Supplementary Information

for

Tetramethylcyclopentadienyl Samarium(II) Chemistry: Isolation of a Bimetallic Sm(II)/Sm(II) Complex

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NMR Spectroscopy

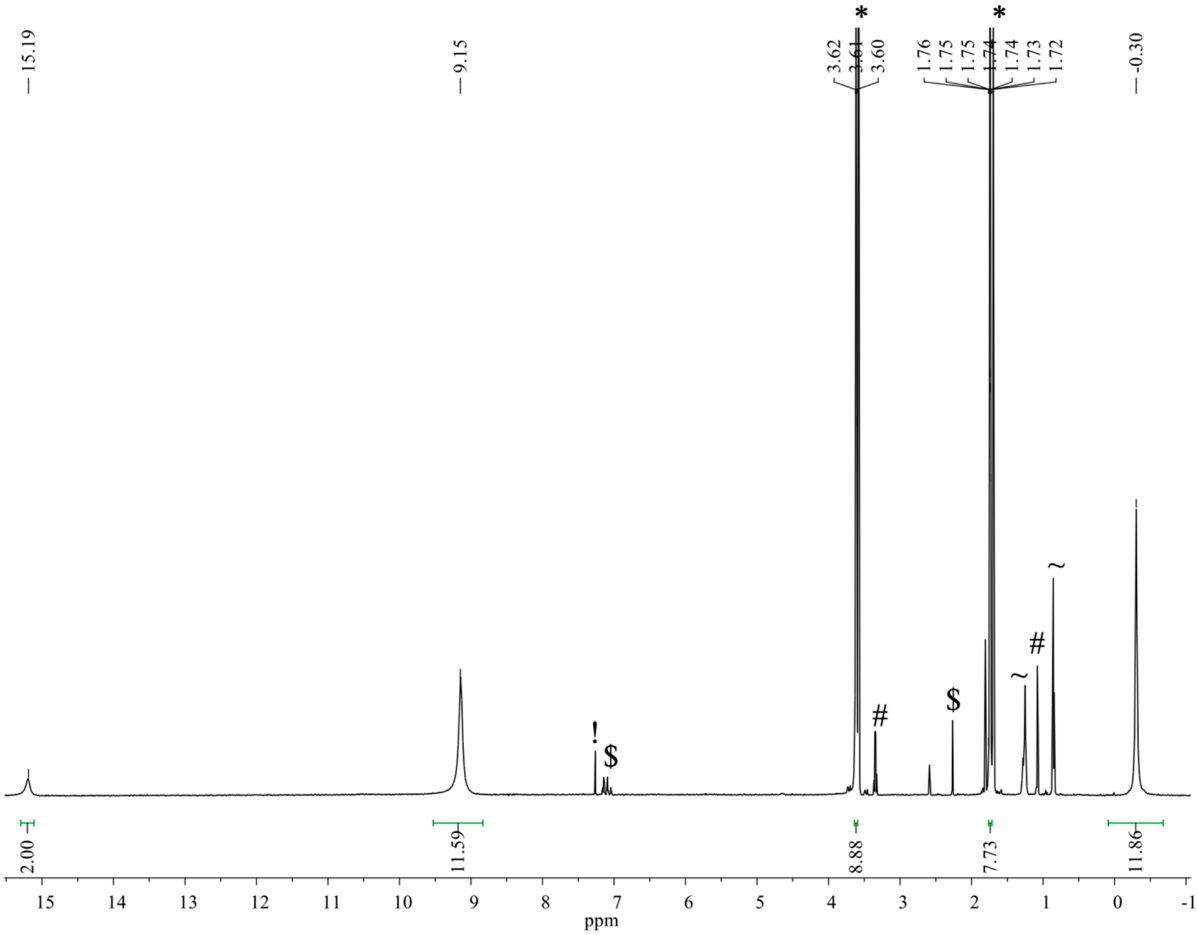

Figure S1. ^{1}H NMR spectrum of $(C_5Me_4H)_2Sm(THF)_2$ in THF-d_8. Assignable solvent impurities include residual benzene labelled (!), toluene labelled ($), diethyl ether labelled (#), hexanes labelled (~) in the sample as well as residual solvent signals for THF-d_8 labelled (*).

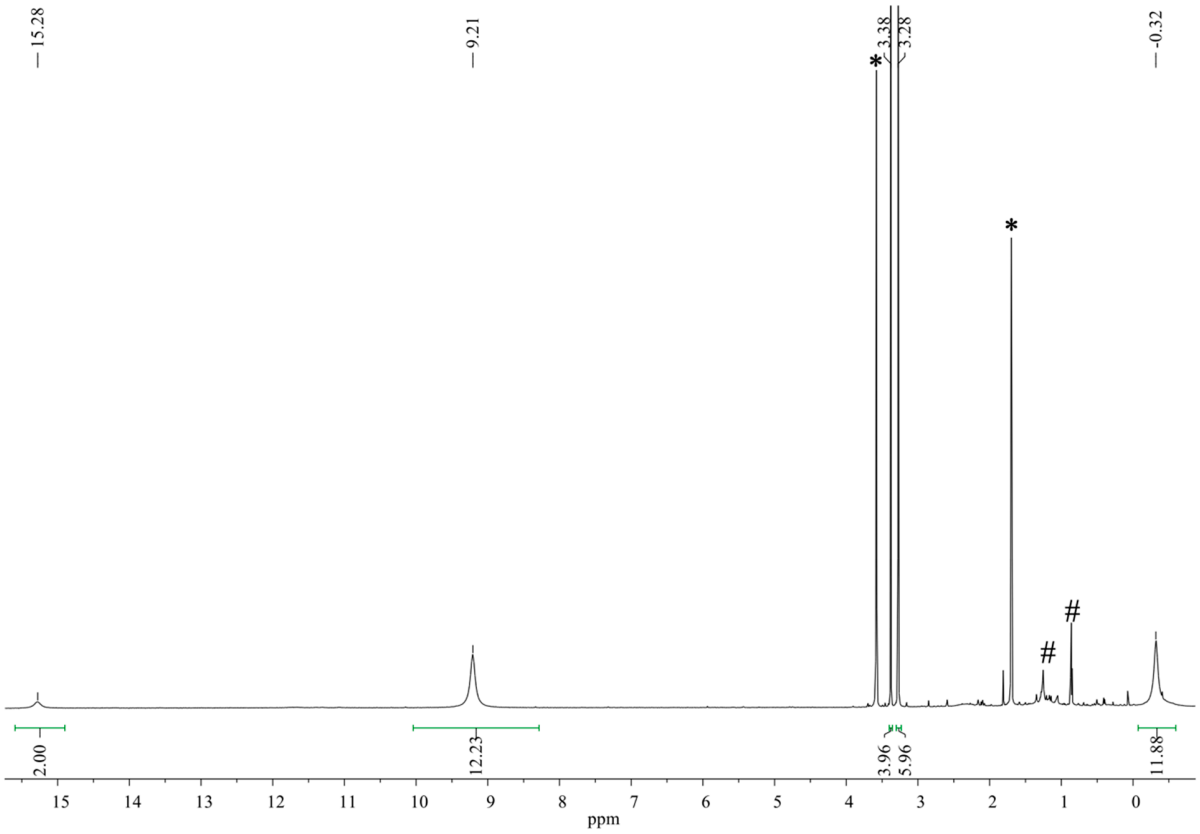

Figure S2. ^{1}H NMR spectrum of complex **2** in THF-d_8. Assignable solvent impurities include residual hexanes labelled (#) in the sample and the solvent residual signals of THF-d_8 labelled (*).

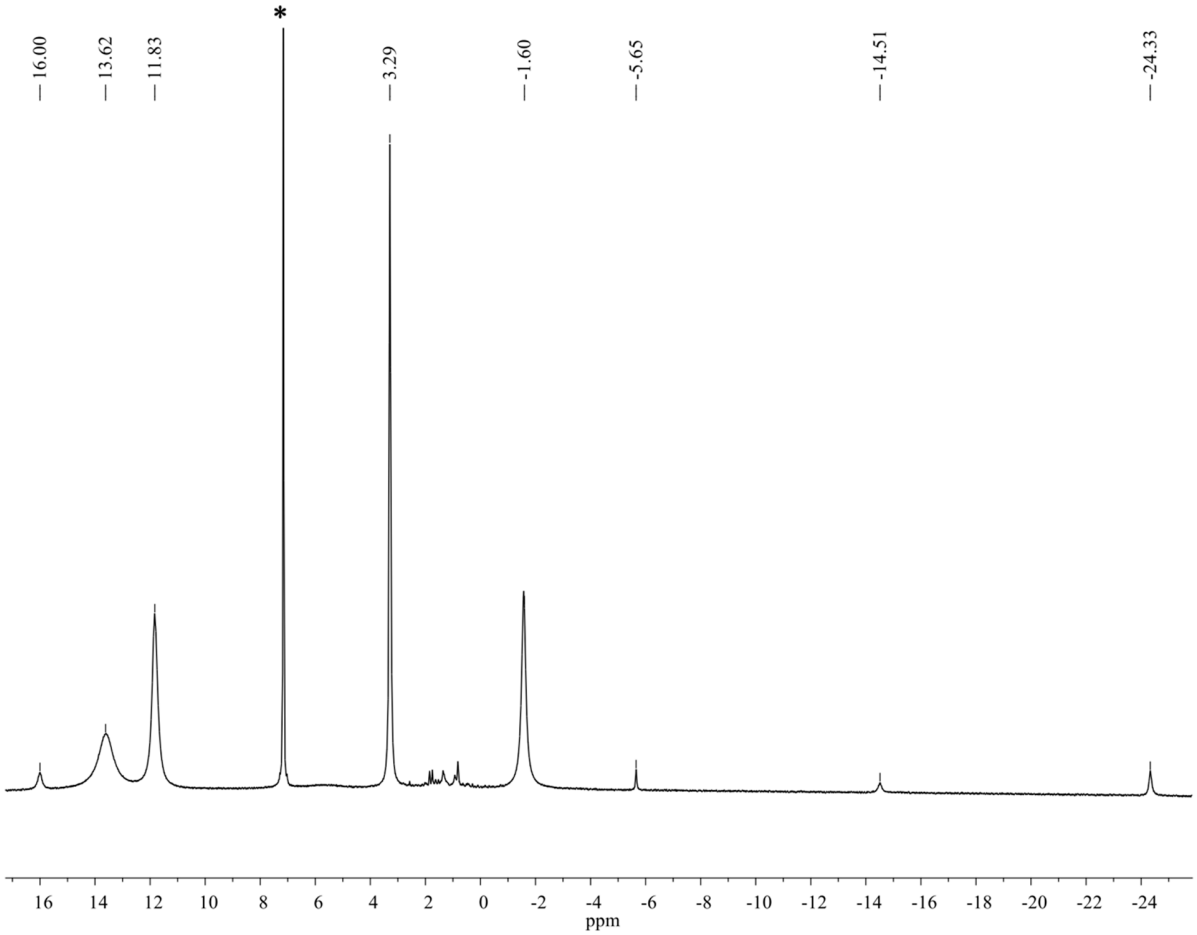

Figure S3. ^{1}H NMR spectrum of complex **3** in C_6D_6. The resonance labelled with (*) was assigned to the solvent residual signal of C_6D_6. The paramagnetism of Sm(II) precluded a definitive assignment.

Infrared Spectroscopy

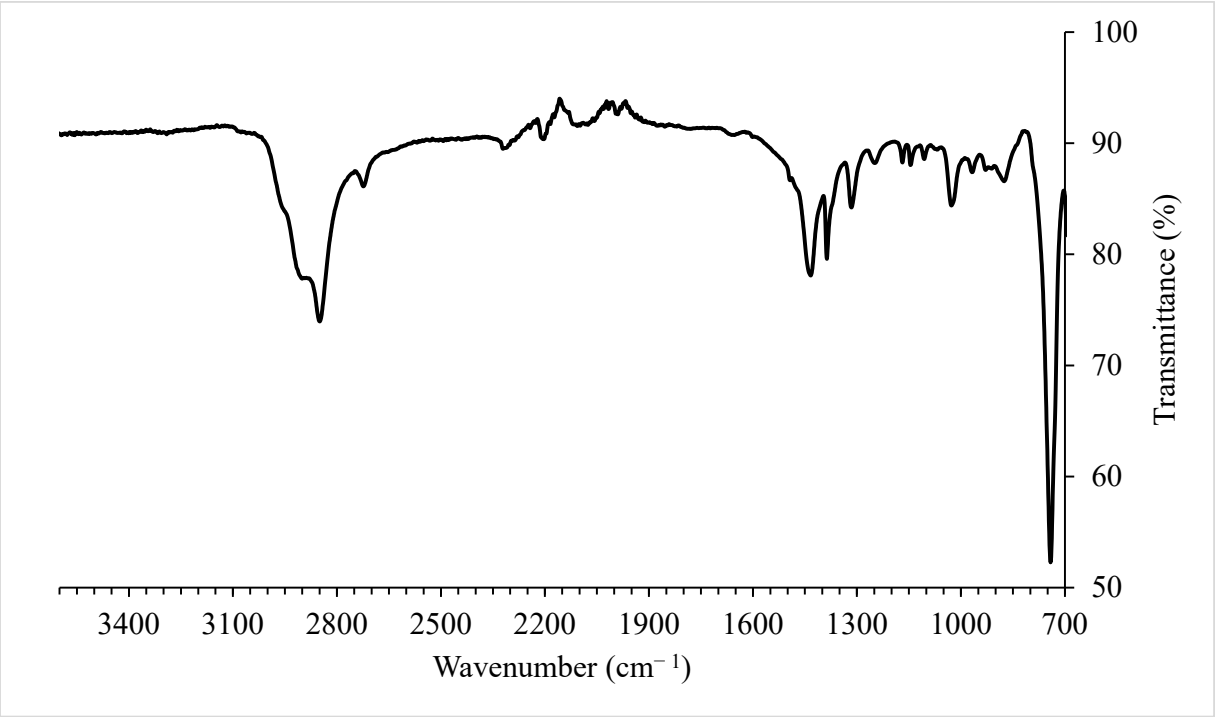

Figure S4. Infrared spectrum of the purple, toluene insoluble solids, **1**.

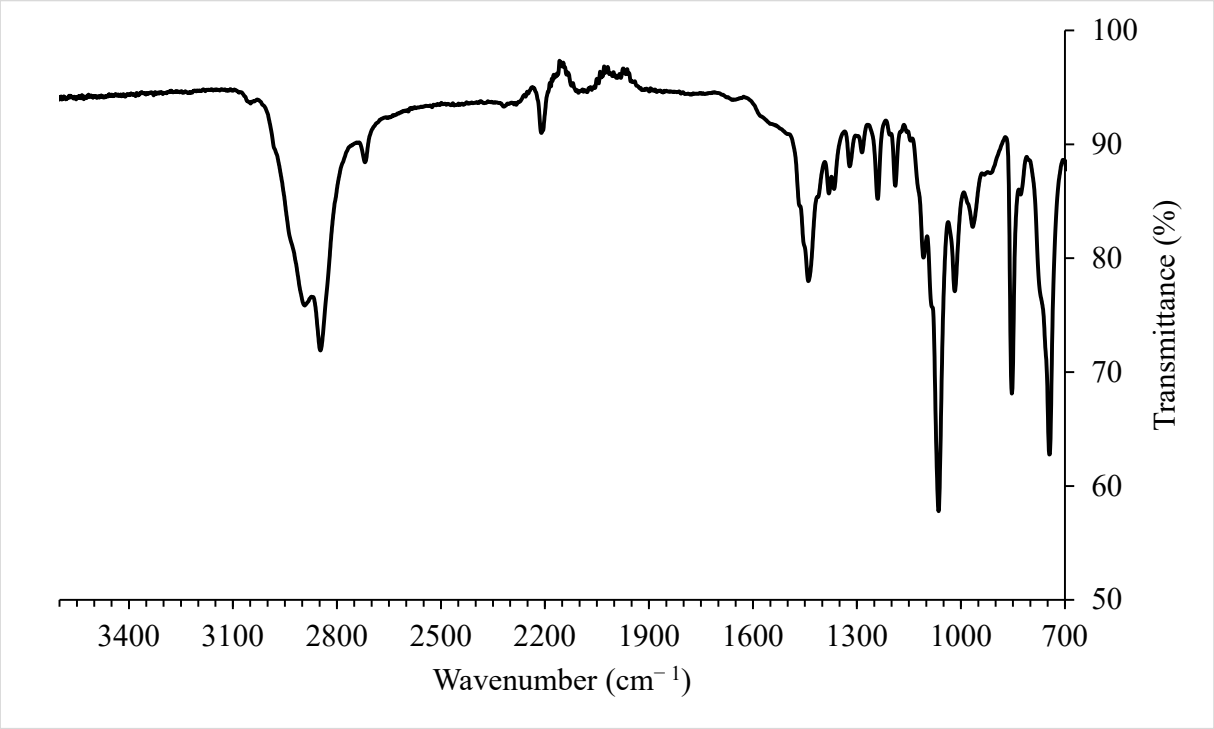

Figure S5. Infrared spectrum of $(C_5Me_4H)_2Sm^{II}(DME)$, **2**.

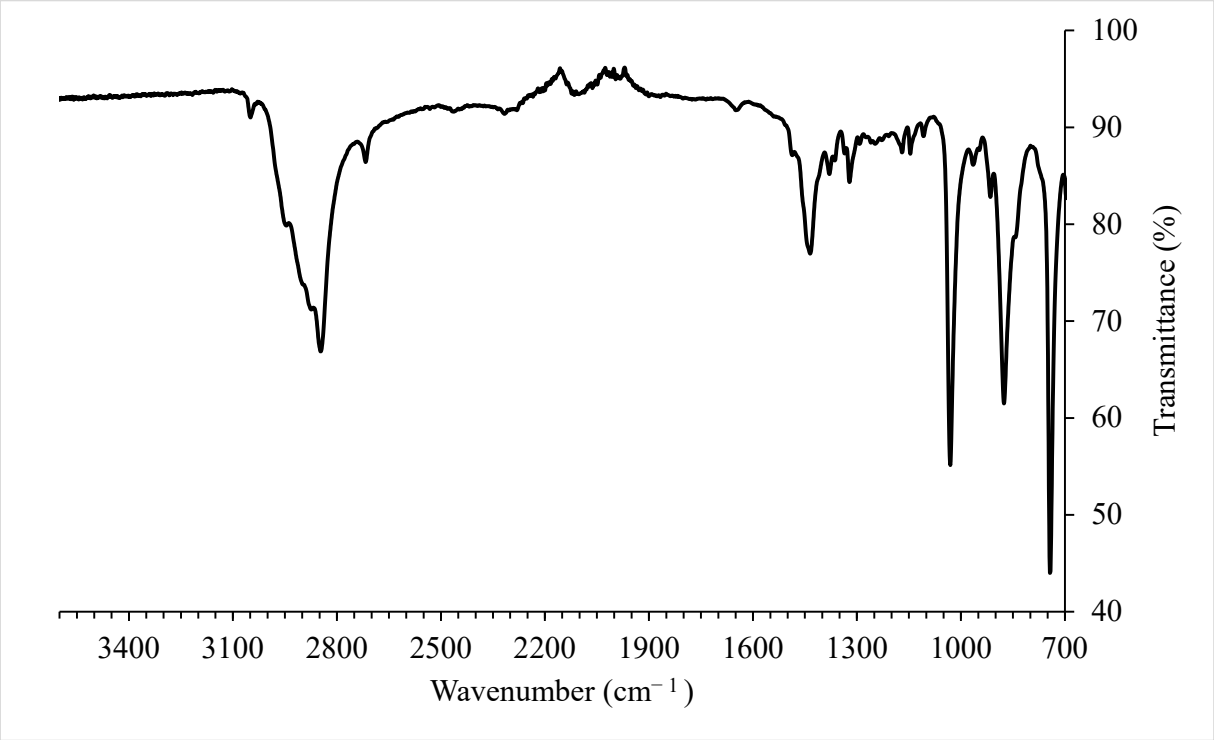

Figure S6. Infrared spectrum of $(C_5Me_4H)_2Sm^{II}(\mu\text{-}\eta^3\text{:}\eta^5\text{-}C_5Me_4H)Sm^{II}(C_5Me_4H)(THF)_2$, **3**.

UV-Visible Spectroscopy

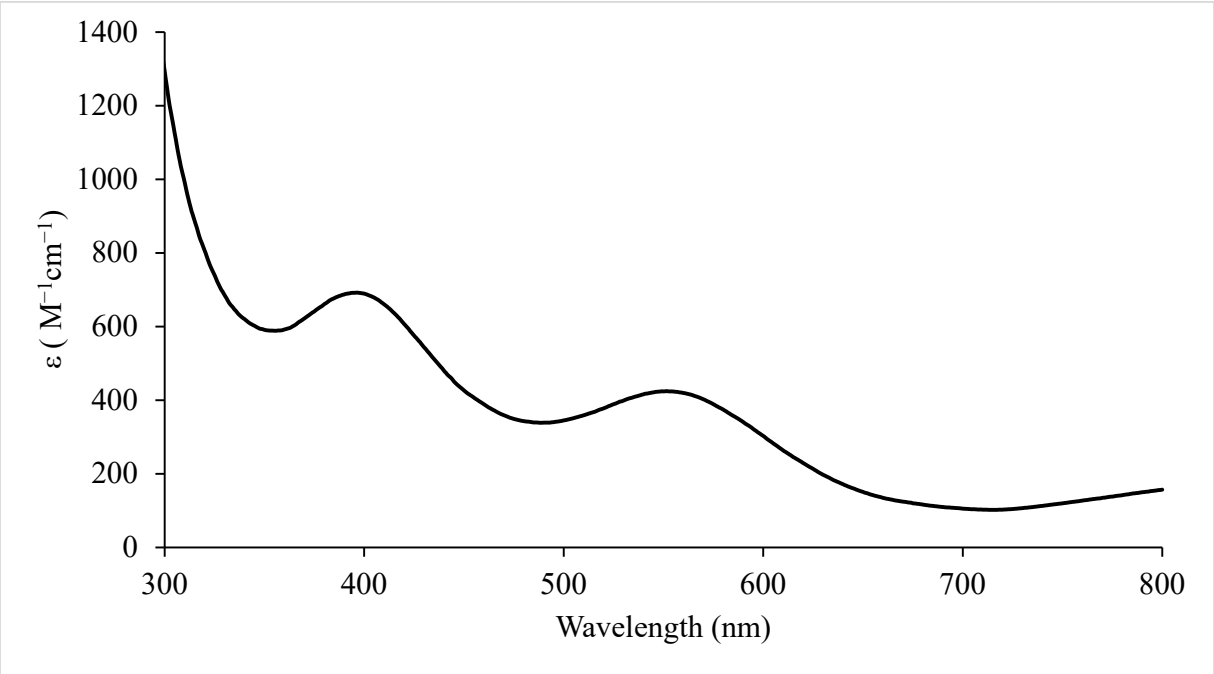

Figure S7. UV-visible spectrum of **1**, presumed to be $[(C_5Me_4H)_2Sm]_n$ as a solid and $(C_5Me_4H)_2Sm(THF)_2$ in THF solution, in THF at room temperature.

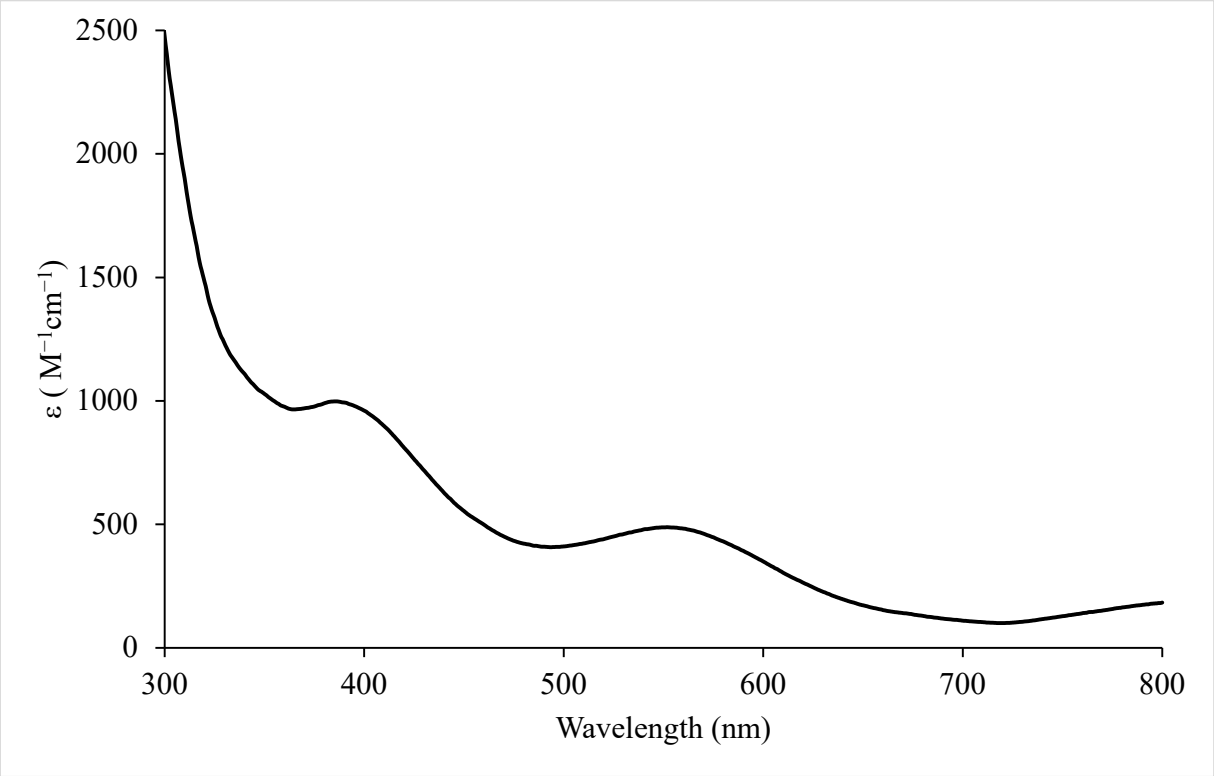

Figure S8. UV-visible spectrum of **2** in THF at room temperature.

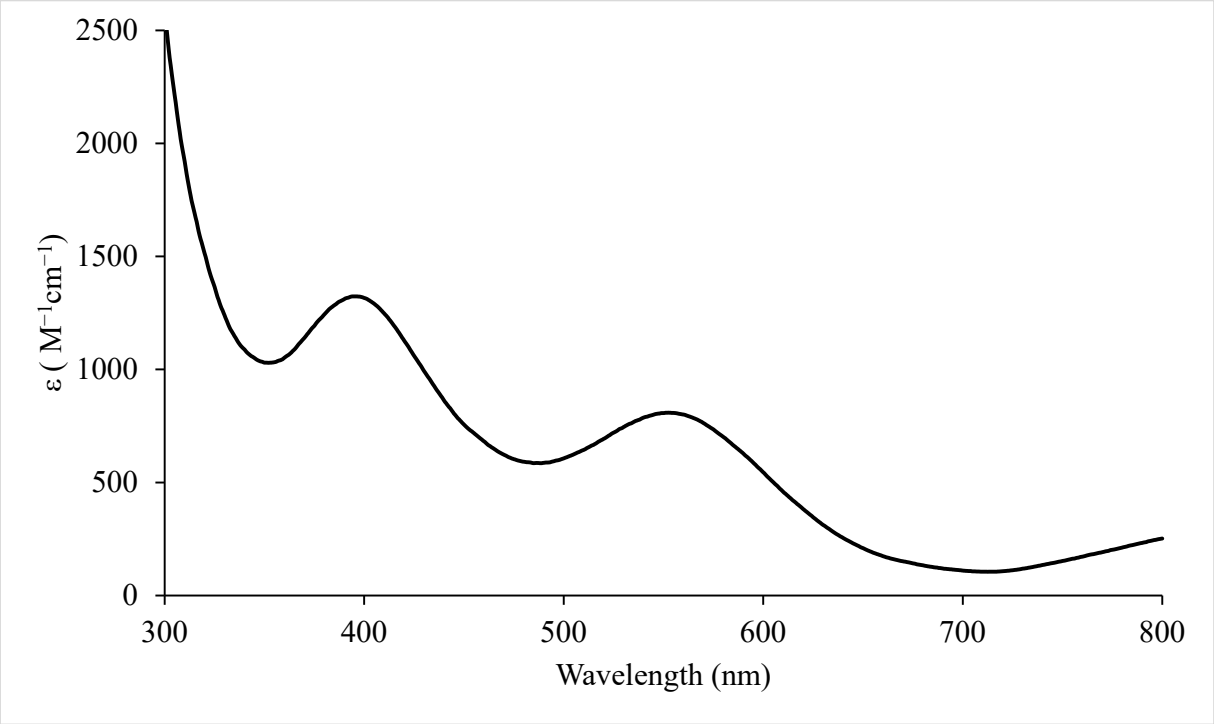

Figure S9. UV-visible spectrum of **3** in THF at room temperature.

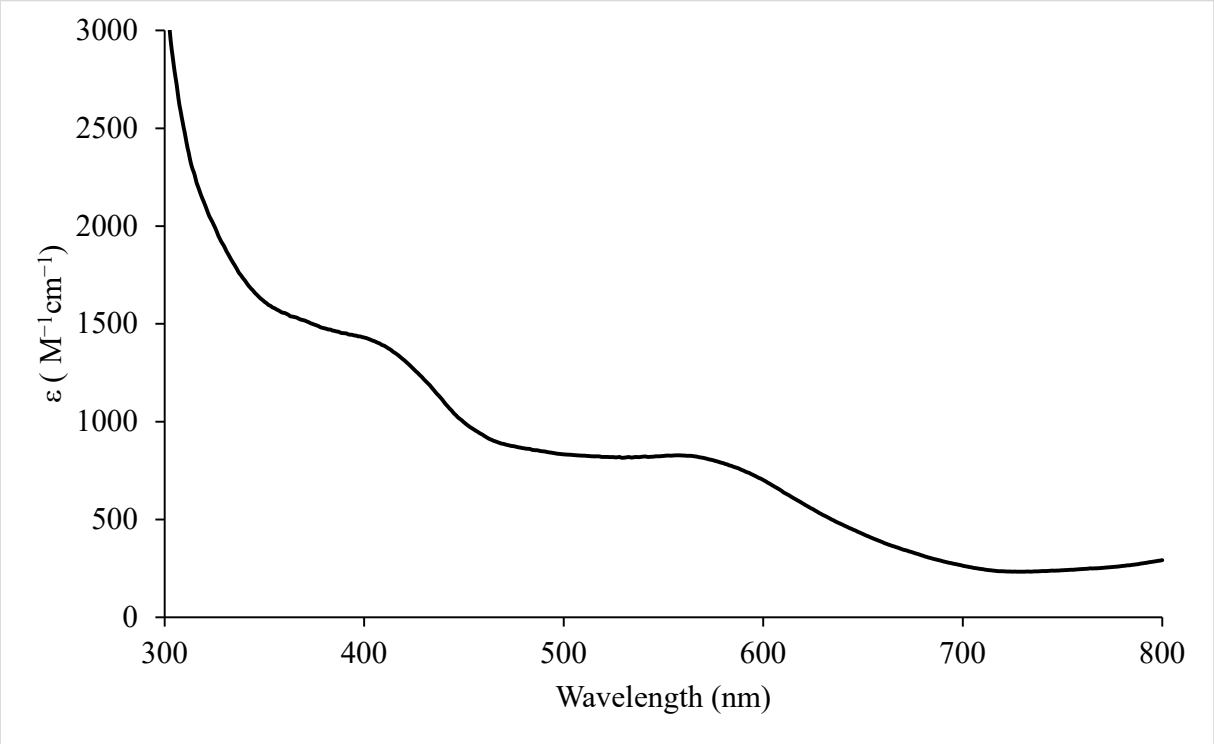

Figure S10. UV-visible spectrum of **3** in toluene at room temperature.

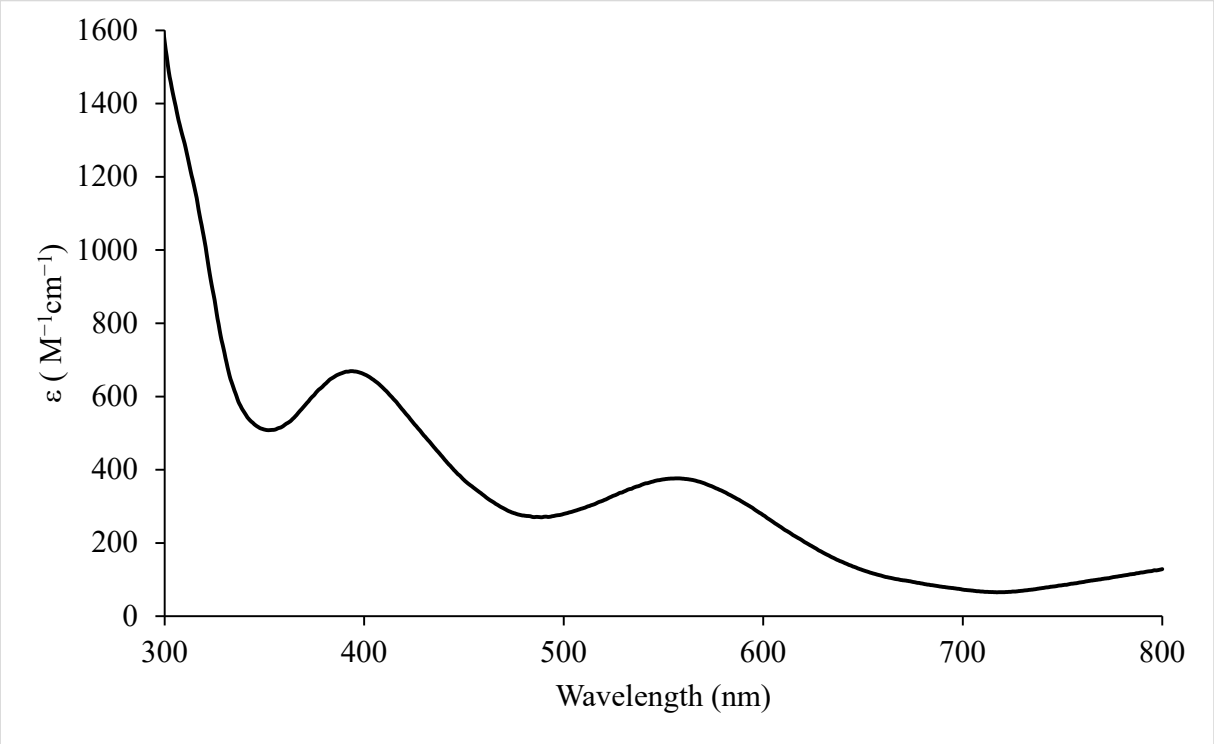

Figure S11. UV-visible spectrum of $(C_5Me_5)_2Sm(THF)_2$ in THF at room temperature.

X-ray Data Collection, Structure Determination, and Refinement for $(C_5Me_4H)_2Sm(DME)$, 2.

A green crystal of approximate dimensions 0.114 x 0.209 x 0.481 mm was mounted in a cryoloop and transferred to a Bruker SMART APEX II diffractometer system. The APEX2[1] program package was used to determine the unit-cell parameters and for data collection (30 sec/frame scan time). The raw frame data was processed using SAINT[2] and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program package. The diffraction symmetry was *mmm* and the systematic absences were consistent with the orthorhombic space group *Pbca* that was later determined to be correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. There were two molecules of the formula unit present.

Least-squares analysis yielded wR2 = 0.0470 and Goof = 1.039 for 469 variables refined against 12415 data (0.72 Å), R1 = 0.0195 for those 10938 data with $I > 2.0\sigma(I)$.

Table S1. Crystal data and structure refinement for jqn48.

Identification code	jqn48 (Joseph Nguyen)
Empirical formula	$C_{44}H_{72}O_4Sm_2$
Formula weight	965.71
Temperature	93(2) K

Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	*Pbca*	
Unit cell dimensions	a = 17.435(4) Å	α = 90°.
	b = 16.479(3) Å	β = 90°.
	c = 30.782(6) Å	γ = 90°.
Volume	8845(3) Å^3	
Z	8	
Density (calculated)	1.450 Mg/m^3	
Absorption coefficient	2.667 mm^{-1}	
F(000)	3936	
Crystal color	green	
Crystal size	0.481 x 0.209 x 0.114 mm^3	
Theta range for data collection	1.323 to 29.575°	
Index ranges	$-24 \leq h \leq 24$, $-22 \leq k \leq 22$, $-42 \leq l \leq 42$	
Reflections collected	211448	
Independent reflections	12415 [R(int) = 0.0439]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.4330 and 0.3062	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12415 / 0 / 469	

Goodness-of-fit on F^2	1.039
Final R indices [I>2σ(I) = 10938 data]	R1 = 0.0195, wR2 = 0.0443
R indices (all data, 0.72 Å)	R1 = 0.0255, wR2 = 0.0470
Largest diff. peak and hole	0.616 and -0.483 e.$Å^{-3}$

Table S2. Bond lengths [Å] and angles [°] for jqn48.

Sm(1)-Cnt1	2.534
Sm(1)-Cnt2	2.527
Sm(1)-O(1)	2.5906(13)
Sm(1)-O(2)	2.6174(13)
Sm(1)-C(14)	2.7408(19)
Sm(1)-C(10)	2.7465(18)
Sm(1)-C(5)	2.7868(18)
Sm(1)-C(4)	2.7962(18)
Sm(1)-C(3)	2.8072(18)
Sm(1)-C(1)	2.8130(18)
Sm(1)-C(13)	2.8189(18)
Sm(1)-C(11)	2.8207(18)
Sm(1)-C(2)	2.8214(18)
Sm(1)-C(12)	2.8666(18)
Sm(2)-Cnt3	2.528
Sm(2)-Cnt4	2.544

Sm(2)-O(4)	2.6014(13)
Sm(2)-O(3)	2.6116(13)
Sm(2)-C(27)	2.7600(18)
Sm(2)-C(26)	2.7859(19)
Sm(2)-C(36)	2.7866(18)
Sm(2)-C(23)	2.7942(19)
Sm(2)-C(32)	2.8101(18)
Sm(2)-C(35)	2.8191(18)
Sm(2)-C(25)	2.824(2)
Sm(2)-C(33)	2.8263(17)
Sm(2)-C(24)	2.830(2)
Sm(2)-C(34)	2.8335(18)
O(1)-C(19)	1.423(2)
O(1)-C(20)	1.439(2)
O(2)-C(22)	1.423(2)
O(2)-C(21)	1.433(2)
O(3)-C(41)	1.427(2)
O(3)-C(42)	1.432(2)
O(4)-C(44)	1.425(2)
O(4)-C(43)	1.441(2)
C(1)-C(5)	1.412(3)
C(1)-C(2)	1.413(3)
C(1)-C(6)	1.507(3)

C(2)-C(3)	1.417(3)
C(2)-C(7)	1.506(3)
C(3)-C(4)	1.414(3)
C(3)-C(8)	1.508(3)
C(4)-C(5)	1.418(3)
C(4)-C(9)	1.503(3)
C(10)-C(14)	1.414(3)
C(10)-C(11)	1.415(3)
C(10)-C(15)	1.502(3)
C(11)-C(12)	1.419(3)
C(11)-C(16)	1.502(3)
C(12)-C(13)	1.416(2)
C(12)-C(17)	1.505(3)
C(13)-C(14)	1.416(3)
C(13)-C(18)	1.502(3)
C(20)-C(21)	1.494(3)
C(23)-C(24)	1.398(3)
C(23)-C(27)	1.411(3)
C(23)-C(28)	1.508(3)
C(24)-C(25)	1.420(3)
C(24)-C(29)	1.512(3)
C(25)-C(26)	1.423(3)
C(25)-C(30)	1.502(3)

C(26)-C(27)	1.409(3)
C(26)-C(31)	1.503(3)
C(32)-C(36)	1.415(3)
C(32)-C(33)	1.417(2)
C(32)-C(37)	1.503(3)
C(33)-C(34)	1.419(3)
C(33)-C(38)	1.508(2)
C(34)-C(35)	1.417(2)
C(34)-C(39)	1.503(2)
C(35)-C(36)	1.414(3)
C(35)-C(40)	1.508(3)
C(42)-C(43)	1.500(3)
Cnt1-Sm(1)-O(1)	111.3
Cnt1-Sm(1)-O(2)	112.6
Cnt2-Sm(1)-O(1)	112.5
Cnt2-Sm(1)-O(2)	107.0
Cnt1-Sm(1)-Cnt2	130.2
O(1)-Sm(1)-O(2)	63.92(4)
O(1)-Sm(1)-C(14)	130.80(5)
O(2)-Sm(1)-C(14)	129.21(5)
O(1)-Sm(1)-C(10)	133.49(5)
O(2)-Sm(1)-C(10)	100.90(5)
C(14)-Sm(1)-C(10)	29.85(5)

O(1)-Sm(1)-C(5)	136.01(5)
O(2)-Sm(1)-C(5)	124.13(5)
C(14)-Sm(1)-C(5)	80.91(5)
C(10)-Sm(1)-C(5)	89.76(5)
O(1)-Sm(1)-C(4)	111.49(5)
O(2)-Sm(1)-C(4)	137.03(5)
C(14)-Sm(1)-C(4)	87.71(6)
C(10)-Sm(1)-C(4)	108.28(6)
C(5)-Sm(1)-C(4)	29.42(5)
O(1)-Sm(1)-C(3)	87.91(5)
O(2)-Sm(1)-C(3)	111.65(5)
C(14)-Sm(1)-C(3)	116.62(6)
C(10)-Sm(1)-C(3)	136.40(6)
C(5)-Sm(1)-C(3)	48.14(5)
C(4)-Sm(1)-C(3)	29.23(6)
O(1)-Sm(1)-C(1)	122.10(5)
O(2)-Sm(1)-C(1)	95.53(5)
C(14)-Sm(1)-C(1)	104.78(6)
C(10)-Sm(1)-C(1)	102.14(5)
C(5)-Sm(1)-C(1)	29.20(6)
C(4)-Sm(1)-C(1)	48.40(6)
C(3)-Sm(1)-C(1)	48.14(5)
O(1)-Sm(1)-C(13)	101.38(5)

O(2)-Sm(1)-C(13)	124.05(5)
C(14)-Sm(1)-C(13)	29.48(5)
C(10)-Sm(1)-C(13)	48.70(5)
C(5)-Sm(1)-C(13)	104.04(6)
C(4)-Sm(1)-C(13)	98.91(6)
C(3)-Sm(1)-C(13)	121.85(6)
C(1)-Sm(1)-C(13)	131.65(6)
O(1)-Sm(1)-C(11)	104.66(5)
O(2)-Sm(1)-C(11)	81.94(5)
C(14)-Sm(1)-C(11)	48.55(5)
C(10)-Sm(1)-C(11)	29.40(5)
C(5)-Sm(1)-C(11)	119.06(5)
C(4)-Sm(1)-C(11)	135.61(5)
C(3)-Sm(1)-C(11)	164.84(5)
C(1)-Sm(1)-C(11)	126.46(5)
C(13)-Sm(1)-C(11)	48.09(5)
O(1)-Sm(1)-C(2)	93.85(5)
O(2)-Sm(1)-C(2)	88.86(5)
C(14)-Sm(1)-C(2)	128.84(6)
C(10)-Sm(1)-C(2)	131.20(5)
C(5)-Sm(1)-C(2)	47.95(6)
C(4)-Sm(1)-C(2)	48.17(6)
C(3)-Sm(1)-C(2)	29.15(6)

C(1)-Sm(1)-C(2)	29.05(5)
C(13)-Sm(1)-C(2)	147.07(6)
C(11)-Sm(1)-C(2)	152.89(5)
O(1)-Sm(1)-C(12)	87.85(5)
O(2)-Sm(1)-C(12)	95.24(5)
C(14)-Sm(1)-C(12)	48.03(5)
C(10)-Sm(1)-C(12)	48.10(5)
C(5)-Sm(1)-C(12)	128.91(5)
C(4)-Sm(1)-C(12)	127.72(5)
C(3)-Sm(1)-C(12)	147.43(5)
C(1)-Sm(1)-C(12)	149.88(5)
C(13)-Sm(1)-C(12)	28.84(5)
C(11)-Sm(1)-C(12)	28.89(5)
C(2)-Sm(1)-C(12)	175.90(5)
Cnt3-Sm(2)-O(3)	117.0
Cnt3-Sm(2)-O(4)	106.6
Cnt4-Sm(2)-O(3)	106.4
Cnt4-Sm(2)-O(4)	114.0
Cnt3-Sm(2)-Cnt4	130.3
O(4)-Sm(2)-O(3)	63.21(4)
O(4)-Sm(2)-C(27)	131.56(5)
O(3)-Sm(2)-C(27)	128.41(5)
O(4)-Sm(2)-C(26)	117.54(6)

O(3)-Sm(2)-C(26)	99.70(5)
C(27)-Sm(2)-C(26)	29.42(6)
O(4)-Sm(2)-C(36)	122.68(5)
O(3)-Sm(2)-C(36)	131.71(5)
C(27)-Sm(2)-C(36)	85.84(6)
C(26)-Sm(2)-C(36)	112.84(6)
O(4)-Sm(2)-C(23)	107.72(5)
O(3)-Sm(2)-C(23)	141.20(5)
C(27)-Sm(2)-C(23)	29.44(6)
C(26)-Sm(2)-C(23)	48.58(6)
C(36)-Sm(2)-C(23)	86.01(6)
O(4)-Sm(2)-C(32)	94.84(5)
O(3)-Sm(2)-C(32)	113.96(5)
C(27)-Sm(2)-C(32)	112.93(6)
C(26)-Sm(2)-C(32)	141.51(6)
C(36)-Sm(2)-C(32)	29.28(5)
C(23)-Sm(2)-C(32)	104.13(6)
O(4)-Sm(2)-C(35)	139.09(5)
O(3)-Sm(2)-C(35)	110.94(5)
C(27)-Sm(2)-C(35)	85.46(6)
C(26)-Sm(2)-C(35)	103.36(6)
C(36)-Sm(2)-C(35)	29.21(5)
C(23)-Sm(2)-C(35)	99.50(6)

C(32)-Sm(2)-C(35)	48.29(5)
O(4)-Sm(2)-C(25)	88.96(6)
O(3)-Sm(2)-C(25)	93.23(5)
C(27)-Sm(2)-C(25)	48.12(6)
C(26)-Sm(2)-C(25)	29.37(7)
C(36)-Sm(2)-C(25)	132.08(6)
C(23)-Sm(2)-C(25)	48.00(6)
C(32)-Sm(2)-C(25)	151.20(6)
C(35)-Sm(2)-C(25)	131.69(6)
O(4)-Sm(2)-C(33)	91.33(5)
O(3)-Sm(2)-C(33)	86.58(5)
C(27)-Sm(2)-C(33)	131.77(6)
C(26)-Sm(2)-C(33)	150.26(6)
C(36)-Sm(2)-C(33)	47.97(5)
C(23)-Sm(2)-C(33)	132.20(6)
C(32)-Sm(2)-C(33)	29.12(5)
C(35)-Sm(2)-C(33)	48.05(5)
C(25)-Sm(2)-C(33)	179.53(7)
O(4)-Sm(2)-C(24)	83.80(5)
O(3)-Sm(2)-C(24)	115.64(6)
C(27)-Sm(2)-C(24)	47.90(6)
C(26)-Sm(2)-C(24)	48.27(7)
C(36)-Sm(2)-C(24)	112.65(6)

C(23)-Sm(2)-C(24)	28.78(6)
C(32)-Sm(2)-C(24)	122.99(6)
C(35)-Sm(2)-C(24)	128.18(6)
C(25)-Sm(2)-C(24)	29.09(7)
C(33)-Sm(2)-C(24)	151.32(6)
O(4)-Sm(2)-C(34)	115.82(5)
O(3)-Sm(2)-C(34)	84.95(5)
C(27)-Sm(2)-C(34)	112.20(6)
C(26)-Sm(2)-C(34)	122.00(6)
C(36)-Sm(2)-C(34)	47.86(5)
C(23)-Sm(2)-C(34)	128.48(6)
C(32)-Sm(2)-C(34)	48.00(5)
C(35)-Sm(2)-C(34)	29.04(5)
C(25)-Sm(2)-C(34)	150.51(6)
C(33)-Sm(2)-C(34)	29.05(5)
C(24)-Sm(2)-C(34)	157.22(6)
C(19)-O(1)-C(20)	110.97(15)
C(19)-O(1)-Sm(1)	123.00(12)
C(20)-O(1)-Sm(1)	115.61(10)
C(22)-O(2)-C(21)	111.56(15)
C(22)-O(2)-Sm(1)	122.97(12)
C(21)-O(2)-Sm(1)	115.72(10)
C(41)-O(3)-C(42)	111.20(14)

C(41)-O(3)-Sm(2)	124.17(11)
C(42)-O(3)-Sm(2)	118.31(10)
C(44)-O(4)-C(43)	111.30(14)
C(44)-O(4)-Sm(2)	119.67(11)
C(43)-O(4)-Sm(2)	116.69(10)
C(5)-C(1)-C(2)	107.56(16)
C(5)-C(1)-C(6)	125.30(18)
C(2)-C(1)-C(6)	126.87(19)
C(5)-C(1)-Sm(1)	74.37(10)
C(2)-C(1)-Sm(1)	75.80(10)
C(6)-C(1)-Sm(1)	120.44(13)
C(1)-C(2)-C(3)	108.20(17)
C(1)-C(2)-C(7)	125.89(19)
C(3)-C(2)-C(7)	125.75(18)
C(1)-C(2)-Sm(1)	75.14(10)
C(3)-C(2)-Sm(1)	74.87(10)
C(7)-C(2)-Sm(1)	119.70(13)
C(4)-C(3)-C(2)	108.19(16)
C(4)-C(3)-C(8)	126.24(18)
C(2)-C(3)-C(8)	125.53(18)
C(4)-C(3)-Sm(1)	74.95(10)
C(2)-C(3)-Sm(1)	75.98(10)
C(8)-C(3)-Sm(1)	117.03(12)

C(3)-C(4)-C(5)	107.35(17)
C(3)-C(4)-C(9)	126.96(18)
C(5)-C(4)-C(9)	125.64(18)
C(3)-C(4)-Sm(1)	75.81(10)
C(5)-C(4)-Sm(1)	74.92(10)
C(9)-C(4)-Sm(1)	117.21(13)
C(1)-C(5)-C(4)	108.70(16)
C(1)-C(5)-Sm(1)	76.43(10)
C(4)-C(5)-Sm(1)	75.66(10)
C(14)-C(10)-C(11)	107.96(16)
C(14)-C(10)-C(15)	126.64(18)
C(11)-C(10)-C(15)	125.34(18)
C(14)-C(10)-Sm(1)	74.85(10)
C(11)-C(10)-Sm(1)	78.21(10)
C(15)-C(10)-Sm(1)	111.35(12)
C(10)-C(11)-C(12)	107.82(15)
C(10)-C(11)-C(16)	126.81(17)
C(12)-C(11)-C(16)	125.34(17)
C(10)-C(11)-Sm(1)	72.39(10)
C(12)-C(11)-Sm(1)	77.35(10)
C(16)-C(11)-Sm(1)	117.59(12)
C(13)-C(12)-C(11)	108.24(16)
C(13)-C(12)-C(17)	125.81(17)

C(11)-C(12)-C(17)	125.84(17)
C(13)-C(12)-Sm(1)	73.71(10)
C(11)-C(12)-Sm(1)	73.76(10)
C(17)-C(12)-Sm(1)	121.52(12)
C(14)-C(13)-C(12)	107.54(16)
C(14)-C(13)-C(18)	126.43(17)
C(12)-C(13)-C(18)	125.92(17)
C(14)-C(13)-Sm(1)	72.21(10)
C(12)-C(13)-Sm(1)	77.45(10)
C(18)-C(13)-Sm(1)	119.27(12)
C(10)-C(14)-C(13)	108.44(16)
C(10)-C(14)-Sm(1)	75.30(10)
C(13)-C(14)-Sm(1)	78.32(10)
O(1)-C(20)-C(21)	108.34(15)
O(2)-C(21)-C(20)	109.03(15)
C(24)-C(23)-C(27)	107.80(18)
C(24)-C(23)-C(28)	126.0(2)
C(27)-C(23)-C(28)	126.2(2)
C(24)-C(23)-Sm(2)	77.04(11)
C(27)-C(23)-Sm(2)	73.94(10)
C(28)-C(23)-Sm(2)	117.30(13)
C(23)-C(24)-C(25)	108.37(19)
C(23)-C(24)-C(29)	124.8(2)

C(25)-C(24)-C(29)	126.7(2)
C(23)-C(24)-Sm(2)	74.18(11)
C(25)-C(24)-Sm(2)	75.21(11)
C(29)-C(24)-Sm(2)	120.01(13)
C(24)-C(25)-C(26)	107.78(18)
C(24)-C(25)-C(30)	125.5(2)
C(26)-C(25)-C(30)	126.7(2)
C(24)-C(25)-Sm(2)	75.70(11)
C(26)-C(25)-Sm(2)	73.83(11)
C(30)-C(25)-Sm(2)	116.76(14)
C(27)-C(26)-C(25)	107.08(19)
C(27)-C(26)-C(31)	124.7(2)
C(25)-C(26)-C(31)	128.2(2)
C(27)-C(26)-Sm(2)	74.27(11)
C(25)-C(26)-Sm(2)	76.80(11)
C(31)-C(26)-Sm(2)	115.02(15)
C(26)-C(27)-C(23)	108.97(19)
C(26)-C(27)-Sm(2)	76.31(11)
C(23)-C(27)-Sm(2)	76.63(10)
C(36)-C(32)-C(33)	107.39(16)
C(36)-C(32)-C(37)	125.18(17)
C(33)-C(32)-C(37)	127.38(18)
C(36)-C(32)-Sm(2)	74.44(10)

C(33)-C(32)-Sm(2)	76.07(10)
C(37)-C(32)-Sm(2)	117.45(12)
C(32)-C(33)-C(34)	108.07(15)
C(32)-C(33)-C(38)	127.30(17)
C(34)-C(33)-C(38)	124.63(16)
C(32)-C(33)-Sm(2)	74.81(10)
C(34)-C(33)-Sm(2)	75.76(10)
C(38)-C(33)-Sm(2)	116.13(11)
C(35)-C(34)-C(33)	108.26(15)
C(35)-C(34)-C(39)	126.11(17)
C(33)-C(34)-C(39)	125.55(16)
C(35)-C(34)-Sm(2)	74.92(10)
C(33)-C(34)-Sm(2)	75.20(10)
C(39)-C(34)-Sm(2)	118.79(12)
C(36)-C(35)-C(34)	107.29(16)
C(36)-C(35)-C(40)	125.76(17)
C(34)-C(35)-C(40)	126.82(17)
C(36)-C(35)-Sm(2)	74.12(10)
C(34)-C(35)-Sm(2)	76.04(10)
C(40)-C(35)-Sm(2)	118.95(13)
C(35)-C(36)-C(32)	108.99(16)
C(35)-C(36)-Sm(2)	76.67(10)
C(32)-C(36)-Sm(2)	76.28(10)

O(3)-C(42)-C(43)	109.24(15)
O(4)-C(43)-C(42)	108.94(15)

X-ray Data Collection, Structure Determination, and Refinement for $(C_5Me_4H)_2Sm(\mu\text{-}\eta^3\text{:}\eta^5\text{-}C_5Me_4H)Sm(C_5Me_4H)(THF)_2$, 3.

A purple crystal of approximate dimensions 0.170 x 0.191 x 0.306 mm was mounted in a cryoloop and transferred to a Bruker SMART APEX II diffractometer system. The APEX2[1] program package was used to determine the unit-cell parameters and for data collection (20 sec/frame scan time). The raw frame data was processed using SAINT[2] and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program package. The diffraction symmetry was 2/*m* and the systematic absences were consistent with the monoclinic space group $P2_1/n$ that was later determined to be correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model.

Least-squares analysis yielded wR2 = 0.0536 and Goof = 1.021 for 449 variables refined against 12542 data (0.70 Å), R1 = 0.0239 for those 10610 data with $I > 2.0\sigma(I)$.

Table S3. Crystal data and structure refinement for jqn20.

Identification code	jqn20 (Joseph Nguyen)
Empirical formula	$C_{44}H_{68}O_2Sm_2$
Formula weight	929.68
Temperature	133(2) K

Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 11.4458(8) Å	α = 90°.
	b = 15.6042(11) Å	β = 92.6546(12)°.
	c = 23.3099(17) Å	γ = 90°.
Volume	4158.7(5) $Å^3$	
Z	4	
Density (calculated)	1.485 Mg/m^3	
Absorption coefficient	2.829 mm^{-1}	
F(000)	1888	
Crystal color	purple	
Crystal size	0.306 x 0.191 x 0.170 mm^3	
Theta range for data collection	1.571 to 30.539°	
Index ranges	$-16 \leq h \leq 16$, $-21 \leq k \leq 22$, $-33 \leq l \leq 33$	
Reflections collected	101857	
Independent reflections	12542 [R(int) = 0.0529]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.5948	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12542 / 0 / 449	

Goodness-of-fit on F^2	1.021
Final R indices [I>2σ(I) = 10610 data]	R1 = 0.0239, wR2 = 0.0496
R indices (all data, 0.70 Å)	R1 = 0.0339, wR2 = 0.0536
Largest diff. peak and hole	0.923 and -0.477 e.$Å^{-3}$

Table S4. Bond lengths [Å] and angles [°] for jqn20.

Sm(1)-Cnt1	2.584
Sm(1)-Cnt2	2.581
Sm(1)-C(14)	2.748(2)
Sm(1)-C(5)	2.751(2)
Sm(1)-C(13)	2.791(2)
Sm(1)-C(4)	2.810(2)
Sm(1)-C(1)	2.819(2)
Sm(1)-C(10)	2.831(2)
Sm(1)-C(32)	2.842(2)
Sm(1)-C(12)	2.919(2)
Sm(1)-C(2)	2.931(2)
Sm(1)-C(3)	2.932(2)
Sm(1)-C(11)	2.940(2)
Sm(1)-C(31)	2.955(2)
Sm(2)-Cnt3	2.537
Sm(2)-Cnt4	2.586

Sm(2)-O(1)	2.5770(15)
Sm(2)-O(2)	2.5970(16)
Sm(2)-C(23)	2.799(2)
Sm(2)-C(21)	2.804(2)
Sm(2)-C(20)	2.806(2)
Sm(2)-C(32)	2.807(2)
Sm(2)-C(22)	2.811(2)
Sm(2)-C(19)	2.814(2)
Sm(2)-C(28)	2.8346(19)
Sm(2)-C(31)	2.864(2)
Sm(2)-C(29)	2.872(2)
Sm(2)-C(30)	2.888(2)
O(1)-C(37)	1.447(3)
O(1)-C(40)	1.448(3)
O(2)-C(44)	1.444(3)
O(2)-C(41)	1.455(3)
C(1)-C(5)	1.409(3)
C(1)-C(2)	1.414(3)
C(1)-C(6)	1.514(3)
C(2)-C(3)	1.415(3)
C(2)-C(7)	1.503(3)
C(3)-C(4)	1.409(3)
C(3)-C(8)	1.506(3)

C(4)-C(5)	1.413(3)
C(4)-C(9)	1.510(3)
C(10)-C(11)	1.409(3)
C(10)-C(14)	1.412(3)
C(10)-C(15)	1.503(3)
C(11)-C(12)	1.416(3)
C(11)-C(16)	1.507(3)
C(12)-C(13)	1.413(3)
C(12)-C(17)	1.505(3)
C(13)-C(14)	1.410(3)
C(13)-C(18)	1.506(3)
C(19)-C(20)	1.403(3)
C(19)-C(23)	1.414(3)
C(19)-C(24)	1.510(3)
C(20)-C(21)	1.421(3)
C(20)-C(25)	1.498(3)
C(21)-C(22)	1.409(3)
C(21)-C(26)	1.501(3)
C(22)-C(23)	1.411(3)
C(22)-C(27)	1.499(3)
C(28)-C(32)	1.412(3)
C(28)-C(29)	1.413(3)
C(28)-C(33)	1.505(3)

C(29)-C(30)	1.421(3)
C(29)-C(34)	1.502(3)
C(30)-C(31)	1.416(3)
C(30)-C(35)	1.503(3)
C(31)-C(32)	1.421(3)
C(31)-C(36)	1.504(3)
C(37)-C(38)	1.513(3)
C(38)-C(39)	1.515(4)
C(39)-C(40)	1.515(3)
C(41)-C(42)	1.515(4)
C(42)-C(43)	1.507(4)
C(43)-C(44)	1.505(4)

Cnt1-Sm(1)-Cnt2	122.8
C(14)-Sm(1)-C(5)	122.82(7)
C(14)-Sm(1)-C(13)	29.48(6)
C(5)-Sm(1)-C(13)	105.96(6)
C(14)-Sm(1)-C(4)	135.21(6)
C(5)-Sm(1)-C(4)	29.41(6)
C(13)-Sm(1)-C(4)	130.99(6)
C(14)-Sm(1)-C(1)	133.88(6)
C(5)-Sm(1)-C(1)	29.27(6)
C(13)-Sm(1)-C(1)	106.65(6)

C(4)-Sm(1)-C(1)	48.06(6)
C(14)-Sm(1)-C(10)	29.27(6)
C(5)-Sm(1)-C(10)	102.34(6)
C(13)-Sm(1)-C(10)	48.12(6)
C(4)-Sm(1)-C(10)	106.76(6)
C(1)-Sm(1)-C(10)	125.39(6)
C(14)-Sm(1)-C(32)	115.82(6)
C(5)-Sm(1)-C(32)	121.25(6)
C(13)-Sm(1)-C(32)	128.02(6)
C(4)-Sm(1)-C(32)	100.75(6)
C(1)-Sm(1)-C(32)	104.71(6)
C(10)-Sm(1)-C(32)	129.32(6)
C(14)-Sm(1)-C(12)	47.29(6)
C(5)-Sm(1)-C(12)	78.76(6)
C(13)-Sm(1)-C(12)	28.54(6)
C(4)-Sm(1)-C(12)	102.45(6)
C(1)-Sm(1)-C(12)	87.10(6)
C(10)-Sm(1)-C(12)	46.92(6)
C(32)-Sm(1)-C(12)	156.20(6)
C(14)-Sm(1)-C(2)	160.97(6)
C(5)-Sm(1)-C(2)	47.12(6)
C(13)-Sm(1)-C(2)	131.66(6)
C(4)-Sm(1)-C(2)	46.90(6)

C(1)-Sm(1)-C(2)	28.39(6)
C(10)-Sm(1)-C(2)	149.40(6)
C(32)-Sm(1)-C(2)	77.50(6)
C(12)-Sm(1)-C(2)	115.42(6)
C(14)-Sm(1)-C(3)	162.70(6)
C(5)-Sm(1)-C(3)	47.10(6)
C(13)-Sm(1)-C(3)	152.02(6)
C(4)-Sm(1)-C(3)	28.31(6)
C(1)-Sm(1)-C(3)	46.87(6)
C(10)-Sm(1)-C(3)	133.44(6)
C(32)-Sm(1)-C(3)	75.22(6)
C(12)-Sm(1)-C(3)	125.86(6)
C(2)-Sm(1)-C(3)	27.93(6)
C(14)-Sm(1)-C(11)	46.98(6)
C(5)-Sm(1)-C(11)	76.94(6)
C(13)-Sm(1)-C(11)	46.92(6)
C(4)-Sm(1)-C(11)	90.13(6)
C(1)-Sm(1)-C(11)	97.33(6)
C(10)-Sm(1)-C(11)	28.18(6)
C(32)-Sm(1)-C(11)	157.38(6)
C(12)-Sm(1)-C(11)	27.96(6)
C(2)-Sm(1)-C(11)	123.31(6)
C(3)-Sm(1)-C(11)	118.27(6)

C(14)-Sm(1)-C(31)	98.23(6)
C(5)-Sm(1)-C(31)	131.47(6)
C(13)-Sm(1)-C(31)	121.78(6)
C(4)-Sm(1)-C(31)	103.08(6)
C(1)-Sm(1)-C(31)	127.42(6)
C(10)-Sm(1)-C(31)	102.98(6)
C(32)-Sm(1)-C(31)	28.30(6)
C(12)-Sm(1)-C(31)	145.44(6)
C(2)-Sm(1)-C(31)	99.04(6)
C(3)-Sm(1)-C(31)	86.12(6)
C(11)-Sm(1)-C(31)	129.88(6)
Cnt3-Sm(2)-Cnt4	130.2
O(1)-Sm(2)-O(2)	97.82(5)
O(1)-Sm(2)-C(23)	90.21(6)
O(2)-Sm(2)-C(23)	130.17(6)
O(1)-Sm(2)-C(21)	104.72(6)
O(2)-Sm(2)-C(21)	82.77(6)
C(23)-Sm(2)-C(21)	47.84(7)
O(1)-Sm(2)-C(20)	130.02(6)
O(2)-Sm(2)-C(20)	93.69(6)
C(23)-Sm(2)-C(20)	47.83(7)
C(21)-Sm(2)-C(20)	29.35(6)
O(1)-Sm(2)-C(32)	118.68(6)

O(2)-Sm(2)-C(32)	120.72(6)
C(23)-Sm(2)-C(32)	96.75(6)
C(21)-Sm(2)-C(32)	124.33(6)
C(20)-Sm(2)-C(32)	95.45(6)
O(1)-Sm(2)-C(22)	81.87(6)
O(2)-Sm(2)-C(22)	103.54(6)
C(23)-Sm(2)-C(22)	29.13(6)
C(21)-Sm(2)-C(22)	29.07(6)
C(20)-Sm(2)-C(22)	48.17(6)
C(32)-Sm(2)-C(22)	125.18(6)
O(1)-Sm(2)-C(19)	119.17(6)
O(2)-Sm(2)-C(19)	122.58(6)
C(23)-Sm(2)-C(19)	29.18(7)
C(21)-Sm(2)-C(19)	48.04(6)
C(20)-Sm(2)-C(19)	28.90(7)
C(32)-Sm(2)-C(19)	79.69(6)
C(22)-Sm(2)-C(19)	48.20(6)
O(1)-Sm(2)-C(28)	126.61(6)
O(2)-Sm(2)-C(28)	91.86(6)
C(23)-Sm(2)-C(28)	121.72(6)
C(21)-Sm(2)-C(28)	128.61(6)
C(20)-Sm(2)-C(28)	101.24(6)
C(32)-Sm(2)-C(28)	28.99(6)

C(22)-Sm(2)-C(28)	145.78(6)
C(19)-Sm(2)-C(28)	97.78(6)
O(1)-Sm(2)-C(31)	89.68(5)
O(2)-Sm(2)-C(31)	130.33(6)
C(23)-Sm(2)-C(31)	98.61(6)
C(21)-Sm(2)-C(31)	142.29(6)
C(20)-Sm(2)-C(31)	118.17(6)
C(32)-Sm(2)-C(31)	29.01(6)
C(22)-Sm(2)-C(31)	126.13(6)
C(19)-Sm(2)-C(31)	94.44(6)
C(28)-Sm(2)-C(31)	47.66(6)
O(1)-Sm(2)-C(29)	100.76(5)
O(2)-Sm(2)-C(29)	83.17(6)
C(23)-Sm(2)-C(29)	143.38(6)
C(21)-Sm(2)-C(29)	152.30(6)
C(20)-Sm(2)-C(29)	128.91(6)
C(32)-Sm(2)-C(29)	47.39(6)
C(22)-Sm(2)-C(29)	172.48(6)
C(19)-Sm(2)-C(29)	125.25(6)
C(28)-Sm(2)-C(29)	28.67(6)
C(31)-Sm(2)-C(29)	47.28(6)
O(1)-Sm(2)-C(30)	79.69(5)
O(2)-Sm(2)-C(30)	104.97(6)

C(23)-Sm(2)-C(30)	124.83(6)
C(21)-Sm(2)-C(30)	170.67(6)
C(20)-Sm(2)-C(30)	142.70(6)
C(32)-Sm(2)-C(30)	47.25(6)
C(22)-Sm(2)-C(30)	147.77(6)
C(19)-Sm(2)-C(30)	122.64(6)
C(28)-Sm(2)-C(30)	47.22(6)
C(31)-Sm(2)-C(30)	28.49(6)
C(29)-Sm(2)-C(30)	28.57(6)
C(37)-O(1)-C(40)	109.09(16)
C(37)-O(1)-Sm(2)	126.29(13)
C(40)-O(1)-Sm(2)	124.14(13)
C(44)-O(2)-C(41)	107.98(18)
C(44)-O(2)-Sm(2)	127.91(14)
C(41)-O(2)-Sm(2)	123.53(14)
C(5)-C(1)-C(2)	107.6(2)
C(5)-C(1)-C(6)	127.8(2)
C(2)-C(1)-C(6)	124.6(2)
C(5)-C(1)-Sm(1)	72.71(12)
C(2)-C(1)-Sm(1)	80.22(12)
C(6)-C(1)-Sm(1)	115.30(14)
C(1)-C(2)-C(3)	108.0(2)
C(1)-C(2)-C(7)	124.7(2)

C(3)-C(2)-C(7)	126.8(2)
C(1)-C(2)-Sm(1)	71.39(12)
C(3)-C(2)-Sm(1)	76.06(12)
C(7)-C(2)-Sm(1)	124.29(14)
C(4)-C(3)-C(2)	108.17(19)
C(4)-C(3)-C(8)	125.4(2)
C(2)-C(3)-C(8)	125.9(2)
C(4)-C(3)-Sm(1)	71.03(12)
C(2)-C(3)-Sm(1)	76.01(12)
C(8)-C(3)-Sm(1)	125.54(14)
C(3)-C(4)-C(5)	107.6(2)
C(3)-C(4)-C(9)	125.7(2)
C(5)-C(4)-C(9)	126.7(2)
C(3)-C(4)-Sm(1)	80.66(12)
C(5)-C(4)-Sm(1)	73.00(12)
C(9)-C(4)-Sm(1)	115.57(15)
C(1)-C(5)-C(4)	108.6(2)
C(1)-C(5)-Sm(1)	78.02(12)
C(4)-C(5)-Sm(1)	77.59(12)
C(11)-C(10)-C(14)	107.44(18)
C(11)-C(10)-C(15)	125.3(2)
C(14)-C(10)-C(15)	127.2(2)
C(11)-C(10)-Sm(1)	80.21(12)

C(14)-C(10)-Sm(1)	72.12(11)
C(15)-C(10)-Sm(1)	116.42(15)
C(10)-C(11)-C(12)	108.38(19)
C(10)-C(11)-C(16)	125.3(2)
C(12)-C(11)-C(16)	126.0(2)
C(10)-C(11)-Sm(1)	71.60(12)
C(12)-C(11)-Sm(1)	75.21(12)
C(16)-C(11)-Sm(1)	124.37(15)
C(13)-C(12)-C(11)	107.82(18)
C(13)-C(12)-C(17)	125.7(2)
C(11)-C(12)-C(17)	126.2(2)
C(13)-C(12)-Sm(1)	70.69(11)
C(11)-C(12)-Sm(1)	76.83(12)
C(17)-C(12)-Sm(1)	123.33(14)
C(14)-C(13)-C(12)	107.65(18)
C(14)-C(13)-C(18)	126.53(19)
C(12)-C(13)-C(18)	125.81(19)
C(14)-C(13)-Sm(1)	73.57(12)
C(12)-C(13)-Sm(1)	80.78(12)
C(18)-C(13)-Sm(1)	111.04(13)
C(13)-C(14)-C(10)	108.69(18)
C(13)-C(14)-Sm(1)	76.95(12)
C(10)-C(14)-Sm(1)	78.62(12)

C(20)-C(19)-C(23)	107.55(19)
C(20)-C(19)-C(24)	125.9(2)
C(23)-C(19)-C(24)	126.1(2)
C(20)-C(19)-Sm(2)	75.22(12)
C(23)-C(19)-Sm(2)	74.81(12)
C(24)-C(19)-Sm(2)	121.87(14)
C(19)-C(20)-C(21)	108.16(19)
C(19)-C(20)-C(25)	125.2(2)
C(21)-C(20)-C(25)	126.5(2)
C(19)-C(20)-Sm(2)	75.88(12)
C(21)-C(20)-Sm(2)	75.28(12)
C(25)-C(20)-Sm(2)	118.27(15)
C(22)-C(21)-C(20)	108.13(19)
C(22)-C(21)-C(26)	124.6(2)
C(20)-C(21)-C(26)	127.1(2)
C(22)-C(21)-Sm(2)	75.71(12)
C(20)-C(21)-Sm(2)	75.37(12)
C(26)-C(21)-Sm(2)	118.68(14)
C(21)-C(22)-C(23)	107.34(19)
C(21)-C(22)-C(27)	125.7(2)
C(23)-C(22)-C(27)	126.8(2)
C(21)-C(22)-Sm(2)	75.22(12)
C(23)-C(22)-Sm(2)	74.96(12)

C(27)-C(22)-Sm(2)	118.68(15)
C(22)-C(23)-C(19)	108.8(2)
C(22)-C(23)-Sm(2)	75.91(13)
C(19)-C(23)-Sm(2)	76.01(12)
C(32)-C(28)-C(29)	107.80(18)
C(32)-C(28)-C(33)	126.25(19)
C(29)-C(28)-C(33)	125.93(19)
C(32)-C(28)-Sm(2)	74.40(11)
C(29)-C(28)-Sm(2)	77.13(11)
C(33)-C(28)-Sm(2)	113.57(14)
C(32)-C(28)-Sm(1)	71.21(11)
C(29)-C(28)-Sm(1)	84.59(12)
C(33)-C(28)-Sm(1)	111.80(13)
Sm(2)-C(28)-Sm(1)	133.52(7)
C(28)-C(29)-C(30)	107.97(18)
C(28)-C(29)-C(34)	125.88(19)
C(30)-C(29)-C(34)	126.04(19)
C(28)-C(29)-Sm(2)	74.20(11)
C(30)-C(29)-Sm(2)	76.35(11)
C(34)-C(29)-Sm(2)	112.61(13)
C(31)-C(30)-C(29)	108.32(18)
C(31)-C(30)-C(35)	126.16(19)
C(29)-C(30)-C(35)	125.48(19)

C(31)-C(30)-Sm(2)	74.80(12)
C(29)-C(30)-Sm(2)	75.09(12)
C(35)-C(30)-Sm(2)	114.63(13)
C(30)-C(31)-C(32)	107.20(18)
C(30)-C(31)-C(36)	126.61(19)
C(32)-C(31)-C(36)	126.19(19)
C(30)-C(31)-Sm(2)	76.70(12)
C(32)-C(31)-Sm(2)	73.26(11)
C(36)-C(31)-Sm(2)	115.60(14)
C(30)-C(31)-Sm(1)	84.54(12)
C(32)-C(31)-Sm(1)	71.42(11)
C(36)-C(31)-Sm(1)	110.64(13)
Sm(2)-C(31)-Sm(1)	132.54(7)
C(28)-C(32)-C(31)	108.70(18)
C(28)-C(32)-Sm(2)	76.61(11)
C(31)-C(32)-Sm(2)	77.73(11)
C(28)-C(32)-Sm(1)	80.73(12)
C(31)-C(32)-Sm(1)	80.28(12)
Sm(2)-C(32)-Sm(1)	141.17(8)
O(1)-C(37)-C(38)	105.27(19)
C(37)-C(38)-C(39)	101.7(2)
C(40)-C(39)-C(38)	102.66(19)
O(1)-C(40)-C(39)	106.13(19)

O(2)-C(41)-C(42)	106.7(2)
C(43)-C(42)-C(41)	103.3(2)
C(44)-C(43)-C(42)	101.8(2)
O(2)-C(44)-C(43)	105.6(2)

References

1. *APEX2* Version 2014.11-0, Bruker AXS, Inc.: Madison, WI, USA, 2014.

2. *SAINT* Version 8.34a, Bruker AXS, Inc.: Madison, WI, USA, 2013.

3. Sheldrick, G. M. *SADABS*, Version 2014/5, Bruker AXS, Inc.: Madison, WI, USA, 2014.

4. Sheldrick, G. M. *SHELXTL*, Version 2014/7, Bruker AXS, Inc.: Madison, WI, USA, 2014.

5. *International Tables for Crystallography 1992*, *Volume C.:* Kluwer Academic Publishers: Dordrecht, The Netherlands, 2004.