Supporting Information

Catalytic production of cyclic carbonates mediated by lanthanide phenolates under mild conditions

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Table S1 Initial TOF of complex **4** under atmospheric pressure[a].

Entry	Time (h)	Conversion[b,c] (%)	TOF[d] (h^{-1})
1	1	44	220
2	2	66	165
3	3	77	128
4	4	84	105
5	5	89	89
6	6	93	78
7	7	95	68
8	9	98	54
9	11	100	45
10[e]	1	36	180
11[f]	1	35	175

[a] Reactions conditions: 0.2 mol% **4**, 0.8 mol% NBu_4I, 1 ml epichlorohydrin (**1b**), 85 °C, 1 bar CO_2 (balloon). [b] Determined by ^1H NMR spectroscopy. [c] Selectivity for the cyclic carbonate product were all >99%. [d] Average TOF/h/mol(**4**). [e] 1-Allyloxy-2,3-epoxypropane (**1c**) was used as substrate. [f] Glycidyl methyl ether (**1e**) was used as substrate.

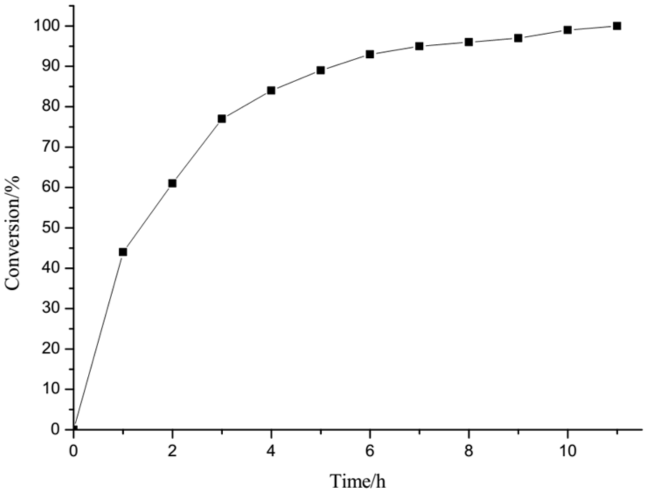


Figure S1 Conversion/time profile for the coupling reaction of epichlorohydrin (**1b**) with CO_2 catalyzed by complex **4** and NBu_4I at atmospheric pressure.

Experimental section

General considerations. Lanthanide complexes (**1-4**) were synthesized under a dry argon atmosphere using standard Schlenk techniques and kept in the glovebox once produced. Solvents (hexane and THF) were freshly distilled by refluxing over sodium/benzophenone ketyl prior to use. $LnCp_3(THF)$ (Ln = Yb, Y, Sm, Nd) and LH_4 were prepared according to the published procedures.[3,4] Propylene oxide was dried over CaH_2 for 2 days and distilled prior to use. Other epoxide substrates, onium salts and carbon dioxide were commercially available and used as received. Carbon, hydrogen, and nitrogen analyses were performed by direct combustion with a Carlo-Erba EA-1110 instrument. The IR spectra were recorded with a Nicolet-550 FT-IR spectrometer as KBr pellets. NMR (^1H, ^{13}C) spectra were recorded on a Unity Varian AC-400 spectrometer. The X-ray structural determination was carried out on a Rigaku Mercury diffract-ometer. The structures were solved by direct methods and refined by full-matrix least-squares procedures based on $|F|^2$. All of the non-hydrogen atoms were refined anisotropically. The hydrogen atoms in these complexes were all generated geometrically, assigned appropriate isotropic thermal parameters, and allowed to ride on their parent carbon atoms. All of the hydrogen atoms were held stationary and included in the structure factor calculation in the final stage of full-matrix least-squares refinement. The structures were solved and refined using *SHELEXL-97* programs.

Complex 1. To a THF solution of $Yb(C_5H_5)_3(THF)$ (1.31 g, 3.00 mmol) was added a THF solution of LH_4 (2.80 g, 3.00 mmol). The reaction mixture was stirred for 4 h at room temperature and then concentrated under vacuum. 14 ml hexane and 0.5 ml THF were added to extract the residue. Yellow crystals were obtained at room temperature after several days from the extract (2.82 g, 2.40 mmol, 80%). Mp: 188-190 °C. Anal. Calcd for $C_{70}H_{109}N_2NdO_6$: C, 67.50; H, 8.94; N, 2.47; Yb, 14.48. Found: C, 67.43; H, 8.66; N, 2.38; Yb, 14.72. IR (KBr pellet, cm^{-1}): 3447(s), 2956(w), 2904(w), 2868(w), 1604(s), 1478(s), 1443(s), 1414(s), 1362(m), 1304(m), 1282(m), 1238(m), 1202(m), 1166(m), 1132(m), 1026(m), 973(s), 912(s), 877(s), 833(s), 806(s), 769(s), 745(s), 671(s), 529(w), 458(w).

Complex 2. Complex **2** was synthesized in analogy to complex **1** from $Y(C_5H_5)_3(THF)$ (1.07 g, 3.00 mmol). Colorless crystals were obtained after several days (2.59 g, 2.37 mmol, 79%). Mp: 178-180 °C. ^1H NMR (C_6D_6, 400 MHz): δ 7.51 (s, 4H, Ar-H), 6.93 (s, 4H, Ar-H), 3.86 (s, 8H, $ArCH_2N$), 2.94 (br, 4H, NCH_2CH_2N), 1.83-1.04 (m, 72H, $C(CH_3)_3$). ^{13}C NMR ($C_6D_6,$ 100 MHz): δ 157.7, 146.8, 141.4, 141.2, 131.0, 130.3 (Ar-C), 76.1($ArCH_2N$), 62.3(NCH_2CH_2N), 40.1, 39.2, 37.0, 36.8, 35.2, 34.9, 30.4($C(CH_3)_3$). Anal.Calcd for $C_{70}H_{109}N_2YO_6$: C, 72.59; H, 9.65; N, 2.62; Y, 8.57. Found: C, 72.63; H, 9.33; N, 2.57; Y, 8.15. IR (KBr pellet, cm^{-1}): 3437(s), 2953(w), 2904(w), 2867(w), 1603(s), 1479(s), 1442(s), 1414(s), 1362(m), 1304(m), 1271(m), 1238(m), 1202(m), 1167(m), 1132(m), 1108(m), 974(s), 912(s), 875(s), 837(s), 805(s), 770(s), 744(s), 669(s), 533(w), 457(w).

Complex 3. Complex **3** was synthesized in analogy to complex **1** from $Sm(C_5H_5)_3(THF)$ (1.25 g, 3.00 mmol). Yellowish crystals were obtained after several days (2.60 g, 2.25 mmol, 75%). Mp: 199-201°C. Anal. Calcd for $C_{70}H_{109}N_2SmO_6$: C, 68.52; H, 8.69; N, 2.53; Sm, 13.27. Found: C, 68.76; H, 8.83; N, 2.43; Sm, 13.04. IR (KBr pellet, cm^{-1}): 3423(s), 2960(w), 2904(w), 2869(w), 1603(s), 1477(s), 1440(s), 1414(s), 1362(m), 1301(m), 1276(m), 1240(m), 1202(m), 1167(m), 997(s), 969(s), 959(s), 913(s), 875(s), 833(s), 808(s), 770(s), 741(s), 691(s), 523(w), 435(w).

Complex 4. Complex **4** was synthesized in analogy to complex **1** from $Nd(C_5H_5)_3(THF)$ (1.23 g, 3.00 mmol). Blue crystals were obtained after several days (2.65 g, 2.25 mmol, 77%). Mp: 182-184 °C. Anal. Calcd for $C_{70}H_{109}N_2NdO_6$: C, 68.80; H, 9.11; N, 2.54; Nd, 12.76. Found: C, 69.13; H, 8.88; N, 2.44; Nd, 12.58. IR (KBr pellet, cm^{-1}): 3436(s), 2957(w), 2904(w), 2869(w), 1609(s), 1479(s), 1442(s), 1411(s), 1362(m), 1304(m), 1276(m), 1235(m), 1204(m), 1165(m), 1132(m), 1026(m), 994(s), 912(s), 877(s), 837(s), 806(s), 759(s), 741(s), 683(s), 529(w), 449(w).

Catalytic procedure for the cycloaddition of CO_2 to epoxides under 1 bar CO_2. In a typical reaction, complex **4** (29.2 mg, 2.55×10^{-2} mmol), NBu_4I (37.7 mg, 1.02×10^{-1} mmol), and **1b** (1 ml, 12.75 mmol) were added to a 20 mL flask equipped with a magnetic stirring bar under argon. The flask was then de-gassed, before being left stirring under 1 bar CO_2, at 85 °C, for 24 h. At the end of the reaction, an aliquot of the resulting mixture was analysed by ^{1}H NMR spectroscopy to determine the conversion and selectivity. Analytically pure product was isolated by column chromatography and confirmed by comparison with literature data.[2,5-7]

Catalytic procedure for the cycloaddition of CO_2 to epoxides under 10 bar CO_2. Reactions were carried out in a 100 mL stainless steel Parr reactor with a stirring bar inside and needle valve for injection. In a typical reaction, complex **4** (67.8 mg, 5.91×10^{-2} mmol), NBu_4Br (76.1 mg, 2.36×10^{-1} mmol) and **1m** (3 ml, 29.5 mmol) were introduced into the reactor which was dried before use. The reactor was pressurized to 10 bar with carbon dioxide, and heated to 85 °C for 45 h. At the end of the reaction, an aliquot of the resulting mixture was analysed by ^{1}H NMR spectroscopy to determine the yield and selectivity, and analytically pure product was isolated by column chromatography and confirmed by comparison with literature data.[2,5-7] Product **2h** which was not synthesized before was characterized by multinuclear NMR spectroscopy, IR and HRMS.

4-chloromethyl-1,3-dioxolan-2-one (2b)[2]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 4.98-4.93 (m, 1H, OCH), 4.59 (dd, J_{HH} = 8.9 and 8.6 Hz, 1H, OCH_2), 4.42 (dd, J_{HH} = 5.7 and 8.9 Hz, 1H, OCH_2), 3.78–3.72 (m, 2H, $ClCH_2$).

4-allyoxymethyl-1,3-dioxan-2-one (2c)[5]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 5.86–5.79 (m, 1H, $CH=CH_2$), 5.26–5.16 (m, 2H, $CH=CH_2$), 4.84–4.80 (m, 1H, OCH), 4.49 (t, J = 8.4 Hz, 1H, OCH_2), 4.36 (t, J = 7.2 Hz, 1H, OCH_2), 4.01–3.97 (m, 2H, OCH_2), 3.63 (m, 2H, OCH_2).

4-phenyl-1,3-dioxolan-2-one (2d)[2]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.48–7.41 (m, 3H, Ar-H), 7.38–7.36 (m, 2H, Ar-H), 5.68 (t, J = 8.0 Hz, 1H, OCH), 4.81 (t, J = 8.4 Hz, 1H, OCH_2), 4.35 (t, J = 8.2 Hz, 1H, OCH_2).

4-methoxymethyl-1,3-dioxolan-2-one (2e)[2]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 4.83–4.78 (m, 1H, OCH), 4.50 (dd, J_{HH} = 8.4 and 8.4Hz, 1H, OCH_2), 4.38 (dd, J_{HH} = 8.4 and 6.1 Hz, 1H, OCH_2), 3.67-3.56 (m, 2H, OCH_2), 3.43 (s, 3H, OCH_3).

4-hydroxymethyl-1,3-dioxolan-2-one (2f)[6]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 4.84–4.78 (m, 1H, OCH), 4.53 (dd, J_{HH} = 8.4 and 8.4 Hz, 1H, OCH_2), 4.46 (dd, J_{HH} = 6.8 and 8.2 Hz, 1H, OCH_2), 4.02-3.97 (m, 1H, OCH_2), 3.76-3.70 (m, 1H, OCH_2).

4-*n*-butyl-1,3-dioxolan-2-one (2g)[2]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 4.70 (m, 1H, OCH), 4.53 (t, J_{HH} = 8.1 Hz, 1H, OCH_2), 4.07 (t, J_{HH} = 8.1 Hz, 1H, OCH_2), 1.86–1.77 (m, 1H, CH_2), 1.73–1.65 (m, 1H, CH_2), 1.50–1.34 (m, 4H, CH_2CH_2), 0.93 (t, J = 6.8 Hz, 3H, CH_3).

4-*tert*-butyl-benzoic acid 2-oxo-[1,3]dioxolan-4-ylmethyl ester (2h). White solid. Mp 57-59 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.95 (d, J = 8.3 Hz, 2H), 7.49 (d, J = 8.3 Hz, 2H), 5.09–5.01 (m, 1H), 4.60-4.64 (m, 1H), 4.58-4.48 (m, 2H), 4.40-4.44 (m, 1H), 1.34 (s, 9H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.2, 157.7, 154.9, 129.9, 126.2, 125.8, 74.3, 66.4, 63.7, 35.4, 31.3. IR (KBr): 2959, 2870, 1789, 1716, 1609, 1572, 1429, 1384, 1315, 1279, 1167, 1119, 1047, 1016, 956, 855, 773, 707, 637 cm^{-1}; HRMS (ESI-TOF) calcd for $C_{15}H_{18}O_5Na^+$: 301.1046 ($[M + Na]^+$), found: 301.1057.

4-phenoxymethyl-1,3-dioxolan-2-one (2i)[2]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.31 (t, J = 7.6 Hz, 2H, Ar-H), 7.01 (t, J = 7.2 Hz, 1H, Ar-H,), 6.91 (d, J = 8.0 Hz, 2H, Ar-H), 5.05–5.00 (m, 1H, OCH), 4.61 (dd, J_{HH} = 8.4 and 5.4 Hz, 1H, OCH_2), 4.54 (dd, J_{HH} = 8.4 and 8.4 Hz, 1H, OCH_2), 4.26-4.13 (m, 2H, OCH_2).

4-(morpholinomethyl)-1,3-dioxolan-2-one (2j)[6]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 4.86–4.79 (m, 2H, CH), 4.53 (dd, J_{HH} = 8.3 and 8.4 Hz, 1H, OCH_2), 4.24 (dd, J = 7.1, 8.4 Hz, 1H, OCH_2), 3.70 (t, J = 4.6 Hz, 4H, OCH_2), 2.70 (d, J = 2.2 Hz, 1H, NCH_2), 2.68 (d, J = 1.9 Hz, 1H, NCH_2), 2.62–2.51 (m, 4H, NCH_2).

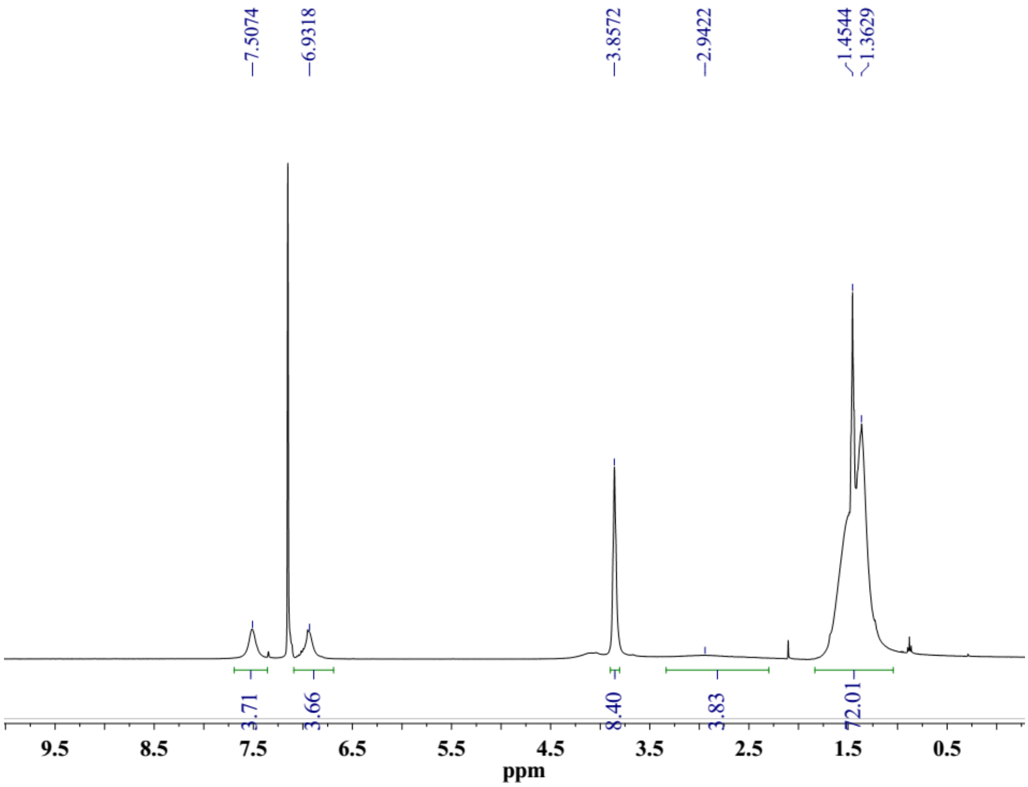
4,4-dimethyl-1,3-dioxolan-2-one (2k)[6]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 4.17 (s, 2H, CH_2), 1.55 (s, 6H, CH_3).

4,5-dimethyl-1,3-dioxolan-2-one (2l)[6]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 4.37–4.30 (m, 2H, CH), 1.47 (d, J = 5.7 Hz, 6H, CH_3).

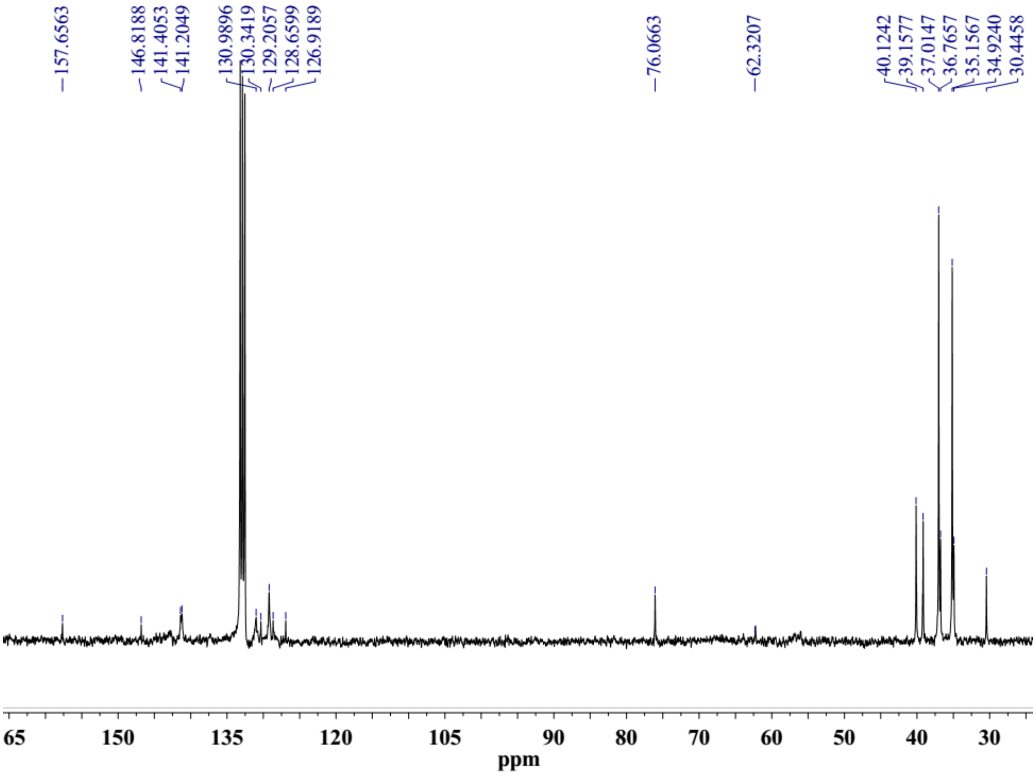
***cis*-1,2-cyclohexene carbonate (2m)**[7]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 4.71–4.66 (m, 2H, OCHCHO), 1.92–1.88 (m, 4H, CH_2), 1.68–1.59 (m, 2H, CH_2), 1.47–1.38 (m, 2H, CH_2).

***cis*-1,2-cyclopentene carbonate (2n)**[7]. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 5.13–5.09 (m, 2H, OCHCHO), 2.19–2.13 (m, 2H, CH_2), 1.84–1.65 (m, 4H, CH_2).

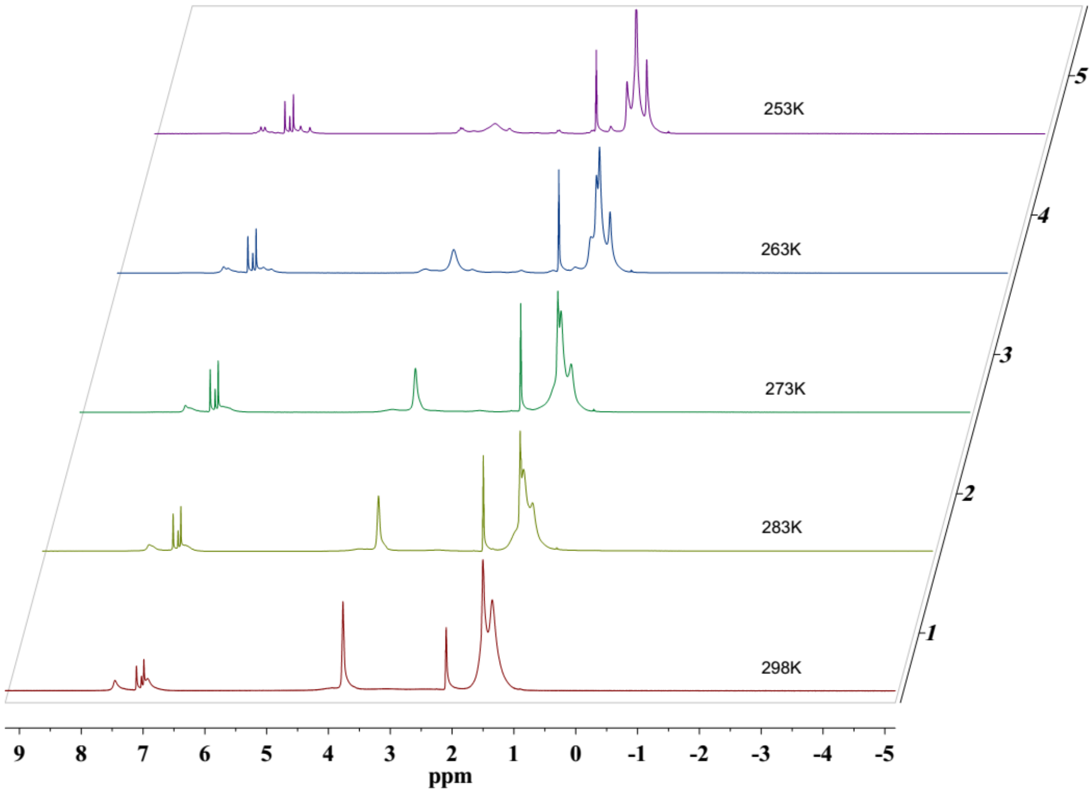
^{1}H NMR spectrum (298 K) of complex 2 in C_6D_6



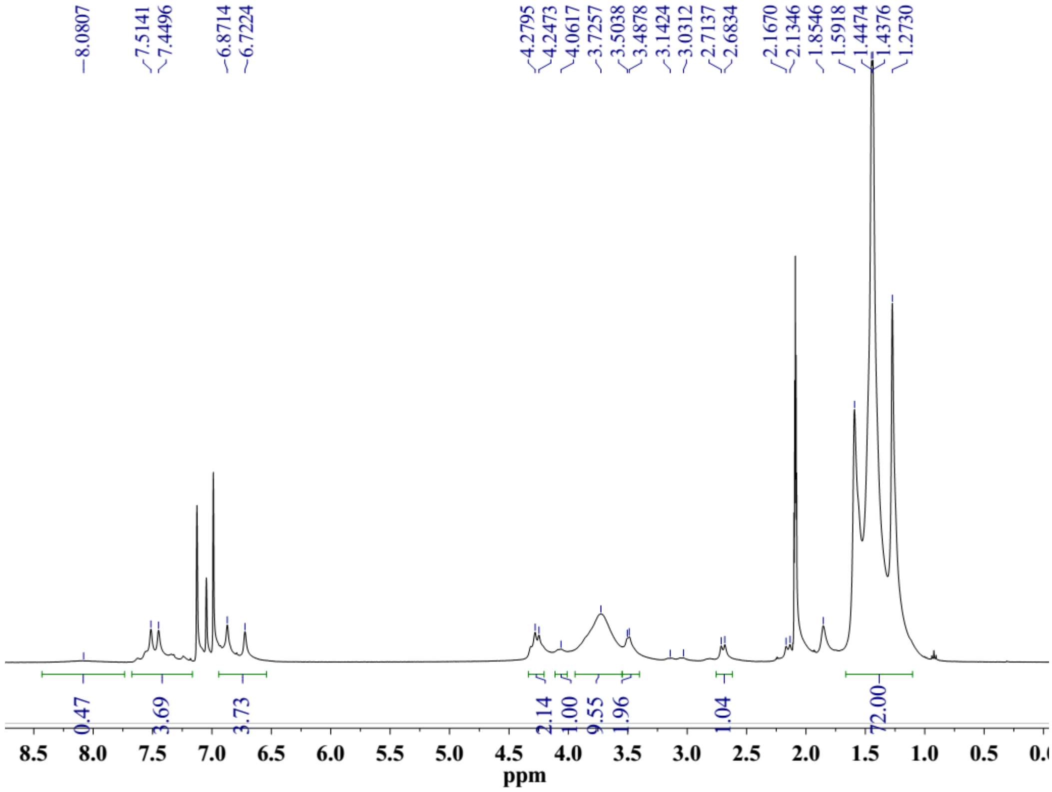
^{13}C NMR spectrum (298 K) of complex 2 in C_6D_6



Variable-temperature ^{1}H NMR spectra of complex 2 (253-298K) in C_7D_8

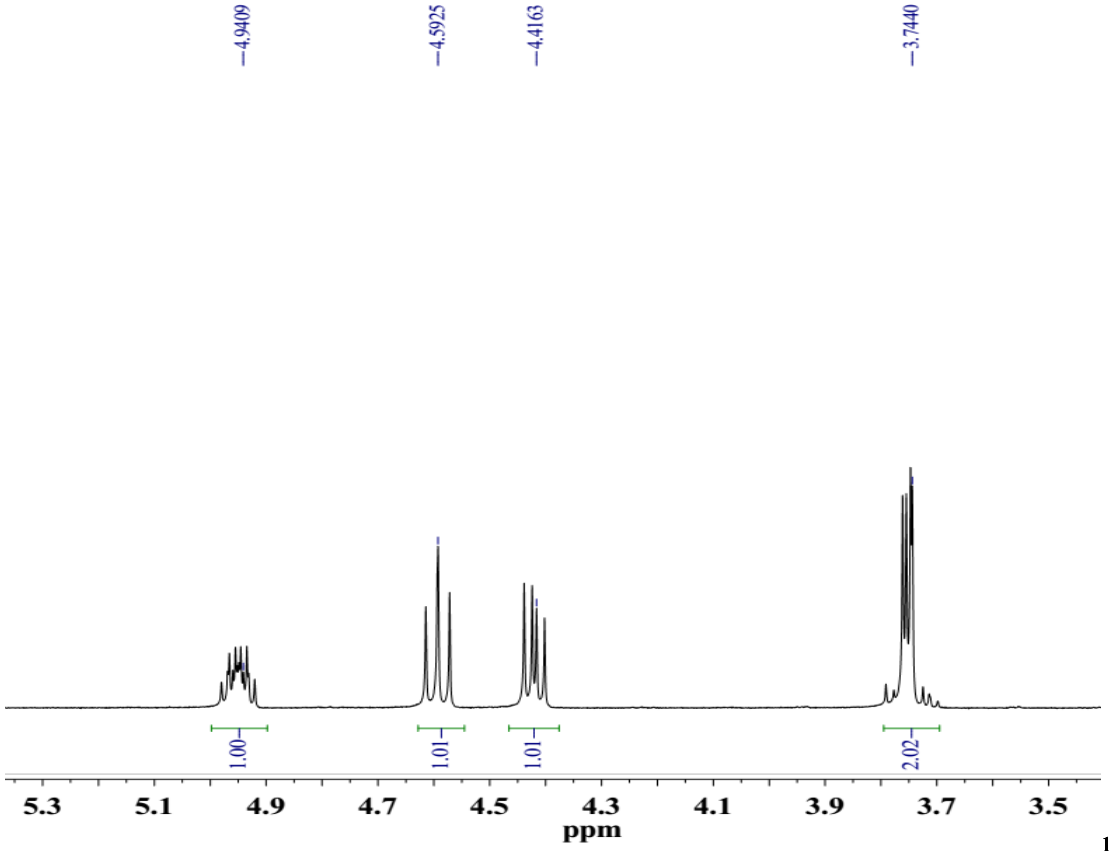


^{1}H NMR spectrum (253 K) of complex 2 in C_7D_8

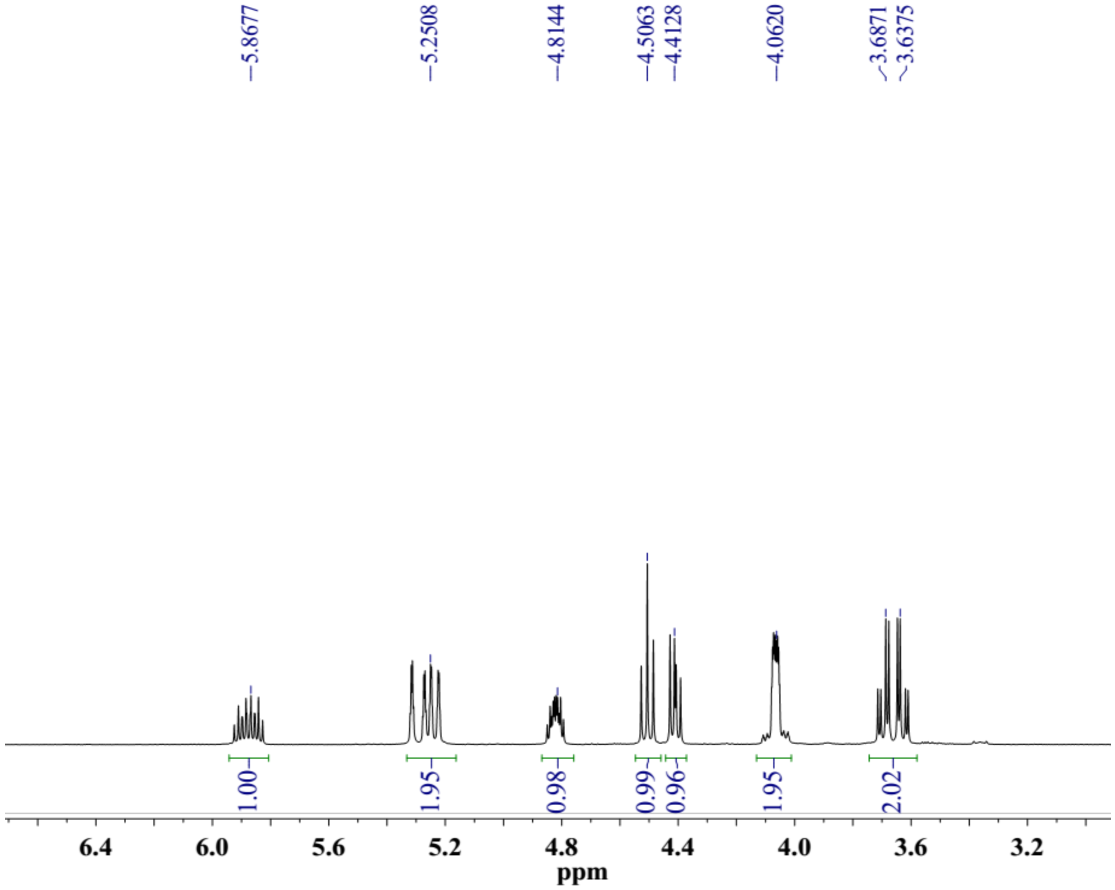


The ^{1}H NMR spectrum recorded at 298 K shows broad signals with the benzylic protons resonating at 3.86 ppm as a singlet. No obvious signal was observed for protons on the bridge. Lowering the temperature to less than 263 K resulted in more complicated spectra with the appearance of additional signals. At 253 K, two doublets at 2.69 and 2.15 ppm with the coupling constant of 12 Hz are observed, corresponding to the diastereotopic protons on the bridge. Signals in the range of 4.5 to 3.2 ppm are assigned to the benzylic protons. In addition, aromatic protons and methyl groups give rise to two sets of signals instead of one broad set at 298 K. More importantly, a signal at 8.09 ppm appears which may be assignable to the pending OH group. Probably, a dynamic process involving the exchange of the OH group and other coordinating pheolate ligand exists in solution, which was slowed down at lower temperature.

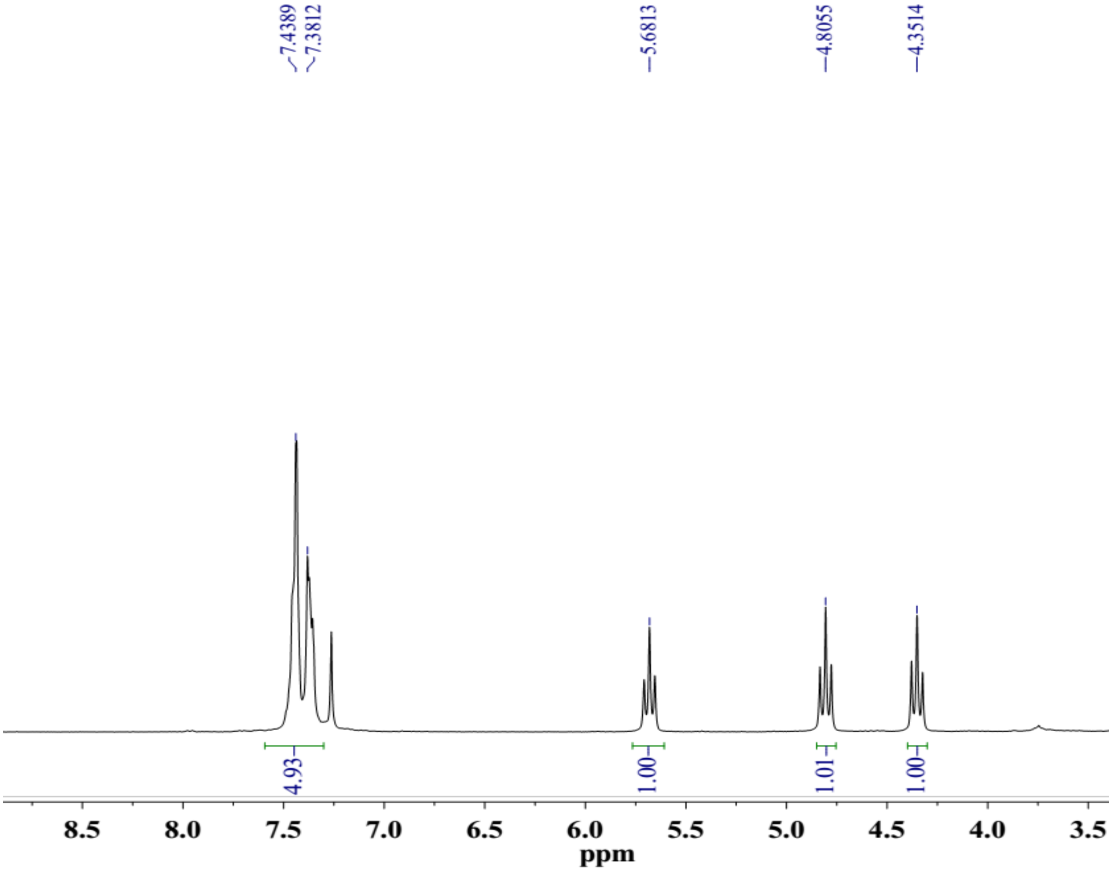
^{1}H NMR spectrum of 2b in CDCl$_3$:



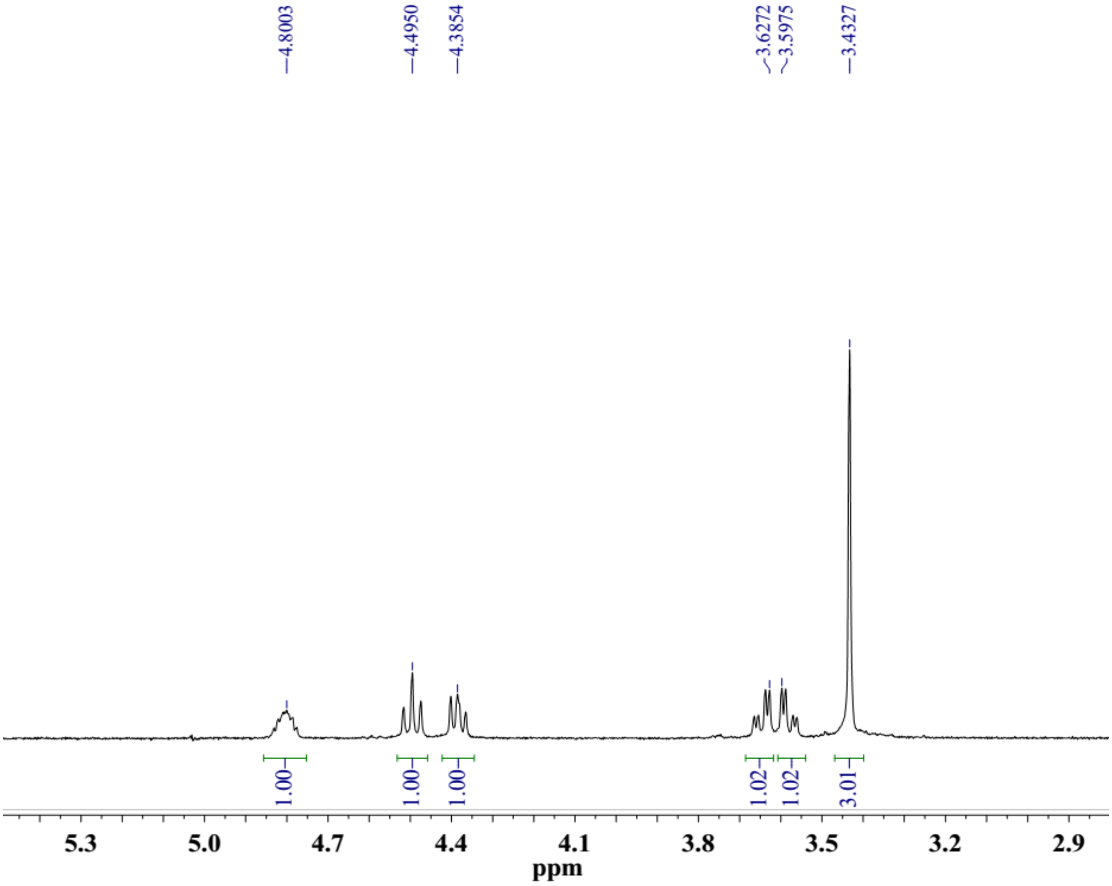
^{1}H NMR spectrum of 2c in CDCl$_3$:



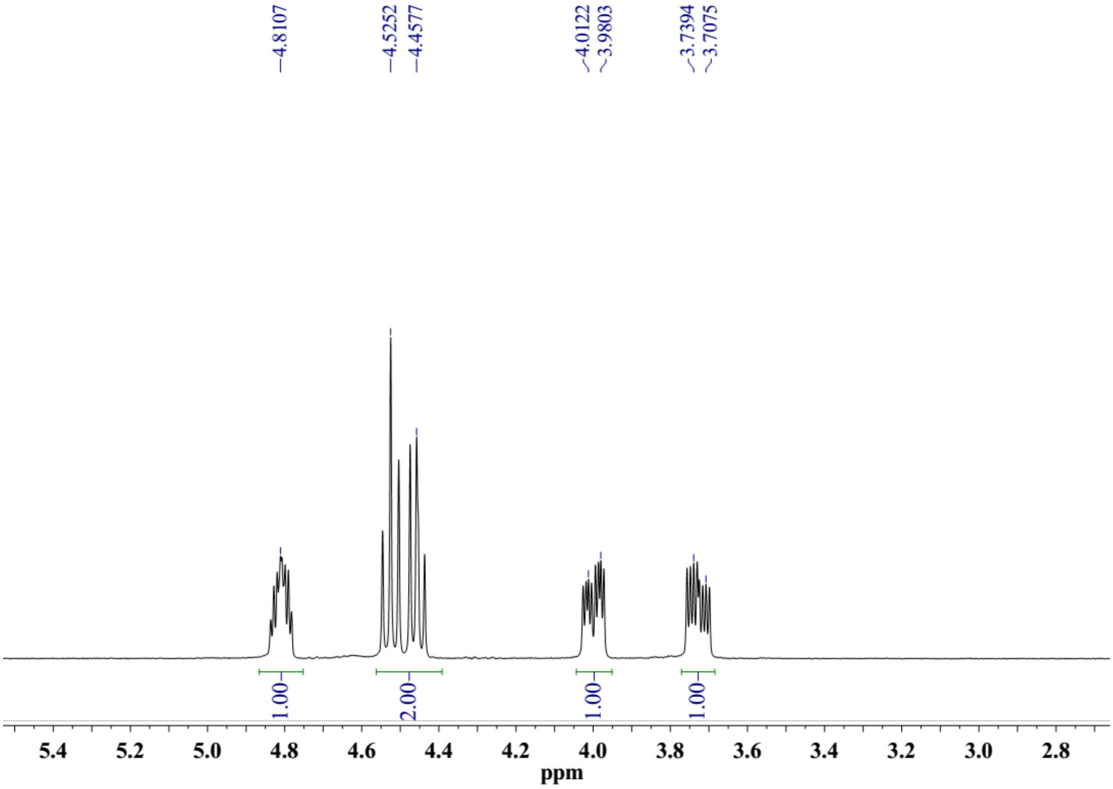
^{1}H NMR spectrum of 2d in CDCl$_3$:



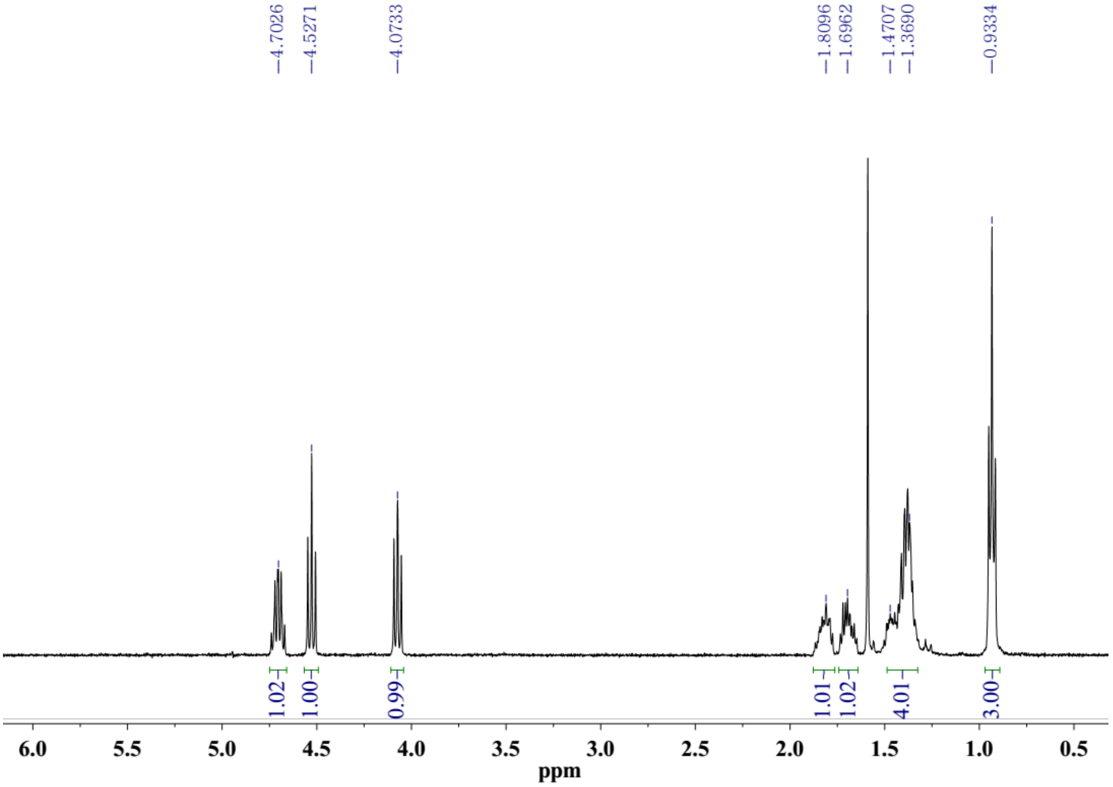
^{1}H NMR spectrum of 2e in CDCl$_3$:



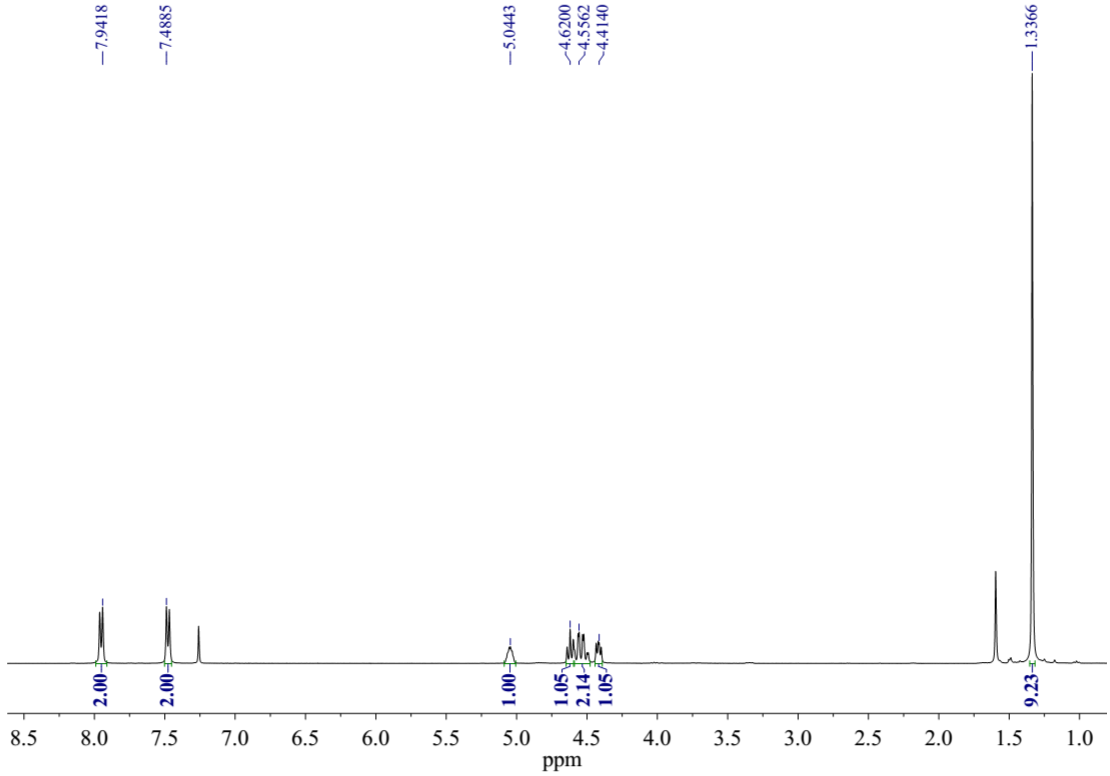
^{1}H NMR spectrum of 2f in $CDCl_3$:



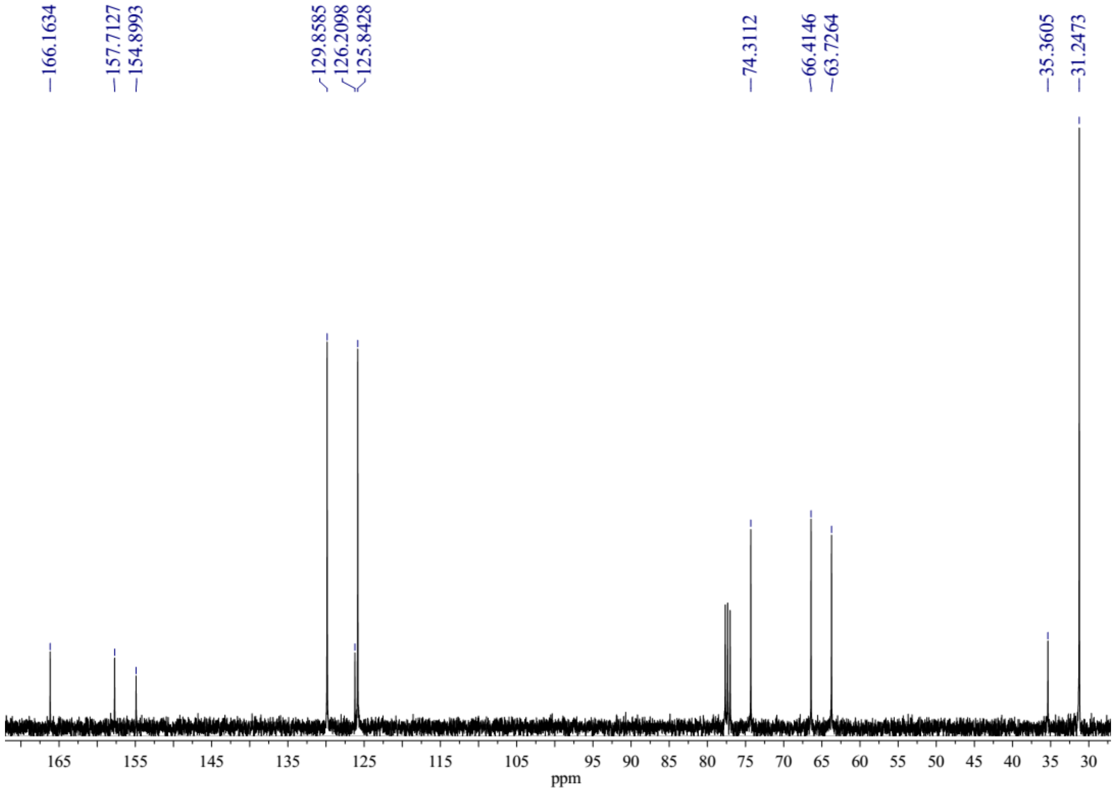
^{1}H NMR spectrum of 2g in $CDCl_3$:



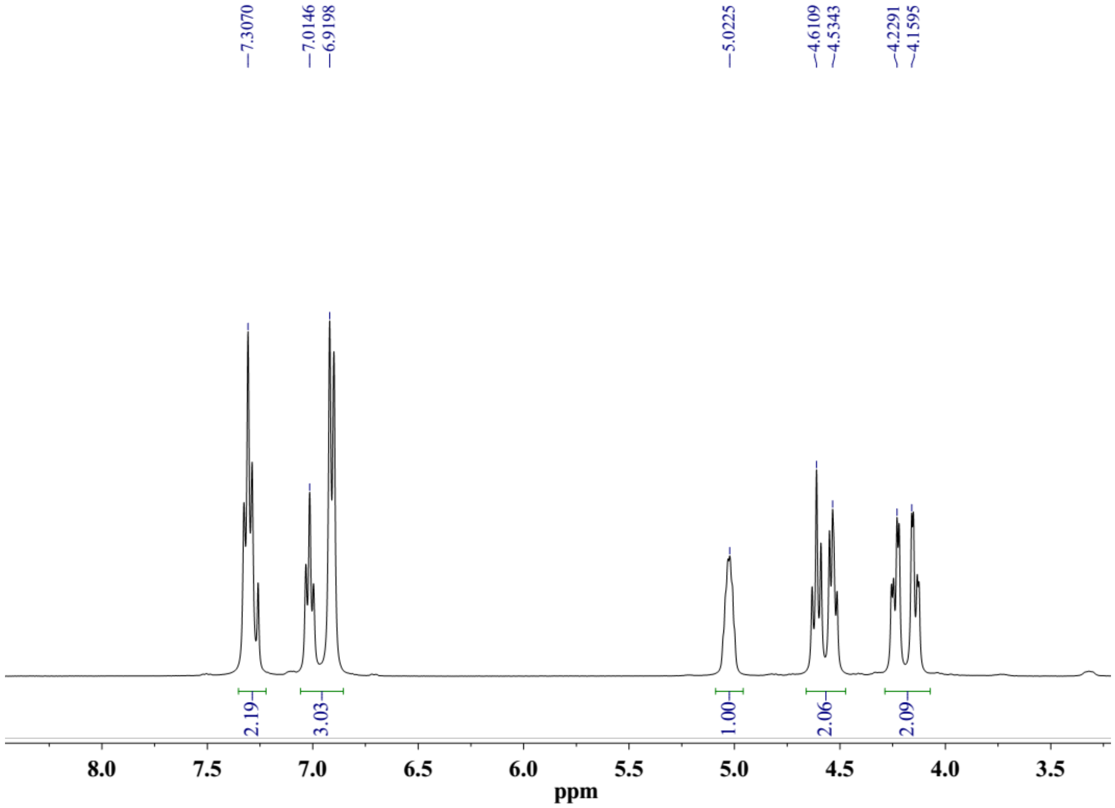
^{1}H NMR spectrum of 2h in $CDCl_3$:



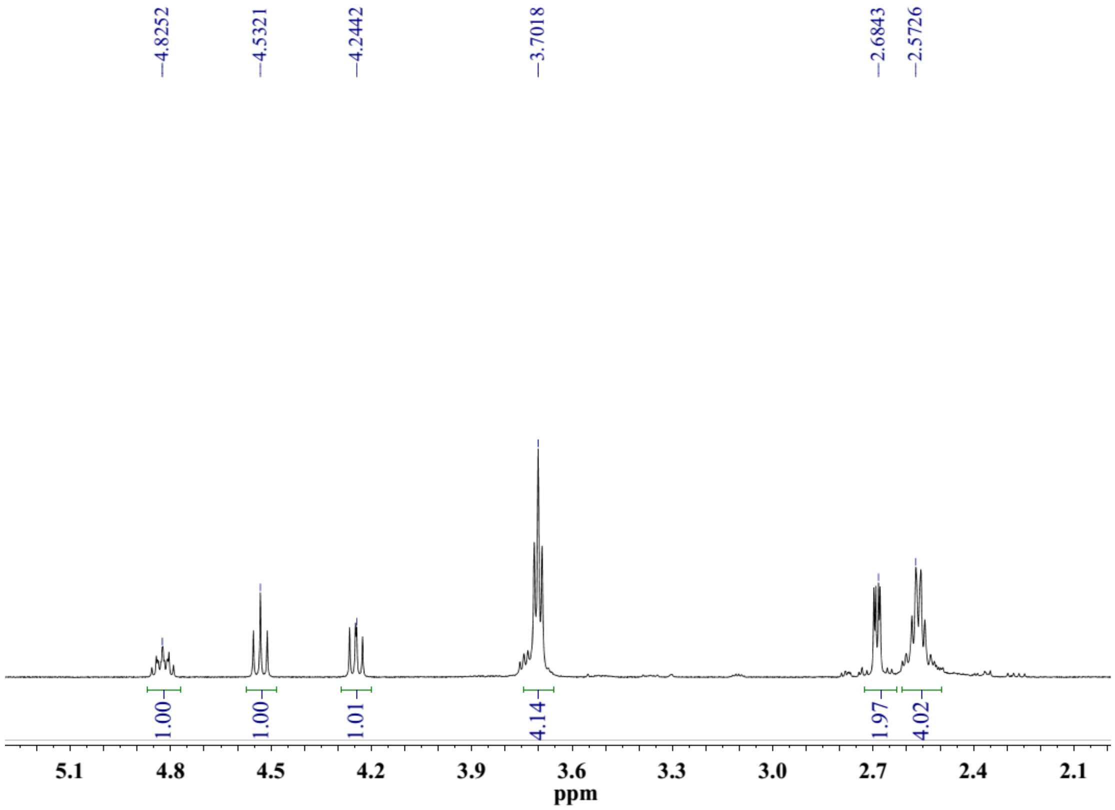
^{13}C NMR spectrum of 2h in $CDCl_3$:



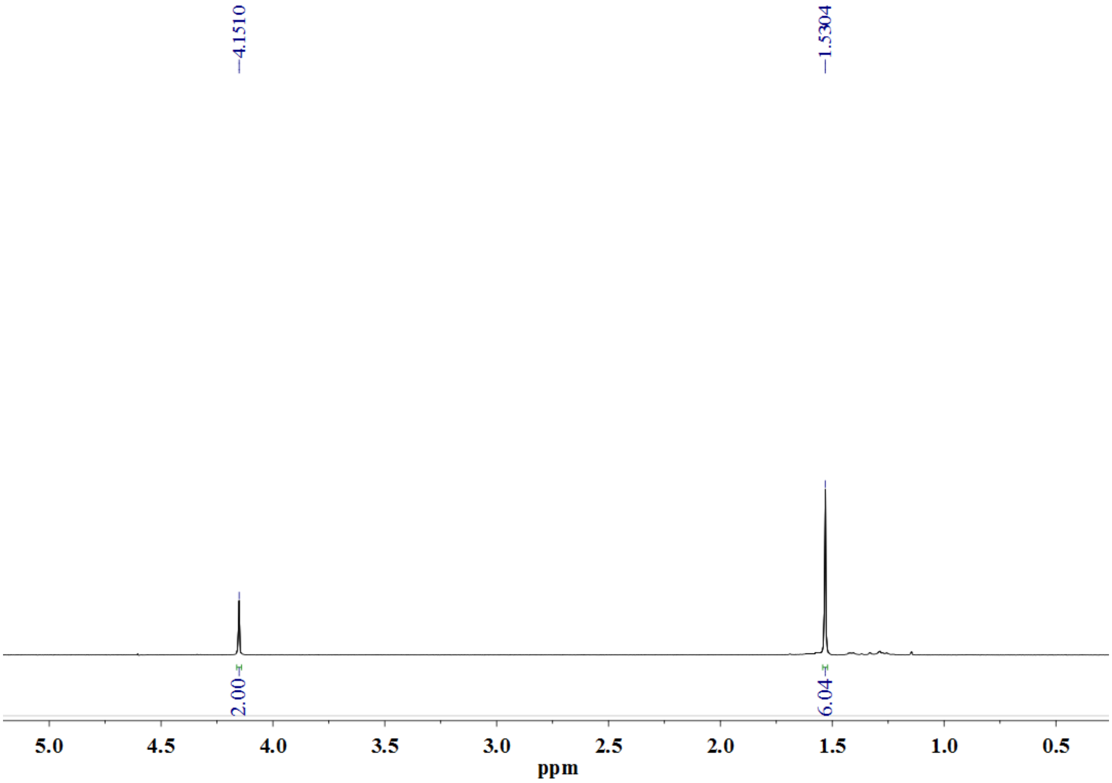
^{1}H NMR spectrum of 2i in $CDCl_3$:



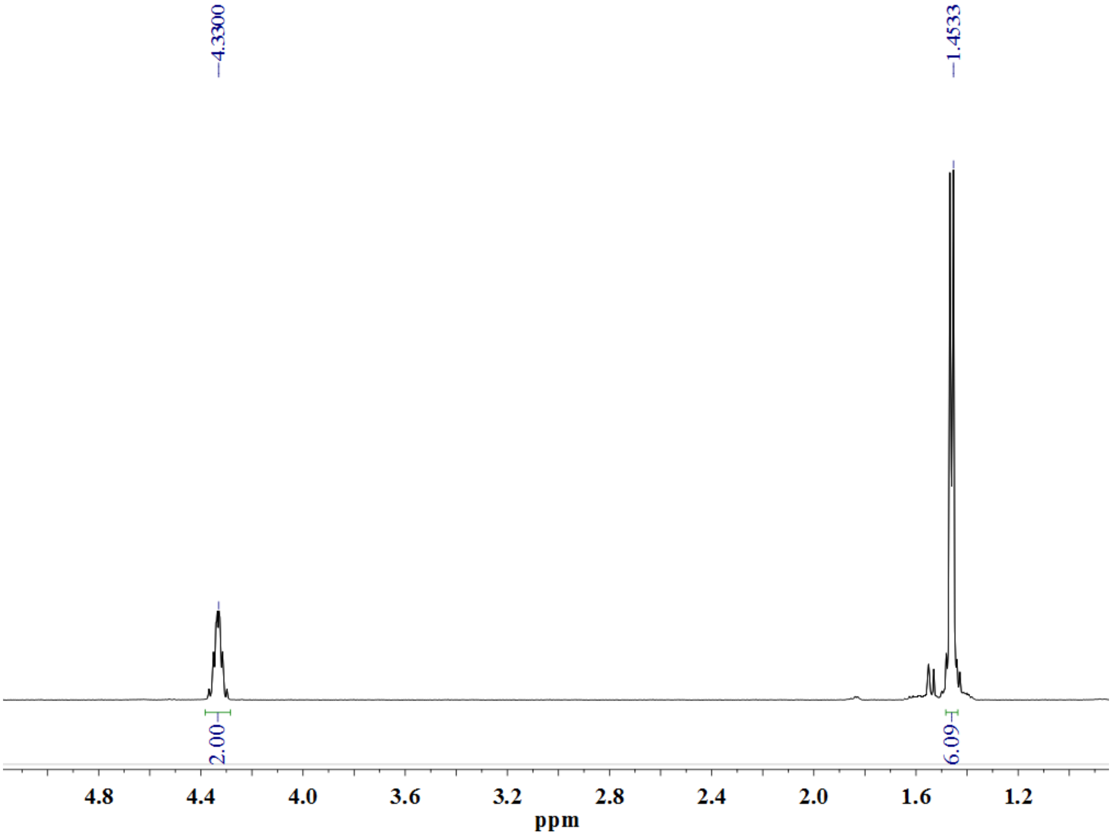
^{1}H NMR spectrum of 2j in $CDCl_3$:



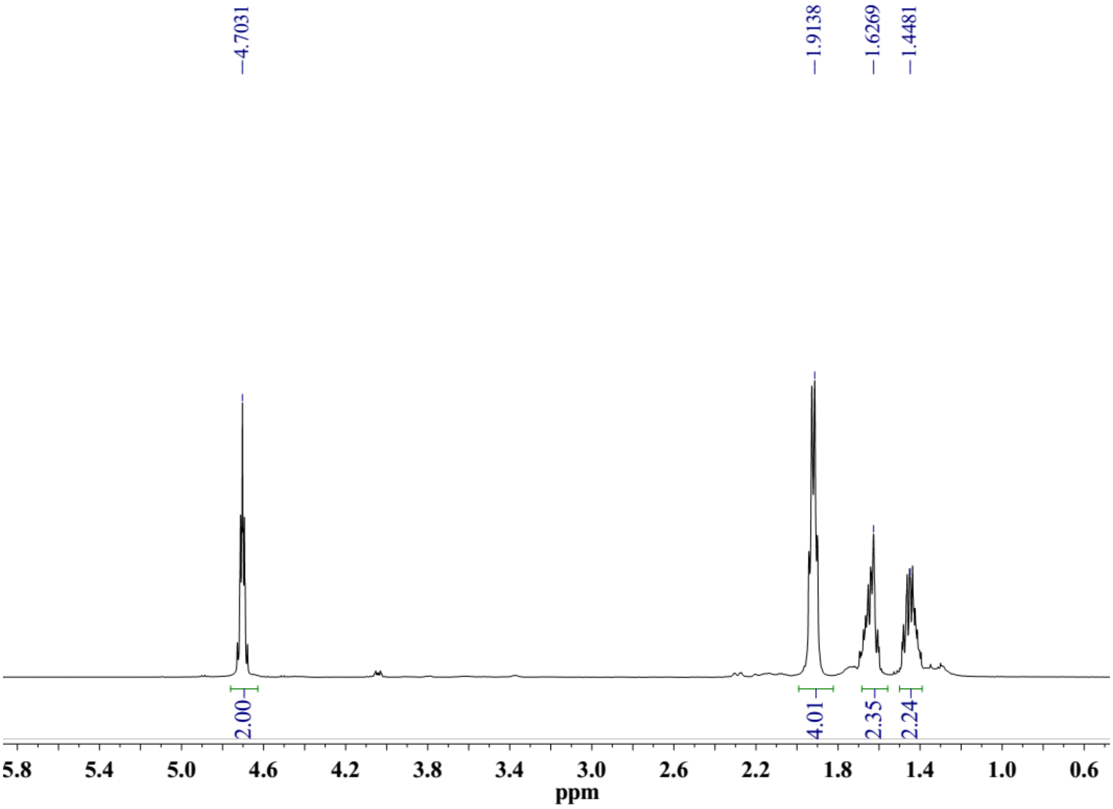
^{1}H NMR spectrum of 2k in CDCl$_3$:



^{1}H NMR spectrum of 2l in CDCl$_3$:



^{1}H NMR spectrum of 2m in CDCl$_3$:



^{1}H NMR spectrum of 2n in CDCl$_3$:

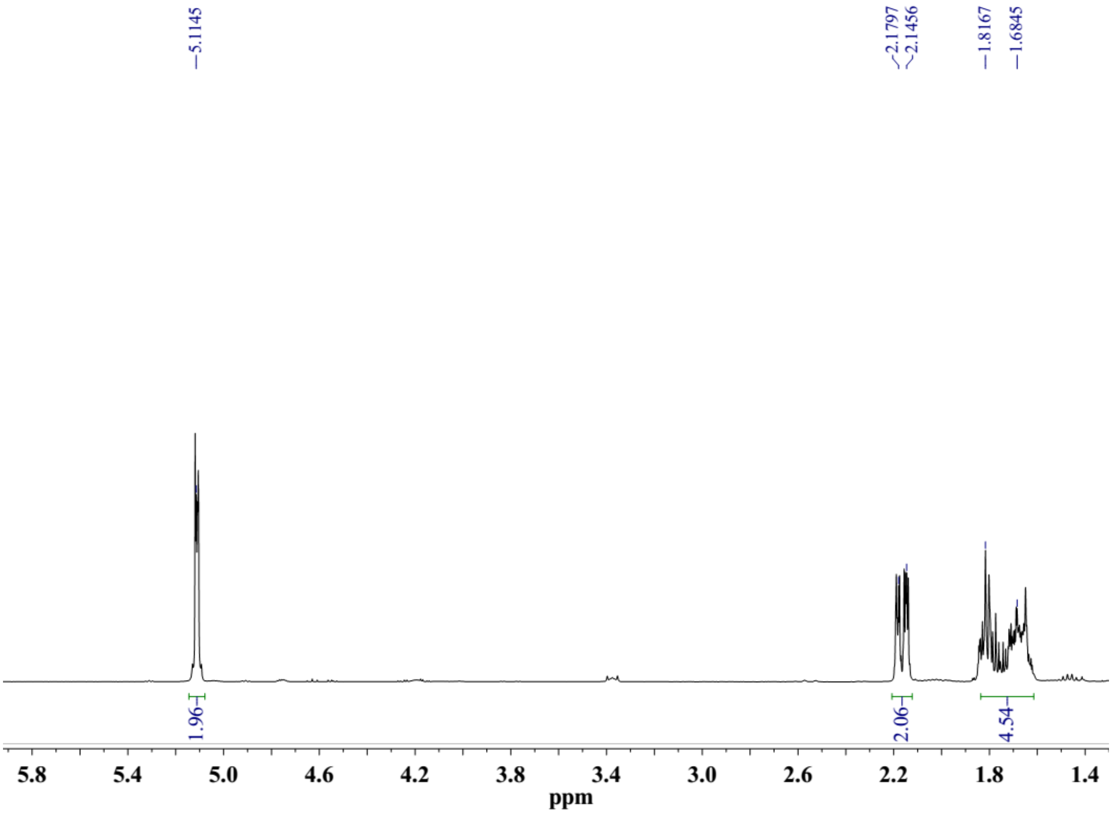


Table S2. Crystallographic data for complexes 1−4

Compound	**1**	**2**	**3**	**4·THF**
formula	$C_{66}H_{101}N_2O_5Yb$	$C_{66}H_{101}N_2O_5Y$	$C_{66}H_{101}N_2O_5Sm$	$C_{70}H_{109}N_2NdO_6$
fw	1175.53	1091.40	1152.84	1218.83
T(K)	223(2)	223(2)	223(2)	223(2)
crystal system	Triclinic	Triclinic	Monoclinic	Triclinic
space group	$P\bar{1}$	$P\bar{1}$	$P\ 2_1/c$	$P\bar{1}$
a (Å)	11.4765(5)	11.6333(4)	13.8842(10)	11.5700(9)
b (Å)	14.790	15.0256(4)	20.6892(17)	13.0084(9)
c (Å)	21.9149(15)	21.5946(8)	22.5022(15)	24.217(2)
α (deg)	93.494(8)	94.787(8)	90	80.278(5)
β (deg)	105.09	104.996(8)	91.478(2)	84.826(5)
γ (deg)	110.393(7)	111.655(9)	90	74.115(5)
V (Å^3)	3318.7(3)	3320.80(19)	6461.7(8)	3451.5(5)
Z	2	2	4	2
D_{calcd} (g cm^{-3})	1.176	1.091	1.185	1.173
μ (mm^{-1})	1.454	0.923	0.955	0.800
F (000)	1242	1180	2452	1302
θ_{max} (deg)	27.48	25.50	25.50	25.50
colldreflns	32210	27389	30100	29331
unique reflns	14962	12279	11947	12723
obsdreflns[I> 2.0σ(I)]	11347	7188	9743	10942
no. of variables	585	585	683	661
GOF	1.146	1.096	1.154	1.100
wR	0.2169	0.3333	0.1585	0.1606
R	0.1001	0.1248	0.0899	0.0585

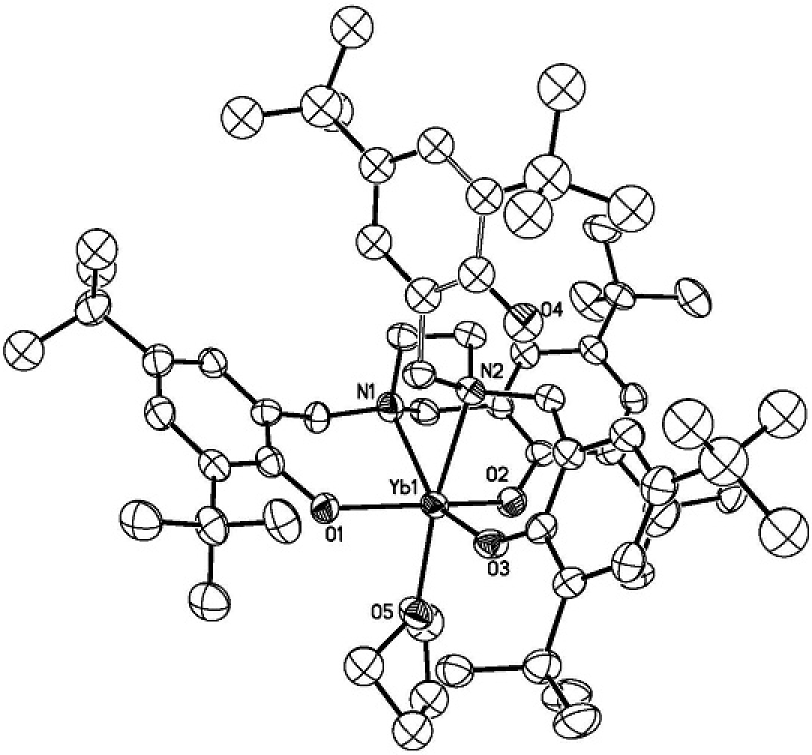


Figure S2 ORTEP diagram of complex **1** showing an atom numbering scheme. Thermal ellipsoids are drawn at the 20% probability level, and hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (deg): Yb(1)-O(3) 2.061(6), Yb(1)-O(1) 2.111(5), Yb(1)-O(2) 2.112(6), Yb(1)-O(5) 2.350(6), Yb(1)-N(1) 2.481(7), Yb(1)-N(2) 2.490(7); O(3)-Yb(1)-O(1) 106.4(2), O(3)-Yb(1)-O(2) 102.1(2), O(1)-Yb(1)-O(2) 149.4(3), O(3)-Yb(1)-O(5) 96.4(2), O(1)-Yb(1)-O(5) 85.9(2), O(2)-Yb(1)-O(5) 80.1(2), O(3)-Yb(1)-N(1) 150.3(2), O(1)-Yb(1)-N(1) 79.7(2), O(2)-Yb(1)-N(1) 81.0(2), O(5)-Yb(1)-N(1) 113.1(2), O(3)-Yb(1)-N(2) 78.0(2), O(1)-Yb(1)-N(2) 100.1(2), O(2)-Yb(1)-N(2) 96.4(2), O(5)-Yb(1)-N(2) 172.7(2), N(1)-Yb(1)-N(2) 72.3(2).

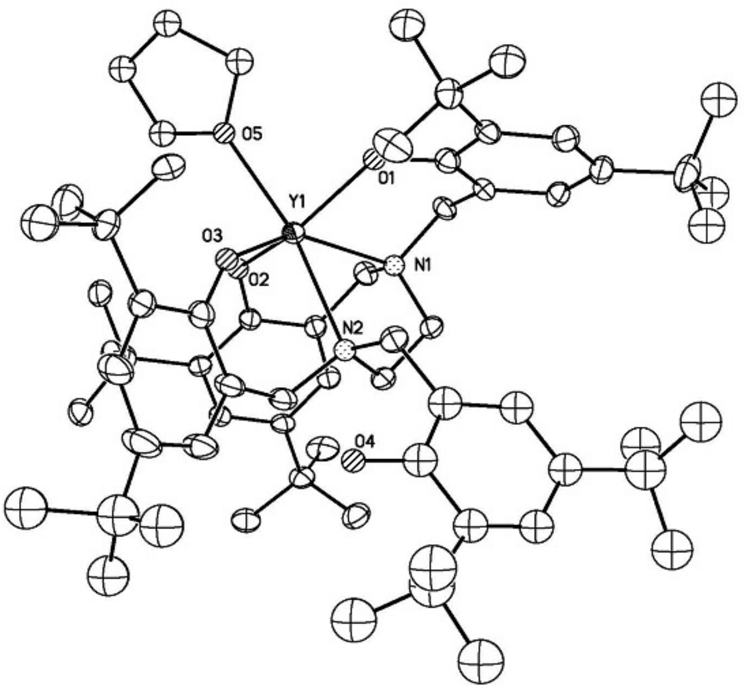


Figure S3 ORTEP diagram of complex **2** showing an atom numbering scheme. Thermal ellipsoids are drawn at the 20% probability level, and hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (deg): Y(1)-O(3) 2.096(5), Y(1)-O(1) 2.148(5), Y(1)-O(2) 2.155(5), Y(1)-O(5) 2.381(6), Y(1)-N(1) 2.528(6), Y(1)-N(2) 2.547(7); O(3)-Y(1)-O(1) 108.0(2), O(3)-Y(1)-O(2) 105.3(2), O(1)-Y(1)-O(2) 143.9(2), O(3)-Y(1)-O(5) 91.9(2), O(1)-Y(1)-O(5) 84.69(19), O(2)-Y(1)-O(5) 80.79(19), O(3)-Y(1)-N(1) 147.1(2), N(1)-Y(1)-N(2) 71.0(2), O(1)-Y(1)-N(1) 79.26(19), O(2)-Y(1)-N(1) 80.31(19), O(5)-Y(1)-N(1) 121.0(2), O(3)-Y(1)-N(2) 76.1(2), O(1)-Y(1)-N(2) 102.5(2), O(2)-Y(1)-N(2) 98.5(2), O(5)-Y(1)-N(2) 167.32(19).

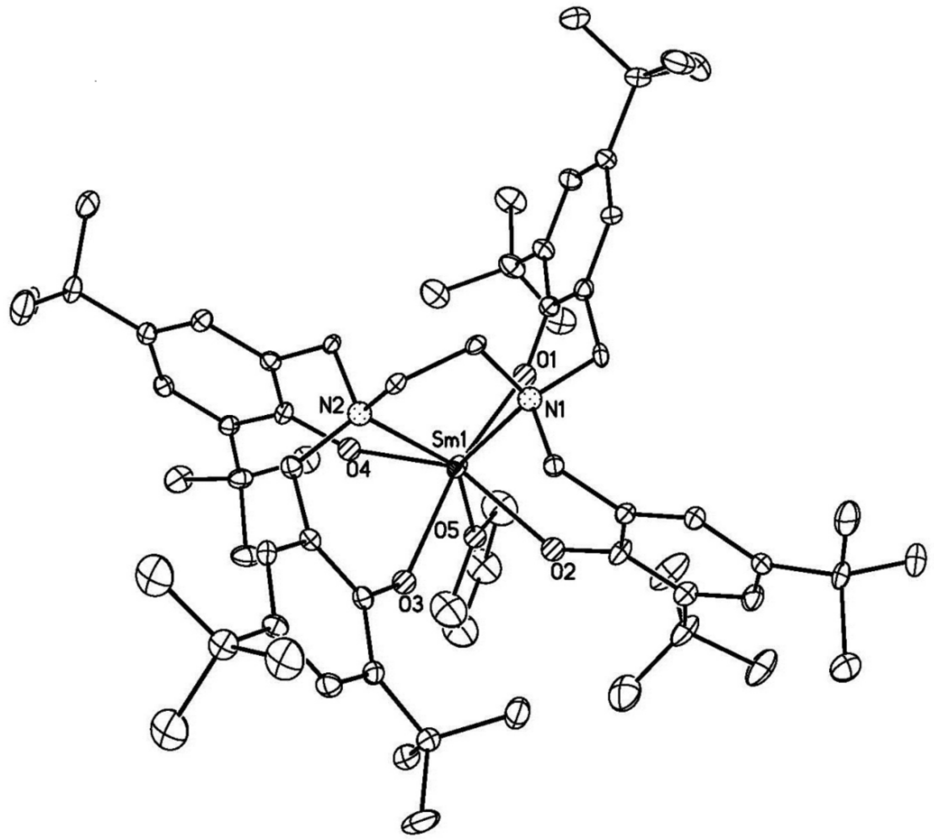


Figure S4 ORTEP diagram of complex **3** showing an atom numbering scheme. Thermal ellipsoids are drawn at the 20% probability level, and hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (deg): Sm(1)-O(1) 2.215(4), Sm(1)-O(4) 2.242(4), Sm(1)-O(2) 2.273(5), Sm(1)-O(5) 2.495(5), Sm(1)-O(3) 2.523(4), Sm(1)-N(2) 2.597(5), Sm(1)-N(1) 2.624(5); O(1)-Sm(1)-O(4) 100.87(17), O(1)-Sm(1)-O(2) 99.1(2), O(4)-Sm(1)-O(2) 147.46(18), O(1)-Sm(1)-O(5) 88.9(2), O(4)-Sm(1)-O(5) 77.67(17), O(2)-Sm(1)-O(5) 77.33(19), O(1)-Sm(1)-O(3) 166.94(17), O(4)-Sm(1)-O(3) 92.17(16), O(1)-Sm(1)-N(2) 111.07(18), O(4)-Sm(1)-N(2) 73.81(16), O(2)-Sm(1)-N(2) 121.61(18), O(2)-Sm(1)-O(3) 69.56(18), O(5)-Sm(1)-O(3) 94.71(19), O(5)-Sm(1)-N(2) 147.67(18), O(3)-Sm(1)-N(2) 71.70(16), O(1)-Sm(1)-N(1) 73.53(17), O(4)-Sm(1)-N(1) 135.25(16), O(2)-Sm(1)-N(1) 75.28(17), O(5)-Sm(1)-N(1) 144.34(17), O(3)-Sm(1)-N(1) 96.66(16), N(2)-Sm(1)-N(1) 67.76(16).

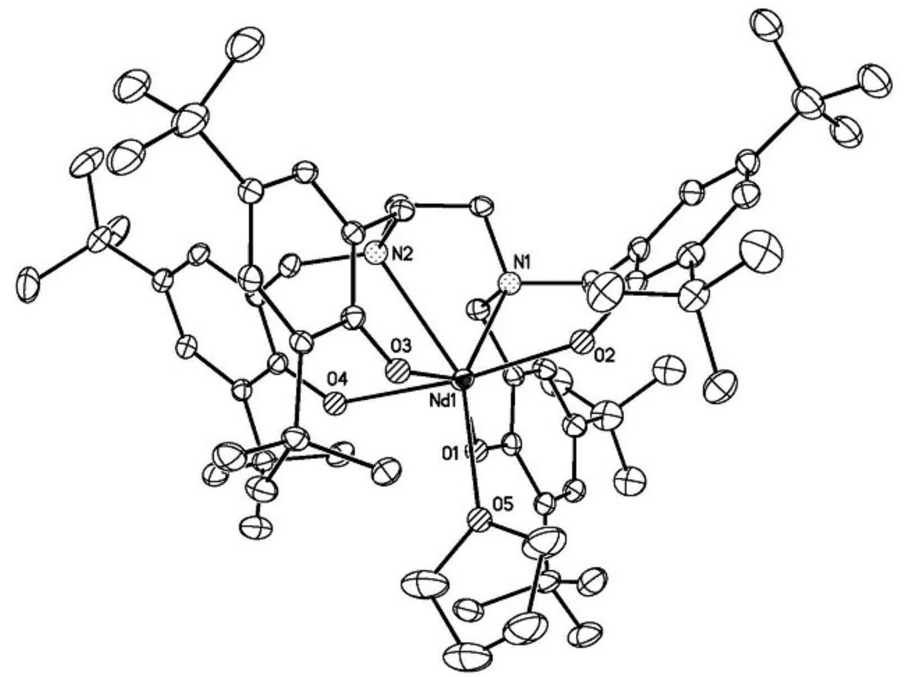


Figure S5 ORTEP diagram of complex **4·THF** showing an atom numbering scheme. Thermal ellipsoids are drawn at the 20% probability level. Hydrogen atoms and a THF molecule are omitted for clarity. Selected bond lengths (Å) and angles (deg): Nd(1)-O(1) 2.317(3), Nd(1)-O(5) 2.530(3), Nd(1)-O(2) 2.205(3), Nd(1)-N(1) 2.647(4), Nd(1)-O(3) 2.268(3), Nd(1)-N(2) 2.632(3), Nd(1)-O(4) 2.649(3); O(2)-Nd(1)-O(3) 98.28(12), O(3)-Nd(1)-N(1) 135.91(11), O(2)-Nd(1)-O(1) 107.76(12), O(1)-Nd(1)-N(1) 74.95(11), O(3)-Nd(1)-O(1) 145.03(11), O(5)-Nd(1)-N(1) 144.99(12), O(2)-Nd(1)-O(5) 93.00(14), N(2)-Nd(1)-N(1) 67.78(11), O(3)-Nd (1)-O(5) 77.44(11), O(2)-Nd(1)-O(4) 165.34(12), O(1)-Nd(1)-O(5) 78.26(12), O(3)-Nd(1)-O(4) 93.70(11), O(2)-N (1)-N(2) 106.68(12), O(1)-Nd(1)-O(4) 65.24(11), O(3)-Nd(1)-N(2) 73.36(10), O(5)-Nd(1)-O(4) 97.83(13), O(1)-Nd(1)-N(2) 118.81(11), N(2)-Nd(1)-O(4) 68.75(10), O(2)-Nd(1)-N(1) 74.47(11), N(1)-Nd(1)-O(4) 91.05(11).

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