

Supporting Information.

**Reductive Disproportionation of CO₂ with Bulky
Divalent Samarium Complexes**

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1. NMR data

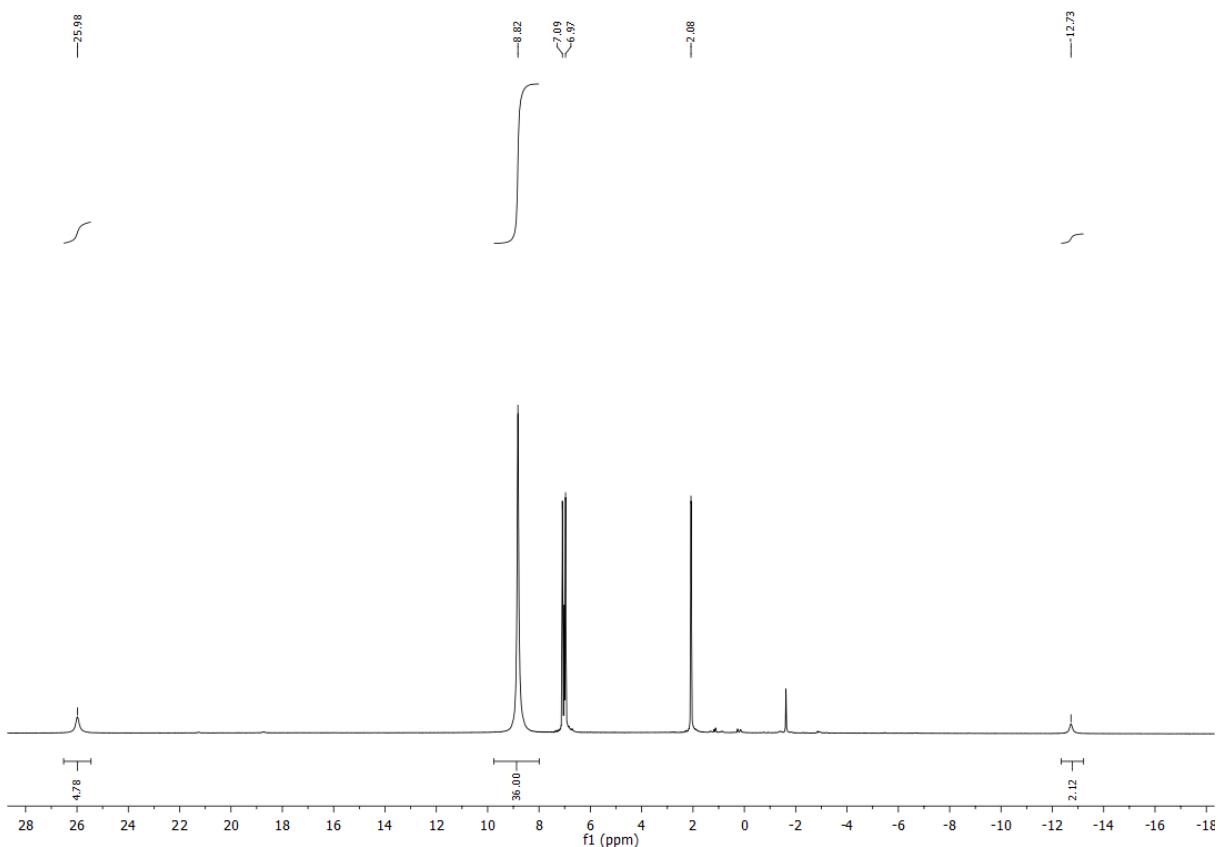


Figure S1: ¹H NMR for **1** in toluene-d₈ measured at 20°C.

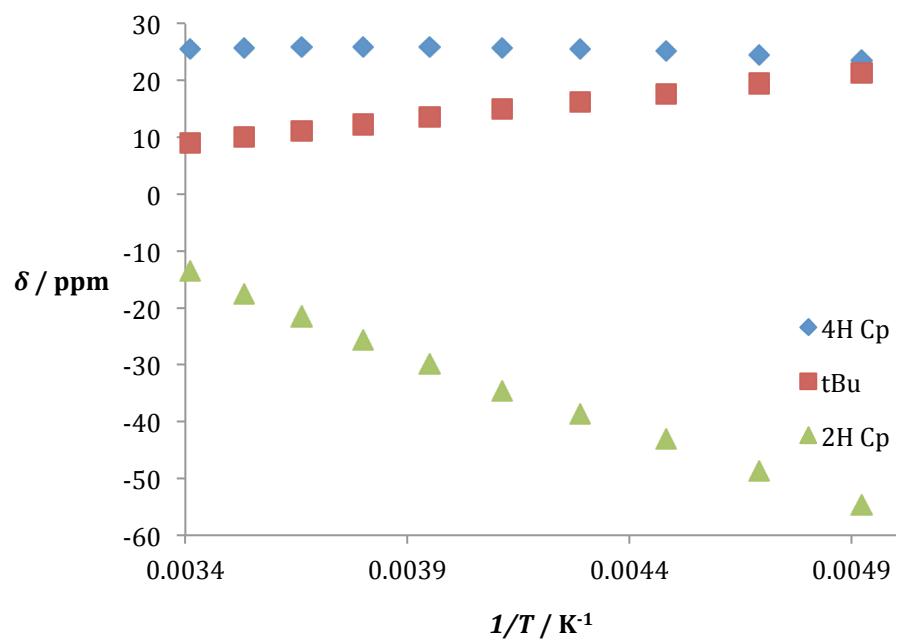


Figure S2: Variable temperature ¹H NMR data for **1** in toluene-d₈.

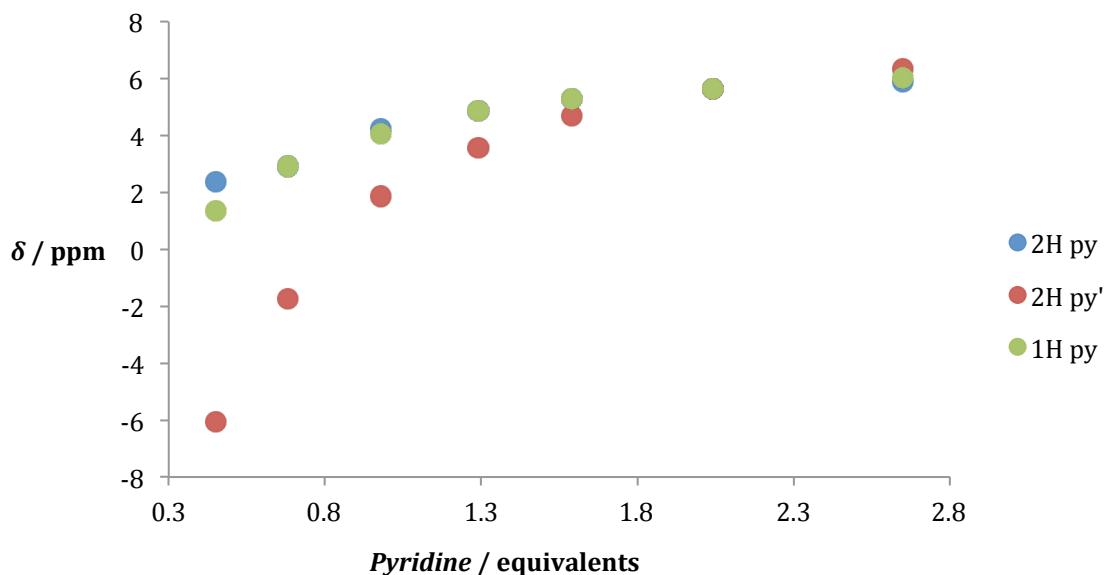


Figure S3: Titration of **1** with pyridine and evolution of the pyridine proton chemical shifts in ^1H NMR at room temperature in toluene-d₈.

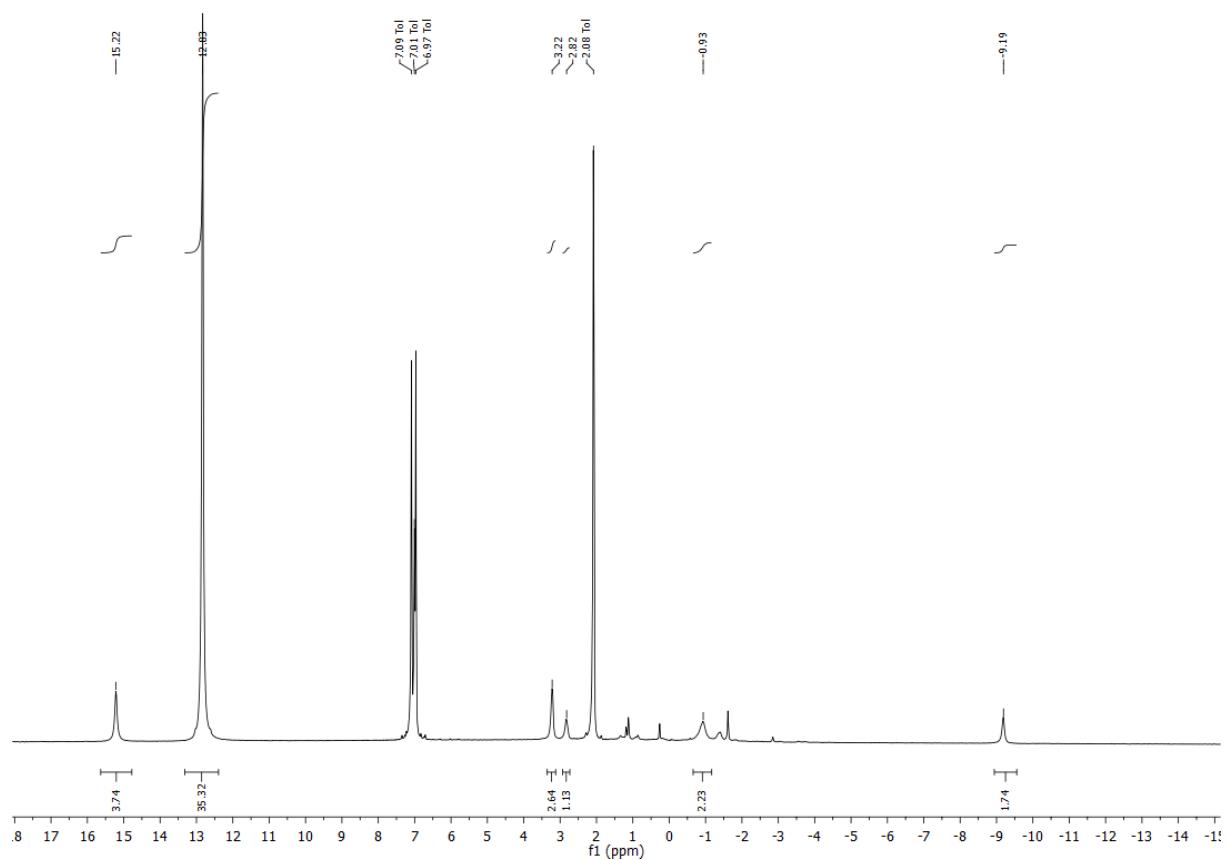


Figure S4: ^1H NMR of **4** in toluene-d₈ at 20°C.

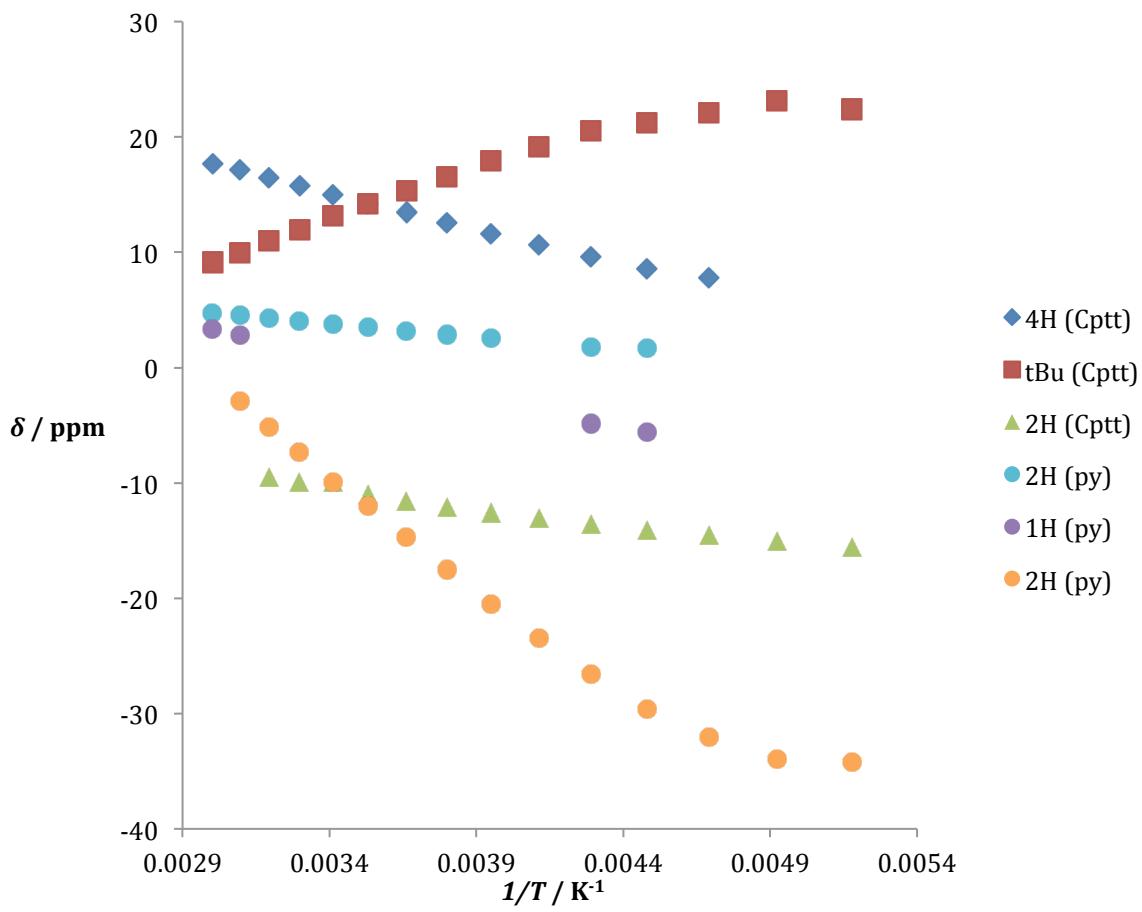


Figure S5: Variable temperature ^1H NMR data for **4** in toluene- d_8 .

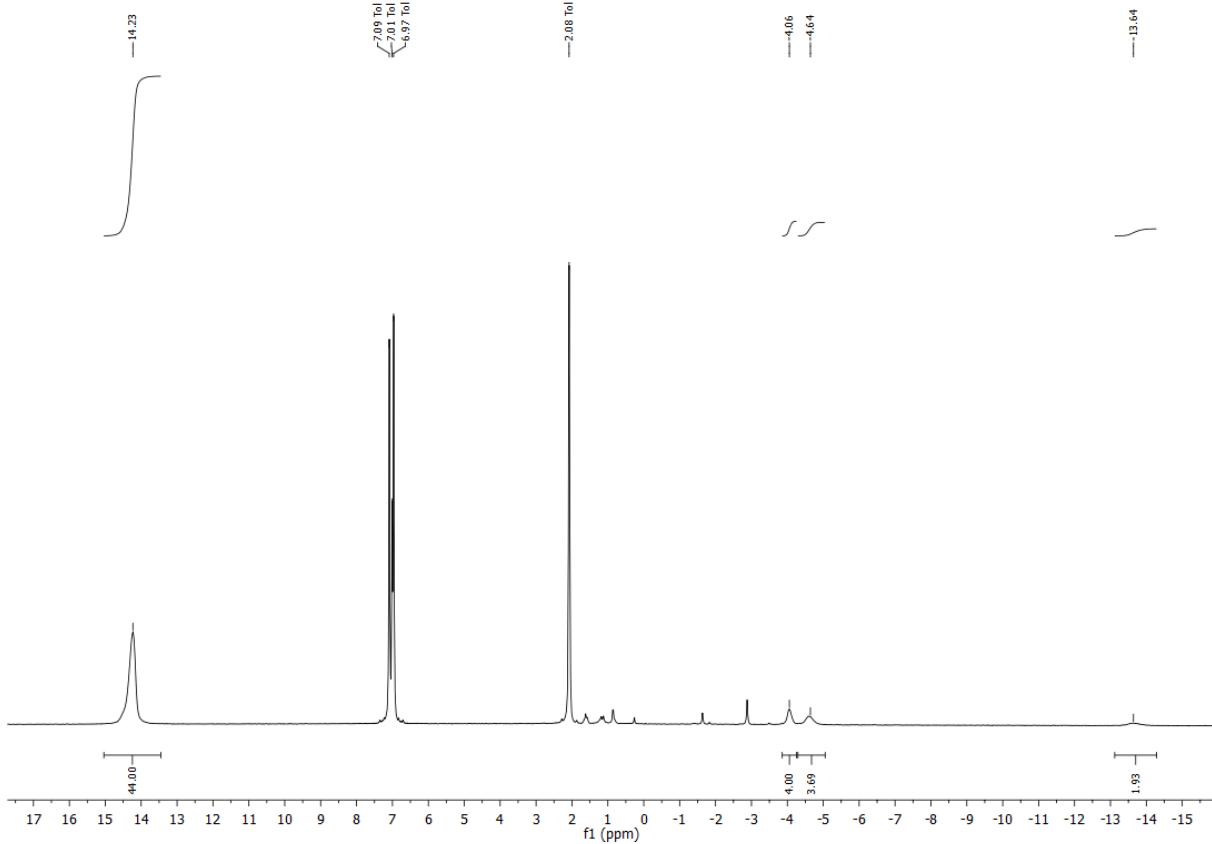


Figure S6: ^1H NMR of **5** in toluene- d_8 at 20°C.

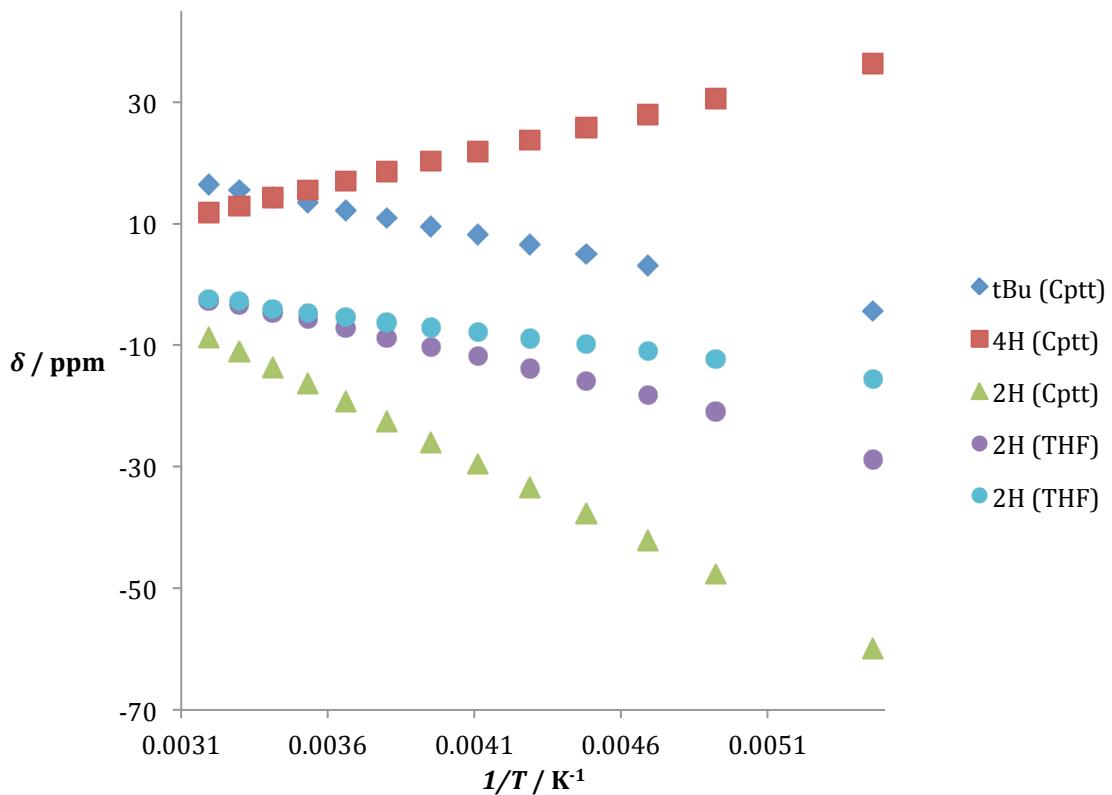


Figure S7: Variable temperature ^1H NMR data for **5** at room temperature in toluene- d_8 .

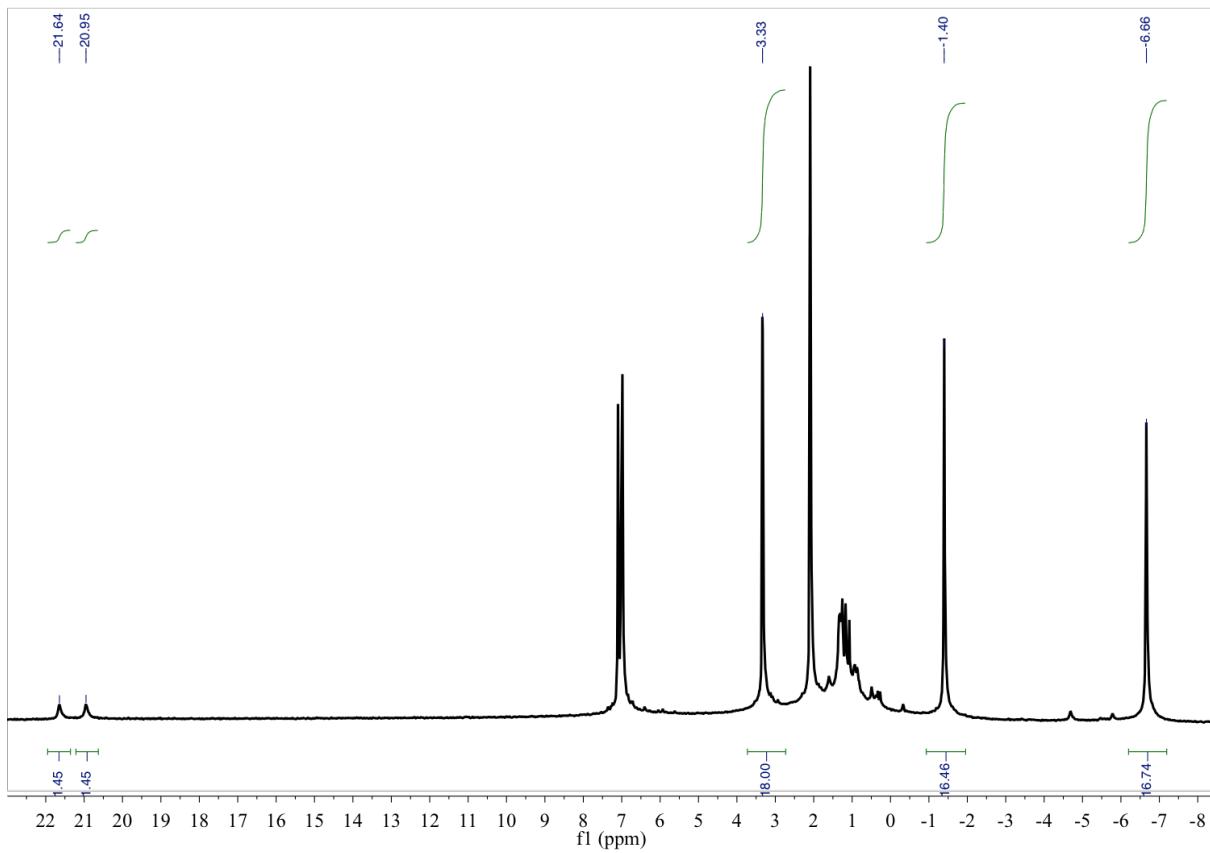


Figure S8: ¹H NMR of **6** in toluene-d₈ at 20°C.

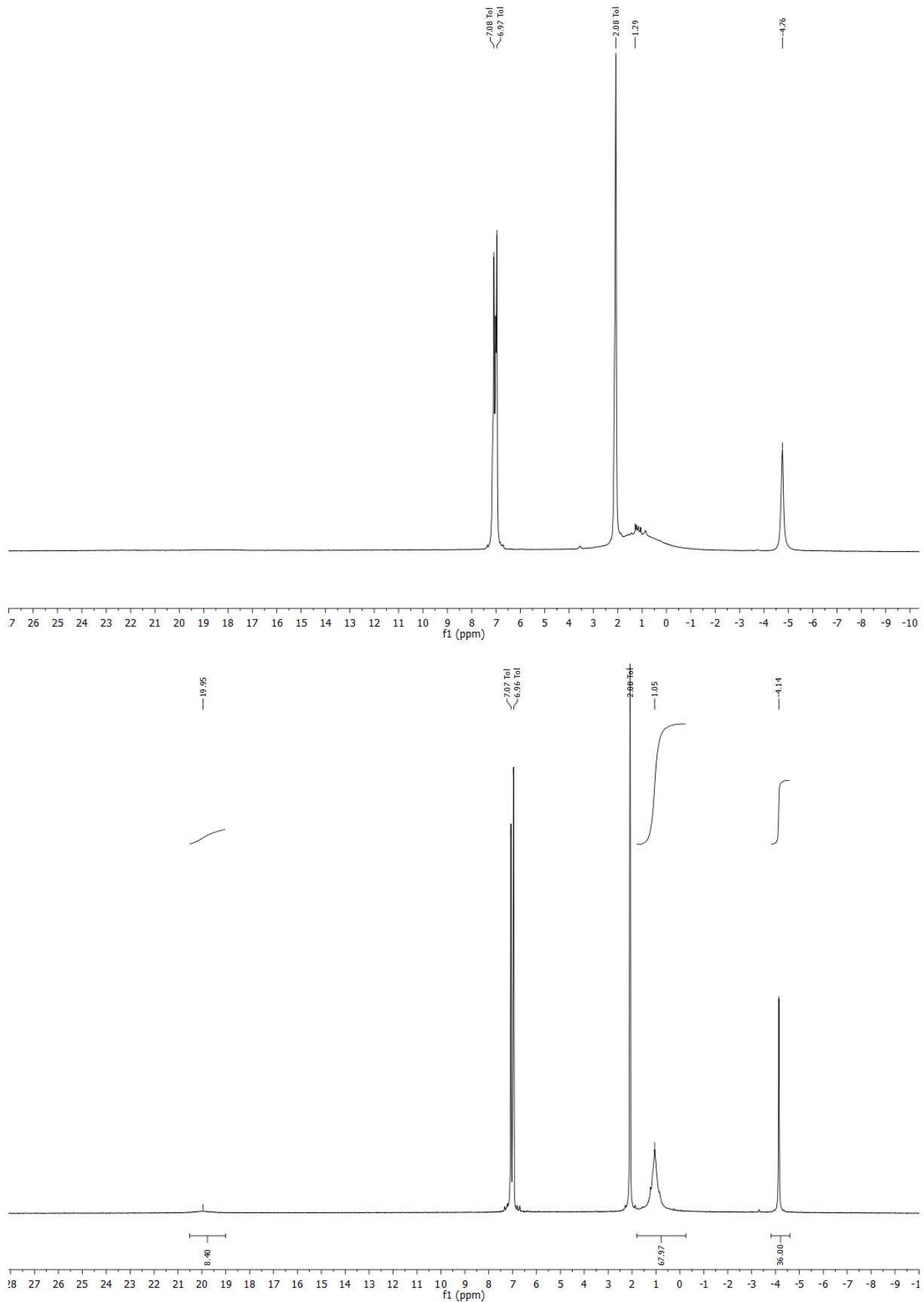


Figure S9: ¹H RMN Spectra of **7** at 20°C (top) and 60°C (bottom) in toluene-d₈.

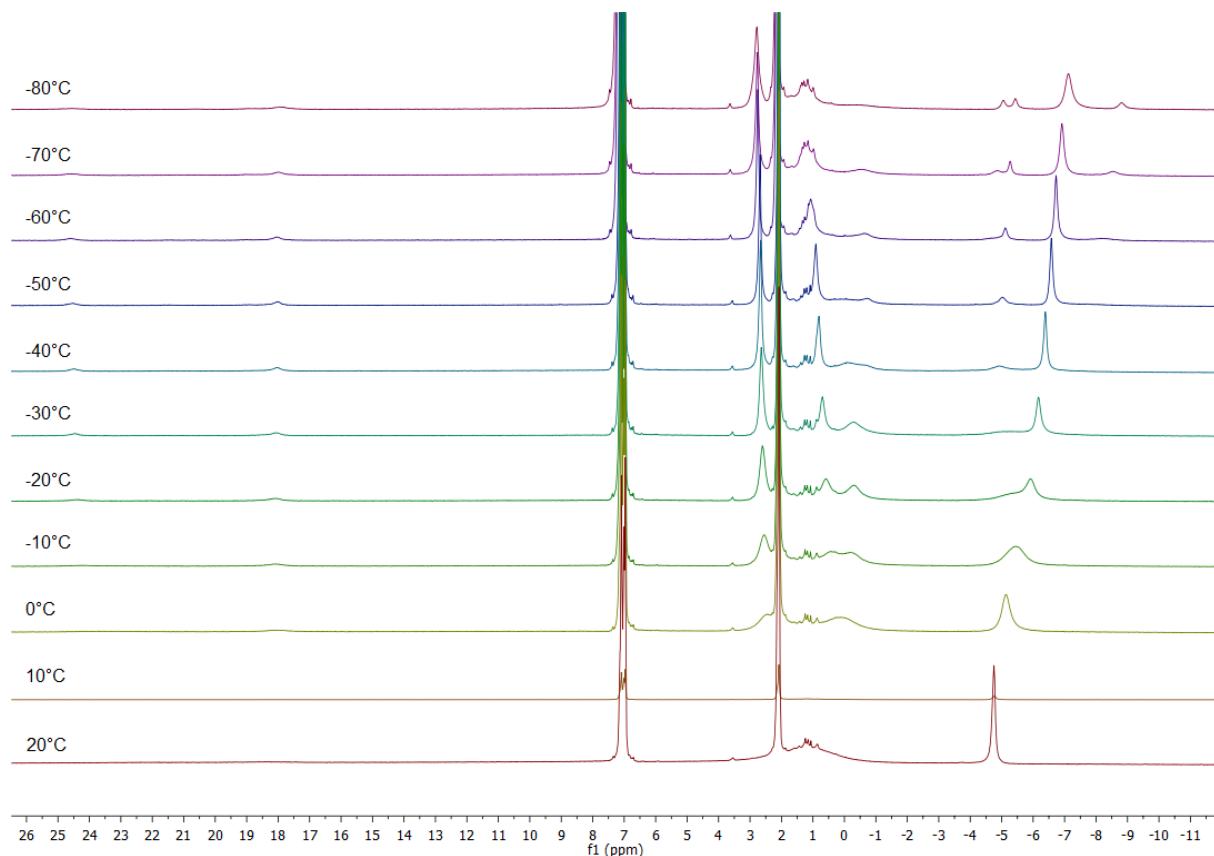


Figure S10: Variable temperature ^1H NMR of **7** in toluene- d_8 .

Table S1. Variable temperature NMR data for **7**.

Group	T_c (en K)	$\Delta\nu$ (en Hz)	ΔG^\ddagger (en kcal/mol)
H (Cp^{ttt})	288	1899	12.1
H (tBu)	280	768	12.2

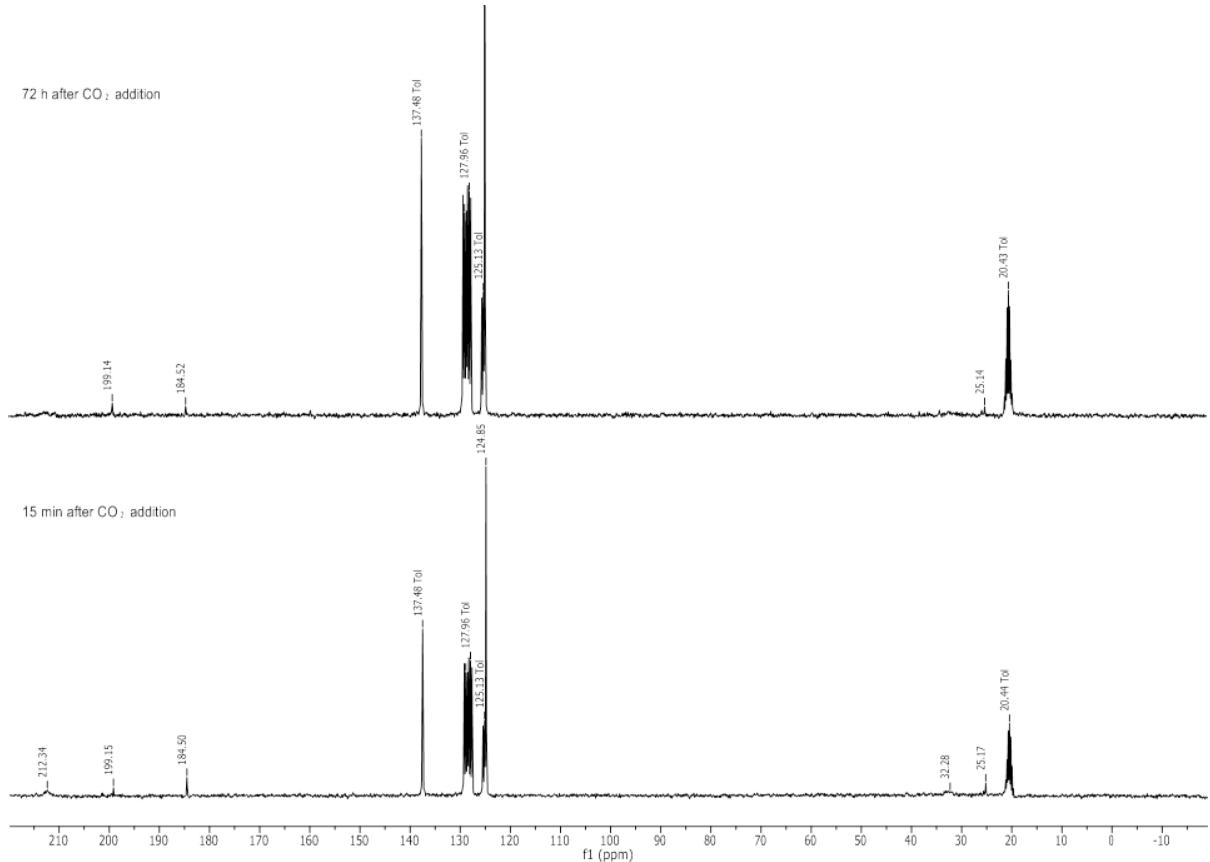


Figure S11: ^{13}C NMR monitoring of the addition of $^{13}\text{CO}_2$ on $\text{Cp}^{\text{ttt}}_2\text{Sm}$ (**2**) in toluene- d_8 .

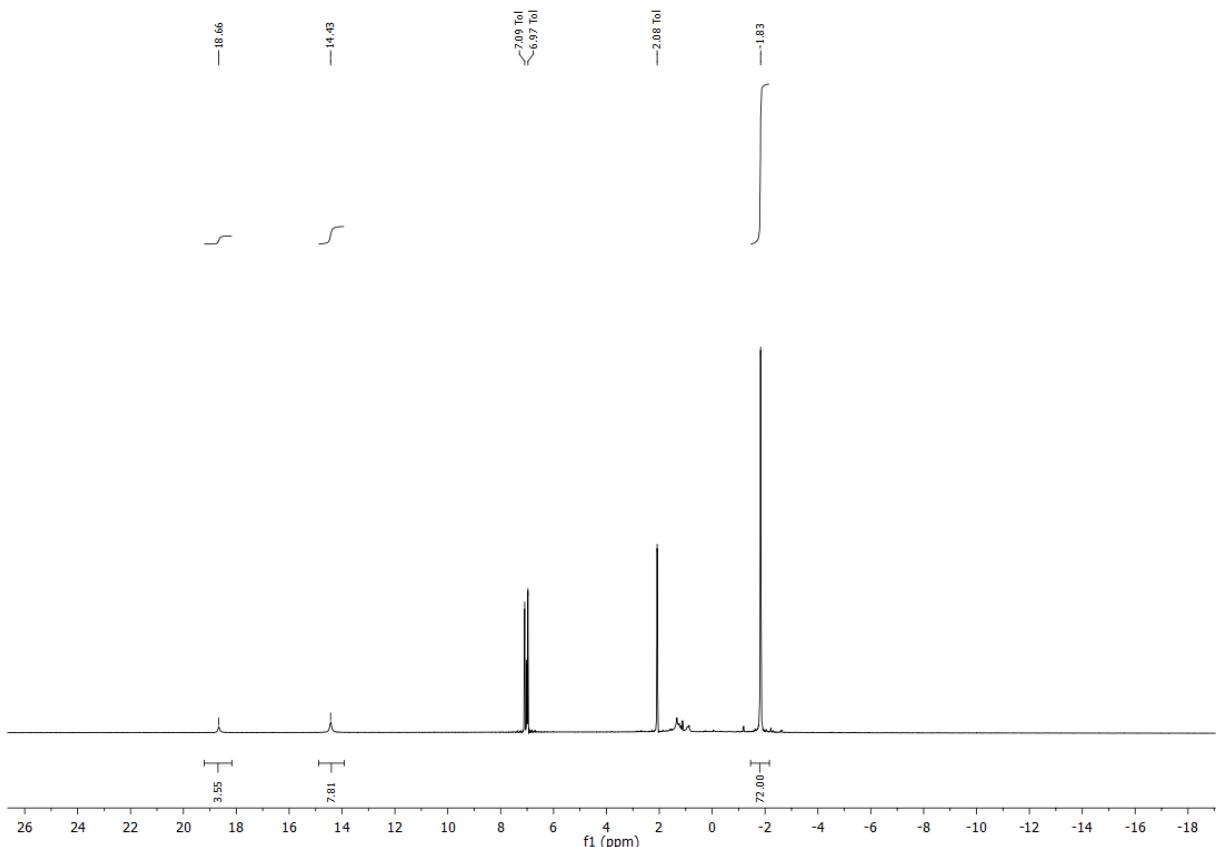


Figure S12: ^1H NMR of **8** in toluene- d_8 measured at 20°C.

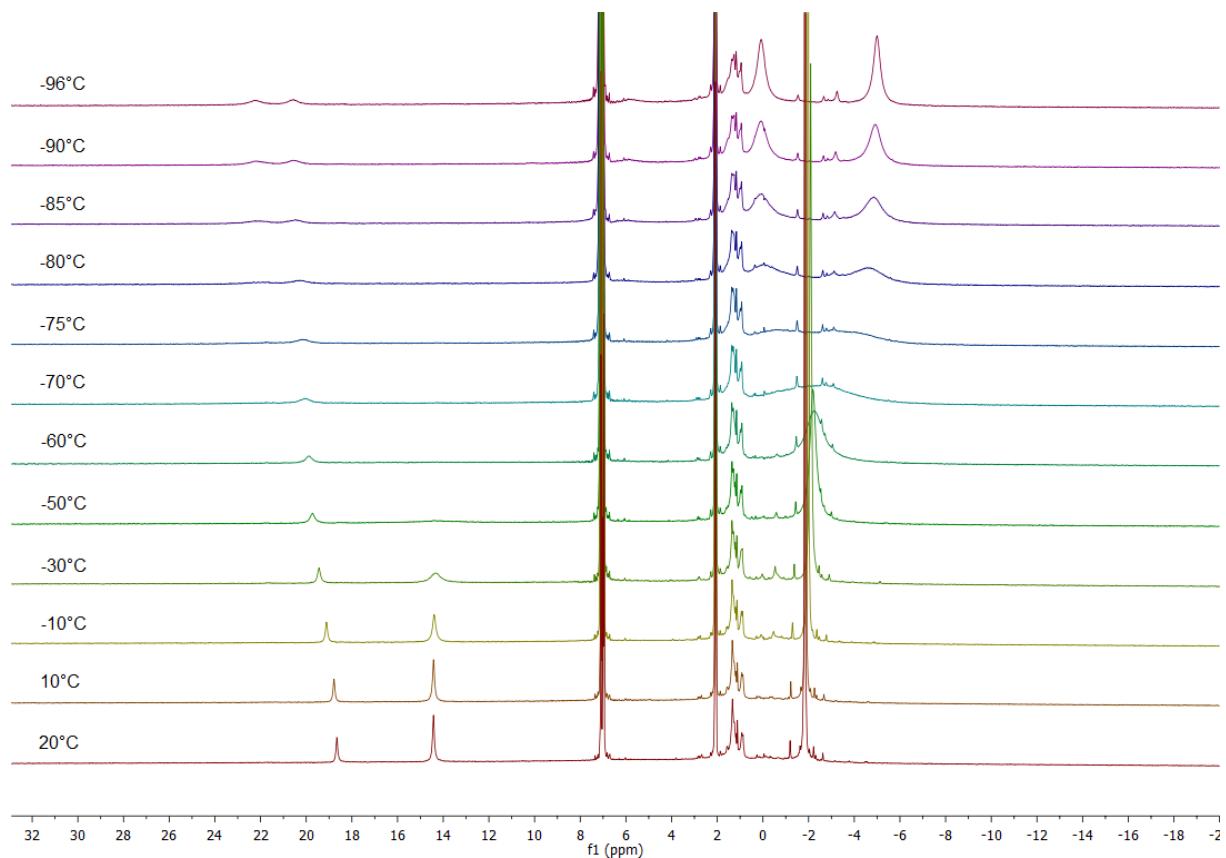


Figure S13: Variable temperature ^1H NMR of **8** in toluene- d_8 .

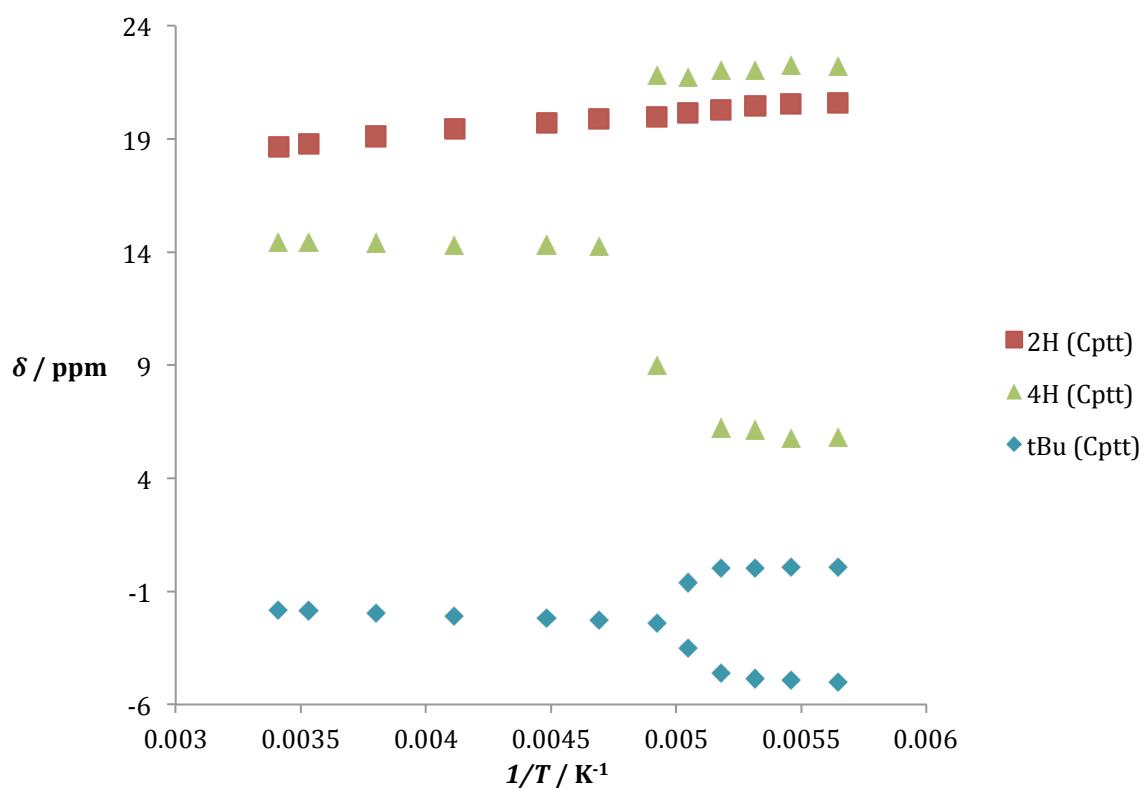


Figure S14: Variable temperature ^1H NMR data of **8** in toluene- d_8 .

Table S2. Variable temperature NMR data for **8**.

Group	T _c (en K)	Δv (en Hz)	ΔG [‡] (en kcal/mol)
H (Cp ^{tt})	213	4929	8.39
H (tBu)	203	1521	8.44

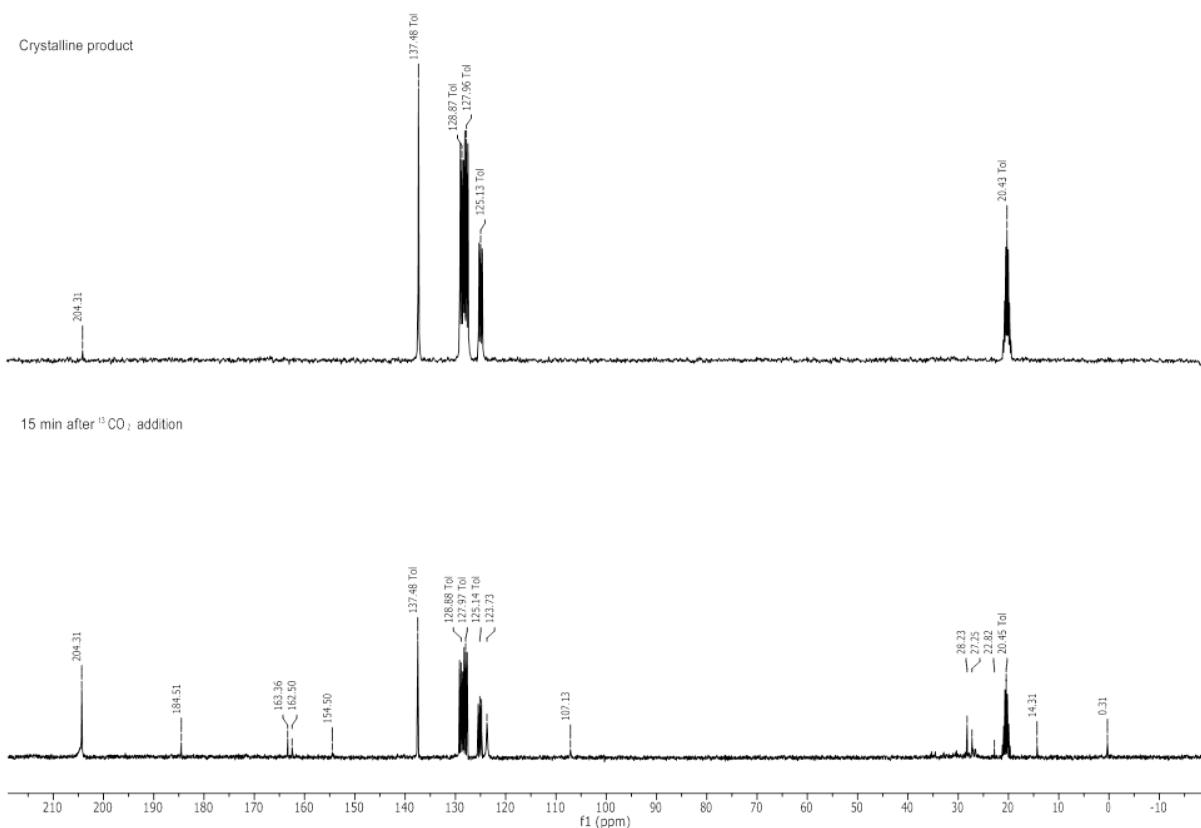


Figure S15: ^{13}C NMR monitoring of the addition of $^{13}\text{CO}_2$ on $\text{Cp}^{\text{tt}}_2\text{Sm}$ (**1**) in toluene-d₈ and ^{13}C NMR of **8**.

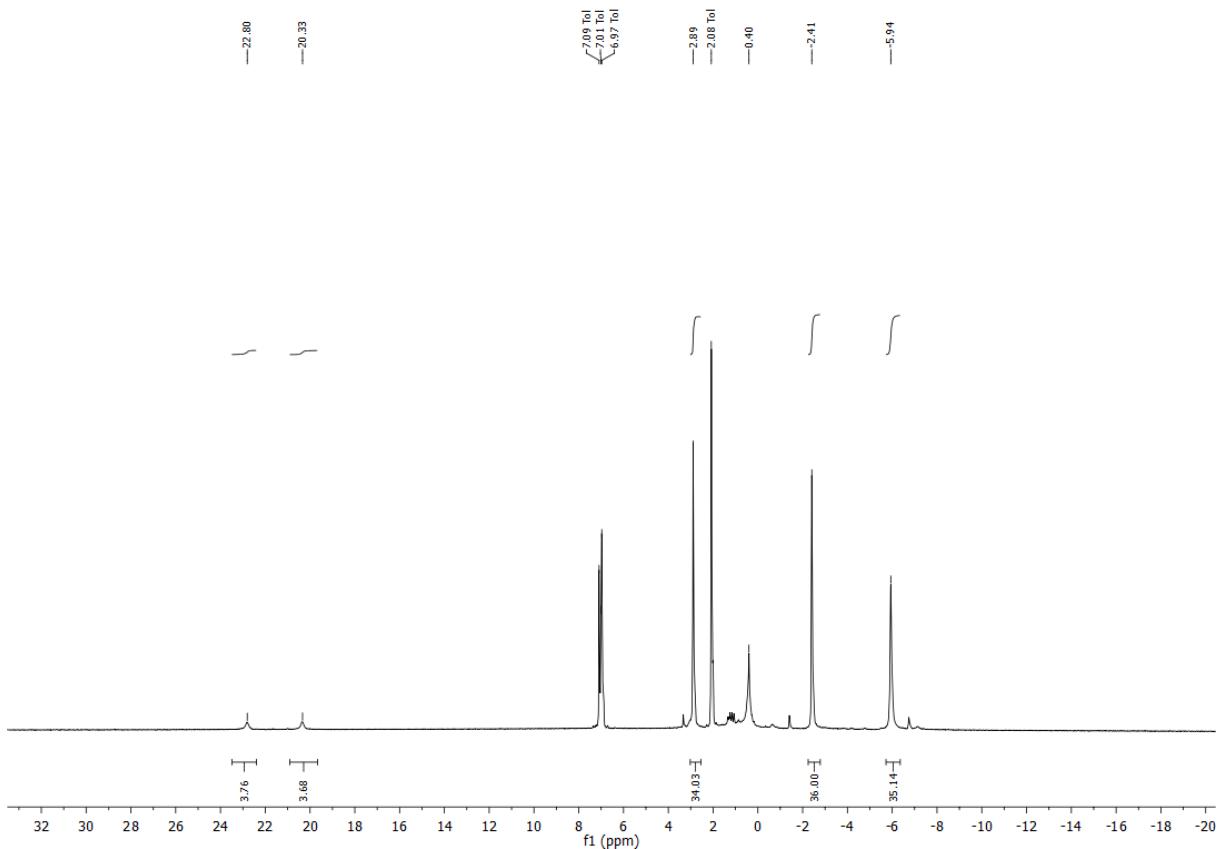


Figure S16: ¹H NMR of **9** in toluene-d₈ measured at 20°C.

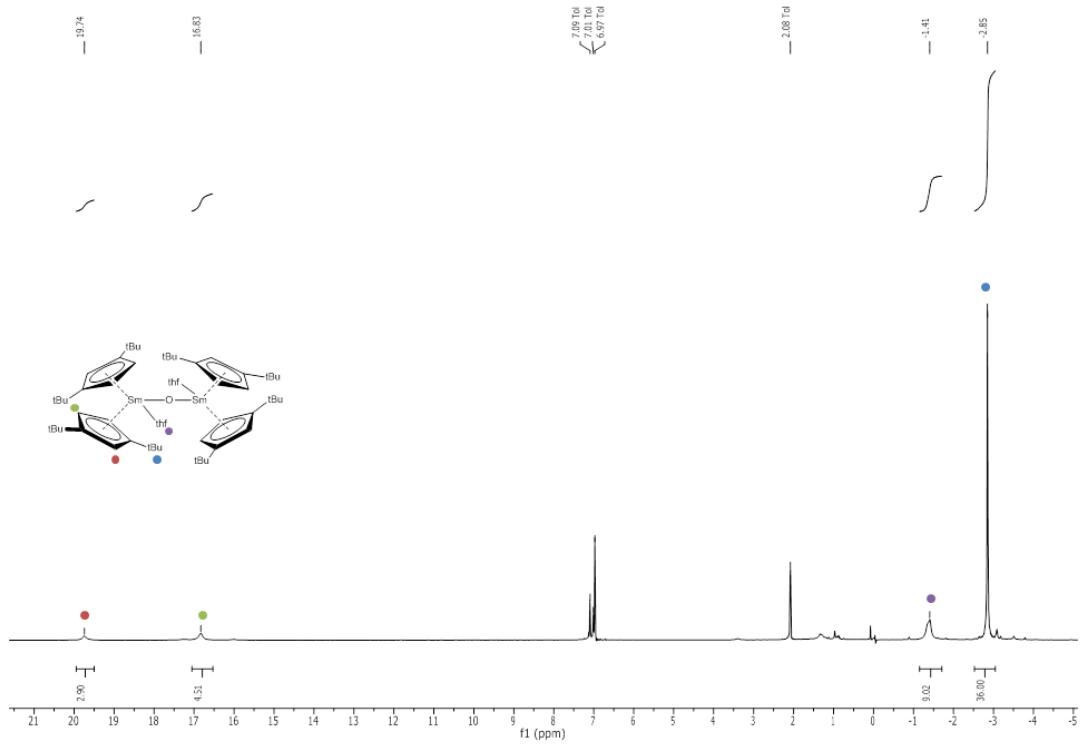
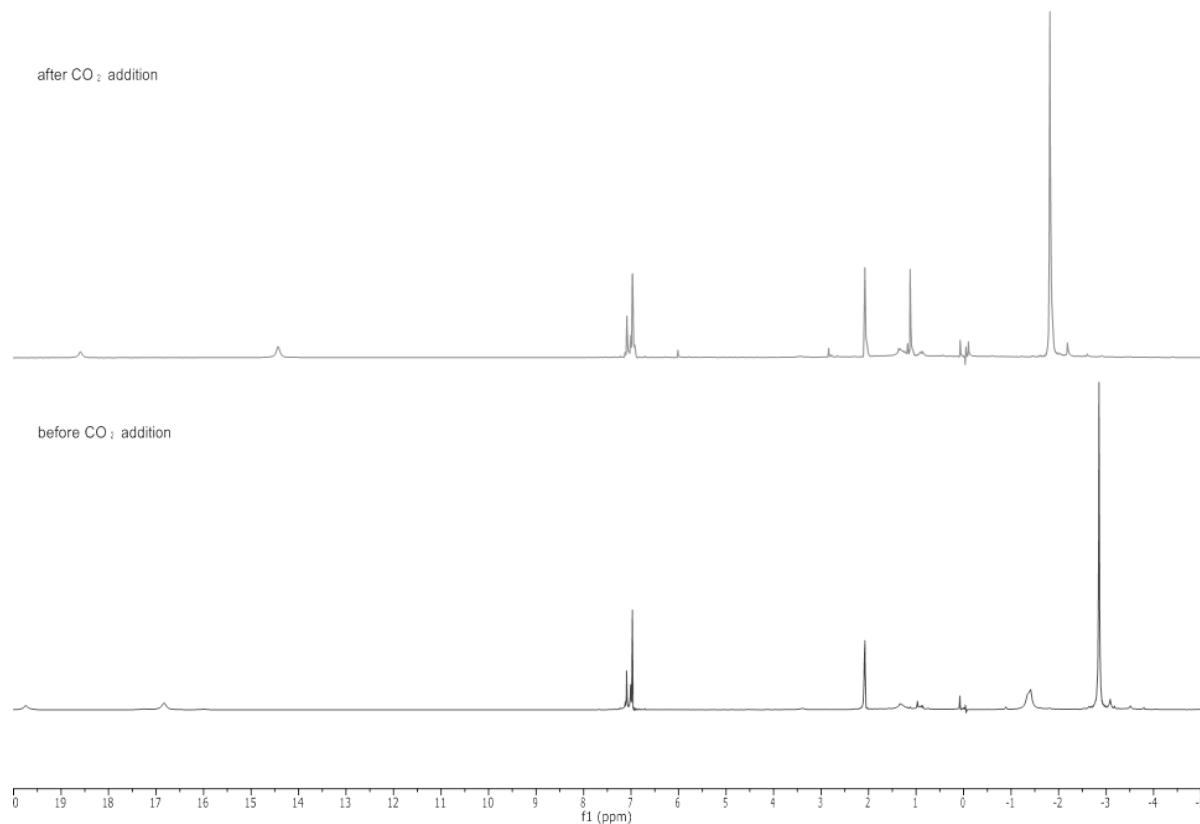
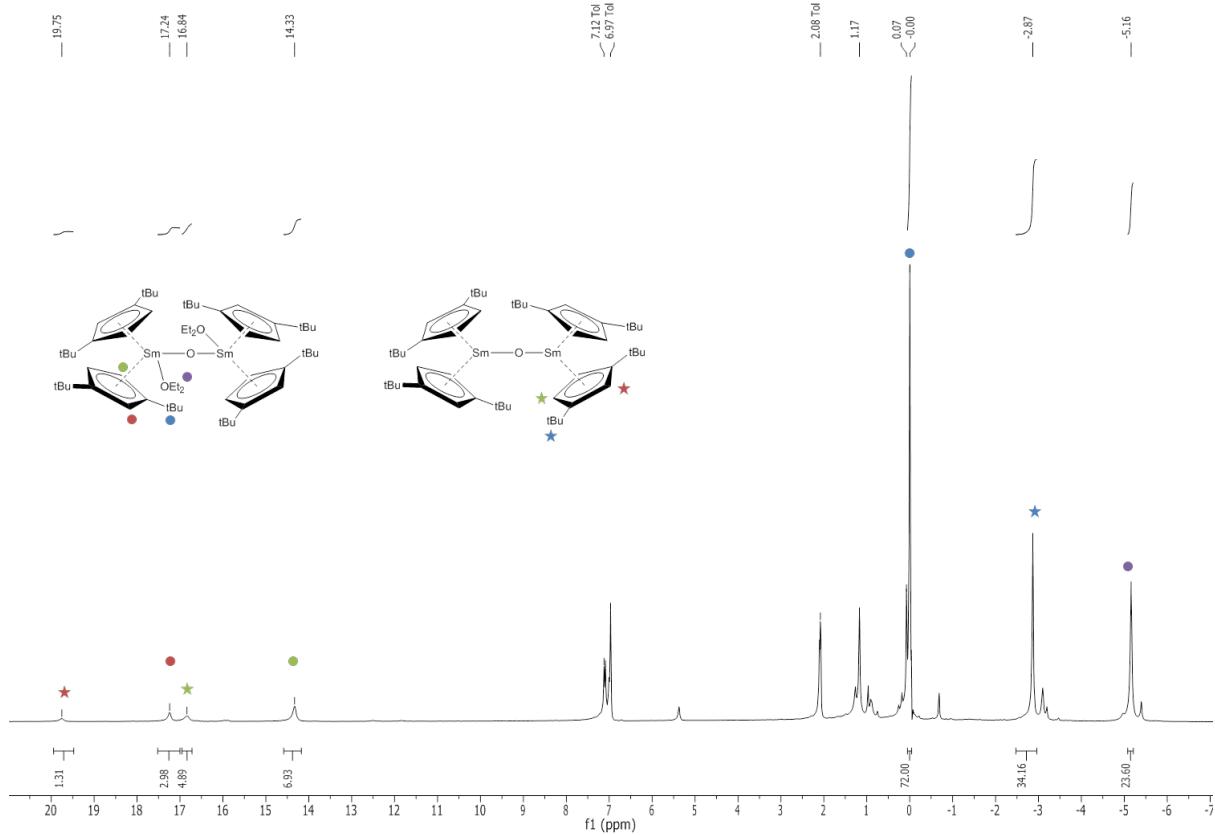


Figure S17: ¹H NMR of **10** in toluene-d₈ measured at 20°C.



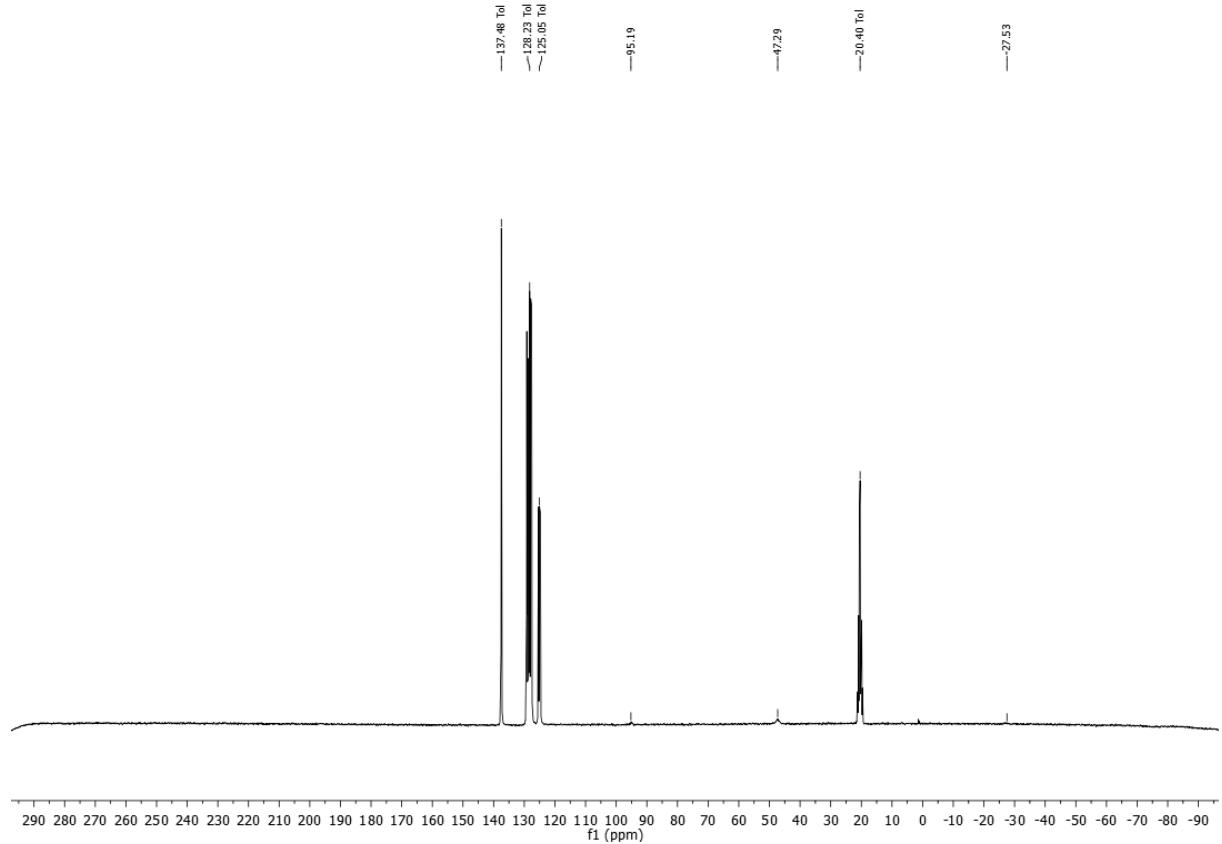


Figure S20: ^{13}H NMR of **1** in toluene- d_8 .

2. IR Data.

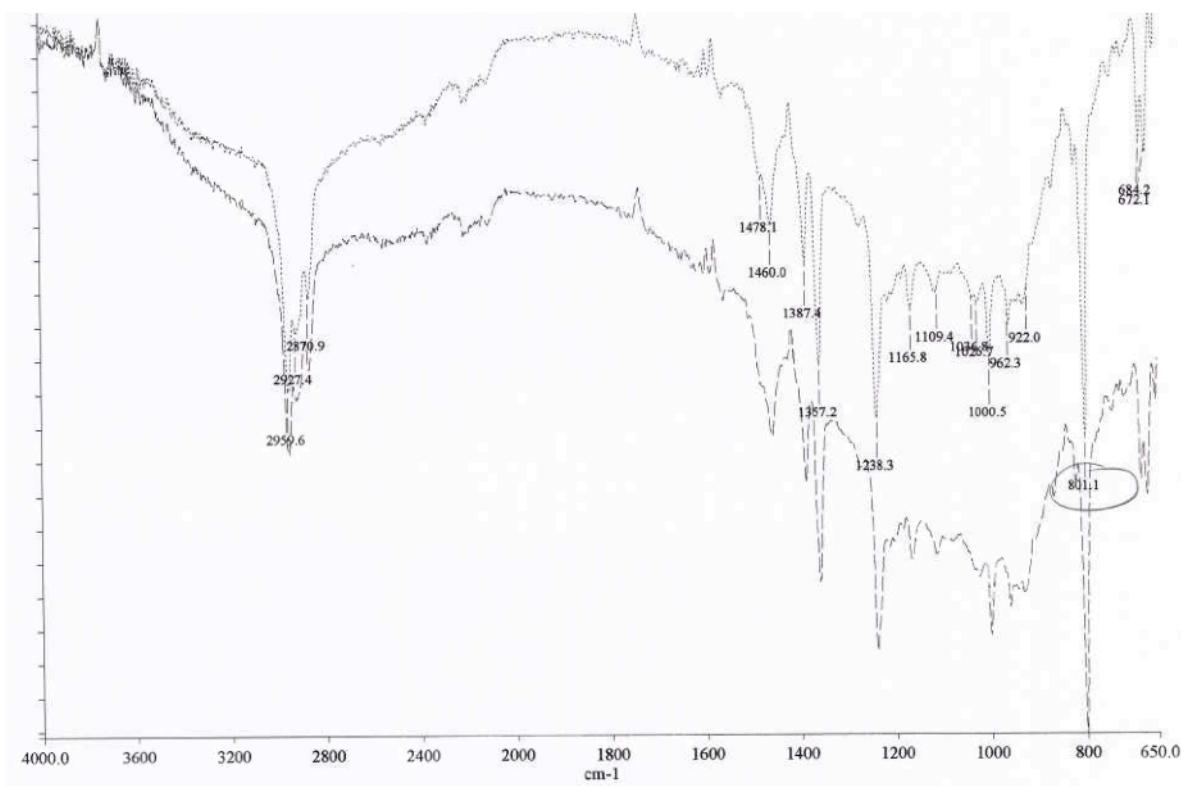


Figure S21: IR spectrum of **6**.

1. X-ray Crystal Structures

Table S3: Selected Crystal Data Collection Parameters for **1**, **3**, **4** and **5**.

	1	3	4.C₇H₈	5
Formula	C ₂₆ H ₄₂ Sm	C ₃₄ H ₅₈ O ₂ Sm	C ₃₁ H ₄₇ NSm,C ₇ H ₈	C ₃₀ H ₅₀ OSm
Crystal size (mm)	0.1 × 0.03 × 0.01	0.150x0.150x0.1 00	0.450x0.120x0.0 40	0.150x0.100x0. 050
Crystal system	Monoclinic	Monoclinic	orthorhombic	Monoclinic
Space group	P 2 ₁ /c	C 2/c	P b c a	P 2 ₁ /c
Volume (Å ³)	2448.24(12)	6716.4(4)	6917.1(2)	5917.0(4)
a (Å)	10.8660 (3)	33.6190 (11)	20.5662 (3)	19.1875 (7)
b (Å)	21.5466 (6)	10.4857 (3)	11.8693 (2)	17.4547 (5)
c (Å)	11.0534 (3)	19.8488 (7)	28.3364 (5)	18.3606 (7)
α (deg)	90	90	90	90
β (deg)	108.908(2)	106.283 (1)	90	105.794 (1)
γ (deg)	90	90	90	90
Z	4	8	8	8
Formula weight – g/mol)	504.94	649.15	676.18	577.05
Density (calcd) (g/cm ³)	1.37	1.284	1.299	1.296
Absorption coefficient (mm ⁻¹)	2.41	1.774	1.722	2.002
F(000)	1040	2720	2816	2400
Temp (K)	150	150	150	150
diffractometer ^a	Kappa APEX II CCD	Kappa APEX II CCD	Kappa APEX II CCD	Kappa APEX II CCD
θ range for data collection (deg)	2.0 – 25	0.998 – 27.485	0.998 – 30.034	0.998 – 30.034
Transmission range	0.795 – 0.976	0.880-1.14	0.876-1.164	0.753-0.907
Absorption correction	Multi-scan	Multi-scan	Multi-scan	Multi-scan
Total no. reflections	21066	33875	31640	30964
Unique reflections	4306 [0.103]	7630 [0.0678]	10075 [0.0541]	10254 [0.0686]
[R _{int}]				
Final R ^b indices	R = 0.0543, R _w = 0.1084	R = 0.0553, R _w = 0.1193	R = 0.0405, R _w = 0.0796	R = 0.1002, R _w = 0.2189
[I>2σ(I)]				
R indices (all data)	R = 0.0828, R _w = 0.1227	R = 0.0706, R _w = 0.1268	R = 0.0625, R _w = 0.0868	R = 0.1245, R _w = 0.2314
Largest diff. peak and hole (e.A ⁻³)	1.51 / -0.67	1.390(0.117) / -0.984(0.117)	0.952(0.108) / -0.828(0.108)	4.129(0.164) / -2.108(0.164)
GooF	0.98	1.180	1.022	1.224

^a Radiation: graphite monochromated Mo Kα ($\lambda = 0.71073 \text{ \AA}$). ^bR = $\Sigma ||\mathbf{F}_o|| - |\mathbf{F}_c|| / \Sigma |\mathbf{F}_o|$.

Table S4: Selected Crystal Data Collection Parameters for **6**, **7** and **8**.

	6.C₇H₈	7	8
Formula	C ₇₅ H ₁₂₄ O ₂ Sm ₂	C ₆₉ H ₁₁₆ O ₃ Sm ₂	C ₅₃ H ₈₄ O ₃ Sm ₂
Crystal size (mm)	0.46 × 0.2 × 0.04	0.120x0.120x0.020	0.120x0.040x0.010
Crystal system	Monoclinic	orthorhombic	monoclinic
Space group	P2/n	P c c n	P 2 ₁
Volume (Å ³)	3476.0 (2)	6641.3(4)	2648.85(8)
a (Å)	18.3970 (7)	28.8648 (10)	10.5388 (2)
b (Å)	10.4587 (4)	11.0573 (4)	23.3764 (4)
c (Å)	19.0071 (7)	20.8084 (7)	11.2759 (2)
α (deg)	90	90	90
β (deg)	108.109 (2)	90	107.534 (1)
γ (deg)	90	90	90
Z	2	4	2
Formula weight – g/mol)	1358.43	1294.31	1069.90
Density (calcd) (g/cm ⁻³)	1.298	1.294	1.341
Absorption coefficient (mm ⁻¹)	1.72	1.793	2.232
F(000)	1428	2712	1100
Temp (K)	150	150	260
diffractometer ^a	Kappa APEX II CCD	Kappa APEX II CCD	Kappa APEX II CCD
θ range for data collection (deg)	1.9 – 26.0	2.4132 – 27.3827	0.998 – 27.485
Transmission range	0.506-0.935	0.814-0.965	0.829-1.213
Absorption correction	Multi-scan	Multi-scan	Multi-scan
Total no. reflections	6571	22335	32004
Unique reflections [R _{int}]	5586 [0.046]	7529 [0.0462]	12079 [0.0736]
Final R ^b indices [I>2σ(I)]	R = 0.0406, R _w = 0.1082	R = 0.0444, R _w = 0.1042	R = 0.0698, R _w = 0.1343
R indices (all data)	R = 0.0519, R _w = 0.1120	R = 0.0752, R _w = 0.1042	R = 0.0854, R _w = 0.1437
Largest diff. peak and hole (e.A ⁻³)	2.134 / -0.801	1.892(0.108) / -0.835(0.108)	2.689(0.170) / -0.838(0.170)
GooF	1.239	1.067	1.104

^a Radiation: graphite monochromated Mo Kα ($\lambda = 0.71073 \text{ \AA}$). ^bR = $\Sigma ||F_o| - |F_c|| / \Sigma |F_o|$.

Table S5: Bond length (in Å) and angles (in °) for **1**.

C12—C10	1.526 (12)	C2—C3	1.428 (11)
C24—C23	1.509 (12)	C2—C6	1.512 (11)
C26—C23	1.522 (11)	C5—C1	1.402 (11)
C25—C23	1.518 (12)	C5—C4	1.417 (11)
C20—C19	1.517 (13)	C5—C10	1.531 (11)
C21—C19	1.545 (13)	C10—C13	1.524 (11)
C22—C19	1.513 (14)	C10—C11	1.539 (11)
Sm1—C16	2.774 (8)	C3—C4	1.422 (11)
Sm1—C17	2.819 (8)	C23—C18	1.506 (11)
Sm1—C15	2.813 (8)	C9—C6	1.527 (11)
Sm1—C3	2.841 (8)	C14—C15	1.413 (11)
Sm1—C14	2.834 (7)	C14—C18	1.426 (11)
Sm1—C4	2.879 (8)	C15—C16	1.425 (11)
Sm1—C18	2.889 (8)	C15—C19	1.509 (12)
Sm1—C2	2.904 (8)	C6—C7	1.521 (11)
Sm1—C1	2.908 (7)	C6—C8	1.536 (11)
Sm1—C5	2.943 (8)	C18—C17	1.436 (11)
C2—C1	1.411 (10)	C16—C17	1.391 (12)
C16—Sm1—C17	28.8 (2)	C10—C5—Sm1	121.9 (5)
C16—Sm1—C15	29.6 (2)	C5—C1—C2	111.2 (7)
C17—Sm1—C15	48.1 (2)	C5—C1—Sm1	77.5 (4)
C16—Sm1—C3	134.9 (2)	C2—C1—Sm1	75.8 (4)
C17—Sm1—C3	121.8 (2)	C12—C10—C13	108.1 (7)
C15—Sm1—C3	110.0 (2)	C12—C10—C5	110.5 (7)
C16—Sm1—C14	47.6 (2)	C13—C10—C5	112.2 (7)
C17—Sm1—C14	47.2 (2)	C12—C10—C11	107.4 (7)
C15—Sm1—C14	29.0 (2)	C13—C10—C11	109.4 (7)
C3—Sm1—C14	87.3 (2)	C5—C10—C11	109.1 (7)
C16—Sm1—C4	129.5 (2)	C2—C3—C4	109.3 (7)
C17—Sm1—C4	134.6 (2)	C2—C3—Sm1	78.1 (4)
C15—Sm1—C4	100.0 (2)	C4—C3—Sm1	77.1 (4)
C3—Sm1—C4	28.8 (2)	C25—C23—C18	110.8 (7)
C14—Sm1—C4	88.6 (2)	C25—C23—C24	110.0 (9)
C16—Sm1—C18	48.1 (2)	C18—C23—C24	112.1 (7)
C17—Sm1—C18	29.1 (2)	C25—C23—C26	107.2 (8)
C15—Sm1—C18	48.4 (2)	C18—C23—C26	109.0 (7)
C3—Sm1—C18	93.2 (2)	C24—C23—C26	107.4 (8)
C14—Sm1—C18	28.8 (2)	C15—C14—C18	110.9 (7)
C4—Sm1—C18	106.9 (2)	C15—C14—Sm1	74.7 (4)

C16—Sm1—C2	157.6 (2)	C18—C14—Sm1	77.7 (4)
C17—Sm1—C2	132.1 (2)	C16—C15—C14	105.8 (7)
C15—Sm1—C2	138.5 (2)	C16—C15—C19	126.2 (7)
C3—Sm1—C2	28.8 (2)	C14—C15—C19	127.9 (8)
C14—Sm1—C2	113.1 (2)	C16—C15—Sm1	73.7 (4)
C4—Sm1—C2	47.4 (2)	C14—C15—Sm1	76.3 (4)
C18—Sm1—C2	109.5 (2)	C19—C15—Sm1	114.8 (5)
C16—Sm1—C1	171.8 (2)	C2—C6—C7	111.2 (7)
C17—Sm1—C1	159.1 (2)	C2—C6—C9	109.8 (7)
C15—Sm1—C1	145.1 (2)	C7—C6—C9	107.5 (7)
C3—Sm1—C1	46.1 (2)	C2—C6—C8	111.0 (7)
C14—Sm1—C1	132.1 (2)	C7—C6—C8	108.9 (7)
C4—Sm1—C1	46.1 (2)	C9—C6—C8	108.3 (7)
C18—Sm1—C1	136.9 (2)	C14—C18—C17	104.6 (7)
C2—Sm1—C1	28.1 (2)	C14—C18—C23	127.0 (7)
C16—Sm1—C5	144.6 (2)	C17—C18—C23	126.2 (7)
C17—Sm1—C5	162.3 (2)	C14—C18—Sm1	73.4 (4)
C15—Sm1—C5	118.5 (2)	C17—C18—Sm1	72.7 (4)
C3—Sm1—C5	46.6 (2)	C23—C18—Sm1	131.2 (5)
C14—Sm1—C5	115.1 (2)	C17—C16—C15	109.0 (7)
C4—Sm1—C5	28.2 (2)	C17—C16—Sm1	77.4 (5)
C18—Sm1—C5	135.0 (2)	C15—C16—Sm1	76.8 (4)
C2—Sm1—C5	46.8 (2)	C16—C17—C18	109.6 (8)
C1—Sm1—C5	27.7 (2)	C16—C17—Sm1	73.8 (5)
C1—C2—C3	105.0 (6)	C18—C17—Sm1	78.2 (4)
C1—C2—C6	125.4 (7)	C5—C4—C3	107.5 (7)
C3—C2—C6	129.4 (7)	C5—C4—Sm1	78.4 (4)
C1—C2—Sm1	76.1 (4)	C3—C4—Sm1	74.1 (4)
C3—C2—Sm1	73.2 (4)	C22—C19—C15	112.0 (8)
C6—C2—Sm1	112.5 (5)	C22—C19—C20	107.9 (9)
C1—C5—C4	106.9 (7)	C15—C19—C20	109.9 (8)
C1—C5—C10	125.4 (7)	C22—C19—C21	110.6 (9)
C4—C5—C10	127.5 (7)	C15—C19—C21	109.3 (8)
C1—C5—Sm1	74.8 (4)	C20—C19—C21	107.1 (8)
C4—C5—Sm1	73.4 (4)		

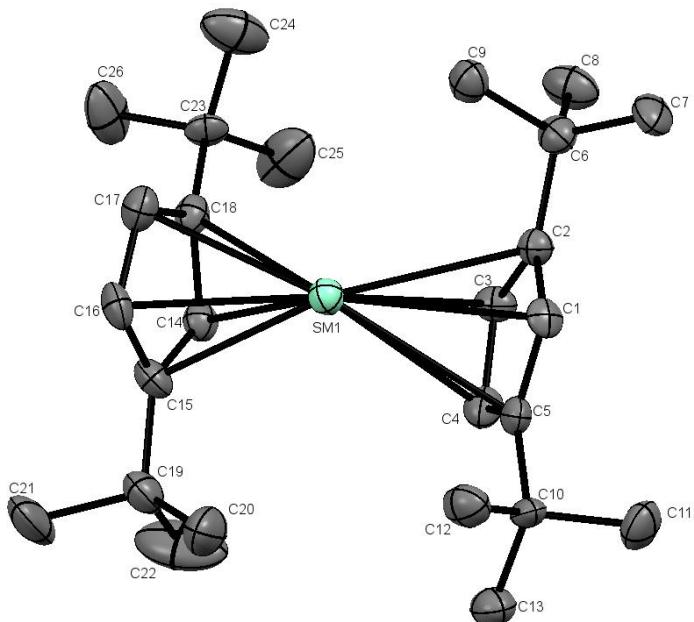


Figure S22: ORTEP of **1** with 50% probability ellipsoids (hydrogen atoms have been removed for clarity).

Table S6: Bond length (in Å) and angles (in °) for **3**.

Sm(1)-O(2)	2.622(4)	Sm(1)-O(1)	2.647(4)
Sm(1)-C(3)	2.825(5)	Sm(1)-C(17)	2.842(5)
Sm(1)-C(16)	2.857(5)	Sm(1)-C(4)	2.863(5)
Sm(1)-C(2)	2.892(5)	Sm(1)-C(1)	2.909(5)
Sm(1)-C(18)	2.909(5)	Sm(1)-C(15)	2.939(5)
Sm(1)-C(14)	2.940(5)	Sm(1)-C(5)	2.941(5)
O(1)-C(27)	1.442(7)	O(1)-C(30)	1.444(7)
O(2)-C(31)	1.435(7)	O(2)-C(34)	1.440(7)
C(1)-C(2)	1.412(7)	C(1)-C(5)	1.419(7)
C(1)-H(1)	0.9500	C(2)-C(3)	1.409(7)
C(2)-C(6)	1.522(7)	C(3)-C(4)	1.412(7)
C(3)-H(3)	0.9500	C(4)-C(5)	1.411(7)
C(4)-H(4)	0.9500	C(5)-C(10)	1.513(7)
C(6)-C(7)	1.519(8)	C(6)-C(8)	1.527(8)
C(6)-C(9)	1.534(8)	C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800	C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800	C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800	C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800	C(9)-H(9C)	0.9800
C(10)-C(11)	1.52(1)	C(10)-C(12)	1.53(1)
C(10)-C(13)	1.535(8)	C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800	C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800	C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800	C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800	C(13)-H(13C)	0.9800
C(14)-C(18)	1.418(8)	C(14)-C(15)	1.424(7)
C(14)-H(14)	0.9500	C(15)-C(16)	1.412(7)
C(15)-C(19)	1.515(8)	C(16)-C(17)	1.414(8)
C(16)-H(16)	0.9500	C(17)-C(18)	1.411(7)
C(17)-H(17)	0.9500	C(18)-C(23)	1.523(7)
C(19)-C(21)	1.533(8)	C(19)-C(22)	1.541(8)
C(19)-C(20)	1.542(8)	C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800	C(20)-H(20C)	0.9800

C(21)-H(21A)	0.9800	C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800	C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800	C(22)-H(22C)	0.9800
C(23)-C(25)	1.524(8)	C(23)-C(24)	1.528(8)
C(23)-C(26)	1.530(8)	C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800	C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800	C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800	C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800	C(26)-H(26C)	0.9800
C(27)-C(28)	1.494(8)	C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900	C(28)-C(29)	1.51(1)
C(28)-H(28A)	0.9900	C(28)-H(28B)	0.9900
C(29)-C(30)	1.527(8)	C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900	C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900	C(31)-C(32)	1.52(1)
C(31)-H(31A)	0.9900	C(31)-H(31B)	0.9900
C(32)-C(33)	1.53(1)	C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900	C(33)-C(34)	1.506(8)
C(33)-H(33A)	0.9900	C(33)-H(33B)	0.9900
C(34)-H(34A)	0.9900	C(34)-H(34B)	0.9900

O(2)-Sm(1)-O(1)	86.8(1)	O(2)-Sm(1)-C(3)	112.7(1)
O(1)-Sm(1)-C(3)	72.9(1)	O(2)-Sm(1)-C(17)	128.4(1)
O(1)-Sm(1)-C(17)	114.8(1)	C(3)-Sm(1)-C(17)	118.2(2)
O(2)-Sm(1)-C(16)	120.3(1)	O(1)-Sm(1)-C(16)	88.0(1)
C(3)-Sm(1)-C(16)	122.1(2)	C(17)-Sm(1)-C(16)	28.7(2)
O(2)-Sm(1)-C(4)	87.6(1)	O(1)-Sm(1)-C(4)	84.2(1)
C(3)-Sm(1)-C(4)	28.7(1)	C(17)-Sm(1)-C(4)	138.0(2)
C(16)-Sm(1)-C(4)	150.5(2)	O(2)-Sm(1)-C(2)	133.6(1)
O(1)-Sm(1)-C(2)	94.7(1)	C(3)-Sm(1)-C(2)	28.5(2)
C(17)-Sm(1)-C(2)	92.7(2)	C(16)-Sm(1)-C(2)	106.0(2)
C(4)-Sm(1)-C(2)	46.8(1)	O(2)-Sm(1)-C(1)	116.6(1)
O(1)-Sm(1)-C(1)	119.2(1)	C(3)-Sm(1)-C(1)	46.4(2)
C(17)-Sm(1)-C(1)	93.8(2)	C(16)-Sm(1)-C(1)	117.5(2)
C(4)-Sm(1)-C(1)	45.9(2)	C(2)-Sm(1)-C(1)	28.2(1)
O(2)-Sm(1)-C(18)	102.8(1)	O(1)-Sm(1)-C(18)	132.5(1)
C(3)-Sm(1)-C(18)	138.0(2)	C(17)-Sm(1)-C(18)	28.4(2)
C(16)-Sm(1)-C(18)	46.9(2)	C(4)-Sm(1)-C(18)	141.7(2)
C(2)-Sm(1)-C(18)	109.5(2)	C(1)-Sm(1)-C(18)	98.0(2)
O(2)-Sm(1)-C(15)	92.2(1)	O(1)-Sm(1)-C(15)	87.2(1)
C(3)-Sm(1)-C(15)	146.5(2)	C(17)-Sm(1)-C(15)	46.8(2)
C(16)-Sm(1)-C(15)	28.2(2)	C(4)-Sm(1)-C(15)	171.3(1)
C(2)-Sm(1)-C(15)	134.1(2)	C(1)-Sm(1)-C(15)	140.4(2)
C(18)-Sm(1)-C(15)	46.7(1)	O(2)-Sm(1)-C(14)	82.5(1)
O(1)-Sm(1)-C(14)	112.7(1)	C(3)-Sm(1)-C(14)	164.4(2)
C(17)-Sm(1)-C(14)	46.2(2)	C(16)-Sm(1)-C(14)	46.2(2)
C(4)-Sm(1)-C(14)	159.8(2)	C(2)-Sm(1)-C(14)	136.9(2)
C(1)-Sm(1)-C(14)	124.9(2)	C(18)-Sm(1)-C(14)	28.1(2)
C(15)-Sm(1)-C(14)	28.0(1)	O(2)-Sm(1)-C(5)	89.9(1)
O(1)-Sm(1)-C(5)	112.2(1)	C(3)-Sm(1)-C(5)	47.1(1)
C(17)-Sm(1)-C(5)	119.1(2)	C(16)-Sm(1)-C(5)	145.2(2)
C(4)-Sm(1)-C(5)	28.1(1)	C(2)-Sm(1)-C(5)	46.9(1)
C(1)-Sm(1)-C(5)	28.1(1)	C(18)-Sm(1)-C(5)	114.1(2)
C(15)-Sm(1)-C(5)	160.6(1)	C(14)-Sm(1)-C(5)	133.8(1)
C(27)-O(1)-C(30)	107.5(4)	C(27)-O(1)-Sm(1)	124.4(3)
C(30)-O(1)-Sm(1)	125.3(3)	C(31)-O(2)-C(34)	108.7(4)
C(31)-O(2)-Sm(1)	127.3(3)	C(34)-O(2)-Sm(1)	124.0(3)
C(2)-C(1)-C(5)	110.2(5)	C(2)-C(1)-Sm(1)	75.2(3)
C(5)-C(1)-Sm(1)	77.2(3)	C(2)-C(1)-H(1)	124.9
C(5)-C(1)-H(1)	124.9	Sm(1)-C(1)-H(1)	114.6
C(3)-C(2)-C(1)	106.6(5)	C(3)-C(2)-C(6)	125.3(5)
C(1)-C(2)-C(6)	127.8(5)	C(3)-C(2)-Sm(1)	73.1(3)

C(1)-C(2)-Sm(1)	76.6(3)	C(6)-C(2)-Sm(1)	120.6(3)
C(2)-C(3)-C(4)	108.1(5)	C(2)-C(3)-Sm(1)	78.4(3)
C(4)-C(3)-Sm(1)	77.1(3)	C(2)-C(3)-H(3)	125.9
C(4)-C(3)-H(3)	125.9	Sm(1)-C(3)-H(3)	111.2
C(5)-C(4)-C(3)	109.5(4)	C(5)-C(4)-Sm(1)	79.1(3)
C(3)-C(4)-Sm(1)	74.2(3)	C(5)-C(4)-H(4)	125.2
C(3)-C(4)-H(4)	125.2	Sm(1)-C(4)-H(4)	113.6
C(4)-C(5)-C(1)	105.5(4)	C(4)-C(5)-C(10)	128.2(5)
C(1)-C(5)-C(10)	126.0(5)	C(4)-C(5)-Sm(1)	72.8(3)
C(1)-C(5)-Sm(1)	74.7(3)	C(10)-C(5)-Sm(1)	122.2(3)
C(7)-C(6)-C(2)	109.6(5)	C(7)-C(6)-C(8)	108.0(5)
C(2)-C(6)-C(8)	110.6(4)	C(7)-C(6)-C(9)	108.7(5)
C(2)-C(6)-C(9)	110.5(5)	C(8)-C(6)-C(9)	109.4(5)
C(6)-C(7)-H(7A)	109.5	C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5	C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5	H(7B)-C(7)-H(7C)	109.5
C(6)-C(8)-H(8A)	109.5	C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5	C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5	H(8B)-C(8)-H(8C)	109.5
C(6)-C(9)-H(9A)	109.5	C(6)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5	C(6)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5	H(9B)-C(9)-H(9C)	109.5
C(5)-C(10)-C(11)	111.1(5)	C(5)-C(10)-C(12)	110.4(5)
C(11)-C(10)-C(12)	109.0(6)	C(5)-C(10)-C(13)	110.8(5)
C(11)-C(10)-C(13)	107.6(5)	C(12)-C(10)-C(13)	107.9(6)
C(10)-C(11)-H(11A)	109.5	C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5	C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5	H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5	C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5	C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5	H(12B)-C(12)-H(12C)	109.5
C(10)-C(13)-H(13A)	109.5	C(10)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5	C(10)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5	H(13B)-C(13)-H(13C)	109.5
C(18)-C(14)-C(15)	109.2(5)	C(18)-C(14)-Sm(1)	74.8(3)
C(15)-C(14)-Sm(1)	76.0(3)	C(18)-C(14)-H(14)	125.4
C(15)-C(14)-H(14)	125.4	Sm(1)-C(14)-H(14)	115.8
C(16)-C(15)-C(14)	106.6(4)	C(16)-C(15)-C(19)	127.8(5)
C(14)-C(15)-C(19)	124.9(5)	C(16)-C(15)-Sm(1)	72.7(3)
C(14)-C(15)-Sm(1)	76.0(3)	C(19)-C(15)-Sm(1)	123.9(3)
C(15)-C(16)-C(17)	108.7(5)	C(15)-C(16)-Sm(1)	79.2(3)
C(17)-C(16)-Sm(1)	75.0(3)	C(15)-C(16)-H(16)	125.7
C(17)-C(16)-H(16)	125.7	Sm(1)-C(16)-H(16)	112.5
C(18)-C(17)-C(16)	108.6(5)	C(18)-C(17)-Sm(1)	78.5(3)
C(16)-C(17)-Sm(1)	76.2(3)	C(18)-C(17)-H(17)	125.7
C(16)-C(17)-H(17)	125.7	Sm(1)-C(17)-H(17)	112.0
C(17)-C(18)-C(14)	106.9(5)	C(17)-C(18)-C(23)	125.4(5)
C(14)-C(18)-C(23)	125.7(5)	C(17)-C(18)-Sm(1)	73.2(3)
C(14)-C(18)-Sm(1)	77.2(3)	C(23)-C(18)-Sm(1)	127.8(4)
C(15)-C(19)-C(21)	110.6(5)	C(15)-C(19)-C(22)	112.6(5)
C(21)-C(19)-C(22)	108.7(5)	C(15)-C(19)-C(20)	109.0(4)
C(21)-C(19)-C(20)	107.3(5)	C(22)-C(19)-C(20)	108.5(5)
C(19)-C(20)-H(20A)	109.5	C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5	C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5	H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5	C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5	C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5	H(21B)-C(21)-H(21C)	109.5
C(19)-C(22)-H(22A)	109.5	C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5	C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5	H(22B)-C(22)-H(22C)	109.5
C(18)-C(23)-C(25)	111.2(5)	C(18)-C(23)-C(24)	111.2(5)
C(25)-C(23)-C(24)	108.5(5)	C(18)-C(23)-C(26)	108.0(5)

C(25)-C(23)-C(26)	108.3(5)	C(24)-C(23)-C(26)	109.6(5)
C(23)-C(24)-H(24A)	109.5	C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5	C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5	H(24B)-C(24)-H(24C)	109.5
C(23)-C(25)-H(25A)	109.5	C(23)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5	C(23)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5	H(25B)-C(25)-H(25C)	109.5
C(23)-C(26)-H(26A)	109.5	C(23)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5	C(23)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5	H(26B)-C(26)-H(26C)	109.5
O(1)-C(27)-C(28)	104.9(5)	O(1)-C(27)-H(27A)	110.8
C(28)-C(27)-H(27A)	110.8	O(1)-C(27)-H(27B)	110.8
C(28)-C(27)-H(27B)	110.8	H(27A)-C(27)-H(27B)	108.9
C(27)-C(28)-C(29)	103.8(5)	C(27)-C(28)-H(28A)	111.0
C(29)-C(28)-H(28A)	111.0	C(27)-C(28)-H(28B)	111.0
C(29)-C(28)-H(28B)	111.0	H(28A)-C(28)-H(28B)	109.0
C(28)-C(29)-C(30)	103.6(5)	C(28)-C(29)-H(29A)	111.0
C(30)-C(29)-H(29A)	111.0	C(28)-C(29)-H(29B)	111.0
C(30)-C(29)-H(29B)	111.0	H(29A)-C(29)-H(29B)	109.0
O(1)-C(30)-C(29)	107.5(5)	O(1)-C(30)-H(30A)	110.2
C(29)-C(30)-H(30A)	110.2	O(1)-C(30)-H(30B)	110.2
C(29)-C(30)-H(30B)	110.2	H(30A)-C(30)-H(30B)	108.5
O(2)-C(31)-C(32)	107.4(5)	O(2)-C(31)-H(31A)	110.2
C(32)-C(31)-H(31A)	110.2	O(2)-C(31)-H(31B)	110.2
C(32)-C(31)-H(31B)	110.2	H(31A)-C(31)-H(31B)	108.5
C(31)-C(32)-C(33)	102.5(5)	C(31)-C(32)-H(32A)	111.3
C(33)-C(32)-H(32A)	111.3	C(31)-C(32)-H(32B)	111.3
C(33)-C(32)-H(32B)	111.3	H(32A)-C(32)-H(32B)	109.2
C(34)-C(33)-C(32)	102.0(5)	C(34)-C(33)-H(33A)	111.4
C(32)-C(33)-H(33A)	111.4	C(34)-C(33)-H(33B)	111.4
C(32)-C(33)-H(33B)	111.4	H(33A)-C(33)-H(33B)	109.2
O(2)-C(34)-C(33)	104.2(5)	O(2)-C(34)-H(34A)	110.9
C(33)-C(34)-H(34A)	110.9	O(2)-C(34)-H(34B)	110.9
C(33)-C(34)-H(34B)	110.9	H(34A)-C(34)-H(34B)	108.9

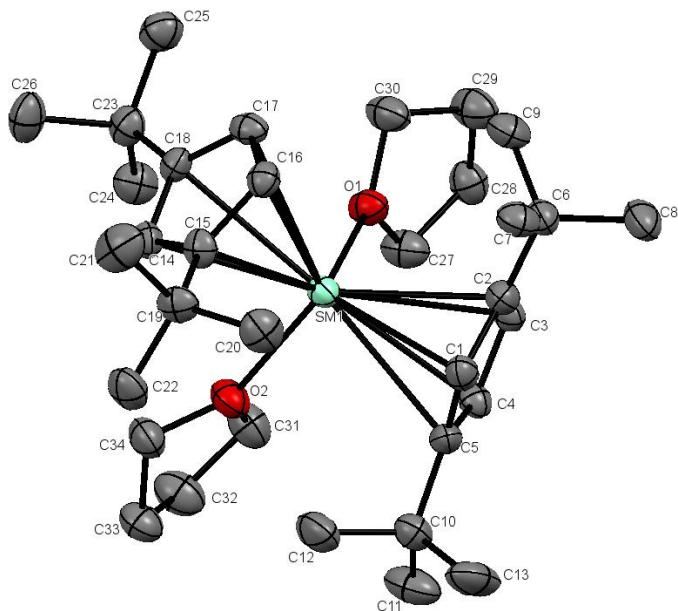


Figure S23: ORTEP of **3** with 50% probability ellipsoids (hydrogen atoms have been removed for clarity).

Table S7: Bond length (in Å) and angles (in °) for **4**.

Sm(1)-N(1)	2.692(2)	Sm(1)-C(5)	2.744(3)
Sm(1)-C(17)	2.773(3)	Sm(1)-C(4)	2.788(3)
Sm(1)-C(16)	2.797(3)	Sm(1)-C(1)	2.800(3)
Sm(1)-C(18)	2.817(3)	Sm(1)-C(15)	2.826(3)
Sm(1)-C(2)	2.844(3)	Sm(1)-C(14)	2.860(3)
Sm(1)-C(3)	2.886(3)	N(1)-C(31)	1.338(4)
N(1)-C(27)	1.349(4)	C(1)-C(5)	1.407(4)
C(1)-C(2)	1.419(4)	C(1)-C(6)	1.515(4)
C(2)-C(3)	1.429(4)	C(2)-H(2)	0.9500
C(3)-C(4)	1.406(4)	C(3)-C(10)	1.510(4)
C(4)-C(5)	1.414(4)	C(4)-H(4)	0.9500
C(5)-H(5)	0.9500	C(6)-C(8)	1.531(4)
C(6)-C(9)	1.531(4)	C(6)-C(7)	1.544(4)
C(7)-H(7A)	0.9800	C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800	C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800	C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800	C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800	C(10)-C(11)	1.535(4)
C(10)-C(12)	1.536(4)	C(10)-C(13)	1.551(4)
C(11)-H(11A)	0.9800	C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800	C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800	C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800	C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800	C(14)-C(18)	1.407(4)
C(14)-C(15)	1.427(4)	C(14)-C(19)	1.518(4)
C(15)-C(16)	1.420(4)	C(15)-H(15)	0.9500
C(16)-C(17)	1.415(4)	C(16)-C(23)	1.511(4)
C(17)-C(18)	1.415(4)	C(17)-H(17)	0.9500
C(18)-H(18)	0.9500	C(19)-C(22)	1.524(4)
C(19)-C(21)	1.537(4)	C(19)-C(20)	1.538(4)
C(20)-H(20A)	0.9800	C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800	C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800	C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800	C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800	C(23)-C(24)	1.530(4)
C(23)-C(26)	1.533(4)	C(23)-C(25)	1.541(4)
C(24)-H(24A)	0.9800	C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800	C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800	C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800	C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800	C(27)-C(28)	1.381(4)
C(27)-H(27)	0.9500	C(28)-C(29)	1.372(4)
C(28)-H(28)	0.9500	C(29)-C(30)	1.386(4)
C(29)-H(29)	0.9500	C(30)-C(31)	1.381(4)
C(30)-H(30)	0.9500	C(31)-H(31)	0.9500
C(32)-C(33)	1.369(5)	C(32)-C(37)	1.418(5)
C(32)-C(38)	1.454(5)	C(33)-C(34)	1.402(5)
C(33)-H(33)	0.9500	C(34)-C(35)	1.354(5)
C(34)-H(34)	0.9500	C(35)-C(36)	1.413(6)
C(35)-H(35)	0.9500	C(36)-C(37)	1.358(6)
C(36)-H(36)	0.9500	C(37)-H(37)	0.9500
C(38)-H(38A)	0.9800	C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800		

N(1)-Sm(1)-C(5)	136.42(8)	N(1)-Sm(1)-C(17)	134.87(8)
C(5)-Sm(1)-C(17)	88.70(8)	N(1)-Sm(1)-C(4)	131.67(8)
C(5)-Sm(1)-C(4)	29.61(8)	C(17)-Sm(1)-C(4)	86.24(8)
N(1)-Sm(1)-C(16)	106.03(8)	C(5)-Sm(1)-C(16)	117.31(8)
C(17)-Sm(1)-C(16)	29.42(8)	C(4)-Sm(1)-C(16)	107.68(8)
N(1)-Sm(1)-C(1)	107.93(8)	C(5)-Sm(1)-C(1)	29.39(8)

C(17)-Sm(1)-C(1)	116.60(8)	C(4)-Sm(1)-C(1)	48.50(8)
C(16)-Sm(1)-C(1)	145.94(8)	N(1)-Sm(1)-C(18)	132.38(8)
C(5)-Sm(1)-C(18)	83.83(8)	C(17)-Sm(1)-C(18)	29.31(8)
C(4)-Sm(1)-C(18)	95.94(8)	C(16)-Sm(1)-C(18)	48.39(8)
C(1)-Sm(1)-C(18)	103.96(8)	N(1)-Sm(1)-C(15)	89.65(8)
C(5)-Sm(1)-C(15)	131.17(8)	C(17)-Sm(1)-C(15)	47.86(8)
C(4)-Sm(1)-C(15)	133.88(8)	C(16)-Sm(1)-C(15)	29.25(8)
C(1)-Sm(1)-C(15)	148.01(8)	C(18)-Sm(1)-C(15)	47.53(8)
N(1)-Sm(1)-C(2)	90.59(7)	C(5)-Sm(1)-C(2)	47.69(8)
C(17)-Sm(1)-C(2)	132.80(8)	C(4)-Sm(1)-C(2)	47.33(8)
C(16)-Sm(1)-C(2)	153.29(8)	C(1)-Sm(1)-C(2)	29.12(8)
C(18)-Sm(1)-C(2)	130.84(8)	C(15)-Sm(1)-C(2)	176.61(8)
N(1)-Sm(1)-C(14)	103.79(8)	C(5)-Sm(1)-C(14)	107.95(8)
C(17)-Sm(1)-C(14)	48.01(8)	C(4)-Sm(1)-C(14)	124.48(8)
C(16)-Sm(1)-C(14)	48.5(1)	C(1)-Sm(1)-C(14)	119.00(8)
C(18)-Sm(1)-C(14)	28.68(8)	C(15)-Sm(1)-C(14)	29.07(8)
C(2)-Sm(1)-C(14)	147.85(8)	N(1)-Sm(1)-C(3)	103.04(7)
C(5)-Sm(1)-C(3)	48.13(8)	C(17)-Sm(1)-C(3)	111.43(8)
C(4)-Sm(1)-C(3)	28.63(7)	C(16)-Sm(1)-C(3)	124.80(8)
C(1)-Sm(1)-C(3)	48.39(8)	C(18)-Sm(1)-C(3)	124.58(8)
C(15)-Sm(1)-C(3)	153.99(8)	C(2)-Sm(1)-C(3)	28.87(8)
C(14)-Sm(1)-C(3)	153.04(8)	C(31)-N(1)-C(27)	116.2(3)
C(31)-N(1)-Sm(1)	125.7(2)	C(27)-N(1)-Sm(1)	118.1(2)
C(5)-C(1)-C(2)	106.2(3)	C(5)-C(1)-C(6)	127.6(3)
C(2)-C(1)-C(6)	126.2(3)	C(5)-C(1)-Sm(1)	73.1(2)
C(2)-C(1)-Sm(1)	77.1(2)	C(6)-C(1)-Sm(1)	114.5(2)
C(1)-C(2)-C(3)	109.9(2)	C(1)-C(2)-Sm(1)	73.7(2)
C(3)-C(2)-Sm(1)	77.2(2)	C(1)-C(2)-H(2)	125.0
C(3)-C(2)-H(2)	125.0	Sm(1)-C(2)-H(2)	115.9
C(4)-C(3)-C(2)	105.8(2)	C(4)-C(3)-C(10)	128.3(3)
C(2)-C(3)-C(10)	125.7(2)	C(4)-C(3)-Sm(1)	71.8(2)
C(2)-C(3)-Sm(1)	73.9(2)	C(10)-C(3)-Sm(1)	122.8(2)
C(3)-C(4)-C(5)	109.2(2)	C(3)-C(4)-Sm(1)	79.6(2)
C(5)-C(4)-Sm(1)	73.5(2)	C(3)-C(4)-H(4)	125.4
C(5)-C(4)-H(4)	125.4	Sm(1)-C(4)-H(4)	113.7
C(1)-C(5)-C(4)	108.9(3)	C(1)-C(5)-Sm(1)	77.5(2)
C(4)-C(5)-Sm(1)	76.9(2)	C(1)-C(5)-H(5)	125.6
C(4)-C(5)-H(5)	125.6	Sm(1)-C(5)-H(5)	112.3
C(1)-C(6)-C(8)	110.1(2)	C(1)-C(6)-C(9)	111.5(2)
C(8)-C(6)-C(9)	108.2(2)	C(1)-C(6)-C(7)	110.0(2)
C(8)-C(6)-C(7)	108.4(2)	C(9)-C(6)-C(7)	108.7(2)
C(6)-C(7)-H(7A)	109.5	C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5	C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5	H(7B)-C(7)-H(7C)	109.5
C(6)-C(8)-H(8A)	109.5	C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5	C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5	H(8B)-C(8)-H(8C)	109.5
C(6)-C(9)-H(9A)	109.5	C(6)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5	C(6)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5	H(9B)-C(9)-H(9C)	109.5
C(3)-C(10)-C(11)	111.2(2)	C(3)-C(10)-C(12)	111.6(2)
C(11)-C(10)-C(12)	108.6(2)	C(3)-C(10)-C(13)	109.1(2)
C(11)-C(10)-C(13)	108.4(2)	C(12)-C(10)-C(13)	107.9(2)
C(10)-C(11)-H(11A)	109.5	C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5	C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5	H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5	C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5	C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5	H(12B)-C(12)-H(12C)	109.5
C(10)-C(13)-H(13A)	109.5	C(10)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5	C(10)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5	H(13B)-C(13)-H(13C)	109.5
C(18)-C(14)-C(15)	106.7(3)	C(18)-C(14)-C(19)	126.4(3)

C(15)-C(14)-C(19)	126.3(3)	C(18)-C(14)-Sm(1)	74.0(2)
C(15)-C(14)-Sm(1)	74.2(2)	C(19)-C(14)-Sm(1)	123.9(2)
C(16)-C(15)-C(14)	109.3(2)	C(16)-C(15)-Sm(1)	74.2(2)
C(14)-C(15)-Sm(1)	76.8(2)	C(16)-C(15)-H(15)	125.4
C(14)-C(15)-H(15)	125.4	Sm(1)-C(15)-H(15)	115.6
C(17)-C(16)-C(15)	106.5(3)	C(17)-C(16)-C(23)	126.5(3)
C(15)-C(16)-C(23)	126.8(3)	C(17)-C(16)-Sm(1)	74.4(2)
C(15)-C(16)-Sm(1)	76.5(2)	C(23)-C(16)-Sm(1)	111.5(2)
C(16)-C(17)-C(18)	108.8(3)	C(16)-C(17)-Sm(1)	76.2(2)
C(18)-C(17)-Sm(1)	77.1(2)	C(16)-C(17)-H(17)	125.6
C(18)-C(17)-H(17)	125.6	Sm(1)-C(17)-H(17)	113.4
C(14)-C(18)-C(17)	108.7(3)	C(14)-C(18)-Sm(1)	77.3(2)
C(17)-C(18)-Sm(1)	73.6(2)	C(14)-C(18)-H(18)	125.6
C(17)-C(18)-H(18)	125.6	Sm(1)-C(18)-H(18)	115.5
C(14)-C(19)-C(22)	111.2(2)	C(14)-C(19)-C(21)	109.1(2)
C(22)-C(19)-C(21)	108.2(3)	C(14)-C(19)-C(20)	110.8(2)
C(22)-C(19)-C(20)	108.6(3)	C(21)-C(19)-C(20)	108.9(2)
C(19)-C(20)-H(20A)	109.5	C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5	C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5	H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5	C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5	C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5	H(21B)-C(21)-H(21C)	109.5
C(19)-C(22)-H(22A)	109.5	C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5	C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5	H(22B)-C(22)-H(22C)	109.5
C(16)-C(23)-C(24)	111.2(3)	C(16)-C(23)-C(26)	110.4(2)
C(24)-C(23)-C(26)	108.8(2)	C(16)-C(23)-C(25)	109.6(2)
C(24)-C(23)-C(25)	108.2(3)	C(26)-C(23)-C(25)	108.5(3)
C(23)-C(24)-H(24A)	109.5	C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5	C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5	H(24B)-C(24)-H(24C)	109.5
C(23)-C(25)-H(25A)	109.5	C(23)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5	C(23)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5	H(25B)-C(25)-H(25C)	109.5
C(23)-C(26)-H(26A)	109.5	C(23)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5	C(23)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5	H(26B)-C(26)-H(26C)	109.5
N(1)-C(27)-C(28)	124.0(3)	N(1)-C(27)-H(27)	118.0
C(28)-C(27)-H(27)	118.0	C(29)-C(28)-C(27)	118.7(3)
C(29)-C(28)-H(28)	120.6	C(27)-C(28)-H(28)	120.6
C(28)-C(29)-C(30)	118.5(3)	C(28)-C(29)-H(29)	120.8
C(30)-C(29)-H(29)	120.8	C(31)-C(30)-C(29)	119.1(3)
C(31)-C(30)-H(30)	120.4	C(29)-C(30)-H(30)	120.4
N(1)-C(31)-C(30)	123.5(3)	N(1)-C(31)-H(31)	118.2
C(30)-C(31)-H(31)	118.2	C(33)-C(32)-C(37)	117.8(4)
C(33)-C(32)-C(38)	122.6(4)	C(37)-C(32)-C(38)	119.7(4)
C(32)-C(33)-C(34)	120.9(3)	C(32)-C(33)-H(33)	119.5
C(34)-C(33)-H(33)	119.5	C(35)-C(34)-C(33)	121.9(4)
C(35)-C(34)-H(34)	119.0	C(33)-C(34)-H(34)	119.0
C(34)-C(35)-C(36)	117.2(4)	C(34)-C(35)-H(35)	121.4
C(36)-C(35)-H(35)	121.4	C(37)-C(36)-C(35)	122.0(4)
C(37)-C(36)-H(36)	119.0	C(35)-C(36)-H(36)	119.0
C(36)-C(37)-C(32)	120.3(4)	C(36)-C(37)-H(37)	119.9
C(32)-C(37)-H(37)	119.9	C(32)-C(38)-H(38A)	109.5
C(32)-C(38)-H(38B)	109.5	H(38A)-C(38)-H(38B)	109.5
C(32)-C(38)-H(38C)	109.5	H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5		

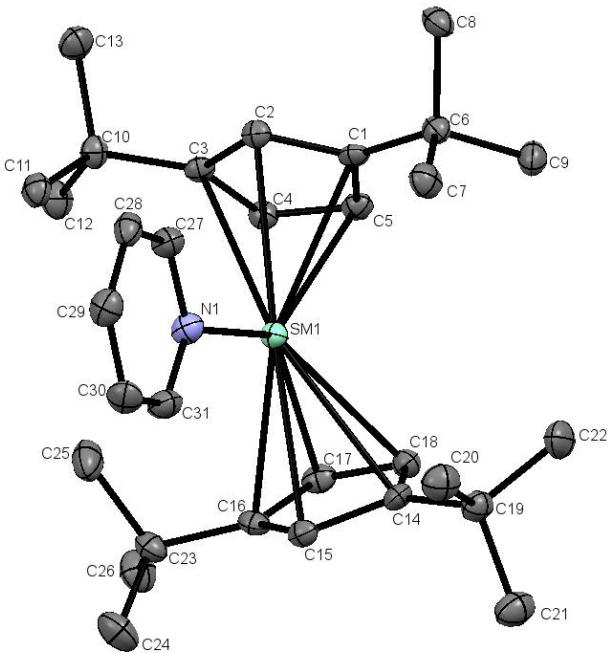


Figure S24: ORTEP of **4** with 50% probability ellipsoids (one molecule of toluene and hydrogen atoms have been removed for clarity).

Table S8: Bond length (in Å) and angles (in °) for **5**.

Sm(1)-O(1)	2.585(7)	Sm(1)-C(5)	2.74(1)
Sm(1)-C(4)	2.77(1)	Sm(1)-C(17)	2.79(1)
Sm(1)-C(16)	2.80(1)	Sm(1)-C(18)	2.81(1)
Sm(1)-C(15)	2.83(1)	Sm(1)-C(1)	2.83(1)
Sm(1)-C(2)	2.84(1)	Sm(1)-C(3)	2.84(1)
Sm(1)-C(14)	2.85(1)	O(1)-C(30)	1.39(2)
O(1)-C(27)	1.44(1)	C(1)-C(5)	1.42(2)
C(1)-C(2)	1.42(2)	C(1)-C(6)	1.49(2)
C(2)-C(3)	1.41(2)	C(2)-H(2)	0.9500
C(3)-C(4)	1.40(2)	C(3)-C(10)	1.53(2)
C(4)-C(5)	1.42(2)	C(4)-H(4)	0.9500
C(5)-H(5)	0.9500	C(6)-C(8)	1.52(2)
C(6)-C(9)	1.54(2)	C(6)-C(7)	1.57(2)
C(7)-H(7A)	0.9800	C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800	C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800	C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800	C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800	C(10)-C(11)	1.48(2)
C(10)-C(13)	1.52(2)	C(10)-C(12)	1.55(2)
C(11)-H(11A)	0.9800	C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800	C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800	C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800	C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800	C(14)-C(18)	1.39(2)
C(14)-C(15)	1.42(2)	C(14)-C(19)	1.51(2)
C(15)-C(16)	1.44(2)	C(15)-H(15)	0.9500
C(16)-C(17)	1.41(2)	C(16)-C(23)	1.52(2)
C(17)-C(18)	1.43(2)	C(17)-H(17)	0.9500
C(18)-H(18)	0.9500	C(19)-C(22)	1.50(2)
C(19)-C(21)	1.53(2)	C(19)-C(20)	1.53(2)
C(20)-H(20A)	0.9800	C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800	C(21)-H(21A)	0.9800

C(21)-H(21B)	0.9800	C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800	C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800	C(23)-C(26)	1.48(2)
C(23)-C(25)	1.51(2)	C(23)-C(24)	1.53(2)
C(24)-H(24A)	0.9800	C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800	C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800	C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800	C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800	C(27)-C(28)	1.48(2)
C(27)-H(27A)	0.9900	C(27)-H(27B)	0.9900
C(28)-C(29)	1.45(2)	C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900	C(29)-C(30)	1.52(2)
C(29)-H(29A)	0.9900	C(29)-H(29B)	0.9900
C(30)-H(30A)	0.9900	C(30)-H(30B)	0.9900
Sm(2)-O(2)	2.558(8)	Sm(2)-C(35)	2.77(1)
Sm(2)-C(34)	2.78(1)	Sm(2)-C(46)	2.79(1)
Sm(2)-C(45)	2.79(1)	Sm(2)-C(32)	2.81(1)
Sm(2)-C(33)	2.81(1)	Sm(2)-C(44)	2.82(1)
Sm(2)-C(47)	2.82(1)	Sm(2)-C(48)	2.83(1)
Sm(2)-C(31)	2.83(1)	O(2)-C(60)	1.44(2)
O(2)-C(57)	1.46(2)	C(31)-C(32)	1.39(2)
C(31)-C(35)	1.40(2)	C(31)-C(36)	1.55(2)
C(32)-C(33)	1.39(2)	C(32)-H(32)	0.9500
C(33)-C(34)	1.40(2)	C(33)-C(40)	1.53(2)
C(34)-C(35)	1.41(2)	C(34)-H(34)	0.9500
C(35)-H(35)	0.9500	C(36)-C(37)	1.36(3)
C(36)-C(39)	1.45(2)	C(36)-C(38)	1.66(4)
C(37)-H(37A)	0.9800	C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800	C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800	C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800	C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800	C(40)-C(41)	1.44(3)
C(40)-C(42)	1.46(2)	C(40)-C(43)	1.54(3)
C(41)-H(41A)	0.9800	C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800	C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800	C(42)-H(42C)	0.9800
C(43)-H(43A)	0.9800	C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800	C(44)-C(48)	1.41(2)
C(44)-C(45)	1.42(2)	C(44)-C(49)	1.53(2)
C(45)-C(46)	1.41(2)	C(45)-H(45)	0.9500
C(46)-C(47)	1.42(2)	C(46)-H(46)	0.9500
C(47)-C(48)	1.40(2)	C(47)-C(53)	1.52(2)
C(48)-H(48)	0.9500	C(49)-C(52)	1.52(2)
C(49)-C(51)	1.55(2)	C(49)-C(50)	1.55(2)
C(50)-H(50A)	0.9800	C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800	C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800	C(51)-H(51C)	0.9800
C(52)-H(52A)	0.9800	C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800	C(53)-C(54)	1.47(2)
C(53)-C(55)	1.49(2)	C(53)-C(56)	1.55(2)
C(54)-H(54A)	0.9800	C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800	C(55)-H(55A)	0.9800
C(55)-H(55B)	0.9800	C(55)-H(55C)	0.9800
C(56)-H(56A)	0.9800	C(56)-H(56B)	0.9800
C(56)-H(56C)	0.9800	C(57)-C(58)	1.52(2)
C(57)-H(57A)	0.9900	C(57)-H(57B)	0.9900
C(58)-C(59)	1.52(3)	C(58)-H(58A)	0.9900
C(58)-H(58B)	0.9900	C(59)-C(60)	1.53(2)
C(59)-H(59A)	0.9900	C(59)-H(59B)	0.9900
C(60)-H(60A)	0.9900	C(60)-H(60B)	0.9900

O(1)-Sm(1)-C(5)

137.1(3)

O(1)-Sm(1)-C(4)

127.0(3)

C(5)-Sm(1)-C(4)	29.8(4)	O(1)-Sm(1)-C(17)	136.1(3)
C(5)-Sm(1)-C(17)	86.5(4)	C(4)-Sm(1)-C(17)	87.0(4)
O(1)-Sm(1)-C(16)	108.2(3)	C(5)-Sm(1)-C(16)	112.6(4)
C(4)-Sm(1)-C(16)	103.3(4)	C(17)-Sm(1)-C(16)	29.1(3)
O(1)-Sm(1)-C(18)	130.1(3)	C(5)-Sm(1)-C(18)	88.4(4)
C(4)-Sm(1)-C(18)	102.7(4)	C(17)-Sm(1)-C(18)	29.6(4)
C(16)-Sm(1)-C(18)	48.2(4)	O(1)-Sm(1)-C(15)	89.8(3)
C(5)-Sm(1)-C(15)	132.9(4)	C(4)-Sm(1)-C(15)	132.2(4)
C(17)-Sm(1)-C(15)	47.9(4)	C(16)-Sm(1)-C(15)	29.6(4)
C(18)-Sm(1)-C(15)	47.1(4)	O(1)-Sm(1)-C(1)	110.1(3)
C(5)-Sm(1)-C(1)	29.5(3)	C(4)-Sm(1)-C(1)	48.6(4)
C(17)-Sm(1)-C(1)	113.5(4)	C(16)-Sm(1)-C(1)	141.5(4)
C(18)-Sm(1)-C(1)	106.0(4)	C(15)-Sm(1)-C(1)	152.4(3)
O(1)-Sm(1)-C(2)	89.7(3)	C(5)-Sm(1)-C(2)	47.8(4)
C(4)-Sm(1)-C(2)	47.4(4)	C(17)-Sm(1)-C(2)	132.3(4)
C(16)-Sm(1)-C(2)	149.6(4)	C(18)-Sm(1)-C(2)	134.1(4)
C(15)-Sm(1)-C(2)	178.4(3)	C(1)-Sm(1)-C(2)	29.1(3)
O(1)-Sm(1)-C(3)	98.4(3)	C(5)-Sm(1)-C(3)	48.3(4)
C(4)-Sm(1)-C(3)	28.8(4)	C(17)-Sm(1)-C(3)	113.6(4)
C(16)-Sm(1)-C(3)	121.8(4)	C(18)-Sm(1)-C(3)	131.5(4)
C(15)-Sm(1)-C(3)	150.0(4)	C(1)-Sm(1)-C(3)	48.4(3)
C(2)-Sm(1)-C(3)	28.7(3)	O(1)-Sm(1)-C(14)	101.7(3)
C(5)-Sm(1)-C(14)	114.8(4)	C(4)-Sm(1)-C(14)	131.0(4)
C(17)-Sm(1)-C(14)	48.4(4)	C(16)-Sm(1)-C(14)	48.8(4)
C(18)-Sm(1)-C(14)	28.4(3)	C(15)-Sm(1)-C(14)	29.0(3)
C(1)-Sm(1)-C(14)	124.5(3)	C(2)-Sm(1)-C(14)	152.6(4)
C(3)-Sm(1)-C(14)	159.8(4)	C(30)-O(1)-C(27)	110(1)
C(30)-O(1)-Sm(1)	129.1(7)	C(27)-O(1)-Sm(1)	121.3(7)
C(5)-C(1)-C(2)	105(1)	C(5)-C(1)-C(6)	127(1)
C(2)-C(1)-C(6)	128(1)	C(5)-C(1)-Sm(1)	71.9(7)
C(2)-C(1)-Sm(1)	75.8(7)	C(6)-C(1)-Sm(1)	118.6(8)
C(3)-C(2)-C(1)	110(1)	C(3)-C(2)-Sm(1)	75.8(8)
C(1)-C(2)-Sm(1)	75.1(7)	C(3)-C(2)-H(2)	124.9
C(1)-C(2)-H(2)	124.9	Sm(1)-C(2)-H(2)	116.1
C(4)-C(3)-C(2)	107(1)	C(4)-C(3)-C(10)	128(1)
C(2)-C(3)-C(10)	126(1)	C(4)-C(3)-Sm(1)	72.8(8)
C(2)-C(3)-Sm(1)	75.5(7)	C(10)-C(3)-Sm(1)	121.3(8)
C(3)-C(4)-C(5)	109(1)	C(3)-C(4)-Sm(1)	78.4(7)
C(5)-C(4)-Sm(1)	74.1(7)	C(3)-C(4)-H(4)	125.6
C(5)-C(4)-H(4)	125.6	Sm(1)-C(4)-H(4)	114.1
C(4)-C(5)-C(1)	109(1)	C(4)-C(5)-Sm(1)	76.1(7)
C(1)-C(5)-Sm(1)	78.6(7)	C(4)-C(5)-H(5)	125.6
C(1)-C(5)-H(5)	125.6	Sm(1)-C(5)-H(5)	112.1
C(1)-C(6)-C(8)	110(1)	C(1)-C(6)-C(9)	113(1)
C(8)-C(6)-C(9)	108(1)	C(1)-C(6)-C(7)	111(1)
C(8)-C(6)-C(7)	109(1)	C(9)-C(6)-C(7)	107(1)
C(6)-C(7)-H(7A)	109.5	C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5	C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5	H(7B)-C(7)-H(7C)	109.5
C(6)-C(8)-H(8A)	109.5	C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5	C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5	H(8B)-C(8)-H(8C)	109.5
C(6)-C(9)-H(9A)	109.5	C(6)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5	C(6)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5	H(9B)-C(9)-H(9C)	109.5
C(11)-C(10)-C(13)	114(2)	C(11)-C(10)-C(3)	112(1)
C(13)-C(10)-C(3)	110(1)	C(11)-C(10)-C(12)	107(2)
C(13)-C(10)-C(12)	104(2)	C(3)-C(10)-C(12)	111(1)
C(10)-C(11)-H(11A)	109.5	C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5	C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5	H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5	C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5	C(10)-C(12)-H(12C)	109.5

H(12A)-C(12)-H(12C)	109.5	H(12B)-C(12)-H(12C)	109.5
C(10)-C(13)-H(13A)	109.5	C(10)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5	C(10)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5	H(13B)-C(13)-H(13C)	109.5
C(18)-C(14)-C(15)	106(1)	C(18)-C(14)-C(19)	128(1)
C(15)-C(14)-C(19)	125(1)	C(18)-C(14)-Sm(1)	74.1(7)
C(15)-C(14)-Sm(1)	74.6(7)	C(19)-C(14)-Sm(1)	116.9(8)
C(14)-C(15)-C(16)	110(1)	C(14)-C(15)-Sm(1)	76.4(7)
C(16)-C(15)-Sm(1)	74.3(7)	C(14)-C(15)-H(15)	125.2
C(16)-C(15)-H(15)	125.2	Sm(1)-C(15)-H(15)	115.9
C(17)-C(16)-C(15)	106(1)	C(17)-C(16)-C(23)	128(1)
C(15)-C(16)-C(23)	126(1)	C(17)-C(16)-Sm(1)	74.8(7)
C(15)-C(16)-Sm(1)	76.1(6)	C(23)-C(16)-Sm(1)	118.4(8)
C(16)-C(17)-C(18)	108(1)	C(16)-C(17)-Sm(1)	76.1(7)
C(18)-C(17)-Sm(1)	76.0(7)	C(16)-C(17)-H(17)	126.1
C(18)-C(17)-H(17)	126.1	Sm(1)-C(17)-H(17)	114.2
C(14)-C(18)-C(17)	110(1)	C(14)-C(18)-Sm(1)	77.4(7)
C(17)-C(18)-Sm(1)	74.4(7)	C(14)-C(18)-H(18)	125.0
C(17)-C(18)-H(18)	125.0	Sm(1)-C(18)-H(18)	115.1
C(22)-C(19)-C(14)	110(1)	C(22)-C(19)-C(21)	107(1)
C(14)-C(19)-C(21)	111(1)	C(22)-C(19)-C(20)	110(2)
C(14)-C(19)-C(20)	110(1)	C(21)-C(19)-C(20)	109(1)
C(19)-C(20)-H(20A)	109.5	C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5	C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5	H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5	C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5	C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5	H(21B)-C(21)-H(21C)	109.5
C(19)-C(22)-H(22A)	109.5	C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5	C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5	H(22B)-C(22)-H(22C)	109.5
C(26)-C(23)-C(25)	109(1)	C(26)-C(23)-C(16)	111(1)
C(25)-C(23)-C(16)	109(1)	C(26)-C(23)-C(24)	109(1)
C(25)-C(23)-C(24)	108(1)	C(16)-C(23)-C(24)	110(1)
C(23)-C(24)-H(24A)	109.5	C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5	C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5	H(24B)-C(24)-H(24C)	109.5
C(23)-C(25)-H(25A)	109.5	C(23)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5	C(23)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5	H(25B)-C(25)-H(25C)	109.5
C(23)-C(26)-H(26A)	109.5	C(23)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5	C(23)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5	H(26B)-C(26)-H(26C)	109.5
O(1)-C(27)-C(28)	104(1)	O(1)-C(27)-H(27A)	111.1
C(28)-C(27)-H(27A)	111.1	O(1)-C(27)-H(27B)	111.1
C(28)-C(27)-H(27B)	111.1	H(27A)-C(27)-H(27B)	109.0
C(29)-C(28)-C(27)	105(1)	C(29)-C(28)-H(28A)	110.8
C(27)-C(28)-H(28A)	110.8	C(29)-C(28)-H(28B)	110.8
C(27)-C(28)-H(28B)	110.8	H(28A)-C(28)-H(28B)	108.8
C(28)-C(29)-C(30)	103(1)	C(28)-C(29)-H(29A)	111.1
C(30)-C(29)-H(29A)	111.1	C(28)-C(29)-H(29B)	111.1
C(30)-C(29)-H(29B)	111.1	H(29A)-C(29)-H(29B)	109.0
O(1)-C(30)-C(29)	107(1)	O(1)-C(30)-H(30A)	110.3
C(29)-C(30)-H(30A)	110.3	O(1)-C(30)-H(30B)	110.3
C(29)-C(30)-H(30B)	110.3	H(30A)-C(30)-H(30B)	108.6
O(2)-Sm(2)-C(35)	126.5(4)	O(2)-Sm(2)-C(34)	135.8(3)
C(35)-Sm(2)-C(34)	29.3(4)	O(2)-Sm(2)-C(46)	140.4(3)
C(35)-Sm(2)-C(46)	88.8(5)	C(34)-Sm(2)-C(46)	83.6(4)
O(2)-Sm(2)-C(45)	127.8(3)	C(35)-Sm(2)-C(45)	105.4(5)
C(34)-Sm(2)-C(45)	87.7(4)	C(46)-Sm(2)-C(45)	29.2(4)
O(2)-Sm(2)-C(32)	88.9(3)	C(35)-Sm(2)-C(32)	47.2(5)
C(34)-Sm(2)-C(32)	47.3(4)	C(46)-Sm(2)-C(32)	130.7(4)
C(45)-Sm(2)-C(32)	130.1(4)	O(2)-Sm(2)-C(33)	109.2(3)

C(35)-Sm(2)-C(33)	48.0(4)	C(34)-Sm(2)-C(33)	29.0(4)
C(46)-Sm(2)-C(33)	108.2(4)	C(45)-Sm(2)-C(33)	101.5(4)
C(32)-Sm(2)-C(33)	28.7(4)	O(2)-Sm(2)-C(44)	99.3(3)
C(35)-Sm(2)-C(44)	134.2(5)	C(34)-Sm(2)-C(44)	116.0(4)
C(46)-Sm(2)-C(44)	48.1(4)	C(45)-Sm(2)-C(44)	29.3(4)
C(32)-Sm(2)-C(44)	149.4(4)	C(33)-Sm(2)-C(44)	122.8(4)
O(2)-Sm(2)-C(47)	114.5(3)	C(35)-Sm(2)-C(47)	103.5(4)
C(34)-Sm(2)-C(47)	108.9(4)	C(46)-Sm(2)-C(47)	29.3(4)
C(45)-Sm(2)-C(47)	48.3(4)	C(32)-Sm(2)-C(47)	150.7(4)
C(33)-Sm(2)-C(47)	136.3(4)	C(44)-Sm(2)-C(47)	48.0(4)
O(2)-Sm(2)-C(48)	92.8(3)	C(35)-Sm(2)-C(48)	132.1(4)
C(34)-Sm(2)-C(48)	130.9(4)	C(46)-Sm(2)-C(48)	47.7(4)
C(45)-Sm(2)-C(48)	47.8(4)	C(32)-Sm(2)-C(48)	177.9(4)
C(33)-Sm(2)-C(48)	149.2(4)	C(44)-Sm(2)-C(48)	28.9(4)
C(47)-Sm(2)-C(48)	28.8(4)	O(2)-Sm(2)-C(31)	97.7(4)
C(35)-Sm(2)-C(31)	29.0(5)	C(34)-Sm(2)-C(31)	48.0(4)
C(46)-Sm(2)-C(31)	117.1(5)	C(45)-Sm(2)-C(31)	133.6(4)
C(32)-Sm(2)-C(31)	28.5(4)	C(33)-Sm(2)-C(31)	47.8(4)
C(44)-Sm(2)-C(31)	162.8(4)	C(47)-Sm(2)-C(31)	125.2(4)
C(48)-Sm(2)-C(31)	152.1(4)	C(60)-O(2)-C(57)	109(1)
C(60)-O(2)-Sm(2)	129.1(8)	C(57)-O(2)-Sm(2)	122(1)
C(32)-C(31)-C(35)	106(1)	C(32)-C(31)-C(36)	124(2)
C(35)-C(31)-C(36)	129(2)	C(32)-C(31)-Sm(2)	74.8(7)
C(35)-C(31)-Sm(2)	73.3(8)	C(36)-C(31)-Sm(2)	120(1)
C(31)-C(32)-C(33)	111(1)	C(31)-C(32)-Sm(2)	76.7(8)
C(33)-C(32)-Sm(2)	75.7(7)	C(31)-C(32)-H(32)	124.8
C(33)-C(32)-H(32)	124.8	Sm(2)-C(32)-H(32)	114.7
C(32)-C(33)-C(34)	107(1)	C(32)-C(33)-C(40)	128(1)
C(34)-C(33)-C(40)	125(1)	C(32)-C(33)-Sm(2)	75.6(7)
C(34)-C(33)-Sm(2)	74.3(7)	C(40)-C(33)-Sm(2)	115.8(8)
C(33)-C(34)-C(35)	108(1)	C(33)-C(34)-Sm(2)	76.7(7)
C(35)-C(34)-Sm(2)	75.1(8)	C(33)-C(34)-H(34)	126.0
C(35)-C(34)-H(34)	126.0	Sm(2)-C(34)-H(34)	114.5
C(31)-C(35)-C(34)	109(1)	C(31)-C(35)-Sm(2)	77.8(8)
C(34)-C(35)-Sm(2)	75.6(8)	C(31)-C(35)-H(35)	125.7
C(34)-C(35)-H(35)	125.7	Sm(2)-C(35)-H(35)	113.3
C(37)-C(36)-C(39)	126(2)	C(37)-C(36)-C(31)	113(2)
C(39)-C(36)-C(31)	112(1)	C(37)-C(36)-C(38)	96(2)
C(39)-C(36)-C(38)	100(2)	C(31)-C(36)-C(38)	104(2)
C(36)-C(37)-H(37A)	109.5	C(36)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5	C(36)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5	H(37B)-C(37)-H(37C)	109.5
C(36)-C(38)-H(38A)	109.5	C(36)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5	C(36)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5	H(38B)-C(38)-H(38C)	109.5
C(36)-C(39)-H(39A)	109.5	C(36)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5	C(36)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5	H(39B)-C(39)-H(39C)	109.5
C(41)-C(40)-C(42)	117(2)	C(41)-C(40)-C(33)	112(1)
C(42)-C(40)-C(33)	111(1)	C(41)-C(40)-C(43)	105(2)
C(42)-C(40)-C(43)	104(2)	C(33)-C(40)-C(43)	108(2)
C(40)-C(41)-H(41A)	109.5	C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5	C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5	H(41B)-C(41)-H(41C)	109.5
C(40)-C(42)-H(42A)	109.5	C(40)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5	C(40)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5	H(42B)-C(42)-H(42C)	109.5
C(40)-C(43)-H(43A)	109.5	C(40)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5	C(40)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5	H(43B)-C(43)-H(43C)	109.5
C(48)-C(44)-C(45)	107(1)	C(48)-C(44)-C(49)	125(1)
C(45)-C(44)-C(49)	127(1)	C(48)-C(44)-Sm(2)	75.8(7)
C(45)-C(44)-Sm(2)	74.3(7)	C(49)-C(44)-Sm(2)	120.7(8)

C(46)-C(45)-C(44)	108(1)	C(46)-C(45)-Sm(2)	75.1(8)
C(44)-C(45)-Sm(2)	76.5(7)	C(46)-C(45)-H(45)	126.1
C(44)-C(45)-H(45)	126.1	Sm(2)-C(45)-H(45)	114.6
C(45)-C(46)-C(47)	109(1)	C(45)-C(46)-Sm(2)	75.6(7)
C(47)-C(46)-Sm(2)	76.8(8)	C(45)-C(46)-H(46)	125.7
C(47)-C(46)-H(46)	125.7	Sm(2)-C(46)-H(46)	114.1
C(48)-C(47)-C(46)	107(1)	C(48)-C(47)-C(53)	128(1)
C(46)-C(47)-C(53)	125(1)	C(48)-C(47)-Sm(2)	75.7(8)
C(46)-C(47)-Sm(2)	73.8(7)	C(53)-C(47)-Sm(2)	119(1)
C(47)-C(48)-C(44)	109(1)	C(47)-C(48)-Sm(2)	75.5(8)
C(44)-C(48)-Sm(2)	75.3(7)	C(47)-C(48)-H(48)	125.3
C(44)-C(48)-H(48)	125.3	Sm(2)-C(48)-H(48)	115.9
C(52)-C(49)-C(44)	112(1)	C(52)-C(49)-C(51)	109(1)
C(44)-C(49)-C(51)	111(1)	C(52)-C(49)-C(50)	108(1)
C(44)-C(49)-C(50)	109(1)	C(51)-C(49)-C(50)	108(1)
C(49)-C(50)-H(50A)	109.5	C(49)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5	C(49)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5	H(50B)-C(50)-H(50C)	109.5
C(49)-C(51)-H(51A)	109.5	C(49)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5	C(49)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5	H(51B)-C(51)-H(51C)	109.5
C(49)-C(52)-H(52A)	109.5	C(49)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5	C(49)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5	H(52B)-C(52)-H(52C)	109.5
C(54)-C(53)-C(55)	114(2)	C(54)-C(53)-C(47)	112(1)
C(55)-C(53)-C(47)	112(1)	C(54)-C(53)-C(56)	106(2)
C(55)-C(53)-C(56)	104(2)	C(47)-C(53)-C(56)	108(1)
C(53)-C(54)-H(54A)	109.5	C(53)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5	C(53)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5	H(54B)-C(54)-H(54C)	109.5
C(53)-C(55)-H(55A)	109.5	C(53)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5	C(53)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5	H(55B)-C(55)-H(55C)	109.5
C(53)-C(56)-H(56A)	109.5	C(53)-C(56)-H(56B)	109.5
H(56A)-C(56)-H(56B)	109.5	C(53)-C(56)-H(56C)	109.5
H(56A)-C(56)-H(56C)	109.5	H(56B)-C(56)-H(56C)	109.5
O(2)-C(57)-C(58)	107(1)	O(2)-C(57)-H(57A)	110.3
C(58)-C(57)-H(57A)	110.3	O(2)-C(57)-H(57B)	110.3
C(58)-C(57)-H(57B)	110.3	H(57A)-C(57)-H(57B)	108.6
C(57)-C(58)-C(59)	103(1)	C(57)-C(58)-H(58A)	111.1
C(59)-C(58)-H(58A)	111.1	C(57)-C(58)-H(58B)	111.1
C(59)-C(58)-H(58B)	111.1	H(58A)-C(58)-H(58B)	109.1
C(58)-C(59)-C(60)	101(1)	C(58)-C(59)-H(59A)	111.5
C(60)-C(59)-H(59A)	111.5	C(58)-C(59)-H(59B)	111.5
C(60)-C(59)-H(59B)	111.5	H(59A)-C(59)-H(59B)	109.3
O(2)-C(60)-C(59)	105(1)	O(2)-C(60)-H(60A)	110.8
C(59)-C(60)-H(60A)	110.8	O(2)-C(60)-H(60B)	110.8
C(59)-C(60)-H(60B)	110.8	H(60A)-C(60)-H(60B)	108.9

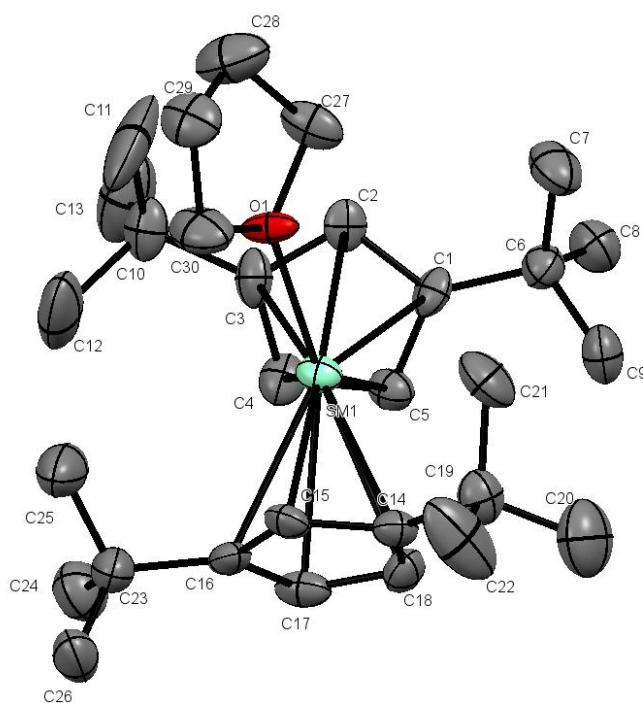


Figure S25: ORTEP of **5** with 50% probability ellipsoids (one of the two molecules and hydrogen atoms have been removed for clarity).

Table S9: Bond length (in Å) and angles (in °) for **6**.

C10—C13	1.535 (7)	O1—Sm1 ⁱ	2.3590 (14)
C10—C12	1.535 (7)	C37—C36	1.363 (10)
C10—C11	1.538 (7)	C37—C38	1.388 (9)
C10—C5	1.551 (6)	C38—C37 ⁱⁱ	1.388 (9)
C24—C23	1.531 (7)	C38—C39	1.532 (14)
C27—C28	1.531 (7)	C36—C35	1.326 (8)
C27—C30	1.531 (7)	C35—C36 ⁱⁱ	1.325 (8)
C27—C29	1.539 (7)	Sm1—C19	2.722 (4)
C27—C20	1.552 (6)	Sm1—C4	2.725 (4)
C31—C33	1.534 (7)	Sm1—C3	2.747 (5)
C31—C21	1.544 (6)	Sm1—C18	2.770 (4)
C31—C32	1.549 (7)	Sm1—C2	2.793 (4)
C31—C34	1.554 (7)	Sm1—C22	2.832 (5)
C15—C14	1.537 (7)	Sm1—C5	2.870 (4)
C8—C6	1.552 (7)	Sm1—C20	2.873 (4)
C6—C7	1.530 (7)	Sm1—C1	2.923 (4)
C6—C1	1.541 (6)	Sm1—C21	2.962 (5)
C6—C9	1.542 (6)	C4—C3	1.420 (6)
C17—C14	1.531 (7)	C4—C5	1.425 (6)
C25—C23	1.526 (7)	C19—C18	1.417 (6)
C23—C18	1.520 (6)	C19—C20	1.426 (6)

C23—C26	1.528 (7)	C2—C3	1.390 (7)
C14—C3	1.520 (6)	C2—C1	1.431 (6)
C14—C16	1.526 (7)	C1—C5	1.430 (6)
O2—O1	1.519 (6)	C22—C18	1.400 (6)
O2—Sm1	2.3576 (14)	C22—C21	1.436 (6)
O2—Sm1 ⁱ	2.3576 (14)	C20—C21	1.433 (7)
O1—Sm1	2.3590 (14)		
C13—C10—C12	106.2 (4)	C18—Sm1—C5	120.84 (13)
C13—C10—C11	105.1 (4)	C2—Sm1—C5	47.61 (13)
C12—C10—C11	110.3 (4)	C22—Sm1—C5	113.57 (13)
C13—C10—C5	109.0 (4)	O2—Sm1—C20	111.64 (11)
C12—C10—C5	112.9 (4)	O1—Sm1—C20	91.04 (11)
C11—C10—C5	112.8 (4)	C19—Sm1—C20	29.38 (13)
C28—C27—C30	110.7 (4)	C4—Sm1—C20	148.89 (13)
C28—C27—C29	105.7 (4)	C3—Sm1—C20	120.28 (13)
C30—C27—C29	106.4 (4)	C18—Sm1—C20	48.75 (13)
C28—C27—C20	111.6 (4)	C2—Sm1—C20	113.03 (13)
C30—C27—C20	113.0 (4)	C22—Sm1—C20	47.24 (13)
C29—C27—C20	109.1 (4)	C5—Sm1—C20	158.78 (13)
C33—C31—C21	117.1 (4)	O2—Sm1—C1	115.03 (12)
C33—C31—C32	105.6 (4)	O1—Sm1—C1	137.29 (10)
C21—C31—C32	112.1 (4)	C19—Sm1—C1	128.90 (13)
C33—C31—C34	109.1 (4)	C4—Sm1—C1	47.77 (13)
C21—C31—C34	106.7 (4)	C3—Sm1—C1	48.30 (13)
C32—C31—C34	105.6 (4)	C18—Sm1—C1	99.22 (13)
C7—C6—C1	112.1 (4)	C2—Sm1—C1	28.88 (12)
C7—C6—C9	105.7 (4)	C22—Sm1—C1	85.69 (13)
C1—C6—C9	116.9 (4)	C5—Sm1—C1	28.57 (13)
C7—C6—C8	106.5 (4)	C20—Sm1—C1	130.38 (13)
C1—C6—C8	105.8 (4)	O2—Sm1—C21	139.68 (10)
C9—C6—C8	109.5 (4)	O1—Sm1—C21	116.56 (12)
C18—C23—C26	109.3 (4)	C19—Sm1—C21	47.55 (13)
C18—C23—C25	108.8 (4)	C4—Sm1—C21	128.88 (13)
C26—C23—C25	111.0 (4)	C3—Sm1—C21	99.02 (13)
C18—C23—C24	110.6 (4)	C18—Sm1—C21	48.01 (13)
C26—C23—C24	108.7 (4)	C2—Sm1—C21	85.41 (13)
C25—C23—C24	108.4 (4)	C22—Sm1—C21	28.58 (13)
C3—C14—C16	109.6 (4)	C5—Sm1—C21	130.52 (13)
C3—C14—C17	109.4 (4)	C20—Sm1—C21	28.37 (13)
C16—C14—C17	111.5 (4)	C1—Sm1—C21	102.58 (13)
C3—C14—C15	110.6 (4)	C3—C4—C5	109.9 (4)

C16—C14—C15	108.2 (4)	C3—C4—Sm1	75.8 (3)
C17—C14—C15	107.5 (4)	C5—C4—Sm1	80.9 (3)
O1—O2—Sm1	71.27 (10)	C18—C19—C20	110.1 (4)
O1—O2—Sm1 ⁱ	71.27 (10)	C18—C19—Sm1	76.9 (3)
Sm1—O2—Sm1 ⁱ	142.5 (2)	C20—C19—Sm1	81.2 (3)
O2—O1—Sm1	71.17 (10)	C3—C2—C1	111.0 (4)
O2—O1—Sm1 ⁱ	71.17 (10)	C3—C2—Sm1	73.7 (3)
Sm1—O1—Sm1 ⁱ	142.3 (2)	C1—C2—Sm1	80.6 (3)
C36—C37—C38	120.7 (6)	C5—C1—C2	106.1 (4)
C37 ⁱⁱ —C38—C37	116.4 (8)	C5—C1—C6	132.1 (4)
C37 ⁱⁱ —C38—C39	121.8 (4)	C2—C1—C6	117.1 (4)
C37—C38—C39	121.8 (4)	C5—C1—Sm1	73.6 (2)
C35—C36—C37	120.4 (7)	C2—C1—Sm1	70.5 (2)
C36 ⁱⁱ —C35—C36	121.2 (10)	C6—C1—Sm1	138.9 (3)
O2—Sm1—O1	37.56 (14)	C18—C22—C21	111.1 (4)
O2—Sm1—C19	95.12 (10)	C18—C22—Sm1	73.1 (3)
O1—Sm1—C19	91.72 (10)	C21—C22—Sm1	80.7 (3)
O2—Sm1—C4	88.92 (10)	C19—C20—C21	107.2 (4)
O1—Sm1—C4	92.17 (10)	C19—C20—C27	120.3 (4)
C19—Sm1—C4	175.81 (14)	C21—C20—C27	131.9 (4)
O2—Sm1—C3	116.40 (10)	C19—C20—Sm1	69.4 (2)
O1—Sm1—C3	106.23 (10)	C21—C20—Sm1	79.2 (3)
C19—Sm1—C3	146.56 (14)	C27—C20—Sm1	122.2 (3)
C4—Sm1—C3	30.07 (13)	C22—C18—C19	105.7 (4)
O2—Sm1—C18	109.14 (10)	C22—C18—C23	127.2 (4)
O1—Sm1—C18	119.16 (10)	C19—C18—C23	127.0 (4)
C19—Sm1—C18	29.89 (13)	C22—C18—Sm1	78.0 (3)
C4—Sm1—C18	146.99 (13)	C19—C18—Sm1	73.2 (2)
C3—Sm1—C18	132.02 (14)	C23—C18—Sm1	117.3 (3)
O2—Sm1—C2	134.87 (10)	C20—C21—C22	105.7 (4)
O1—Sm1—C2	135.17 (10)	C20—C21—C31	133.0 (4)
C19—Sm1—C2	127.88 (14)	C22—C21—C31	117.0 (4)
C4—Sm1—C2	47.93 (14)	C20—C21—Sm1	72.4 (2)
C3—Sm1—C2	29.05 (14)	C22—C21—Sm1	70.7 (3)
C18—Sm1—C2	104.71 (14)	C31—C21—Sm1	138.6 (3)
O2—Sm1—C22	137.97 (10)	C4—C5—C1	106.9 (4)
O1—Sm1—C22	137.02 (10)	C4—C5—C10	121.0 (4)
C19—Sm1—C22	47.62 (14)	C1—C5—C10	131.7 (4)
C4—Sm1—C22	128.21 (14)	C4—C5—Sm1	69.7 (2)
C3—Sm1—C22	104.75 (14)	C1—C5—Sm1	77.8 (2)
C18—Sm1—C22	28.91 (13)	C10—C5—Sm1	122.3 (3)
C2—Sm1—C22	80.52 (14)	C2—C3—C4	105.9 (4)

O2—Sm1—C5	88.92 (11)	C2—C3—C14	126.9 (4)
O1—Sm1—C5	109.20 (10)	C4—C3—C14	127.0 (4)
C19—Sm1—C5	149.30 (13)	C2—C3—Sm1	77.3 (3)
C4—Sm1—C5	29.37 (13)	C4—C3—Sm1	74.1 (3)
C3—Sm1—C5	48.94 (13)	C14—C3—Sm1	118.2 (3)

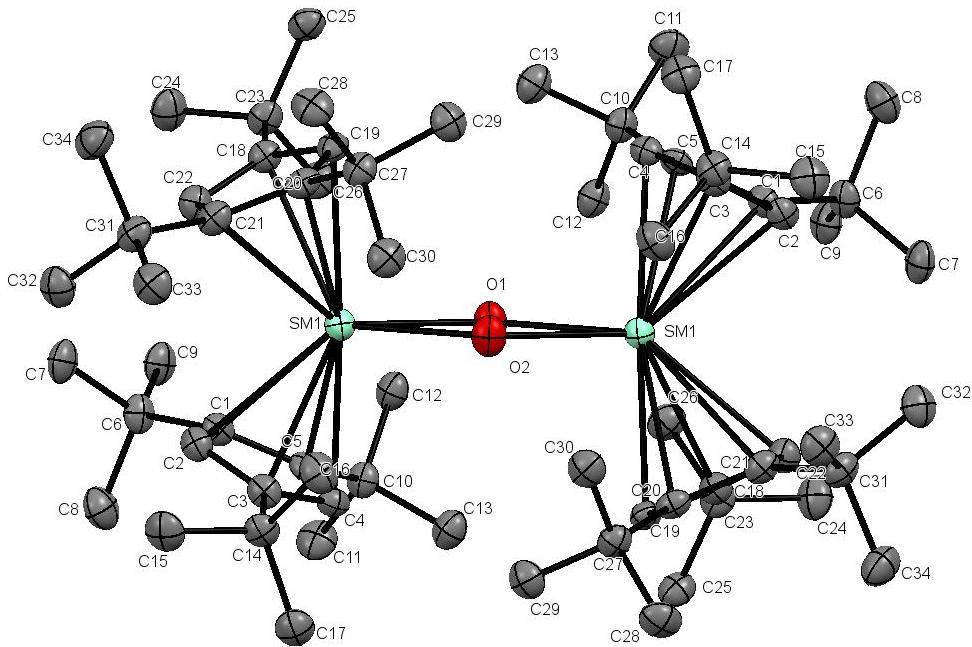


Figure S26: ORTEP of **6** with 50% probability ellipsoids (one molecule of toluene and hydrogen atoms have been removed for clarity).

Table S10: Bond length (in Å) and angles (in °) for **7**.

Sm(1)-O(3)	2.379 (7)	Sm(1)-O(1)	2.386 (6)
Sm(1)-C(23)	2.702 (5)	Sm(1)-C(6)	2.715 (5)
Sm(1)-C(20)	2.738 (5)	Sm(1)-C(19)	2.744 (5)
Sm(1)-C(4)	2.745 (5)	Sm(1)-C(1)	2.756 (6)
Sm(1)-C(5)	2.758 (5)	Sm(1)-C(22)	2.782 (5)
Sm(1)-C(2)	2.795 (5)	Sm(1)-C(21)	2.803 (5)
O(1)-C(1)	1.297 (4)	O(2)-C(1)	1.300 (4)
O(3)-C(1)	1.297 (4)	C(2)-C(6)	1.399 (7)
C(2)-C(3)	1.442 (7)	C(2)-C(7)	1.571 (7)
C(3)-C(4)	1.428 (7)	C(3)-C(11)	1.537 (7)
C(4)-C(5)	1.411 (7)	C(4)-H(4)	0.9500
C(5)-C(6)	1.413 (7)	C(5)-C(15)	1.526 (7)
C(6)-H(6)	0.9500	C(7)-C(9)	1.531 (8)
C(7)-C(8)	1.532 (7)	C(7)-C(10)	1.555 (8)
C(8)-H(8A)	0.9800	C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800	C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800	C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800	C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800	C(11)-C(14)	1.537 (7)
C(11)-C(12)	1.538 (8)	C(11)-C(13)	1.558 (7)

C(12)-H(12A)	0.9800	C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800	C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800	C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800	C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800	C(15)-C(18)	1.505(8)
C(15)-C(16)	1.521(8)	C(15)-C(17)	1.531(7)
C(16)-H(16A)	0.9800	C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800	C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800	C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800	C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800	C(19)-C(20)	1.407(7)
C(19)-C(23)	1.409(7)	C(19)-C(24)	1.536(7)
C(20)-C(21)	1.429(7)	C(20)-H(20)	0.9500
C(21)-C(22)	1.464(7)	C(21)-C(28)	1.539(7)
C(22)-C(23)	1.405(7)	C(22)-C(32)	1.536(7)
C(23)-H(23)	0.9500	C(24)-C(25)	1.496(8)
C(24)-C(26)	1.524(8)	C(24)-C(27)	1.53(1)
C(25)-H(25A)	0.9800	C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800	C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800	C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800	C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800	C(28)-C(30)	1.538(7)
C(28)-C(29)	1.544(7)	C(28)-C(31)	1.551(8)
C(29)-H(29A)	0.9800	C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800	C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800	C(30)-H(30C)	0.9800
C(31)-H(31A)	0.9800	C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800	C(32)-C(35)	1.531(7)
C(32)-C(33)	1.534(8)	C(32)-C(34)	1.567(7)
C(33)-H(33A)	0.9800	C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800	C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800	C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800	C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800		

O(3)-Sm(1)-O(1)	56.1(2)	O(3)-Sm(1)-C(23)	90.4(2)
O(1)-Sm(1)-C(23)	79.1(2)	O(3)-Sm(1)-C(6)	77.9(2)
O(1)-Sm(1)-C(6)	87.4(2)	C(23)-Sm(1)-C(6)	165.7(1)
O(3)-Sm(1)-C(20)	132.9(2)	O(1)-Sm(1)-C(20)	121.3(2)
C(23)-Sm(1)-C(20)	48.8(2)	C(6)-Sm(1)-C(20)	145.3(2)
O(3)-Sm(1)-C(19)	119.7(2)	O(1)-Sm(1)-C(19)	91.6(2)
C(23)-Sm(1)-C(19)	30.0(1)	C(6)-Sm(1)-C(19)	157.5(2)
C(20)-Sm(1)-C(19)	29.8(1)	O(3)-Sm(1)-C(4)	118.1(2)
O(1)-Sm(1)-C(4)	131.5(2)	C(23)-Sm(1)-C(4)	145.8(1)
C(6)-Sm(1)-C(4)	48.5(2)	C(20)-Sm(1)-C(4)	97.1(1)
C(19)-Sm(1)-C(4)	120.8(1)	O(3)-Sm(1)-C(1)	28.0(1)
O(1)-Sm(1)-C(1)	28.0(1)	C(23)-Sm(1)-C(1)	83.4(4)
C(6)-Sm(1)-C(1)	82.4(4)	C(20)-Sm(1)-C(1)	132.2(4)
C(19)-Sm(1)-C(1)	106.7(4)	C(4)-Sm(1)-C(1)	130.6(4)
O(3)-Sm(1)-C(5)	88.4(2)	O(1)-Sm(1)-C(5)	116.2(2)
C(23)-Sm(1)-C(5)	160.1(2)	C(6)-Sm(1)-C(5)	29.9(2)
C(20)-Sm(1)-C(5)	121.4(2)	C(19)-Sm(1)-C(5)	149.2(1)
C(4)-Sm(1)-C(5)	29.7(1)	C(1)-Sm(1)-C(5)	104.1(4)
O(3)-Sm(1)-C(22)	83.5(2)	O(1)-Sm(1)-C(22)	98.9(2)
C(23)-Sm(1)-C(22)	29.6(1)	C(6)-Sm(1)-C(22)	152.4(2)
C(20)-Sm(1)-C(22)	49.5(2)	C(19)-Sm(1)-C(22)	49.8(2)
C(4)-Sm(1)-C(22)	129.4(2)	C(1)-Sm(1)-C(22)	90.7(4)
C(5)-Sm(1)-C(22)	130.7(2)	O(3)-Sm(1)-C(2)	99.6(2)
O(1)-Sm(1)-C(2)	83.2(2)	C(23)-Sm(1)-C(2)	150.0(2)
C(6)-Sm(1)-C(2)	29.4(2)	C(20)-Sm(1)-C(2)	127.5(2)
C(19)-Sm(1)-C(2)	128.2(2)	C(4)-Sm(1)-C(2)	48.7(2)
C(1)-Sm(1)-C(2)	92.2(4)	C(5)-Sm(1)-C(2)	49.3(2)

C(22)-Sm(1)-C(2)	176.9(1)	O(3)-Sm(1)-C(21)	108.2(2)
O(1)-Sm(1)-C(21)	127.3(2)	C(23)-Sm(1)-C(21)	49.2(1)
C(6)-Sm(1)-C(21)	142.6(2)	C(20)-Sm(1)-C(21)	29.9(2)
C(19)-Sm(1)-C(21)	49.6(1)	C(4)-Sm(1)-C(21)	100.9(1)
C(1)-Sm(1)-C(21)	120.8(4)	C(5)-Sm(1)-C(21)	112.7(1)
C(22)-Sm(1)-C(21)	30.4(1)	C(2)-Sm(1)-C(21)	146.8(1)
C(1)-O(1)-Sm(1)	92.0(4)	C(1)-O(3)-Sm(1)	92.4(4)
O(3)-C(1)-O(1)	119.5(6)	O(3)-C(1)-O(2)	119.0(8)
O(1)-C(1)-O(2)	122(1)	O(3)-C(1)-Sm(1)	59.6(4)
O(1)-C(1)-Sm(1)	59.9(4)	O(2)-C(1)-Sm(1)	179(1)
C(6)-C(2)-C(3)	107.4(5)	C(6)-C(2)-C(7)	120.6(4)
C(3)-C(2)-C(7)	131.8(5)	C(6)-C(2)-Sm(1)	72.1(3)
C(3)-C(2)-Sm(1)	75.9(3)	C(7)-C(2)-Sm(1)	121.5(3)
C(4)-C(3)-C(2)	105.5(4)	C(4)-C(3)-C(11)	117.8(4)
C(2)-C(3)-C(11)	134.8(5)	C(4)-C(3)-Sm(1)	72.4(3)
C(2)-C(3)-Sm(1)	74.3(3)	C(11)-C(3)-Sm(1)	129.6(3)
C(5)-C(4)-C(3)	110.9(4)	C(5)-C(4)-Sm(1)	75.6(3)
C(3)-C(4)-Sm(1)	77.9(3)	C(5)-C(4)-H(4)	124.6
C(3)-C(4)-H(4)	124.6	Sm(1)-C(4)-H(4)	113.8
C(4)-C(5)-C(6)	105.1(5)	C(4)-C(5)-C(15)	128.1(5)
C(6)-C(5)-C(15)	126.8(4)	C(4)-C(5)-Sm(1)	74.6(3)
C(6)-C(5)-Sm(1)	73.4(3)	C(15)-C(5)-Sm(1)	116.9(3)
C(2)-C(6)-C(5)	111.0(5)	C(2)-C(6)-Sm(1)	78.5(3)
C(5)-C(6)-Sm(1)	76.7(3)	C(2)-C(6)-H(6)	124.5
C(5)-C(6)-H(6)	124.5	Sm(1)-C(6)-H(6)	112.3
C(9)-C(7)-C(8)	110.9(5)	C(9)-C(7)-C(10)	105.9(5)
C(8)-C(7)-C(10)	105.7(4)	C(9)-C(7)-C(2)	114.2(4)
C(8)-C(7)-C(2)	110.5(4)	C(10)-C(7)-C(2)	109.1(5)
C(7)-C(8)-H(8A)	109.5	C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5	C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5	H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5	C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5	C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5	H(9B)-C(9)-H(9C)	109.5
C(7)-C(10)-H(10A)	109.5	C(7)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5	C(7)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5	H(10B)-C(10)-H(10C)	109.5
C(3)-C(11)-C(14)	111.1(4)	C(3)-C(11)-C(12)	117.5(5)
C(14)-C(11)-C(12)	105.7(5)	C(3)-C(11)-C(13)	107.5(5)
C(14)-C(11)-C(13)	106.6(5)	C(12)-C(11)-C(13)	107.9(5)
C(11)-C(12)-H(12A)	109.5	C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5	C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5	H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5	C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5	C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5	H(13B)-C(13)-H(13C)	109.5
C(11)-C(14)-H(14A)	109.5	C(11)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5	C(11)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5	H(14B)-C(14)-H(14C)	109.5
C(18)-C(15)-C(16)	110.6(5)	C(18)-C(15)-C(5)	110.4(4)
C(16)-C(15)-C(5)	109.8(5)	C(18)-C(15)-C(17)	108.0(5)
C(16)-C(15)-C(17)	108.5(5)	C(5)-C(15)-C(17)	109.5(5)
C(15)-C(16)-H(16A)	109.5	C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5	C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5	H(16B)-C(16)-H(16C)	109.5
C(15)-C(17)-H(17A)	109.5	C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5	C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5	H(17B)-C(17)-H(17C)	109.5
C(15)-C(18)-H(18A)	109.5	C(15)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5	C(15)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5	H(18B)-C(18)-H(18C)	109.5
C(20)-C(19)-C(23)	105.9(4)	C(20)-C(19)-C(24)	128.5(5)
C(23)-C(19)-C(24)	125.2(4)	C(20)-C(19)-Sm(1)	74.9(3)

C(23)-C(19)-Sm(1)	73.4(3)	C(24)-C(19)-Sm(1)	121.7(3)
C(19)-C(20)-C(21)	110.4(4)	C(19)-C(20)-Sm(1)	75.4(3)
C(21)-C(20)-Sm(1)	77.6(3)	C(19)-C(20)-H(20)	124.8
C(21)-C(20)-H(20)	124.8	Sm(1)-C(20)-H(20)	114.2
C(20)-C(21)-C(22)	106.0(4)	C(20)-C(21)-C(28)	117.5(4)
C(22)-C(21)-C(28)	134.6(5)	C(20)-C(21)-Sm(1)	72.5(3)
C(22)-C(21)-Sm(1)	74.0(3)	C(28)-C(21)-Sm(1)	129.7(3)
C(23)-C(22)-C(21)	106.1(4)	C(23)-C(22)-C(32)	121.3(4)
C(21)-C(22)-C(32)	132.0(5)	C(23)-C(22)-Sm(1)	72.0(3)
C(21)-C(22)-Sm(1)	75.6(3)	C(32)-C(22)-Sm(1)	124.3(3)
C(22)-C(23)-C(19)	111.4(4)	C(22)-C(23)-Sm(1)	78.4(3)
C(19)-C(23)-Sm(1)	76.6(3)	C(22)-C(23)-H(23)	124.3
C(19)-C(23)-H(23)	124.3	Sm(1)-C(23)-H(23)	112.6
C(25)-C(24)-C(26)	109.6(5)	C(25)-C(24)-C(27)	109.9(6)
C(26)-C(24)-C(27)	107.7(6)	C(25)-C(24)-C(19)	111.2(5)
C(26)-C(24)-C(19)	111.1(5)	C(27)-C(24)-C(19)	107.3(5)
C(24)-C(25)-H(25A)	109.5	C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5	C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5	H(25B)-C(25)-H(25C)	109.5
C(24)-C(26)-H(26A)	109.5	C(24)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5	C(24)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5	H(26B)-C(26)-H(26C)	109.5
C(24)-C(27)-H(27A)	109.5	C(24)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5	C(24)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5	H(27B)-C(27)-H(27C)	109.5
C(30)-C(28)-C(21)	107.7(4)	C(30)-C(28)-C(29)	107.9(4)
C(21)-C(28)-C(29)	110.4(4)	C(30)-C(28)-C(31)	108.6(5)
C(21)-C(28)-C(31)	115.8(4)	C(29)-C(28)-C(31)	106.2(5)
C(28)-C(29)-H(29A)	109.5	C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5	C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5	H(29B)-C(29)-H(29C)	109.5
C(28)-C(30)-H(30A)	109.5	C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5	C(28)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5	H(30B)-C(30)-H(30C)	109.5
C(28)-C(31)-H(31A)	109.5	C(28)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5	C(28)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5	H(31B)-C(31)-H(31C)	109.5
C(35)-C(32)-C(33)	110.1(5)	C(35)-C(32)-C(22)	111.2(4)
C(33)-C(32)-C(22)	115.1(4)	C(35)-C(32)-C(34)	106.1(4)
C(33)-C(32)-C(34)	104.6(5)	C(22)-C(32)-C(34)	109.2(4)
C(32)-C(33)-H(33A)	109.5	C(32)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5	C(32)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5	H(33B)-C(33)-H(33C)	109.5
C(32)-C(34)-H(34A)	109.5	C(32)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5	C(32)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5	H(34B)-C(34)-H(34C)	109.5
C(32)-C(35)-H(35A)	109.5	C(32)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5	C(32)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5	H(35B)-C(35)-H(35C)	109.5

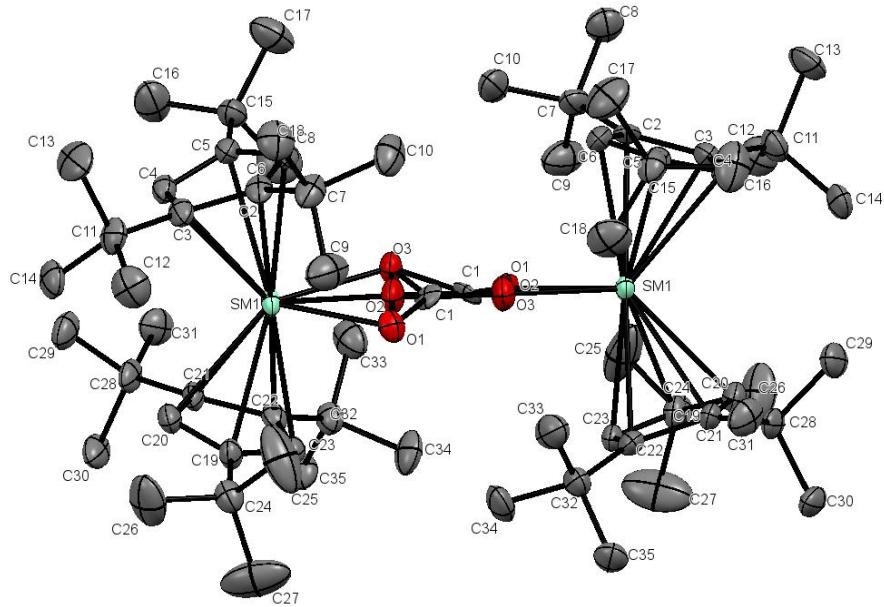


Figure S27: ORTEP of **7** with 50% probability ellipsoids (hydrogen atoms have been removed for clarity).

Table S11: Bond length (in Å) and angles (in °) for **8**.

Sm(1)-O(2)	2.36(1)	Sm(1)-O(1)	2.49(1)
Sm(1)-C(5)	2.66(2)	Sm(1)-C(17)	2.67(1)
Sm(1)-C(18)	2.69(2)	Sm(1)-C(4)	2.71(2)
Sm(1)-C(16)	2.73(1)	Sm(1)-C(14)	2.75(1)
Sm(1)-C(15)	2.75(1)	Sm(1)-C(1)	2.76(1)
Sm(1)-C(2)	2.77(2)	Sm(1)-C(3)	2.79(1)
Sm(2)-O(3)	2.35(1)	Sm(2)-O(1)	2.48(1)
Sm(2)-C(43)	2.65(2)	Sm(2)-C(31)	2.67(2)
Sm(2)-C(44)	2.68(2)	Sm(2)-C(30)	2.71(2)
Sm(2)-C(42)	2.72(1)	Sm(2)-C(41)	2.73(1)
Sm(2)-C(40)	2.75(2)	Sm(2)-C(29)	2.76(2)
Sm(2)-C(28)	2.76(2)	Sm(2)-C(27)	2.76(2)
O(1)-C(53)	1.57(2)	O(2)-C(53)	1.18(2)
O(3)-C(53)	1.15(2)	C(1)-C(5)	1.40(3)
C(1)-C(2)	1.41(2)	C(1)-C(6)	1.54(2)
C(2)-C(3)	1.39(3)	C(2)-H(2)	0.9300
C(3)-C(4)	1.44(2)	C(3)-C(10)	1.51(2)
C(4)-C(5)	1.37(2)	C(4)-H(4)	0.9300
C(5)-H(5)	0.9300	C(6)-C(7)	1.50(2)
C(6)-C(8)	1.53(3)	C(6)-C(9)	1.54(2)
C(7)-H(7A)	0.9600	C(7)-H(7B)	0.9600
C(7)-H(7C)	0.9600	C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600	C(8)-H(8C)	0.9600
C(9)-H(9A)	0.9600	C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600	C(10)-C(11)	1.51(3)
C(10)-C(12)	1.53(3)	C(10)-C(13)	1.57(3)
C(11)-H(11A)	0.9600	C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600	C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600	C(12)-H(12C)	0.9600
C(13)-H(13A)	0.9600	C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600	C(14)-C(18)	1.41(2)
C(14)-C(15)	1.44(2)	C(14)-C(19)	1.51(2)
C(15)-C(16)	1.43(2)	C(15)-H(15)	0.9300
C(16)-C(17)	1.42(2)	C(16)-C(23)	1.52(2)

C(17)-C(18)	1.37(2)	C(17)-H(17)	0.9300
C(18)-H(18)	0.9300	C(19)-C(20)	1.53(2)
C(19)-C(21)	1.53(2)	C(19)-C(22)	1.56(2)
C(20)-H(20A)	0.9600	C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600	C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600	C(21)-H(21C)	0.9600
C(22)-H(22A)	0.9600	C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600	C(23)-C(26)	1.50(2)
C(23)-C(24)	1.52(3)	C(23)-C(25)	1.53(2)
C(24)-H(24A)	0.9600	C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600	C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600	C(25)-H(25C)	0.9600
C(26)-H(26A)	0.9600	C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600	C(27)-C(28)	1.41(2)
C(27)-C(31)	1.42(3)	C(27)-C(32)	1.50(2)
C(28)-C(29)	1.43(2)	C(28)-H(28)	0.9300
C(29)-C(30)	1.40(2)	C(29)-C(36)	1.52(2)
C(30)-C(31)	1.41(3)	C(30)-H(30)	0.9300
C(31)-H(31)	0.9300	C(32)-C(33)	1.51(2)
C(32)-C(34)	1.53(2)	C(32)-C(35)	1.53(2)
C(33)-H(33A)	0.9600	C(33)-H(33B)	0.9600
C(33)-H(33C)	0.9600	C(34)-H(34A)	0.9600
C(34)-H(34B)	0.9600	C(34)-H(34C)	0.9600
C(35)-H(35A)	0.9600	C(35)-H(35B)	0.9600
C(35)-H(35C)	0.9600	C(36)-C(39)	1.48(3)
C(36)-C(37)	1.51(3)	C(36)-C(38)	1.56(3)
C(37)-H(37A)	0.9600	C(37)-H(37B)	0.9600
C(37)-H(37C)	0.9600	C(38)-H(38A)	0.9600
C(38)-H(38B)	0.9600	C(38)-H(38C)	0.9600
C(39)-H(39A)	0.9600	C(39)-H(39B)	0.9600
C(39)-H(39C)	0.9600	C(40)-C(41)	1.43(2)
C(40)-C(44)	1.44(3)	C(40)-C(45)	1.51(2)
C(41)-C(42)	1.38(2)	C(41)-H(41)	0.9300
C(42)-C(43)	1.41(2)	C(42)-C(49)	1.55(2)
C(43)-C(44)	1.39(2)	C(43)-H(43)	0.9300
C(44)-H(44)	0.9300	C(45)-C(46)	1.50(3)
C(45)-C(47)	1.51(2)	C(45)-C(48)	1.55(2)
C(46)-H(46A)	0.9600	C(46)-H(46B)	0.9600
C(46)-H(46C)	0.9600	C(47)-H(47A)	0.9600
C(47)-H(47B)	0.9600	C(47)-H(47C)	0.9600
C(48)-H(48A)	0.9600	C(48)-H(48B)	0.9600
C(48)-H(48C)	0.9600	C(49)-C(52)	1.49(3)
C(49)-C(51)	1.51(3)	C(49)-C(50)	1.61(3)
C(50)-H(50A)	0.9600	C(50)-H(50B)	0.9600
C(50)-H(50C)	0.9600	C(51)-H(51A)	0.9600
C(51)-H(51B)	0.9600	C(51)-H(51C)	0.9600
C(52)-H(52A)	0.9600	C(52)-H(52B)	0.9600
C(52)-H(52C)	0.9600		

O(2)-Sm(1)-O(1)	54.2(4)	O(2)-Sm(1)-C(5)	99.2(5)
O(1)-Sm(1)-C(5)	131.7(5)	O(2)-Sm(1)-C(17)	131.2(4)
O(1)-Sm(1)-C(17)	131.2(5)	C(5)-Sm(1)-C(17)	97.0(5)
O(2)-Sm(1)-C(18)	109.7(4)	O(1)-Sm(1)-C(18)	141.9(5)
C(5)-Sm(1)-C(18)	81.2(6)	C(17)-Sm(1)-C(18)	29.6(5)
O(2)-Sm(1)-C(4)	128.6(5)	O(1)-Sm(1)-C(4)	142.6(5)
C(5)-Sm(1)-C(4)	29.6(5)	C(17)-Sm(1)-C(4)	78.3(5)
C(18)-Sm(1)-C(4)	75.5(5)	O(2)-Sm(1)-C(16)	113.8(4)
O(1)-Sm(1)-C(16)	101.1(5)	C(5)-Sm(1)-C(16)	127.2(5)
C(17)-Sm(1)-C(16)	30.4(5)	C(18)-Sm(1)-C(16)	49.9(5)
C(4)-Sm(1)-C(16)	107.5(5)	O(2)-Sm(1)-C(14)	82.8(4)
O(1)-Sm(1)-C(14)	114.2(5)	C(5)-Sm(1)-C(14)	98.4(6)
C(17)-Sm(1)-C(14)	49.4(5)	C(18)-Sm(1)-C(14)	30.0(5)

C(4)-Sm(1)-C(14)	102.6(5)	C(16)-Sm(1)-C(14)	50.2(4)
O(2)-Sm(1)-C(15)	85.3(4)	O(1)-Sm(1)-C(15)	92.5(5)
C(5)-Sm(1)-C(15)	128.0(6)	C(17)-Sm(1)-C(15)	49.5(5)
C(18)-Sm(1)-C(15)	49.6(6)	C(4)-Sm(1)-C(15)	124.1(5)
C(16)-Sm(1)-C(15)	30.2(5)	C(14)-Sm(1)-C(15)	30.3(4)
O(2)-Sm(1)-C(1)	84.3(5)	O(1)-Sm(1)-C(1)	102.5(5)
C(5)-Sm(1)-C(1)	29.7(6)	C(17)-Sm(1)-C(1)	125.6(5)
C(18)-Sm(1)-C(1)	110.4(6)	C(4)-Sm(1)-C(1)	49.1(6)
C(16)-Sm(1)-C(1)	155.9(5)	C(14)-Sm(1)-C(1)	121.9(5)
C(15)-Sm(1)-C(1)	151.7(5)	O(2)-Sm(1)-C(2)	102.4(5)
O(1)-Sm(1)-C(2)	94.2(5)	C(5)-Sm(1)-C(2)	48.6(6)
C(17)-Sm(1)-C(2)	122.4(5)	C(18)-Sm(1)-C(2)	123.9(6)
C(4)-Sm(1)-C(2)	48.7(6)	C(16)-Sm(1)-C(2)	143.1(5)
C(14)-Sm(1)-C(2)	146.9(5)	C(15)-Sm(1)-C(2)	171.9(6)
C(1)-Sm(1)-C(2)	29.6(5)	O(2)-Sm(1)-C(3)	130.8(5)
O(1)-Sm(1)-C(3)	114.6(5)	C(5)-Sm(1)-C(3)	49.0(6)
C(17)-Sm(1)-C(3)	93.7(5)	C(18)-Sm(1)-C(3)	101.7(5)
C(4)-Sm(1)-C(3)	30.2(5)	C(16)-Sm(1)-C(3)	115.4(5)
C(14)-Sm(1)-C(3)	131.0(5)	C(15)-Sm(1)-C(3)	142.9(6)
C(1)-Sm(1)-C(3)	48.8(5)	C(2)-Sm(1)-C(3)	29.0(5)
O(3)-Sm(2)-O(1)	54.4(4)	O(3)-Sm(2)-C(43)	132.6(5)
O(1)-Sm(2)-C(43)	129.8(5)	O(3)-Sm(2)-C(31)	98.2(5)
O(1)-Sm(2)-C(31)	130.3(5)	C(43)-Sm(2)-C(31)	99.7(5)
O(3)-Sm(2)-C(44)	112.0(5)	O(1)-Sm(2)-C(44)	143.3(5)
C(43)-Sm(2)-C(44)	30.1(5)	C(31)-Sm(2)-C(44)	82.2(6)
O(3)-Sm(2)-C(30)	128.4(5)	O(1)-Sm(2)-C(30)	140.5(5)
C(43)-Sm(2)-C(30)	80.2(6)	C(31)-Sm(2)-C(30)	30.5(5)
C(44)-Sm(2)-C(30)	76.0(6)	O(3)-Sm(2)-C(42)	113.2(4)
O(1)-Sm(2)-C(42)	100.4(5)	C(43)-Sm(2)-C(42)	30.3(5)
C(31)-Sm(2)-C(42)	129.4(5)	C(44)-Sm(2)-C(42)	50.1(5)
C(30)-Sm(2)-C(42)	109.7(5)	O(3)-Sm(2)-C(41)	86.0(5)
O(1)-Sm(2)-C(41)	93.8(5)	C(43)-Sm(2)-C(41)	49.0(6)
C(31)-Sm(2)-C(41)	128.2(5)	C(44)-Sm(2)-C(41)	49.6(5)
C(30)-Sm(2)-C(41)	124.9(5)	C(42)-Sm(2)-C(41)	29.4(5)
O(3)-Sm(2)-C(40)	84.0(4)	O(1)-Sm(2)-C(40)	115.8(5)
C(43)-Sm(2)-C(40)	50.2(5)	C(31)-Sm(2)-C(40)	98.4(5)
C(44)-Sm(2)-C(40)	30.8(5)	C(30)-Sm(2)-C(40)	103.2(5)
C(42)-Sm(2)-C(40)	50.1(5)	C(41)-Sm(2)-C(40)	30.3(5)
O(3)-Sm(2)-C(29)	130.3(5)	O(1)-Sm(2)-C(29)	113.2(5)
C(43)-Sm(2)-C(29)	93.9(6)	C(31)-Sm(2)-C(29)	49.9(6)
C(44)-Sm(2)-C(29)	100.9(6)	C(30)-Sm(2)-C(29)	29.6(5)
C(42)-Sm(2)-C(29)	116.4(5)	C(41)-Sm(2)-C(29)	142.8(5)
C(40)-Sm(2)-C(29)	130.8(5)	O(3)-Sm(2)-C(28)	101.0(4)
O(1)-Sm(2)-C(28)	92.1(5)	C(43)-Sm(2)-C(28)	123.7(5)
C(31)-Sm(2)-C(28)	49.2(5)	C(44)-Sm(2)-C(28)	124.6(5)
C(30)-Sm(2)-C(28)	48.8(5)	C(42)-Sm(2)-C(28)	144.6(5)
C(41)-Sm(2)-C(28)	172.7(5)	C(40)-Sm(2)-C(28)	147.5(5)
C(29)-Sm(2)-C(28)	30.0(5)	O(3)-Sm(2)-C(27)	83.0(5)
O(1)-Sm(2)-C(27)	100.4(5)	C(43)-Sm(2)-C(27)	128.4(5)
C(31)-Sm(2)-C(27)	30.3(5)	C(44)-Sm(2)-C(27)	112.1(6)
C(30)-Sm(2)-C(27)	49.7(6)	C(42)-Sm(2)-C(27)	158.7(5)
C(41)-Sm(2)-C(27)	152.1(5)	C(40)-Sm(2)-C(27)	122.6(5)
C(29)-Sm(2)-C(27)	49.7(6)	C(28)-Sm(2)-C(27)	29.5(5)
C(53)-O(1)-Sm(2)	89.4(8)	C(53)-O(1)-Sm(1)	90.7(8)
Sm(2)-O(1)-Sm(1)	178.6(6)	C(53)-O(2)-Sm(1)	109(1)
C(53)-O(3)-Sm(2)	109(1)	C(5)-C(1)-C(2)	106(2)
C(5)-C(1)-C(6)	127(2)	C(2)-C(1)-C(6)	127(2)
C(5)-C(1)-Sm(1)	71(1)	C(2)-C(1)-Sm(1)	75(1)
C(6)-C(1)-Sm(1)	126(1)	C(3)-C(2)-C(1)	110(2)
C(3)-C(2)-Sm(1)	76(1)	C(1)-C(2)-Sm(1)	75.1(8)
C(3)-C(2)-H(2)	125.0	C(1)-C(2)-H(2)	125.0
Sm(1)-C(2)-H(2)	115.4	C(2)-C(3)-C(4)	106(2)
C(2)-C(3)-C(10)	129(2)	C(4)-C(3)-C(10)	124(2)

C(2)-C(3)-Sm(1)	75(1)	C(4)-C(3)-Sm(1)	72(1)
C(10)-C(3)-Sm(1)	128(1)	C(5)-C(4)-C(3)	108(2)
C(5)-C(4)-Sm(1)	73(1)	C(3)-C(4)-Sm(1)	78(1)
C(5)-C(4)-H(4)	126.2	C(3)-C(4)-H(4)	126.2
Sm(1)-C(4)-H(4)	115.1	C(4)-C(5)-C(1)	111(2)
C(4)-C(5)-Sm(1)	77(1)	C(1)-C(5)-Sm(1)	79(1)
C(4)-C(5)-H(5)	124.8	C(1)-C(5)-H(5)	124.8
Sm(1)-C(5)-H(5)	111.0	C(7)-C(6)-C(8)	110(2)
C(7)-C(6)-C(1)	112(1)	C(8)-C(6)-C(1)	112(2)
C(7)-C(6)-C(9)	108(2)	C(8)-C(6)-C(9)	108(2)
C(1)-C(6)-C(9)	108(1)	C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5	H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5	H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5	C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5	H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5	H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5	C(6)-C(9)-H(9A)	109.5
C(6)-C(9)-H(9B)	109.5	H(9A)-C(9)-H(9B)	109.5
C(6)-C(9)-H(9C)	109.5	H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5	C(11)-C(10)-C(3)	115(2)
C(11)-C(10)-C(12)	111(2)	C(3)-C(10)-C(12)	106(2)
C(11)-C(10)-C(13)	107(2)	C(3)-C(10)-C(13)	110(2)
C(12)-C(10)-C(13)	108(2)	C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5	H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5	H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5	C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5	H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5	H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5	C(10)-C(13)-H(13A)	109.5
C(10)-C(13)-H(13B)	109.5	H(13A)-C(13)-H(13B)	109.5
C(10)-C(13)-H(13C)	109.5	H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5	C(18)-C(14)-C(15)	107(1)
C(18)-C(14)-C(19)	126(2)	C(15)-C(14)-C(19)	127(2)
C(18)-C(14)-Sm(1)	73(1)	C(15)-C(14)-Sm(1)	74.9(8)
C(19)-C(14)-Sm(1)	124(1)	C(16)-C(15)-C(14)	108(2)
C(16)-C(15)-Sm(1)	74(1)	C(14)-C(15)-Sm(1)	74.8(8)
C(16)-C(15)-H(15)	125.9	C(14)-C(15)-H(15)	125.9
Sm(1)-C(15)-H(15)	117.3	C(17)-C(16)-C(15)	106(1)
C(17)-C(16)-C(23)	127(2)	C(15)-C(16)-C(23)	127(2)
C(17)-C(16)-Sm(1)	72.4(8)	C(15)-C(16)-Sm(1)	75.8(8)
C(23)-C(16)-Sm(1)	116(1)	C(18)-C(17)-C(16)	110(1)
C(18)-C(17)-Sm(1)	76(1)	C(16)-C(17)-Sm(1)	77.2(8)
C(18)-C(17)-H(17)	124.8	C(16)-C(17)-H(17)	124.8
Sm(1)-C(17)-H(17)	113.8	C(17)-C(18)-C(14)	109(2)
C(17)-C(18)-Sm(1)	74(1)	C(14)-C(18)-Sm(1)	77(1)
C(17)-C(18)-H(18)	125.5	C(14)-C(18)-H(18)	125.5
Sm(1)-C(18)-H(18)	115.1	C(14)-C(19)-C(20)	111(1)
C(14)-C(19)-C(21)	108(1)	C(20)-C(19)-C(21)	108(2)
C(14)-C(19)-C(22)	111(1)	C(20)-C(19)-C(22)	109(1)
C(21)-C(19)-C(22)	109(2)	C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5	H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5	H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5	C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5	H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5	H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5	C(19)-C(22)-H(22A)	109.5
C(19)-C(22)-H(22B)	109.5	H(22A)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5	H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5	C(26)-C(23)-C(16)	111(1)
C(26)-C(23)-C(24)	109(2)	C(16)-C(23)-C(24)	111(1)
C(26)-C(23)-C(25)	110(2)	C(16)-C(23)-C(25)	108(1)
C(24)-C(23)-C(25)	108(2)	C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5	H(24A)-C(24)-H(24B)	109.5

C(23)-C(24)-H(24C)	109.5	H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5	C(23)-C(25)-H(25A)	109.5
C(23)-C(25)-H(25B)	109.5	H(25A)-C(25)-H(25B)	109.5
C(23)-C(25)-H(25C)	109.5	H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5	C(23)-C(26)-H(26A)	109.5
C(23)-C(26)-H(26B)	109.5	H(26A)-C(26)-H(26B)	109.5
C(23)-C(26)-H(26C)	109.5	H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5	C(28)-C(27)-C(31)	106(2)
C(28)-C(27)-C(32)	127(2)	C(31)-C(27)-C(32)	126(2)
C(28)-C(27)-Sm(2)	75(1)	C(31)-C(27)-Sm(2)	71(1)
C(32)-C(27)-Sm(2)	127(1)	C(27)-C(28)-C(29)	110(2)
C(27)-C(28)-Sm(2)	75(1)	C(29)-C(28)-Sm(2)	75(1)
C(27)-C(28)-H(28)	125.0	C(29)-C(28)-H(28)	125.0
Sm(2)-C(28)-H(28)	116.6	C(30)-C(29)-C(28)	106(2)
C(30)-C(29)-C(36)	126(2)	C(28)-C(29)-C(36)	127(2)
C(30)-C(29)-Sm(2)	73(1)	C(28)-C(29)-Sm(2)	75(1)
C(36)-C(29)-Sm(2)	126(1)	C(29)-C(30)-C(31)	109(2)
C(29)-C(30)-Sm(2)	77(1)	C(31)-C(30)-Sm(2)	73(1)
C(29)-C(30)-H(30)	125.5	C(31)-C(30)-H(30)	125.5
Sm(2)-C(30)-H(30)	116.4	C(30)-C(31)-C(27)	109(2)
C(30)-C(31)-Sm(2)	77(1)	C(27)-C(31)-Sm(2)	78(1)
C(30)-C(31)-H(31)	125.8	C(27)-C(31)-H(31)	125.8
Sm(2)-C(31)-H(31)	111.8	C(27)-C(32)-C(33)	113(1)
C(27)-C(32)-C(34)	106(2)	C(33)-C(32)-C(34)	108(2)
C(27)-C(32)-C(35)	113(2)	C(33)-C(32)-C(35)	108(2)
C(34)-C(32)-C(35)	109(2)	C(32)-C(33)-H(33A)	109.5
C(32)-C(33)-H(33B)	109.5	H(33A)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5	H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5	C(32)-C(34)-H(34A)	109.5
C(32)-C(34)-H(34B)	109.5	H(34A)-C(34)-H(34B)	109.5
C(32)-C(34)-H(34C)	109.5	H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5	C(32)-C(35)-H(35A)	109.5
C(32)-C(35)-H(35B)	109.5	H(35A)-C(35)-H(35B)	109.5
C(32)-C(35)-H(35C)	109.5	H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5	C(39)-C(36)-C(37)	109(2)
C(39)-C(36)-C(29)	113(2)	C(37)-C(36)-C(29)	112(2)
C(39)-C(36)-C(38)	109(2)	C(37)-C(36)-C(38)	107(2)
C(29)-C(36)-C(38)	107(2)	C(36)-C(37)-H(37A)	109.5
C(36)-C(37)-H(37B)	109.5	H(37A)-C(37)-H(37B)	109.5
C(36)-C(37)-H(37C)	109.5	H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5	C(36)-C(38)-H(38A)	109.5
C(36)-C(38)-H(38B)	109.5	H(38A)-C(38)-H(38B)	109.5
C(36)-C(38)-H(38C)	109.5	H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5	C(36)-C(39)-H(39A)	109.5
C(36)-C(39)-H(39B)	109.5	H(39A)-C(39)-H(39B)	109.5
C(36)-C(39)-H(39C)	109.5	H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5	C(41)-C(40)-C(44)	105(2)
C(41)-C(40)-C(45)	129(2)	C(44)-C(40)-C(45)	126(2)
C(41)-C(40)-Sm(2)	74(1)	C(44)-C(40)-Sm(2)	72(1)
C(45)-C(40)-Sm(2)	124(1)	C(42)-C(41)-C(40)	111(2)
C(42)-C(41)-Sm(2)	75(1)	C(40)-C(41)-Sm(2)	76(1)
C(42)-C(41)-H(41)	124.5	C(40)-C(41)-H(41)	124.5
Sm(2)-C(41)-H(41)	116.4	C(41)-C(42)-C(43)	106(2)
C(41)-C(42)-C(49)	127(2)	C(43)-C(42)-C(49)	127(2)
C(41)-C(42)-Sm(2)	75(1)	C(43)-C(42)-Sm(2)	72(1)
C(49)-C(42)-Sm(2)	118(1)	C(44)-C(43)-C(42)	110(2)
C(44)-C(43)-Sm(2)	77(1)	C(42)-C(43)-Sm(2)	78(1)
C(44)-C(43)-H(43)	124.9	C(42)-C(43)-H(43)	124.9
Sm(2)-C(43)-H(43)	112.7	C(43)-C(44)-C(40)	108(2)
C(43)-C(44)-Sm(2)	73(1)	C(40)-C(44)-Sm(2)	77(1)
C(43)-C(44)-H(44)	126.0	C(40)-C(44)-H(44)	126.0
Sm(2)-C(44)-H(44)	115.7	C(46)-C(45)-C(47)	110(2)
C(46)-C(45)-C(40)	110(2)	C(47)-C(45)-C(40)	112(1)

C(46)-C(45)-C(48)	109(2)	C(47)-C(45)-C(48)	109(2)
C(40)-C(45)-C(48)	107(2)	C(45)-C(46)-H(46A)	109.5
C(45)-C(46)-H(46B)	109.5	H(46A)-C(46)-H(46B)	109.5
C(45)-C(46)-H(46C)	109.5	H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5	C(45)-C(47)-H(47A)	109.5
C(45)-C(47)-H(47B)	109.5	H(47A)-C(47)-H(47B)	109.5
C(45)-C(47)-H(47C)	109.5	H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5	C(45)-C(48)-H(48A)	109.5
C(45)-C(48)-H(48B)	109.5	H(48A)-C(48)-H(48B)	109.5
C(45)-C(48)-H(48C)	109.5	H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5	C(52)-C(49)-C(51)	115(2)
C(52)-C(49)-C(42)	110(2)	C(51)-C(49)-C(42)	110(2)
C(52)-C(49)-C(50)	108(2)	C(51)-C(49)-C(50)	107(2)
C(42)-C(49)-C(50)	107(2)	C(49)-C(50)-H(50A)	109.5
C(49)-C(50)-H(50B)	109.5	H(50A)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50C)	109.5	H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5	C(49)-C(51)-H(51A)	109.5
C(49)-C(51)-H(51B)	109.5	H(51A)-C(51)-H(51B)	109.5
C(49)-C(51)-H(51C)	109.5	H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5	C(49)-C(52)-H(52A)	109.5
C(49)-C(52)-H(52B)	109.5	H(52A)-C(52)-H(52B)	109.5
C(49)-C(52)-H(52C)	109.5	H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5	O(3)-C(53)-O(2)	147(2)
O(3)-C(53)-O(1)	107(1)	O(2)-C(53)-O(1)	106(1)
O(3)-C(53)-Sm(2)	49.5(8)	O(2)-C(53)-Sm(2)	164(1)
O(1)-C(53)-Sm(2)	58.0(7)	O(3)-C(53)-Sm(1)	165(1)
O(2)-C(53)-Sm(1)	48.7(8)	O(1)-C(53)-Sm(1)	57.2(7)
Sm(2)-C(53)-Sm(1)	115.2(5)		

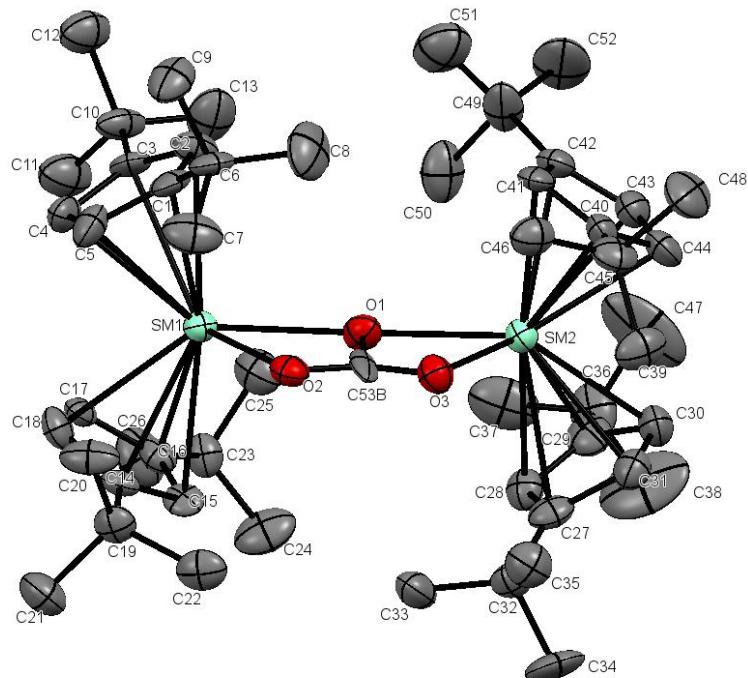


Figure S28: ORTEP of **8** with 50% probability ellipsoids (hydrogen atoms have been removed for clarity).

2. Quantum calculations

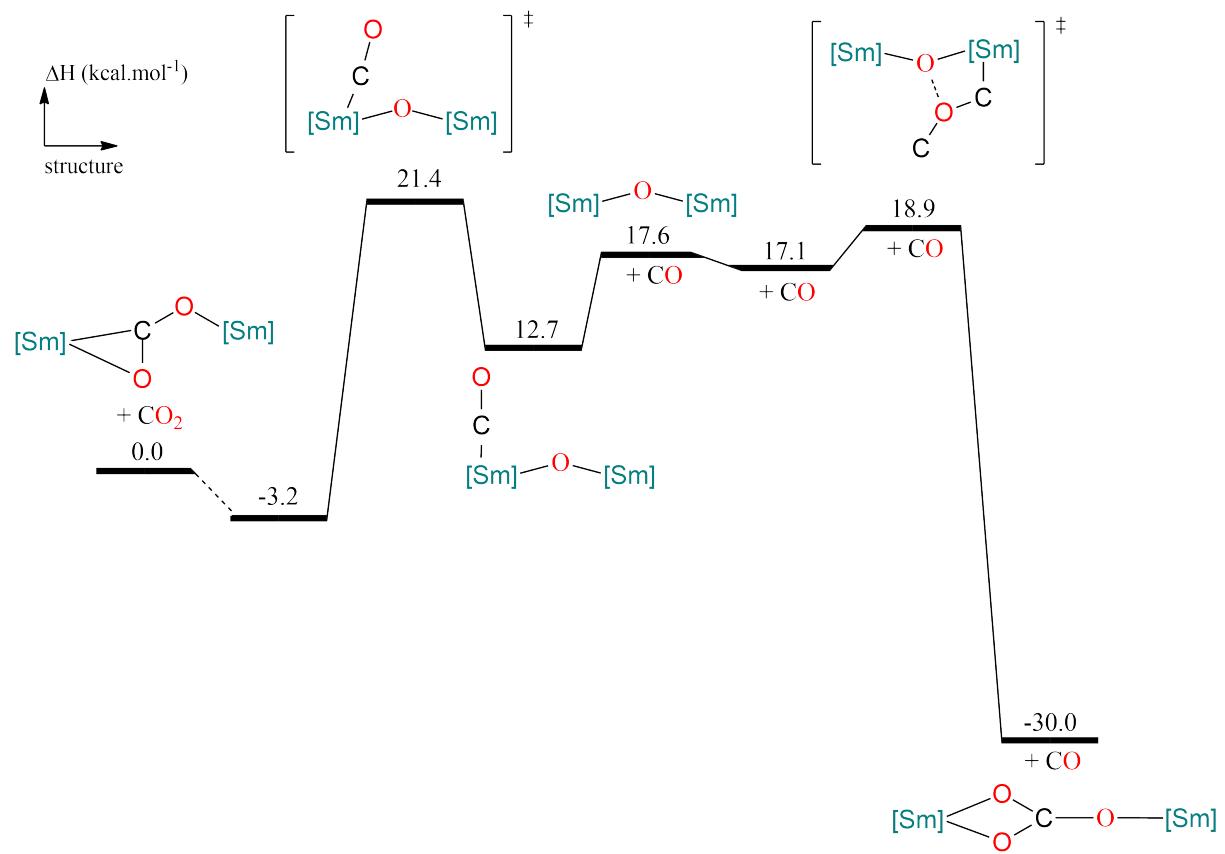


Figure S29: Computed Enthalpy profile for the oxo formation and its subsequent reaction with CO_2 for the $\text{Cp}^{\text{t}2}\text{Sm}$ complex.

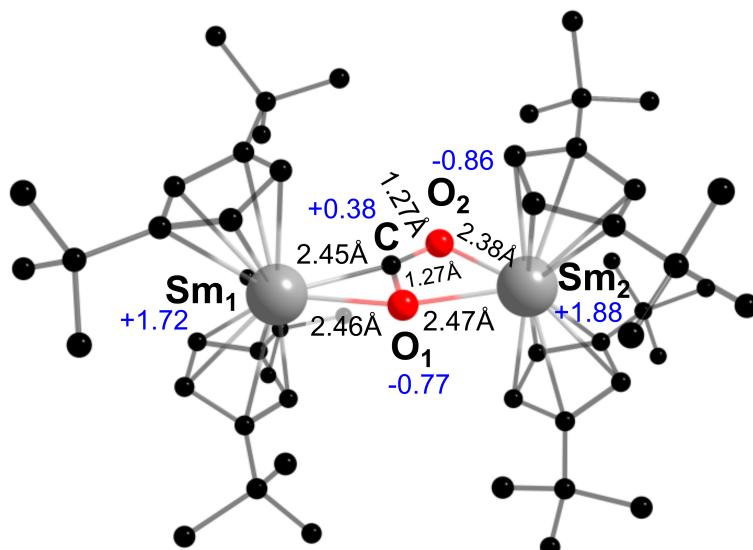


Figure S30: Complex $[\text{Cp}^{\text{t}2}\text{Sm}]_2(\mu\text{-CO}_2^{2-})$, geometrical parameters and NPA charges ($\text{Sm}_1\text{-O}_1\text{-C} = 73^\circ$, $\text{C-Sm}_1\text{-O}_1 = 32^\circ$, $\text{O}_1\text{-C-O}_2 = 117^\circ$, $\text{C-O}_2\text{-Sm}_2 = 98^\circ$, $\text{O}_2\text{-Sm}_2\text{-O}_1 = 54^\circ$).

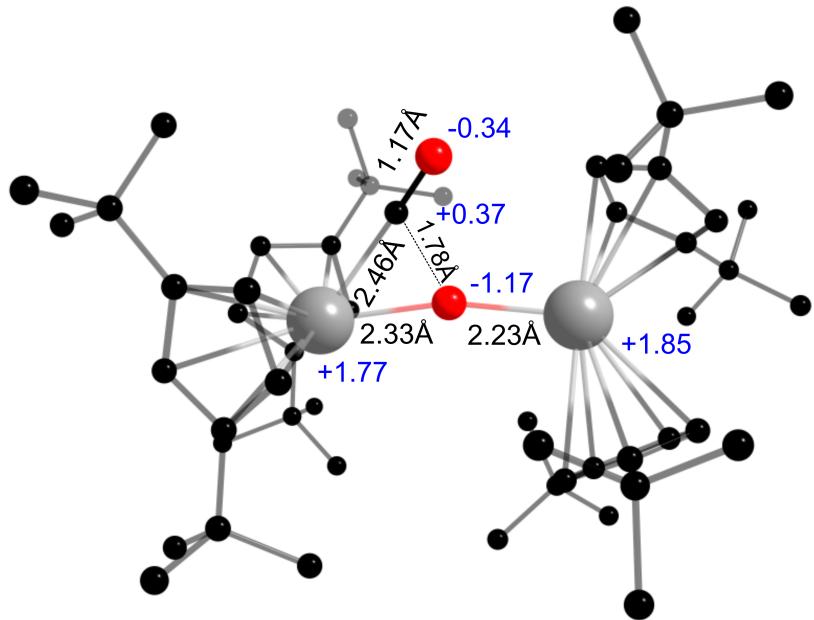


Figure S31: Transition state **I**, geometrical parameters and NPA charges.

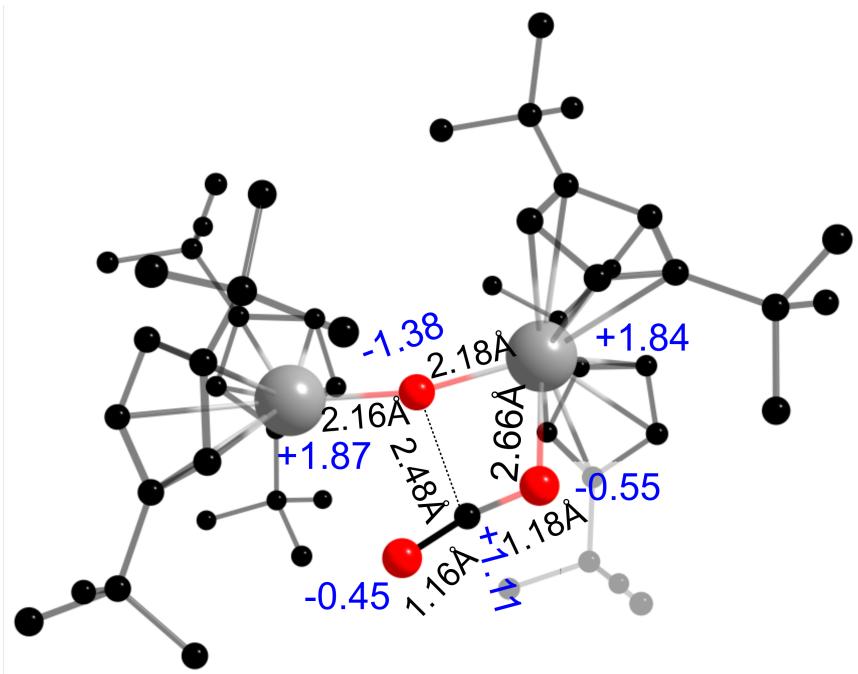


Figure S32: Transition state **II**, geometrical parameters and NPA charges (Sm-O-Sm angle: 161°, CO₂: 169°).

The optimized structures are given on a separate xyz file: structure .xyz