## **ELECTRONIC SUPPORTING INFORMATION**

For

## Synthesis and Structural Characterization of Amido Scorpionate Rare Earth Metals Complexes

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**Figure S1.** (a) <sup>1</sup>H NMR spectrum of reaction mixture of bpztcpH and  $[Y{N(SiHMe_2)_2}_3(thf)_2]$  in toluene- $d_8$  at 25 °C. (b) <sup>1</sup>H NMR spectrum of reaction mixture after 3 h at 60 °C in toluene- $d_8$ . (c) <sup>1</sup>H NMR spectrum of reaction mixture after 15 h at 60 °C in toluene- $d_8$ .

	1	$3 \cdot C_7 H_8$	5·C <sub>7</sub> H <sub>8</sub>
Empirical formula	$C_{35}H_{49}N_6Si_3Y$	C <sub>30.5</sub> H <sub>53</sub> N <sub>6</sub> Si <sub>3</sub> Y	C44H65N6NdSi4
Formula weight	726.98	676.97	934.62
Temperature (K)	180(2)	180(2)	180(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	P 2 <sub>1</sub> /n	C 2/c	$P 2_1/c$
a(Å)	13.609(7)	24.434(2)	17.107(7)
b(Å)	17.854(3)	9.9080(7)	17.353(3)
c(Å)	16.652(3)	31.4640(10)	16.089(6)
β(°)	108.76(2)	105.003(4)	98.231(13)
Volume(Å <sup>3</sup> )	3831(2)	7357.5(8)	4727(3)
Z	4	8	4
Density (calculated) $(g/cm^3)$	1.260	1.222	1.313
Absorption coefficient (mm <sup>-1</sup> )	1.648	1.711	1.236
F(000)	1528	2872	1948
Crystal size mm <sup>3</sup>	0.38 x 0.30 x 0.17	0.27 x 0.18 x 0.12	0.52 x 0.44 x 0.11
Index ranges	-16≤h≤17	-28≤h≤28	-20≤h≤20
-	-22≤k≤20	-11≤k≤11	-20≤k≤16
	-20≤l≤20	-37≤l≤37	-19 <u>≤</u> 1 <u>≤</u> 19
Reflections collected	26465	35070	28922
Independent reflections	7822	6293	8104
	[R(int) = 0.1502]	$[R(int) = 0.0000]^{a}$	[R(int) = 0.2220]
Data / restraints / parameters	7822 / 2 / 424	6293 / 2 / 355	8104 / 4 / 524
Goodness-of-fit on F <sup>2</sup>	0.863	0.994	0.843
Final R indices $[I > 2\sigma(I)]$	R1 = 0.0553	R1 = 0.0767	R1 = 0.0629
	wR2 = 0.1053	wR2 = 0.1523	wR2 = 0.1109
Largest diff. peak and hole (e.Å $^{-3}$ )	0.521 and -1.738	0.671 and -0.619	1.457 and -1.108

## Table S1. Crystal data and structure refinement for 1, $3 \cdot C_7 H_8$ and $5 \cdot C_7 H_8$ .

<sup>a</sup> The value of R(int) = 0.000 was caused by the application of Squeeze.