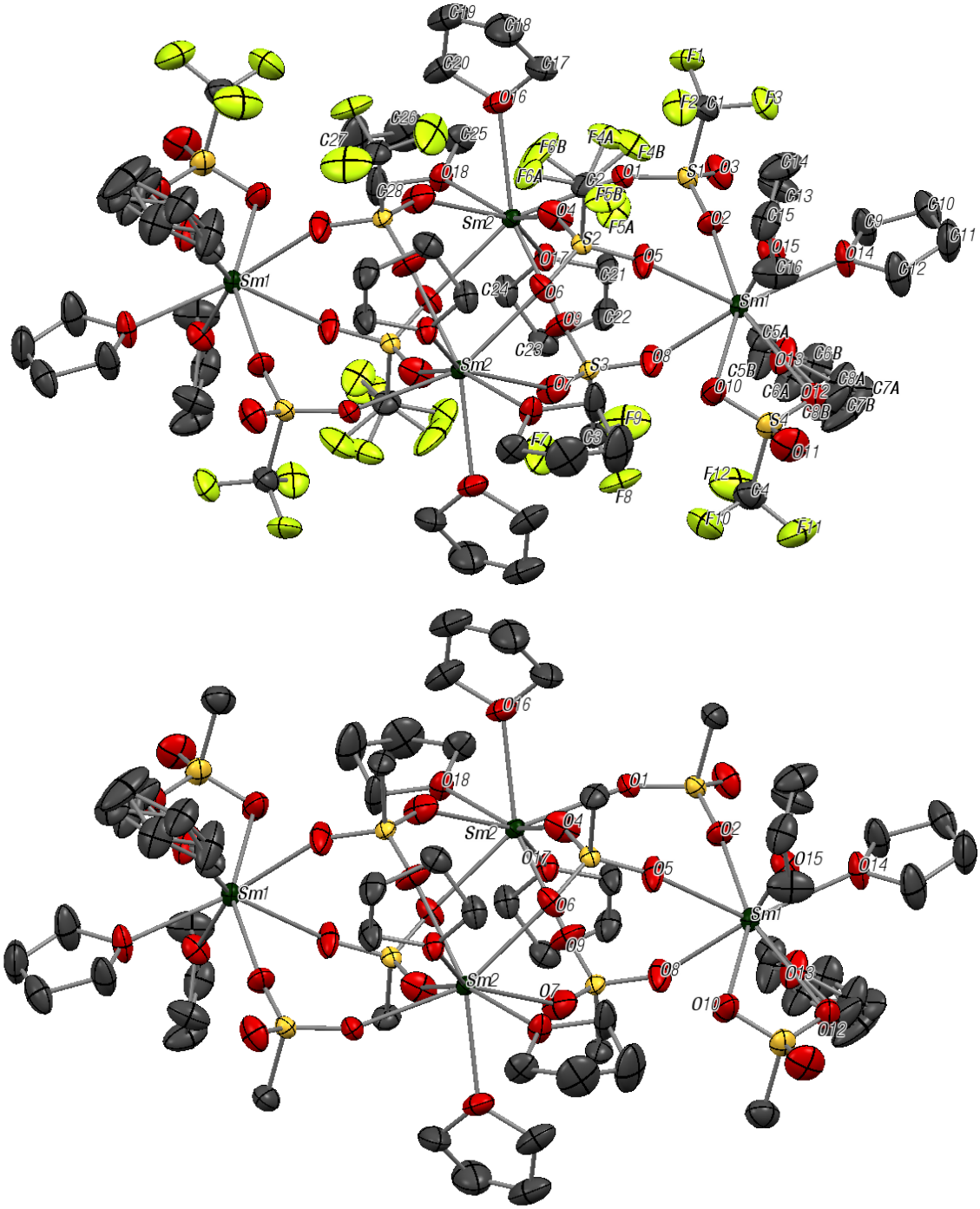
Table S4: Bond lengths (Å) and angles (deg) in **2-py**.

Sm(1)-O(14)	2.275(5)	Sm(1)-O(15)	2.373(4)
Sm(1)-O(9)	2.439(5)	Sm(1)-O(4)	2.441(5)
Sm(1)-O(1)	2.480(5)	Sm(1)-O(7)	2.484(5)
Sm(1)-N(1)	2.573(5)	Sm(1)-N(2)	2.662(6)
Sm(2)-O(10)	2.342(6)	Sm(2)-O(13)#3	2.373(5)
Sm(2)-O(15)	2.399(4)	Sm(2)-O(3)	2.425(5)
Sm(2)-O(5)	2.501(5)	Sm(2)-N(5)	2.557(6)
Sm(2)-N(3)	2.583(7)	Sm(2)-N(4)	2.614(6)
Sm(2)-C(5)#3	2.794(6)	S(1)-O(1)	1.428(5)
S(1)-O(3)	1.447(6)	S(1)-O(2)	1.452(7)
S(1)-C(1)	1.80(1)	S(2)-O(6)	1.411(6)
S(2)-O(4)	1.436(5)	S(2)-O(5)	1.449(6)
S(2)-C(2)	1.86(1)	S(3)-O(8)	1.420(5)
S(3)-O(7)	1.445(5)	S(3)-O(9)#3	1.457(5)
S(3)-C(3)	1.834(8)	S(4)-O(11)	1.403(8)
S(4)-O(12)	1.43(1)	S(4)-O(10)	1.444(6)
S(4)-C(4)	1.83(1)	F(1)-C(1)	1.29(1)
F(2)-C(1)	1.31(1)	F(3)-C(1)	1.39(1)
F(4)-C(2)	1.33(1)	F(5)-C(2)	1.31(1)
F(6)-C(2)	1.30(1)	F(7)-C(3)	1.33(1)
F(8)-C(3)	1.33(1)	F(9)-C(3)	1.30(1)
F(10A)-C(4)	1.337(4)	F(11A)-C(4)	1.325(4)
F(12A)-C(4)	1.334(4)	F(11B)-C(4)	1.335(4)
F(10B)-C(4)	1.328(4)	F(12B)-C(4)	1.324(4)
O(13)-C(5)	1.266(8)	O(14)-C(5)	1.264(8)
O(15)-C(5)#3	1.301(8)	N(1)-C(10)	1.33(1)
N(1)-C(6)	1.34(1)	N(2)-C(15)	1.34(1)
N(2)-C(11)	1.35(1)	N(3)-C(20)	1.32(1)
N(3)-C(16)	1.35(1)	N(4)-C(25)	1.36(1)
N(4)-C(21)	1.36(1)	N(5)-C(30)	1.34(1)
N(5)-C(26)	1.34(1)	C(6)-C(7)	1.38(1)
C(6)-H(6)	0.9500	C(7)-C(8)	1.36(1)
C(7)-H(7)	0.9500	C(8)-C(9)	1.38(1)
C(8)-H(8)	0.9500	C(9)-C(10)	1.38(1)
C(9)-H(9)	0.9500	C(10)-H(10)	0.9500
C(11)-C(12)	1.37(1)	C(11)-H(11)	0.9500
C(12)-C(13)	1.36(1)	C(12)-H(12)	0.9500
C(13)-C(14)	1.38(1)	C(13)-H(13)	0.9500
C(14)-C(15)	1.37(1)	C(14)-H(14)	0.9500
C(15)-H(15)	0.9500	C(16)-C(17)	1.38(1)
C(16)-H(16)	0.9500	C(17)-C(18)	1.33(2)
C(17)-H(17)	0.9500	C(18)-C(19)	1.39(2)
C(18)-H(18)	0.9500	C(19)-C(20)	1.38(1)
C(19)-H(19)	0.9500	C(20)-H(20)	0.9500
C(21)-C(22)	1.37(1)	C(21)-H(21)	0.9500
C(22)-C(23)	1.36(1)	C(22)-H(22)	0.9500
C(23)-C(24)	1.36(1)	C(23)-H(23)	0.9500
C(24)-C(25)	1.36(1)	C(24)-H(24)	0.9500
C(25)-H(25)	0.9500	C(26)-C(27)	1.37(1)
C(26)-H(26)	0.9500	C(27)-C(28)	1.36(1)
C(27)-H(27)	0.9500	C(28)-C(29)	1.38(1)
C(28)-H(28)	0.9500	C(29)-C(30)	1.38(1)
C(29)-H(29)	0.9500	C(30)-H(30)	0.9500

O(14)-Sm(1)-O(15)	113.4(2)	O(14)-Sm(1)-O(9)	76.4(2)
O(15)-Sm(1)-O(9)	76.9(2)	O(14)-Sm(1)-O(4)	146.9(2)
O(15)-Sm(1)-O(4)	74.4(2)	O(9)-Sm(1)-O(4)	74.4(2)
O(14)-Sm(1)-O(1)	140.8(2)	O(15)-Sm(1)-O(1)	76.6(2)

O(9)-Sm(1)-O(1)	141.3(2)	O(4)-Sm(1)-O(1)	71.6(2)
O(14)-Sm(1)-O(7)	73.9(2)	O(15)-Sm(1)-O(7)	75.3(2)
O(9)-Sm(1)-O(7)	126.2(2)	O(4)-Sm(1)-O(7)	137.3(2)
O(1)-Sm(1)-O(7)	72.5(2)	O(14)-Sm(1)-N(1)	81.7(2)
O(15)-Sm(1)-N(1)	143.6(2)	O(9)-Sm(1)-N(1)	139.4(2)
O(4)-Sm(1)-N(1)	111.6(2)	O(1)-Sm(1)-N(1)	72.1(2)
O(7)-Sm(1)-N(1)	77.9(2)	O(14)-Sm(1)-N(2)	83.1(2)
O(15)-Sm(1)-N(2)	140.3(2)	O(9)-Sm(1)-N(2)	72.3(2)
O(4)-Sm(1)-N(2)	73.5(2)	O(1)-Sm(1)-N(2)	114.0(2)
O(7)-Sm(1)-N(2)	144.0(2)	N(1)-Sm(1)-N(2)	71.5(2)
O(10)-Sm(2)-O(13)#3	153.4(2)	O(10)-Sm(2)-O(15)	151.9(2)
O(13)#3-Sm(2)-O(15)	54.5(2)	O(10)-Sm(2)-O(3)	87.5(2)
O(13)#3-Sm(2)-O(3)	105.5(2)	O(15)-Sm(2)-O(3)	74.7(2)
O(10)-Sm(2)-O(5)	80.4(2)	O(13)#3-Sm(2)-O(5)	124.9(2)
O(15)-Sm(2)-O(5)	74.3(2)	O(3)-Sm(2)-O(5)	75.7(2)
O(10)-Sm(2)-N(5)	98.9(2)	O(13)#3-Sm(2)-N(5)	82.7(2)
O(15)-Sm(2)-N(5)	85.9(2)	O(3)-Sm(2)-N(5)	147.5(2)
O(5)-Sm(2)-N(5)	74.1(2)	O(10)-Sm(2)-N(3)	83.3(2)
O(13)#3-Sm(2)-N(3)	79.4(2)	O(15)-Sm(2)-N(3)	110.1(2)
O(3)-Sm(2)-N(3)	70.9(2)	O(5)-Sm(2)-N(3)	143.2(2)
N(5)-Sm(2)-N(3)	141.4(2)	O(10)-Sm(2)-N(4)	83.1(2)
O(13)#3-Sm(2)-N(4)	72.5(2)	O(15)-Sm(2)-N(4)	124.1(2)
O(3)-Sm(2)-N(4)	142.4(2)	O(5)-Sm(2)-N(4)	137.3(2)
N(5)-Sm(2)-N(4)	70.1(2)	N(3)-Sm(2)-N(4)	72.0(2)
O(10)-Sm(2)-C(5)#3	176.7(2)	O(13)#3-Sm(2)-C(5)#3	26.8(2)
O(15)-Sm(2)-C(5)#3	27.7(2)	O(3)-Sm(2)-C(5)#3	89.6(2)
O(5)-Sm(2)-C(5)#3	100.5(2)	N(5)-Sm(2)-C(5)#3	84.4(2)
N(3)-Sm(2)-C(5)#3	94.2(2)	N(4)-Sm(2)-C(5)#3	98.3(2)
O(1)-S(1)-O(3)	113.1(3)	O(1)-S(1)-O(2)	116.3(4)
O(3)-S(1)-O(2)	115.2(4)	O(1)-S(1)-C(1)	103.7(4)
O(3)-S(1)-C(1)	102.9(4)	O(2)-S(1)-C(1)	103.3(4)
O(6)-S(2)-O(4)	117.0(4)	O(6)-S(2)-O(5)	114.6(4)
O(4)-S(2)-O(5)	113.4(3)	O(6)-S(2)-C(2)	103.5(4)
O(4)-S(2)-C(2)	101.7(4)	O(5)-S(2)-C(2)	104.4(4)
O(8)-S(3)-O(7)	115.6(3)	O(8)-S(3)-O(9)#3	114.4(3)
O(7)-S(3)-O(9)#3	113.7(3)	O(8)-S(3)-C(3)	105.5(4)
O(7)-S(3)-C(3)	103.3(3)	O(9)#3-S(3)-C(3)	102.3(3)
O(11)-S(4)-O(12)	116.7(6)	O(11)-S(4)-O(10)	114.2(5)
O(12)-S(4)-O(10)	112.5(5)	O(11)-S(4)-C(4)	103.7(5)
O(12)-S(4)-C(4)	105.8(5)	O(10)-S(4)-C(4)	102.0(4)
S(1)-O(1)-Sm(1)	138.3(3)	S(1)-O(3)-Sm(2)	146.1(4)
S(2)-O(4)-Sm(1)	145.5(3)	S(2)-O(5)-Sm(2)	139.3(3)
S(3)-O(7)-Sm(1)	144.4(3)	S(3)#3-O(9)-Sm(1)	145.5(3)
S(4)-O(10)-Sm(2)	163.3(4)	C(5)-O(13)-Sm(2)#3	95.5(4)
C(5)-O(14)-Sm(1)	170.3(5)	C(5)#3-O(15)-Sm(1)	118.1(4)
C(5)#3-O(15)-Sm(2)	93.3(3)	Sm(1)-O(15)-Sm(2)	146.8(2)
C(10)-N(1)-C(6)	117.1(6)	C(10)-N(1)-Sm(1)	123.7(5)
C(6)-N(1)-Sm(1)	118.2(5)	C(15)-N(2)-C(11)	116.6(7)
C(15)-N(2)-Sm(1)	124.3(5)	C(11)-N(2)-Sm(1)	118.9(5)
C(20)-N(3)-C(16)	117.9(8)	C(20)-N(3)-Sm(2)	120.1(6)
C(16)-N(3)-Sm(2)	121.3(6)	C(25)-N(4)-C(21)	115.1(7)
C(25)-N(4)-Sm(2)	121.3(5)	C(21)-N(4)-Sm(2)	123.6(6)
C(30)-N(5)-C(26)	116.7(7)	C(30)-N(5)-Sm(2)	119.6(5)
C(26)-N(5)-Sm(2)	123.5(5)	F(1)-C(1)-F(2)	110(1)
F(1)-C(1)-F(3)	108.2(8)	F(2)-C(1)-F(3)	106.5(8)
F(1)-C(1)-S(1)	112.6(7)	F(2)-C(1)-S(1)	112.1(6)
F(3)-C(1)-S(1)	106.8(7)	F(6)-C(2)-F(5)	111.4(8)
F(6)-C(2)-F(4)	108(1)	F(5)-C(2)-F(4)	107.2(7)
F(6)-C(2)-S(2)	111.3(6)	F(5)-C(2)-S(2)	108.6(7)
F(4)-C(2)-S(2)	110.3(6)	F(9)-C(3)-F(7)	108.9(7)
F(9)-C(3)-F(8)	109.5(7)	F(7)-C(3)-F(8)	108.0(7)
F(9)-C(3)-S(3)	111.2(6)	F(7)-C(3)-S(3)	109.6(6)
F(8)-C(3)-S(3)	109.5(6)	F(12B)-C(4)-F(10B)	106.5(4)

F(11A)-C(4)-F(12A)	117(2)	F(12B)-C(4)-F(11B)	105.7(4)
F(10B)-C(4)-F(11B)	105.3(4)	F(11A)-C(4)-F(10A)	112(1)
F(12A)-C(4)-F(10A)	108(1)	F(12B)-C(4)-S(4)	115.8(8)
F(11A)-C(4)-S(4)	110(1)	F(10B)-C(4)-S(4)	113.8(8)
F(12A)-C(4)-S(4)	107(1)	F(11B)-C(4)-S(4)	108.9(8)
F(10A)-C(4)-S(4)	103(1)	O(14)-C(5)-O(13)	123.5(6)
O(14)-C(5)-O(15)#3	119.8(6)	O(13)-C(5)-O(15)#3	116.7(6)
O(14)-C(5)-Sm(2)#3	177.9(4)	O(13)-C(5)-Sm(2)#3	57.7(3)
O(15)#3-C(5)-Sm(2)#3	59.0(3)	N(1)-C(6)-C(7)	122.7(8)
N(1)-C(6)-H(6)	118.7	C(7)-C(6)-H(6)	118.7
C(8)-C(7)-C(6)	120.0(8)	C(8)-C(7)-H(7)	120.0
C(6)-C(7)-H(7)	120.0	C(7)-C(8)-C(9)	118.2(7)
C(7)-C(8)-H(8)	120.9	C(9)-C(8)-H(8)	120.9
C(8)-C(9)-C(10)	119.0(8)	C(8)-C(9)-H(9)	120.5
C(10)-C(9)-H(9)	120.5	N(1)-C(10)-C(9)	123.0(7)
N(1)-C(10)-H(10)	118.5	C(9)-C(10)-H(10)	118.5
N(2)-C(11)-C(12)	123.2(8)	N(2)-C(11)-H(11)	118.4
C(12)-C(11)-H(11)	118.4	C(13)-C(12)-C(11)	119.0(7)
C(13)-C(12)-H(12)	120.5	C(11)-C(12)-H(12)	120.5
C(12)-C(13)-C(14)	119.1(8)	C(12)-C(13)-H(13)	120.4
C(14)-C(13)-H(13)	120.4	C(15)-C(14)-C(13)	119(1)
C(15)-C(14)-H(14)	120.6	C(13)-C(14)-H(14)	120.6
N(2)-C(15)-C(14)	123.2(8)	N(2)-C(15)-H(15)	118.4
C(14)-C(15)-H(15)	118.4	N(3)-C(16)-C(17)	122(1)
N(3)-C(16)-H(16)	119.2	C(17)-C(16)-H(16)	119.2
C(18)-C(17)-C(16)	120(1)	C(18)-C(17)-H(17)	119.9
C(16)-C(17)-H(17)	119.9	C(17)-C(18)-C(19)	119(1)
C(17)-C(18)-H(18)	120.6	C(19)-C(18)-H(18)	120.6
C(20)-C(19)-C(18)	119(1)	C(20)-C(19)-H(19)	120.7
C(18)-C(19)-H(19)	120.7	N(3)-C(20)-C(19)	123(1)
N(3)-C(20)-H(20)	118.7	C(19)-C(20)-H(20)	118.7
N(4)-C(21)-C(22)	123(1)	N(4)-C(21)-H(21)	118.8
C(22)-C(21)-H(21)	118.8	C(23)-C(22)-C(21)	121(1)
C(23)-C(22)-H(22)	119.4	C(21)-C(22)-H(22)	119.4
C(22)-C(23)-C(24)	117(1)	C(22)-C(23)-H(23)	121.5
C(24)-C(23)-H(23)	121.5	C(25)-C(24)-C(23)	121(1)
C(25)-C(24)-H(24)	119.8	C(23)-C(24)-H(24)	119.8
N(4)-C(25)-C(24)	124(1)	N(4)-C(25)-H(25)	118.2
C(24)-C(25)-H(25)	118.2	N(5)-C(26)-C(27)	123.5(8)
N(5)-C(26)-H(26)	118.3	C(27)-C(26)-H(26)	118.3
C(28)-C(27)-C(26)	120(1)	C(28)-C(27)-H(27)	120.0
C(26)-C(27)-H(27)	120.0	C(27)-C(28)-C(29)	117.6(8)
C(27)-C(28)-H(28)	121.2	C(29)-C(28)-H(28)	121.2
C(28)-C(29)-C(30)	119.7(8)	C(28)-C(29)-H(29)	120.1
C(30)-C(29)-H(29)	120.1	N(5)-C(30)-C(29)	122.5(8)
N(5)-C(30)-H(30)	118.8	C(29)-C(30)-H(30)	118.8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C2
O1
S1
O3
C14
O18
C28
F5B
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O2
C10
C9
C11
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Sm2
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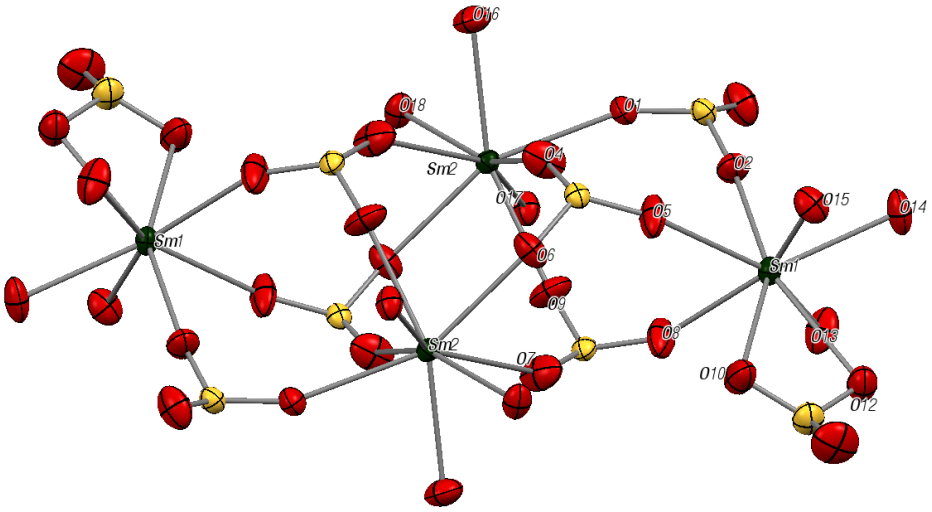

Figure S15: ORTEP of **3**. Top, complete structure where only hydrogen atoms are removed for clarity. Middle, hydrogen atoms and CF_3 groups are removed for clarity. Bottom, hydrogen, carbon and fluorine atoms are removed for clarity. Carbon atoms are shown in grey, oxygen atoms in red, fluoride in green, sulfur in yellow and samarium in green.

Table S5: Bond lengths (Å) and angles (deg) in **3**.

Sm(1)-O(8)	2.511(3)	Sm(1)-O(2)	2.519(2)
Sm(1)-O(5)	2.578(2)	Sm(1)-O(15)	2.579(2)
Sm(1)-O(13)	2.602(3)	Sm(1)-O(14)	2.609(2)
Sm(1)-O(10)	2.663(3)	Sm(1)-O(12)	2.781(3)
Sm(1)-S(4)	3.267(1)	Sm(2)-O(18)	2.595(2)
Sm(2)-O(4)	2.597(2)	Sm(2)-O(6)#2	2.604(2)
Sm(2)-O(9)	2.609(2)	Sm(2)-O(16)	2.612(2)
Sm(2)-O(1)	2.632(2)	Sm(2)-O(17)	2.642(2)
Sm(2)-O(7)#2	2.687(3)	S(1)-O(3)	1.423(3)
S(1)-O(2)	1.437(2)	S(1)-O(1)	1.444(2)
S(1)-C(1)	1.827(4)	S(2)-O(5)	1.421(3)
S(2)-O(6)	1.432(2)	S(2)-O(4)	1.432(3)
S(2)-C(2)	1.822(4)	S(3)-O(7)	1.418(3)
S(3)-O(9)	1.423(3)	S(3)-O(8)	1.428(3)
S(3)-C(3)	1.821(4)	S(4)-O(11)	1.427(3)
S(4)-O(10)	1.441(3)	S(4)-O(12)	1.442(3)
S(4)-C(4)	1.815(5)	F(1)-C(1)	1.317(5)
F(2)-C(1)	1.332(5)	F(3)-C(1)	1.329(4)
F(4A)-C(2)	1.24(1)	F(5A)-C(2)	1.34(2)
F(6A)-C(2)	1.37(1)	F(4B)-C(2)	1.45(2)
F(5B)-C(2)	1.28(3)	F(6B)-C(2)	1.26(1)
F(7)-C(3)	1.291(5)	F(8)-C(3)	1.315(5)
F(9)-C(3)	1.311(5)	F(10)-C(4)	1.330(5)
F(11)-C(4)	1.329(5)	F(12)-C(4)	1.325(5)
O(13)-C(8A)	1.43(1)	O(13)-C(5A)	1.45(1)
O(13)-C(5B)	1.449(4)	O(13)-C(8B)	1.450(4)
O(14)-C(9)	1.431(5)	O(14)-C(12)	1.439(5)
O(15)-C(16)	1.415(5)	O(15)-C(13)	1.425(5)
O(16)-C(17)	1.437(5)	O(16)-C(20)	1.452(5)
O(17)-C(24)	1.440(4)	O(17)-C(21)	1.440(4)
O(18)-C(28)	1.431(4)	O(18)-C(25)	1.444(4)
C(5A)-C(6A)	1.53(1)	C(5A)-H(5A)	0.9900
C(5A)-H(5B)	0.9900	C(6A)-C(7A)	1.71(2)
C(6A)-H(6A)	0.9900	C(6A)-H(6B)	0.9900
C(7A)-C(8A)	1.32(1)	C(7A)-H(7A)	0.9900

C(7A)-H(7B)	0.9900	C(8A)-H(8A)	0.9900
C(8A)-H(8B)	0.9900	C(5B)-C(6B)	1.450(4)
C(5B)-H(5C)	0.9900	C(5B)-H(5D)	0.9900
C(6B)-C(7B)	1.451(4)	C(6B)-H(6C)	0.9900
C(6B)-H(6D)	0.9900	C(7B)-C(8B)	1.449(4)
C(7B)-H(7C)	0.9900	C(7B)-H(7D)	0.9900
C(8B)-H(8C)	0.9900	C(8B)-H(8D)	0.9900
C(9)-C(10)	1.470(6)	C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900	C(10)-C(11)	1.489(7)
C(10)-H(10A)	0.9900	C(10)-H(10B)	0.9900
C(11)-C(12)	1.444(6)	C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900	C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900	C(13)-C(14)	1.464(6)
C(13)-H(13A)	0.9900	C(13)-H(13B)	0.9900
C(14)-C(15)	1.489(7)	C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900	C(15)-C(16)	1.475(6)
C(15)-H(15A)	0.9900	C(15)-H(15B)	0.9900
C(16)-H(16A)	0.9900	C(16)-H(16B)	0.9900
C(17)-C(18)	1.497(7)	C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900	C(18)-C(19)	1.519(8)
C(18)-H(18A)	0.9900	C(18)-H(18B)	0.9900
C(19)-C(20)	1.491(6)	C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900	C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900	C(21)-C(22)	1.507(5)
C(21)-H(21A)	0.9900	C(21)-H(21B)	0.9900
C(22)-C(23)	1.510(6)	C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900	C(23)-C(24)	1.505(5)
C(23)-H(23A)	0.9900	C(23)-H(23B)	0.9900
C(24)-H(24A)	0.9900	C(24)-H(24B)	0.9900
C(25)-C(26)	1.495(6)	C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900	C(26)-C(27)	1.494(8)
C(26)-H(26A)	0.9900	C(26)-H(26B)	0.9900
C(27)-C(28)	1.496(6)	C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900	C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900	O(19)-C(32B)	1.25(2)
O(19)-C(29A)	1.34(1)	O(19)-C(29B)	1.54(3)
O(19)-C(32A)	1.56(1)	C(29A)-C(30A)	1.49(1)
C(29A)-H(29A)	0.9900	C(29A)-H(29B)	0.9900
C(30A)-C(31A)	1.52(1)	C(30A)-H(30A)	0.9900
C(30A)-H(30B)	0.9900	C(31A)-C(32A)	1.52(1)
C(31A)-H(31A)	0.9900	C(31A)-H(31B)	0.9900
C(32A)-H(32A)	0.9900	C(32A)-H(32B)	0.9900
C(29B)-C(30B)	1.450(4)	C(29B)-H(29C)	0.9900
C(29B)-H(29D)	0.9900	C(30B)-C(31B)	1.51(3)
C(30B)-H(30C)	0.9900	C(30B)-H(30D)	0.9900
C(31B)-C(32B)	1.48(3)	C(31B)-H(31C)	0.9900
C(31B)-H(31D)	0.9900	C(32B)-H(32C)	0.9900
C(32B)-H(32D)	0.9900		

O(8)-Sm(1)-O(2)	84.3(1)	O(8)-Sm(1)-O(5)	73.9(1)
O(2)-Sm(1)-O(5)	77.2(1)	O(8)-Sm(1)-O(15)	141.9(1)
O(2)-Sm(1)-O(15)	105.1(1)	O(5)-Sm(1)-O(15)	72.5(1)
O(8)-Sm(1)-O(13)	75.4(1)	O(2)-Sm(1)-O(13)	82.9(1)
O(5)-Sm(1)-O(13)	144.8(1)	O(15)-Sm(1)-O(13)	141.6(1)
O(8)-Sm(1)-O(14)	145.8(1)	O(2)-Sm(1)-O(14)	80.17(8)
O(5)-Sm(1)-O(14)	130.6(1)	O(15)-Sm(1)-O(14)	72.0(1)
O(13)-Sm(1)-O(14)	72.6(1)	O(8)-Sm(1)-O(10)	76.7(1)
O(2)-Sm(1)-O(10)	153.34(8)	O(5)-Sm(1)-O(10)	79.7(1)
O(15)-Sm(1)-O(10)	80.1(1)	O(13)-Sm(1)-O(10)	109.6(1)
O(14)-Sm(1)-O(10)	125.59(8)	O(8)-Sm(1)-O(12)	104.2(1)
O(2)-Sm(1)-O(12)	153.70(8)	O(5)-Sm(1)-O(12)	128.9(1)
O(15)-Sm(1)-O(12)	83.7(1)	O(13)-Sm(1)-O(12)	75.5(1)

O(14)-Sm(1)-O(12)	79.16(8)	O(10)-Sm(1)-O(12)	51.62(8)
O(8)-Sm(1)-S(4)	89.60(8)	O(2)-Sm(1)-S(4)	172.91(7)
O(5)-Sm(1)-S(4)	104.50(7)	O(15)-Sm(1)-S(4)	81.91(6)
O(13)-Sm(1)-S(4)	92.17(7)	O(14)-Sm(1)-S(4)	103.22(6)
O(10)-Sm(1)-S(4)	25.62(6)	O(12)-Sm(1)-S(4)	26.03(5)
O(18)-Sm(2)-O(4)	151.7(1)	O(18)-Sm(2)-O(6)#2	73.18(8)
O(4)-Sm(2)-O(6)#2	114.66(8)	O(18)-Sm(2)-O(9)	129.6(1)
O(4)-Sm(2)-O(9)	77.3(1)	O(6)#2-Sm(2)-O(9)	72.3(1)
O(18)-Sm(2)-O(16)	72.0(1)	O(4)-Sm(2)-O(16)	83.3(1)
O(6)#2-Sm(2)-O(16)	128.7(1)	O(9)-Sm(2)-O(16)	156.6(1)
O(18)-Sm(2)-O(1)	112.11(7)	O(4)-Sm(2)-O(1)	74.13(8)
O(6)#2-Sm(2)-O(1)	152.64(8)	O(9)-Sm(2)-O(1)	85.4(1)
O(16)-Sm(2)-O(1)	76.70(8)	O(18)-Sm(2)-O(17)	68.84(8)
O(4)-Sm(2)-O(17)	137.7(1)	O(6)#2-Sm(2)-O(17)	80.74(8)
O(9)-Sm(2)-O(17)	70.33(8)	O(16)-Sm(2)-O(17)	118.83(8)
O(1)-Sm(2)-O(17)	76.83(7)	O(18)-Sm(2)-O(7)#2	85.4(1)
O(4)-Sm(2)-O(7)#2	73.2(1)	O(6)#2-Sm(2)-O(7)#2	70.1(1)
O(9)-Sm(2)-O(7)#2	115.1(1)	O(16)-Sm(2)-O(7)#2	70.6(1)
O(1)-Sm(2)-O(7)#2	135.7(1)	O(17)-Sm(2)-O(7)#2	145.7(1)
O(3)-S(1)-O(2)	114.8(2)	O(3)-S(1)-O(1)	115.2(2)
O(2)-S(1)-O(1)	114.4(2)	O(3)-S(1)-C(1)	104.2(2)
O(2)-S(1)-C(1)	102.0(2)	O(1)-S(1)-C(1)	103.9(2)
O(5)-S(2)-O(6)	115.4(2)	O(5)-S(2)-O(4)	115.8(2)
O(6)-S(2)-O(4)	114.0(2)	O(5)-S(2)-C(2)	102.2(2)
O(6)-S(2)-C(2)	102.7(2)	O(4)-S(2)-C(2)	104.3(2)
O(7)-S(3)-O(9)	114.7(2)	O(7)-S(3)-O(8)	115.2(2)
O(9)-S(3)-O(8)	114.6(2)	O(7)-S(3)-C(3)	104.8(2)
O(9)-S(3)-C(3)	104.7(2)	O(8)-S(3)-C(3)	100.5(2)
O(11)-S(4)-O(10)	115.8(2)	O(11)-S(4)-O(12)	116.2(2)
O(10)-S(4)-O(12)	110.8(2)	O(11)-S(4)-C(4)	104.0(2)
O(10)-S(4)-C(4)	104.0(2)	O(12)-S(4)-C(4)	104.3(2)
O(11)-S(4)-Sm(1)	143.2(2)	O(10)-S(4)-Sm(1)	53.0(1)
O(12)-S(4)-Sm(1)	57.8(1)	C(4)-S(4)-Sm(1)	112.7(2)
S(1)-O(1)-Sm(2)	156.6(1)	S(1)-O(2)-Sm(1)	173.3(2)
S(2)-O(4)-Sm(2)	151.6(2)	S(2)-O(5)-Sm(1)	158.4(2)
S(2)-O(6)-Sm(2)#2	146.0(2)	S(3)-O(7)-Sm(2)#2	149.2(2)
S(3)-O(8)-Sm(1)	154.0(2)	S(3)-O(9)-Sm(2)	150.5(2)
S(4)-O(10)-Sm(1)	101.3(1)	S(4)-O(12)-Sm(1)	96.2(1)
C(8A)-O(13)-C(5A)	109.4(8)	C(5B)-O(13)-C(8B)	102(1)
C(8A)-O(13)-Sm(1)	127.7(6)	C(5A)-O(13)-Sm(1)	120.2(6)
C(5B)-O(13)-Sm(1)	131.4(8)	C(8B)-O(13)-Sm(1)	125.4(8)
C(9)-O(14)-C(12)	108.1(3)	C(9)-O(14)-Sm(1)	126.2(2)
C(12)-O(14)-Sm(1)	123.7(2)	C(16)-O(15)-C(13)	108.2(3)
C(16)-O(15)-Sm(1)	130.8(2)	C(13)-O(15)-Sm(1)	120.2(2)
C(17)-O(16)-C(20)	108.7(3)	C(17)-O(16)-Sm(2)	121.4(2)
C(20)-O(16)-Sm(2)	126.4(3)	C(24)-O(17)-C(21)	109.0(3)
C(24)-O(17)-Sm(2)	122.8(2)	C(21)-O(17)-Sm(2)	124.1(2)
C(28)-O(18)-C(25)	109.4(3)	C(28)-O(18)-Sm(2)	125.4(2)
C(25)-O(18)-Sm(2)	125.1(2)	F(1)-C(1)-F(3)	107.7(3)
F(1)-C(1)-F(2)	108.2(4)	F(3)-C(1)-F(2)	108.0(3)
F(1)-C(1)-S(1)	111.3(3)	F(3)-C(1)-S(1)	110.8(3)
F(2)-C(1)-S(1)	110.8(3)	F(6B)-C(2)-F(5B)	115(2)
F(4A)-C(2)-F(5A)	115(2)	F(4A)-C(2)-F(6A)	108.5(6)
F(5A)-C(2)-F(6A)	103(1)	F(6B)-C(2)-F(4B)	104(2)
F(5B)-C(2)-F(4B)	99(2)	F(4A)-C(2)-S(2)	115.2(6)
F(6B)-C(2)-S(2)	112.1(6)	F(5B)-C(2)-S(2)	119(1)
F(5A)-C(2)-S(2)	105(1)	F(6A)-C(2)-S(2)	109.7(5)
F(4B)-C(2)-S(2)	105(1)	F(7)-C(3)-F(9)	108.0(4)
F(7)-C(3)-F(8)	107.5(4)	F(9)-C(3)-F(8)	107.1(3)
F(7)-C(3)-S(3)	112.3(3)	F(9)-C(3)-S(3)	111.2(3)
F(8)-C(3)-S(3)	110.6(3)	F(12)-C(4)-F(11)	108.0(4)
F(12)-C(4)-F(10)	108.7(4)	F(11)-C(4)-F(10)	106.9(4)
F(12)-C(4)-S(4)	111.0(3)	F(11)-C(4)-S(4)	110.7(3)

F(10)-C(4)-S(4)	111.3(4)	O(13)-C(5A)-C(6A)	104(1)
O(13)-C(5A)-H(5A)	111.0	C(6A)-C(5A)-H(5A)	111.0
O(13)-C(5A)-H(5B)	111.0	C(6A)-C(5A)-H(5B)	111.0
H(5A)-C(5A)-H(5B)	109.0	C(5A)-C(6A)-C(7A)	97(1)
C(5A)-C(6A)-H(6A)	112.3	C(7A)-C(6A)-H(6A)	112.3
C(5A)-C(6A)-H(6B)	112.3	C(7A)-C(6A)-H(6B)	112.3
H(6A)-C(6A)-H(6B)	109.9	C(8A)-C(7A)-C(6A)	102(1)
C(8A)-C(7A)-H(7A)	111.3	C(6A)-C(7A)-H(7A)	111.3
C(8A)-C(7A)-H(7B)	111.3	C(6A)-C(7A)-H(7B)	111.3
H(7A)-C(7A)-H(7B)	109.2	C(7A)-C(8A)-O(13)	113(1)
C(7A)-C(8A)-H(8A)	108.9	O(13)-C(8A)-H(8A)	108.9
C(7A)-C(8A)-H(8B)	108.9	O(13)-C(8A)-H(8B)	108.9
H(8A)-C(8A)-H(8B)	107.8	O(13)-C(5B)-C(6B)	106(1)
O(13)-C(5B)-H(5C)	110.5	C(6B)-C(5B)-H(5C)	110.5
O(13)-C(5B)-H(5D)	110.5	C(6B)-C(5B)-H(5D)	110.5
H(5C)-C(5B)-H(5D)	108.7	C(5B)-C(6B)-C(7B)	99(2)
C(5B)-C(6B)-H(6C)	111.9	C(7B)-C(6B)-H(6C)	111.9
C(5B)-C(6B)-H(6D)	111.9	C(7B)-C(6B)-H(6D)	111.9
H(6C)-C(6B)-H(6D)	109.6	C(8B)-C(7B)-C(6B)	108(1)
C(8B)-C(7B)-H(7C)	110.2	C(6B)-C(7B)-H(7C)	110.2
C(8B)-C(7B)-H(7D)	110.2	C(6B)-C(7B)-H(7D)	110.2
H(7C)-C(7B)-H(7D)	108.5	C(7B)-C(8B)-O(13)	107(1)
C(7B)-C(8B)-H(8C)	110.4	O(13)-C(8B)-H(8C)	110.4
C(7B)-C(8B)-H(8D)	110.4	O(13)-C(8B)-H(8D)	110.4
H(8C)-C(8B)-H(8D)	108.6	O(14)-C(9)-C(10)	108.4(4)
O(14)-C(9)-H(9A)	110.0	C(10)-C(9)-H(9A)	110.0
O(14)-C(9)-H(9B)	110.0	C(10)-C(9)-H(9B)	110.0
H(9A)-C(9)-H(9B)	108.4	C(9)-C(10)-C(11)	105.8(4)
C(9)-C(10)-H(10A)	110.6	C(11)-C(10)-H(10A)	110.6
C(9)-C(10)-H(10B)	110.6	C(11)-C(10)-H(10B)	110.6
H(10A)-C(10)-H(10B)	108.7	C(12)-C(11)-C(10)	107.5(4)
C(12)-C(11)-H(11A)	110.2	C(10)-C(11)-H(11A)	110.2
C(12)-C(11)-H(11B)	110.2	C(10)-C(11)-H(11B)	110.2
H(11A)-C(11)-H(11B)	108.5	O(14)-C(12)-C(11)	108.5(4)
O(14)-C(12)-H(12A)	110.0	C(11)-C(12)-H(12A)	110.0
O(14)-C(12)-H(12B)	110.0	C(11)-C(12)-H(12B)	110.0
H(12A)-C(12)-H(12B)	108.4	O(15)-C(13)-C(14)	108.9(4)
O(15)-C(13)-H(13A)	109.9	C(14)-C(13)-H(13A)	109.9
O(15)-C(13)-H(13B)	109.9	C(14)-C(13)-H(13B)	109.9
H(13A)-C(13)-H(13B)	108.3	C(13)-C(14)-C(15)	105.8(4)
C(13)-C(14)-H(14A)	110.6	C(15)-C(14)-H(14A)	110.6
C(13)-C(14)-H(14B)	110.6	C(15)-C(14)-H(14B)	110.6
H(14A)-C(14)-H(14B)	108.7	C(16)-C(15)-C(14)	104.7(4)
C(16)-C(15)-H(15A)	110.8	C(14)-C(15)-H(15A)	110.8
C(16)-C(15)-H(15B)	110.8	C(14)-C(15)-H(15B)	110.8
H(15A)-C(15)-H(15B)	108.9	O(15)-C(16)-C(15)	108.0(4)
O(15)-C(16)-H(16A)	110.1	C(15)-C(16)-H(16A)	110.1
O(15)-C(16)-H(16B)	110.1	C(15)-C(16)-H(16B)	110.1
H(16A)-C(16)-H(16B)	108.4	O(16)-C(17)-C(18)	105.7(4)
O(16)-C(17)-H(17A)	110.6	C(18)-C(17)-H(17A)	110.6
O(16)-C(17)-H(17B)	110.6	C(18)-C(17)-H(17B)	110.6
H(17A)-C(17)-H(17B)	108.7	C(17)-C(18)-C(19)	102.8(5)
C(17)-C(18)-H(18A)	111.2	C(19)-C(18)-H(18A)	111.2
C(17)-C(18)-H(18B)	111.2	C(19)-C(18)-H(18B)	111.2
H(18A)-C(18)-H(18B)	109.1	C(20)-C(19)-C(18)	105.7(4)
C(20)-C(19)-H(19A)	110.6	C(18)-C(19)-H(19A)	110.6
C(20)-C(19)-H(19B)	110.6	C(18)-C(19)-H(19B)	110.6
H(19A)-C(19)-H(19B)	108.7	O(16)-C(20)-C(19)	106.8(4)
O(16)-C(20)-H(20A)	110.4	C(19)-C(20)-H(20A)	110.4
O(16)-C(20)-H(20B)	110.4	C(19)-C(20)-H(20B)	110.4
H(20A)-C(20)-H(20B)	108.6	O(17)-C(21)-C(22)	107.0(3)
O(17)-C(21)-H(21A)	110.3	C(22)-C(21)-H(21A)	110.3
O(17)-C(21)-H(21B)	110.3	C(22)-C(21)-H(21B)	110.3

H(21A)-C(21)-H(21B)	108.6	C(21)-C(22)-C(23)	103.8(3)
C(21)-C(22)-H(22A)	111.0	C(23)-C(22)-H(22A)	111.0
C(21)-C(22)-H(22B)	111.0	C(23)-C(22)-H(22B)	111.0
H(22A)-C(22)-H(22B)	109.0	C(24)-C(23)-C(22)	102.5(3)
C(24)-C(23)-H(23A)	111.3	C(22)-C(23)-H(23A)	111.3
C(24)-C(23)-H(23B)	111.3	C(22)-C(23)-H(23B)	111.3
H(23A)-C(23)-H(23B)	109.2	O(17)-C(24)-C(23)	105.1(3)
O(17)-C(24)-H(24A)	110.7	C(23)-C(24)-H(24A)	110.7
O(17)-C(24)-H(24B)	110.7	C(23)-C(24)-H(24B)	110.7
H(24A)-C(24)-H(24B)	108.8	O(18)-C(25)-C(26)	105.9(4)
O(18)-C(25)-H(25A)	110.5	C(26)-C(25)-H(25A)	110.5
O(18)-C(25)-H(25B)	110.5	C(26)-C(25)-H(25B)	110.5
H(25A)-C(25)-H(25B)	108.7	C(27)-C(26)-C(25)	103.3(4)
C(27)-C(26)-H(26A)	111.1	C(25)-C(26)-H(26A)	111.1
C(27)-C(26)-H(26B)	111.1	C(25)-C(26)-H(26B)	111.1
H(26A)-C(26)-H(26B)	109.1	C(26)-C(27)-C(28)	103.0(4)
C(26)-C(27)-H(27A)	111.2	C(28)-C(27)-H(27A)	111.2
C(26)-C(27)-H(27B)	111.2	C(28)-C(27)-H(27B)	111.2
H(27A)-C(27)-H(27B)	109.1	O(18)-C(28)-C(27)	105.8(4)
O(18)-C(28)-H(28A)	110.6	C(27)-C(28)-H(28A)	110.6
O(18)-C(28)-H(28B)	110.6	C(27)-C(28)-H(28B)	110.6
H(28A)-C(28)-H(28B)	108.7	C(32B)-O(19)-C(29B)	114(1)
C(29A)-O(19)-C(32A)	104.9(8)	O(19)-C(29A)-C(30A)	110(1)
O(19)-C(29A)-H(29A)	109.7	C(30A)-C(29A)-H(29A)	109.7
O(19)-C(29A)-H(29B)	109.7	C(30A)-C(29A)-H(29B)	109.7
H(29A)-C(29A)-H(29B)	108.2	C(29A)-C(30A)-C(31A)	104(1)
C(29A)-C(30A)-H(30A)	110.9	C(31A)-C(30A)-H(30A)	110.9
C(29A)-C(30A)-H(30B)	110.9	C(31A)-C(30A)-H(30B)	110.9
H(30A)-C(30A)-H(30B)	108.9	C(32A)-C(31A)-C(30A)	102(1)
C(32A)-C(31A)-H(31A)	111.3	C(30A)-C(31A)-H(31A)	111.3
C(32A)-C(31A)-H(31B)	111.3	C(30A)-C(31A)-H(31B)	111.3
H(31A)-C(31A)-H(31B)	109.2	C(31A)-C(32A)-O(19)	107.1(8)
C(31A)-C(32A)-H(32A)	110.3	O(19)-C(32A)-H(32A)	110.3
C(31A)-C(32A)-H(32B)	110.3	O(19)-C(32A)-H(32B)	110.3
H(32A)-C(32A)-H(32B)	108.5	C(30B)-C(29B)-O(19)	99(2)
C(30B)-C(29B)-H(29C)	111.9	O(19)-C(29B)-H(29C)	111.9
C(30B)-C(29B)-H(29D)	111.9	O(19)-C(29B)-H(29D)	111.9
H(29C)-C(29B)-H(29D)	109.6	C(29B)-C(30B)-C(31B)	101(2)
C(29B)-C(30B)-H(30C)	111.5	C(31B)-C(30B)-H(30C)	111.5
C(29B)-C(30B)-H(30D)	111.5	C(31B)-C(30B)-H(30D)	111.5
H(30C)-C(30B)-H(30D)	109.3	C(32B)-C(31B)-C(30B)	102(2)
C(32B)-C(31B)-H(31C)	111.4	C(30B)-C(31B)-H(31C)	111.4
C(32B)-C(31B)-H(31D)	111.4	C(30B)-C(31B)-H(31D)	111.4
H(31C)-C(31B)-H(31D)	109.3	O(19)-C(32B)-C(31B)	104(2)
O(19)-C(32B)-H(32C)	110.9	C(31B)-C(32B)-H(32C)	110.9
O(19)-C(32B)-H(32D)	110.9	C(31B)-C(32B)-H(32D)	110.9
H(32C)-C(32B)-H(32D)	109.0		

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