Variable Coordination of Carbazolyl-*bis*(tetrazole) Ligands in Lanthanide Chemistry

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Table S1. Summary of crystallographic data for compounds **2-5**.

Compound	**2 • 0.5 C_3H_7OH** [a]	**3 • 2 C_7H_8** [a]	**4 • 2 C_7H_8** [b]	**5 • 2.5 C_7H_8** [a]
CCDC Dep. No.	1853581	1853585	1853582	1853587
Emp. formula	$C_{29.5}H_{41}N_9O_{0.5}$	$C_{54}H_{88}ErN_{11}Si_4$	$C_{54}H_{88}YbN_{11}Si_4$	$C_{79.5}H_{110}CeN_{19}Si_2$
Formula wgt.	529.71	1170.97	1176.75	1528.16
Temp. (K)	90(2)	120(2)	150(2)	120(2)
Crystal system	Monoclinic	Triclinic	Triclinic	Monoclinic
Space group	*P2₁/n* (No. 14)	*P-1* (No. 2)	*P-1* (No. 2)	*C2/c* (No. 15)
a (Å)	11.5895(14)	11.1978(5)	11.2711(9)	40.053(7)
b (Å)	18.322(2)	15.7727(8)	15.7793(12)	18.203(3)
c (Å)	14.424(2)	19.3549(9)	19.4540(14)	28.621(5)
α (º)	90	108.997(2)	108.834(2)	90
β (º)	104.335(7)	104.761(2)	104.839(2)	128.185(4)
γ (º)	90	97.811(2)	97.646(2)	90
Volume (Å^3)	2967.5(6)	3034.7(3)	3076.2(4)	16401(5)
Z	4	2	2	8
Density (g/cm^3)	1.186	1.281	1.270	1.238
Abs. coeff. μ (mm^{-1})	0.075	1.505	2.045	0.638
F(000)	1140	1226	1230	6448
Crystal size (mm)	0.18 x 0.15 x 0.05	0.20 x 0.10 x 0.05	0.12 x 0.07 x 0.07	0.31 x 0.22 x 0.17
Colour and habit	colourless needle	yellow block	yellow needle	yellow block
Theta range (º)	1.833-27.806	1.406-27.215	2.077-31.151	1.793-27.10
Refl. collected	29581	65917	57212	175948
Independent refl.	7007	13522	15021	18106
Goodness-of-fit (F^2)	1.040	1.015	0.981	1.082
Final R [I>2σ(I)]	0.055	0.044	0.027	0.041
Final wR2	0.135	0.076	0.065	0.094
R (all data)	0.090	0.074	0.031	0.054
wR2 (all data)	0.155	0.085	0.067	0.101
Max peak/hole (e/Å^3)	0.31/-0.22	0.83/-1.27	1.38/-0.30	1.41/-0.68

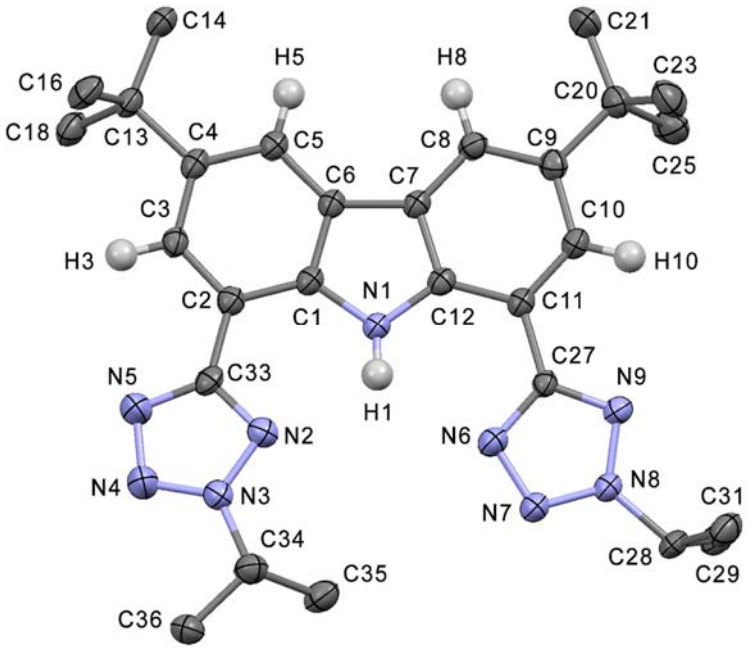
[a] Data collected on a Bruker Kappa X8-Apex II diffractometer using Mo Kα radiation (λ = 0.71073 Å) at the University of Notre Dame; [b] Data collected at the Advanced Light Source (ALS) synchrotron facility (λ = 0.7749 Å) , Lawrence Berkeley National Laboratory, Berkeley, CA.

Table S2. Summary of crystallographic data for compounds **3a, 4a, 6a** and **7**.

Compound	**3a** • 2.5 C_7H_8 [a]	**4a** • 2.33 C_7H_8 [b,c]	**6a** • 0.5 C_7H_8 [b]	**7** • 0.87 C_7H_8 [a,c,d]
CCDC Dep. No.	1853586	1853583	1853584	1853588
Emp. formula	$C_{76.5}H_{101}ErN_{18}OSi$	$C_{75.31}H_{99.64}N_{18}OSiYb$	$C_{115.5}H_{148}N_{36}O_2Sm_2$	$C_{90.09}H_{114.96}N_{27}Y$
Formula wgt.	1484.10	1474.21	2373.39	1665.03
Temp. (K)	90(2)	150(2)	150(2)	120(2)
Crystal system	Triclinic	Triclinic	Triclinic	Monoclinic
Space group	*P-1* (No. 2)	*P-1* (No. 2)	*P-1* (No. 2)	C2/c (No. 15)
a (Å)	13.0938(7)	13.0237(13)	16.490(2)	36.2178(14)
b (Å)	15.8303(8)	15.846(2)	19.382(2)	16.7410(7)
c (Å)	18.8209(9)	18.841(2)	21.328(2)	31.6549(12)
α (º)	82.643(3)	82.905(3)	73.382(3)	90
β (º)	88.231(3)	88.389(3)	72.642(3)	102.2743(13)
γ (º)	88.254(3)	87.902(3)	89.771(3)	90
Volume (Å^3)	3865.7(3)	3854.9(7)	6209.8(12)	18754.3(13)
Z	2	2	2	8
Density (g/cm^3)	1.275	1.270	1.269	1.179
Abs. coeff. μ (mm^{-1})	1.156	1.580	2.746	0.680
F(000)	1552	1593	2466	7068
Crystal size (mm)	0.25 x 0.21 x 0.08	0.11 x 0.04 x 0.02	0.05 x 0.05 x 0.01	0.17 x 0.17 x 0.14
Colour and habit	yellow block	yellow block	yellow-orange tablet	yellow prism
Theta range (º)	2.176-28.282	1.954-29.224	2.365-35.632	1.317-26.043
Refl. collected	74280	59476	50956	214690
Independent refl.	19078	15886	18131	18490
Goodness-of-fit (F^2)	1.076	1.055	1.032	1.044
Final R [I>2σ(I)]	0.045	0.056	0.093	0.045
Final wR2	0.098	0.126	0.243	0.119
R (all data)	0.060	0.078	0.144	0.064
wR2 (all data)	0.106	0.142	0.281	0.129
Max peak/hole (e/Å^3)	3.30/-0.82	2.22/-1.08	2.61/-1.37	0.69/-0.40

[a] Data collected on a Bruker Kappa X8-Apex II diffractometer using Mo Kα radiation (λ = 0.71073 Å) at the University of Notre Dame; [b] Data collected at the Advanced Light Source (ALS) synchrotron facility (λ = 0.7749 Å **4a**; 1.0332 Å **6a**) , Lawrence Berkeley National Laboratory, Berkeley, CA. [c] SQUEEZED solvent is included in the formula which leads to fractional equivalents of solvent as noted. The structures were refined both with discreet, severely disordered toluene molecules of crystallization and using the SQUEEZE routine; the latter gave marginally better refinements. Since the structure of the solvate is not relevant to the discussion, the results of the SQUEEZED refinement are presented. [d] Formula contains one 0.67 occupancy toluene that was modelled and residual solvent equating to 0.2 equivlents of toluene per asymmetric unit (masked) for a total of 0.87 equivalents of toluene.

Figure S1 Labeled ORTEP drawing of **H-CzT^{iPr} 2 • 0.5 C_3H_7OH**



Disordered t-Bu group carbons C15, C17, C19 and C22, C24, C26 not shown.

Disordered i-Pr group carbons C30, C32 not shown.

Disordered i-PrOH of solvation not shown: C37-C39 and O1

Only select H are shown.

Table S3 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **2 • 0.5 C_3H_7OH**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
N1	3896.5(13)	2776.1(8)	4571.8(10)	25.0(3)
N2	211.2(13)	2041.5(8)	3623.9(10)	27.5(3)
N3	1507.7(13)	2938.9(8)	3571.0(11)	31.6(4)
N4	475.5(13)	3121.9(8)	2985.0(11)	30.6(3)
N5	-269.7(12)	2582.4(8)	3027.2(10)	26.3(3)
C1	3451.7(14)	2131.8(9)	4841.3(11)	23.9(4)
C2	2276.1(14)	1872.3(9)	4617.5(12)	23.7(3)
C3	2064.8(15)	1209.1(9)	5019.5(12)	26.5(4)
C4	2980.3(15)	793.6(9)	5623.5(12)	27.2(4)
C5	4152.2(15)	1057.3(9)	5811.6(12)	26.6(4)
C6	4396.0(14)	1726.7(9)	5429.8(12)	24.3(4)
C7	2681.2(17)	79.4(10)	6073.4(14)	34.4(4)
C8	2010(3)	-441.8(17)	5293(3)	43.4(9)
C9	1767(3)	290.7(18)	6700(3)	44.6(9)
C10	3710(3)	-286.8(18)	6707(3)	43.0(10)
C11	1319.0(14)	2285.4(9)	3957.6(11)	22.4(3)
C12	-1534.3(15)	2581.6(10)	2477.6(13)	30.2(4)
C13	-1797.8(17)	1881.2(11)	1898.3(14)	36.9(5)
C14	-2328.5(17)	2698.7(12)	3161.0(14)	39.5(5)
C15	3165(7)	117(4)	7172(5)	56(2)
C16	1464(6)	-168(4)	5777(6)	58(2)
C17	3524(6)	-552(3)	5743(5)	55.6(19)
C18	8842.7(15)	2507.0(10)	6443.0(13)	28.8(4)
C19	9290(20)	1821(11)	6054(19)	55(8)
C20	9590(20)	3143(13)	6150(20)	65(9)
C21	8980(20)	2538(15)	7508(9)	47(7)
C22	3456(11)	5335(6)	2075(8)	62(3)
C23	2362(9)	4924(6)	3243(9)	53(3)
N2'	4399.6(13)	4201.5(8)	4053.1(11)	31.0(3)
N3'	6274.1(15)	4522.6(9)	4126.8(13)	46.1(5)
N4'	5562.9(15)	5043.0(10)	3652.7(13)	45.5(5)
N5'	4461.5(13)	4838.8(8)	3616.8(11)	30.6(3)

C1'	5113.7(15)	2800.1(9)	4973.5(11)	24.5(4)
C2'	5470.0(14)	2159.8(9)	5512.7(12)	24.6(4)
C3'	6667.7(14)	2062.0(9)	5991.9(12)	25.7(4)
C4'	7515.1(15)	2588.1(9)	5929.8(12)	26.2(4)
C5'	7131.8(15)	3218.1(9)	5374.8(12)	26.3(4)
C6'	5945.1(15)	3342.1(9)	4899.2(12)	25.3(4)
C8'	9095.2(17)	1781.1(11)	6990.9(15)	34.7(5)
C9'	9221.6(18)	3129.2(12)	7171.5(16)	37.6(6)
C10'	9599.6(18)	2523.3(13)	5704.9(15)	38.0(6)
C11'	5550.4(15)	4025.4(9)	4355.0(12)	26.5(4)
C12'	3390.1(17)	5279.1(10)	3177.4(14)	33.7(4)
C13'	2432(2)	4815.3(14)	2534(2)	37.9(7)
C14'	3737(2)	5938.1(13)	2697.5(18)	35.2(7)
O1	8832(3)	4350.4(17)	4333(3)	62.2(10)
C25	9690(5)	4866(3)	4746(5)	76.8(18)
C24	9244(8)	5370(5)	5355(6)	73(2)
C26	10827(8)	4485(6)	5174(7)	100(3)

Table S4 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **2 • 0.5 C_3H_7OH**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
N1	20.7(7)	26.1(7)	26.7(7)	2.3(6)	3.3(6)	-0.3(6)
N2	23.2(8)	30.8(8)	26.5(7)	2.2(6)	2.3(6)	1.4(6)
N3	23.0(8)	32.6(8)	36.0(8)	4.2(7)	1.3(6)	0.5(6)
N4	23.9(8)	31.5(8)	33.1(8)	4.5(6)	0.7(6)	-1.9(6)
N5	21.0(7)	28.3(7)	27.9(7)	1.4(6)	2.7(6)	-0.2(6)
C1	21.5(8)	26.7(8)	23.4(8)	-1.4(7)	5.2(7)	0.8(7)
C2	20.3(8)	26.5(8)	23.7(8)	-1.8(7)	4.5(7)	-0.1(7)
C3	20.8(8)	29.3(9)	28.3(9)	-2.1(7)	3.6(7)	-1.9(7)
C4	28.0(9)	25.0(9)	28.1(9)	-1.2(7)	6.1(7)	-2.3(7)
C5	23.7(9)	26.2(9)	27.9(9)	0.9(7)	2.5(7)	2.5(7)
C6	19.9(8)	27.1(8)	25.2(8)	-0.7(7)	4.5(7)	0.2(7)
C7	34.6(10)	29.4(9)	36.2(10)	4.2(8)	3.1(8)	-6.6(8)
C8	49(2)	26.0(16)	49(2)	3.7(14)	1.7(17)	-4.4(15)

C9	48(2)	41.3(18)	52(2)	10.4(16)	24.9(17)	-1.4(15)
C10	35.7(18)	32.7(17)	57(2)	16.5(16)	3.5(16)	-3.7(14)
C11	18.6(8)	25.7(8)	21.8(8)	-1.4(6)	2.9(6)	-3.0(6)
C12	18.2(9)	37.6(10)	31.0(9)	6.0(8)	-1.3(7)	0.6(7)
C13	30.0(10)	41.3(11)	33.6(10)	0.6(8)	-3.2(8)	-1.2(8)
C14	23.3(10)	53.6(12)	39.5(11)	2.7(9)	3.8(8)	3.0(8)
C15	71(5)	50(4)	49(4)	11(3)	18(3)	-22(3)
C16	35(3)	49(4)	83(5)	26(4)	-2(3)	-10(3)
C17	58(4)	31(3)	80(5)	5(3)	19(4)	-1(3)
C18	19.4(9)	33.7(9)	31.0(9)	-0.4(7)	1.7(7)	-0.7(7)
C19	44(15)	59(11)	59(15)	-1(12)	6(13)	30(11)
C20	23(11)	73(14)	90(20)	44(16)	-5(13)	-6(11)
C21	24(12)	70(20)	33(6)	-6(9)	-13(7)	1(12)
C22	68(8)	59(7)	59(7)	15(6)	14(6)	14(6)
C23	41(6)	57(6)	54(7)	9(5)	-3(5)	9(5)
N2'	31.4(8)	28.6(8)	31.6(8)	4.7(6)	5.1(7)	-1.0(6)
N3'	32.2(9)	43.2(10)	59.1(11)	20.6(9)	4.3(8)	-3.6(8)
N4'	31.3(9)	43.6(10)	58.4(11)	18.1(9)	5.0(8)	-5.1(7)
N5'	29.8(8)	30.0(8)	30.1(8)	4.6(6)	3.9(6)	-3.1(6)
C1'	20.5(8)	29.4(9)	22.7(8)	-2.2(7)	3.9(7)	0.1(7)
C2'	20.6(8)	28.1(9)	24.9(8)	-1.4(7)	5.3(7)	-0.9(7)
C3'	22.8(9)	28.7(9)	24.5(8)	-0.8(7)	3.8(7)	0.5(7)
C4'	19.2(8)	33.1(9)	25.4(8)	-3.2(7)	3.5(7)	-0.6(7)
C5'	22.6(9)	31.0(9)	24.8(8)	-1.6(7)	5.0(7)	-5.1(7)
C6'	23.8(9)	27.5(8)	24.5(8)	-0.9(7)	5.5(7)	-0.6(7)
C8'	20.8(10)	38.6(11)	40.5(12)	4.8(9)	-0.6(9)	0.1(8)
C9'	26.8(11)	38.9(12)	40.1(12)	-6.7(10)	-5.4(9)	0.7(9)
C10'	21.4(10)	52.5(14)	39.1(12)	4.3(10)	5.6(9)	1.0(9)
C11'	22.6(9)	31.9(9)	22.2(8)	-3.7(7)	0.7(7)	-1.0(7)
C12'	32.0(10)	30.9(9)	35.4(10)	3.8(8)	3.0(8)	2.8(8)
C13'	31.8(14)	34.1(14)	41.6(17)	-2.4(12)	-2.9(12)	2.6(11)
C14'	35.2(14)	33.5(13)	36.3(14)	10.0(11)	7.9(11)	2.4(10)
O1	36.3(17)	48.5(18)	105(3)	-21.1(18)	24.2(19)	-13.7(14)
C25	66(4)	72(4)	95(5)	-40(3)	26(3)	-35(3)
C24	57(4)	82(5)	84(5)	-20(4)	27(4)	-7(3)
C26	79(6)	96(6)	124(8)	-31(7)	27(7)	-19(5)

Table S5 Bond Lengths for **2 • 0.5 C_3H_7OH**.

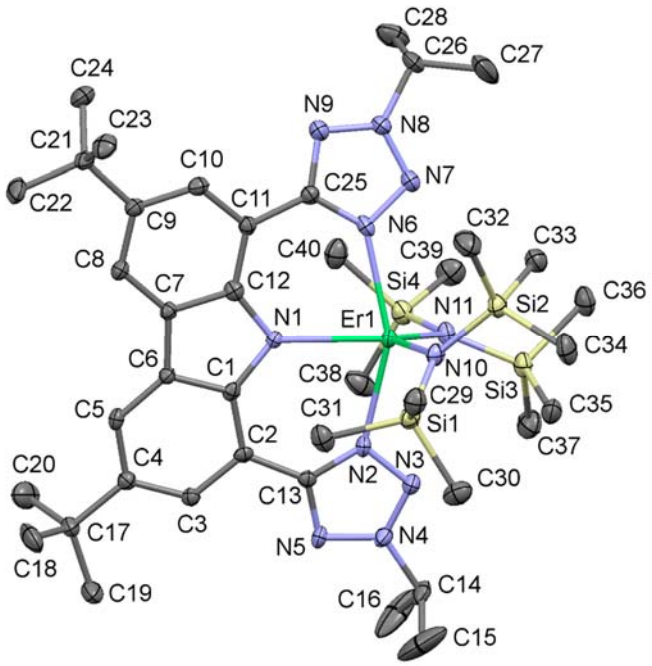
Atom	Atom	Length/Å	Atom	Atom	Length/ Å
N1	C1	1.382(2)	C18	C20	1.569(13)
N1	C1'	1.387(2)	C18	C21	1.506(13)
N2	N5	1.3401(19)	C18	C4'	1.541(2)
N2	C11	1.332(2)	C18	C8'	1.538(3)
N3	N4	1.3255(19)	C18	C9'	1.539(3)
N3	C11	1.361(2)	C18	C10'	1.538(3)
N4	N5	1.324(2)	C22	C12'	1.614(11)
N5	C12	1.484(2)	C23	C12'	1.381(10)
C1	C2	1.403(2)	N2'	N5'	1.337(2)
C1	C6	1.417(2)	N2'	C11'	1.336(2)
C2	C3	1.394(2)	N3'	N4'	1.333(2)
C2	C11	1.479(2)	N3'	C11'	1.334(2)
C3	C4	1.416(2)	N4'	N5'	1.319(2)
C4	C5	1.403(2)	N5'	C12'	1.485(2)
C4	C7	1.538(2)	C1'	C2'	1.412(2)
C5	C6	1.402(2)	C1'	C6'	1.406(2)
C6	C2'	1.456(2)	C2'	C3'	1.401(2)
C7	C8	1.533(4)	C3'	C4'	1.395(2)
C7	C9	1.601(4)	C4'	C5'	1.412(2)
C7	C10	1.472(4)	C5'	C6'	1.395(2)
C7	C15	1.546(7)	C6'	C11'	1.488(2)
C7	C16	1.442(6)	C12'	C13'	1.518(3)
C7	C17	1.659(6)	C12'	C14'	1.496(3)
C12	C13	1.521(3)	O1	C25	1.394(5)
C12	C14	1.521(3)	C25	C24	1.454(7)
C18	C19	1.521(13)	C25	C26	1.484(8)

Table S6 Bond Angles for **2 • 0.5 C_3H_7OH**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	C1'	108.74(14)	C21	C18	C20	108.8(13)
C11	N2	N5	101.21(13)	C21	C18	C4'	108.9(10)
N4	N3	C11	105.81(14)	C4'	C18	C20	110.4(10)
N5	N4	N3	106.14(13)	C8'	C18	C4'	111.76(14)
N2	N5	C12	122.77(14)	C8'	C18	C9'	107.70(16)
N4	N5	N2	114.16(14)	C8'	C18	C10'	107.69(16)
N4	N5	C12	123.06(14)	C9'	C18	C4'	109.80(15)
N1	C1	C2	129.29(15)	C10'	C18	C4'	109.78(15)
N1	C1	C6	109.23(14)	C10'	C18	C9'	110.06(16)
C2	C1	C6	121.48(15)	C11'	N2'	N5'	101.46(14)
C1	C2	C11	120.37(15)	N4'	N3'	C11'	105.57(15)
C3	C2	C1	117.40(15)	N5'	N4'	N3'	106.66(15)
C3	C2	C11	122.21(15)	N2'	N5'	C12'	122.60(14)
C2	C3	C4	122.84(15)	N4'	N5'	N2'	113.18(14)
C3	C4	C7	120.27(15)	N4'	N5'	C12'	124.17(15)
C5	C4	C3	118.40(15)	N1	C1'	C2'	109.41(14)
C5	C4	C7	121.32(15)	N1	C1'	C6'	129.49(15)
C6	C5	C4	120.33(15)	C6'	C1'	C2'	121.10(15)
C1	C6	C2'	106.35(14)	C1'	C2'	C6	106.27(14)
C5	C6	C1	119.51(15)	C3'	C2'	C6	133.91(16)
C5	C6	C2'	134.12(15)	C3'	C2'	C1'	119.81(15)
C4	C7	C9	106.40(17)	C4'	C3'	C2'	120.49(16)
C4	C7	C15	109.4(3)	C3'	C4'	C18	122.53(15)
C4	C7	C17	105.2(3)	C3'	C4'	C5'	118.28(15)
C8	C7	C4	110.29(18)	C5'	C4'	C18	119.20(15)
C8	C7	C9	106.2(2)	C6'	C5'	C4'	123.04(16)
C10	C7	C4	114.66(18)	C1'	C6'	C11'	120.49(15)
C10	C7	C8	111.0(2)	C5'	C6'	C1'	117.27(15)
C10	C7	C9	107.9(2)	C5'	C6'	C11'	122.22(15)
C15	C7	C17	103.6(4)	N2'	C11'	C6'	121.78(15)
C16	C7	C4	116.6(3)	N3'	C11'	N2'	113.13(16)
C16	C7	C15	113.5(4)	N3'	C11'	C6'	125.09(16)
C16	C7	C17	107.4(4)	C23	C12'	C22	110.5(7)
N2	C11	N3	112.66(14)	C23	C12'	N5'	111.1(4)

N2	C11	C2	124.28(14)	N5'	C12'	C22	102.5(4)
N3	C11	C2	122.89(14)	N5'	C12'	C13'	111.36(16)
N5	C12	C13	109.38(14)	N5'	C12'	C14'	110.10(16)
N5	C12	C14	109.26(15)	C14'	C12'	C13'	114.11(19)
C13	C12	C14	113.81(16)	O1	C25	C24	111.4(6)
C19	C18	C20	104.7(14)	O1	C25	C26	109.0(6)
C19	C18	C4'	107.2(11)	C24	C25	C26	117.4(6)
C21	C18	C19	116.7(13)				

Figure S2 Labeled ORTEP drawing of **Er(CzT^{iPr})[N(SiMe$_3$)$_2$]$_2$ 3 • 2 C$_7$H$_8$**



Toluenes of solvation not shown.

Table S7 Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$)[1] for **$Er(CzT^{iPr})[N(SiMe_3)_2]_2$ 3 • 2 C_7H_8**

Atom	x	y	z	U(eq)
Er(1)	0.41402(2)	0.18241(2)	0.78858(2)	0.015(1)
Si(1)	0.59762(11)	0.32329(8)	0.97097(6)	0.020(1)
Si(2)	0.61832(11)	0.12738(8)	0.92269(6)	0.023(1)
Si(3)	0.16916(11)	0.02357(8)	0.79429(6)	0.022(1)
Si(4)	0.14964(11)	0.04973(8)	0.64738(6)	0.022(1)
N(1)	0.4586(3)	0.2901(2)	0.73176(16)	0.013(1)
N(2)	0.2782(3)	0.2833(2)	0.81984(17)	0.017(1)
N(3)	0.1965(3)	0.2621(2)	0.85436(18)	0.020(1)
N(4)	0.1272(3)	0.3221(2)	0.85762(18)	0.021(1)
N(5)	0.1569(3)	0.3837(2)	0.82781(17)	0.019(1)
N(6)	0.5359(3)	0.1094(2)	0.71140(18)	0.018(1)
N(7)	0.5387(3)	0.0217(2)	0.69676(18)	0.021(1)
N(8)	0.6105(3)	0.0043(2)	0.65269(18)	0.021(1)
N(9)	0.6559(3)	0.0753(2)	0.63647(18)	0.022(1)
N(10)	0.5537(3)	0.2132(2)	0.90230(17)	0.018(1)
N(11)	0.2369(3)	0.0704(2)	0.74057(17)	0.019(1)
C(1)	0.4154(3)	0.3704(2)	0.73680(19)	0.014(1)
C(2)	0.3216(3)	0.4028(2)	0.76645(19)	0.014(1)
C(3)	0.2921(4)	0.4847(2)	0.7606(2)	0.016(1)
C(4)	0.3517(3)	0.5366(2)	0.7276(2)	0.016(1)
C(5)	0.4483(3)	0.5055(3)	0.7015(2)	0.016(1)
C(6)	0.4803(3)	0.4251(2)	0.7060(2)	0.014(1)
C(7)	0.5693(3)	0.3772(2)	0.6802(2)	0.014(1)
C(8)	0.6593(3)	0.3982(3)	0.6462(2)	0.016(1)
C(9)	0.7347(3)	0.3383(3)	0.6257(2)	0.016(1)
C(10)	0.7148(3)	0.2563(3)	0.6384(2)	0.017(1)
C(11)	0.6250(3)	0.2329(2)	0.6711(2)	0.015(1)
C(12)	0.5518(3)	0.2954(3)	0.6957(2)	0.016(1)
C(13)	0.2529(3)	0.3579(2)	0.8038(2)	0.015(1)
C(14)	0.0283(4)	0.3239(3)	0.8958(2)	0.024(1)
C(15)	0.0783(5)	0.4005(4)	0.9721(3)	0.074(2)
C(16)	-0.0919(5)	0.3273(5)	0.8442(3)	0.078(2)
C(17)	0.3113(4)	0.6219(3)	0.7181(2)	0.021(1)
C(18)	0.4264(4)	0.7052(3)	0.7564(3)	0.038(1)
C(19)	0.2074(4)	0.6457(3)	0.7526(3)	0.034(1)
C(20)	0.2610(5)	0.6028(3)	0.6313(2)	0.041(1)
C(21)	0.8406(4)	0.3600(3)	0.5923(2)	0.018(1)
C(22)	0.8413(4)	0.4489(3)	0.5769(3)	0.030(1)
C(23)	0.9687(4)	0.3716(3)	0.6510(2)	0.028(1)
C(24)	0.8235(4)	0.2803(3)	0.5170(2)	0.029(1)
C(25)	0.6077(4)	0.1414(3)	0.6743(2)	0.017(1)
C(26)	0.6320(4)	-0.0886(3)	0.6188(2)	0.028(1)

C(27)	0.6166(7)	-0.1422(4)	0.6685(3)	0.068(2)
C(28)	0.5443(5)	-0.1337(3)	0.5364(3)	0.040(1)
C(29)	0.7656(4)	0.3577(3)	1.0353(2)	0.027(1)
C(30)	0.4933(4)	0.3383(3)	1.0331(2)	0.032(1)
C(31)	0.5885(4)	0.4132(3)	0.9277(2)	0.028(1)
C(32)	0.7802(4)	0.1334(3)	0.9127(3)	0.038(1)
C(33)	0.5193(4)	0.0094(3)	0.8564(2)	0.029(1)
C(34)	0.6307(4)	0.1287(3)	1.0216(2)	0.035(1)
C(35)	0.2509(4)	0.0839(3)	0.9003(2)	0.029(1)
C(36)	0.1697(4)	-0.1015(3)	0.7701(2)	0.031(1)
C(37)	-0.0015(4)	0.0297(3)	0.7812(3)	0.034(1)
C(38)	0.0417(5)	0.1305(3)	0.6431(3)	0.037(1)
C(39)	0.0509(4)	-0.0705(3)	0.5928(2)	0.033(1)
C(40)	0.2544(4)	0.0683(3)	0.5894(2)	0.031(1)
C(41)	0.2388(4)	0.3187(3)	0.4742(2)	0.022(1)
C(42)	0.1440(4)	0.2875(3)	0.4041(2)	0.029(1)
C(43)	0.1647(4)	0.3050(3)	0.3419(2)	0.034(1)
C(44)	0.2815(4)	0.3540(3)	0.3489(2)	0.027(1)
C(45)	0.3767(4)	0.3863(3)	0.4191(2)	0.027(1)
C(46)	0.3558(4)	0.3689(3)	0.4809(2)	0.025(1)
C(47)	0.2165(4)	0.2982(3)	0.5412(2)	0.032(1)
C(48)	0.8849(5)	0.7700(4)	0.8883(3)	0.049(1)
C(49)	0.9634(5)	0.7183(4)	0.8620(3)	0.044(1)
C(50)	0.9242(5)	0.6202(4)	0.8320(3)	0.045(1)
C(51)	0.8091(5)	0.5788(4)	0.8298(3)	0.046(1)
C(52)	0.7298(5)	0.6326(4)	0.8566(3)	0.052(2)
C(53)	0.7679(5)	0.7265(4)	0.8852(3)	0.048(1)
C(54)	0.9242(6)	0.8740(4)	0.9195(4)	0.075(2)
H(3)	0.22765	0.50573	0.78044	0.019
H(5)	0.49339	0.54008	0.68009	0.019
H(8)	0.66870	0.45399	0.63705	0.020
H(10)	0.76540	0.21418	0.62394	0.021
H(14)	0.01315	0.26486	0.90457	0.029
H(15A)	0.16278	0.39687	0.99967	0.111
H(15B)	0.02074	0.39568	1.00199	0.111
H(15C)	0.08441	0.45961	0.96524	0.111
H(16A)	-0.08028	0.38518	0.83548	0.117
H(16B)	-0.15884	0.32383	0.86816	0.117
H(16C)	-0.11652	0.27496	0.79487	0.117
H(18A)	0.45595	0.72031	0.81213	0.056
H(18B)	0.40165	0.75839	0.74621	0.056
H(18C)	0.49495	0.69026	0.73519	0.056
H(19A)	0.13254	0.59354	0.72775	0.051
H(19B)	0.18439	0.70026	0.74432	0.051
H(19C)	0.23794	0.65883	0.80803	0.051
H(20A)	0.32923	0.59218	0.60867	0.062

H(20B)	0.23185	0.65605	0.62401	0.062
H(20C)	0.18987	0.54792	0.60585	0.062
H(22A)	0.75916	0.44308	0.54019	0.044
H(22B)	0.90931	0.46002	0.55522	0.044
H(22C)	0.85586	0.50072	0.62530	0.044
H(23A)	0.97889	0.42141	0.69982	0.042
H(23B)	1.03765	0.38689	0.63128	0.042
H(23C)	0.97144	0.31383	0.65953	0.042
H(24A)	0.82365	0.22296	0.52657	0.044
H(24B)	0.89352	0.29326	0.49732	0.044
H(24C)	0.74250	0.27347	0.47887	0.044
H(26)	0.72161	-0.08096	0.61792	0.034
H(27A)	0.67054	-0.10589	0.72177	0.102
H(27B)	0.64160	-0.20042	0.64960	0.102
H(27C)	0.52744	-0.15519	0.66662	0.102
H(28A)	0.45566	-0.14263	0.53585	0.060
H(28B)	0.56129	-0.19371	0.51176	0.060
H(28C)	0.55904	-0.09401	0.50808	0.060
H(29A)	0.77991	0.31354	1.06054	0.041
H(29B)	0.78228	0.41958	1.07451	0.041
H(29C)	0.82307	0.35794	1.00466	0.041
H(30A)	0.40534	0.32855	1.00131	0.048
H(30B)	0.52187	0.40101	1.07252	0.048
H(30C)	0.49783	0.29338	1.05808	0.048
H(31A)	0.64047	0.40617	0.89330	0.042
H(31B)	0.62041	0.47473	0.96883	0.042
H(31C)	0.49994	0.40596	0.89825	0.042
H(32A)	0.77579	0.12938	0.86044	0.057
H(32B)	0.81210	0.08193	0.92199	0.057
H(32C)	0.83768	0.19198	0.95029	0.057
H(33A)	0.45903	-0.01183	0.87958	0.044
H(33B)	0.57464	-0.03344	0.84776	0.044
H(33C)	0.47241	0.01153	0.80699	0.044
H(34A)	0.68761	0.18684	1.06047	0.052
H(34B)	0.66479	0.07678	1.02822	0.052
H(34C)	0.54619	0.12314	1.02786	0.052
H(35A)	0.34313	0.09903	0.91061	0.043
H(35B)	0.22962	0.04351	0.92684	0.043
H(35C)	0.22285	0.14087	0.91915	0.043
H(36A)	0.11536	-0.13729	0.71677	0.046
H(36B)	0.13720	-0.12373	0.80507	0.046
H(36C)	0.25674	-0.10879	0.77566	0.046
H(37A)	-0.00771	0.09385	0.79187	0.051
H(37B)	-0.03179	0.00741	0.81686	0.051
H(37C)	-0.05386	-0.00884	0.72805	0.051
H(38A)	-0.01341	0.12564	0.67432	0.056

H(38B)	-0.01067	0.11394	0.58948	0.056
H(38C)	0.09297	0.19399	0.66317	0.056
H(39A)	0.10553	-0.11406	0.59309	0.050
H(39B)	0.00813	-0.07814	0.53948	0.050
H(39C)	-0.01289	-0.08269	0.61706	0.050
H(40A)	0.30907	0.13102	0.61491	0.047
H(40B)	0.20154	0.06019	0.53772	0.047
H(40C)	0.30735	0.02343	0.58514	0.047
H(42)	0.06301	0.25328	0.39824	0.035
H(43)	0.09778	0.28316	0.29418	0.041
H(44)	0.29644	0.36542	0.30615	0.033
H(45)	0.45755	0.42078	0.42494	0.032
H(46)	0.42241	0.39169	0.52878	0.030
H(47A)	0.28334	0.27036	0.56168	0.049
H(47B)	0.13341	0.25521	0.52400	0.049
H(47C)	0.21839	0.35570	0.58170	0.049
H(49)	1.04459	0.74765	0.86371	0.052
H(50)	0.97896	0.58409	0.81354	0.053
H(51)	0.78229	0.51337	0.81001	0.055
H(52)	0.64853	0.60371	0.85510	0.063
H(53)	0.71248	0.76236	0.90314	0.058
H(54A)	0.92598	0.89856	0.97329	0.112
H(54B)	0.86322	0.89741	0.88879	0.112
H(54C)	1.00912	0.89369	0.91662	0.112

[1] U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

Table S8 Anisotropic displacement parameters $(Å^2)^2$ for **Er(CzT^{iPr})[N(SiMe$_3$)$_2$]$_2$ 3 • 2 C$_7$H$_8$**

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Er(1)	0.0178(1)	0.0142(1)	0.0144(1)	0.0079(1)	0.0065(1)	0.0041(1)
Si(1)	0.0217(6)	0.0209(6)	0.0171(5)	0.0077(5)	0.0053(5)	0.0050(5)
Si(2)	0.0256(6)	0.0242(6)	0.0224(6)	0.0137(5)	0.0075(5)	0.0081(5)
Si(3)	0.0241(6)	0.0189(6)	0.0249(6)	0.0109(5)	0.0077(5)	0.0016(5)
Si(4)	0.0244(6)	0.0198(6)	0.0197(6)	0.0073(5)	0.0024(5)	0.0037(5)
N(1)	0.0131(16)	0.0137(16)	0.0118(15)	0.0055(13)	0.0046(13)	0.0023(13)
N(2)	0.0214(18)	0.0165(17)	0.0196(17)	0.0114(14)	0.0095(15)	0.0041(14)
N(3)	0.0256(19)	0.0205(18)	0.0238(18)	0.0130(15)	0.0146(16)	0.0083(15)
N(4)	0.0211(18)	0.0266(19)	0.0218(18)	0.0136(15)	0.0125(15)	0.0081(15)
N(5)	0.0232(18)	0.0203(18)	0.0184(17)	0.0124(14)	0.0106(15)	0.0047(14)
N(6)	0.0216(18)	0.0133(17)	0.0222(17)	0.0094(14)	0.0060(15)	0.0064(14)
N(7)	0.029(2)	0.0165(17)	0.0246(18)	0.0109(15)	0.0123(16)	0.0092(15)
N(8)	0.0274(19)	0.0171(17)	0.0228(18)	0.0096(15)	0.0122(16)	0.0104(15)
N(9)	0.029(2)	0.0178(18)	0.0224(18)	0.0099(15)	0.0116(16)	0.0089(15)

N(10)	0.0200(18)	0.0217(18)	0.0139(16)	0.0090(14)	0.0033(14)	0.0057(14)
N(11)	0.0207(18)	0.0165(17)	0.0195(17)	0.0091(14)	0.0030(14)	0.0006(14)
C(1)	0.0149(19)	0.0142(19)	0.0096(17)	0.0032(15)	0.0025(15)	0.0004(15)
C(2)	0.015(2)	0.0151(19)	0.0093(17)	0.0021(15)	0.0031(15)	0.0032(16)
C(3)	0.018(2)	0.0147(19)	0.0146(18)	0.0051(15)	0.0055(16)	0.0045(16)
C(4)	0.017(2)	0.0157(19)	0.0139(18)	0.0052(16)	0.0038(16)	0.0041(16)
C(5)	0.017(2)	0.018(2)	0.0138(18)	0.0093(16)	0.0044(16)	0.0023(16)
C(6)	0.0135(19)	0.0152(19)	0.0136(18)	0.0062(15)	0.0056(16)	0.0038(15)
C(7)	0.0138(19)	0.0157(19)	0.0129(18)	0.0063(15)	0.0039(15)	0.0039(15)
C(8)	0.016(2)	0.018(2)	0.0163(19)	0.0077(16)	0.0066(16)	0.0030(16)
C(9)	0.016(2)	0.019(2)	0.0149(19)	0.0066(16)	0.0057(16)	0.0050(16)
C(10)	0.017(2)	0.021(2)	0.0151(19)	0.0062(16)	0.0056(16)	0.0074(17)
C(11)	0.017(2)	0.0136(19)	0.0149(19)	0.0055(15)	0.0046(16)	0.0024(16)
C(12)	0.014(2)	0.016(2)	0.0154(19)	0.0052(16)	0.0020(16)	0.0022(15)
C(13)	0.016(2)	0.0132(19)	0.0127(18)	0.0035(15)	0.0045(16)	0.0027(16)
C(14)	0.022(2)	0.034(2)	0.029(2)	0.020(2)	0.0153(19)	0.0081(19)
C(15)	0.056(4)	0.097(5)	0.042(3)	-0.010(3)	0.036(3)	-0.013(3)
C(16)	0.023(3)	0.186(8)	0.061(4)	0.082(5)	0.023(3)	0.037(4)
C(17)	0.026(2)	0.019(2)	0.026(2)	0.0134(18)	0.0134(19)	0.0103(18)
C(18)	0.040(3)	0.021(2)	0.060(3)	0.023(2)	0.019(3)	0.010(2)
C(19)	0.043(3)	0.032(3)	0.049(3)	0.027(2)	0.029(2)	0.023(2)
C(20)	0.058(3)	0.050(3)	0.029(3)	0.023(2)	0.016(2)	0.032(3)
C(21)	0.017(2)	0.023(2)	0.020(2)	0.0101(17)	0.0092(17)	0.0088(17)
C(22)	0.029(2)	0.034(3)	0.041(3)	0.025(2)	0.021(2)	0.010(2)
C(23)	0.019(2)	0.036(3)	0.033(2)	0.016(2)	0.012(2)	0.0067(19)
C(24)	0.035(3)	0.031(3)	0.027(2)	0.011(2)	0.020(2)	0.010(2)
C(25)	0.018(2)	0.016(2)	0.0137(18)	0.0051(16)	0.0037(16)	0.0037(16)
C(26)	0.040(3)	0.018(2)	0.039(3)	0.015(2)	0.021(2)	0.016(2)
C(27)	0.138(6)	0.037(3)	0.060(4)	0.031(3)	0.051(4)	0.052(4)
C(28)	0.050(3)	0.024(3)	0.037(3)	0.000(2)	0.012(2)	0.012(2)
C(29)	0.027(2)	0.028(2)	0.023(2)	0.0106(19)	0.0045(19)	0.0018(19)
C(30)	0.032(3)	0.034(3)	0.026(2)	0.005(2)	0.012(2)	0.006(2)
C(31)	0.033(3)	0.022(2)	0.024(2)	0.0090(18)	0.002(2)	0.0036(19)
C(32)	0.038(3)	0.037(3)	0.051(3)	0.023(2)	0.019(2)	0.019(2)
C(33)	0.039(3)	0.025(2)	0.028(2)	0.013(2)	0.013(2)	0.013(2)
C(34)	0.045(3)	0.031(3)	0.032(3)	0.021(2)	0.006(2)	0.008(2)
C(35)	0.039(3)	0.025(2)	0.027(2)	0.0133(19)	0.016(2)	0.006(2)
C(36)	0.037(3)	0.021(2)	0.035(3)	0.014(2)	0.009(2)	0.000(2)
C(37)	0.030(3)	0.033(3)	0.041(3)	0.017(2)	0.015(2)	0.003(2)
C(38)	0.047(3)	0.033(3)	0.028(2)	0.010(2)	0.003(2)	0.021(2)
C(39)	0.032(3)	0.031(3)	0.027(2)	0.005(2)	0.005(2)	0.002(2)
C(40)	0.034(3)	0.033(3)	0.024(2)	0.013(2)	0.005(2)	0.001(2)
C(41)	0.026(2)	0.020(2)	0.020(2)	0.0063(17)	0.0076(18)	0.0029(18)
C(42)	0.024(2)	0.031(2)	0.028(2)	0.012(2)	0.005(2)	-0.0028(19)
C(43)	0.037(3)	0.035(3)	0.023(2)	0.012(2)	-0.001(2)	0.002(2)
C(44)	0.041(3)	0.023(2)	0.024(2)	0.0123(19)	0.014(2)	0.009(2)

C(45)	0.026(2)	0.025(2)	0.035(3)	0.015(2)	0.015(2)	0.0077(19)
C(46)	0.027(2)	0.023(2)	0.021(2)	0.0056(18)	0.0055(19)	0.0065(19)
C(47)	0.032(3)	0.037(3)	0.029(2)	0.013(2)	0.013(2)	0.000(2)
C(48)	0.044(3)	0.070(4)	0.043(3)	0.034(3)	0.011(3)	0.014(3)
C(49)	0.026(3)	0.079(4)	0.036(3)	0.030(3)	0.011(2)	0.019(3)
C(50)	0.038(3)	0.071(4)	0.028(3)	0.021(3)	0.009(2)	0.020(3)
C(51)	0.042(3)	0.053(3)	0.032(3)	0.009(2)	0.005(2)	0.004(3)
C(52)	0.030(3)	0.075(4)	0.041(3)	0.013(3)	0.011(3)	0.000(3)
C(53)	0.030(3)	0.069(4)	0.047(3)	0.022(3)	0.015(3)	0.011(3)
C(54)	0.082(5)	0.060(4)	0.080(5)	0.040(4)	0.012(4)	0.002(4)

[2] The anisotropic displacement factor exponent takes the form $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

Table S9 Bond lengths [Å] for **Er(CzT^{iPr})[N(SiMe$_3$)$_2$]$_2$ 3 • 2 C$_7$H$_8$**

atom-atom	**distance**	**atom-atom**	**distance**
Er(1)-N(10)	2.207(3)	Er(1)-N(11)	2.226(3)
Er(1)-N(1)	2.368(3)	Er(1)-N(2)	2.390(3)
Er(1)-N(6)	2.401(3)	Er(1)-Si(4)	3.3290(11)
Si(1)-N(10)	1.719(3)	Si(1)-C(30)	1.863(4)
Si(1)-C(29)	1.864(4)	Si(1)-C(31)	1.869(4)
Si(2)-N(10)	1.726(3)	Si(2)-C(32)	1.864(5)
Si(2)-C(33)	1.871(4)	Si(2)-C(34)	1.877(4)
Si(3)-N(11)	1.718(3)	Si(3)-C(35)	1.868(4)
Si(3)-C(36)	1.874(4)	Si(3)-C(37)	1.883(4)
Si(4)-N(11)	1.717(3)	Si(4)-C(39)	1.862(4)
Si(4)-C(40)	1.875(4)	Si(4)-C(38)	1.877(4)
N(1)-C(1)	1.400(5)	N(1)-C(12)	1.403(5)
N(2)-N(3)	1.330(4)	N(2)-C(13)	1.357(5)
N(3)-N(4)	1.298(4)	N(4)-N(5)	1.327(4)
N(4)-C(14)	1.478(5)	N(5)-C(13)	1.337(5)
N(6)-N(7)	1.325(4)	N(6)-C(25)	1.356(5)
N(7)-N(8)	1.306(4)	N(8)-N(9)	1.329(4)
N(8)-C(26)	1.478(5)	N(9)-C(25)	1.332(5)
C(1)-C(2)	1.398(5)	C(1)-C(6)	1.418(5)
C(2)-C(3)	1.408(5)	C(2)-C(13)	1.445(5)
C(3)-C(4)	1.389(5)	C(3)-H(3)	0.9500
C(4)-C(5)	1.388(5)	C(4)-C(17)	1.528(5)
C(5)-C(6)	1.388(5)	C(5)-H(5)	0.9500
C(6)-C(7)	1.424(5)	C(7)-C(8)	1.395(5)
C(7)-C(12)	1.416(5)	C(8)-C(9)	1.380(5)
C(8)-H(8)	0.9500	C(9)-C(10)	1.394(5)
C(9)-C(21)	1.539(5)	C(10)-C(11)	1.387(5)
C(10)-H(10)	0.9500	C(11)-C(12)	1.408(5)

C(11)-C(25)	1.453(5)	C(14)-C(16)	1.477(6)
C(14)-C(15)	1.479(6)	C(14)-H(14)	1.0000
C(15)-H(15A)	0.9800	C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800	C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800	C(16)-H(16C)	0.9800
C(17)-C(19)	1.514(6)	C(17)-C(18)	1.536(6)
C(17)-C(20)	1.541(5)	C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800	C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800	C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800	C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800	C(20)-H(20C)	0.9800
C(21)-C(22)	1.525(5)	C(21)-C(24)	1.530(5)
C(21)-C(23)	1.531(5)	C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800	C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800	C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800	C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800	C(24)-H(24C)	0.9800
C(26)-C(27)	1.497(6)	C(26)-C(28)	1.513(6)
C(26)-H(26)	1.0000	C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800	C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800	C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800	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)-H(32A)	0.9800	C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800	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
C(36)-H(36A)	0.9800	C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800	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)-H(40A)	0.9800	C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800	C(41)-C(42)	1.378(5)
C(41)-C(46)	1.388(6)	C(41)-C(47)	1.505(5)
C(42)-C(43)	1.385(6)	C(42)-H(42)	0.9500
C(43)-C(44)	1.376(6)	C(43)-H(43)	0.9500
C(44)-C(45)	1.382(6)	C(44)-H(44)	0.9500
C(45)-C(46)	1.377(5)	C(45)-H(45)	0.9500
C(46)-H(46)	0.9500	C(47)-H(47A)	0.9800

C(47)-H(47B)	0.9800	C(47)-H(47C)	0.9800
C(48)-C(49)	1.361(7)	C(48)-C(53)	1.371(7)
C(48)-C(54)	1.507(8)	C(49)-C(50)	1.422(7)
C(49)-H(49)	0.9500	C(50)-C(51)	1.348(7)
C(50)-H(50)	0.9500	C(51)-C(52)	1.389(7)
C(51)-H(51)	0.9500	C(52)-C(53)	1.362(7)
C(52)-H(52)	0.9500	C(53)-H(53)	0.9500
C(54)-H(54A)	0.9800	C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800		

Table S10 Bond angles [°] for **Er(CzT^{iPr})[N(SiMe$_3$)$_2$]$_2$ 3 • 2 C$_7$H$_8$**

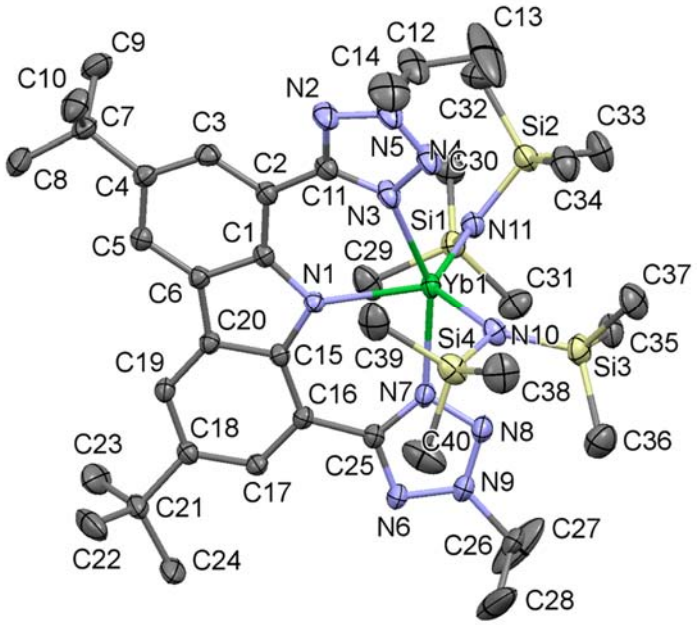
atom-atom-atom	angle	atom-atom-atom	angle
N(10)-Er(1)-N(11)	121.98(11)	N(10)-Er(1)-N(1)	113.63(11)
N(11)-Er(1)-N(1)	123.98(10)	N(10)-Er(1)-N(2)	102.44(11)
N(11)-Er(1)-N(2)	84.83(11)	N(1)-Er(1)-N(2)	77.20(10)
N(10)-Er(1)-N(6)	97.23(11)	N(11)-Er(1)-N(6)	99.74(11)
N(1)-Er(1)-N(6)	78.68(10)	N(2)-Er(1)-N(6)	153.46(10)
N(10)-Er(1)-Si(4)	149.66(8)	N(11)-Er(1)-Si(4)	27.97(8)
N(1)-Er(1)-Si(4)	96.71(7)	N(2)-Er(1)-Si(4)	83.14(8)
N(6)-Er(1)-Si(4)	88.86(8)	N(10)-Si(1)-C(30)	111.18(18)
N(10)-Si(1)-C(29)	114.14(18)	C(30)-Si(1)-C(29)	107.8(2)
N(10)-Si(1)-C(31)	112.47(17)	C(30)-Si(1)-C(31)	107.2(2)
C(29)-Si(1)-C(31)	103.51(19)	N(10)-Si(2)-C(32)	111.65(19)
N(10)-Si(2)-C(33)	112.02(18)	C(32)-Si(2)-C(33)	106.7(2)
N(10)-Si(2)-C(34)	114.14(19)	C(32)-Si(2)-C(34)	107.6(2)
C(33)-Si(2)-C(34)	104.1(2)	N(11)-Si(3)-C(35)	112.95(17)
N(11)-Si(3)-C(36)	112.34(19)	C(35)-Si(3)-C(36)	106.95(19)
N(11)-Si(3)-C(37)	113.63(18)	C(35)-Si(3)-C(37)	104.3(2)
C(36)-Si(3)-C(37)	106.0(2)	N(11)-Si(4)-C(39)	114.13(18)
N(11)-Si(4)-C(40)	111.63(18)	C(39)-Si(4)-C(40)	105.2(2)
N(11)-Si(4)-C(38)	111.76(19)	C(39)-Si(4)-C(38)	107.9(2)
C(40)-Si(4)-C(38)	105.7(2)	N(11)-Si(4)-Er(1)	37.47(10)
C(39)-Si(4)-Er(1)	145.02(15)	C(40)-Si(4)-Er(1)	79.85(13)
C(38)-Si(4)-Er(1)	103.70(15)	C(1)-N(1)-C(12)	103.7(3)
C(1)-N(1)-Er(1)	128.9(2)	C(12)-N(1)-Er(1)	126.6(2)
N(3)-N(2)-C(13)	106.8(3)	N(3)-N(2)-Er(1)	118.4(2)
C(13)-N(2)-Er(1)	134.5(3)	N(4)-N(3)-N(2)	105.7(3)
N(3)-N(4)-N(5)	114.8(3)	N(3)-N(4)-C(14)	121.9(3)
N(5)-N(4)-C(14)	123.2(3)	N(4)-N(5)-C(13)	102.2(3)
N(7)-N(6)-C(25)	107.3(3)	N(7)-N(6)-Er(1)	121.3(2)
C(25)-N(6)-Er(1)	131.4(2)	N(8)-N(7)-N(6)	105.2(3)
N(7)-N(8)-N(9)	114.6(3)	N(7)-N(8)-C(26)	122.8(3)
N(9)-N(8)-C(26)	122.5(3)	N(8)-N(9)-C(25)	102.3(3)

Si(1)-N(10)-Si(2)	119.95(17)	Si(1)-N(10)-Er(1)	119.65(16)
Si(2)-N(10)-Er(1)	120.40(16)	Si(4)-N(11)-Si(3)	119.17(18)
Si(4)-N(11)-Er(1)	114.56(16)	Si(3)-N(11)-Er(1)	124.79(16)
C(2)-C(1)-N(1)	130.4(3)	C(2)-C(1)-C(6)	117.6(3)
N(1)-C(1)-C(6)	112.0(3)	C(1)-C(2)-C(3)	118.7(3)
C(1)-C(2)-C(13)	124.1(3)	C(3)-C(2)-C(13)	117.2(3)
C(4)-C(3)-C(2)	124.0(4)	C(4)-C(3)-H(3)	118.0
C(2)-C(3)-H(3)	118.0	C(5)-C(4)-C(3)	116.6(3)
C(5)-C(4)-C(17)	121.2(3)	C(3)-C(4)-C(17)	122.2(4)
C(6)-C(5)-C(4)	121.3(3)	C(6)-C(5)-H(5)	119.3
C(4)-C(5)-H(5)	119.3	C(5)-C(6)-C(1)	121.7(4)
C(5)-C(6)-C(7)	131.9(3)	C(1)-C(6)-C(7)	106.3(3)
C(8)-C(7)-C(12)	122.3(4)	C(8)-C(7)-C(6)	132.0(3)
C(12)-C(7)-C(6)	105.7(3)	C(9)-C(8)-C(7)	120.4(4)
C(9)-C(8)-H(8)	119.8	C(7)-C(8)-H(8)	119.8
C(8)-C(9)-C(10)	117.5(3)	C(8)-C(9)-C(21)	122.9(3)
C(10)-C(9)-C(21)	119.6(3)	C(11)-C(10)-C(9)	123.4(4)
C(11)-C(10)-H(10)	118.3	C(9)-C(10)-H(10)	118.3
C(10)-C(11)-C(12)	119.6(3)	C(10)-C(11)-C(25)	116.9(4)
C(12)-C(11)-C(25)	123.5(3)	N(1)-C(12)-C(11)	131.0(3)
N(1)-C(12)-C(7)	112.3(3)	C(11)-C(12)-C(7)	116.7(3)
N(5)-C(13)-N(2)	110.6(3)	N(5)-C(13)-C(2)	125.3(3)
N(2)-C(13)-C(2)	124.1(3)	C(16)-C(14)-N(4)	109.7(3)
C(16)-C(14)-C(15)	115.2(5)	N(4)-C(14)-C(15)	108.5(4)
C(16)-C(14)-H(14)	107.7	N(4)-C(14)-H(14)	107.7
C(15)-C(14)-H(14)	107.7	C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5	H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5	H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5	C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5	H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5	H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5	C(19)-C(17)-C(4)	112.9(3)
C(19)-C(17)-C(18)	108.7(4)	C(4)-C(17)-C(18)	109.8(3)
C(19)-C(17)-C(20)	108.2(4)	C(4)-C(17)-C(20)	108.4(3)
C(18)-C(17)-C(20)	108.8(4)	C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5	H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5	H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5	C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5	H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5	H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5	C(17)-C(20)-H(20A)	109.5
C(17)-C(20)-H(20B)	109.5	H(20A)-C(20)-H(20B)	109.5
C(17)-C(20)-H(20C)	109.5	H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5	C(22)-C(21)-C(24)	109.1(3)
C(22)-C(21)-C(23)	108.5(3)	C(24)-C(21)-C(23)	109.2(3)
C(22)-C(21)-C(9)	111.9(3)	C(24)-C(21)-C(9)	110.0(3)

C(23)-C(21)-C(9)	108.2(3)	C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5	H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5	H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5	C(21)-C(23)-H(23A)	109.5
C(21)-C(23)-H(23B)	109.5	H(23A)-C(23)-H(23B)	109.5
C(21)-C(23)-H(23C)	109.5	H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5	C(21)-C(24)-H(24A)	109.5
C(21)-C(24)-H(24B)	109.5	H(24A)-C(24)-H(24B)	109.5
C(21)-C(24)-H(24C)	109.5	H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5	N(9)-C(25)-N(6)	110.6(3)
N(9)-C(25)-C(11)	123.5(3)	N(6)-C(25)-C(11)	125.9(4)
N(8)-C(26)-C(27)	109.8(4)	N(8)-C(26)-C(28)	108.3(3)
C(27)-C(26)-C(28)	114.5(4)	N(8)-C(26)-H(26)	108.0
C(27)-C(26)-H(26)	108.0	C(28)-C(26)-H(26)	108.0
C(26)-C(27)-H(27A)	109.5	C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5	C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5	H(27B)-C(27)-H(27C)	109.5
C(26)-C(28)-H(28A)	109.5	C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5	C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5	H(28B)-C(28)-H(28C)	109.5
Si(1)-C(29)-H(29A)	109.5	Si(1)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5	Si(1)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5	H(29B)-C(29)-H(29C)	109.5
Si(1)-C(30)-H(30A)	109.5	Si(1)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5	Si(1)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5	H(30B)-C(30)-H(30C)	109.5
Si(1)-C(31)-H(31A)	109.5	Si(1)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5	Si(1)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5	H(31B)-C(31)-H(31C)	109.5
Si(2)-C(32)-H(32A)	109.5	Si(2)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5	Si(2)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5	H(32B)-C(32)-H(32C)	109.5
Si(2)-C(33)-H(33A)	109.5	Si(2)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5	Si(2)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5	H(33B)-C(33)-H(33C)	109.5
Si(2)-C(34)-H(34A)	109.5	Si(2)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5	Si(2)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5	H(34B)-C(34)-H(34C)	109.5
Si(3)-C(35)-H(35A)	109.5	Si(3)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5	Si(3)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5	H(35B)-C(35)-H(35C)	109.5
Si(3)-C(36)-H(36A)	109.5	Si(3)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5	Si(3)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5	H(36B)-C(36)-H(36C)	109.5
Si(3)-C(37)-H(37A)	109.5	Si(3)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5	Si(3)-C(37)-H(37C)	109.5

H(37A)-C(37)-H(37C)	109.5	H(37B)-C(37)-H(37C)	109.5
Si(4)-C(38)-H(38A)	109.5	Si(4)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5	Si(4)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5	H(38B)-C(38)-H(38C)	109.5
Si(4)-C(39)-H(39A)	109.5	Si(4)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5	Si(4)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5	H(39B)-C(39)-H(39C)	109.5
Si(4)-C(40)-H(40A)	109.5	Si(4)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5	Si(4)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5	H(40B)-C(40)-H(40C)	109.5
C(42)-C(41)-C(46)	117.9(4)	C(42)-C(41)-C(47)	121.1(4)
C(46)-C(41)-C(47)	121.0(4)	C(41)-C(42)-C(43)	121.3(4)
C(41)-C(42)-H(42)	119.3	C(43)-C(42)-H(42)	119.3
C(44)-C(43)-C(42)	120.4(4)	C(44)-C(43)-H(43)	119.8
C(42)-C(43)-H(43)	119.8	C(43)-C(44)-C(45)	118.7(4)
C(43)-C(44)-H(44)	120.6	C(45)-C(44)-H(44)	120.6
C(46)-C(45)-C(44)	120.7(4)	C(46)-C(45)-H(45)	119.6
C(44)-C(45)-H(45)	119.6	C(45)-C(46)-C(41)	121.0(4)
C(45)-C(46)-H(46)	119.5	C(41)-C(46)-H(46)	119.5
C(41)-C(47)-H(47A)	109.5	C(41)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5	C(41)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5	H(47B)-C(47)-H(47C)	109.5
C(49)-C(48)-C(53)	119.2(6)	C(49)-C(48)-C(54)	120.9(5)
C(53)-C(48)-C(54)	119.9(6)	C(48)-C(49)-C(50)	120.1(5)
C(48)-C(49)-H(49)	119.9	C(50)-C(49)-H(49)	119.9
C(51)-C(50)-C(49)	119.7(5)	C(51)-C(50)-H(50)	120.1
C(49)-C(50)-H(50)	120.1	C(50)-C(51)-C(52)	119.5(5)
C(50)-C(51)-H(51)	120.3	C(52)-C(51)-H(51)	120.3
C(53)-C(52)-C(51)	120.5(5)	C(53)-C(52)-H(52)	119.7
C(51)-C(52)-H(52)	119.7	C(52)-C(53)-C(48)	121.0(6)
C(52)-C(53)-H(53)	119.5	C(48)-C(53)-H(53)	119.5
C(48)-C(54)-H(54A)	109.5	C(48)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5	C(48)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5	H(54B)-C(54)-H(54C)	109.5

Figure S3 Labeled ORTEP drawing of **Yb(CzT^{iPr})[N(SiMe$_3$)$_2$]$_2$ 4 • 2 C$_7$H$_8$**



Toluenes of solvation not shown.

Table S11 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$)[1] for **Yb(CzT^{iPr})[N(SiMe$_3$)$_2$]$_2$ 4 • 2 C$_7$H$_8$**

Atom	*x*	*y*	*z*	U(eq)
Yb1	5882.2(2)	3162.1(2)	2113.1(2)	21.14(3)
Si1	4041.7(6)	1773.5(4)	307.9(4)	27.20(13)
Si2	3830.6(7)	3731.9(5)	793.6(4)	32.64(14)
Si3	8285.1(7)	4751.6(4)	2056.8(4)	33.66(15)
Si4	8492.3(7)	4491.4(4)	3521.4(4)	33.88(15)
N1	5435.0(16)	2097.1(11)	2674(1)	19.6(3)
N2	3486(2)	4259.2(13)	3624.0(12)	34.3(5)
N3	4694.9(19)	3904.5(12)	2884.3(11)	28.3(4)
N4	4680(2)	4789.9(13)	3035.3(12)	33.8(5)
N5	3958(2)	4962.4(13)	3466.1(12)	35.5(5)
N6	8435.4(17)	1152.7(13)	1718.1(11)	26.1(4)
N7	7228.0(17)	2157.2(12)	1793.6(11)	25.5(4)
N8	8035.6(18)	2369.8(13)	1445.8(12)	29.3(4)
N9	8724.6(18)	1768.4(13)	1415.5(11)	27.3(4)
N10	7605.7(18)	4276.0(12)	2591.7(11)	27.3(4)
N11	4487.9(18)	2874.1(12)	1001.3(10)	26.3(4)
C1	4507.9(19)	2045.0(13)	3031.6(11)	20.0(4)
C2	3780(2)	2676.0(14)	3272.1(12)	22.6(4)
C3	2884(2)	2441.9(15)	3603.5(12)	24.9(4)
C4	2681.7(19)	1619.8(14)	3731.6(12)	23.1(4)
C5	3437.8(19)	1018.1(14)	3529.3(12)	22.7(4)
C6	4327.6(19)	1226.6(13)	3188.3(12)	20.6(4)
C7	1632(2)	1409.1(16)	4063.8(13)	28.0(5)
C8	1619(3)	522.1(19)	4224.8(17)	41.6(6)
C9	356(2)	1286(2)	3478.1(16)	41.2(6)
C10	1798(3)	2202.9(19)	4814.0(15)	41.9(6)
C11	3969(2)	3592.4(14)	3248.3(12)	24.8(4)
C12	3740(3)	5898.1(17)	3803.5(17)	48.5(7)
C13	3903(7)	6423(3)	3315(3)	122(2)
C14	4553(4)	6315(2)	4637.1(19)	59.7(9)
C15	5864.3(19)	1293.0(13)	2626.3(11)	19.2(4)
C16	6805.7(19)	959.5(13)	2330.9(11)	20.1(4)
C17	7101.9(19)	146.9(14)	2390.7(11)	21.2(4)
C18	6504(2)	-373.1(14)	2719.4(12)	21.8(4)
C19	5540(2)	-62.5(14)	2982.9(12)	22.2(4)
C20	5228.0(19)	743.3(13)	2934.5(11)	20.1(4)
C21	6899(2)	-1232.3(15)	2816.1(13)	27.8(5)
C22	7397(4)	-1046(2)	3670.2(18)	50.5(9)

C23	5765(3)	-2055.4(19)	2429(2)	47.5(8)
C24	7944(3)	-1466.8(19)	2475.3(19)	39.5(7)
C25	7482.9(19)	1415.6(14)	1955.5(12)	21.3(4)
C26	9725(2)	1756.2(18)	1045.4(14)	33.7(5)
C27	9240(4)	1006(3)	291(2)	101.0(18)
C28	10918(3)	1766(4)	1574(2)	89.4(16)
C29	4117(3)	862.3(17)	733.2(15)	41.3(6)
C30	2363(2)	1442.3(18)	-334.6(15)	37.6(6)
C31	5071(3)	1622.6(19)	-315.0(15)	42.2(6)
C32	2227(3)	3679(2)	917(2)	55.4(8)
C33	3680(3)	3713(2)	-197.7(16)	49.3(7)
C34	4826(3)	4916.6(18)	1441.0(17)	44.9(7)
C35	7464(3)	4150.1(18)	992.7(15)	40.0(6)
C36	9981(3)	4692(2)	2192(2)	51.6(7)
C37	8278(3)	6005.6(17)	2302.8(18)	47.1(7)
C38	9461(3)	5699.6(19)	4063.8(17)	50.1(7)
C39	7458(3)	4313(2)	4106.4(16)	47.7(7)
C40	9576(3)	3693(2)	3571.5(18)	58.5(9)
C55	8267(15)	-1020(20)	3312(16)	47(6)
C56	6100(20)	-1741(17)	3166(16)	37(6)
C57	6710(30)	-1952(17)	2020(10)	45(6)
C41	2366(2)	8195.7(16)	4735.8(14)	32.5(5)
C42	1431(3)	7888.2(19)	4027.7(16)	43.7(6)
C43	1660(3)	8042(2)	3410.9(16)	46.3(7)
C44	2828(3)	8521.3(18)	3485.7(16)	40.5(6)
C45	3767(2)	8850.0(17)	4190.1(16)	37.7(6)
C46	3542(2)	8680.7(16)	4804.1(14)	31.1(5)
C47	2132(3)	8000(2)	5404.8(16)	48.6(7)
C48	1161(4)	-2702(3)	1116(2)	65.5(9)
C49	2338(3)	-2251(3)	1160(2)	65.3(10)
C50	2709(3)	-1321(3)	1432(2)	69.6(11)
C51	1904(3)	-789(3)	1690.0(18)	62.8(9)
C52	764(3)	-1202(3)	1666.3(18)	60.8(9)
C53	372(3)	-2182(3)	1370.8(19)	59.2(9)
C54	756(5)	-3727(3)	808(3)	102.8(17)

[1] U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Table S12 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **$Yb(CzT^{iPr})[N(SiMe_3)_2]_2$ 4 • 2 C_7H_8**

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Yb1	26.37(5)	16.90(5)	21.97(5)	8.79(3)	9.05(3)	4.47(3)
Si1	29.0(3)	27.6(3)	23.8(3)	9.3(2)	7.2(2)	5.7(2)
Si2	37.8(4)	32.4(3)	34.8(3)	19.2(3)	12.4(3)	12.7(3)
Si3	37.2(4)	24.3(3)	41.0(4)	14.8(3)	14.0(3)	2.5(3)
Si4	36.1(3)	25.0(3)	31.3(3)	6.9(3)	2.0(3)	3.7(3)
N1	22.7(8)	16.9(7)	21.4(8)	7.8(7)	9.3(7)	5.8(6)
N2	48.4(12)	26.7(9)	39.2(11)	15.9(9)	23.4(10)	18.8(9)
N3	41.3(11)	19.4(8)	28.6(10)	10.6(7)	14.2(8)	11.2(8)
N4	53.5(13)	21.7(9)	35.9(11)	14.5(8)	21.5(10)	16.9(9)
N5	56.3(13)	24.7(9)	37.2(11)	15.1(9)	23.9(10)	20.9(9)
N6	28.3(9)	30.7(9)	28.8(9)	17.2(8)	15.5(8)	9.6(8)
N7	29.3(9)	23.3(8)	30.6(10)	13.7(8)	15.8(8)	5.5(7)
N8	32.7(10)	28.0(9)	36.1(11)	17.3(8)	18.6(9)	7.3(8)
N9	27.8(9)	31.8(10)	30.5(10)	16.9(8)	15.5(8)	7.0(8)
N10	32.2(10)	18.1(8)	29.2(10)	8.5(7)	7.5(8)	3.6(7)
N11	29.7(9)	27.0(9)	25.2(9)	12.4(8)	10.0(8)	7.0(8)
C1	21.6(9)	18.9(9)	18.7(9)	6.9(7)	5.3(7)	4.3(7)
C2	26(1)	21.4(9)	21.8(10)	8.9(8)	7.9(8)	7.3(8)
C3	25.9(10)	24.9(10)	26(1)	8.5(9)	10.6(9)	10.7(8)
C4	21.5(10)	26.1(10)	22.1(10)	8.6(8)	7.8(8)	5.7(8)
C5	22.6(10)	22.5(9)	23.3(10)	8.9(8)	7.7(8)	4.4(8)
C6	21.2(9)	19.1(9)	21.5(9)	7.4(8)	7.1(8)	4.2(8)
C7	24.5(10)	31.4(11)	32.4(12)	11.7(9)	15.0(9)	8.9(9)
C8	42.5(14)	45.0(14)	56.8(17)	28.4(13)	33.3(13)	15.2(12)
C9	26.6(12)	54.1(16)	46.2(15)	20.4(13)	15.0(11)	8.7(11)
C10	48.5(15)	44.5(14)	37.3(14)	12.0(12)	26.2(12)	9.7(12)
C11	30.2(11)	23.7(10)	22.9(10)	9.8(8)	9.0(9)	10.4(9)
C12	83(2)	26.6(12)	50.1(16)	15.6(12)	34.7(16)	30.4(14)
C13	271(8)	59(2)	109(4)	58(3)	116(5)	98(4)
C14	78(2)	30.1(14)	62(2)	2.0(14)	24.4(18)	17.3(15)
C15	21.5(9)	17.1(9)	18.3(9)	6.5(7)	5.8(7)	3.9(7)
C16	20.9(9)	21.2(9)	19.0(9)	7.9(8)	7.5(8)	4.4(8)
C17	23.4(10)	22.3(9)	21.3(9)	8.9(8)	10.1(8)	8.1(8)
C18	25.2(10)	20.3(9)	21.6(10)	9.1(8)	7.6(8)	7.4(8)
C19	26.2(10)	20.3(9)	23.2(10)	9.8(8)	11.3(8)	4.5(8)
C20	21.5(9)	18.4(9)	20.6(9)	6.9(8)	8.0(8)	3.9(7)
C21	35.5(12)	25.1(10)	35.2(12)	18.1(9)	19(1)	14.2(9)
C22	72(2)	58.8(19)	42.7(17)	34.0(15)	23.2(16)	40.6(18)
C23	48.3(17)	26.2(13)	78(2)	25.3(14)	26.5(16)	13.0(12)

C24	49.7(17)	33.9(14)	60.3(19)	30.1(14)	34.9(15)	25.9(13)
C25	22.5(9)	21.2(9)	20.7(9)	7.9(8)	8.1(8)	4.1(8)
C26	30.5(12)	45.3(14)	38.5(13)	23.3(11)	22.5(10)	10.2(10)
C27	75(3)	127(4)	63(2)	-17(2)	53(2)	-26(3)
C28	31.3(16)	202(5)	76(3)	91(3)	28.4(17)	39(2)
C29	47.5(15)	28.5(12)	37.8(14)	12.9(11)	-0.2(12)	2.0(11)
C30	35.6(13)	39.5(13)	33.9(13)	13.1(11)	7.2(10)	6.1(11)
C31	41.2(14)	44.4(15)	36.5(14)	7.0(12)	16.0(11)	9.1(12)
C32	44.6(16)	55.0(18)	80(2)	32.2(17)	25.1(16)	25.2(14)
C33	67(2)	45.7(16)	38.6(15)	27.0(13)	9.4(14)	11.1(14)
C34	63.2(18)	32.3(13)	45.1(16)	16.9(12)	22.3(14)	14.5(13)
C35	53.0(16)	35.8(13)	40.2(14)	21.3(11)	20.3(12)	10.7(12)
C36	40.6(15)	51.6(17)	65(2)	24.1(15)	20.1(14)	4.9(13)
C37	56.3(17)	25.7(12)	58.1(18)	19.4(12)	14.6(14)	3.0(12)
C38	55.5(17)	35.1(14)	39.6(15)	1.2(12)	5.8(13)	-3.2(13)
C39	51.5(17)	50.9(16)	32.2(14)	17.7(12)	2.3(12)	0.9(13)
C40	67(2)	55.0(18)	45.6(17)	14.5(15)	2.4(15)	29.9(16)
C55	41(7)	47(13)	64(12)	35(10)	14(6)	19(7)
C56	48(11)	31(10)	59(13)	32(10)	32(10)	28(8)
C57	64(15)	33(9)	50(7)	20(6)	27(7)	23(9)
C41	36.1(12)	26.3(11)	31.8(12)	8.0(9)	11.7(10)	2.5(9)
C42	37.1(14)	42.2(14)	41.7(15)	13.9(12)	6.6(11)	-7.0(11)
C43	51.1(16)	43.5(15)	35.0(14)	16.3(12)	2.4(12)	-0.4(13)
C44	55.3(16)	34.2(13)	37.1(14)	18.1(11)	17.9(12)	8.4(12)
C45	35.9(13)	35.1(13)	46.3(15)	17.7(12)	17.8(11)	6.2(11)
C46	31.2(12)	28.4(11)	31.5(12)	9.9(10)	8.8(10)	5.9(9)
C47	45.4(16)	53.9(17)	40.3(15)	14.3(13)	16.8(13)	-6.0(13)
C48	61(2)	81(3)	60(2)	35.8(19)	16.7(17)	15.9(19)
C49	42.0(17)	92(3)	65(2)	30(2)	20.8(16)	14.5(18)
C50	44.1(18)	98(3)	54(2)	17(2)	16.5(15)	2.0(19)
C51	59(2)	71(2)	38.7(16)	9.0(16)	3.3(15)	3.3(17)
C52	52.5(19)	91(3)	39.9(16)	21.7(17)	15.9(14)	26.0(19)
C53	38.6(15)	98(3)	48.1(18)	38.1(19)	12.5(13)	14.7(17)
C54	126(4)	71(3)	109(4)	48(3)	23(3)	8(3)

[2] The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Table S13 Bond Lengths for **Yb(CzT^{iPr})[N(SiMe$_3$)$_2$]$_2$ 4 • 2 C$_7$H$_8$**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Yb1	Si1	3.3952(7)	C2	C11	1.451(3)
Yb1	Si2	3.4275(7)	C3	C4	1.399(3)
Yb1	Si3	3.4871(7)	C4	C5	1.389(3)
Yb1	Si4	3.3287(7)	C4	C7	1.534(3)
Yb1	N1	2.3471(16)	C5	C6	1.396(3)
Yb1	N3	2.3926(19)	C6	C20	1.440(3)
Yb1	N7	2.3850(19)	C7	C8	1.529(3)
Yb1	N10	2.1997(18)	C7	C9	1.532(3)
Yb1	N11	2.1882(18)	C7	C10	1.533(3)
Si1	N11	1.7310(19)	C12	C13	1.476(5)
Si1	C29	1.877(3)	C12	C14	1.514(5)
Si1	C30	1.876(3)	C15	C16	1.414(3)
Si1	C31	1.865(3)	C15	C20	1.420(3)
Si2	N11	1.735(2)	C16	C17	1.400(3)
Si2	C32	1.878(3)	C16	C25	1.454(3)
Si2	C33	1.882(3)	C17	C18	1.396(3)
Si2	C34	1.881(3)	C18	C19	1.396(3)
Si3	N10	1.730(2)	C18	C21	1.534(3)
Si3	C35	1.887(3)	C19	C20	1.389(3)
Si3	C36	1.881(3)	C21	C22	1.525(4)
Si3	C37	1.881(3)	C21	C23	1.524(4)
Si4	N10	1.724(2)	C21	C24	1.523(3)
Si4	C38	1.870(3)	C21	C55	1.521(13)
Si4	C39	1.880(3)	C21	C56	1.547(13)
Si4	C40	1.876(3)	C21	C57	1.539(13)
N1	C1	1.403(3)	C26	C27	1.466(4)
N1	C15	1.401(3)	C26	C28	1.463(4)
N2	N5	1.325(3)	C41	C42	1.390(4)
N2	C11	1.341(3)	C41	C46	1.391(3)
N3	N4	1.335(2)	C41	C47	1.507(4)
N3	C11	1.352(3)	C42	C43	1.377(4)
N4	N5	1.304(3)	C43	C44	1.376(4)
N5	C12	1.492(3)	C44	C45	1.385(4)
N6	N9	1.334(2)	C45	C46	1.380(4)
N6	C25	1.337(3)	C48	C49	1.387(5)
N7	N8	1.334(2)	C48	C53	1.367(5)
N7	C25	1.354(3)	C48	C54	1.491(6)
N8	N9	1.300(3)	C49	C50	1.353(6)
N9	C26	1.484(3)	C50	C51	1.394(5)

C1	C2	1.413(3)	C51	C52	1.344(5)
C1	C6	1.421(3)	C52	C53	1.426(5)
C2	C3	1.400(3)			

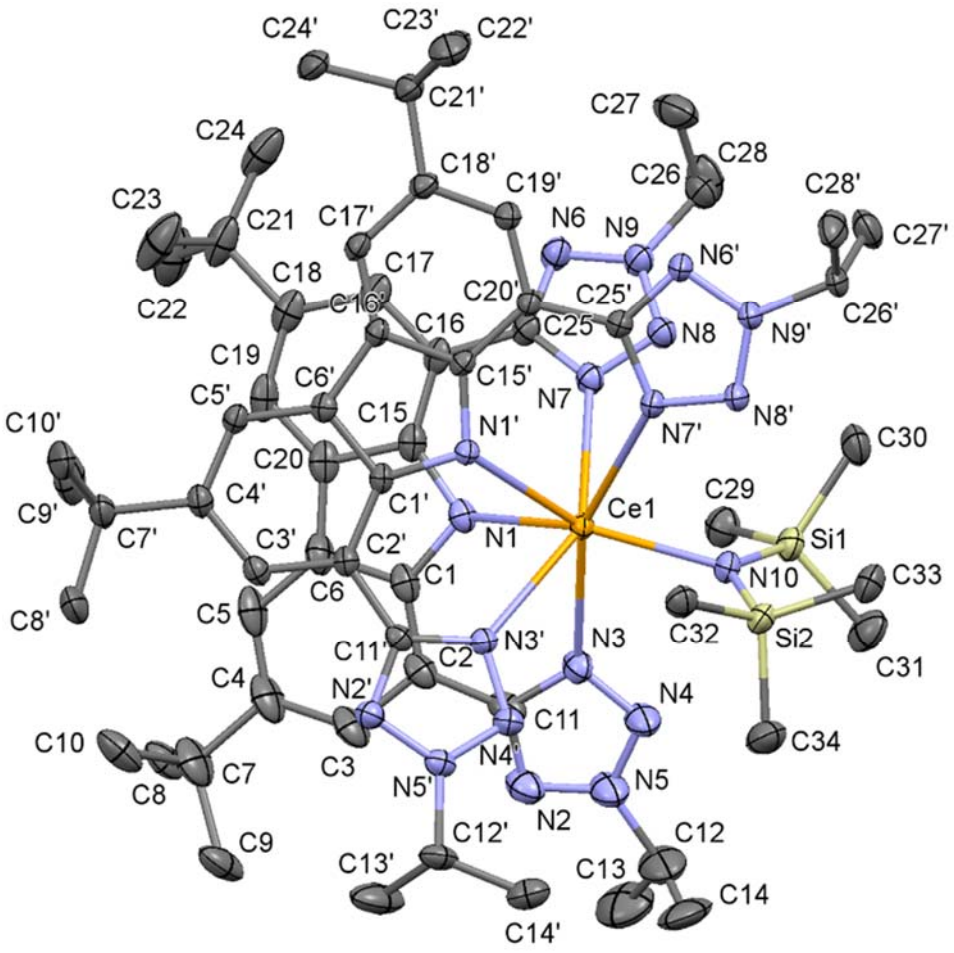
Table S14 Bond Angles for **Yb(CzT^{iPr})[N(SiMe$_3$)$_2$]$_2$ 4 • 2 C$_7$H$_8$**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Si1	Yb1	Si2	51.931(17)	N8	N7	Yb1	118.58(14)
Si1	Yb1	Si3	110.280(17)	N8	N7	C25	107.02(18)
Si2	Yb1	Si3	87.375(18)	C25	N7	Yb1	134.00(14)
Si4	Yb1	Si1	157.831(18)	N9	N8	N7	105.25(17)
Si4	Yb1	Si2	128.851(17)	N6	N9	C26	123.06(19)
Si4	Yb1	Si3	51.480(18)	N8	N9	N6	115.00(18)
N1	Yb1	Si1	95.20(4)	N8	N9	C26	121.91(19)
N1	Yb1	Si2	128.41(4)	Si3	N10	Yb1	124.68(10)
N1	Yb1	Si3	144.22(4)	Si4	N10	Yb1	115.53(10)
N1	Yb1	Si4	96.91(4)	Si4	N10	Si3	118.19(11)
N1	Yb1	N3	78.79(6)	Si1	N11	Yb1	119.61(10)
N1	Yb1	N7	77.91(6)	Si1	N11	Si2	119.05(11)
N3	Yb1	Si1	112.77(5)	Si2	N11	Yb1	121.33(10)
N3	Yb1	Si2	80.45(5)	N1	C1	C2	130.62(18)
N3	Yb1	Si3	111.64(5)	N1	C1	C6	112.56(17)
N3	Yb1	Si4	87.82(5)	C2	C1	C6	116.79(18)
N7	Yb1	Si1	80.68(5)	C1	C2	C11	123.55(19)
N7	Yb1	Si2	123.50(5)	C3	C2	C1	119.07(19)
N7	Yb1	Si3	81.81(4)	C3	C2	C11	117.22(19)
N7	Yb1	Si4	83.79(5)	C4	C3	C2	123.7(2)
N7	Yb1	N3	154.06(6)	C3	C4	C7	119.56(19)
N10	Yb1	Si1	134.20(5)	C5	C4	C3	117.34(19)
N10	Yb1	Si2	105.21(5)	C5	C4	C7	123.09(19)
N10	Yb1	Si3	24.07(5)	C4	C5	C6	120.28(19)
N10	Yb1	Si4	27.86(5)	C1	C6	C20	105.48(17)
N10	Yb1	N1	124.19(6)	C5	C6	C1	122.71(19)
N10	Yb1	N3	98.35(7)	C5	C6	C20	131.81(19)
N10	Yb1	N7	85.49(7)	C8	C7	C4	112.22(19)
N11	Yb1	Si1	26.31(5)	C8	C7	C9	107.8(2)
N11	Yb1	Si2	25.62(5)	C8	C7	C10	108.4(2)
N11	Yb1	Si3	99.65(5)	C9	C7	C4	108.51(19)
N11	Yb1	Si4	149.67(5)	C9	C7	C10	109.6(2)
N11	Yb1	N1	113.40(6)	C10	C7	C4	110.32(19)

N11	Yb1	N3	96.69(7)	N2	C11	N3	111.07(19)
N11	Yb1	N7	102.93(7)	N2	C11	C2	123.5(2)
N11	Yb1	N10	122.21(7)	N3	C11	C2	125.36(19)
N11	Si1	Yb1	34.08(6)	N5	C12	C14	107.7(2)
N11	Si1	C29	112.34(11)	C13	C12	N5	109.4(2)
N11	Si1	C30	114.17(11)	C13	C12	C14	117.4(4)
N11	Si1	C31	111.42(11)	N1	C15	C16	130.75(18)
C29	Si1	Yb1	82.50(8)	N1	C15	C20	112.48(17)
C30	Si1	Yb1	140.59(9)	C16	C15	C20	116.77(18)
C30	Si1	C29	103.33(12)	C15	C16	C25	123.12(18)
C31	Si1	Yb1	107.62(9)	C17	C16	C15	119.22(18)
C31	Si1	C29	107.55(14)	C17	C16	C25	117.66(18)
C31	Si1	C30	107.49(12)	C18	C17	C16	123.71(19)
N11	Si2	Yb1	33.05(6)	C17	C18	C19	116.97(18)
N11	Si2	C32	111.41(12)	C17	C18	C21	122.47(19)
N11	Si2	C33	114.36(12)	C19	C18	C21	120.53(18)
N11	Si2	C34	111.98(12)	C20	C19	C18	120.66(18)
C32	Si2	Yb1	112.81(11)	C15	C20	C6	105.75(17)
C32	Si2	C33	108.02(16)	C19	C20	C6	131.60(19)
C32	Si2	C34	106.72(15)	C19	C20	C15	122.58(19)
C33	Si2	Yb1	135.59(11)	C18	C21	C56	115.3(10)
C34	Si2	Yb1	80.73(9)	C18	C21	C57	108.9(12)
C34	Si2	C33	103.81(13)	C22	C21	C18	108.5(2)
N10	Si3	Yb1	31.25(6)	C23	C21	C18	109.8(2)
N10	Si3	C35	112.79(11)	C23	C21	C22	109.7(2)
N10	Si3	C36	113.54(12)	C24	C21	C18	112.29(18)
N10	Si3	C37	112.25(12)	C24	C21	C22	107.9(2)
C35	Si3	Yb1	81.63(8)	C24	C21	C23	108.7(2)
C36	Si3	Yb1	127.15(10)	C55	C21	C18	112.6(12)
C36	Si3	C35	104.72(14)	C55	C21	C56	106.3(13)
C36	Si3	C37	105.87(14)	C55	C21	C57	109.2(15)
C37	Si3	Yb1	122.53(10)	C57	C21	C56	104.2(13)
C37	Si3	C35	107.05(13)	N6	C25	N7	110.93(18)
N10	Si4	Yb1	36.60(6)	N6	C25	C16	124.42(19)
N10	Si4	C38	114.55(12)	N7	C25	C16	124.64(19)
N10	Si4	C39	111.28(11)	C27	C26	N9	108.2(2)
N10	Si4	C40	112.07(12)	C28	C26	N9	109.9(2)
C38	Si4	Yb1	144.83(11)	C28	C26	C27	117.7(4)
C38	Si4	C39	104.50(14)	C42	C41	C46	117.5(2)
C38	Si4	C40	107.96(15)	C42	C41	C47	121.7(2)
C39	Si4	Yb1	80.54(9)	C46	C41	C47	120.8(2)
C40	Si4	Yb1	103.78(10)	C43	C42	C41	121.6(2)

C40	Si4	C39	105.85(16)	C44	C43	C42	120.3(3)
C1	N1	Yb1	126.80(13)	C43	C44	C45	119.1(2)
C15	N1	Yb1	128.77(13)	C46	C45	C44	120.4(2)
C15	N1	C1	103.70(16)	C45	C46	C41	121.0(2)
N5	N2	C11	101.64(19)	C49	C48	C54	121.6(4)
N4	N3	Yb1	121.52(15)	C53	C48	C49	118.4(4)
N4	N3	C11	106.88(18)	C53	C48	C54	120.0(4)
C11	N3	Yb1	131.60(14)	C50	C49	C48	122.0(4)
N5	N4	N3	105.07(18)	C49	C50	C51	119.8(3)
N2	N5	C12	121.7(2)	C52	C51	C50	119.9(4)
N4	N5	N2	115.35(18)	C51	C52	C53	120.1(3)
N4	N5	C12	122.8(2)	C48	C53	C52	119.8(3)
N9	N6	C25	101.80(17)				

Figure S4 Labeled ORTEP drawing of **$Ce(CzT^{iPr})_2[N(SiMe_3)_2]$ 5 • 2.5 C_7H_8**



Toluenes of solvation not shown.

Table S15 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$)[1] for **$Ce(CzT^{iPr})_2[N(SiMe_3)_2]$ 5 • 2.5 C_7H_8**

Atom	*x*	*y*	*z*	U(eq)
Ce1	3631.3(2)	6186.3(2)	3960.1(2)	17.34(5)
Si1	2821.6(3)	6004.4(5)	4103.7(4)	28.52(18)
Si2	3416.9(3)	4719.7(5)	4497.4(4)	26.90(17)
N1	3858.3(7)	7509.8(12)	3990.8(10)	22.9(5)
N2	4421.8(8)	7340.9(17)	5877.6(12)	37.6(6)
N3	3944.4(8)	6817.4(14)	5003.8(11)	27.8(5)
N4	3863.7(9)	6596.1(17)	5365.2(12)	38.3(7)
N5	4152.2(9)	6916.7(19)	5876.0(12)	43.4(7)
N6	2665.2(8)	7575.3(14)	2179.3(11)	28.5(5)
N7	3023.2(7)	6893.6(13)	2997(1)	23.3(5)
N8	2618.1(7)	6683.8(14)	2666.5(10)	25.4(5)
N9	2420.1(7)	7095.2(14)	2190.5(11)	26.5(5)
N10	3244.1(7)	5580.5(13)	4212.4(10)	24.3(5)
C1	4253.6(9)	7770.8(15)	4476.1(14)	26.4(6)
C2	4469.5(9)	7658.3(16)	5086.3(13)	28.4(6)
C3	4871.2(10)	7988.4(18)	5496.7(16)	37.5(8)
C4	5060.5(11)	8434.1(19)	5325.7(17)	42.6(9)
C5	4841.2(11)	8563.1(17)	4722.6(17)	38.3(8)
C6	4442.5(10)	8247.7(16)	4303.8(15)	31.7(7)
C7	5495.2(12)	8796(2)	5792.0(18)	49.6(10)
C8	5464.7(17)	9584(3)	5846(3)	35.8(15)
C9	5743.1(19)	8457(4)	6467(3)	47.9(19)
C10	5823.9(17)	8594(4)	5683(3)	44.6(18)
C11	4282.5(9)	7267.5(17)	5320.0(13)	28.2(6)
C12	4159.9(15)	6832(3)	6399.3(18)	62.7(13)
C13	4296(4)	7565(6)	6742(4)	73(3)
C14	4332(4)	6191(6)	6685(4)	68(3)
C15	3793.0(9)	7845.0(15)	3503.2(13)	24.1(6)
C16	3433.1(9)	7829.5(15)	2901.7(13)	23.9(6)
C17	3434.8(10)	8232.7(16)	2487.5(15)	29.7(6)
C18	3781.9(10)	8658.7(16)	2644.0(16)	31.6(7)
C19	4135.7(10)	8686.5(15)	3245.1(16)	31.4(7)
C20	4142.7(9)	8295.0(15)	3665.9(14)	27.5(6)
C21	3776.7(12)	9083.6(19)	2177.2(18)	41.8(9)
C22	4111.8(15)	8754(3)	2136(2)	65.0(14)
C23	3874.1(15)	9895(2)	2350(2)	59.8(12)
C24	3346.5(13)	9040(2)	1559.6(18)	51.6(10)
C25	3047.7(9)	7433.3(15)	2693.7(12)	23.1(6)

C26	1956.4(9)	7055.5(19)	1719.6(14)	32.5(7)
C27	1760.9(11)	7778(2)	1700.8(18)	46.9(9)
C28	1868.9(11)	6853(3)	1139.0(16)	53.5(11)
C29	2861.1(11)	7029.5(18)	4067.2(15)	36.3(7)
C30	2302.8(10)	5707(2)	3392.6(15)	38.8(8)
C31	2776.1(12)	5842(2)	4708.7(17)	45.3(9)
C32	3779.8(9)	4371.0(17)	4334.2(13)	29.3(6)
C33	2981.9(11)	4026.7(18)	4206.0(15)	34.0(7)
C34	3752.4(11)	4707(2)	5331.1(14)	42.5(8)
C35	5418(3)	9353(6)	6124(5)	57(3)
C36	5783(3)	8236(6)	6082(6)	71(5)
C37	5591(3)	9332(6)	5446(4)	62(3)
C38	4011(4)	6028(6)	6417(4)	70(3)
C39	4644(3)	6834(7)	6976(4)	86(4)
N1'	3943.3(7)	6021.2(12)	3408.5(9)	17.7(4)
N2'	5148.1(7)	5974.2(13)	5227.6(10)	23.4(5)
N3'	4450.2(7)	5922.8(13)	4725.3(10)	21.2(5)
N4'	4628.3(7)	5681.0(13)	5270.4(10)	22.6(5)
N5'	5038.9(7)	5717.9(12)	5552.6(10)	21.8(5)
N6'	2656.6(7)	5075.3(14)	2059.8(10)	24.4(5)
N7'	3146.8(7)	5258.2(12)	3031.3(10)	20.7(5)
N8'	2847.7(7)	4831.7(13)	2957(1)	21.3(5)
N9'	2565.7(7)	4737.1(13)	2380.7(10)	22.0(5)
C1'	4325.2(8)	6347.5(14)	3608.4(12)	18.0(5)
C2'	4711.3(8)	6406.5(14)	4186.8(12)	19.6(5)
C3'	5056.9(8)	6755.0(15)	4269.0(12)	21.9(5)
C4'	5037.4(8)	7048.0(15)	3802.1(13)	23.2(6)
C5'	4657.1(8)	6974.6(15)	3228.0(12)	20.5(5)
C6'	4309.7(8)	6626.3(14)	3129.5(12)	19.0(5)
C7'	5414.1(9)	7445.7(17)	3896.3(14)	29.5(6)
C8'	5820.5(10)	7400(2)	4540.4(15)	43.4(9)
C9'	5297.1(12)	8257(2)	3729(2)	55.4(11)
C10'	5507.5(10)	7103(2)	3500.3(15)	43.1(9)
C11'	4769.6(8)	6104.7(14)	4704.6(11)	19.3(5)
C12'	5362.3(9)	5512.7(16)	6186.6(12)	28.6(6)
C13'	5615.7(14)	6196(2)	6527.7(16)	60.5(13)
C14'	5151.7(11)	5163.5(19)	6424.6(14)	35.4(7)
C15'	3686.1(8)	6081.0(14)	2792.3(11)	17.7(5)
C16'	3892.4(8)	6455.1(15)	2597.7(12)	18.9(5)
C17'	3690.1(8)	6595.8(15)	2000.7(12)	21.2(5)
C18'	3270.6(9)	6371.5(15)	1568.1(12)	22.2(6)
C19'	3073.3(8)	5991.5(15)	1759.2(12)	22.3(6)

C20'	3267.5(8)	5831.3(14)	2354.4(11)	19.1(5)
C21'	3020.4(9)	6520.7(18)	904.1(13)	29.0(6)
C22'	2624.1(11)	6979(2)	677.1(16)	46.6(10)
C23'	2877.1(12)	5786(2)	568.4(15)	43.8(9)
C24'	3284.3(10)	6930(2)	764.5(13)	33.5(7)
C25'	3028.3(8)	5395.1(15)	2481.8(12)	20.4(5)
C26'	2175.0(9)	4292.8(16)	2107.7(13)	26.2(6)
C27'	1791.7(9)	4792(2)	1797.0(16)	39.7(8)
C28'	2148.3(11)	3731.4(19)	1692.9(15)	36.8(8)
C53	5269(5)	9357(8)	8476(4)	158(3)
C47	5003(3)	9345(5)	7809(4)	158(3)
C48	5068(4)	9863(5)	7509(5)	158(3)
C49	4829(5)	9843(6)	6891(5)	158(3)
C50	4519(4)	9303(8)	6561(4)	158(3)
C51	4450(3)	8785(7)	6853(5)	158(3)
C52	4690(4)	8808(5)	7470(6)	158(3)
C60	850(2)	4572(5)	29(4)	75(3)
C54	1210.1(18)	4591(3)	-5(3)	42(2)
C55	1338(3)	5254(4)	-101(4)	54(3)
C56	1666(3)	5271(6)	-147(5)	63(4)
C57	1872(3)	4623(7)	-97(6)	72(5)
C58	1749(4)	3960(6)	0(8)	119(10)
C59	1421(3)	3946(4)	46(6)	72(6)
C40	3333(3)	1946(5)	1252(3)	130(3)
C41	3550(2)	2021(3)	1865(3)	102(2)
C42	3488.1(17)	2666(3)	2027(3)	76.9(15)
C43	3256.2(17)	3242(3)	1664(3)	89(2)
C44	3038(2)	3142(5)	1034(3)	104(2)
C45	3084(2)	2486(5)	835(3)	113(3)
C46	3191(3)	3930(4)	1807(4)	133(3)
C61	1524(4)	5192(7)	-148(5)	45(3)
C62	1768(5)	4624(9)	-69(7)	62(4)
C63	1732(3)	3947(6)	63(6)	47(4)
C64	1423(4)	3832(11)	125(9)	71(6)
C65	1162(6)	4338(8)	67(8)	75(5)
C66	1218(4)	5049(9)	-72(6)	58(4)
C67	1568(3)	5937(5)	-324(4)	55(3)

[1] U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor

Table S16 Anisotropic Displacement Parameters ($Å^2 \times 10^3$)^2 for **$Ce(CzT^{iPr})_2[N(SiMe_3)_2]$ 5 • 2.5 C_7H_8**

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ce1	16.58(7)	18.81(8)	18.63(7)	-0.81(6)	11.89(6)	-1.75(6)
Si1	26.0(4)	36.7(5)	30.5(4)	3.6(3)	21.2(4)	0.3(3)
Si2	27.2(4)	32.4(4)	25.6(4)	5.8(3)	18.6(3)	-0.9(3)
N1	22.0(11)	19.5(11)	28.6(12)	-3.5(9)	16.3(10)	-1.7(9)
N2	30.3(14)	48.4(17)	29.3(14)	-10.6(12)	16.0(12)	-3.7(12)
N3	25.0(12)	34.1(14)	28.8(13)	-4.7(11)	18.8(11)	-2.3(10)
N4	33.6(14)	57.8(19)	26.8(14)	-12.7(13)	20.2(12)	-10.4(13)
N5	37.6(15)	66(2)	28.9(14)	-14.0(14)	21.6(13)	-9.4(14)
N6	26.4(12)	31.6(13)	32.8(14)	8.7(11)	21.0(11)	4.8(10)
N7	20.2(11)	25.5(12)	26.4(12)	1.9(10)	15.5(10)	2.4(9)
N8	21.4(11)	28.7(13)	26.1(12)	3.5(10)	14.8(10)	1.9(10)
N9	21.9(11)	30.4(13)	28.6(13)	6.4(10)	16.2(11)	4.4(10)
N10	22.7(11)	30.0(13)	24.9(12)	0.5(10)	17(1)	-2.8(10)
C1	26.4(14)	17.2(13)	38.0(16)	-8.5(12)	21.1(13)	-4.3(11)
C2	26.4(14)	22.9(14)	31.8(16)	-10.3(12)	15.9(13)	-4.6(11)
C3	33.0(16)	30.8(17)	40.4(18)	-18.6(14)	18.5(15)	-12.8(13)
C4	38.7(18)	31.4(18)	57(2)	-24.2(16)	29.0(18)	-18.4(15)
C5	39.8(18)	19.9(14)	63(2)	-15.3(15)	35.4(18)	-14.8(13)
C6	35.8(16)	21.9(14)	42.7(18)	-10.4(13)	26.9(15)	-11.7(12)
C7	44(2)	38(2)	58(2)	-23.1(18)	26.6(19)	-22.3(17)
C8	26(3)	24(3)	38(3)	-8(2)	10(2)	-6(2)
C9	32(3)	34(3)	35(3)	1(3)	0(3)	-10(2)
C10	22(3)	39(3)	45(4)	-9(3)	7(2)	0(2)
C11	23.9(14)	29.7(15)	25.6(14)	-8.6(12)	12.7(12)	3.2(12)
C12	62(3)	101(4)	34(2)	-18(2)	34(2)	-15(3)
C13	93(8)	95(8)	52(6)	-9(5)	55(6)	3(6)
C14	96(9)	78(7)	25(4)	1(5)	35(5)	-19(6)
C15	27.3(14)	15.7(13)	36.9(16)	-1.1(11)	23.6(13)	0.5(11)
C16	25.8(14)	20.6(13)	34.7(15)	2.3(11)	23.4(13)	4.2(11)
C17	34.0(16)	26.0(15)	42.6(18)	8.1(13)	30.5(15)	10.6(12)
C18	41.8(17)	20.7(14)	53(2)	9.3(13)	39.7(17)	11.7(12)
C19	35.2(16)	13.6(13)	60(2)	2.6(13)	37.2(17)	2.6(11)
C20	33.0(15)	14.2(12)	46.2(18)	-5.3(12)	29.9(15)	-0.7(11)
C21	50(2)	32.4(17)	69(2)	22.3(17)	50(2)	17.9(15)
C22	78(3)	71(3)	95(3)	45(3)	78(3)	40(2)
C23	73(3)	34(2)	95(3)	27(2)	63(3)	9.4(19)
C24	70(3)	48(2)	67(3)	28.4(19)	57(2)	21.8(19)
C25	23.3(13)	24.8(14)	26.9(14)	4.3(11)	18.2(12)	5.8(11)

C26	20.2(14)	41.1(18)	32.3(16)	5.6(14)	14.1(13)	3.4(13)
C27	28.3(16)	42(2)	65(2)	11.2(18)	26.5(17)	9.0(15)
C28	28.3(17)	89(3)	30.9(18)	-1.6(19)	12.3(15)	3.5(19)
C29	36.0(17)	36.5(18)	41.8(19)	1.6(14)	26.8(16)	2.4(14)
C30	25.5(15)	47(2)	46(2)	1.9(16)	23.2(15)	-5.1(14)
C31	47(2)	59(2)	50(2)	12.8(18)	40.0(19)	12.6(18)
C32	26.7(14)	30.8(16)	29.6(15)	8.5(12)	17.0(13)	3.4(12)
C33	39.9(17)	33.2(17)	39.8(18)	3.7(14)	30.2(16)	-4.4(14)
C34	40.9(19)	56(2)	31.0(17)	11.7(16)	22.5(16)	5.8(17)
C35	49(6)	45(6)	43(6)	-20(5)	11(5)	-28(5)
C36	20(4)	52(6)	72(9)	-2(6)	-6(5)	-3(4)
C37	31(5)	68(7)	61(7)	-17(5)	15(5)	-29(5)
C38	75(7)	97(8)	45(5)	4(5)	41(5)	16(6)
C39	59(6)	139(11)	37(5)	-15(6)	19(4)	12(6)
N1'	16.6(10)	20.6(11)	16.7(10)	-1.2(8)	10.7(9)	-1.9(8)
N2'	21.1(11)	24.5(12)	20.4(11)	0.6(9)	10.7(10)	-0.9(9)
N3'	20.2(11)	24.5(11)	18.2(11)	0.5(9)	11.6(9)	0.0(9)
N4'	21.0(11)	24.9(12)	19.0(11)	0.7(9)	11(1)	0.1(9)
N5'	21.0(11)	20.8(11)	19.3(11)	0.4(9)	10.2(10)	1.0(9)
N6'	21.5(11)	32.9(13)	19.8(11)	-0.8(10)	13.2(10)	-8.4(10)
N7'	20.3(11)	23.0(12)	20.1(11)	0.2(9)	13.1(9)	-4.6(9)
N8'	20.6(11)	22.8(12)	19.9(11)	-0.8(9)	12.2(9)	-5.7(9)
N9'	20.2(11)	25.5(12)	19.8(11)	-1.1(9)	12.0(9)	-6.5(9)
C1'	18.5(12)	16.0(12)	23.2(13)	-0.6(10)	14.8(11)	-0.7(9)
C2'	19.0(12)	18.3(12)	22.7(13)	-0.9(10)	13.6(11)	-1.3(10)
C3'	18.0(12)	20.2(13)	24.4(14)	-0.9(11)	11.6(11)	-2.6(10)
C4'	20.1(13)	20.9(13)	29.2(14)	0.6(11)	15.6(12)	-2.3(10)
C5'	20.9(12)	20.5(13)	25.0(13)	3.9(10)	16.5(11)	1.4(10)
C6'	19.5(12)	17.8(12)	21.9(13)	-0.3(10)	13.9(11)	1(1)
C7'	21.0(13)	31.4(16)	31.9(16)	5.9(13)	14.2(13)	-5.0(12)
C8'	26.0(16)	55(2)	36.9(18)	2.4(16)	13.3(15)	-17.1(15)
C9'	40(2)	35(2)	83(3)	14(2)	34(2)	-7.0(16)
C10'	23.2(15)	71(3)	39.4(19)	5.4(17)	21.5(15)	-6.3(16)
C11'	18.0(12)	17.2(12)	20.0(12)	-1.6(10)	10.4(10)	-0.4(10)
C12'	29.1(15)	25.0(15)	16.4(13)	2.4(11)	6.3(12)	1.2(12)
C13'	70(3)	44(2)	23.4(17)	-3.9(16)	7.0(18)	-22(2)
C14'	41.7(18)	38.5(18)	24.3(15)	4.3(13)	19.5(14)	6.5(14)
C15'	19.6(12)	18.4(13)	18.4(12)	1.3(10)	13.4(10)	1.2(10)
C16'	18.7(12)	20.2(12)	22.0(13)	1(1)	14.7(11)	0.6(10)
C17'	22.6(13)	24.3(14)	23.4(13)	4.6(11)	17.7(11)	2.4(11)
C18'	23.5(13)	27.4(14)	19.4(13)	2.8(11)	15.1(11)	2.9(11)
C19'	19.0(12)	28.9(15)	19.6(13)	-0.8(11)	12.2(11)	-1.6(11)

C20'	20.1(12)	19.9(13)	20.5(13)	-0.6(10)	14.1(11)	-2.2(10)
C21'	23.0(14)	44.5(18)	21.4(14)	5.9(13)	14.8(12)	3.0(13)
C22'	32.5(17)	74(3)	40.9(19)	30.3(19)	26.6(16)	18.6(17)
C23'	43.8(19)	65(2)	25.4(16)	-5.5(16)	22.6(15)	-10.0(18)
C24'	29.6(15)	53(2)	24.6(15)	8.6(14)	20.1(13)	3.7(14)
C25'	19.9(12)	22.4(13)	19.6(13)	0.2(10)	12.6(11)	-1.7(10)
C26'	20.8(13)	31.5(15)	25.2(14)	-3.0(12)	13.6(12)	-12.0(12)
C27'	20.9(14)	45(2)	42.4(19)	1.4(15)	14.0(14)	-7.8(14)
C28'	41.4(18)	39.5(18)	35.5(17)	-14.4(14)	26.7(15)	-21.6(15)
C53	183(8)	150(7)	157(7)	-21(6)	114(7)	30(6)
C47	183(8)	150(7)	157(7)	-21(6)	114(7)	30(6)
C48	183(8)	150(7)	157(7)	-21(6)	114(7)	30(6)
C49	183(8)	150(7)	157(7)	-21(6)	114(7)	30(6)
C50	183(8)	150(7)	157(7)	-21(6)	114(7)	30(6)
C51	183(8)	150(7)	157(7)	-21(6)	114(7)	30(6)
C52	183(8)	150(7)	157(7)	-21(6)	114(7)	30(6)
C60	72(6)	72(6)	112(8)	-17(6)	73(6)	-18(5)
C54	43(4)	21(5)	54(5)	-8(5)	26(4)	-9(5)
C55	53(8)	43(5)	69(6)	-1(4)	40(6)	-8(5)
C56	71(9)	56(6)	78(7)	-1(5)	54(7)	-21(6)
C57	63(8)	71(8)	108(10)	-22(6)	67(7)	-11(6)
C58	119(17)	93(17)	170(20)	-23(14)	100(16)	-16(12)
C59	79(13)	46(8)	89(12)	-9(7)	52(10)	0(7)
C40	125(6)	131(7)	72(4)	-8(4)	30(4)	-58(5)
C41	92(4)	63(4)	126(6)	-5(4)	54(4)	-8(3)
C42	74(3)	64(3)	102(4)	18(3)	59(3)	11(3)
C43	61(3)	56(3)	154(6)	-2(3)	68(4)	-6(2)
C44	77(4)	169(8)	70(4)	-10(4)	47(3)	-50(5)
C45	100(5)	144(7)	70(4)	-6(5)	40(4)	-51(5)
C46	135(6)	96(5)	242(10)	30(6)	153(7)	35(5)
C61	46(8)	52(7)	39(5)	-3(4)	26(5)	-3(5)
C62	43(6)	82(11)	57(7)	-15(6)	30(6)	7(7)
C63	31(6)	39(8)	49(6)	-12(5)	13(5)	11(5)
C64	31(8)	73(9)	72(10)	-35(8)	13(7)	-13(6)
C65	76(10)	48(9)	69(8)	-4(7)	29(7)	-25(7)
C66	51(8)	69(11)	51(6)	-6(9)	30(6)	8(8)
C67	55(6)	63(6)	43(5)	2(4)	28(4)	8(5)

[2] Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$

Table S17 Bond Lengths for **Ce(CzT^{iPr})$_2$[N(SiMe$_3$)$_2$] 5 • 2.5 C$_7$H$_8$**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ce1	Si2	3.4442(9)	N3'	N4'	1.327(3)
Ce1	N1	2.557(2)	N3'	C11'	1.358(3)
Ce1	N3	2.680(2)	N4'	N5'	1.311(3)
Ce1	N7	2.624(2)	N5'	C12'	1.485(3)
Ce1	N10	2.351(2)	N6'	N9'	1.330(3)
Ce1	N1'	2.566(2)	N6'	C25'	1.338(3)
Ce1	N3'	2.627(2)	N7'	N8'	1.330(3)
Ce1	N7'	2.703(2)	N7'	C25'	1.356(3)
Si1	N10	1.704(2)	N8'	N9'	1.312(3)
Si1	C29	1.881(3)	N9'	C26'	1.484(3)
Si1	C30	1.877(3)	C1'	C2'	1.406(4)
Si1	C31	1.873(3)	C1'	C6'	1.427(4)
Si2	N10	1.703(3)	C2'	C3'	1.404(4)
Si2	C32	1.890(3)	C2'	C11'	1.458(4)
Si2	C33	1.878(3)	C3'	C4'	1.396(4)
Si2	C34	1.880(3)	C4'	C5'	1.394(4)
N1	C1	1.394(4)	C4'	C7'	1.539(4)
N1	C15	1.392(4)	C5'	C6'	1.390(4)
N2	N5	1.325(4)	C6'	C16'	1.436(4)
N2	C11	1.332(4)	C7'	C8'	1.531(4)
N3	N4	1.323(4)	C7'	C9'	1.533(5)
N3	C11	1.345(4)	C7'	C10'	1.529(5)
N4	N5	1.313(4)	C12'	C13'	1.518(4)
N5	C12	1.487(5)	C12'	C14'	1.513(4)
N6	N9	1.329(3)	C15'	C16'	1.423(3)
N6	C25	1.339(4)	C15'	C20'	1.411(4)
N7	N8	1.332(3)	C16'	C17'	1.389(4)
N7	C25	1.354(4)	C17'	C18'	1.397(4)
N8	N9	1.308(3)	C18'	C19'	1.392(4)
N9	C26	1.475(4)	C18'	C21'	1.528(4)
C1	C2	1.404(4)	C19'	C20'	1.398(4)
C1	C6	1.425(4)	C20'	C25'	1.454(4)
C2	C3	1.412(4)	C21'	C22'	1.537(4)
C2	C11	1.461(4)	C21'	C23'	1.536(5)
C3	C4	1.390(5)	C21'	C24'	1.534(4)
C4	C5	1.390(5)	C26'	C27'	1.512(4)
C4	C7	1.540(4)	C26'	C28'	1.519(4)
C5	C6	1.396(4)	C53	C47	1.5072
C6	C20	1.439(5)	C47	C48	1.4021

C7	C8	1.457(6)	C47	C52	1.4021
C7	C9	1.652(8)	C48	C49	1.3961
C7	C10	1.573(7)	C49	C50	1.3963
C7	C35	1.545(10)	C50	C51	1.3964
C7	C36	1.368(9)	C51	C52	1.3968
C7	C37	1.597(10)	C60	C54	1.5064
C12	C13	1.542(11)	C54	C55	1.4026
C12	C14	1.344(11)	C54	C59	1.4022
C12	C38	1.593(13)	C55	C56	1.3961
C12	C39	1.589(10)	C56	C57	1.3958
C15	C16	1.405(4)	C57	C58	1.3960
C15	C20	1.429(4)	C58	C59	1.3966
C16	C17	1.398(4)	C40	C41	1.401(9)
C16	C25	1.457(4)	C40	C45	1.384(10)
C17	C18	1.402(4)	C41	C42	1.341(8)
C18	C19	1.399(5)	C42	C43	1.359(8)
C18	C21	1.533(4)	C43	C44	1.447(9)
C19	C20	1.385(4)	C43	C46	1.393(8)
C21	C22	1.540(5)	C44	C45	1.382(10)
C21	C23	1.529(5)	C61	C62	1.341(18)
C21	C24	1.528(6)	C61	C66	1.397(16)
C26	C27	1.515(5)	C61	C67	1.493(16)
C26	C28	1.517(5)	C62	C63	1.322(18)
N1'	C1'	1.392(3)	C63	C64	1.37(2)
N1'	C15'	1.392(3)	C64	C65	1.33(2)
N2'	N5'	1.333(3)	C65	C66	1.411(17)
N2'	C11'	1.338(3)			

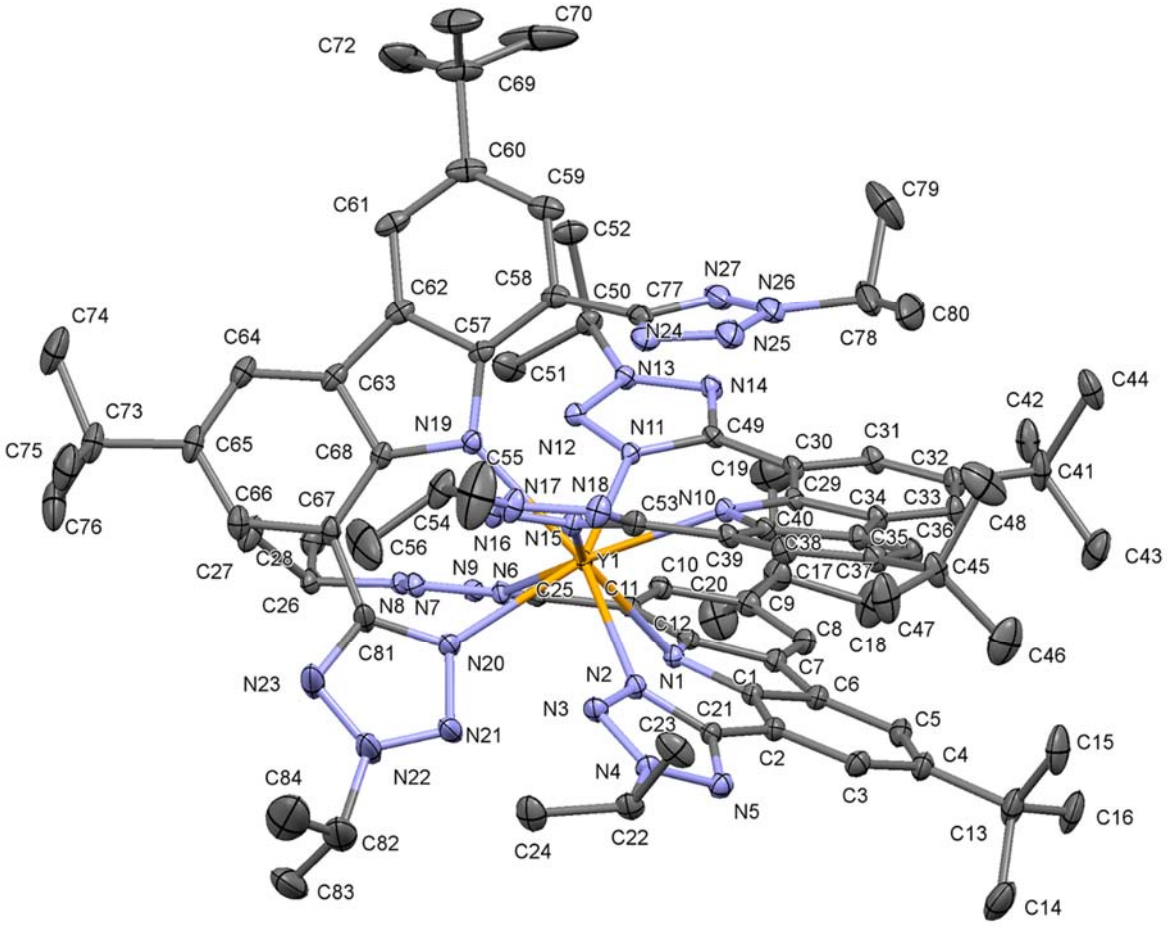
Table S18 Bond Angles for **$Ce(CzT^{iPr})_2[N(SiMe_3)_2]$ 5 • 2.5 C_7H_8**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Ce1	Si2	153.69(5)	C18	C21	C22	109.2(3)
N1	Ce1	N3	69.30(8)	C23	C21	C18	110.0(3)
N1	Ce1	N7	69.72(7)	C23	C21	C22	109.9(3)
N1	Ce1	N1'	80.41(7)	C24	C21	C18	112.3(3)
N1	Ce1	N3'	84.79(7)	C24	C21	C22	107.7(3)
N1	Ce1	N7'	130.26(7)	C24	C21	C23	107.7(3)
N3	Ce1	Si2	84.76(6)	N6	C25	N7	111.0(2)
N3	Ce1	N7'	157.02(7)	N6	C25	C16	123.9(3)
N7	Ce1	Si2	121.57(5)	N7	C25	C16	125.2(3)
N7	Ce1	N3	116.82(8)	N9	C26	C27	108.7(3)
N7	Ce1	N3'	146.61(7)	N9	C26	C28	108.7(3)
N7	Ce1	N7'	68.77(7)	C27	C26	C28	114.1(3)
N10	Ce1	Si2	26.54(6)	C1'	N1'	Ce1	121.78(16)
N10	Ce1	N1	136.00(8)	C15'	N1'	Ce1	120.68(16)
N10	Ce1	N3	78.56(8)	C15'	N1'	C1'	104.6(2)
N10	Ce1	N7	101.10(8)	N5'	N2'	C11'	102.1(2)
N10	Ce1	N1'	143.01(8)	N4'	N3'	Ce1	121.84(16)
N10	Ce1	N3'	112.27(8)	N4'	N3'	C11'	107.2(2)
N10	Ce1	N7'	78.47(8)	C11'	N3'	Ce1	130.05(17)
N1'	Ce1	Si2	122.33(5)	N5'	N4'	N3'	105.4(2)
N1'	Ce1	N3	131.74(7)	N2'	N5'	C12'	121.7(2)
N1'	Ce1	N7	84.26(7)	N4'	N5'	N2'	114.6(2)
N1'	Ce1	N3'	70.11(7)	N4'	N5'	C12'	123.7(2)
N1'	Ce1	N7'	69.41(7)	N9'	N6'	C25'	101.8(2)
N3'	Ce1	Si2	90.78(5)	N8'	N7'	Ce1	123.38(16)
N3'	Ce1	N3	70.51(7)	N8'	N7'	C25'	106.7(2)
N3'	Ce1	N7'	118.23(7)	C25'	N7'	Ce1	123.34(17)
N7'	Ce1	Si2	74.29(5)	N9'	N8'	N7'	105.5(2)
N10	Si1	C29	110.56(14)	N6'	N9'	C26'	122.6(2)
N10	Si1	C30	112.08(14)	N8'	N9'	N6'	114.6(2)
N10	Si1	C31	114.38(14)	N8'	N9'	C26'	122.8(2)
C30	Si1	C29	107.52(16)	N1'	C1'	C2'	130.2(2)
C31	Si1	C29	105.48(17)	N1'	C1'	C6'	111.9(2)
C31	Si1	C30	106.37(17)	C2'	C1'	C6'	117.8(2)
N10	Si2	Ce1	38.08(8)	C1'	C2'	C11'	122.4(2)
N10	Si2	C32	109.72(13)	C3'	C2'	C1'	119.0(2)
N10	Si2	C33	114.49(14)	C3'	C2'	C11'	118.6(2)
N10	Si2	C34	112.26(15)	C4'	C3'	C2'	123.1(3)
C32	Si2	Ce1	73.01(10)	C3'	C4'	C7'	122.9(2)

C33	Si2	Ce1	137.85(11)	C5'	C4'	C3'	117.7(2)
C33	Si2	C32	107.98(15)	C5'	C4'	C7'	119.3(2)
C33	Si2	C34	107.14(16)	C6'	C5'	C4'	120.7(2)
C34	Si2	Ce1	113.33(12)	C1'	C6'	C16'	105.8(2)
C34	Si2	C32	104.71(15)	C5'	C6'	C1'	121.6(2)
C1	N1	Ce1	121.06(18)	C5'	C6'	C16'	132.6(2)
C15	N1	Ce1	122.42(17)	C8'	C7'	C4'	112.5(2)
C15	N1	C1	104.1(2)	C8'	C7'	C9'	108.7(3)
N5	N2	C11	101.6(3)	C9'	C7'	C4'	108.7(3)
N4	N3	Ce1	124.66(19)	C10'	C7'	C4'	109.9(3)
N4	N3	C11	106.9(2)	C10'	C7'	C8'	107.8(3)
C11	N3	Ce1	126.42(19)	C10'	C7'	C9'	109.2(3)
N5	N4	N3	105.3(3)	N2'	C11'	N3'	110.8(2)
N2	N5	C12	123.2(3)	N2'	C11'	C2'	124.3(2)
N4	N5	N2	114.6(3)	N3'	C11'	C2'	125.0(2)
N4	N5	C12	122.1(3)	N5'	C12'	C13'	108.1(2)
N9	N6	C25	101.9(2)	N5'	C12'	C14'	110.4(2)
N8	N7	Ce1	122.49(17)	C14'	C12'	C13'	113.1(3)
N8	N7	C25	107.0(2)	N1'	C15'	C16'	112.3(2)
C25	N7	Ce1	129.88(18)	N1'	C15'	C20'	130.0(2)
N9	N8	N7	105.3(2)	C20'	C15'	C16'	117.7(2)
N6	N9	C26	122.8(2)	C15'	C16'	C6'	105.4(2)
N8	N9	N6	114.9(2)	C17'	C16'	C6'	132.5(2)
N8	N9	C26	122.3(2)	C17'	C16'	C15'	122.1(2)
Si1	N10	Ce1	120.04(13)	C16'	C17'	C18'	120.2(2)
Si2	N10	Ce1	115.37(12)	C17'	C18'	C21'	123.7(2)
Si2	N10	Si1	124.59(14)	C19'	C18'	C17'	117.5(2)
N1	C1	C2	129.5(3)	C19'	C18'	C21'	118.8(2)
N1	C1	C6	112.4(3)	C18'	C19'	C20'	124.0(2)
C2	C1	C6	118.0(3)	C15'	C20'	C25'	124.0(2)
C1	C2	C3	118.8(3)	C19'	C20'	C15'	118.4(2)
C1	C2	C11	123.0(3)	C19'	C20'	C25'	117.6(2)
C3	C2	C11	118.0(3)	C18'	C21'	C22'	109.5(2)
C4	C3	C2	123.0(3)	C18'	C21'	C23'	109.1(3)
C3	C4	C7	121.0(4)	C18'	C21'	C24'	112.5(2)
C5	C4	C3	118.2(3)	C23'	C21'	C22'	108.6(3)
C5	C4	C7	120.8(3)	C24'	C21'	C22'	108.9(3)
C4	C5	C6	120.4(3)	C24'	C21'	C23'	108.2(3)
C1	C6	C20	105.7(3)	N6'	C25'	N7'	111.3(2)
C5	C6	C1	121.6(3)	N6'	C25'	C20'	123.3(2)
C5	C6	C20	132.7(3)	N7'	C25'	C20'	125.4(2)
C4	C7	C9	113.2(3)	N9'	C26'	C27'	109.8(2)

C4	C7	C10	111.4(3)	N9'	C26'	C28'	108.7(2)
C4	C7	C35	105.4(4)	C27'	C26'	C28'	112.9(3)
C4	C7	C37	107.5(4)	C48	C47	C53	120.9
C8	C7	C4	112.9(4)	C52	C47	C53	120.9
C8	C7	C9	105.9(4)	C52	C47	C48	118.1
C8	C7	C10	112.7(4)	C49	C48	C47	121.1
C10	C7	C9	100.0(4)	C48	C49	C50	120.2
C35	C7	C37	101.3(6)	C49	C50	C51	119.4
C36	C7	C4	106.5(5)	C50	C51	C52	120.1
C36	C7	C35	121.8(8)	C51	C52	C47	121.1
C36	C7	C37	113.4(8)	C55	C54	C60	120.9
N2	C11	N3	111.7(3)	C59	C54	C60	121.0
N2	C11	C2	123.1(3)	C59	C54	C55	118.1
N3	C11	C2	125.2(3)	C56	C55	C54	121.1
N5	C12	C13	109.2(5)	C57	C56	C55	120.1
N5	C12	C38	110.6(4)	C56	C57	C58	119.5
N5	C12	C39	107.4(5)	C57	C58	C59	120.1
C14	C12	N5	112.7(5)	C58	C59	C54	121.1
C14	C12	C13	121.2(6)	C45	C40	C41	124.6(9)
C39	C12	C38	102.0(7)	C42	C41	C40	114.4(7)
N1	C15	C16	129.4(3)	C41	C42	C43	126.5(7)
N1	C15	C20	112.7(3)	C42	C43	C44	117.2(6)
C16	C15	C20	117.8(3)	C42	C43	C46	129.2(8)
C15	C16	C25	122.4(3)	C46	C43	C44	113.6(7)
C17	C16	C15	119.3(3)	C45	C44	C43	119.3(7)
C17	C16	C25	118.2(3)	C44	C45	C40	117.8(7)
C16	C17	C18	122.9(3)	C62	C61	C66	116.5(12)
C17	C18	C21	121.6(3)	C62	C61	C67	122.1(13)
C19	C18	C17	117.6(3)	C66	C61	C67	121.3(12)
C19	C18	C21	120.8(3)	C63	C62	C61	124.9(15)
C20	C19	C18	120.8(3)	C62	C63	C64	116.4(13)
C15	C20	C6	105.1(3)	C65	C64	C63	126(2)
C19	C20	C6	133.4(3)	C64	C65	C66	114.9(18)
C19	C20	C15	121.5(3)	C61	C66	C65	121.6(14)

Figure S5 Labeled ORTEP drawing of **$Y(CzT^{iPr})_3$ 7 • 0.87 C_7H_8**



Note: 0.87 equiv of toluene not shown

Table S19 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **$Y(CzT^{iPr})_3$ 7 • 0.87 C_7H_8**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Y1	3031.2(2)	5933.1(2)	3615.3(2)	17.00(7)
N1	3367.0(5)	7149.6(11)	3923.5(6)	20.6(4)
N2	3049.2(5)	6896.5(12)	3002.8(6)	21.9(4)
N3	2811.8(6)	6841.6(12)	2619.6(6)	25.6(4)
N4	2941.7(6)	7340.2(12)	2367.5(6)	25.9(4)
N5	3254.0(6)	7729.5(12)	2555.5(7)	27.3(5)
N6	2760.6(5)	6417.3(11)	4248.4(6)	20.5(4)
N7	2420.2(5)	6222.3(12)	4305.7(6)	22.5(4)
N8	2422.5(5)	6386.6(11)	4711.5(6)	21.0(4)
N9	2747.1(5)	6693.2(11)	4930.8(6)	21.1(4)
N10	3635.3(5)	5652.4(11)	3469.1(6)	18.9(4)
N11	3415.4(5)	5378.8(11)	4294.0(6)	18.3(4)
N12	3265.9(5)	5082.1(11)	4610.1(6)	19.6(4)
N13	3550.9(5)	4994.0(11)	4937.9(6)	21.2(4)
N14	3886.0(5)	5205.8(12)	4864.4(6)	22.6(4)
N15	2913.6(5)	5224.4(12)	2908.5(6)	22.1(4)
N16	2581.0(6)	4899.7(13)	2742.3(6)	27.6(5)
N17	2602.2(6)	4670.1(14)	2352.0(7)	31.3(5)
N18	2933.8(6)	4820.5(13)	2246.9(7)	30.3(5)
N19	2686.4(5)	4699.6(11)	3712.0(6)	20.9(4)
N20	2366.7(5)	6342.0(12)	3324.2(6)	25.4(4)
N21	2268.9(7)	7028.5(15)	3120.1(9)	45.0(7)
N22	1892.4(9)	6953(2)	2961.6(14)	33.7(9)
N23	1738.0(11)	6290(3)	3074.9(15)	35.2(10)
N22A	1968(3)	7271(8)	3193(5)	33(3)
N23A	1777(4)	6611(10)	3265(5)	40(4)
N24	3424.0(6)	3818.4(13)	3276.2(7)	32.3(5)
N25	3759.3(7)	3883.9(14)	3180.3(9)	39.6(6)
N26	4004.4(7)	3919.5(14)	3552.9(9)	41.6(6)
N27	3849.3(7)	3883.7(13)	3897.9(8)	38.2(6)
C1	3632.9(6)	7544.0(13)	3739.1(8)	21.7(5)
C2	3629.1(6)	7682.3(14)	3299.8(8)	23.3(5)

C3	3927.7(7)	8094.6(15)	3190.8(8)	29.5(6)
C4	4235.7(7)	8387.3(16)	3496.5(9)	31.3(6)
C5	4237.0(7)	8257.1(15)	3929.8(9)	29.7(6)
C6	3940.9(7)	7846.9(14)	4051.5(8)	25.1(5)
C7	3859.9(7)	7639.7(14)	4463.0(8)	24.1(5)
C8	4057.7(7)	7730.7(15)	4888.2(8)	27.5(5)
C9	3909.0(7)	7445.0(15)	5229.7(8)	27.4(5)
C10	3548.2(7)	7100.2(14)	5129.7(8)	23.3(5)
C11	3341.8(6)	7003.8(13)	4707.9(7)	20.5(5)
C12	3506.3(6)	7240.6(13)	4363.9(7)	20.7(5)
C13	4549.1(8)	8836(2)	3335.4(10)	44.3(7)
C14	4375.4(10)	9533(2)	3046.0(12)	62.4(10)
C15	4744.7(9)	8257(3)	3076.9(12)	63.8(10)
C16	4843.0(9)	9180(2)	3711.0(11)	56.3(9)
C17	4123.5(8)	7474.9(17)	5703.2(8)	35.3(6)
C18	4494.8(10)	7935(2)	5757.2(10)	60.1(10)
C19	4206.4(11)	6624(2)	5866.1(11)	58.9(10)
C20	3883.3(10)	7904(2)	5979.3(10)	55.4(9)
C21	3316.3(7)	7436.4(14)	2958.2(8)	22.8(5)
C22	2765.6(7)	7430.6(16)	1903.8(8)	30.3(6)
C23	2962.5(9)	6863(2)	1651.7(9)	46.7(8)
C24	2345.4(8)	7290(2)	1838.2(9)	41.1(7)
C25	2955.6(6)	6704.4(13)	4630.9(7)	19.4(5)
C26	2080.3(7)	6304.5(14)	4896.2(8)	24.8(5)
C27	1837.6(8)	5640.2(18)	4663.5(10)	41.0(7)
C28	2192.1(8)	6183.7(17)	5379.7(8)	32.7(6)
C29	3971.9(6)	5819.5(13)	3758.2(7)	19.3(5)
C30	4061.0(6)	5752.9(14)	4210.5(7)	20.2(5)
C31	4427.4(7)	5937.4(15)	4432.5(8)	24.3(5)
C32	4713.2(7)	6177.3(16)	4226.0(8)	27.3(5)
C33	4626.4(7)	6216.2(15)	3775.8(8)	25.4(5)
C34	4266.3(6)	6034.2(14)	3546.7(7)	21.6(5)
C35	4106.3(6)	5943.4(14)	3090.5(7)	21.8(5)
C36	4260.7(7)	5989.9(15)	2727.4(8)	25.2(5)
C37	4045.7(7)	5780.8(15)	2322.4(8)	25.7(5)
C38	3674.9(7)	5528.0(15)	2298.8(7)	24.6(5)

C39	3508.6(6)	5483.6(14)	2656.9(7)	21.8(5)
C40	3726.1(6)	5696.0(14)	3066.1(7)	20.8(5)
C41	5113.6(7)	6350(2)	4480.4(9)	41.7(7)
C42	5157.2(11)	6301(3)	4959.5(12)	40.6(12)
C43	5253.5(19)	7105(4)	4338(2)	50.9(16)
C44	5370.1(10)	5631(3)	4356.2(13)	42.7(12)
C42A	5363(5)	6802(15)	4235(6)	68(6)
C43A	5276(3)	5813(7)	4792(4)	48(3)
C44A	5041(3)	7204(6)	4811(3)	40(3)
C45	4226.0(7)	5790.5(18)	1925.7(8)	32.6(6)
C46	4448.1(11)	6572(3)	1915.9(10)	62.8(10)
C47	3934.6(9)	5748(3)	1505.8(9)	56.6(10)
C48	4497.0(12)	5090(3)	1956.4(11)	70.0(12)
C49	3792.4(6)	5451.6(13)	4453.1(7)	19.0(5)
C50	3509.3(7)	4633.7(14)	5350.8(7)	24.9(5)
C51	3160.8(9)	4966.6(19)	5483.0(10)	47.0(8)
C52	3498.0(9)	3734.5(16)	5303.2(9)	35.9(6)
C53	3124.8(7)	5176.0(14)	2604.0(7)	22.9(5)
C54	2280.2(8)	4246(2)	2068.0(9)	43.5(7)
C55	2357.6(14)	4131(3)	1624.7(12)	98.2(19)
C56	1920.9(10)	4641(3)	2107.1(17)	87.6(15)
C57	2829.6(7)	3983.6(13)	3906.5(7)	22.1(5)
C58	3187.7(7)	3618.2(14)	3951.1(8)	26.5(5)
C59	3256.9(8)	2901.9(15)	4184.2(8)	31.7(6)
C60	2985.4(9)	2496.5(15)	4357.9(8)	35.7(7)
C61	2627.3(8)	2820.6(14)	4283.7(8)	31.8(6)
C62	2549.2(7)	3541.6(14)	4058.0(7)	25.2(5)
C63	2204.2(7)	3959.6(14)	3910.8(7)	25.0(5)
C64	1833.5(7)	3753.7(16)	3913.6(8)	30.3(6)
C65	1538.8(7)	4228.0(17)	3710.4(8)	32.8(6)
C66	1630.7(7)	4932.6(17)	3519.4(8)	30.6(6)
C67	2000.9(7)	5167.5(15)	3512.9(7)	24.8(5)
C68	2302.1(6)	4660.7(14)	3703.1(7)	21.3(5)
C69	3073.0(11)	1678.1(17)	4578.2(10)	49.8(9)
C70	3106(2)	1050(4)	4215(2)	34.9(15)
C71	2695.6(17)	1340(4)	4742(2)	43.1(14)

C72	3374(2)	1654(5)	4920(2)	55.6(18)
C70A	2989(2)	1044(4)	4277(2)	47.1(19)
C71A	2911(2)	1666(5)	4969(2)	58.2(18)
C72A	3541.0(18)	1646(4)	4799(2)	38.5(13)
C73	1120.9(8)	4023.3(19)	3683.1(10)	42.9(7)
C74	1074.0(10)	3218(2)	3900.6(11)	59.5(10)
C75	922.1(9)	3962(2)	3213.0(11)	58.9(10)
C76	945.7(9)	4656(3)	3923.8(14)	66.3(11)
C77	3482.9(7)	3824.1(14)	3712.6(8)	26.4(5)
C78	4417.7(9)	4001(2)	3584.7(17)	67.4(12)
C79	4608.0(14)	3324(5)	3892(2)	86(2)
C80	4518.0(15)	3990(4)	3173(2)	76(2)
C79A	4637(5)	4013(13)	3934(6)	57(6)
C80A	4528(5)	3406(17)	3181(7)	71(7)
C81	2040.2(7)	5932.7(17)	3312.3(9)	32.5(6)
C82	1663.9(11)	7561(3)	2678.7(16)	47.9(13)
C83	1472(3)	8081(7)	2937(4)	130(5)
C84	1413.3(13)	7136(3)	2305.3(17)	73.4(18)
C82A	1782(5)	8055(11)	3064(8)	85(9)
C83A	1405(6)	8010(13)	2916(4)	25(4)
C84A	1763(8)	8480(12)	3508(11)	138(16)
C1S	4209(3)	10952(5)	4176(5)	124(2)
C2S	4010(2)	10248(4)	4204(4)	111(2)
C3S	4109(3)	9901(4)	4593(4)	110(2)
C4S	4375(3)	10155(6)	4937(4)	137(2)
C5S	4562(4)	10769(6)	4888(5)	146(2)
C6S	4472(3)	11218(6)	4473(4)	132(2)
C7S	4079(3)	11339(7)	3793(4)	159(4)

Table S20 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **$Y(CzT^{iPr})_3$ 7 • 0.87 C_7H_8**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Y1	14.22(11)	20.16(11)	17.17(11)	0.92(8)	4.58(8)	-0.53(8)
N1	17.7(10)	21.7(10)	23.5(10)	0.0(8)	7.2(8)	-0.6(8)
N2	17.9(10)	27.0(10)	20.6(10)	2.9(8)	3.5(8)	0.2(8)
N3	23.7(11)	30.5(11)	22.1(10)	6.8(9)	4.2(8)	0.8(9)
N4	25.4(11)	31.0(11)	21.5(10)	7.6(9)	5.4(8)	0.9(9)
N5	26.2(11)	29.8(11)	26.3(11)	4.6(9)	6.3(9)	-2.5(9)
N6	15.1(9)	23.7(10)	23.6(10)	-1.1(8)	6.0(8)	1.0(8)
N7	20.3(10)	23.9(10)	25.4(10)	-0.2(8)	9.7(8)	0.9(8)
N8	21.3(10)	19.3(10)	24.5(10)	0.0(8)	9.3(8)	1.0(8)
N9	21.5(10)	19.0(9)	24.2(10)	0.5(8)	7.7(8)	1.4(8)
N10	18.3(9)	23.1(9)	16.0(9)	-0.5(8)	4.9(7)	0.5(8)
N11	19.2(10)	18.6(9)	18.7(9)	-1.3(7)	7.8(8)	0.2(7)
N12	20.6(10)	21.1(9)	18.1(9)	0.7(8)	6.5(8)	1.2(8)
N13	21.8(10)	23.5(10)	19.4(10)	1.6(8)	7.0(8)	2.4(8)
N14	18.7(10)	28.8(11)	21.5(10)	1.3(8)	7.2(8)	3.2(8)
N15	18.5(10)	26.7(10)	20.7(10)	1.4(8)	3.4(8)	-3.5(8)
N16	23.6(11)	35.8(12)	22.6(10)	-1.6(9)	3.6(8)	-8.0(9)
N17	28.7(12)	41.9(13)	22.4(11)	-3.8(9)	3.1(9)	-12.8(10)
N18	29.4(12)	39.4(12)	22.2(11)	-5.1(9)	5.4(9)	-10.2(10)
N19	19.7(10)	23.0(10)	18.9(9)	0.7(8)	1.5(8)	-2.8(8)
N20	21.1(10)	30.0(11)	26.7(11)	10.4(9)	8.7(8)	3.9(8)
N21	29.6(13)	44.5(14)	67.7(17)	33.0(13)	25.7(12)	16.0(11)
N22	16.6(15)	40(2)	44(2)	20.9(17)	3.4(15)	4.2(13)
N23	19.4(16)	43(2)	42(2)	19.7(18)	4.8(17)	0.2(16)
N22A	21(6)	44(7)	36(7)	25(6)	9(5)	1(5)
N23A	19(6)	58(10)	45(9)	31(7)	16(6)	14(6)
N24	33.2(12)	27.5(11)	37.2(13)	-4.2(10)	9.7(10)	2.6(9)
N25	33.2(13)	32.0(12)	54.9(16)	-6.6(11)	12.7(12)	2.5(10)
N26	29.4(13)	29.9(12)	65.8(18)	-4.1(11)	10.9(12)	6.3(10)
N27	30.3(12)	27.9(12)	52.7(15)	-1.4(11)	0.4(11)	6.0(9)
C1	19.0(11)	19.3(11)	27.8(12)	1.8(9)	7.1(10)	0.4(9)
C2	19.6(12)	22.8(12)	28.6(13)	2.7(10)	7.3(10)	-0.1(9)
C3	27.8(13)	32.0(13)	30.4(13)	6.5(11)	10.2(11)	-1.8(11)

C4	23.1(13)	34.1(14)	37.9(15)	5.7(11)	9.0(11)	-6.3(11)
C5	22.1(13)	31.3(13)	34.9(14)	0.7(11)	4.2(11)	-7.1(10)
C6	23.1(12)	24.2(12)	28.3(13)	0.7(10)	5.7(10)	-1.8(10)
C7	22.3(12)	21.9(12)	28.6(13)	-1.8(10)	6.6(10)	-1.8(9)
C8	22.9(12)	27.1(13)	31.0(13)	-0.7(10)	2.3(10)	-3.8(10)
C9	26.5(13)	28.0(13)	26.0(13)	-2.5(10)	2.0(10)	0.4(10)
C10	23.1(12)	23.3(12)	24.4(12)	-0.7(9)	7.5(10)	3.1(9)
C11	19.7(11)	18.0(11)	24.7(12)	-1.3(9)	6.8(9)	3.3(9)
C12	19.5(11)	18.9(11)	24.3(12)	-1.0(9)	6.0(9)	2.5(9)
C13	31.8(15)	56.8(19)	45.9(17)	11.2(15)	11.8(13)	-17.2(14)
C14	52(2)	68(2)	65(2)	28.1(19)	7.6(17)	-25.6(18)
C15	37.5(18)	95(3)	67(2)	2(2)	31.0(17)	-16.1(18)
C16	33.5(17)	74(2)	59(2)	13.9(18)	6.3(15)	-29.1(16)
C17	31.5(15)	44.3(16)	26.9(14)	1.8(12)	-0.9(11)	-4.3(12)
C18	48(2)	88(3)	34.8(17)	2.6(17)	-10.8(14)	-25.2(19)
C19	60(2)	58(2)	45.3(19)	11.8(16)	-19.1(16)	1.2(17)
C20	54(2)	78(2)	29.0(16)	-15.5(16)	-0.8(14)	-1.5(18)
C21	22.5(12)	22.6(12)	25.0(12)	5.2(9)	8.7(10)	3.0(9)
C22	31.8(14)	37.0(14)	21.0(12)	10.2(11)	2.9(10)	3.8(11)
C23	48.3(18)	67(2)	24.0(14)	7.2(14)	5.3(13)	21.8(16)
C24	31.8(15)	62(2)	26.6(14)	11.8(13)	-1.0(12)	4.4(14)
C25	21.5(12)	15.8(10)	22.0(11)	0.3(9)	7.3(9)	3.8(9)
C26	22.1(12)	24.8(12)	32.0(13)	0.2(10)	15.7(10)	0.8(10)
C27	36.0(16)	44.7(16)	48.5(17)	-9.1(14)	22.9(14)	-15.1(13)
C28	32.9(14)	36.7(14)	33.9(14)	4.0(12)	18.8(12)	0.4(11)
C29	17.1(11)	20.7(11)	20.7(11)	-1.6(9)	5.5(9)	3.0(9)
C30	15.6(11)	25.9(12)	19.6(11)	-0.4(9)	4.8(9)	3.7(9)
C31	19.7(12)	34.8(13)	18.0(11)	-0.7(10)	3.5(9)	3.0(10)
C32	18.5(12)	39.8(14)	23.9(12)	0.1(11)	5.3(10)	0.4(10)
C33	17.1(12)	37.6(14)	23.2(12)	0.5(10)	8.1(9)	-1.1(10)
C34	19.5(11)	27.5(12)	19.1(11)	-0.1(9)	6.8(9)	2.5(9)
C35	18.3(11)	27.8(12)	20.4(11)	0.2(9)	6.7(9)	0.9(9)
C36	19.8(12)	33.9(13)	23.7(12)	2.6(10)	8.3(10)	0.7(10)
C37	25.0(13)	34.7(14)	18.5(11)	2.3(10)	7.3(10)	3.5(10)
C38	23.9(12)	32.8(13)	17.5(11)	-1.3(10)	5.0(9)	3.3(10)
C39	20.1(12)	25.8(12)	19.6(11)	-0.6(9)	4.1(9)	1.5(9)

C40	19.6(11)	24.2(11)	19.4(11)	1.0(9)	6.2(9)	1.9(9)
C41	17.9(13)	77(2)	29.1(14)	9.0(14)	1.1(11)	-8.0(13)
C42	22(2)	77(3)	22.1(19)	-6(2)	1.7(15)	-9(2)
C43	37(4)	65(4)	44(4)	5(3)	-6(3)	-25(3)
C44	20.2(19)	76(3)	32(2)	3(2)	3.8(16)	9.5(19)
C42A	22(8)	140(20)	44(10)	6(10)	-2(6)	-26(10)
C43A	23(5)	61(8)	55(7)	-8(6)	-2(5)	3(5)
C44A	32(5)	46(6)	38(6)	-18(5)	-3(4)	-6(4)
C45	25.5(13)	54.7(17)	19.8(12)	2.1(11)	9.9(10)	4.6(12)
C46	67(2)	93(3)	34.0(17)	4.4(18)	23.8(16)	-25(2)
C47	36.6(17)	114(3)	22.0(14)	4.5(17)	12.5(13)	-0.7(18)
C48	79(3)	99(3)	40.8(19)	9.6(19)	33.8(19)	46(2)
C49	17.9(11)	20.9(11)	18.1(11)	-0.6(9)	4.0(9)	4.2(9)
C50	29.6(13)	28.7(13)	17.4(11)	5.5(9)	7.4(10)	0.9(10)
C51	54.8(19)	50.2(18)	46.4(17)	20.4(15)	34.6(15)	16.9(15)
C52	51.2(18)	29.8(14)	26.2(13)	6.8(11)	6.8(12)	2.0(12)
C53	23.6(12)	26.6(12)	18.3(11)	-0.4(9)	4.3(9)	-1.5(10)
C54	39.6(17)	56.6(19)	30.7(15)	-4.7(13)	-1.0(12)	-24.5(14)
C55	82(3)	164(5)	42(2)	-33(3)	0(2)	-66(3)
C56	35(2)	88(3)	121(4)	-39(3)	-25(2)	-7(2)
C57	27.7(12)	19.4(11)	17.0(11)	-1.9(9)	0.0(9)	-3.5(9)
C58	31.2(14)	21.8(12)	23.1(12)	-4.0(10)	-1.8(10)	0.4(10)
C59	43.7(16)	25.4(13)	22.6(12)	-3.6(10)	-0.6(11)	7.4(11)
C60	64(2)	22.8(13)	19.6(12)	-1.4(10)	8.4(12)	5.9(13)
C61	57.2(18)	19.8(12)	21.4(12)	-1.7(10)	14.9(12)	-6.0(12)
C62	36.0(14)	21.5(12)	18.4(11)	-3.3(9)	6.6(10)	-4.9(10)
C63	31.9(13)	25.5(12)	18.6(11)	-3.8(9)	7.4(10)	-9.6(10)
C64	32.6(14)	32.4(13)	28.1(13)	-5.3(11)	11.3(11)	-15.0(11)
C65	27.3(14)	46.7(16)	26.4(13)	-9.7(12)	10.0(11)	-17.8(12)
C66	20.1(12)	47.4(16)	23.9(12)	-1.3(11)	3.9(10)	-5.5(11)
C67	18.4(12)	36.0(14)	18.7(11)	2.8(10)	1.0(9)	-4.8(10)
C68	20.9(12)	27.0(12)	15.6(11)	-1.5(9)	3.1(9)	-5.6(9)
C69	91(3)	27.4(15)	34.9(16)	10.1(12)	22.1(17)	16.3(15)
C73	27.9(15)	58.0(19)	44.5(17)	-10.1(14)	11.3(13)	-20.4(13)
C74	46.0(19)	81(3)	51(2)	3.2(18)	9.2(16)	-37.7(18)
C75	34.0(17)	84(3)	54(2)	1.3(18)	-2.5(15)	-26.6(17)

C76	30.2(17)	90(3)	84(3)	-27(2)	24.6(18)	-21.3(18)
C77	25.0(13)	17.8(11)	33.1(14)	-3.7(10)	-1.0(10)	4.2(9)
C78	26.1(17)	44(2)	131(4)	-14(2)	15(2)	4.7(14)
C79	36(3)	111(6)	107(5)	8(4)	6(3)	37(3)
C80	51(3)	54(4)	143(6)	7(3)	63(4)	11(3)
C79A	40(9)	67(14)	67(12)	-8(9)	17(8)	5(8)
C80A	37(10)	91(18)	87(14)	-25(12)	20(9)	11(10)
C81	18.9(12)	47.2(16)	31.8(14)	18.3(12)	6.7(10)	3.0(11)
C82	31(2)	50(3)	65(3)	36(2)	15(2)	10.1(18)
C83	56(6)	78(6)	271(14)	93(7)	67(7)	30(5)
C84	48(3)	81(4)	78(4)	52(3)	-19(2)	-4(2)
C82A	46(11)	67(12)	160(20)	92(15)	60(13)	44(9)
C83A	14(7)	52(11)	12(6)	6(6)	7(5)	27(7)
C84A	160(30)	53(12)	260(40)	75(18)	170(30)	67(15)
C1S	133(5)	66(3)	206(6)	-1(4)	111(5)	13(3)
C2S	119(4)	49(3)	201(6)	-13(3)	117(4)	24(3)
C3S	122(4)	42(3)	199(6)	-15(3)	109(4)	17(3)
C4S	155(5)	71(4)	208(6)	-7(4)	93(5)	23(4)
C5S	155(5)	83(4)	221(6)	-9(4)	85(5)	9(4)
C6S	139(5)	69(4)	215(6)	0(4)	95(5)	-9(4)
C7S	172(8)	119(7)	221(9)	-21(7)	117(7)	22(6)

Table S21 Bond Lengths for **$Y(CzT^{iPr})_3$ 7 • 0.87 C_7H_8**.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Y1	N10	2.3775(18)	C17	C20	1.537(4)
Y1	N1	2.4647(19)	C22	C24	1.510(4)
Y1	N19	2.4658(19)	C22	C23	1.513(4)
Y1	N11	2.4784(19)	C26	C27	1.509(4)
Y1	N20	2.4831(19)	C26	C28	1.511(4)
Y1	N15	2.4878(19)	C29	C30	1.403(3)
Y1	N2	2.5334(19)	C29	C34	1.420(3)
Y1	N6	2.5436(19)	C30	C31	1.398(3)
N1	C12	1.386(3)	C30	C49	1.452(3)
N1	C1	1.394(3)	C31	C32	1.396(3)

N2	N3	1.332(3)	C32	C33	1.394(3)
N2	C21	1.353(3)	C32	C41	1.530(3)
N3	N4	1.309(3)	C33	C34	1.385(3)
N4	N5	1.331(3)	C34	C35	1.445(3)
N4	C22	1.479(3)	C35	C36	1.383(3)
N5	C21	1.339(3)	C35	C40	1.424(3)
N6	N7	1.324(3)	C36	C37	1.395(3)
N6	C25	1.354(3)	C37	C38	1.395(3)
N7	N8	1.312(3)	C37	C45	1.534(3)
N8	N9	1.334(3)	C38	C39	1.394(3)
N8	C26	1.485(3)	C39	C40	1.411(3)
N9	C25	1.333(3)	C39	C53	1.458(3)
N10	C40	1.385(3)	C41	C43A	1.372(12)
N10	C29	1.388(3)	C41	C43	1.467(8)
N11	N12	1.331(3)	C41	C42	1.493(5)
N11	C49	1.357(3)	C41	C42A	1.514(19)
N12	N13	1.307(3)	C41	C44	1.619(5)
N13	N14	1.331(3)	C41	C44A	1.822(10)
N13	C50	1.476(3)	C45	C47	1.513(4)
N14	C49	1.338(3)	C45	C48	1.520(4)
N15	N16	1.325(3)	C45	C46	1.539(5)
N15	C53	1.354(3)	C50	C52	1.513(4)
N16	N17	1.312(3)	C50	C51	1.518(4)
N17	N18	1.337(3)	C54	C56	1.489(5)
N17	C54	1.492(3)	C54	C55	1.501(5)
N18	C53	1.334(3)	C57	C58	1.414(3)
N19	C68	1.388(3)	C57	C62	1.420(3)
N19	C57	1.396(3)	C58	C59	1.402(3)
N20	N21	1.329(3)	C58	C77	1.475(4)
N20	C81	1.360(3)	C59	C60	1.400(4)
N21	N22A	1.231(11)	C60	C61	1.379(4)
N21	N22	1.355(4)	C60	C69	1.539(4)
N22	N23	1.325(5)	C61	C62	1.401(3)
N22	C82	1.486(5)	C62	C63	1.421(4)
N23	C81	1.331(5)	C63	C64	1.388(3)
N22A	N23A	1.348(19)	C63	C68	1.426(3)

N22A	C82A	1.490(17)	C64	C65	1.375(4)
N23A	C81	1.470(14)	C65	C66	1.398(4)
N24	N25	1.317(3)	C65	C73	1.536(4)
N24	C77	1.352(3)	C66	C67	1.401(3)
N25	N26	1.318(4)	C67	C68	1.412(3)
N26	N27	1.331(4)	C67	C81	1.450(4)
N26	C78	1.485(4)	C69	C72	1.365(8)
N27	C77	1.336(3)	C69	C70A	1.416(8)
C1	C2	1.407(3)	C69	C71A	1.477(8)
C1	C6	1.418(3)	C69	C70	1.581(7)
C2	C3	1.387(3)	C69	C71	1.661(7)
C2	C21	1.450(3)	C69	C72A	1.691(7)
C3	C4	1.401(4)	C73	C75	1.513(4)
C4	C5	1.388(4)	C73	C76	1.520(5)
C4	C13	1.536(4)	C73	C74	1.540(5)
C5	C6	1.395(3)	C78	C79A	1.217(18)
C6	C7	1.437(3)	C78	C80	1.425(7)
C7	C8	1.392(3)	C78	C79	1.556(7)
C7	C12	1.419(3)	C78	C80A	1.73(2)
C8	C9	1.391(4)	C82	C83	1.467(13)
C9	C10	1.402(3)	C82	C84	1.507(7)
C9	C17	1.535(3)	C82A	C83A	1.35(3)
C10	C11	1.394(3)	C82A	C84A	1.59(4)
C11	C12	1.405(3)	C1S	C6S	1.267(15)
C11	C25	1.457(3)	C1S	C7S	1.367(15)
C13	C16	1.529(4)	C1S	C2S	1.394(12)
C13	C14	1.533(5)	C2S	C3S	1.340(13)
C13	C15	1.536(5)	C3S	C4S	1.359(14)
C17	C19	1.523(4)	C4S	C5S	1.259(13)
C17	C18	1.527(4)	C5S	C6S	1.488(16)

Table S22 Bond Angles for **$Y(CzT^{iPr})_3$ 7 • 0.87 C_7H_8**.

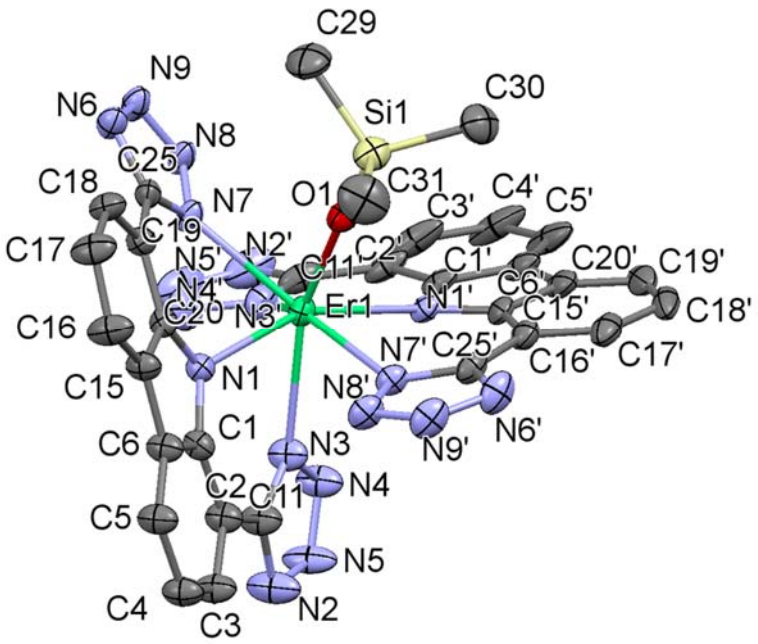
Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N10	Y1	N1	80.98(6)	N6	C25	C11	124.9(2)
N10	Y1	N19	111.71(6)	N8	C26	C27	108.93(19)
N1	Y1	N19	149.67(6)	N8	C26	C28	110.2(2)
N10	Y1	N11	74.00(6)	C27	C26	C28	113.5(2)
N1	Y1	N11	80.06(6)	N10	C29	C30	129.5(2)
N19	Y1	N11	77.56(6)	N10	C29	C34	112.47(19)
N10	Y1	N20	147.31(6)	C30	C29	C34	117.9(2)
N1	Y1	N20	106.07(7)	C31	C30	C29	118.9(2)
N19	Y1	N20	78.50(6)	C31	C30	C49	118.8(2)
N11	Y1	N20	138.26(6)	C29	C30	C49	122.2(2)
N10	Y1	N15	73.70(6)	C32	C31	C30	123.2(2)
N1	Y1	N15	136.53(6)	C33	C32	C31	117.6(2)
N19	Y1	N15	73.62(6)	C33	C32	C41	120.8(2)
N11	Y1	N15	123.93(6)	C31	C32	C41	121.5(2)
N20	Y1	N15	80.26(7)	C34	C33	C32	120.5(2)
N10	Y1	N2	78.61(6)	C33	C34	C29	121.8(2)
N1	Y1	N2	71.71(6)	C33	C34	C35	132.8(2)
N19	Y1	N2	136.41(6)	C29	C34	C35	105.2(2)
N11	Y1	N2	143.20(6)	C36	C35	C40	121.9(2)
N20	Y1	N2	73.80(6)	C36	C35	C34	132.7(2)
N15	Y1	N2	69.07(6)	C40	C35	C34	105.20(19)
N10	Y1	N6	137.82(6)	C35	C36	C37	120.3(2)
N1	Y1	N6	70.43(6)	C38	C37	C36	117.9(2)
N19	Y1	N6	83.04(6)	C38	C37	C45	122.1(2)
N11	Y1	N6	71.07(6)	C36	C37	C45	119.9(2)
N20	Y1	N6	72.50(6)	C39	C38	C37	123.4(2)
N15	Y1	N6	147.11(6)	C38	C39	C40	118.7(2)
N2	Y1	N6	118.49(6)	C38	C39	C53	119.4(2)
C12	N1	C1	103.47(18)	C40	C39	C53	121.8(2)
C12	N1	Y1	122.17(14)	N10	C40	C39	129.5(2)
C1	N1	Y1	123.53(14)	N10	C40	C35	112.4(2)
N3	N2	C21	106.76(18)	C39	C40	C35	117.9(2)
N3	N2	Y1	122.42(14)	C43	C41	C42	113.0(4)
C21	N2	Y1	129.82(15)	C43A	C41	C42A	119.0(10)

N4	N3	N2	105.36(19)	C43A	C41	C32	117.9(5)
N3	N4	N5	114.90(19)	C43	C41	C32	110.6(3)
N3	N4	C22	122.4(2)	C42	C41	C32	114.1(2)
N5	N4	C22	122.67(19)	C42A	C41	C32	115.3(8)
N4	N5	C21	101.60(19)	C43	C41	C44	108.2(4)
N7	N6	C25	106.79(18)	C42	C41	C44	105.3(3)
N7	N6	Y1	123.72(14)	C32	C41	C44	105.1(3)
C25	N6	Y1	127.07(14)	C43A	C41	C44A	101.2(7)
N8	N7	N6	105.68(18)	C42A	C41	C44A	94.5(10)
N7	N8	N9	114.29(18)	C32	C41	C44A	102.3(4)
N7	N8	C26	122.28(19)	C47	C45	C48	109.9(3)
N9	N8	C26	123.21(18)	C47	C45	C37	112.3(2)
C25	N9	N8	101.81(18)	C48	C45	C37	108.7(2)
C40	N10	C29	104.43(18)	C47	C45	C46	107.0(3)
C40	N10	Y1	125.26(14)	C48	C45	C46	108.9(3)
C29	N10	Y1	123.19(14)	C37	C45	C46	109.9(2)
N12	N11	C49	107.01(18)	N14	C49	N11	111.10(19)
N12	N11	Y1	123.26(14)	N14	C49	C30	124.2(2)
C49	N11	Y1	128.57(14)	N11	C49	C30	124.7(2)
N13	N12	N11	105.07(17)	N13	C50	C52	108.92(19)
N12	N13	N14	115.26(18)	N13	C50	C51	110.0(2)
N12	N13	C50	122.47(19)	C52	C50	C51	112.7(2)
N14	N13	C50	122.14(19)	N18	C53	N15	111.1(2)
N13	N14	C49	101.55(18)	N18	C53	C39	124.4(2)
N16	N15	C53	107.25(19)	N15	C53	C39	124.5(2)
N16	N15	Y1	121.34(14)	C56	C54	N17	108.9(3)
C53	N15	Y1	130.85(15)	C56	C54	C55	118.4(4)
N17	N16	N15	105.30(19)	N17	C54	C55	110.3(3)
N16	N17	N18	114.51(19)	N19	C57	C58	131.5(2)
N16	N17	C54	120.8(2)	N19	C57	C62	111.8(2)
N18	N17	C54	124.6(2)	C58	C57	C62	116.6(2)
C53	N18	N17	101.81(19)	C59	C58	C57	118.7(2)
C68	N19	C57	104.23(18)	C59	C58	C77	113.7(2)
C68	N19	Y1	124.68(15)	C57	C58	C77	126.7(2)
C57	N19	Y1	128.56(15)	C60	C59	C58	124.0(3)
N21	N20	C81	106.4(2)	C61	C60	C59	117.1(2)

N21	N20	Y1	123.78(16)	C61	C60	C69	121.5(3)
C81	N20	Y1	129.76(16)	C59	C60	C69	121.0(3)
N22A	N21	N20	110.5(5)	C60	C61	C62	120.4(2)
N20	N21	N22	104.0(2)	C61	C62	C57	122.7(2)
N23	N22	N21	115.3(3)	C61	C62	C63	131.3(2)
N23	N22	C82	121.6(3)	C57	C62	C63	105.9(2)
N21	N22	C82	123.2(3)	C64	C63	C62	131.3(2)
N22	N23	C81	100.7(3)	C64	C63	C68	122.9(2)
N21	N22A	N23A	105.5(11)	C62	C63	C68	105.6(2)
N21	N22A	C82A	127.3(10)	C65	C64	C63	120.6(2)
N23A	N22A	C82A	123.4(11)	C64	C65	C66	117.2(2)
N22A	N23A	C81	107.9(10)	C64	C65	C73	123.7(3)
N25	N24	C77	106.4(2)	C66	C65	C73	119.1(3)
N24	N25	N26	106.0(2)	C65	C66	C67	124.0(3)
N25	N26	N27	114.2(2)	C66	C67	C68	118.7(2)
N25	N26	C78	122.8(3)	C66	C67	C81	116.0(2)
N27	N26	C78	122.9(3)	C68	C67	C81	125.4(2)
N26	N27	C77	101.3(2)	N19	C68	C67	131.4(2)
N1	C1	C2	129.0(2)	N19	C68	C63	112.1(2)
N1	C1	C6	112.9(2)	C67	C68	C63	116.5(2)
C2	C1	C6	118.1(2)	C70A	C69	C71A	119.1(5)
C3	C2	C1	118.9(2)	C72	C69	C60	116.1(4)
C3	C2	C21	118.9(2)	C70A	C69	C60	111.6(4)
C1	C2	C21	122.2(2)	C71A	C69	C60	108.1(4)
C2	C3	C4	123.4(2)	C72	C69	C70	112.8(5)
C5	C4	C3	117.6(2)	C60	C69	C70	107.6(3)
C5	C4	C13	123.9(2)	C72	C69	C71	108.3(4)
C3	C4	C13	118.6(2)	C60	C69	C71	109.9(3)
C4	C5	C6	120.6(2)	C70	C69	C71	101.2(4)
C5	C6	C1	121.4(2)	C70A	C69	C72A	107.9(4)
C5	C6	C7	133.3(2)	C71A	C69	C72A	101.3(4)
C1	C6	C7	105.3(2)	C60	C69	C72A	107.9(3)
C8	C7	C12	121.3(2)	C75	C73	C76	112.2(3)
C8	C7	C6	133.4(2)	C75	C73	C65	109.1(2)
C12	C7	C6	105.2(2)	C76	C73	C65	109.1(2)
C9	C8	C7	120.6(2)	C75	C73	C74	107.8(3)

C8	C9	C10	117.5(2)	C76	C73	C74	106.8(3)
C8	C9	C17	123.2(2)	C65	C73	C74	111.8(3)
C10	C9	C17	119.2(2)	N27	C77	N24	112.0(2)
C11	C10	C9	123.3(2)	N27	C77	C58	123.6(2)
C10	C11	C12	118.7(2)	N24	C77	C58	123.2(2)
C10	C11	C25	120.0(2)	C79A	C78	N26	121.2(9)
C12	C11	C25	121.2(2)	C80	C78	N26	112.7(4)
N1	C12	C11	128.7(2)	C80	C78	C79	113.4(4)
N1	C12	C7	113.1(2)	N26	C78	C79	106.3(4)
C11	C12	C7	118.2(2)	C79A	C78	C80A	118.1(11)
C16	C13	C14	107.9(3)	N26	C78	C80A	106.5(7)
C16	C13	C4	111.6(2)	N23	C81	N20	113.2(3)
C14	C13	C4	109.4(2)	N23	C81	C67	120.0(3)
C16	C13	C15	109.2(3)	N20	C81	C67	126.8(2)
C14	C13	C15	109.8(3)	N20	C81	N23A	98.9(6)
C4	C13	C15	108.9(3)	C67	C81	N23A	127.3(5)
C19	C17	C18	109.2(3)	C83	C82	N22	109.9(6)
C19	C17	C9	108.8(2)	C83	C82	C84	116.1(6)
C18	C17	C9	112.1(2)	N22	C82	C84	108.3(4)
C19	C17	C20	109.8(3)	C83A	C82A	N22A	114.2(17)
C18	C17	C20	107.0(3)	C83A	C82A	C84A	95.8(17)
C9	C17	C20	109.9(2)	N22A	C82A	C84A	104.8(16)
N5	C21	N2	111.4(2)	C6S	C1S	C7S	123.5(11)
N5	C21	C2	123.6(2)	C6S	C1S	C2S	124.6(13)
N2	C21	C2	125.1(2)	C7S	C1S	C2S	111.9(13)
N4	C22	C24	109.3(2)	C3S	C2S	C1S	112.6(11)
N4	C22	C23	107.9(2)	C2S	C3S	C4S	127.3(10)
C24	C22	C23	113.8(3)	C5S	C4S	C3S	117.7(13)
N9	C25	N6	111.4(2)	C4S	C5S	C6S	119.9(14)
N9	C25	C11	123.7(2)	C1S	C6S	C5S	117.8(10)

Figure S6 Labeled ORTEP drawing of **Er(CzT^{iPr})$_2$(OSiMe$_3$) 3a • 2.5 C$_7$H$_8$**



Toluenes of solvation, t-butyl and isopropyl groups not shown.

Table S23 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **Er(CzT^{iPr})$_2$(OSiMe$_3$) 3a • 2.5 C$_7$H$_8$**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ}tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	4362(2)	2337(2)	6955.4(18)	25.5(7)
C1'	1105(3)	5486(2)	7315.6(17)	28.4(7)
C2	4919(3)	2690(2)	7469.0(19)	29.5(7)
C2'	1446(3)	6105(2)	6757.7(19)	37.3(9)
C3	5650(3)	2179(2)	7862(2)	33.8(8)
C3'	1021(4)	6936(2)	6701(2)	55.3(13)
C4	5848(3)	1319(2)	7781(2)	34.5(8)
C4'	251(5)	7192(3)	7164(2)	64.2(16)
C5	5291(3)	973(2)	7267(2)	32.6(8)
C5'	-104(4)	6583(3)	7702(2)	54.4(13)
C6	4570(3)	1468(2)	6860.4(19)	29.1(7)
C6'	304(3)	5746(2)	7780.9(19)	37.6(9)
C7	6629(3)	756(2)	8226(2)	41.3(9)
C7'	84(6)	8200(4)	6987(4)	32.9(14)
C8	7117(4)	1233(3)	8792(3)	57.0(13)
C8'	942(6)	8740(4)	7204(4)	39.4(19)
C9	7489(4)	465(3)	7726(3)	57.2(13)
C9'	-238(13)	8447(7)	6200(6)	87(6)
C10	6105(4)	-25(3)	8626(3)	62.4(14)
C10'	-885(7)	8359(5)	7473(5)	57(3)
C11	4736(3)	3576(2)	7607(2)	34.5(8)
C11'	2240(3)	5927(2)	6233.6(19)	35.8(9)
C12	5115(11)	5418(10)	8479(7)	29(3)
C12'	4092(9)	6289(6)	4730(6)	45(3)
C13	5073(6)	5144(4)	9275(4)	32.0(15)
C13'	3799(12)	5912(8)	4111(6)	92(5)
C14	6206(6)	5664(5)	8186(4)	35.2(16)
C14'	4166(11)	7243(6)	4662(8)	90(5)
C15	3909(3)	1292(2)	6299.1(19)	29.6(7)
C15'	776(3)	4352(2)	8080.3(16)	25.8(7)
C16	3734(3)	564(2)	5982(2)	39.2(9)
C16'	740(3)	3551(2)	8509.3(17)	29.3(7)

C17	3058(3)	596(2)	5420(2)	40.0(9)
C17'	21(3)	3441(3)	9077.5(19)	37.9(9)
C18	2604(3)	1388(2)	5171.8(19)	31.2(7)
C18'	-666(3)	4082(3)	9259(2)	43.7(10)
C19	2755(3)	2133(2)	5481.9(17)	26.0(7)
C19'	-617(3)	4870(3)	8848(2)	42.3(10)
C20	3390(2)	2071(2)	6086.9(17)	24.1(6)
C20'	84(3)	5007(2)	8275.5(18)	33.5(8)
C21	2718(8)	-200(7)	5128(5)	45(2)
C21'	-1440(3)	3889(4)	9888(3)	65.2(16)
C22	3158(13)	-1009(8)	5553(8)	100(6)
C22'	-902(4)	3388(4)	10534(2)	77.6(19)
C23	3093(7)	-120(5)	4349(4)	55(2)
C23'	-1923(4)	4710(4)	10120(3)	85(2)
C24	1537(6)	-256(5)	5158(4)	62(2)
C24'	-2288(4)	3340(5)	9644(3)	89(2)
C25	2311(2)	2943(2)	5154.1(16)	25.3(7)
C25'	1435(3)	2827(2)	8415.5(17)	28.5(7)
C26	1149(3)	4330(2)	3786.2(18)	36.4(9)
C26'	2474(4)	757(2)	8887(2)	51.1(11)
C27	509(3)	5104(2)	3960.2(19)	35.9(8)
C27'	3337(6)	824(3)	9388(3)	101(3)
C28	1983(4)	4545(4)	3221(2)	64.4(15)
C28'	2741(5)	223(3)	8309(3)	61.6(14)
C29	-366(4)	2449(3)	5668(2)	51.9(11)
C30	-1083(3)	2765(3)	7175(2)	45.8(10)
C31	453(4)	1332(3)	6964(3)	60.8(13)
C200	-416(6)	8030(4)	7191(4)	32.9(14)
C201	-46(9)	8580(7)	6504(7)	67(3)
C202	-1592(7)	7959(7)	7142(6)	61(3)
C203	-189(8)	8399(6)	7871(5)	62(3)
C204	2997(17)	-192(15)	4967(11)	45(2)
C205	2141(12)	-76(8)	4420(8)	61(4)
C206	3979(10)	-401(8)	4565(7)	54(4)
C207	2785(16)	-977(14)	5530(9)	53(5)
C208	5355(12)	5473(10)	8256(7)	32(3)

C209	4479(8)	5745(6)	8733(5)	52(2)
C210	6298(7)	5204(6)	8638(6)	50(2)
C211	3856(7)	6633(6)	4858(5)	35.2(19)
C212	3185(6)	6971(6)	4236(4)	39.9(18)
C213	4704(9)	6070(7)	4659(7)	71(4)
Er1	2326.2(2)	3719.9(2)	6760.4(2)	22.37(5)
N1	3620(2)	2713.2(17)	6498.6(14)	23.8(5)
N1'	1396(2)	4635.0(16)	7489.4(13)	23.7(5)
N2	5355(3)	3986(2)	7999(2)	46.7(9)
N2'	2614(3)	6523(2)	5727(2)	52.7(10)
N3	3919(2)	4071.5(17)	7378.3(16)	30.9(6)
N3'	2717(2)	5161.5(19)	6199.2(16)	32.9(7)
N4	4012(2)	4819.7(18)	7631.6(19)	38.1(7)
N4'	3419(3)	5272(2)	5674.0(19)	48.5(9)
N5	4863(3)	4742.3(19)	7991(2)	45.3(9)
N5'	3325(3)	6079(3)	5413(2)	59.9(12)
N6	1909(2)	3063.5(19)	4499.9(15)	30.9(6)
N6'	1397(3)	2079(2)	8842.0(16)	39.7(8)
N7	2274(2)	3673.9(17)	5458.0(14)	26.8(6)
N7'	2200(2)	2812.8(17)	7913.4(14)	26.2(6)
N8	1820(2)	4269.8(19)	4999.9(14)	30.3(6)
N8'	2653(2)	2040.8(18)	8019.3(15)	31.9(6)
N9	1613(2)	3886.1(19)	4441.4(15)	31.9(7)
N9'	2156(3)	1631.8(18)	8565.8(16)	37.0(7)
O1	976.5(18)	3090.0(14)	6643.3(12)	28.0(5)
Si1	45.3(8)	2449.2(6)	6614.0(6)	33.0(2)
C122	5413(5)	1954(4)	10671(4)	55(2)
C123	4405(4)	2372(3)	10445(2)	37(2)
C124	4296(5)	2826(4)	9759(2)	42(2)
C125	3368(6)	3229(4)	9553(3)	45(3)
C126	2529(5)	3184(4)	10032(4)	50(2)
C127	2623(4)	2732(4)	10715(3)	46(2)
C128	3554(5)	2330(3)	10917(2)	39.4(19)
C129	5920(20)	7480(30)	6433(17)	64(4)
C130	5022(15)	7649(14)	6914(10)	52(4)
C131	4252(19)	7061(11)	7059(12)	60.1(17)

C132	3427(17)	7230(13)	7507(13)	58(5)
C133	3373(15)	7986(14)	7810(11)	63(6)
C134	4143(18)	8574(12)	7665(13)	55(5)
C142	4968(16)	8405(13)	7217(13)	55.3(16)
C100	3050(6)	7600(6)	7796(5)	141(5)
C101	4015(5)	7651(4)	7338(3)	63.8(17)
C102	4625(5)	8370(4)	7282(3)	55.3(16)
C103	5533(5)	8411(4)	6872(3)	52.2(19)
C104	5847(5)	7730(4)	6505(4)	58(2)
C105	5245(6)	7011(4)	6554(5)	61.6(16)
C106	4339(5)	6973(4)	6966(4)	60.1(17)
C107	2257(8)	2475(7)	11021(6)	62(3)
C108	3174(7)	2646(5)	10529(5)	36.5(19)
C109	3083(9)	3076(7)	9830(5)	34(2)
C110	3907(7)	3203(6)	9379(5)	37(2)
C111	4859(7)	2916(5)	9589(4)	36.5(18)
C112	4993(7)	2493(5)	10277(5)	37.7(18)
C113	4142(9)	2376(6)	10732(5)	35(2)
C115	5420(20)	6369(15)	6175(14)	48(4)
C116	5150(20)	7120(20)	6570(20)	61.6(16)
C121	4200(20)	7170(20)	6920(20)	60.1(17)
C120	3990(20)	7810(20)	7350(20)	63.8(17)
C119	4730(30)	8400(20)	7433(18)	55.3(16)
C118	5680(30)	8347(19)	7087(16)	48(4)
C117	5890(20)	7710(20)	6660(20)	64(4)
C07	573(19)	-1223(11)	9711(10)	136(8)
C01	255(7)	-530(5)	10105(4)	62(3)
C02	-155(7)	185(6)	9694(3)	66(3)
C03	-478(6)	892(4)	10017(3)	62(3)
C04	-390(5)	884(4)	10752(3)	58(2)
C05	20(5)	169(4)	11164(2)	45.7(18)
C06	343(5)	-538(4)	10840(4)	59(2)

Table S24 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **Er(CzT^{iPr})$_2$(OSiMe$_3$) 3a • 2.5 C$_7$H$_8$**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	24.0(16)	19.9(15)	33.1(17)	-4.7(13)	-1.8(13)	-1.0(12)
C1'	43(2)	22.0(16)	21.9(15)	-9.9(12)	-12.2(14)	5.4(14)
C2	31.6(18)	18.9(16)	39.1(19)	-6.2(14)	-7.3(15)	-1.2(13)
C2'	69(3)	19.3(16)	25.5(17)	-5.8(13)	-18.0(17)	2.7(16)
C3	37(2)	21.0(16)	45(2)	-8.2(15)	-16.7(16)	-0.1(14)
C3'	111(4)	21.6(19)	36(2)	-7.7(16)	-34(2)	13(2)
C4	35(2)	24.9(17)	44(2)	-6.4(15)	-13.2(16)	2.5(15)
C4'	123(5)	33(2)	41(2)	-21.9(19)	-46(3)	41(3)
C5	34.5(19)	19.7(16)	45(2)	-9.6(14)	-12.9(16)	3.8(14)
C5'	79(3)	52(3)	39(2)	-33(2)	-31(2)	40(2)
C6	29.6(18)	19.9(16)	39.3(19)	-8.2(14)	-8.7(14)	0.6(13)
C6'	52(2)	39(2)	24.9(17)	-17.2(15)	-15.0(16)	18.8(17)
C7	43(2)	28.1(19)	55(2)	-8.9(17)	-26.3(19)	5.1(16)
C7'	51(5)	16(3)	32(3)	-4(2)	-7(3)	8(3)
C8	63(3)	38(2)	75(3)	-18(2)	-46(3)	17(2)
C8'	73(6)	13(3)	34(4)	-7(3)	-16(4)	8(3)
C9	48(3)	46(3)	81(3)	-18(2)	-29(2)	20(2)
C9'	182(15)	19(5)	65(7)	-17(4)	-94(9)	33(6)
C10	77(3)	41(2)	68(3)	9(2)	-41(3)	-8(2)
C10'	71(6)	19(4)	87(7)	-29(4)	-42(6)	25(4)
C11	37(2)	20.4(16)	48(2)	-8.1(15)	-12.5(16)	-1.7(14)
C11'	56(2)	21.1(17)	29.9(18)	4.1(14)	-16.1(17)	-10.6(16)
C12	28(6)	24(5)	41(8)	-23(6)	1(5)	-3(4)
C12'	51(7)	23(5)	56(6)	2(4)	33(5)	2(4)
C13	42(4)	24(3)	34(4)	-16(3)	-2(3)	-3(3)
C13'	144(13)	75(8)	53(6)	5(6)	34(8)	-46(8)
C14	46(5)	28(4)	34(4)	-8(3)	-1(3)	-14(3)
C14'	107(10)	36(6)	118(10)	9(6)	64(9)	-12(6)
C15	31.1(18)	24.2(17)	34.1(18)	-5.1(14)	-7.0(14)	2.7(14)
C15'	29.1(17)	31.6(17)	18.7(14)	-10.7(12)	-1.6(12)	0.0(13)
C16	52(2)	20.0(17)	47(2)	-8.3(15)	-21.9(19)	7.5(16)
C16'	34.5(19)	32.8(18)	22.1(15)	-8.6(13)	0.5(13)	-5.2(14)

C17	52(2)	25.3(18)	46(2)	-10.6(16)	-19.3(18)	-0.5(16)
C17'	40(2)	49(2)	27.5(17)	-13.3(16)	2.4(15)	-18.9(18)
C18	36.1(19)	29.0(18)	29.2(17)	-4.3(14)	-10.4(14)	1.0(15)
C18'	28.1(19)	76(3)	34(2)	-31(2)	6.8(15)	-17.0(19)
C19	27.7(17)	24.4(16)	25.9(16)	-3.5(13)	-1.3(13)	0.6(13)
C19'	31(2)	65(3)	38(2)	-34(2)	-3.8(16)	3.9(18)
C20	25.7(16)	20.2(15)	27.2(16)	-6.7(12)	0.6(13)	-0.7(12)
C20'	36(2)	44(2)	24.4(16)	-17.6(15)	-8.2(14)	10.0(16)
C21	76(6)	20.6(19)	42(5)	-10(3)	-27(4)	1(4)
C21'	39(2)	116(4)	53(3)	-53(3)	21(2)	-37(3)
C22	191(15)	18(4)	100(9)	-22(4)	-94(10)	9(7)
C22'	73(4)	132(5)	35(2)	-33(3)	26(2)	-60(4)
C23	76(6)	43(4)	53(4)	-28(3)	-19(4)	12(4)
C23'	40(3)	146(6)	85(4)	-81(4)	31(3)	-28(3)
C24	88(5)	43(4)	59(5)	-14(3)	-18(4)	-33(4)
C24'	50(3)	146(6)	89(4)	-74(4)	28(3)	-59(4)
C25	25.7(16)	29.3(17)	20.3(15)	-2.8(12)	2.3(12)	2.2(13)
C25'	37.0(19)	26.3(17)	21.7(15)	0.4(13)	-0.5(13)	-9.4(14)
C26	46(2)	40(2)	22.9(16)	-4.0(15)	-7.3(15)	14.9(17)
C26'	82(3)	19.3(18)	49(2)	10.2(17)	-3(2)	-4.7(19)
C27	49(2)	29.2(19)	29.4(18)	-1.5(14)	-10.2(16)	7.5(16)
C27'	195(8)	35(3)	74(4)	1(3)	-77(5)	23(4)
C28	62(3)	99(4)	24(2)	10(2)	4.6(19)	29(3)
C28'	100(4)	26(2)	58(3)	1.8(19)	-22(3)	4(2)
C29	52(3)	58(3)	50(3)	-19(2)	-12(2)	-16(2)
C30	40(2)	47(2)	48(2)	1.6(19)	3.5(18)	-12.7(19)
C31	69(3)	30(2)	80(4)	6(2)	-2(3)	-11(2)
C200	51(5)	16(3)	32(3)	-4(2)	-7(3)	8(3)
C201	67(8)	32(6)	98(11)	-4(7)	-4(7)	19(5)
C202	70(7)	52(6)	66(6)	-25(5)	-12(5)	26(5)
C203	75(7)	39(5)	77(7)	-28(5)	-5(6)	13(5)
C204	76(6)	20.6(19)	42(5)	-10(3)	-27(4)	1(4)
C205	74(11)	50(7)	67(9)	-32(7)	-34(7)	0(7)
C206	60(8)	52(8)	55(8)	-32(6)	2(6)	1(6)
C207	78(12)	53(10)	29(7)	-7(6)	8(8)	-41(9)
C208	40(9)	24(4)	34(7)	-12(5)	-1(5)	-2(5)

C209	63(6)	43(5)	55(5)	-20(4)	-1(5)	-6(4)
C210	48(5)	43(5)	66(6)	-30(5)	-12(4)	-4(4)
C211	33(5)	31(5)	39(5)	1(4)	15(3)	0(4)
C212	33(4)	52(5)	31(4)	12(3)	4(3)	-9(3)
C213	63(7)	58(7)	78(8)	30(6)	40(6)	3(6)
Er1	27.49(8)	18.45(7)	20.83(7)	-1.93(5)	1.74(5)	0.29(5)
N1	23.8(14)	22.7(13)	24.8(13)	-3.0(10)	-0.4(11)	-0.7(11)
N1'	32.4(15)	19.8(13)	19.6(12)	-5.1(10)	-3.7(11)	1.4(11)
N2	48(2)	21.9(15)	74(2)	-14.5(16)	-29.7(18)	5.7(14)
N2'	79(3)	34.4(19)	43(2)	9.7(16)	-16(2)	-24.7(19)
N3	36.8(17)	15.5(13)	41.5(17)	-5.7(12)	-9.1(13)	-0.4(11)
N3'	39.2(17)	28.1(15)	30.4(15)	1.4(12)	1.6(13)	-9.6(13)
N4	41.2(18)	18.9(14)	56(2)	-9.1(13)	-17.8(15)	0.7(13)
N4'	48(2)	51(2)	42.7(19)	11.0(16)	10.3(16)	-16.6(17)
N5	48(2)	21.3(15)	71(2)	-14.2(15)	-33.9(18)	3.7(14)
N5'	72(3)	59(3)	45(2)	20.6(19)	-7(2)	-38(2)
N6	36.2(16)	30.6(15)	25.1(14)	-2.2(12)	-1.7(12)	9.7(13)
N6'	59(2)	28.3(16)	30.4(16)	1.6(13)	6.3(15)	-10.2(15)
N7	35.2(16)	24.3(14)	20.1(13)	-2.1(10)	0.1(11)	5.8(12)
N7'	33.7(15)	19.6(13)	24.3(13)	1.8(10)	-2.3(11)	-0.6(11)
N8	39.5(17)	32.9(16)	17.3(13)	-0.9(11)	-0.1(11)	9.7(13)
N8'	43.8(18)	22.1(14)	28.1(15)	3.3(11)	-2.5(13)	-1.2(12)
N9	41.3(17)	30.8(16)	22.7(14)	-3.5(11)	0.4(12)	11.3(13)
N9'	58(2)	19.6(14)	31.5(16)	4.8(12)	-0.9(14)	-5.0(14)
O1	34.5(13)	23.6(12)	26.6(12)	-4.6(9)	-1.4(10)	-4.3(10)
Si1	38.9(6)	25.1(5)	35.1(5)	-1.8(4)	-3.5(4)	-10.5(4)
C122	58(6)	50(5)	56(6)	-3(4)	-8(5)	-7(5)
C123	39(6)	35(5)	40(6)	-11(4)	3(5)	-10(4)
C124	52(6)	36(5)	39(5)	0(4)	1(5)	-20(4)
C125	65(10)	32(5)	36(8)	1(5)	-8(6)	-10(6)
C126	61(7)	42(5)	50(6)	-12(4)	-11(5)	-9(5)
C127	52(7)	43(6)	44(6)	-11(4)	6(5)	-6(5)
C128	52(6)	34(5)	32(5)	-4(4)	5(4)	-5(4)
C129	84(8)	63(8)	46(10)	-12(7)	-2(7)	2(6)
C130	72(8)	45(7)	39(8)	-2(6)	-12(7)	2(6)
C131	89(4)	48(4)	44(3)	0(3)	-23(3)	-14(3)

C132	72(10)	55(10)	50(11)	-7(9)	-25(7)	-19(8)
C133	70(11)	62(10)	60(12)	-13(9)	0(10)	-18(9)
C134	68(10)	50(10)	53(11)	-22(9)	1(8)	-11(8)
C142	60(4)	58(3)	51(4)	-17(3)	-1(3)	-12(3)
C100	107(8)	202(14)	133(10)	-81(10)	50(7)	-92(8)
C101	75(4)	75(4)	46(3)	-16(3)	-2(3)	-28(3)
C102	60(4)	58(3)	51(4)	-17(3)	-1(3)	-12(3)
C103	60(4)	42(3)	53(5)	-2(3)	4(3)	-5(3)
C104	77(5)	57(4)	38(4)	-2(3)	6(4)	8(3)
C105	96(4)	45(3)	46(3)	-12(3)	-28(3)	13(3)
C106	89(4)	48(4)	44(3)	0(3)	-23(3)	-14(3)
C107	57(6)	62(7)	70(7)	-17(6)	30(5)	-12(5)
C108	46(5)	25(4)	40(5)	-12(3)	17(4)	-13(4)
C109	44(6)	29(5)	32(6)	-13(4)	-7(5)	-2(4)
C110	45(6)	35(5)	35(5)	-16(4)	-4(4)	5(5)
C111	45(5)	33(4)	33(4)	-12(3)	10(4)	-16(4)
C112	36(5)	31(4)	49(5)	-14(4)	-10(4)	-2(4)
C113	49(6)	22(4)	36(6)	-4(4)	3(5)	-8(4)
C115	69(7)	38(7)	34(8)	8(6)	-3(7)	1(6)
C116	96(4)	45(3)	46(3)	-12(3)	-28(3)	13(3)
C121	89(4)	48(4)	44(3)	0(3)	-23(3)	-14(3)
C120	75(4)	75(4)	46(3)	-16(3)	-2(3)	-28(3)
C119	60(4)	58(3)	51(4)	-17(3)	-1(3)	-12(3)
C118	69(7)	38(7)	34(8)	8(6)	-3(7)	1(6)
C117	84(8)	63(8)	46(10)	-12(7)	-2(7)	2(6)
C07	190(20)	109(15)	115(16)	-43(12)	66(15)	-50(14)
C01	45(6)	83(10)	64(6)	-35(5)	18(5)	-14(6)
C02	45(6)	101(10)	53(6)	-16(5)	10(5)	-31(6)
C03	49(7)	85(10)	50(6)	5(5)	-3(5)	-15(7)
C04	55(6)	71(6)	49(5)	-3(4)	-1(4)	-15(4)
C05	35(4)	65(5)	38(4)	-10(3)	-5(3)	-9(4)
C06	39(5)	77(6)	67(5)	-22(5)	-9(4)	-1(4)

Table S25 Bond Lengths for **Er(CzT^{iPr})$_2$(OSiMe$_3$) 3a • 2.5 C$_7$H$_8$**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	N1	1.387(4)	C200	C203	1.514(10)
C1	C2	1.408(5)	C200	C201	1.536(11)
C1	C6	1.427(4)	C200	C202	1.554(10)
C1'	N1'	1.389(4)	C204	C206	1.52(2)
C1'	C2'	1.413(5)	C204	C205	1.54(3)
C1'	C6'	1.430(5)	C204	C207	1.55(3)
C2	C3	1.401(5)	C208	C210	1.47(2)
C2	C11	1.470(5)	C208	N5	1.488(17)
C2'	C3'	1.404(5)	C208	C209	1.521(13)
C2'	C11'	1.457(6)	C211	N5'	1.449(9)
C3	C4	1.405(5)	C211	C213	1.471(13)
C3'	C4'	1.397(7)	C211	C212	1.518(12)
C4	C5	1.404(5)	Er1	O1	2.087(2)
C4	C7	1.532(5)	Er1	N1	2.374(3)
C4'	C5'	1.385(8)	Er1	N1'	2.401(3)
C4'	C200	1.572(7)	Er1	N7'	2.448(3)
C4'	C7'	1.598(7)	Er1	N3'	2.451(3)
C5	C6	1.391(5)	Er1	N7	2.465(3)
C5'	C6'	1.405(5)	Er1	N3	2.530(3)
C6	C15	1.446(5)	N2	N5	1.341(4)
C6'	C20'	1.430(6)	N2'	N5'	1.320(6)
C7	C10	1.533(6)	N3	N4	1.342(4)
C7	C9	1.541(7)	N3'	N4'	1.327(4)
C7	C8	1.546(5)	N4	N5	1.316(4)
C7'	C8'	1.528(9)	N4'	N5'	1.313(5)
C7'	C9'	1.551(9)	N6	N9	1.339(4)
C7'	C10'	1.574(10)	N6'	N9'	1.333(5)
C11	N2	1.346(5)	N7	N8	1.333(4)
C11	N3	1.354(5)	N7'	N8'	1.336(4)
C11'	N2'	1.344(5)	N8	N9	1.319(4)
C11'	N3'	1.354(5)	N8'	N9'	1.309(4)
C12	C13	1.505(15)	O1	Si1	1.616(2)
C12	N5	1.545(15)	C122	C123	1.5071

C12	C14	1.558(14)	C123	C128	1.4017
C12'	C13'	1.441(16)	C123	C124	1.4027
C12'	C14'	1.505(13)	C124	C125	1.3969
C12'	N5'	1.614(10)	C125	C126	1.3973
C15	C16	1.392(5)	C126	C127	1.3967
C15	C20	1.408(5)	C127	C128	1.3975
C15'	N1'	1.391(4)	C129	C130	1.504(18)
C15'	C16'	1.414(5)	C130	C131	1.3900
C15'	C20'	1.432(5)	C130	C142	1.3900
C16	C17	1.395(5)	C131	C132	1.3900
C16'	C17'	1.400(5)	C132	C133	1.3900
C16'	C25'	1.467(5)	C133	C134	1.3900
C17	C18	1.401(5)	C134	C142	1.3900
C17	C21	1.522(11)	C100	C101	1.5066
C17	C204	1.61(2)	C101	C106	1.4021
C17'	C18'	1.403(6)	C101	C102	1.4023
C18	C19	1.403(5)	C102	C103	1.3962
C18'	C19'	1.384(6)	C103	C104	1.3971
C18'	C21'	1.540(6)	C104	C105	1.3962
C19	C20	1.422(5)	C105	C106	1.3968
C19	C25	1.463(5)	C107	C108	1.503(12)
C19'	C20'	1.392(5)	C108	C113	1.376(14)
C20	N1	1.399(4)	C108	C109	1.408(13)
C21	C23	1.523(10)	C109	C110	1.355(13)
C21	C22	1.527(12)	C110	C111	1.366(13)
C21	C24	1.549(11)	C111	C112	1.393(12)
C21'	C23'	1.537(8)	C112	C113	1.386(13)
C21'	C22'	1.541(8)	C115	C116	1.514(14)
C21'	C24'	1.546(6)	C116	C121	1.3900
C25	N6	1.343(4)	C116	C117	1.3900
C25	N7	1.353(4)	C121	C120	1.3900
C25'	N6'	1.344(4)	C120	C119	1.3900
C25'	N7'	1.357(4)	C119	C118	1.3900
C26	N9	1.477(4)	C118	C117	1.3900
C26	C28	1.516(6)	C07	C01	1.445(13)
C26	C27	1.529(5)	C01	C02	1.3900

C26'	C28'	1.488(7)	C01	C06	1.3900
C26'	N9'	1.491(5)	C02	C03	1.3900
C26'	C27'	1.509(8)	C03	C04	1.3900
C29	Si1	1.875(4)	C04	C05	1.3900
C30	Si1	1.882(4)	C05	C06	1.3900
C31	Si1	1.875(5)			

Table S26 Bond Angles for **Er(CzT^{iPr})$_2$(OSiMe$_3$) 3a • 2.5 C$_7$H$_8$**

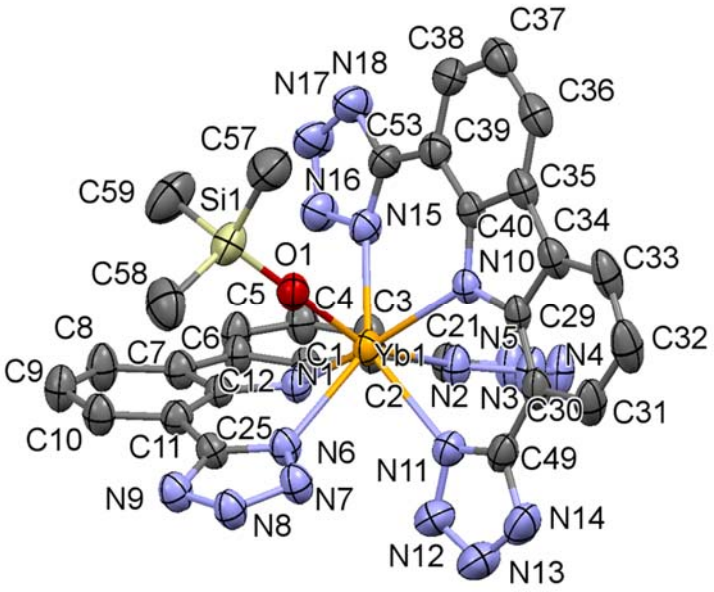
Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
N1	C1	C2	129.7(3)	N5	C208	C209	98.5(9)
N1	C1	C6	112.2(3)	N5'	C211	C213	101.5(7)
C2	C1	C6	118.1(3)	N5'	C211	C212	113.2(7)
N1'	C1'	C2'	130.9(3)	C213	C211	C212	113.6(9)
N1'	C1'	C6'	112.3(3)	O1	Er1	N1	103.28(9)
C2'	C1'	C6'	116.7(3)	O1	Er1	N1'	89.05(9)
C3	C2	C1	119.0(3)	N1	Er1	N1'	155.73(9)
C3	C2	C11	119.6(3)	O1	Er1	N7'	78.99(9)
C1	C2	C11	121.4(3)	N1	Er1	N7'	83.71(9)
C3'	C2'	C1'	119.6(4)	N1'	Er1	N7'	78.16(9)
C3'	C2'	C11'	117.6(4)	O1	Er1	N3'	125.38(10)
C1'	C2'	C11'	122.8(3)	N1	Er1	N3'	111.67(10)
C2	C3	C4	123.3(3)	N1'	Er1	N3'	75.86(10)
C4'	C3'	C2'	123.5(4)	N7'	Er1	N3'	143.46(10)
C5	C4	C3	117.3(3)	O1	Er1	N7	76.64(9)
C5	C4	C7	119.6(3)	N1	Er1	N7	74.27(9)
C3	C4	C7	123.1(3)	N1'	Er1	N7	129.50(9)
C5'	C4'	C3'	117.2(4)	N7'	Er1	N7	142.11(9)
C5'	C4'	C200	108.2(5)	N3'	Er1	N7	74.25(10)
C3'	C4'	C200	134.4(5)	O1	Er1	N3	156.29(9)
C5'	C4'	C7'	134.3(5)	N1	Er1	N3	72.99(9)
C3'	C4'	C7'	108.0(5)	N1'	Er1	N3	87.27(9)
C6	C5	C4	120.8(3)	N7'	Er1	N3	77.32(10)
C4'	C5'	C6'	121.2(4)	N3'	Er1	N3	76.21(10)
C5	C6	C1	121.5(3)	N7	Er1	N3	122.87(10)

C5	C6	C15	132.8(3)	C1	N1	C20	103.8(3)
C1	C6	C15	105.7(3)	C1	N1	Er1	127.1(2)
C5'	C6'	C20'	132.7(4)	C20	N1	Er1	119.6(2)
C5'	C6'	C1'	121.8(4)	C1'	N1'	C15'	104.4(3)
C20'	C6'	C1'	105.6(3)	C1'	N1'	Er1	128.4(2)
C4	C7	C10	109.9(3)	C15'	N1'	Er1	124.7(2)
C4	C7	C9	109.5(3)	N5	N2	C11	101.4(3)
C10	C7	C9	109.7(4)	N5'	N2'	C11'	101.4(3)
C4	C7	C8	112.0(3)	N4	N3	C11	106.7(3)
C10	C7	C8	107.5(4)	N4	N3	Er1	121.8(2)
C9	C7	C8	108.3(4)	C11	N3	Er1	130.9(2)
C8'	C7'	C9'	113.4(7)	N4'	N3'	C11'	107.0(3)
C8'	C7'	C10'	107.7(6)	N4'	N3'	Er1	119.9(2)
C9'	C7'	C10'	106.6(8)	C11'	N3'	Er1	132.2(2)
C8'	C7'	C4'	115.8(6)	N5	N4	N3	105.3(3)
C9'	C7'	C4'	110.9(6)	N5'	N4'	N3'	104.9(4)
C10'	C7'	C4'	101.3(6)	N4	N5	N2	114.9(3)
N2	C11	N3	111.7(3)	N4	N5	C208	123.2(7)
N2	C11	C2	123.5(3)	N2	N5	C208	121.0(7)
N3	C11	C2	124.8(3)	N4	N5	C12	119.8(7)
N2'	C11'	N3'	111.1(4)	N2	N5	C12	124.3(7)
N2'	C11'	C2'	123.4(4)	N4'	N5'	N2'	115.5(3)
N3'	C11'	C2'	125.5(3)	N4'	N5'	C211	134.7(6)
C13	C12	N5	117.0(10)	N2'	N5'	C211	109.7(5)
C13	C12	C14	113.1(11)	N4'	N5'	C12'	110.2(5)
N5	C12	C14	100.4(7)	N2'	N5'	C12'	134.2(5)
C13'	C12'	C14'	118.2(11)	N9	N6	C25	102.0(3)
C13'	C12'	N5'	113.3(8)	N9'	N6'	C25'	101.9(3)
C14'	C12'	N5'	103.1(8)	N8	N7	C25	107.3(3)
C16	C15	C20	121.8(3)	N8	N7	Er1	124.1(2)
C16	C15	C6	133.4(3)	C25	N7	Er1	123.7(2)
C20	C15	C6	104.8(3)	N8'	N7'	C25'	107.0(3)
N1'	C15'	C16'	130.8(3)	N8'	N7'	Er1	122.0(2)
N1'	C15'	C20'	112.2(3)	C25'	N7'	Er1	126.8(2)
C16'	C15'	C20'	116.9(3)	N9	N8	N7	105.3(3)
C15	C16	C17	120.3(3)	N9'	N8'	N7'	105.2(3)

C17'	C16'	C15'	118.6(3)	N8	N9	N6	114.3(3)
C17'	C16'	C25'	117.1(3)	N8	N9	C26	123.4(3)
C15'	C16'	C25'	124.3(3)	N6	N9	C26	122.2(3)
C16	C17	C18	117.8(3)	N8'	N9'	N6'	115.0(3)
C16	C17	C21	122.5(5)	N8'	N9'	C26'	122.0(3)
C18	C17	C21	119.4(5)	N6'	N9'	C26'	122.8(3)
C16	C17	C204	120.4(9)	Si1	O1	Er1	169.59(15)
C18	C17	C204	120.5(9)	O1	Si1	C31	110.44(19)
C16'	C17'	C18'	124.2(4)	O1	Si1	C29	110.71(17)
C17	C18	C19	123.4(3)	C31	Si1	C29	107.7(2)
C19'	C18'	C17'	117.2(3)	O1	Si1	C30	110.89(16)
C19'	C18'	C21'	122.8(4)	C31	Si1	C30	108.2(2)
C17'	C18'	C21'	120.0(4)	C29	Si1	C30	108.9(2)
C18	C19	C20	117.8(3)	C128	C123	C124	118.1
C18	C19	C25	119.6(3)	C128	C123	C122	121.0
C20	C19	C25	122.5(3)	C124	C123	C122	120.9
C18'	C19'	C20'	120.6(4)	C125	C124	C123	121.1
N1	C20	C15	113.3(3)	C124	C125	C126	120.1
N1	C20	C19	128.1(3)	C127	C126	C125	119.5
C15	C20	C19	118.5(3)	C126	C127	C128	120.0
C19'	C20'	C6'	132.0(4)	C127	C128	C123	121.2
C19'	C20'	C15'	122.5(4)	C131	C130	C142	120.0
C6'	C20'	C15'	105.5(3)	C131	C130	C129	121(2)
C17	C21	C23	106.2(7)	C142	C130	C129	119(2)
C17	C21	C22	111.6(9)	C130	C131	C132	120.0
C23	C21	C22	110.8(10)	C131	C132	C133	120.0
C17	C21	C24	111.2(7)	C134	C133	C132	120.0
C23	C21	C24	109.1(8)	C142	C134	C133	120.0
C22	C21	C24	107.9(10)	C134	C142	C130	120.0
C23'	C21'	C18'	111.6(5)	C106	C101	C102	118.1
C23'	C21'	C22'	108.6(4)	C106	C101	C100	120.9
C18'	C21'	C22'	109.8(4)	C102	C101	C100	120.9
C23'	C21'	C24'	109.3(4)	C103	C102	C101	121.1
C18'	C21'	C24'	108.3(3)	C102	C103	C104	120.1
C22'	C21'	C24'	109.2(5)	C105	C104	C103	119.5
N6	C25	N7	111.1(3)	C104	C105	C106	120.1

N6	C25	C19	124.1(3)	C105	C106	C101	121.1
N7	C25	C19	124.8(3)	C113	C108	C109	116.5(8)
N6'	C25'	N7'	110.9(3)	C113	C108	C107	121.7(10)
N6'	C25'	C16'	123.0(3)	C109	C108	C107	121.7(10)
N7'	C25'	C16'	126.1(3)	C110	C109	C108	121.5(10)
N9	C26	C28	109.1(3)	C109	C110	C111	120.9(10)
N9	C26	C27	110.4(3)	C110	C111	C112	120.0(8)
C28	C26	C27	113.6(4)	C113	C112	C111	118.2(8)
C28'	C26'	N9'	109.8(3)	C108	C113	C112	122.8(9)
C28'	C26'	C27'	113.4(5)	C121	C116	C117	120.0
N9'	C26'	C27'	108.7(4)	C121	C116	C115	119.9(8)
C203	C200	C201	113.6(8)	C117	C116	C115	119.7(8)
C203	C200	C202	108.7(7)	C120	C121	C116	120.0
C201	C200	C202	107.0(8)	C121	C120	C119	120.0
C203	C200	C4'	108.7(6)	C120	C119	C118	120.0
C201	C200	C4'	101.6(6)	C117	C118	C119	120.0
C202	C200	C4'	117.2(6)	C118	C117	C116	120.0
C206	C204	C205	107.2(15)	C02	C01	C06	120.0
C206	C204	C207	106.5(16)	C02	C01	C07	115.2(10)
C205	C204	C207	109.8(17)	C06	C01	C07	124.8(10)
C206	C204	C17	115.0(14)	C03	C02	C01	120.0
C205	C204	C17	112.8(15)	C02	C03	C04	120.0
C207	C204	C17	105.2(15)	C05	C04	C03	120.0
C210	C208	N5	111.7(11)	C04	C05	C06	120.0
C210	C208	C209	114.4(11)	C05	C06	C01	120.0

Figure S7 Labeled ORTEP drawing of **Yb(CzT^{iPr})$_2$(OSiMe$_3$), 4a • 2.33 C$_7$H$_8$**



t-Bu (C13-C16, C17-C20, C41-C44, C45-C48) and i-Pr groups (C22-C24, C26-C28, C50-C52, C54-C56) omitted for clarity.

Table S27 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **Yb(CzT^{iPr})$_2$(OSiMe$_3$), 4a • 2.33 C$_7$H$_8$**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Yb1	7669.6(2)	6298.1(2)	3236.2(2)	40.50(8)
Si1	9946.8(14)	7526.6(10)	3391.0(10)	55.5(4)
O1	9016(3)	6905(2)	3353.4(19)	47.4(9)
N1	6384(3)	7291(2)	3496(2)	38.7(9)
N2	6101(4)	5941(3)	2624(2)	45.6(11)
N3	6014(4)	5189(3)	2375(3)	50.5(12)
N4	5164(4)	5262(3)	2022(3)	55.1(13)
N5	4660(4)	6016(3)	2010(3)	54.8(13)
N6	7744(4)	6345(3)	4531(2)	42.3(10)
N7	8204(4)	5755(3)	4982(2)	46.2(11)
N8	8418(4)	6132(3)	5540(2)	46.8(11)
N9	8110(4)	6948(3)	5486(2)	46.6(11)
N10	8573(3)	5386(2)	2517(2)	35.4(9)
N11	7256(4)	4889(3)	3796(2)	46.2(11)
N12	6560(4)	4807(3)	4326(3)	62.1(14)
N13	6618(5)	4010(4)	4592(3)	67.3(15)
N14	7323(5)	3547(3)	4273(3)	67.2(15)
N15	7793(4)	7197(2)	2094(2)	43.0(10)
N16	7336(4)	7969(3)	1990(3)	54.8(13)
N17	7825(4)	8368(3)	1448(3)	58.8(14)
N18	8583(4)	7921(3)	1174(3)	60.6(14)
C1	5634(4)	7668(3)	3043(3)	38.5(11)
C2	5074(4)	7315(3)	2538(3)	41.7(12)
C3	4340(4)	7815(3)	2144(3)	45.7(13)
C4	4132(4)	8673(3)	2221(3)	48.0(13)
C5	4686(4)	9019(3)	2734(3)	46.1(13)
C6	5424(4)	8531(3)	3141(3)	39.6(11)
C7	6082(4)	8709(3)	3695(3)	42.0(12)
C8	6258(5)	9437(3)	4015(3)	51.2(14)
C9	6937(5)	9408(3)	4567(3)	50.7(14)
C10	7403(4)	8620(3)	4816(3)	45.6(13)
C11	7244(4)	7880(3)	4506(3)	40.0(11)

C12	6611(4)	7931(3)	3908(3)	33.9(10)
C13	3337(5)	9229(4)	1780(4)	59.7(17)
C14	2863(6)	8752(5)	1222(4)	88(3)
C15	3855(8)	10001(5)	1380(5)	115(4)
C16	2491(6)	9516(5)	2280(4)	90(3)
C17	7196(6)	10198(4)	4915(4)	75(2)
C18	7110(50)	11000(30)	4390(30)	106(14)
C19	8282(11)	10204(15)	5186(11)	124(5)
C20	7062(19)	10065(15)	5719(6)	121(5)
C18A	6720(50)	11000(30)	4520(30)	108(14)
C19A	8363(10)	10268(11)	4811(8)	100(5)
C20A	6458(17)	10215(15)	5549(9)	131(6)
C21	5271(4)	6429(3)	2396(3)	44.1(12)
C22	4809(6)	4562(4)	1639(4)	71(2)
C23	3778(9)	4335(7)	1861(6)	67(3)
C24	4915(9)	4826(6)	807(6)	70(3)
C23A	3731(19)	4758(15)	1415(14)	75(4)
C24A	5552(18)	4263(14)	1280(13)	77(4)
C25	7698(4)	7071(3)	4835(3)	38.0(11)
C26	8886(5)	5688(4)	6191(3)	52.0(14)
C27	8065(6)	5500(5)	6761(4)	79(2)
C28	9507(5)	4908(4)	6024(3)	60.9(17)
C29	8859(4)	4536(3)	2686(3)	37.7(11)
C30	8509(5)	3923(3)	3245(3)	46.0(13)
C31	8926(5)	3093(3)	3298(3)	57.1(17)
C32	9690(6)	2827(4)	2838(3)	64.1(19)
C33	10051(5)	3427(4)	2304(3)	59.7(17)
C34	9650(5)	4261(3)	2229(3)	45.5(13)
C35	9890(4)	4997(3)	1739(3)	42.3(12)
C36	10591(4)	5125(4)	1175(3)	49.2(14)
C37	10659(5)	5908(4)	766(3)	51.2(14)
C38	9977(5)	6552(4)	946(3)	50.0(14)
C39	9245(4)	6454(3)	1507(3)	43.2(12)
C40	9198(4)	5658(3)	1936(3)	37.5(11)
C41	10070(6)	1886(4)	2921(4)	92(3)
C42	10340(20)	1619(16)	3706(7)	106(6)

C43	10980(11)	1714(8)	2429(9)	96(4)
C44	9155(10)	1334(6)	2755(8)	80(4)
C42A	9920(20)	1435(17)	3681(8)	117(7)
C43A	11261(9)	1946(9)	2916(11)	109(4)
C44A	10052(17)	1568(9)	2183(7)	101(4)
C45	11442(5)	6095(5)	154(4)	65.8(18)
C46	11918(6)	5270(5)	-90(4)	84(2)
C47	12290(6)	6627(6)	403(5)	94(3)
C48	10927(6)	6591(5)	-499(4)	81(2)
C49	7715(5)	4113(3)	3764(3)	49.2(14)
C50	5939(8)	3695(6)	5236(4)	111(4)
C51	5868(18)	2767(8)	5307(11)	113(5)
C52	6195(16)	4120(10)	5858(7)	101(5)
C51A	6659(12)	3190(11)	5744(8)	103(4)
C52A	5114(16)	3249(15)	4939(12)	145(6)
C53	8545(4)	7180(3)	1595(3)	44.3(12)
C54	7520(7)	9250(4)	1123(4)	83(2)
C55	6675(11)	9194(6)	623(6)	160(6)
C56	7260(9)	9776(5)	1700(5)	112(3)
C57	11076(6)	7199(5)	2836(4)	78(2)
C58	10357(6)	7519(5)	4341(4)	79(2)
C59	9535(7)	8645(4)	3036(5)	89(3)

Table S28 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **Yb(CzT^{iPr})$_2$(OSiMe$_3$), 4a • 2.33 C$_7$H$_8$**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Yb1	50.99(15)	29.43(11)	41.59(14)	-7.39(8)	-1.44(10)	2.20(9)
Si1	58.9(11)	40.0(8)	69.0(11)	-8.7(7)	-3.9(9)	-10.9(7)
O1	59(2)	39.4(19)	45(2)	-10.7(16)	-3.5(18)	-4.9(17)
N1	48(3)	32(2)	38(2)	-7.8(17)	-3.6(19)	0.2(18)
N2	57(3)	29(2)	53(3)	-12.4(19)	-8(2)	1.8(19)
N3	52(3)	32(2)	70(3)	-14(2)	-18(2)	1(2)
N4	61(3)	35(2)	73(3)	-22(2)	-22(3)	5(2)

N5	61(3)	36(2)	71(3)	-19(2)	-19(3)	6(2)
N6	55(3)	34(2)	39(2)	-6.0(18)	-8(2)	6.5(19)
N7	60(3)	39(2)	41(2)	-11.5(19)	-8(2)	8(2)
N8	61(3)	38(2)	42(2)	-8.0(19)	-7(2)	7(2)
N9	56(3)	40(2)	44(3)	-7.9(19)	-5(2)	9(2)
N10	45(2)	28.3(19)	34(2)	-6.1(16)	-6.2(18)	2.5(17)
N11	59(3)	36(2)	43(3)	-5.5(19)	1(2)	-5(2)
N12	74(4)	51(3)	60(3)	-2(2)	12(3)	-15(3)
N13	79(4)	58(3)	64(3)	3(3)	8(3)	-22(3)
N14	98(5)	41(3)	62(3)	1(2)	-4(3)	-21(3)
N15	54(3)	30(2)	45(2)	-4.3(18)	-1(2)	4.8(19)
N16	73(4)	33(2)	56(3)	0(2)	5(3)	8(2)
N17	83(4)	33(2)	56(3)	6(2)	8(3)	7(2)
N18	82(4)	38(2)	59(3)	-1(2)	18(3)	4(2)
C1	43(3)	35(2)	39(3)	-12(2)	1(2)	0(2)
C2	48(3)	32(2)	47(3)	-10(2)	-5(2)	-3(2)
C3	50(3)	41(3)	48(3)	-14(2)	-11(3)	1(2)
C4	52(3)	40(3)	54(3)	-13(2)	-10(3)	6(2)
C5	53(3)	30(2)	57(3)	-12(2)	-11(3)	6(2)
C6	44(3)	31(2)	45(3)	-10(2)	-6(2)	2(2)
C7	49(3)	34(2)	43(3)	-8(2)	-7(2)	4(2)
C8	68(4)	31(3)	57(3)	-12(2)	-21(3)	9(2)
C9	59(4)	36(3)	60(4)	-15(2)	-18(3)	1(2)
C10	56(4)	40(3)	43(3)	-8(2)	-16(3)	2(2)
C11	45(3)	35(2)	41(3)	-6(2)	-5(2)	1(2)
C12	38(3)	30(2)	36(3)	-8.9(19)	1(2)	-1.3(19)
C13	65(4)	44(3)	73(4)	-15(3)	-28(3)	13(3)
C14	94(6)	74(5)	102(6)	-33(4)	-67(5)	33(4)
C15	143(9)	76(5)	120(7)	38(5)	-79(7)	-26(5)
C16	89(6)	89(5)	98(6)	-35(5)	-37(5)	48(5)
C17	112(6)	37(3)	80(5)	-19(3)	-49(5)	-2(3)
C18	180(40)	39(6)	105(17)	-23(8)	-50(20)	-3(13)
C19	213(13)	73(6)	98(9)	-41(8)	-49(8)	-26(8)
C20	217(13)	71(7)	88(8)	-49(7)	-39(8)	-23(9)
C18A	190(40)	38(6)	106(17)	-30(8)	-70(20)	6(13)
C19A	191(13)	58(7)	61(9)	-28(8)	-46(9)	-37(8)

C20A	237(16)	80(9)	93(10)	-62(8)	-1(11)	-40(11)
C21	54(3)	31(2)	50(3)	-13(2)	-5(3)	-4(2)
C22	77(5)	38(3)	105(6)	-34(3)	-28(4)	3(3)
C23	74(6)	50(5)	81(7)	-21(5)	1(6)	-14(5)
C24	80(6)	56(5)	84(6)	-38(5)	-8(5)	-10(4)
C23A	82(8)	60(7)	89(8)	-33(6)	-9(7)	-9(7)
C24A	85(10)	62(8)	93(10)	-40(8)	-1(9)	-11(8)
C25	42(3)	39(3)	34(3)	-8(2)	-5(2)	4(2)
C26	61(4)	51(3)	44(3)	-8(3)	-14(3)	13(3)
C27	89(6)	93(5)	51(4)	9(4)	-3(4)	12(4)
C28	82(5)	50(3)	52(4)	-8(3)	-23(3)	8(3)
C29	52(3)	28(2)	35(3)	-10.6(19)	-11(2)	4(2)
C30	68(4)	31(2)	41(3)	-10(2)	-15(3)	4(2)
C31	96(5)	28(3)	48(3)	-4(2)	-22(3)	5(3)
C32	104(6)	37(3)	53(4)	-13(3)	-34(4)	23(3)
C33	84(5)	47(3)	52(3)	-26(3)	-22(3)	28(3)
C34	63(4)	37(3)	38(3)	-12(2)	-11(3)	11(2)
C35	48(3)	43(3)	39(3)	-15(2)	-11(2)	10(2)
C36	46(3)	56(3)	48(3)	-22(3)	-9(3)	11(3)
C37	49(4)	64(4)	45(3)	-20(3)	-2(3)	-4(3)
C38	55(4)	47(3)	50(3)	-10(3)	-1(3)	-12(3)
C39	49(3)	38(3)	44(3)	-9(2)	0(2)	0(2)
C40	41(3)	38(3)	35(3)	-10(2)	-7(2)	2(2)
C41	143(8)	47(4)	92(6)	-32(4)	-63(5)	42(4)
C42	144(14)	40(9)	131(9)	1(6)	-31(8)	28(9)
C43	139(10)	36(5)	118(9)	-41(5)	-41(7)	36(6)
C44	127(11)	25(5)	94(9)	-27(5)	-51(7)	21(6)
C42A	146(17)	45(11)	150(10)	21(8)	-12(10)	35(10)
C43A	154(11)	51(6)	121(9)	-19(6)	-24(8)	42(7)
C44A	147(10)	49(6)	113(9)	-34(6)	-41(7)	27(7)
C45	55(4)	88(5)	61(4)	-31(4)	8(3)	-18(3)
C46	63(5)	111(6)	87(5)	-47(5)	26(4)	-11(4)
C47	64(5)	122(7)	107(6)	-47(5)	16(5)	-43(5)
C48	87(6)	100(6)	60(4)	-24(4)	22(4)	-28(5)
C49	72(4)	31(3)	45(3)	-2(2)	-13(3)	-8(3)
C50	153(9)	108(7)	67(5)	30(5)	-5(5)	-83(7)

C51	149(12)	81(9)	102(9)	11(7)	42(9)	-26(8)
C52	149(12)	85(8)	68(8)	2(7)	33(8)	-48(9)
C51A	140(11)	90(8)	77(8)	2(7)	37(8)	-44(8)
C52A	177(15)	118(11)	132(12)	19(10)	33(11)	-23(11)
C53	58(4)	33(3)	41(3)	-1(2)	3(3)	-3(2)
C54	115(7)	32(3)	95(6)	11(3)	17(5)	10(3)
C55	295(17)	64(5)	120(8)	-2(5)	-108(10)	59(8)
C56	179(10)	41(4)	115(7)	-7(4)	-23(7)	23(5)
C57	82(5)	66(4)	85(5)	-8(4)	5(4)	-16(4)
C58	75(5)	84(5)	85(5)	-37(4)	-16(4)	-12(4)
C59	94(6)	45(4)	128(7)	0(4)	-3(5)	-8(4)

Table S29 Bond Lengths for **Yb(CzT^{iPr})$_2$(OSiMe$_3$), 4a • 2.33 C$_7$H$_8$**

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Yb1	O1	2.061(4)	C9	C17	1.536(7)
Yb1	N1	2.338(4)	C10	C11	1.397(7)
Yb1	N2	2.491(5)	C11	C12	1.408(7)
Yb1	N6	2.455(4)	C11	C25	1.464(7)
Yb1	N10	2.361(4)	C13	C14	1.525(9)
Yb1	N11	2.421(4)	C13	C15	1.525(10)
Yb1	N15	2.434(4)	C13	C16	1.524(10)
Si1	O1	1.598(4)	C17	C18	1.513(10)
Si1	C57	1.876(8)	C17	C19	1.517(10)
Si1	C58	1.881(7)	C17	C20	1.509(10)
Si1	C59	1.880(7)	C17	C18A	1.512(10)
N1	C1	1.385(6)	C17	C19A	1.533(10)
N1	C12	1.396(6)	C17	C20A	1.515(10)
N2	N3	1.342(6)	C19	C20	1.86(3)
N2	C21	1.354(7)	C22	C23	1.441(13)
N3	N4	1.302(6)	C22	C24	1.574(13)
N4	N5	1.340(6)	C22	C23A	1.49(2)
N4	C22	1.491(7)	C22	C24A	1.27(2)
N5	C21	1.334(7)	C26	C27	1.505(9)
N6	N7	1.322(6)	C26	C28	1.513(8)

N6	C25	1.347(6)	C29	C30	1.419(7)
N7	N8	1.313(6)	C29	C34	1.415(7)
N8	N9	1.332(6)	C30	C31	1.397(7)
N8	C26	1.473(7)	C30	C49	1.453(8)
N9	C25	1.341(6)	C31	C32	1.390(9)
N10	C29	1.385(6)	C32	C33	1.381(10)
N10	C40	1.381(6)	C32	C41	1.544(8)
N11	N12	1.327(7)	C33	C34	1.395(7)
N11	C49	1.356(7)	C34	C35	1.433(8)
N12	N13	1.301(7)	C35	C36	1.382(8)
N13	N14	1.330(8)	C35	C40	1.434(7)
N13	C50	1.526(9)	C36	C37	1.381(8)
N14	C49	1.334(7)	C37	C38	1.395(8)
N15	N16	1.335(6)	C37	C45	1.528(9)
N15	C53	1.341(7)	C38	C39	1.402(8)
N16	N17	1.296(7)	C39	C40	1.413(7)
N17	N18	1.324(7)	C39	C53	1.464(7)
N17	C54	1.499(7)	C41	C42	1.536(9)
N18	C53	1.335(7)	C41	C43	1.521(9)
C1	C2	1.397(7)	C41	C44	1.565(9)
C1	C6	1.418(6)	C41	C42A	1.531(9)
C2	C3	1.390(7)	C41	C43A	1.556(9)
C2	C21	1.474(7)	C41	C44A	1.537(9)
C3	C4	1.401(7)	C45	C46	1.541(10)
C4	C5	1.398(7)	C45	C47	1.531(9)
C4	C13	1.529(8)	C45	C48	1.532(10)
C5	C6	1.396(7)	C50	C51	1.467(11)
C6	C7	1.429(7)	C50	C52	1.474(11)
C7	C8	1.396(7)	C50	C51A	1.497(11)
C7	C12	1.410(7)	C50	C52A	1.468(12)
C8	C9	1.379(8)	C54	C55	1.480(13)
C9	C10	1.400(7)	C54	C56	1.475(11)

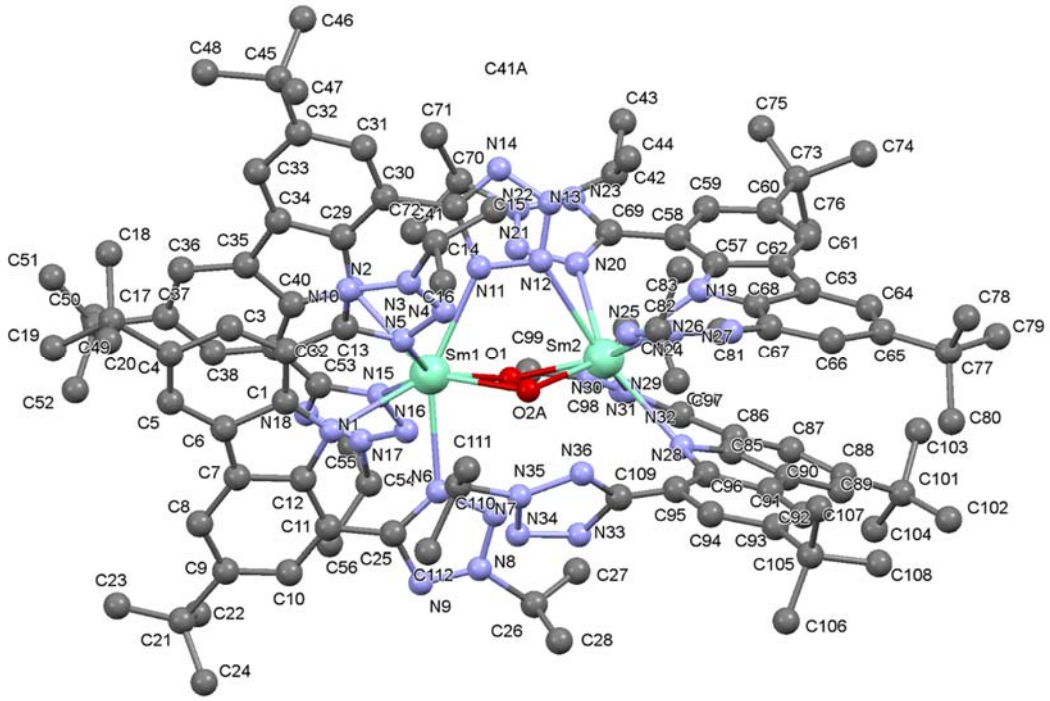
Table S30 Bond Angles for **Yb(CzT^{iPr})$_2$(OSiMe$_3$), 4a • 2.33 C$_7$H$_8$**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Yb1	N1	103.91(14)	C15	C13	C4	109.5(6)
O1	Yb1	N2	156.65(15)	C15	C13	C14	107.3(7)
O1	Yb1	N6	76.27(15)	C16	C13	C4	109.0(5)
O1	Yb1	N10	89.25(14)	C16	C13	C14	109.2(6)
O1	Yb1	N11	125.65(15)	C16	C13	C15	110.0(7)
O1	Yb1	N15	79.05(15)	C18	C17	C9	112(3)
N1	Yb1	N2	73.54(14)	C18	C17	C19	104(3)
N1	Yb1	N6	74.74(14)	C19	C17	C9	115.4(9)
N1	Yb1	N10	155.37(14)	C20	C17	C9	112.5(9)
N1	Yb1	N11	110.42(15)	C20	C17	C18	131(3)
N1	Yb1	N15	83.79(14)	C20	C17	C19	75.9(12)
N6	Yb1	N2	123.64(15)	C18A	C17	C9	112(3)
N10	Yb1	N2	86.09(14)	C18A	C17	C19A	106(3)
N10	Yb1	N6	129.27(13)	C18A	C17	C20A	93(3)
N10	Yb1	N11	76.49(14)	C19A	C17	C9	104.7(7)
N10	Yb1	N15	78.31(13)	C20A	C17	C9	105.7(9)
N11	Yb1	N2	75.33(15)	C20A	C17	C19A	134.4(12)
N11	Yb1	N6	73.87(14)	C17	C19	C20	51.9(7)
N11	Yb1	N15	143.93(14)	C17	C20	C19	52.3(7)
N15	Yb1	N2	77.60(15)	N2	C21	C2	124.6(5)
N15	Yb1	N6	141.99(14)	N5	C21	N2	111.7(4)
O1	Si1	C57	110.8(3)	N5	C21	C2	123.7(5)
O1	Si1	C58	110.7(3)	N4	C22	C24	109.5(6)
O1	Si1	C59	109.8(3)	N4	C22	C23A	109.0(9)
C57	Si1	C58	108.9(4)	C23	C22	N4	111.2(7)
C57	Si1	C59	108.2(4)	C23	C22	C24	112.3(8)
C59	Si1	C58	108.4(4)	C24A	C22	N4	110.2(11)
Si1	O1	Yb1	169.8(2)	C24A	C22	C23A	128.2(15)
C1	N1	Yb1	127.3(3)	N6	C25	C11	124.7(4)
C1	N1	C12	103.6(4)	N9	C25	N6	110.5(4)
C12	N1	Yb1	119.7(3)	N9	C25	C11	124.8(4)
N3	N2	Yb1	122.0(3)	N8	C26	C27	109.4(5)
N3	N2	C21	106.6(4)	N8	C26	C28	110.8(5)
C21	N2	Yb1	130.9(3)	C27	C26	C28	113.7(6)

N4	N3	N2	105.1(4)	N10	C29	C30	130.5(5)
N3	N4	N5	115.2(4)	N10	C29	C34	113.1(4)
N3	N4	C22	121.7(5)	C34	C29	C30	116.4(4)
N5	N4	C22	123.0(5)	C29	C30	C49	122.9(4)
C21	N5	N4	101.4(4)	C31	C30	C29	119.3(5)
N7	N6	Yb1	124.3(3)	C31	C30	C49	117.8(5)
N7	N6	C25	107.5(4)	C32	C31	C30	123.7(6)
C25	N6	Yb1	123.6(3)	C31	C32	C41	119.9(6)
N8	N7	N6	105.7(4)	C33	C32	C31	117.2(5)
N7	N8	N9	113.8(4)	C33	C32	C41	122.9(6)
N7	N8	C26	123.6(4)	C32	C33	C34	120.9(6)
N9	N8	C26	122.5(4)	C29	C34	C35	105.4(4)
N8	N9	C25	102.4(4)	C33	C34	C29	122.5(5)
C29	N10	Yb1	128.6(3)	C33	C34	C35	132.2(6)
C40	N10	Yb1	124.6(3)	C34	C35	C40	105.0(5)
C40	N10	C29	104.0(4)	C36	C35	C34	132.4(5)
N12	N11	Yb1	119.3(3)	C36	C35	C40	122.6(5)
N12	N11	C49	107.4(5)	C37	C36	C35	121.2(5)
C49	N11	Yb1	132.4(4)	C36	C37	C38	116.7(5)
N13	N12	N11	105.5(5)	C36	C37	C45	123.5(6)
N12	N13	N14	114.3(5)	C38	C37	C45	119.8(6)
N12	N13	C50	119.6(7)	C37	C38	C39	124.4(5)
N14	N13	C50	126.0(6)	C38	C39	C40	118.7(5)
N13	N14	C49	102.7(5)	C38	C39	C53	117.4(5)
N16	N15	Yb1	122.0(3)	C40	C39	C53	123.9(5)
N16	N15	C53	106.8(4)	N10	C40	C35	112.5(4)
C53	N15	Yb1	127.1(3)	N10	C40	C39	131.1(4)
N17	N16	N15	105.2(4)	C39	C40	C35	116.4(5)
N16	N17	N18	115.0(4)	C32	C41	C44	108.0(6)
N16	N17	C54	122.9(5)	C32	C41	C43A	103.2(8)
N18	N17	C54	122.0(5)	C42	C41	C32	108.4(11)
N17	N18	C53	101.8(5)	C42	C41	C44	107.0(12)
N1	C1	C2	129.4(4)	C43	C41	C32	113.5(7)
N1	C1	C6	112.2(4)	C43	C41	C42	110.6(14)
C2	C1	C6	118.4(5)	C43	C41	C44	109.1(9)
C1	C2	C21	121.2(5)	C42A	C41	C32	113.2(12)

C3	C2	C1	119.5(4)	C42A	C41	C43A	98.2(14)
C3	C2	C21	119.2(5)	C42A	C41	C44A	132.3(13)
C2	C3	C4	123.2(5)	C44A	C41	C32	108.2(7)
C3	C4	C13	123.3(5)	C44A	C41	C43A	94.3(12)
C5	C4	C3	116.9(5)	C37	C45	C46	111.7(6)
C5	C4	C13	119.8(5)	C37	C45	C47	108.7(5)
C6	C5	C4	121.2(5)	C37	C45	C48	110.5(6)
C1	C6	C7	106.1(4)	C47	C45	C46	109.7(6)
C5	C6	C1	120.7(5)	C48	C45	C46	106.9(6)
C5	C6	C7	133.1(4)	C48	C45	C47	109.3(7)
C8	C7	C6	133.8(5)	N11	C49	C30	124.9(5)
C8	C7	C12	121.3(5)	N14	C49	N11	110.1(6)
C12	C7	C6	104.8(4)	N14	C49	C30	125.0(5)
C9	C8	C7	120.7(5)	C51	C50	N13	110.7(10)
C8	C9	C10	118.0(5)	C51	C50	C52	120.3(12)
C8	C9	C17	122.7(5)	C52	C50	N13	110.2(8)
C10	C9	C17	119.3(5)	C51A	C50	N13	104.5(9)
C11	C10	C9	122.7(5)	C52A	C50	N13	104.8(11)
C10	C11	C12	118.8(4)	C52A	C50	C51A	118.3(13)
C10	C11	C25	119.0(5)	N15	C53	C39	125.6(5)
C12	C11	C25	122.1(4)	N18	C53	N15	111.1(5)
N1	C12	C7	113.1(4)	N18	C53	C39	123.2(5)
N1	C12	C11	128.7(4)	C55	C54	N17	108.7(6)
C11	C12	C7	118.2(4)	C56	C54	N17	109.0(6)
C14	C13	C4	111.8(5)	C56	C54	C55	114.1(8)

Figure S8 Labeled ORTEP drawing of **[Sm(CzT^{iPr})$_2$]$_2$(μ-OH)$_2$, 6a • 0.5 C$_7$H$_8$**



Toluene of solvation not shown; depicted as ball and stick for clarity since the peripheral groups show excessive thermal motion.

Table S31 Atomic coordinates and equivalent isotropic displacement parameters (Å^2)[1] for **[Sm(CzT^{iPr})$_2$]$_2$(μ-OH)$_2$, 6a • 0.5 C$_7$H$_8$**

Atom	x	y	z	U(eq)
Sm(1)	0.64839(3)	0.74678(3)	0.24782(3)	0.056(1)
Sm(2)	0.49792(3)	0.88489(3)	0.28704(3)	0.052(1)
O(1)	0.5152(5)	0.7807(4)	0.2608(5)	0.085(3)
O(2A)	0.6391(6)	0.8705(5)	0.2341(5)	0.058(3)
O(2B)	0.6114(18)	0.8270(15)	0.3182(16)	0.092(8)
N(1)	0.7695(7)	0.6986(5)	0.1711(5)	0.074(3)
N(2)	0.9009(6)	0.7524(8)	0.3047(7)	0.093(4)
N(3)	0.8653(8)	0.8089(7)	0.3185(6)	0.086(3)
N(4)	0.7999(7)	0.8267(6)	0.2973(6)	0.082(3)
N(5)	0.7910(6)	0.7767(6)	0.2668(5)	0.074(3)
N(6)	0.6381(9)	0.7813(6)	0.1255(5)	0.097(4)
N(7)	0.5792(13)	0.8283(8)	0.1097(7)	0.140(6)
N(8)	0.5732(15)	0.8195(9)	0.0533(8)	0.160(8)
N(9)	0.6125(16)	0.7690(9)	0.0321(8)	0.173(9)
N(10)	0.6561(5)	0.6303(4)	0.3360(4)	0.052(2)
N(15)	0.5627(6)	0.6431(5)	0.2346(5)	0.069(3)
N(16)	0.4996(8)	0.6538(6)	0.2052(6)	0.084(3)
N(17)	0.4862(9)	0.5915(7)	0.1955(7)	0.101(4)
N(18)	0.5340(9)	0.5406(6)	0.2169(6)	0.095(4)
N(19)	0.3966(5)	0.9370(4)	0.3741(4)	0.051(2)
N(20)	0.4120(6)	0.7823(5)	0.3967(5)	0.070(3)
N(21)	0.4395(6)	0.7169(6)	0.4084(7)	0.096(4)
N(22)	0.3755(7)	0.6743(5)	0.4579(6)	0.091(4)
N(23)	0.3063(6)	0.7064(6)	0.4784(6)	0.092(4)
N(24)	0.5766(5)	0.9881(4)	0.3056(4)	0.049(2)
N(25)	0.6597(6)	0.9930(5)	0.2947(5)	0.065(2)
N(26)	0.6792(6)	1.0587(6)	0.2953(5)	0.077(3)
N(27)	0.6115(7)	1.0977(5)	0.3055(5)	0.072(3)
N(28)	0.4689(6)	0.9911(4)	0.1990(4)	0.058(2)
N(29)	0.3597(6)	0.8523(5)	0.2692(5)	0.070(3)
N(30)	0.3283(7)	0.7836(6)	0.2869(8)	0.105(4)
N(31)	0.2499(8)	0.7861(7)	0.2836(8)	0.111(4)
N(32)	0.2271(7)	0.8533(6)	0.2611(7)	0.100(4)
C(1)	0.8295(9)	0.6643(7)	0.1937(7)	0.085(4)
C(2)	0.8679(7)	0.6727(7)	0.2425(7)	0.076(4)
C(3)	0.9289(9)	0.6266(9)	0.2586(9)	0.107(5)
C(4)	0.9533(10)	0.5702(10)	0.2267(11)	0.120(6)
C(5)	0.9170(12)	0.5640(10)	0.1802(10)	0.114(6)
C(6)	0.8584(10)	0.6083(8)	0.1599(8)	0.092(5)
C(7)	0.8142(11)	0.6143(8)	0.1144(7)	0.097(5)
C(8)	0.8175(14)	0.5804(9)	0.0638(9)	0.126(7)
C(9)	0.764(2)	0.5973(10)	0.0216(9)	0.164(11)

C(10)	0.7157(13)	0.6532(9)	0.0273(7)	0.121(7)
C(11)	0.7115(12)	0.6892(7)	0.0758(7)	0.095(5)
C(12)	0.7601(10)	0.6702(6)	0.1206(7)	0.085(4)
C(13)	0.8533(8)	0.7330(7)	0.2718(7)	0.072(3)
C(14)	0.8964(11)	0.8490(10)	0.3573(11)	0.125(6)
C(15)	0.8237(14)	0.8771(11)	0.4020(13)	0.158(8)
C(16)	0.964(2)	0.9032(17)	0.3073(11)	0.28(2)
C(17)	1.0216(13)	0.5231(13)	0.2522(14)	0.153(9)
C(18)	0.995(2)	0.489(2)	0.3259(18)	0.31(3)
C(19)	1.0239(15)	0.4573(14)	0.2213(18)	0.228(15)
C(20)	1.1052(13)	0.5675(15)	0.221(2)	0.29(2)
C(21)	0.770(3)	0.5571(13)	-0.0325(11)	0.206(15)
C(22)	0.672(3)	0.525(2)	-0.013(2)	0.29(2)
C(23)	0.814(3)	0.4945(12)	-0.0238(11)	0.31(3)
C(24)	0.789(3)	0.6111(12)	-0.0993(10)	0.38(3)
C(25)	0.6599(13)	0.7461(9)	0.0771(8)	0.113(6)
C(26)	0.507(3)	0.8634(14)	0.0250(16)	0.188(14)
C(27)	0.428(2)	0.868(2)	0.0708(19)	0.227(18)
C(28)	0.5615(18)	0.9327(12)	-0.0194(10)	0.193(14)
C(29)	0.6944(6)	0.6256(5)	0.3855(5)	0.053(3)
C(30)	0.6943(7)	0.6684(5)	0.4283(6)	0.057(3)
C(31)	0.7380(7)	0.6518(6)	0.4744(6)	0.063(3)
C(32)	0.7876(7)	0.5914(7)	0.4828(7)	0.075(3)
C(33)	0.7876(8)	0.5484(7)	0.4412(6)	0.074(3)
C(34)	0.7399(6)	0.5628(6)	0.3956(5)	0.055(3)
C(35)	0.7260(7)	0.5260(6)	0.3497(5)	0.059(3)
C(36)	0.7531(8)	0.4594(6)	0.3398(7)	0.079(4)
C(37)	0.7224(9)	0.4354(7)	0.2939(7)	0.079(4)
C(38)	0.6664(9)	0.4755(7)	0.2636(7)	0.080(4)
C(39)	0.6421(8)	0.5407(6)	0.2735(6)	0.064(3)
C(40)	0.6736(7)	0.5669(5)	0.3158(6)	0.058(3)
C(42)	0.5317(8)	0.8695(7)	0.4781(6)	0.071(3)
C(43)	0.4643(9)	0.8319(9)	0.5413(7)	0.104(5)
C(44)	0.5995(11)	0.9176(8)	0.4862(7)	0.103(5)
C(45)	0.8390(9)	0.5792(9)	0.5330(8)	0.098(5)
C(46)	0.7787(10)	0.5634(10)	0.6039(8)	0.111(5)
C(47)	0.9052(17)	0.6376(15)	0.5121(16)	0.27(2)
C(48)	0.8876(15)	0.5094(15)	0.5320(12)	0.199(13)
C(49)	0.7445(12)	0.3605(7)	0.2807(8)	0.102(5)
C(50)	0.6622(11)	0.3136(7)	0.2989(9)	0.120(6)
C(51)	0.7997(12)	0.3218(8)	0.3231(9)	0.118(6)
C(52)	0.7947(13)	0.3770(9)	0.2049(8)	0.126(7)
C(53)	0.5829(8)	0.5742(6)	0.2414(6)	0.065(3)
C(54)	0.4252(14)	0.5811(11)	0.1579(12)	0.139(7)
C(55)	0.3625(14)	0.5165(11)	0.2049(12)	0.149(8)
C(56)	0.4794(19)	0.5743(17)	0.0874(12)	0.218(14)

C(57)	0.3136(7)	0.9068(6)	0.4120(6)	0.066(3)
C(58)	0.2809(7)	0.8351(6)	0.4432(6)	0.065(3)
C(59)	0.1949(7)	0.8200(7)	0.4842(7)	0.079(4)
C(60)	0.1402(8)	0.8724(8)	0.4907(7)	0.083(4)
C(61)	0.1721(8)	0.9436(8)	0.4596(6)	0.081(4)
C(62)	0.2563(6)	0.9607(6)	0.4209(5)	0.060(3)
C(63)	0.3085(7)	1.0276(6)	0.3868(6)	0.061(3)
C(64)	0.2901(8)	1.1007(6)	0.3727(6)	0.068(3)
C(65)	0.3526(7)	1.1552(6)	0.3401(6)	0.062(3)
C(66)	0.4376(8)	1.1379(6)	0.3194(5)	0.065(3)
C(67)	0.4580(6)	1.0657(5)	0.3294(5)	0.049(2)
C(68)	0.3934(7)	1.0105(6)	0.3608(5)	0.058(3)
C(69)	0.3339(6)	0.7746(7)	0.4402(7)	0.073(3)
C(70)	0.3826(9)	0.5971(7)	0.4849(10)	0.106(6)
C(71)	0.4454(9)	0.5866(9)	0.5247(9)	0.130(7)
C(72)	0.4064(11)	0.5644(8)	0.4282(11)	0.122(6)
C(73)	0.0458(7)	0.8497(9)	0.5360(9)	0.102(5)
C(74)	0.0110(15)	0.9103(14)	0.5684(19)	0.29(2)
C(75)	0.0323(11)	0.7851(13)	0.5899(13)	0.223(16)
C(76)	0.0012(14)	0.854(3)	0.4861(16)	0.35(3)
C(77)	0.3387(9)	1.2372(7)	0.3225(7)	0.081(4)
C(78)	0.3869(12)	1.2767(8)	0.3526(10)	0.117(6)
C(79)	0.2452(11)	1.2465(10)	0.3510(13)	0.157(9)
C(80)	0.3650(16)	1.2725(9)	0.2448(10)	0.155(9)
C(81)	0.5482(7)	1.0513(6)	0.3131(5)	0.054(3)
C(82)	0.7652(9)	1.0847(9)	0.2870(11)	0.113(6)
C(83)	0.7712(10)	1.1005(9)	0.3501(9)	0.107(5)
C(84)	0.7966(12)	1.1372(13)	0.2288(14)	0.163(9)
C(85)	0.3863(8)	1.0128(6)	0.2056(6)	0.066(3)
C(86)	0.3062(8)	0.9713(7)	0.2297(6)	0.075(3)
C(87)	0.2330(8)	1.0077(8)	0.2267(7)	0.082(4)
C(88)	0.2335(10)	1.0813(8)	0.2006(8)	0.090(4)
C(89)	0.3118(10)	1.1221(8)	0.1762(7)	0.089(4)
C(90)	0.3866(8)	1.0899(6)	0.1795(5)	0.068(3)
C(91)	0.4745(8)	1.1168(7)	0.1541(6)	0.071(3)
C(92)	0.5139(9)	1.1851(7)	0.1246(7)	0.079(4)
C(93)	0.6007(11)	1.1980(8)	0.1009(7)	0.099(5)
C(94)	0.6476(9)	1.1371(8)	0.1069(6)	0.084(4)
C(95)	0.6074(8)	1.0663(6)	0.1371(6)	0.068(3)
C(96)	0.5198(7)	1.0555(6)	0.1645(5)	0.059(3)
C(97)	0.2969(8)	0.8926(7)	0.2534(6)	0.075(3)
C(98)	0.1936(12)	0.7201(9)	0.3022(14)	0.142(8)
C(99)	0.2409(18)	0.6596(12)	0.302(3)	0.44(5)
C(100)	0.1308(18)	0.7153(16)	0.3640(18)	0.262(19)
C(101)	0.1523(12)	1.1174(11)	0.1936(13)	0.134(7)
C(102)	0.167(2)	1.191(2)	0.165(2)	0.130(12)

C(103)	0.091(2)	1.091(2)	0.267(2)	0.131(12)
C(104)	0.110(2)	1.070(2)	0.160(2)	0.122(11)
C(02A)	0.083(2)	1.077(2)	0.218(2)	0.118(11)
C(03A)	0.171(2)	1.165(2)	0.116(2)	0.133(12)
C(04A)	0.1475(19)	1.1868(17)	0.2249(17)	0.097(9)
C(105)	0.6499(10)	1.2748(8)	0.0663(8)	0.114(5)
C(106)	0.691(2)	1.2822(19)	-0.0085(12)	0.108(10)
C(107)	0.694(3)	1.297(2)	0.110(2)	0.156(15)
C(108)	0.585(2)	1.3301(18)	0.067(2)	0.129(12)
C(06A)	0.616(3)	1.324(2)	0.110(2)	0.135(13)
C(07A)	0.645(3)	1.304(2)	-0.0051(13)	0.135(14)
C(08A)	0.7416(15)	1.2780(19)	0.0661(19)	0.111(10)
C(110)	0.8514(13)	0.9158(15)	0.1063(10)	0.159(10)
C(111)	0.9151(16)	0.9558(18)	0.1157(16)	0.219(15)
C(112)	0.867(2)	0.9022(19)	0.0346(15)	0.31(2)
C(41)	0.6432(9)	0.7331(8)	0.4258(7)	0.089(4)
N(11)	0.6209(7)	0.7676(6)	0.3655(5)	0.043(3)
N(12)	0.5795(7)	0.8224(6)	0.3793(6)	0.045(3)
N(13)	0.5790(8)	0.8190(6)	0.4406(7)	0.054(4)
N(14)	0.6129(7)	0.7640(6)	0.4706(6)	0.045(3)
C(41A)	0.6432(9)	0.7331(8)	0.4258(7)	0.089(4)
N(11A)	0.5562(18)	0.7045(18)	0.467(2)	0.115(6)
N(12A)	0.5209(19)	0.756(2)	0.492(2)	0.133(8)
N(13A)	0.584(3)	0.8053(18)	0.471(3)	0.117(9)
N(14A)	0.657(2)	0.7779(19)	0.456(2)	0.102(6)
C(109)	0.6602(8)	1.0231(8)	0.1208(8)	0.095(7)
N(33)	0.6509(8)	0.9774(8)	0.0814(8)	0.096(5)
N(34)	0.7233(9)	0.9371(7)	0.0718(7)	0.111(6)
N(35)	0.7775(7)	0.9579(8)	0.1052(8)	0.105(6)
N(36)	0.7385(8)	1.0110(7)	0.1355(7)	0.086(5)
C(09A)	0.6641(11)	1.0026(8)	0.1387(10)	0.042(7)
N(36A)	0.7511(10)	0.9986(9)	0.1037(9)	0.056(7)
N(35A)	0.7729(9)	0.9279(11)	0.1318(12)	0.103(12)
N(34A)	0.6993(12)	0.8883(8)	0.1841(10)	0.063(7)
N(33A)	0.6320(9)	0.9344(9)	0.1883(9)	0.054(6)
C(1S)	0.9320(12)	1.2080(10)	-0.0366(9)	0.106(10)
C(2S)	0.9554(10)	1.2418(8)	-0.1071(9)	0.086(7)
C(3S)	0.9222(11)	1.2137(9)	-0.1483(7)	0.079(7)
C(4S)	0.8657(11)	1.1518(9)	-0.1190(9)	0.090(8)
C(5S)	0.8424(11)	1.1180(8)	-0.0485(9)	0.108(10)
C(6S)	0.8755(12)	1.1461(10)	-0.0073(7)	0.092(8)
C(7S)	0.975(3)	1.243(2)	0.007(2)	0.141(14)
H(3)	0.95473	0.63248	0.29124	0.128
H(5)	0.93265	0.52643	0.15969	0.137
H(8)	0.85685	0.54510	0.05767	0.151
H(10)	0.68319	0.66864	-0.00342	0.145

H(14)	0.92296	0.81411	0.38830	0.150
H(15A)	0.78217	0.83669	0.43338	0.237
H(15B)	0.84537	0.90167	0.42881	0.237
H(15C)	0.79602	0.91128	0.37305	0.237
H(16A)	0.98648	0.93103	0.33134	0.416
H(16B)	1.01029	0.87905	0.28340	0.416
H(16C)	0.94105	0.93592	0.27375	0.416
H(18A)	0.93972	0.46117	0.34037	0.465
H(18B)	1.03753	0.45610	0.33770	0.465
H(18C)	0.99060	0.52585	0.34956	0.465
H(19A)	1.04133	0.47563	0.17099	0.342
H(19B)	1.06465	0.42428	0.23551	0.342
H(19C)	0.96694	0.43139	0.23849	0.342
H(20A)	1.11623	0.58785	0.17144	0.439
H(20B)	1.10372	0.60688	0.24179	0.439
H(20C)	1.15064	0.53712	0.22993	0.439
H(22A)	0.63556	0.56442	-0.01749	0.440
H(22B)	0.66868	0.49701	-0.04411	0.440
H(22C)	0.65384	0.49290	0.03457	0.440
H(23A)	0.79321	0.46437	0.02431	0.461
H(23B)	0.80557	0.46708	-0.05371	0.461
H(23C)	0.87538	0.50862	-0.03588	0.461
H(24A)	0.75158	0.65035	-0.09564	0.567
H(24B)	0.84840	0.63041	-0.11473	0.567
H(24C)	0.77859	0.58887	-0.13255	0.567
H(26)	0.49497	0.83967	-0.00748	0.226
H(27A)	0.39970	0.81961	0.09622	0.341
H(27B)	0.43621	0.89246	0.10328	0.341
H(27C)	0.39233	0.89615	0.04496	0.341
H(28A)	0.61488	0.92148	-0.04876	0.290
H(28B)	0.53053	0.96269	-0.04835	0.290
H(28C)	0.57441	0.95900	0.00996	0.290
H(31)	0.73555	0.68221	0.50273	0.075
H(33)	0.82077	0.50807	0.44363	0.088
H(36)	0.78983	0.43257	0.36263	0.094
H(38)	0.64389	0.45719	0.23479	0.096
H(42A)	0.50337	0.90183	0.44676	0.085
H(42B)	0.51090	0.89218	0.43797	0.085
H(43A)	0.43587	0.86719	0.56344	0.155
H(43B)	0.42264	0.80539	0.53029	0.155
H(43C)	0.48928	0.79790	0.57265	0.155
H(44A)	0.64152	0.94029	0.44118	0.154
H(44B)	0.57200	0.95518	0.50542	0.154
H(44C)	0.62818	0.88797	0.51733	0.154
H(46A)	0.73698	0.52325	0.61245	0.167
H(46B)	0.81047	0.55009	0.63719	0.167

H(46C)	0.74905	0.60635	0.60879	0.167
H(47A)	0.94100	0.64325	0.46482	0.405
H(47B)	0.87896	0.68258	0.51454	0.405
H(47C)	0.94038	0.62633	0.54294	0.405
H(48A)	0.84625	0.46745	0.54569	0.298
H(48B)	0.92602	0.51526	0.48541	0.298
H(48C)	0.92088	0.50188	0.56416	0.298
H(50A)	0.62687	0.33883	0.27138	0.180
H(50B)	0.67568	0.26778	0.28899	0.180
H(50C)	0.63116	0.30405	0.34788	0.180
H(51A)	0.76807	0.31080	0.37221	0.176
H(51B)	0.81484	0.27669	0.31219	0.176
H(51C)	0.85180	0.35283	0.31238	0.176
H(52A)	0.75978	0.40207	0.17690	0.189
H(52B)	0.84681	0.40790	0.19451	0.189
H(52C)	0.80986	0.33177	0.19432	0.189
H(54)	0.39309	0.62503	0.15004	0.167
H(55A)	0.32157	0.50795	0.18225	0.223
H(55B)	0.39370	0.47362	0.21478	0.223
H(55C)	0.33200	0.52636	0.24811	0.223
H(56A)	0.44171	0.56743	0.06137	0.327
H(56B)	0.51775	0.61834	0.06156	0.327
H(56C)	0.51317	0.53263	0.09452	0.327
H(59)	0.17401	0.77112	0.50865	0.095
H(61)	0.13570	0.98098	0.46502	0.097
H(64)	0.23245	1.11176	0.38653	0.082
H(66)	0.48222	1.17588	0.29809	0.078
H(70)	0.32560	0.57388	0.51714	0.127
H(71A)	0.45049	0.53488	0.54296	0.195
H(71B)	0.50121	0.61082	0.49430	0.195
H(71C)	0.42549	0.60742	0.56293	0.195
H(72A)	0.41100	0.51265	0.44677	0.183
H(72B)	0.36259	0.57127	0.40498	0.183
H(72C)	0.46134	0.58766	0.39529	0.183
H(74A)	0.01951	0.95637	0.53190	0.441
H(74B)	-0.05003	0.89853	0.59330	0.441
H(74C)	0.04152	0.91432	0.60036	0.441
H(75A)	0.06564	0.78905	0.62002	0.335
H(75B)	-0.02845	0.77600	0.61646	0.335
H(75C)	0.05020	0.74507	0.57088	0.335
H(76A)	0.01568	0.90116	0.45127	0.532
H(76B)	0.01815	0.81583	0.46385	0.532
H(76C)	-0.06050	0.84676	0.50942	0.532
H(78A)	0.44795	1.27159	0.33485	0.175
H(78B)	0.37697	1.32806	0.33981	0.175
H(78C)	0.36747	1.25658	0.40282	0.175

H(79A)	0.21194	1.22095	0.33203	0.236
H(79B)	0.22676	1.22655	0.40130	0.236
H(79C)	0.23626	1.29802	0.33828	0.236
H(80A)	0.33360	1.24687	0.22459	0.232
H(80B)	0.35206	1.32317	0.23500	0.232
H(80C)	0.42642	1.27025	0.22490	0.232
H(82)	0.80083	1.04344	0.28225	0.136
H(83A)	0.74639	1.05856	0.39041	0.160
H(83B)	0.83118	1.11097	0.34541	0.160
H(83C)	0.73986	1.14252	0.35598	0.160
H(84A)	0.85466	1.15377	0.22441	0.245
H(84B)	0.79786	1.11930	0.18994	0.245
H(84C)	0.76059	1.17756	0.22870	0.245
H(87)	0.17970	0.97954	0.24381	0.098
H(89)	0.31424	1.17296	0.15694	0.107
H(92)	0.48001	1.22488	0.12043	0.095
H(94)	0.70811	1.14392	0.09019	0.100
H(98)	0.16474	0.72629	0.26605	0.170
H(99A)	0.28330	0.66803	0.25623	0.658
H(99B)	0.26985	0.65188	0.33673	0.658
H(99C)	0.20232	0.61682	0.31156	0.658
H(10A)	0.10151	0.75969	0.35934	0.393
H(10B)	0.08952	0.67384	0.37544	0.393
H(10C)	0.15705	0.70890	0.40061	0.393
H(10D)	0.20677	1.20272	0.11810	0.195
H(10E)	0.11333	1.21219	0.16377	0.195
H(10F)	0.19232	1.21163	0.19288	0.195
H(10G)	0.08488	1.03821	0.28295	0.196
H(10H)	0.11468	1.10898	0.29757	0.196
H(10I)	0.03568	1.10954	0.26846	0.196
H(10J)	0.10391	1.01859	0.18713	0.182
H(10K)	0.05302	1.08518	0.15989	0.182
H(10L)	0.14552	1.07560	0.11277	0.182
H(02A)	0.03607	1.10639	0.21050	0.177
H(02B)	0.08709	1.03956	0.19521	0.177
H(02C)	0.07185	1.05472	0.26761	0.177
H(03A)	0.22518	1.19430	0.10019	0.199
H(03B)	0.17384	1.13280	0.08693	0.199
H(03C)	0.12482	1.19629	0.11189	0.199
H(04A)	0.20242	1.21620	0.20456	0.146
H(04B)	0.10248	1.21635	0.21380	0.146
H(04C)	0.13487	1.16890	0.27502	0.146
H(10M)	0.65035	1.26436	-0.02665	0.162
H(10N)	0.70964	1.33320	-0.03394	0.162
H(10O)	0.74094	1.25392	-0.01369	0.162
H(10P)	0.65442	1.28691	0.15701	0.233

H(10Q)	0.74360	1.26923	0.11135	0.233
H(10R)	0.71230	1.34851	0.09109	0.233
H(10S)	0.54883	1.32343	0.03934	0.194
H(10T)	0.54898	1.32384	0.11424	0.194
H(10U)	0.61420	1.37887	0.04710	0.194
H(06A)	0.62090	1.30200	0.15618	0.203
H(06B)	0.64999	1.37075	0.08901	0.203
H(06C)	0.55651	1.33033	0.11312	0.203
H(07A)	0.66778	1.27012	-0.03115	0.202
H(07B)	0.58578	1.31032	-0.00355	0.202
H(07C)	0.67927	1.35075	-0.02766	0.202
H(08A)	0.74366	1.25864	0.11336	0.167
H(08B)	0.77415	1.24907	0.03795	0.167
H(08C)	0.76648	1.32826	0.04696	0.167
H(110)	0.83408	0.86906	0.14406	0.191
H(11Z)	0.85355	0.86629	0.13658	0.191
H(11A)	0.97116	0.94157	0.09412	0.329
H(11B)	0.91248	1.00750	0.09464	0.329
H(11C)	0.90615	0.94639	0.16509	0.329
H(11D)	0.92710	0.89328	0.01672	0.461
H(11E)	0.83027	0.86011	0.04008	0.461
H(11F)	0.85447	0.94484	0.00238	0.461
H(2S)	0.99398	1.28416	-0.12715	0.103
H(3S)	0.93816	1.23678	-0.19652	0.095
H(4S)	0.84304	1.13252	-0.14718	0.108
H(5S)	0.80373	1.07563	-0.02848	0.130
H(6S)	0.85955	1.12301	0.04089	0.111
H(7S1)	0.95363	1.21429	0.05613	0.211
H(7S2)	1.03708	1.24217	-0.00928	0.211
H(7S3)	0.96030	1.29260	0.00237	0.211

[1] U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

Table S32 Anisotropic displacement parameters $(Å^2)^2$ for **$[Sm(CzT^{iPr})_2]_2(\mu\text{-}OH)_2$, 6a • 0.5 C_7H_8**

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Sm(1)	0.0674(4)	0.0458(3)	0.0474(3)	-0.0102(2)	-0.0117(3)	0.0006(3)
Sm(2)	0.0543(4)	0.0468(3)	0.0499(3)	-0.0067(2)	-0.0145(3)	0.0019(2)
O(1)	0.072(5)	0.067(5)	0.134(8)	-0.047(5)	-0.046(5)	0.021(4)
N(1)	0.094(8)	0.057(6)	0.048(6)	-0.013(5)	0.009(5)	-0.006(5)
N(2)	0.051(6)	0.114(10)	0.108(9)	-0.039(8)	-0.011(6)	-0.005(6)
N(3)	0.075(7)	0.083(8)	0.105(9)	-0.030(7)	-0.033(7)	-0.014(6)
N(4)	0.073(7)	0.078(7)	0.097(8)	-0.026(6)	-0.030(6)	0.002(6)

N(5)	0.071(7)	0.068(6)	0.074(7)	-0.021(5)	-0.009(5)	0.008(5)
N(6)	0.174(12)	0.063(7)	0.057(7)	-0.024(6)	-0.035(7)	0.019(7)
N(7)	0.27(2)	0.102(10)	0.083(9)	-0.043(8)	-0.094(11)	0.065(12)
N(8)	0.33(3)	0.112(12)	0.104(11)	-0.055(10)	-0.141(14)	0.065(14)
N(9)	0.38(3)	0.090(10)	0.079(10)	-0.027(8)	-0.111(14)	0.022(14)
N(10)	0.054(5)	0.045(5)	0.050(5)	-0.007(4)	-0.012(4)	0.001(4)
N(15)	0.077(7)	0.064(6)	0.059(6)	-0.011(5)	-0.016(5)	-0.003(5)
N(16)	0.102(8)	0.072(7)	0.090(8)	-0.017(6)	-0.052(7)	-0.003(6)
N(17)	0.131(10)	0.084(9)	0.106(9)	-0.017(7)	-0.073(8)	-0.008(8)
N(18)	0.134(10)	0.066(7)	0.090(8)	-0.008(6)	-0.054(8)	-0.002(7)
N(19)	0.048(5)	0.048(5)	0.050(5)	-0.007(4)	-0.011(4)	0.001(4)
N(20)	0.053(6)	0.049(5)	0.088(7)	0.009(5)	-0.020(5)	0.014(4)
N(21)	0.063(6)	0.060(6)	0.126(10)	0.007(6)	-0.005(6)	0.010(5)
N(22)	0.067(7)	0.054(6)	0.105(8)	0.023(6)	-0.004(6)	0.003(5)
N(23)	0.054(6)	0.059(6)	0.119(9)	0.015(6)	-0.002(6)	0.003(5)
N(24)	0.049(5)	0.049(5)	0.048(5)	-0.015(4)	-0.015(4)	0.006(4)
N(25)	0.066(6)	0.057(6)	0.065(6)	-0.015(5)	-0.013(5)	-0.005(5)
N(26)	0.060(6)	0.088(8)	0.080(7)	-0.028(6)	-0.017(5)	-0.004(6)
N(27)	0.080(7)	0.060(6)	0.077(7)	-0.028(5)	-0.019(5)	0.008(5)
N(28)	0.074(6)	0.053(5)	0.044(5)	-0.007(4)	-0.019(4)	-0.004(5)
N(29)	0.063(6)	0.060(6)	0.072(6)	-0.005(5)	-0.017(5)	0.003(5)
N(30)	0.069(7)	0.070(8)	0.152(12)	0.006(7)	-0.038(7)	-0.011(6)
N(31)	0.095(9)	0.076(8)	0.157(13)	0.001(8)	-0.067(9)	-0.013(7)
N(32)	0.071(7)	0.077(8)	0.145(11)	0.000(7)	-0.055(7)	-0.007(6)
C(1)	0.069(8)	0.076(9)	0.076(9)	-0.003(7)	0.008(7)	0.021(7)
C(2)	0.047(7)	0.077(8)	0.082(9)	-0.017(7)	0.005(7)	0.002(6)
C(3)	0.059(8)	0.130(14)	0.119(13)	-0.045(11)	-0.002(8)	0.005(9)
C(4)	0.071(10)	0.126(14)	0.146(17)	-0.062(13)	0.009(10)	0.044(10)
C(5)	0.102(13)	0.109(13)	0.118(15)	-0.050(12)	-0.001(11)	0.023(11)
C(6)	0.099(11)	0.079(9)	0.079(10)	-0.051(8)	0.024(9)	0.000(8)
C(7)	0.139(14)	0.074(9)	0.053(8)	-0.025(7)	0.013(9)	-0.008(9)
C(8)	0.20(2)	0.073(10)	0.074(11)	-0.032(9)	0.010(12)	0.011(11)
C(9)	0.33(3)	0.077(12)	0.059(11)	-0.029(9)	-0.011(15)	-0.003(16)
C(10)	0.23(2)	0.076(10)	0.046(8)	-0.023(7)	-0.025(10)	-0.012(11)
C(11)	0.151(14)	0.053(8)	0.049(8)	0.006(6)	-0.003(9)	-0.003(8)
C(12)	0.121(11)	0.047(7)	0.055(8)	-0.018(6)	0.020(8)	-0.008(7)
C(13)	0.053(7)	0.075(8)	0.070(8)	-0.016(7)	0.006(6)	-0.016(6)
C(14)	0.101(12)	0.097(12)	0.176(19)	-0.040(13)	-0.041(13)	-0.008(10)
C(15)	0.167(19)	0.141(17)	0.22(2)	-0.102(18)	-0.096(18)	0.023(15)
C(16)	0.33(4)	0.33(4)	0.102(16)	-0.03(2)	-0.01(2)	-0.25(4)
C(17)	0.109(15)	0.17(2)	0.18(2)	-0.083(18)	-0.012(14)	0.070(14)
C(18)	0.33(4)	0.48(6)	0.21(3)	-0.18(4)	-0.15(3)	0.35(5)
C(19)	0.138(19)	0.15(2)	0.36(4)	-0.06(3)	-0.04(2)	0.073(17)
C(20)	0.060(13)	0.21(3)	0.57(7)	-0.06(4)	-0.10(2)	0.028(15)
C(21)	0.41(5)	0.110(18)	0.082(14)	-0.054(13)	-0.03(2)	-0.02(2)
C(22)	0.40(6)	0.25(4)	0.34(6)	-0.19(4)	-0.16(5)	0.05(5)

C(23)	0.74(9)	0.074(14)	0.092(15)	-0.048(12)	-0.08(3)	0.02(3)
C(24)	0.96(10)	0.103(16)	0.059(12)	-0.046(12)	-0.12(3)	0.04(3)
C(25)	0.194(18)	0.084(11)	0.053(9)	-0.002(8)	-0.043(10)	-0.014(11)
C(26)	0.36(4)	0.105(16)	0.18(3)	-0.022(18)	-0.21(3)	0.04(2)
C(27)	0.25(4)	0.21(4)	0.26(4)	-0.04(3)	-0.16(3)	0.00(3)
C(28)	0.37(4)	0.13(2)	0.110(16)	-0.038(15)	-0.12(2)	0.11(2)
C(29)	0.042(5)	0.053(6)	0.055(6)	-0.017(5)	-0.005(5)	0.010(5)
C(30)	0.062(6)	0.050(6)	0.053(6)	-0.012(5)	-0.010(5)	0.011(5)
C(31)	0.067(7)	0.061(7)	0.058(7)	-0.021(5)	-0.013(6)	0.015(5)
C(32)	0.066(7)	0.082(8)	0.076(8)	-0.017(7)	-0.029(6)	0.019(6)
C(33)	0.081(8)	0.072(8)	0.066(8)	-0.027(7)	-0.014(7)	0.033(6)
C(34)	0.051(6)	0.058(6)	0.048(6)	-0.011(5)	-0.009(5)	0.003(5)
C(35)	0.068(7)	0.053(6)	0.052(6)	-0.020(5)	-0.008(5)	0.005(5)
C(36)	0.096(9)	0.061(7)	0.082(9)	-0.029(7)	-0.025(7)	0.023(7)
C(37)	0.099(9)	0.068(8)	0.065(8)	-0.032(7)	-0.007(7)	0.009(7)
C(38)	0.113(11)	0.062(8)	0.071(8)	-0.022(6)	-0.033(8)	0.004(7)
C(39)	0.077(8)	0.056(7)	0.055(7)	-0.013(6)	-0.019(6)	0.000(6)
C(40)	0.056(6)	0.040(6)	0.061(7)	-0.002(5)	-0.005(5)	-0.006(5)
C(42)	0.080(8)	0.068(8)	0.062(7)	-0.026(6)	-0.013(6)	0.027(7)
C(43)	0.101(11)	0.135(13)	0.060(8)	-0.028(8)	-0.005(8)	0.016(9)
C(44)	0.161(14)	0.074(9)	0.076(10)	-0.030(8)	-0.033(9)	0.017(10)
C(45)	0.093(10)	0.129(13)	0.092(11)	-0.043(9)	-0.048(9)	0.047(9)
C(46)	0.129(13)	0.139(14)	0.091(11)	-0.048(10)	-0.059(10)	0.061(11)
C(47)	0.26(3)	0.24(3)	0.31(4)	0.08(3)	-0.23(3)	-0.14(3)
C(48)	0.22(2)	0.29(3)	0.20(2)	-0.15(2)	-0.16(2)	0.20(2)
C(49)	0.156(15)	0.056(8)	0.088(10)	-0.025(7)	-0.024(10)	0.013(9)
C(50)	0.162(16)	0.053(8)	0.137(14)	-0.032(9)	-0.031(12)	-0.002(9)
C(51)	0.167(16)	0.086(10)	0.121(13)	-0.049(10)	-0.059(12)	0.068(11)
C(52)	0.196(18)	0.086(11)	0.095(12)	-0.049(9)	-0.023(12)	0.046(11)
C(53)	0.103(9)	0.040(6)	0.054(7)	-0.011(5)	-0.032(6)	-0.015(6)
C(54)	0.174(19)	0.114(14)	0.158(19)	-0.021(13)	-0.112(16)	0.001(13)
C(55)	0.174(19)	0.113(15)	0.17(2)	-0.031(14)	-0.085(16)	-0.022(14)
C(56)	0.28(3)	0.28(4)	0.112(18)	-0.05(2)	-0.09(2)	-0.05(3)
C(57)	0.066(7)	0.063(7)	0.056(7)	0.001(6)	-0.019(6)	0.014(6)
C(58)	0.050(6)	0.058(7)	0.065(7)	0.012(5)	-0.012(5)	0.009(5)
C(59)	0.051(7)	0.073(8)	0.086(9)	0.008(7)	-0.011(6)	0.000(6)
C(60)	0.061(8)	0.090(10)	0.091(10)	-0.020(8)	-0.019(7)	0.011(7)
C(61)	0.073(9)	0.093(10)	0.067(8)	-0.014(7)	-0.018(7)	0.021(7)
C(62)	0.041(6)	0.079(8)	0.052(6)	-0.008(6)	-0.015(5)	-0.001(5)
C(63)	0.054(6)	0.078(8)	0.059(7)	-0.032(6)	-0.018(5)	0.023(6)
C(64)	0.074(8)	0.065(7)	0.062(7)	-0.019(6)	-0.018(6)	0.018(6)
C(65)	0.064(7)	0.066(7)	0.056(7)	-0.020(6)	-0.020(6)	0.016(6)
C(66)	0.087(9)	0.060(7)	0.048(6)	-0.013(5)	-0.022(6)	0.004(6)
C(67)	0.054(6)	0.051(6)	0.035(5)	-0.007(4)	-0.010(5)	0.009(5)
C(68)	0.071(7)	0.070(7)	0.038(6)	-0.017(5)	-0.023(5)	0.024(6)
C(69)	0.035(6)	0.077(8)	0.081(8)	-0.002(7)	-0.001(6)	-0.006(5)

C(70)	0.069(9)	0.056(8)	0.142(14)	0.023(9)	-0.011(9)	0.008(7)
C(71)	0.076(9)	0.106(12)	0.148(15)	0.047(11)	-0.029(10)	0.020(8)
C(72)	0.110(12)	0.052(8)	0.178(19)	-0.009(10)	-0.034(12)	0.000(8)
C(73)	0.027(6)	0.129(13)	0.132(13)	-0.025(11)	-0.010(7)	0.007(7)
C(74)	0.126(18)	0.15(2)	0.41(5)	-0.01(3)	0.12(3)	0.045(16)
C(75)	0.066(11)	0.20(2)	0.23(3)	0.10(2)	0.045(13)	0.029(12)
C(76)	0.073(14)	0.79(10)	0.18(3)	-0.15(4)	0.001(16)	-0.13(3)
C(77)	0.099(10)	0.068(8)	0.082(9)	-0.025(7)	-0.033(8)	0.033(7)
C(78)	0.150(15)	0.064(9)	0.152(15)	-0.046(10)	-0.059(12)	0.046(9)
C(79)	0.116(14)	0.089(12)	0.24(3)	-0.038(14)	-0.024(15)	0.033(11)
C(80)	0.27(3)	0.076(11)	0.131(16)	-0.015(11)	-0.087(16)	0.066(13)
C(81)	0.071(7)	0.054(6)	0.035(5)	-0.007(5)	-0.017(5)	-0.010(6)
C(82)	0.068(10)	0.087(11)	0.166(17)	-0.032(11)	-0.015(10)	-0.032(8)
C(83)	0.097(11)	0.117(13)	0.133(14)	-0.050(11)	-0.064(10)	-0.011(9)
C(84)	0.096(14)	0.153(19)	0.24(3)	-0.06(2)	-0.043(16)	-0.024(13)
C(85)	0.085(9)	0.058(7)	0.054(7)	-0.009(5)	-0.028(6)	0.006(6)
C(86)	0.076(8)	0.074(8)	0.067(8)	-0.004(6)	-0.029(6)	-0.005(7)
C(87)	0.061(8)	0.093(10)	0.084(9)	-0.011(8)	-0.026(7)	0.005(7)
C(88)	0.097(11)	0.080(10)	0.100(11)	-0.019(8)	-0.046(9)	0.022(8)
C(89)	0.118(12)	0.080(9)	0.093(10)	-0.026(8)	-0.065(9)	0.021(9)
C(90)	0.091(9)	0.069(8)	0.043(6)	-0.008(5)	-0.029(6)	0.002(7)
C(91)	0.088(9)	0.070(8)	0.043(6)	0.008(6)	-0.028(6)	-0.005(7)
C(92)	0.095(10)	0.063(8)	0.080(9)	-0.008(7)	-0.041(8)	0.002(7)
C(93)	0.125(13)	0.085(10)	0.078(9)	0.010(8)	-0.052(9)	-0.040(10)
C(94)	0.083(9)	0.092(10)	0.061(8)	-0.001(7)	-0.021(7)	-0.016(8)
C(95)	0.093(9)	0.053(7)	0.049(6)	-0.007(5)	-0.016(6)	-0.002(6)
C(96)	0.072(8)	0.063(7)	0.037(6)	-0.009(5)	-0.015(5)	-0.005(6)
C(97)	0.058(7)	0.082(9)	0.073(8)	-0.005(7)	-0.018(6)	-0.010(7)
C(98)	0.100(13)	0.073(11)	0.24(3)	-0.020(13)	-0.055(15)	-0.015(10)
C(99)	0.16(2)	0.075(15)	1.04(14)	-0.05(4)	-0.23(5)	-0.014(15)
C(100)	0.17(3)	0.21(3)	0.29(4)	-0.05(3)	0.06(3)	-0.08(2)
C(101)	0.111(13)	0.111(14)	0.19(2)	-0.030(14)	-0.071(14)	0.002(11)
C(105)	0.138(14)	0.091(11)	0.091(11)	0.009(9)	-0.037(10)	-0.036(10)
C(110)	0.103(14)	0.21(2)	0.100(14)	0.006(14)	0.004(11)	0.057(15)
C(111)	0.14(2)	0.32(4)	0.25(3)	-0.10(3)	-0.11(2)	0.01(2)
C(112)	0.40(5)	0.25(4)	0.16(3)	-0.09(2)	0.10(3)	0.06(3)
C(41)	0.090(6)	0.082(6)	0.103(7)	-0.037(6)	-0.034(6)	0.012(5)
N(11)	0.046(7)	0.050(7)	0.023(6)	0.003(5)	-0.007(5)	0.008(5)
N(12)	0.060(7)	0.048(7)	0.028(7)	-0.017(5)	-0.009(5)	0.011(6)
N(13)	0.064(8)	0.036(7)	0.052(9)	-0.010(6)	-0.009(7)	0.021(6)
N(14)	0.033(6)	0.053(7)	0.042(7)	-0.023(6)	0.009(5)	0.018(6)
C(41A)	0.090(6)	0.082(6)	0.103(7)	-0.037(6)	-0.034(6)	0.012(5)

[2] The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

Table S33 Bond lengths [Å] for **[Sm(CzT^{iPr})$_2$]$_2$(μ-OH)$_2$, 6a • 0.5 C$_7$H$_8$**

atom-atom	distance	atom-atom	distance
Sm(1)-O(1)	2.250(8)	Sm(1)-O(2A)	2.342(10)
Sm(1)-O(2B)	2.41(3)	Sm(1)-N(10)	2.522(8)
Sm(1)-N(1)	2.539(9)	Sm(1)-N(6)	2.559(11)
Sm(1)-N(11)	2.563(11)	Sm(1)-N(15)	2.588(10)
Sm(1)-N(5)	2.597(11)	Sm(1)-N(34A)	2.699(15)
Sm(1)-Sm(2)	3.7432(8)	Sm(2)-O(1)	2.241(8)
Sm(2)-O(2A)	2.319(10)	Sm(2)-O(2B)	2.35(3)
Sm(2)-N(28)	2.512(8)	Sm(2)-N(33A)	2.515(13)
Sm(2)-N(29)	2.531(10)	Sm(2)-N(19)	2.543(8)
Sm(2)-N(24)	2.573(8)	Sm(2)-N(20)	2.611(9)
Sm(2)-N(12)	2.711(12)	N(1)-C(1)	1.323(17)
N(1)-C(12)	1.389(17)	N(2)-N(3)	1.308(15)
N(2)-C(13)	1.315(17)	N(3)-N(4)	1.298(15)
N(3)-C(14)	1.47(2)	N(4)-N(5)	1.343(14)
N(5)-C(13)	1.339(16)	N(6)-C(25)	1.356(19)
N(6)-N(7)	1.380(18)	N(7)-N(8)	1.293(17)
N(8)-N(9)	1.29(2)	N(8)-C(26)	1.53(3)
N(9)-C(25)	1.39(2)	N(10)-C(29)	1.366(13)
N(10)-C(40)	1.416(13)	N(15)-C(53)	1.352(14)
N(15)-N(16)	1.354(14)	N(16)-N(17)	1.312(15)
N(17)-N(18)	1.325(16)	N(17)-C(54)	1.51(2)
N(18)-C(53)	1.342(16)	N(19)-C(68)	1.375(13)
N(19)-C(57)	1.395(13)	N(20)-C(69)	1.323(13)
N(20)-N(21)	1.326(13)	N(21)-N(22)	1.324(13)
N(22)-N(23)	1.316(14)	N(22)-C(70)	1.460(16)
N(23)-C(69)	1.337(15)	N(24)-N(25)	1.319(12)
N(24)-C(81)	1.345(13)	N(25)-N(26)	1.319(13)
N(26)-N(27)	1.343(13)	N(26)-C(82)	1.451(17)
N(27)-C(81)	1.323(14)	N(28)-C(96)	1.384(13)
N(28)-C(85)	1.402(14)	N(29)-N(30)	1.336(14)
N(29)-C(97)	1.359(15)	N(30)-N(31)	1.315(15)
N(31)-N(32)	1.346(15)	N(31)-C(98)	1.468(19)
N(32)-C(97)	1.324(15)	C(1)-C(2)	1.41(2)
C(1)-C(6)	1.470(18)	C(2)-C(3)	1.40(2)
C(2)-C(13)	1.463(18)	C(3)-C(4)	1.44(2)
C(3)-H(3)	0.9500	C(4)-C(5)	1.33(2)
C(4)-C(17)	1.57(3)	C(5)-C(6)	1.37(2)
C(5)-H(5)	0.9500	C(6)-C(7)	1.36(2)
C(7)-C(8)	1.40(2)	C(7)-C(12)	1.41(2)
C(8)-C(9)	1.42(3)	C(8)-H(8)	0.9500
C(9)-C(10)	1.35(3)	C(9)-C(21)	1.55(3)
C(10)-C(11)	1.39(2)	C(10)-H(10)	0.9500
C(11)-C(25)	1.39(2)	C(11)-C(12)	1.39(2)

C(14)-C(16)	1.47(2)	C(14)-C(15)	1.50(2)
C(14)-H(14)	1.0000	C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800	C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800	C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800	C(17)-C(18)	1.45(4)
C(17)-C(20)	1.49(3)	C(17)-C(19)	1.59(3)
C(18)-H(18A)	0.9800	C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800	C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800	C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800	C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800	C(21)-C(23)	1.41(5)
C(21)-C(24)	1.45(3)	C(21)-C(22)	1.61(5)
C(22)-H(22A)	0.9800	C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800	C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800	C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800	C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800	C(26)-C(27)	1.40(4)
C(26)-C(28)	1.51(3)	C(26)-H(26)	1.0000
C(27)-H(27A)	0.9800	C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800	C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800	C(28)-H(28C)	0.9800
C(29)-C(30)	1.396(15)	C(29)-C(34)	1.426(14)
C(30)-C(31)	1.353(16)	C(30)-C(41A)	1.506(17)
C(30)-C(41)	1.506(17)	C(31)-C(32)	1.426(16)
C(31)-H(31)	0.9500	C(32)-C(33)	1.382(17)
C(32)-C(45)	1.521(19)	C(33)-C(34)	1.392(16)
C(33)-H(33)	0.9500	C(34)-C(35)	1.434(15)
C(35)-C(40)	1.390(15)	C(35)-C(36)	1.416(15)
C(36)-C(37)	1.410(18)	C(36)-H(36)	0.9500
C(37)-C(38)	1.394(18)	C(37)-C(49)	1.576(17)
C(38)-C(39)	1.379(16)	C(38)-H(38)	0.9500
C(39)-C(40)	1.373(16)	C(39)-C(53)	1.406(16)
C(42)-C(43)	1.462(17)	C(42)-N(13)	1.508(15)
C(42)-N(13A)	1.53(3)	C(42)-C(44)	1.538(19)
C(42)-H(42A)	1.0000	C(42)-H(42B)	1.0000
C(43)-H(43A)	0.9800	C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800	C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800	C(44)-H(44C)	0.9800
C(45)-C(47)	1.45(2)	C(45)-C(46)	1.49(2)
C(45)-C(48)	1.57(2)	C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800	C(46)-H(46C)	0.9800
C(47)-H(47A)	0.9800	C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800	C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800	C(48)-H(48C)	0.9800
C(49)-C(51)	1.52(2)	C(49)-C(52)	1.52(2)
C(49)-C(50)	1.52(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(54)-C(55)	1.52(3)	C(54)-C(56)	1.55(3)
C(54)-H(54)	1.0000	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)	1.389(15)
C(57)-C(62)	1.421(15)	C(58)-C(59)	1.406(15)
C(58)-C(69)	1.465(16)	C(59)-C(60)	1.365(17)
C(59)-H(59)	0.9500	C(60)-C(61)	1.376(19)
C(60)-C(73)	1.554(18)	C(61)-C(62)	1.372(16)
C(61)-H(61)	0.9500	C(62)-C(63)	1.430(16)
C(63)-C(64)	1.413(16)	C(63)-C(68)	1.420(14)
C(64)-C(65)	1.350(16)	C(64)-H(64)	0.9500
C(65)-C(66)	1.407(16)	C(65)-C(77)	1.559(16)
C(66)-C(67)	1.409(15)	C(66)-H(66)	0.9500
C(67)-C(68)	1.379(15)	C(67)-C(81)	1.468(14)
C(70)-C(72)	1.47(2)	C(70)-C(71)	1.50(2)
C(70)-H(70)	1.0000	C(71)-H(71A)	0.9800
C(71)-H(71B)	0.9800	C(71)-H(71C)	0.9800
C(72)-H(72A)	0.9800	C(72)-H(72B)	0.9800
C(72)-H(72C)	0.9800	C(73)-C(75)	1.40(2)
C(73)-C(76)	1.45(3)	C(73)-C(74)	1.55(3)
C(74)-H(74A)	0.9800	C(74)-H(74B)	0.9800
C(74)-H(74C)	0.9800	C(75)-H(75A)	0.9800
C(75)-H(75B)	0.9800	C(75)-H(75C)	0.9800
C(76)-H(76A)	0.9800	C(76)-H(76B)	0.9800
C(76)-H(76C)	0.9800	C(77)-C(78)	1.49(2)
C(77)-C(79)	1.51(2)	C(77)-C(80)	1.53(2)
C(78)-H(78A)	0.9800	C(78)-H(78B)	0.9800
C(78)-H(78C)	0.9800	C(79)-H(79A)	0.9800
C(79)-H(79B)	0.9800	C(79)-H(79C)	0.9800
C(80)-H(80A)	0.9800	C(80)-H(80B)	0.9800
C(80)-H(80C)	0.9800	C(82)-C(84)	1.32(3)
C(82)-C(83)	1.49(2)	C(82)-H(82)	1.0000
C(83)-H(83A)	0.9800	C(83)-H(83B)	0.9800
C(83)-H(83C)	0.9800	C(84)-H(84A)	0.9800
C(84)-H(84B)	0.9800	C(84)-H(84C)	0.9800
C(85)-C(86)	1.422(17)	C(85)-C(90)	1.437(16)
C(86)-C(87)	1.402(17)	C(86)-C(97)	1.457(18)
C(87)-C(88)	1.375(19)	C(87)-H(87)	0.9500
C(88)-C(89)	1.39(2)	C(88)-C(101)	1.54(2)
C(89)-C(90)	1.392(17)	C(89)-H(89)	0.9500
C(90)-C(91)	1.430(17)	C(91)-C(92)	1.362(17)

C(91)-C(96)	1.400(16)	C(92)-C(93)	1.366(19)
C(92)-H(92)	0.9500	C(93)-C(94)	1.40(2)
C(93)-C(105)	1.563(19)	C(94)-C(95)	1.409(17)
C(94)-H(94)	0.9500	C(95)-C(109)	1.249(14)
C(95)-C(96)	1.380(16)	C(95)-C(09A)	1.543(17)
C(98)-C(100)	1.39(3)	C(98)-C(99)	1.41(3)
C(98)-H(98)	1.0000	C(99)-H(99A)	0.9800
C(99)-H(99B)	0.9800	C(99)-H(99C)	0.9800
C(100)-H(10A)	0.9800	C(100)-H(10B)	0.9800
C(100)-H(10C)	0.9800	C(101)-C(02A)	1.27(4)
C(101)-C(102)	1.38(4)	C(101)-C(103)	1.53(4)
C(101)-C(03A)	1.59(4)	C(101)-C(104)	1.60(4)
C(101)-C(04A)	1.66(4)	C(102)-H(10D)	0.9800
C(102)-H(10E)	0.9800	C(102)-H(10F)	0.9800
C(103)-H(10G)	0.9800	C(103)-H(10H)	0.9800
C(103)-H(10I)	0.9800	C(104)-H(10J)	0.9800
C(104)-H(10K)	0.9800	C(104)-H(10L)	0.9800
C(02A)-H(02A)	0.9800	C(02A)-H(02B)	0.9800
C(02A)-H(02C)	0.9800	C(03A)-H(03A)	0.9800
C(03A)-H(03B)	0.9800	C(03A)-H(03C)	0.9800
C(04A)-H(04A)	0.9800	C(04A)-H(04B)	0.9800
C(04A)-H(04C)	0.9800	C(105)-C(107)	1.489(19)
C(105)-C(07A)	1.491(18)	C(105)-C(106)	1.501(18)
C(105)-C(06A)	1.505(18)	C(105)-C(08A)	1.513(18)
C(105)-C(108)	1.515(18)	C(106)-H(10M)	0.9800
C(106)-H(10N)	0.9800	C(106)-H(10O)	0.9800
C(107)-H(10P)	0.9800	C(107)-H(10Q)	0.9800
C(107)-H(10R)	0.9800	C(108)-H(10S)	0.9800
C(108)-H(10T)	0.9800	C(108)-H(10U)	0.9800
C(06A)-H(06A)	0.9800	C(06A)-H(06B)	0.9800
C(06A)-H(06C)	0.9800	C(07A)-H(07A)	0.9800
C(07A)-H(07B)	0.9800	C(07A)-H(07C)	0.9800
C(08A)-H(08A)	0.9800	C(08A)-H(08B)	0.9800
C(08A)-H(08C)	0.9800	C(110)-N(35A)	1.29(2)
C(110)-C(111)	1.40(3)	C(110)-N(35)	1.47(2)
C(110)-C(112)	1.57(4)	C(110)-H(110)	1.0000
C(110)-H(11Z)	1.0000	C(111)-H(11A)	0.9800
C(111)-H(11B)	0.9800	C(111)-H(11C)	0.9800
C(112)-H(11D)	0.9800	C(112)-H(11E)	0.9800
C(112)-H(11F)	0.9800	C(41)-N(14)	1.250(16)
C(41)-N(11)	1.422(16)	N(11)-N(12)	1.316(15)
N(12)-N(13)	1.287(17)	N(13)-N(14)	1.296(15)
C(41A)-N(14A)	1.27(2)	C(41A)-N(11A)	1.45(2)
N(11A)-N(12A)	1.32(2)	N(12A)-N(13A)	1.30(2)
N(13A)-N(14A)	1.29(2)	C(109)-N(33)	1.4200
C(109)-N(36)	1.4200	N(33)-N(34)	1.4200

N(34)-N(35)	1.4200	N(35)-N(36)	1.4200
C(09A)-N(36A)	1.4200	C(09A)-N(33A)	1.4200
N(36A)-N(35A)	1.4200	N(35A)-N(34A)	1.4200
N(34A)-N(33A)	1.4200	C(1S)-C(2S)	1.3900
C(1S)-C(6S)	1.3900	C(1S)-C(7S)	1.61(4)
C(2S)-C(3S)	1.3900	C(2S)-H(2S)	0.9500
C(3S)-C(4S)	1.3900	C(3S)-H(3S)	0.9500
C(4S)-C(5S)	1.3900	C(4S)-H(4S)	0.9500
C(5S)-C(6S)	1.3900	C(5S)-H(5S)	0.9500
C(6S)-H(6S)	0.9500	C(7S)-H(7S1)	0.9800
C(7S)-H(7S2)	0.9800	C(7S)-H(7S3)	0.9800

Table S34 Bond angles [°] for **[Sm(CzT^{iPr})$_2$]$_2$(μ-OH)$_2$, 6a • 0.5 C$_7$H$_8$**

atom-atom-atom	angle	atom-atom-atom	angle
O(1)-Sm(1)-O(2A)	66.2(3)	O(1)-Sm(1)-O(2B)	66.9(7)
O(1)-Sm(1)-N(10)	113.6(3)	O(2A)-Sm(1)-N(10)	141.2(3)
O(2B)-Sm(1)-N(10)	101.1(7)	O(1)-Sm(1)-N(1)	143.3(4)
O(2A)-Sm(1)-N(1)	122.5(3)	O(2B)-Sm(1)-N(1)	145.5(7)
N(10)-Sm(1)-N(1)	82.1(3)	O(1)-Sm(1)-N(6)	76.5(4)
O(2A)-Sm(1)-N(6)	83.5(4)	O(2B)-Sm(1)-N(6)	121.8(8)
N(10)-Sm(1)-N(6)	135.3(3)	N(1)-Sm(1)-N(6)	70.0(4)
O(1)-Sm(1)-N(11)	82.3(3)	O(2A)-Sm(1)-N(11)	71.4(4)
N(10)-Sm(1)-N(11)	70.2(3)	N(1)-Sm(1)-N(11)	134.1(4)
N(6)-Sm(1)-N(11)	152.1(4)	O(1)-Sm(1)-N(15)	74.3(3)
O(2A)-Sm(1)-N(15)	136.9(3)	O(2B)-Sm(1)-N(15)	133.0(7)
N(10)-Sm(1)-N(15)	70.9(3)	N(1)-Sm(1)-N(15)	80.8(3)
N(6)-Sm(1)-N(15)	70.7(3)	N(11)-Sm(1)-N(15)	120.5(3)
O(1)-Sm(1)-N(5)	142.2(3)	O(2A)-Sm(1)-N(5)	81.1(3)
O(2B)-Sm(1)-N(5)	76.1(7)	N(10)-Sm(1)-N(5)	80.2(3)
N(1)-Sm(1)-N(5)	70.5(3)	N(6)-Sm(1)-N(5)	119.5(4)
N(11)-Sm(1)-N(5)	69.3(3)	N(15)-Sm(1)-N(5)	141.7(3)
O(1)-Sm(1)-N(34A)	85.4(4)	O(2B)-Sm(1)-N(34A)	63.5(8)
N(10)-Sm(1)-N(34A)	149.7(5)	N(1)-Sm(1)-N(34A)	96.6(5)
N(6)-Sm(1)-N(34A)	70.1(5)	N(15)-Sm(1)-N(34A)	139.1(5)
N(5)-Sm(1)-N(34A)	71.0(5)	O(1)-Sm(1)-Sm(2)	33.5(2)
O(2A)-Sm(1)-Sm(2)	36.4(2)	O(2B)-Sm(1)-Sm(2)	37.5(7)
N(10)-Sm(1)-Sm(2)	123.59(18)	N(1)-Sm(1)-Sm(2)	154.3(2)
N(6)-Sm(1)-Sm(2)	89.6(3)	N(11)-Sm(1)-Sm(2)	63.1(2)
N(15)-Sm(1)-Sm(2)	107.7(2)	N(5)-Sm(1)-Sm(2)	109.1(2)
N(34A)-Sm(1)-Sm(2)	60.7(4)	O(1)-Sm(2)-O(2A)	66.8(3)
O(1)-Sm(2)-O(2B)	68.2(7)	O(1)-Sm(2)-N(28)	117.1(3)
O(2A)-Sm(2)-N(28)	102.0(3)	O(2B)-Sm(2)-N(28)	141.1(7)
O(1)-Sm(2)-N(33A)	86.3(5)	O(2B)-Sm(2)-N(33A)	72.4(8)
N(28)-Sm(2)-N(33A)	69.7(5)	O(1)-Sm(2)-N(29)	74.4(3)
O(2A)-Sm(2)-N(29)	132.5(3)	O(2B)-Sm(2)-N(29)	138.8(7)
N(28)-Sm(2)-N(29)	72.3(3)	N(33A)-Sm(2)-N(29)	122.3(5)
O(1)-Sm(2)-N(19)	139.6(3)	O(2A)-Sm(2)-N(19)	145.8(3)
O(2B)-Sm(2)-N(19)	117.0(7)	N(28)-Sm(2)-N(19)	84.6(3)
N(33A)-Sm(2)-N(19)	134.1(5)	N(29)-Sm(2)-N(19)	81.6(3)
O(1)-Sm(2)-N(24)	143.5(3)	O(2A)-Sm(2)-N(24)	78.4(3)
O(2B)-Sm(2)-N(24)	78.7(7)	N(28)-Sm(2)-N(24)	79.9(3)
N(33A)-Sm(2)-N(24)	68.9(5)	N(29)-Sm(2)-N(24)	141.5(3)
N(19)-Sm(2)-N(24)	69.6(2)	O(1)-Sm(2)-N(20)	73.0(3)
O(2A)-Sm(2)-N(20)	118.0(3)	O(2B)-Sm(2)-N(20)	80.4(7)
N(28)-Sm(2)-N(20)	138.5(3)	N(33A)-Sm(2)-N(20)	150.5(5)
N(29)-Sm(2)-N(20)	72.6(3)	N(19)-Sm(2)-N(20)	69.0(3)
N(24)-Sm(2)-N(20)	117.1(3)	O(1)-Sm(2)-N(12)	83.2(3)

O(2A)-Sm(2)-N(12)	67.7(3)	N(28)-Sm(2)-N(12)	152.6(3)
N(29)-Sm(2)-N(12)	133.9(3)	N(19)-Sm(2)-N(12)	90.9(3)
N(24)-Sm(2)-N(12)	73.2(3)	N(20)-Sm(2)-N(12)	62.4(3)
O(1)-Sm(2)-Sm(1)	33.6(2)	O(2A)-Sm(2)-Sm(1)	36.8(3)
O(2B)-Sm(2)-Sm(1)	38.8(7)	N(28)-Sm(2)-Sm(1)	125.3(2)
N(33A)-Sm(2)-Sm(1)	65.3(4)	N(29)-Sm(2)-Sm(1)	107.8(2)
N(19)-Sm(2)-Sm(1)	150.02(18)	N(24)-Sm(2)-Sm(1)	109.86(18)
N(20)-Sm(2)-Sm(1)	86.37(19)	N(12)-Sm(2)-Sm(1)	61.7(2)
Sm(2)-O(1)-Sm(1)	112.9(3)	Sm(2)-O(2A)-Sm(1)	106.9(4)
Sm(2)-O(2B)-Sm(1)	103.7(11)	C(1)-N(1)-C(12)	106.5(12)
C(1)-N(1)-Sm(1)	122.1(8)	C(12)-N(1)-Sm(1)	123.5(9)
N(3)-N(2)-C(13)	102.1(12)	N(4)-N(3)-N(2)	115.9(11)
N(4)-N(3)-C(14)	122.1(14)	N(2)-N(3)-C(14)	122.0(14)
N(3)-N(4)-N(5)	103.7(10)	C(13)-N(5)-N(4)	106.9(11)
C(13)-N(5)-Sm(1)	126.7(9)	N(4)-N(5)-Sm(1)	122.6(8)
C(25)-N(6)-N(7)	107.4(13)	C(25)-N(6)-Sm(1)	130.6(10)
N(7)-N(6)-Sm(1)	118.5(8)	N(8)-N(7)-N(6)	103.3(14)
N(9)-N(8)-N(7)	118.2(16)	N(9)-N(8)-C(26)	126.2(17)
N(7)-N(8)-C(26)	114.8(19)	N(8)-N(9)-C(25)	102.0(14)
C(29)-N(10)-C(40)	105.4(8)	C(29)-N(10)-Sm(1)	124.0(6)
C(40)-N(10)-Sm(1)	119.6(7)	C(53)-N(15)-N(16)	108.1(10)
C(53)-N(15)-Sm(1)	127.1(8)	N(16)-N(15)-Sm(1)	123.4(7)
N(17)-N(16)-N(15)	103.8(10)	N(16)-N(17)-N(18)	115.3(11)
N(16)-N(17)-C(54)	121.7(14)	N(18)-N(17)-C(54)	122.9(14)
N(17)-N(18)-C(53)	103.0(11)	C(68)-N(19)-C(57)	105.7(8)
C(68)-N(19)-Sm(2)	120.6(6)	C(57)-N(19)-Sm(2)	123.5(7)
C(69)-N(20)-N(21)	105.7(9)	C(69)-N(20)-Sm(2)	133.6(7)
N(21)-N(20)-Sm(2)	119.2(7)	N(22)-N(21)-N(20)	105.1(9)
N(23)-N(22)-N(21)	115.2(9)	N(23)-N(22)-C(70)	123.9(10)
N(21)-N(22)-C(70)	120.8(10)	N(22)-N(23)-C(69)	99.7(9)
N(25)-N(24)-C(81)	107.6(8)	N(25)-N(24)-Sm(2)	122.8(6)
C(81)-N(24)-Sm(2)	128.3(7)	N(26)-N(25)-N(24)	105.4(9)
N(25)-N(26)-N(27)	113.3(9)	N(25)-N(26)-C(82)	122.5(11)
N(27)-N(26)-C(82)	124.2(12)	C(81)-N(27)-N(26)	102.3(9)
C(96)-N(28)-C(85)	102.9(9)	C(96)-N(28)-Sm(2)	126.8(7)
C(85)-N(28)-Sm(2)	121.5(6)	N(30)-N(29)-C(97)	105.3(10)
N(30)-N(29)-Sm(2)	121.6(8)	C(97)-N(29)-Sm(2)	132.3(8)
N(31)-N(30)-N(29)	105.9(11)	N(30)-N(31)-N(32)	114.6(11)
N(30)-N(31)-C(98)	121.6(13)	N(32)-N(31)-C(98)	123.8(13)
C(97)-N(32)-N(31)	100.7(10)	N(1)-C(1)-C(2)	131.6(13)
N(1)-C(1)-C(6)	110.5(16)	C(2)-C(1)-C(6)	117.9(14)
C(3)-C(2)-C(1)	119.5(13)	C(3)-C(2)-C(13)	117.7(15)
C(1)-C(2)-C(13)	122.5(13)	C(2)-C(3)-C(4)	121.3(17)
C(2)-C(3)-H(3)	119.4	C(4)-C(3)-H(3)	119.4
C(5)-C(4)-C(3)	118.0(17)	C(5)-C(4)-C(17)	128.1(18)
C(3)-C(4)-C(17)	114(2)	C(4)-C(5)-C(6)	124.5(17)

C(4)-C(5)-H(5)	117.7	C(6)-C(5)-H(5)	117.7
C(7)-C(6)-C(5)	136.0(15)	C(7)-C(6)-C(1)	105.2(16)
C(5)-C(6)-C(1)	118.7(18)	C(6)-C(7)-C(8)	132.9(17)
C(6)-C(7)-C(12)	107.6(14)	C(8)-C(7)-C(12)	119.3(19)
C(7)-C(8)-C(9)	121.8(18)	C(7)-C(8)-H(8)	119.1
C(9)-C(8)-H(8)	119.1	C(10)-C(9)-C(8)	116.6(17)
C(10)-C(9)-C(21)	124(3)	C(8)-C(9)-C(21)	119(3)
C(9)-C(10)-C(11)	123(2)	C(9)-C(10)-H(10)	118.3
C(11)-C(10)-H(10)	118.3	C(25)-C(11)-C(10)	118.5(18)
C(25)-C(11)-C(12)	120.9(14)	C(10)-C(11)-C(12)	120.5(16)
N(1)-C(12)-C(11)	131.7(13)	N(1)-C(12)-C(7)	110.1(16)
C(11)-C(12)-C(7)	118.2(14)	N(2)-C(13)-N(5)	111.4(12)
N(2)-C(13)-C(2)	124.5(14)	N(5)-C(13)-C(2)	124.1(13)
C(16)-C(14)-N(3)	107.2(17)	C(16)-C(14)-C(15)	116(2)
N(3)-C(14)-C(15)	110.8(14)	C(16)-C(14)-H(14)	107.5
N(3)-C(14)-H(14)	107.5	C(15)-C(14)-H(14)	107.5
C(14)-C(15)-H(15A)	109.5	C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5	C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5	H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5	C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5	C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5	H(16B)-C(16)-H(16C)	109.5
C(18)-C(17)-C(20)	117(3)	C(18)-C(17)-C(4)	113.7(16)
C(20)-C(17)-C(4)	108(2)	C(18)-C(17)-C(19)	104(3)
C(20)-C(17)-C(19)	110(2)	C(4)-C(17)-C(19)	104(2)
C(17)-C(18)-H(18A)	109.5	C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5	C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5	H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5	C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5	C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5	H(19B)-C(19)-H(19C)	109.5
C(17)-C(20)-H(20A)	109.5	C(17)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5	C(17)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5	H(20B)-C(20)-H(20C)	109.5
C(23)-C(21)-C(24)	121(3)	C(23)-C(21)-C(9)	114(3)
C(24)-C(21)-C(9)	107.7(18)	C(23)-C(21)-C(22)	103(3)
C(24)-C(21)-C(22)	106(4)	C(9)-C(21)-C(22)	102(3)
C(21)-C(22)-H(22A)	109.5	C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5	C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5	H(22B)-C(22)-H(22C)	109.5
C(21)-C(23)-H(23A)	109.5	C(21)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5	C(21)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5	H(23B)-C(23)-H(23C)	109.5
C(21)-C(24)-H(24A)	109.5	C(21)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5	C(21)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5	H(24B)-C(24)-H(24C)	109.5

N(6)-C(25)-C(11)	127.5(16)	N(6)-C(25)-N(9)	108.7(17)
C(11)-C(25)-N(9)	123.3(17)	C(27)-C(26)-C(28)	118(3)
C(27)-C(26)-N(8)	119(3)	C(28)-C(26)-N(8)	101(2)
C(27)-C(26)-H(26)	106.0	C(28)-C(26)-H(26)	106.0
N(8)-C(26)-H(26)	106.0	C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5	H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5	H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5	C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5	H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5	H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5	N(10)-C(29)-C(30)	132.5(9)
N(10)-C(29)-C(34)	111.4(9)	C(30)-C(29)-C(34)	116.1(10)
C(31)-C(30)-C(29)	121.1(10)	C(31)-C(30)-C(41A)	118.1(11)
C(29)-C(30)-C(41A)	120.8(11)	C(31)-C(30)-C(41)	118.1(11)
C(29)-C(30)-C(41)	120.8(11)	C(30)-C(31)-C(32)	123.7(11)
C(30)-C(31)-H(31)	118.1	C(32)-C(31)-H(31)	118.1
C(33)-C(32)-C(31)	115.6(11)	C(33)-C(32)-C(45)	124.1(11)
C(31)-C(32)-C(45)	120.3(12)	C(32)-C(33)-C(34)	121.4(10)
C(32)-C(33)-H(33)	119.3	C(34)-C(33)-H(33)	119.3
C(33)-C(34)-C(29)	121.8(10)	C(33)-C(34)-C(35)	132.6(10)
C(29)-C(34)-C(35)	105.6(10)	C(40)-C(35)-C(36)	123.1(11)
C(40)-C(35)-C(34)	106.6(9)	C(36)-C(35)-C(34)	130.2(11)
C(37)-C(36)-C(35)	115.9(12)	C(37)-C(36)-H(36)	122.0
C(35)-C(36)-H(36)	122.0	C(38)-C(37)-C(36)	119.7(11)
C(38)-C(37)-C(49)	119.0(13)	C(36)-C(37)-C(49)	121.1(13)
C(39)-C(38)-C(37)	122.9(12)	C(39)-C(38)-H(38)	118.6
C(37)-C(38)-H(38)	118.6	C(40)-C(39)-C(38)	118.6(12)
C(40)-C(39)-C(53)	124.6(10)	C(38)-C(39)-C(53)	116.7(11)
C(39)-C(40)-C(35)	119.6(10)	C(39)-C(40)-N(10)	129.3(11)
C(35)-C(40)-N(10)	110.9(10)	C(43)-C(42)-N(13)	113.0(11)
C(43)-C(42)-N(13A)	97.8(19)	C(43)-C(42)-C(44)	115.8(12)
N(13)-C(42)-C(44)	106.8(11)	N(13A)-C(42)-C(44)	98.1(19)
C(43)-C(42)-H(42A)	106.9	N(13)-C(42)-H(42A)	106.9
C(44)-C(42)-H(42A)	106.9	C(43)-C(42)-H(42B)	114.3
N(13A)-C(42)-H(42B)	114.3	C(44)-C(42)-H(42B)	114.3
C(42)-C(43)-H(43A)	109.5	C(42)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5	C(42)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5	H(43B)-C(43)-H(43C)	109.5
C(42)-C(44)-H(44A)	109.5	C(42)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5	C(42)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5	H(44B)-C(44)-H(44C)	109.5
C(47)-C(45)-C(46)	116(2)	C(47)-C(45)-C(32)	111.2(15)
C(46)-C(45)-C(32)	108.5(12)	C(47)-C(45)-C(48)	105.2(19)
C(46)-C(45)-C(48)	105.5(15)	C(32)-C(45)-C(48)	109.7(13)
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

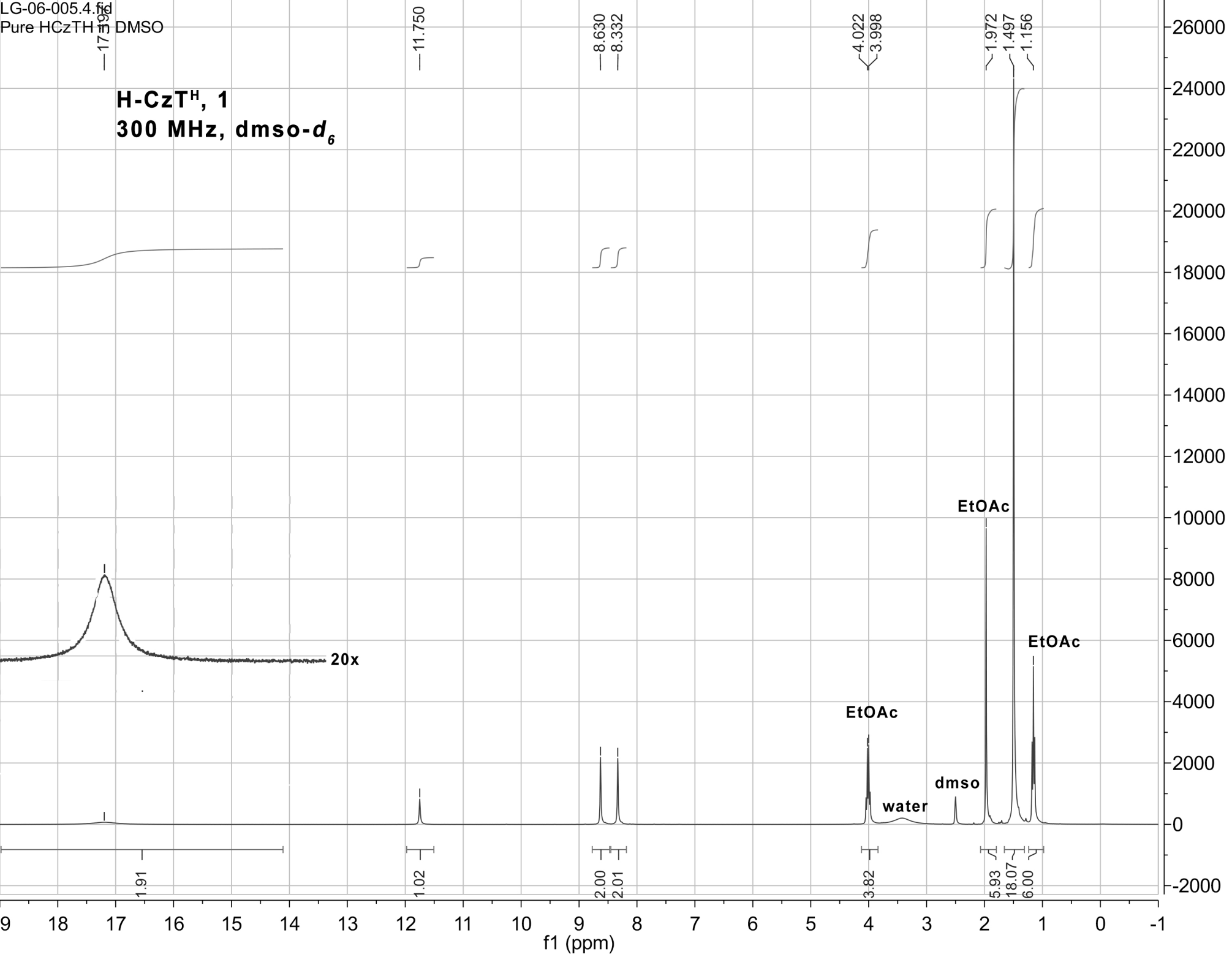
H(46A)-C(46)-H(46C)	109.5	H(46B)-C(46)-H(46C)	109.5
C(45)-C(47)-H(47A)	109.5	C(45)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5	C(45)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5	H(47B)-C(47)-H(47C)	109.5
C(45)-C(48)-H(48A)	109.5	C(45)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5	C(45)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5	H(48B)-C(48)-H(48C)	109.5
C(51)-C(49)-C(52)	108.6(15)	C(51)-C(49)-C(50)	109.8(13)
C(52)-C(49)-C(50)	111.2(15)	C(51)-C(49)-C(37)	111.2(13)
C(52)-C(49)-C(37)	106.7(11)	C(50)-C(49)-C(37)	109.2(13)
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
N(18)-C(53)-N(15)	109.8(12)	N(18)-C(53)-C(39)	124.5(11)
N(15)-C(53)-C(39)	125.6(10)	N(17)-C(54)-C(55)	106.9(15)
N(17)-C(54)-C(56)	107.2(18)	C(55)-C(54)-C(56)	116(2)
N(17)-C(54)-H(54)	108.8	C(55)-C(54)-H(54)	108.8
C(56)-C(54)-H(54)	108.8	C(54)-C(55)-H(55A)	109.5
C(54)-C(55)-H(55B)	109.5	H(55A)-C(55)-H(55B)	109.5
C(54)-C(55)-H(55C)	109.5	H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5	C(54)-C(56)-H(56A)	109.5
C(54)-C(56)-H(56B)	109.5	H(56A)-C(56)-H(56B)	109.5
C(54)-C(56)-H(56C)	109.5	H(56A)-C(56)-H(56C)	109.5
H(56B)-C(56)-H(56C)	109.5	C(58)-C(57)-N(19)	130.7(10)
C(58)-C(57)-C(62)	117.4(10)	N(19)-C(57)-C(62)	111.8(9)
C(57)-C(58)-C(59)	118.6(11)	C(57)-C(58)-C(69)	122.7(10)
C(59)-C(58)-C(69)	118.4(10)	C(60)-C(59)-C(58)	123.1(12)
C(60)-C(59)-H(59)	118.5	C(58)-C(59)-H(59)	118.5
C(59)-C(60)-C(61)	118.4(12)	C(59)-C(60)-C(73)	119.0(13)
C(61)-C(60)-C(73)	122.6(12)	C(62)-C(61)-C(60)	120.3(12)
C(62)-C(61)-H(61)	119.8	C(60)-C(61)-H(61)	119.8
C(61)-C(62)-C(57)	122.0(11)	C(61)-C(62)-C(63)	133.3(11)
C(57)-C(62)-C(63)	104.5(9)	C(64)-C(63)-C(68)	119.6(11)
C(64)-C(63)-C(62)	133.0(10)	C(68)-C(63)-C(62)	107.2(10)
C(65)-C(64)-C(63)	121.4(11)	C(65)-C(64)-H(64)	119.3
C(63)-C(64)-H(64)	119.3	C(64)-C(65)-C(66)	118.6(11)
C(64)-C(65)-C(77)	125.1(11)	C(66)-C(65)-C(77)	116.2(11)
C(65)-C(66)-C(67)	121.5(11)	C(65)-C(66)-H(66)	119.2
C(67)-C(66)-H(66)	119.2	C(68)-C(67)-C(66)	119.4(9)
C(68)-C(67)-C(81)	121.6(9)	C(66)-C(67)-C(81)	118.6(10)

N(19)-C(68)-C(67)	130.3(9)	N(19)-C(68)-C(63)	110.7(10)
C(67)-C(68)-C(63)	119.0(10)	N(20)-C(69)-N(23)	114.1(11)
N(20)-C(69)-C(58)	122.7(10)	N(23)-C(69)-C(58)	123.1(10)
N(22)-C(70)-C(72)	110.0(14)	N(22)-C(70)-C(71)	109.1(15)
C(72)-C(70)-C(71)	112.7(14)	N(22)-C(70)-H(70)	108.3
C(72)-C(70)-H(70)	108.3	C(71)-C(70)-H(70)	108.3
C(70)-C(71)-H(71A)	109.5	C(70)-C(71)-H(71B)	109.5
H(71A)-C(71)-H(71B)	109.5	C(70)-C(71)-H(71C)	109.5
H(71A)-C(71)-H(71C)	109.5	H(71B)-C(71)-H(71C)	109.5
C(70)-C(72)-H(72A)	109.5	C(70)-C(72)-H(72B)	109.5
H(72A)-C(72)-H(72B)	109.5	C(70)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5	H(72B)-C(72)-H(72C)	109.5
C(75)-C(73)-C(76)	117(2)	C(75)-C(73)-C(74)	107(2)
C(76)-C(73)-C(74)	104(2)	C(75)-C(73)-C(60)	115.2(13)
C(76)-C(73)-C(60)	103.3(15)	C(74)-C(73)-C(60)	109.1(15)
C(73)-C(74)-H(74A)	109.5	C(73)-C(74)-H(74B)	109.5
H(74A)-C(74)-H(74B)	109.5	C(73)-C(74)-H(74C)	109.5
H(74A)-C(74)-H(74C)	109.5	H(74B)-C(74)-H(74C)	109.5
C(73)-C(75)-H(75A)	109.5	C(73)-C(75)-H(75B)	109.5
H(75A)-C(75)-H(75B)	109.5	C(73)-C(75)-H(75C)	109.5
H(75A)-C(75)-H(75C)	109.5	H(75B)-C(75)-H(75C)	109.5
C(73)-C(76)-H(76A)	109.5	C(73)-C(76)-H(76B)	109.5
H(76A)-C(76)-H(76B)	109.5	C(73)-C(76)-H(76C)	109.5
H(76A)-C(76)-H(76C)	109.5	H(76B)-C(76)-H(76C)	109.5
C(78)-C(77)-C(79)	107.8(14)	C(78)-C(77)-C(80)	108.9(15)
C(79)-C(77)-C(80)	107.3(15)	C(78)-C(77)-C(65)	112.1(11)
C(79)-C(77)-C(65)	109.6(12)	C(80)-C(77)-C(65)	110.9(11)
C(77)-C(78)-H(78A)	109.5	C(77)-C(78)-H(78B)	109.5
H(78A)-C(78)-H(78B)	109.5	C(77)-C(78)-H(78C)	109.5
H(78A)-C(78)-H(78C)	109.5	H(78B)-C(78)-H(78C)	109.5
C(77)-C(79)-H(79A)	109.5	C(77)-C(79)-H(79B)	109.5
H(79A)-C(79)-H(79B)	109.5	C(77)-C(79)-H(79C)	109.5
H(79A)-C(79)-H(79C)	109.5	H(79B)-C(79)-H(79C)	109.5
C(77)-C(80)-H(80A)	109.5	C(77)-C(80)-H(80B)	109.5
H(80A)-C(80)-H(80B)	109.5	C(77)-C(80)-H(80C)	109.5
H(80A)-C(80)-H(80C)	109.5	H(80B)-C(80)-H(80C)	109.5
N(27)-C(81)-N(24)	111.3(10)	N(27)-C(81)-C(67)	124.8(10)
N(24)-C(81)-C(67)	124.0(9)	C(84)-C(82)-N(26)	111.1(18)
C(84)-C(82)-C(83)	115.6(16)	N(26)-C(82)-C(83)	111.7(14)
C(84)-C(82)-H(82)	105.9	N(26)-C(82)-H(82)	105.9
C(83)-C(82)-H(82)	105.9	C(82)-C(83)-H(83A)	109.5
C(82)-C(83)-H(83B)	109.5	H(83A)-C(83)-H(83B)	109.5
C(82)-C(83)-H(83C)	109.5	H(83A)-C(83)-H(83C)	109.5
H(83B)-C(83)-H(83C)	109.5	C(82)-C(84)-H(84A)	109.5
C(82)-C(84)-H(84B)	109.5	H(84A)-C(84)-H(84B)	109.5
C(82)-C(84)-H(84C)	109.5	H(84A)-C(84)-H(84C)	109.5

H(84B)-C(84)-H(84C)	109.5	N(28)-C(85)-C(86)	130.8(10)
N(28)-C(85)-C(90)	111.9(10)	C(86)-C(85)-C(90)	117.2(11)
C(87)-C(86)-C(85)	118.6(12)	C(87)-C(86)-C(97)	118.2(11)
C(85)-C(86)-C(97)	123.1(11)	C(88)-C(87)-C(86)	124.3(13)
C(88)-C(87)-H(87)	117.9	C(86)-C(87)-H(87)	117.9
C(87)-C(88)-C(89)	117.4(13)	C(87)-C(88)-C(101)	121.9(14)
C(89)-C(88)-C(101)	120.6(14)	C(88)-C(89)-C(90)	121.4(13)
C(88)-C(89)-H(89)	119.3	C(90)-C(89)-H(89)	119.3
C(89)-C(90)-C(91)	133.2(12)	C(89)-C(90)-C(85)	121.1(12)
C(91)-C(90)-C(85)	105.3(11)	C(92)-C(91)-C(96)	122.6(12)
C(92)-C(91)-C(90)	132.1(13)	C(96)-C(91)-C(90)	105.3(10)
C(91)-C(92)-C(93)	121.9(13)	C(91)-C(92)-H(92)	119.0
C(93)-C(92)-H(92)	119.0	C(92)-C(93)-C(94)	116.6(12)
C(92)-C(93)-C(105)	124.5(16)	C(94)-C(93)-C(105)	118.8(15)
C(93)-C(94)-C(95)	121.9(13)	C(93)-C(94)-H(94)	119.1
C(95)-C(94)-H(94)	119.1	C(109)-C(95)-C(96)	129.7(12)
C(109)-C(95)-C(94)	108.7(13)	C(96)-C(95)-C(94)	119.8(12)
C(96)-C(95)-C(09A)	121.9(11)	C(94)-C(95)-C(09A)	118.3(13)
C(95)-C(96)-N(28)	128.8(11)	C(95)-C(96)-C(91)	116.8(10)
N(28)-C(96)-C(91)	114.4(10)	N(32)-C(97)-N(29)	113.4(12)
N(32)-C(97)-C(86)	123.5(12)	N(29)-C(97)-C(86)	123.0(11)
C(100)-C(98)-C(99)	115(3)	C(100)-C(98)-N(31)	108(2)
C(99)-C(98)-N(31)	111.0(17)	C(100)-C(98)-H(98)	107.4
C(99)-C(98)-H(98)	107.4	N(31)-C(98)-H(98)	107.4
C(98)-C(99)-H(99A)	109.5	C(98)-C(99)-H(99B)	109.5
H(99A)-C(99)-H(99B)	109.5	C(98)-C(99)-H(99C)	109.5
H(99A)-C(99)-H(99C)	109.5	H(99B)-C(99)-H(99C)	109.5
C(98)-C(100)-H(10A)	109.5	C(98)-C(100)-H(10B)	109.5
H(10A)-C(100)-H(10B)	109.5	C(98)-C(100)-H(10C)	109.5
H(10A)-C(100)-H(10C)	109.5	H(10B)-C(100)-H(10C)	109.5
C(102)-C(101)-C(103)	116(3)	C(02A)-C(101)-C(88)	117(2)
C(102)-C(101)-C(88)	112(2)	C(103)-C(101)-C(88)	102(2)
C(02A)-C(101)-C(03A)	114(3)	C(88)-C(101)-C(03A)	108(2)
C(102)-C(101)-C(104)	121(3)	C(103)-C(101)-C(104)	99(2)
C(88)-C(101)-C(104)	104.6(19)	C(02A)-C(101)-C(04A)	112(3)
C(88)-C(101)-C(04A)	107.2(17)	C(03A)-C(101)-C(04A)	96(2)
C(101)-C(102)-H(10D)	109.5	C(101)-C(102)-H(10E)	109.5
H(10D)-C(102)-H(10E)	109.5	C(101)-C(102)-H(10F)	109.5
H(10D)-C(102)-H(10F)	109.5	H(10E)-C(102)-H(10F)	109.5
C(101)-C(103)-H(10G)	109.5	C(101)-C(103)-H(10H)	109.5
H(10G)-C(103)-H(10H)	109.5	C(101)-C(103)-H(10I)	109.5
H(10G)-C(103)-H(10I)	109.5	H(10H)-C(103)-H(10I)	109.5
C(101)-C(104)-H(10J)	109.5	C(101)-C(104)-H(10K)	109.5
H(10J)-C(104)-H(10K)	109.5	C(101)-C(104)-H(10L)	109.5
H(10J)-C(104)-H(10L)	109.5	H(10K)-C(104)-H(10L)	109.5
C(101)-C(02A)-H(02A)	109.5	C(101)-C(02A)-H(02B)	109.5

H(02A)-C(02A)-H(02B)	109.5	C(101)-C(02A)-H(02C)	109.5
H(02A)-C(02A)-H(02C)	109.5	H(02B)-C(02A)-H(02C)	109.5
C(101)-C(03A)-H(03A)	109.5	C(101)-C(03A)-H(03B)	109.5
H(03A)-C(03A)-H(03B)	109.5	C(101)-C(03A)-H(03C)	109.5
H(03A)-C(03A)-H(03C)	109.5	H(03B)-C(03A)-H(03C)	109.5
C(101)-C(04A)-H(04A)	109.5	C(101)-C(04A)-H(04B)	109.5
H(04A)-C(04A)-H(04B)	109.5	C(101)-C(04A)-H(04C)	109.5
H(04A)-C(04A)-H(04C)	109.5	H(04B)-C(04A)-H(04C)	109.5
C(107)-C(105)-C(106)	124(3)	C(07A)-C(105)-C(06A)	113(3)
C(07A)-C(105)-C(08A)	110(2)	C(06A)-C(105)-C(08A)	99(2)
C(107)-C(105)-C(108)	98(3)	C(106)-C(105)-C(108)	104(2)
C(107)-C(105)-C(93)	113(2)	C(07A)-C(105)-C(93)	109.7(19)
C(106)-C(105)-C(93)	107.4(18)	C(06A)-C(105)-C(93)	110.5(19)
C(08A)-C(105)-C(93)	114.5(18)	C(108)-C(105)-C(93)	108(2)
C(105)-C(106)-H(10M)	109.5	C(105)-C(106)-H(10N)	109.5
H(10M)-C(106)-H(10N)	109.5	C(105)-C(106)-H(10O)	109.5
H(10M)-C(106)-H(10O)	109.5	H(10N)-C(106)-H(10O)	109.5
C(105)-C(107)-H(10P)	109.5	C(105)-C(107)-H(10Q)	109.5
H(10P)-C(107)-H(10Q)	109.5	C(105)-C(107)-H(10R)	109.5
H(10P)-C(107)-H(10R)	109.5	H(10Q)-C(107)-H(10R)	109.5
C(105)-C(108)-H(10S)	109.5	C(105)-C(108)-H(10T)	109.5
H(10S)-C(108)-H(10T)	109.5	C(105)-C(108)-H(10U)	109.5
H(10S)-C(108)-H(10U)	109.5	H(10T)-C(108)-H(10U)	109.5
C(105)-C(06A)-H(06A)	109.5	C(105)-C(06A)-H(06B)	109.5
H(06A)-C(06A)-H(06B)	109.5	C(105)-C(06A)-H(06C)	109.5
H(06A)-C(06A)-H(06C)	109.5	H(06B)-C(06A)-H(06C)	109.5
C(105)-C(07A)-H(07A)	109.5	C(105)-C(07A)-H(07B)	109.5
H(07A)-C(07A)-H(07B)	109.5	C(105)-C(07A)-H(07C)	109.5
H(07A)-C(07A)-H(07C)	109.5	H(07B)-C(07A)-H(07C)	109.5
C(105)-C(08A)-H(08A)	109.5	C(105)-C(08A)-H(08B)	109.5
H(08A)-C(08A)-H(08B)	109.5	C(105)-C(08A)-H(08C)	109.5
H(08A)-C(08A)-H(08C)	109.5	H(08B)-C(08A)-H(08C)	109.5
N(35A)-C(110)-C(111)	118(3)	C(111)-C(110)-N(35)	110(2)
N(35A)-C(110)-C(112)	111(3)	C(111)-C(110)-C(112)	119(2)
N(35)-C(110)-C(112)	98(2)	C(111)-C(110)-H(110)	110.1
N(35)-C(110)-H(110)	110.1	C(112)-C(110)-H(110)	110.1
N(35A)-C(110)-H(11Z)	101.8	C(111)-C(110)-H(11Z)	101.8
C(112)-C(110)-H(11Z)	101.8	C(110)-C(111)-H(11A)	109.5
C(110)-C(111)-H(11B)	109.5	H(11A)-C(111)-H(11B)	109.5
C(110)-C(111)-H(11C)	109.5	H(11A)-C(111)-H(11C)	109.5
H(11B)-C(111)-H(11C)	109.5	C(110)-C(112)-H(11D)	109.5
C(110)-C(112)-H(11E)	109.5	H(11D)-C(112)-H(11E)	109.5
C(110)-C(112)-H(11F)	109.5	H(11D)-C(112)-H(11F)	109.5
H(11E)-C(112)-H(11F)	109.5	N(14)-C(41)-N(11)	109.7(12)
N(14)-C(41)-C(30)	130.3(13)	N(11)-C(41)-C(30)	120.0(12)
N(12)-N(11)-C(41)	104.7(10)	N(12)-N(11)-Sm(1)	120.6(8)

C(41)-N(11)-Sm(1)	134.6(9)	N(13)-N(12)-N(11)	105.3(10)
N(13)-N(12)-Sm(2)	139.8(8)	N(11)-N(12)-Sm(2)	113.2(8)
N(12)-N(13)-N(14)	115.1(11)	N(12)-N(13)-C(42)	122.2(11)
N(14)-N(13)-C(42)	122.3(12)	C(41)-N(14)-N(13)	105.0(12)
N(14A)-C(41A)-N(11A)	101(2)	N(14A)-C(41A)-C(30)	119(2)
N(11A)-C(41A)-C(30)	105.6(18)	N(12A)-N(11A)-C(41A)	106.0(19)
N(13A)-N(12A)-N(11A)	103(2)	N(14A)-N(13A)-N(12A)	111(2)
N(14A)-N(13A)-C(42)	151(3)	N(12A)-N(13A)-C(42)	98(3)
C(41A)-N(14A)-N(13A)	103(2)	C(95)-C(109)-N(33)	123.7(12)
C(95)-C(109)-N(36)	128.3(12)	N(33)-C(109)-N(36)	108.0
C(109)-N(33)-N(34)	108.0	N(35)-N(34)-N(33)	108.0
N(34)-N(35)-N(36)	108.0	N(34)-N(35)-C(110)	114.9(15)
N(36)-N(35)-C(110)	136.7(15)	N(35)-N(36)-C(109)	108.0
N(36A)-C(09A)-N(33A)	108.0	N(36A)-C(09A)-C(95)	132.2(12)
N(33A)-C(09A)-C(95)	119.3(12)	C(09A)-N(36A)-N(35A)	108.0
C(110)-N(35A)-N(34A)	136.2(18)	C(110)-N(35A)-N(36A)	115.7(18)
N(34A)-N(35A)-N(36A)	108.0	N(33A)-N(34A)-N(35A)	108.0
N(33A)-N(34A)-Sm(1)	114.4(10)	N(35A)-N(34A)-Sm(1)	135.1(10)
N(34A)-N(33A)-C(09A)	108.0	N(34A)-N(33A)-Sm(2)	115.5(10)
C(09A)-N(33A)-Sm(2)	135.8(10)	C(2S)-C(1S)-C(6S)	120.0
C(2S)-C(1S)-C(7S)	117.1(19)	C(6S)-C(1S)-C(7S)	122.9(19)
C(3S)-C(2S)-C(1S)	120.0	C(3S)-C(2S)-H(2S)	120.0
C(1S)-C(2S)-H(2S)	120.0	C(2S)-C(3S)-C(4S)	120.0
C(2S)-C(3S)-H(3S)	120.0	C(4S)-C(3S)-H(3S)	120.0
C(5S)-C(4S)-C(3S)	120.0	C(5S)-C(4S)-H(4S)	120.0
C(3S)-C(4S)-H(4S)	120.0	C(6S)-C(5S)-C(4S)	120.0
C(6S)-C(5S)-H(5S)	120.0	C(4S)-C(5S)-H(5S)	120.0
C(5S)-C(6S)-C(1S)	120.0	C(5S)-C(6S)-H(6S)	120.0
C(1S)-C(6S)-H(6S)	120.0	C(1S)-C(7S)-H(7S1)	109.5
C(1S)-C(7S)-H(7S2)	109.5	H(7S1)-C(7S)-H(7S2)	109.5
C(1S)-C(7S)-H(7S3)	109.5	H(7S1)-C(7S)-H(7S3)	109.5
H(7S2)-C(7S)-H(7S3)	109.5		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4.022
3.998
1.972
1.497
1.156
20x
EtOAc
EtOAc
EtOAc
water
dmso
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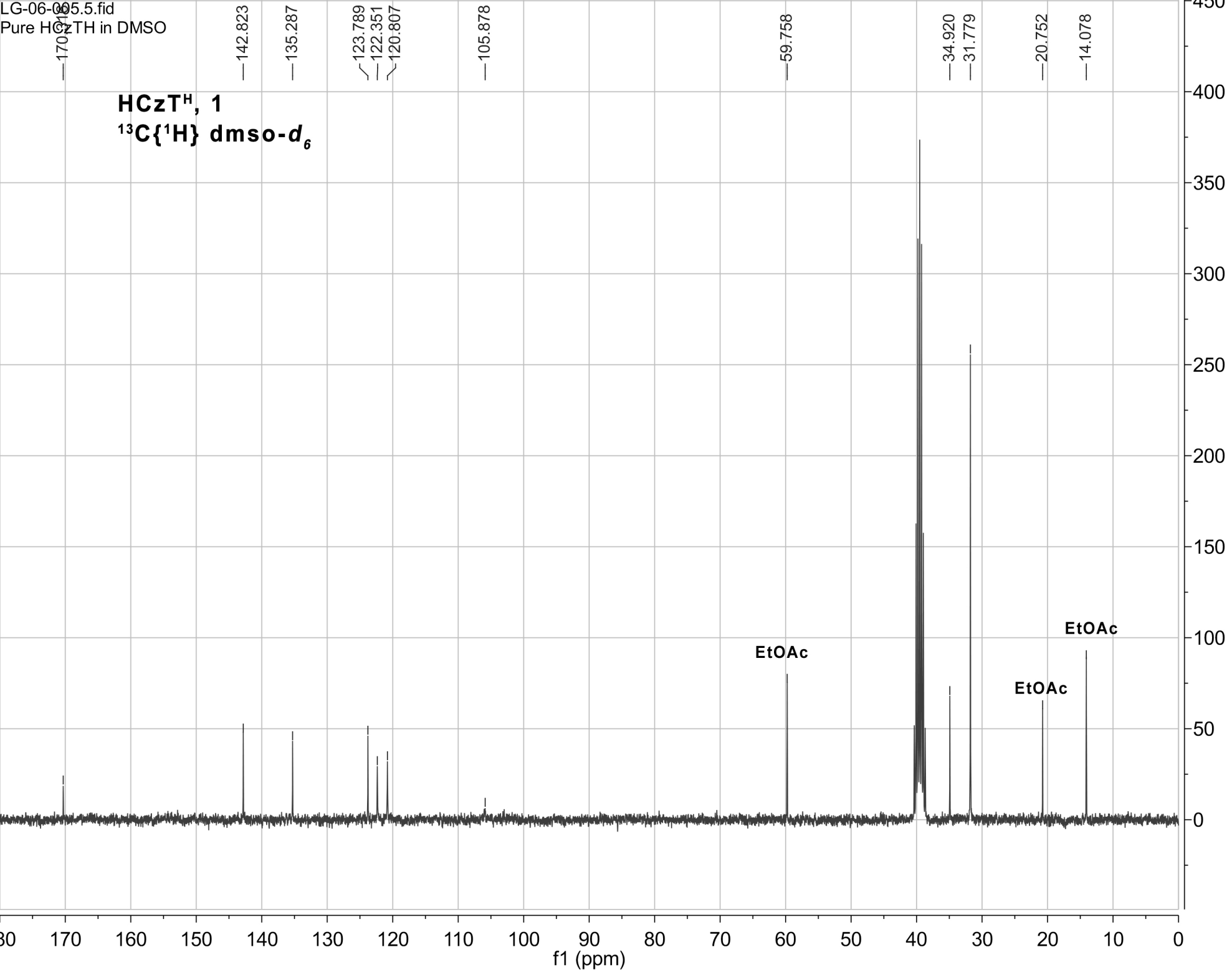
1.02
2.00
2.01
3.82
5.93
18.07
6.00
f1 (ppm)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Pure HCzTH in DMSO
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122.351
120.807
105.878
59.758
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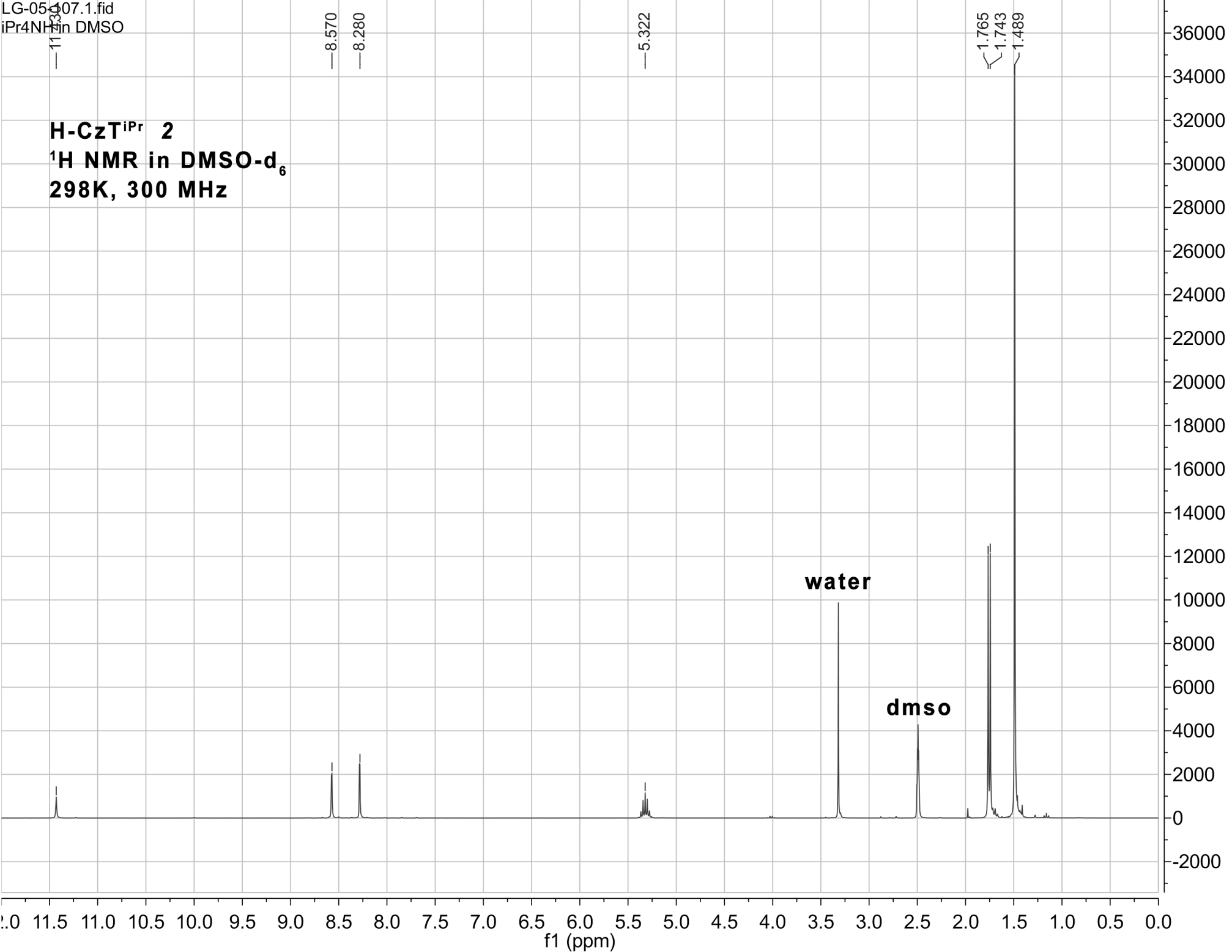
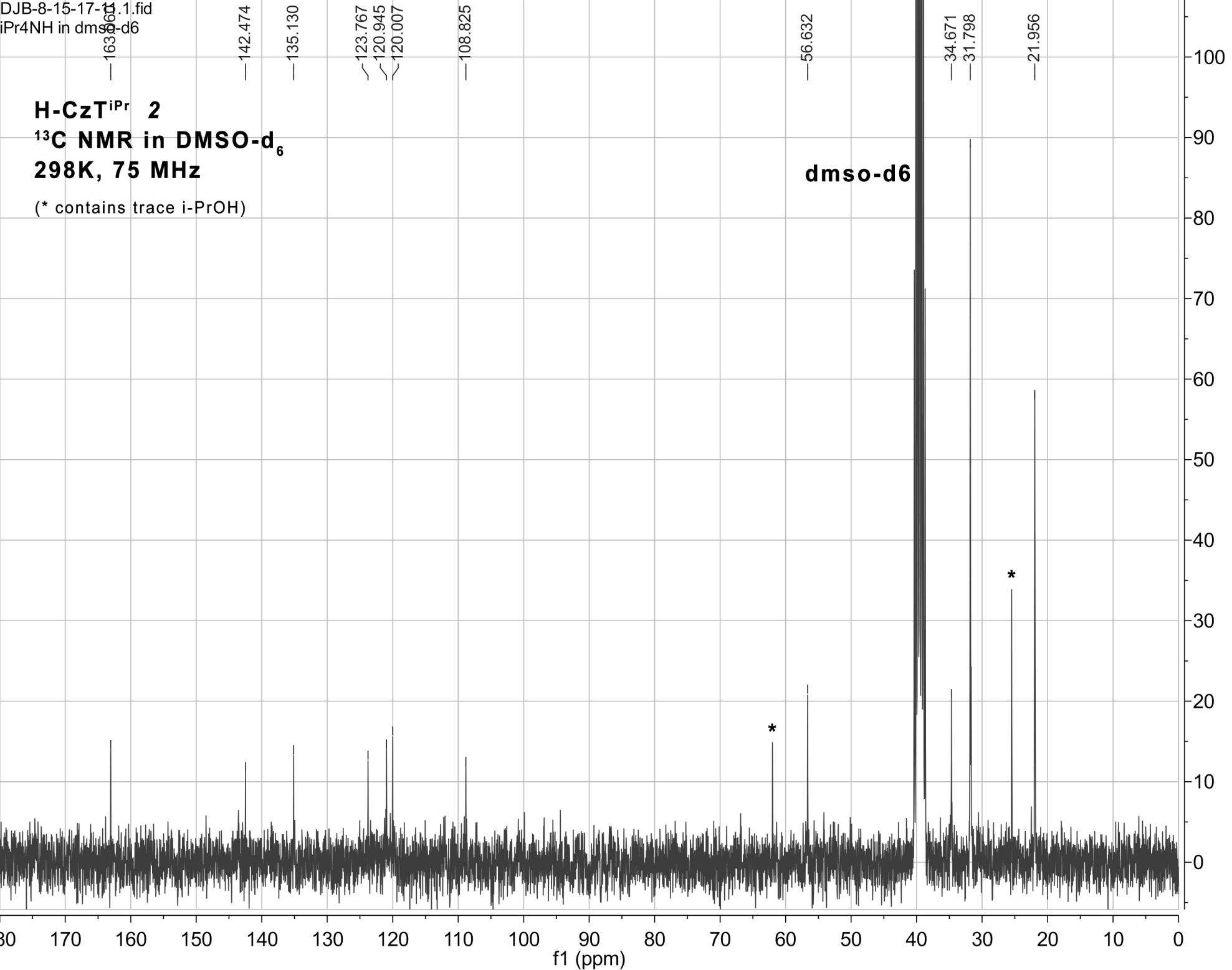
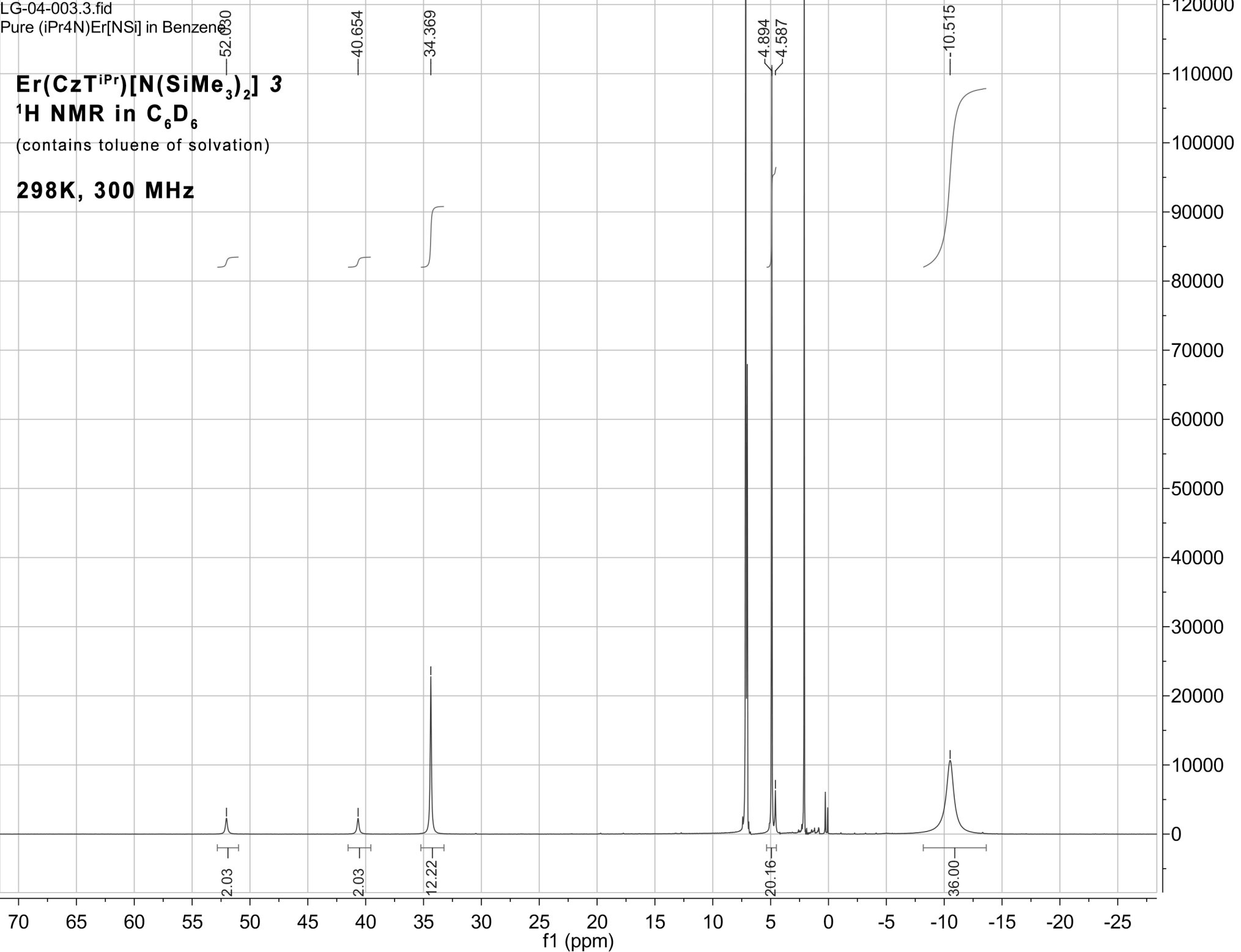
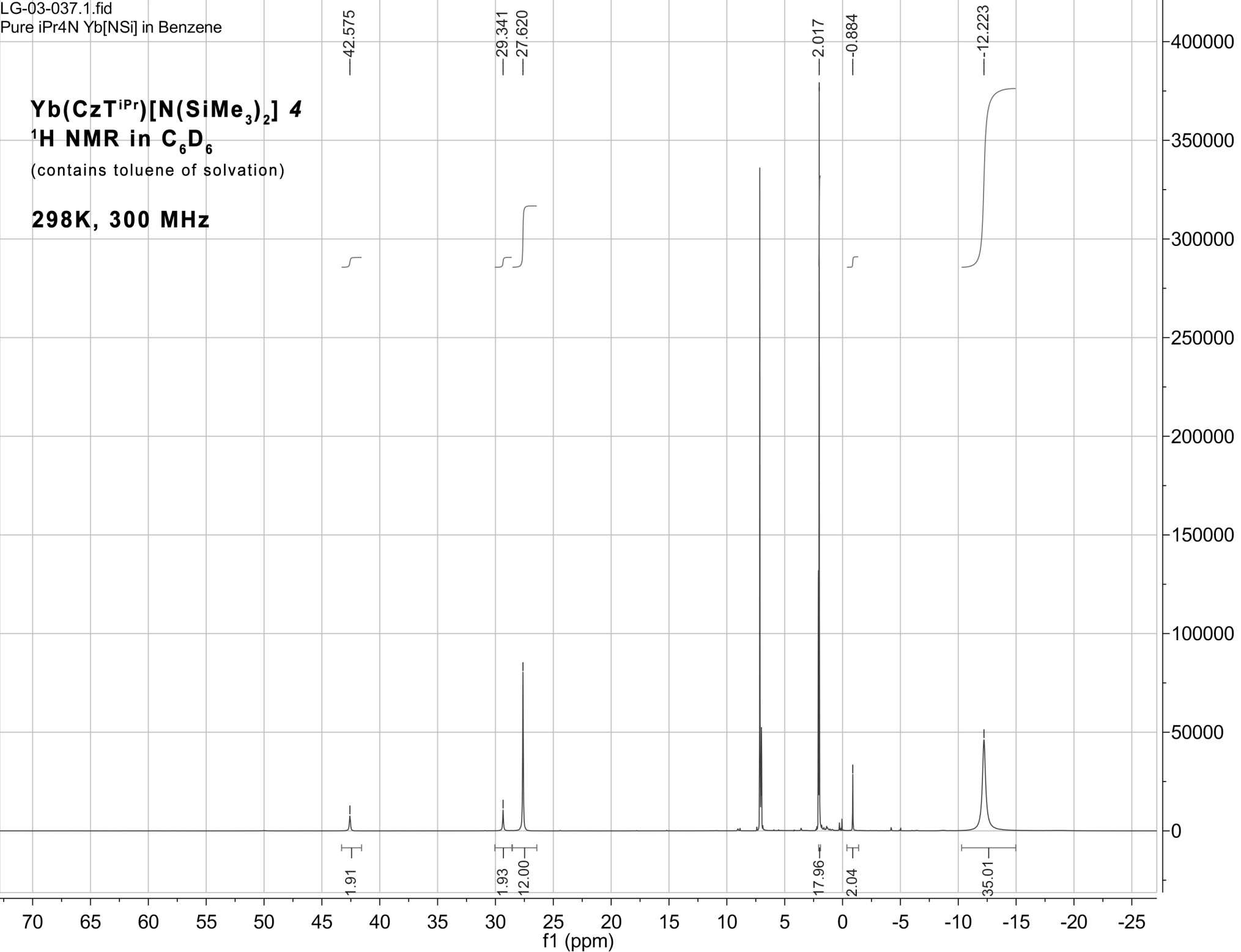
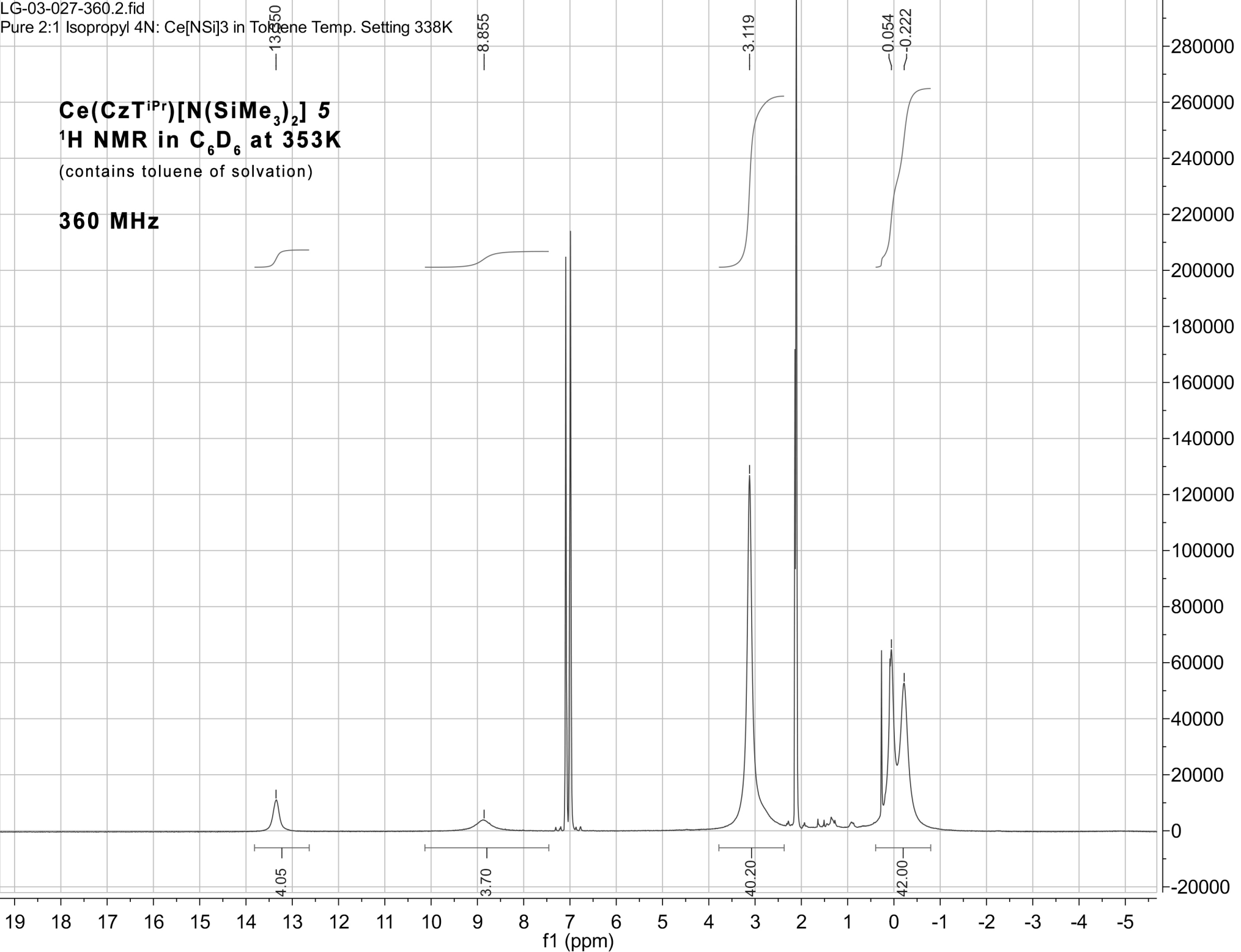
20.752
14.078
HCzTH, 1
13C{1H} dmso-d6
EtOAc
EtOAc
EtOAc
f1 (ppm)

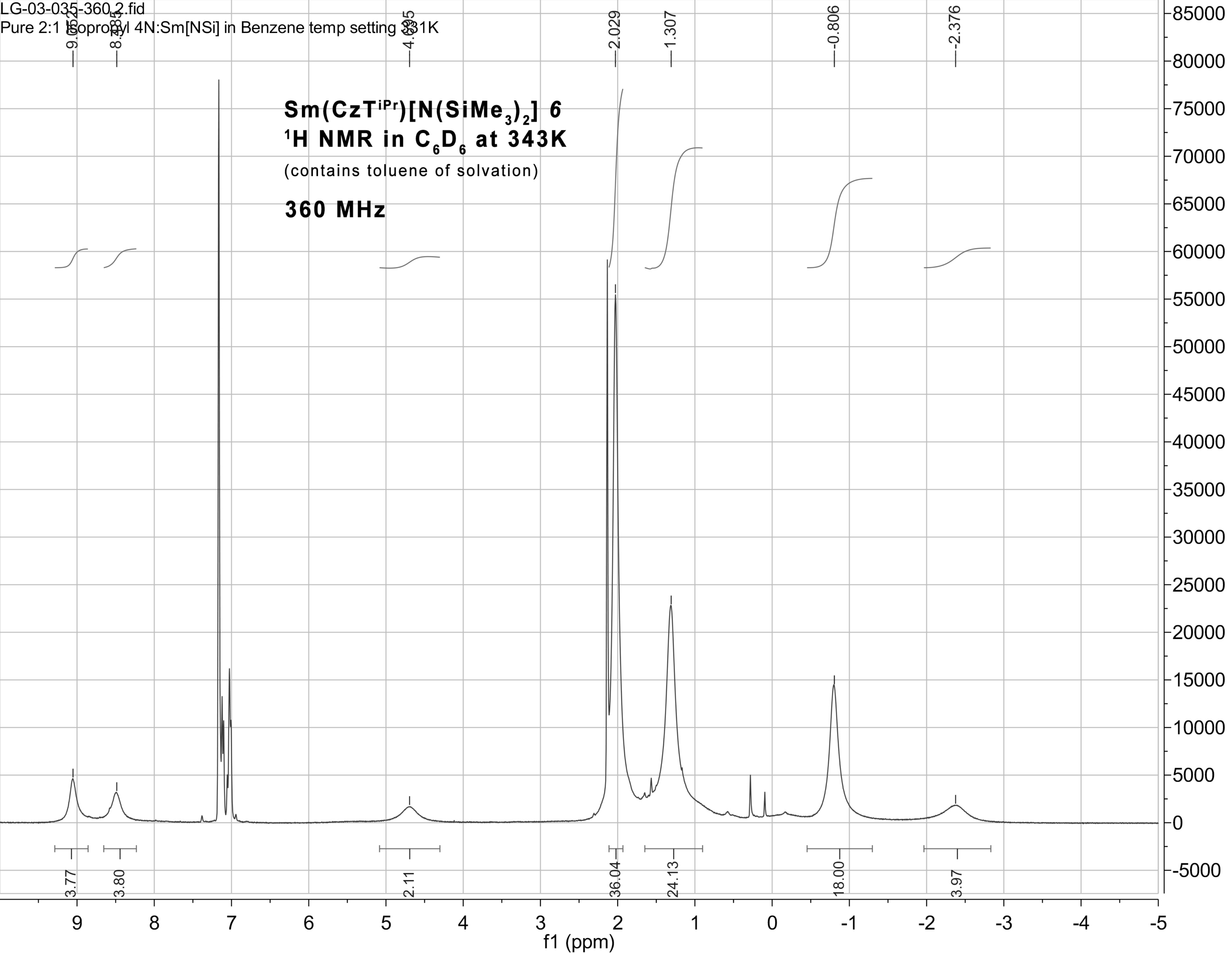

LG-05-107.1.fid
iPr4NH in DMSO
11.430
8.570
8.280
5.322
1.765
1.743
1.489
H-CzT^iPr 2
^1H NMR in DMSO-d_6
298K, 300 MHz
water
dmso
36000
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

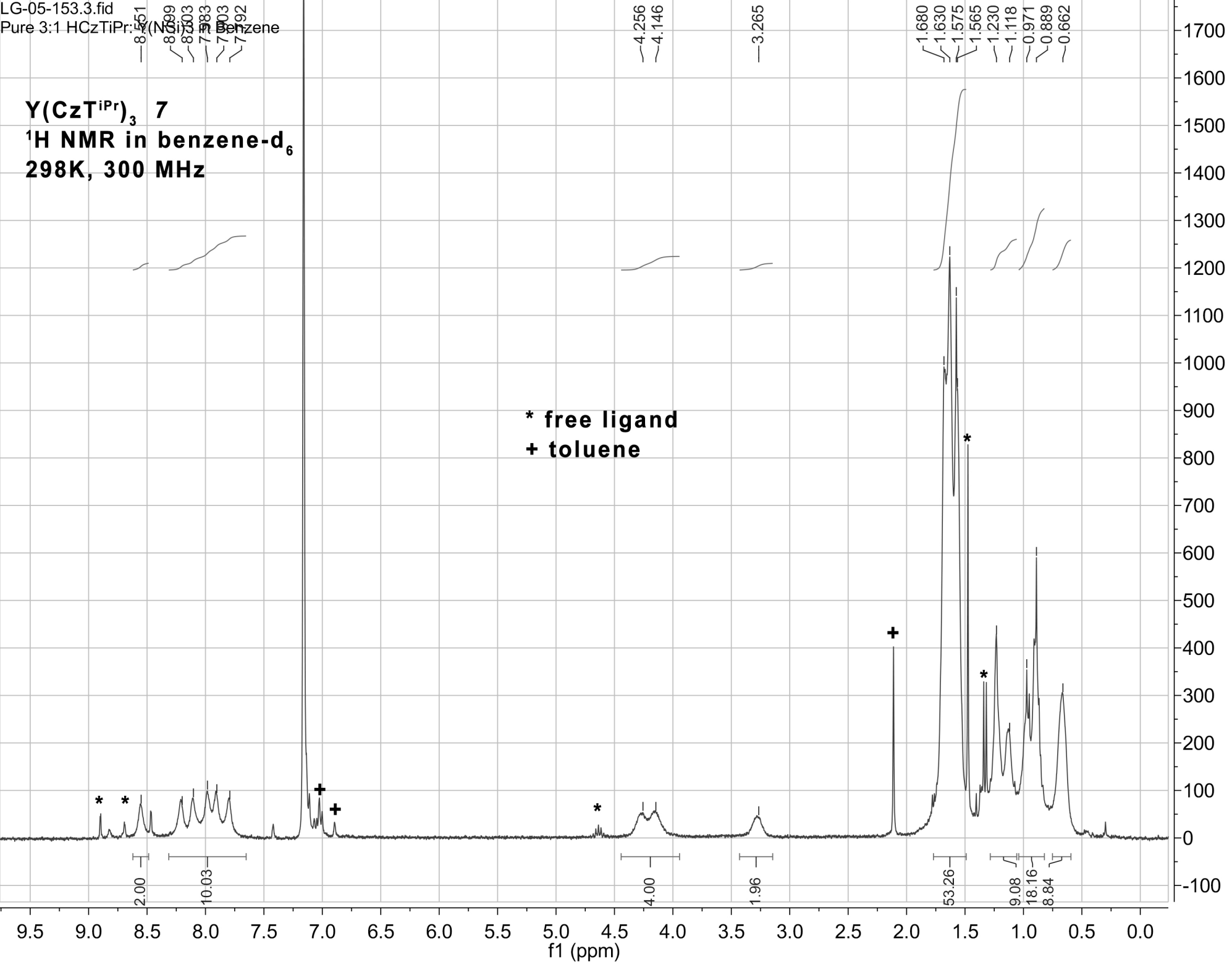

DJB-8-15-17-1.1.fid
iPr4NH in dmso-d6
163.961
142.474
135.130
123.767
120.945
120.007
108.825
56.632
34.671
31.798
21.956
H-CzT^iPr 2
13C NMR in DMSO-d6
298K, 75 MHz
(* contains trace i-PrOH)
dmso-d6
*
*
f1 (ppm)


LG-04-003.3.fid
Pure (iPr4N)Er[NSi] in Benzene
52.030
40.654
34.369
4.894
4.587
-10.515
Er(CzT^iPr)[N(SiMe3)2] 3
1H NMR in C6D6
(contains toluene of solvation)
298K, 300 MHz
2.03
2.03
12.22
20.16
36.00
f1 (ppm)


LG-03-037.1.fid
Pure iPr4N Yb[NSi] in Benzene
Yb(CzT^iPr)[N(SiMe3)2] 4
1H NMR in C6D6
(contains toluene of solvation)
298K, 300 MHz
42.575
29.341
27.620
2.017
-0.884
-12.223
1.91
1.93
12.00
17.96
2.04
35.01
400000
350000
300000
250000
200000
150000
100000
50000
0
70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25
f1 (ppm)


LG-03-027-360.2.fid
Pure 2:1 Isopropyl 4N: Ce[NSi]3 in Toluene Temp. Setting 338K
13.550
8.855
3.119
0.054
-0.222
Ce(CzT^iPr)[N(SiMe3)2] 5
1H NMR in C6D6 at 353K
(contains toluene of solvation)
360 MHz
4.05
3.70
40.20
42.00
f1 (ppm)


LG-03-035-360_2.fid
Pure 2:1 Isopropyl 4N:Sm[NSi] in Benzene temp setting 331K
Sm(CzT^iPr)[N(SiMe3)2] 6
1H NMR in C6D6 at 343K
(contains toluene of solvation)
360 MHz
2.029
1.307
-0.806
-2.376
3.77
3.80
2.11
36.04
24.13
18.00
3.97
f1 (ppm)


LG-05-153.3.fid
Pure 3:1 HCzTiPr:Y(NSi)3 in Benzene
8.551
8.509
8.503
7.983
7.803
7.792
4.256
4.146
3.265
1.680
1.630
1.575
1.565
1.230
1.118
0.971
0.889
0.662
Y(CzT^iPr)3 7
1H NMR in benzene-d6
298K, 300 MHz
* free ligand
+ toluene
2.00
10.03
4.00
1.96
53.26
9.08
18.16
8.84
f1 (ppm)