Supporting information for

Coordination of 1,4-Diazabutadiene Ligands to Decamethylytterbocene: Additional Examples of Spin Coupling in Ytterbocene Complexes

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1. Crystal Structure Data of $(C_5Me_5)_2Yb(dad(H)\text{-}p\text{-}tolyl)$

1.1 Labeling Diagram

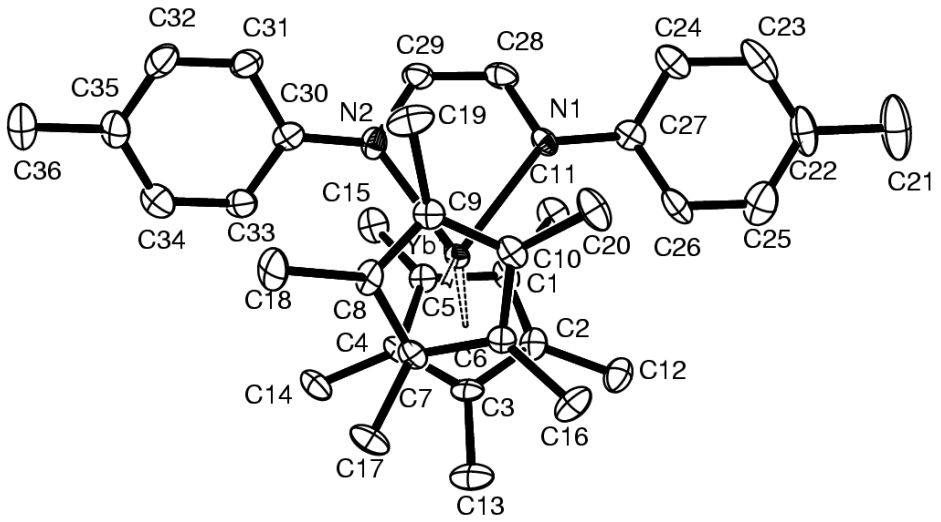


Figure S1. ORTEP diagram of $(C_5Me_5)_2Yb(dad(H)\text{-}p\text{-}tolyl)$ (50% probability ellipsoids).

1.2 Experimental Details

Data Collection

A fragment of a dark green block-like crystal of $C_{36}H_{46}N_2Yb$ having approximate dimensions of 0.38 x 0.11 x 0.09 mm was mounted on a glass fiber using Paratone N hydrocarbon oil. All measurements were made on a Bruker SMART CCD 1k [10] CCD area detector with graphite monochromated MoK_α radiation.

Cell constants and an orientation matrix, obtained from a least-squares refinement using the measured positions of 6184 centered reflections with $I > 10\sigma(I)$ in the range $2.1 < \theta < 24.7^{o}$ corresponded to a primitive monoclinic cell with dimensions:

a = 11.417(1) Å	$\alpha = 90^{o}$
b = 14.070(1) Å	$\beta = 104.413(1)^{o}$
c = 19.878(1) Å	$\gamma = 90^{o}$
V = 3092.6(3) $Å^3$	

For Z = 4 and F.W. = 679.79, the calculated density is 1.460 g/cm^3.

Analysis of the systematic absences allowed the space group to be uniquely determined to be:

$P2_1/c$

The data were collected at a temperature of 134(2) K. Frames corresponding to an arbitrary hemisphere of data were collected using ω scans of 0.3^{o} counted for a total of 10 seconds per frame.

Data Reduction

Data were integrated by the program SAINT[11] to a maximum θ value of 24.75°. The data were corrected for Lorentz and polarization effects. Data were analyzed for agreement and possible absorption using XPREP[12]. An empirical absorption correction based on comparison of redundant and equivalent reflections was applied using SADABS[13]. (Tmax = 0.7709, Tmin = 0.3903). Of the 13484 reflections that were collected, 5092 were unique (R_{int} = 0.0491); equivalent reflections were merged. No decay correction was applied.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in calculated positions using a riding model, but not refined. The final cycle of full-matrix least-squares refinement[3] was based on 5092 reflections (all data) and 364 variable parameters and converged (largest parameter shift was 0.000 times its esd) with conventional unweighted and weighted agreement factors of:

$$R_1 = \Sigma||Fo| - |Fc|| / \Sigma|Fo| = 0.0467 \text{ for 4045 data with } I > 2\sigma(I)$$

$$wR_2 = [(\Sigma w (|Fo|^2 - |Fc|^2)^2 / \Sigma w |Fo|^2)]^{1/2} = 0.1121$$

The standard deviation of an observation of unit weight[4] was 1.000. The weighting scheme was based on counting statistics and included a factor (q = 0.0829) to downweight the intense reflections. The maximum and minimum peaks on the final difference Fourier map corresponded to 2.013 and -4.890 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the SHELXTL[9] crystallographic software package of Bruker Analytical X-ray Systems Inc.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{36}H_{46}N_2Yb$
Formula Weight	679.79
Crystal Color, Habit	dark green, block
Crystal Dimensions	0.38 x 0.11 x 0.09 mm
Crystal System	monoclinic
Lattice Type	primitive
Lattice Parameters	a = 11.417(1) Å b = 14.070(1) Å c = 19.878(1) Å α= 90 ^{o} β= 104.413(1) ^{o} γ = 90^o V = 3092.6(3) Å^3
Space Group	$P2_1/c$
Z value	4
D_{calc}	1.460 g/cm^3
F_{000}	1384
μ(MoK)	3.05 cm^{-1}

B. Intensity Measurements

Diffractometer	Bruker SMART CCD 1k
Radiation	MoK$_\alpha$ (λ = 0.71069 Å) graphite monochromated
Detector Position	60.00 mm
Exposure Time	10 seconds per frame.
Scan Type	ω (0.3 degrees per frame)
θ_{max}	24.75^o
No. of Reflections Measured	Total: 13484 Unique: 5092 (R_{int} = 0.0491)
Corrections	Lorentz-polarization Absorption (Tmax = 0.7709, Tmin = 0.3903)

C. Structure Solution and Refinement

Structure Solution	direct (SHELXS-97 (Sheldrick, 1997))
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\|F_o\|^2 - \|F_c\|^2)^2$
Least Squares Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (qP)^2 + 0.000P]$ where $P = [F_o^2 + 2F_c^2]/3$
q-factor	0.0829
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>2.00σ(I))	4045
No. Variables	364
Reflection/Parameter Ratio	11.11
Residuals: R; wR_2; Rall	0.0467; 0.1121; 0.0607
Goodness of Fit Indicator	1.000
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	2.013 $e^-/Å^3$
Minimum peak in Final Diff. Map	-4.890 $e^-/Å^3$

1.3 Tables

Table 1. Atomic coordinates and U_{iso}/U_{eq} and occupancy

atom	x	y	z	U_{eq}	Occupancy
Yb1	0.1965(1)	0.3307(1)	0.1993(1)	0.015(1)	1
N1	0.2470(5)	0.2129(4)	0.2868(2)	0.019(1)	1
N2	0.0682(5)	0.2014(4)	0.1609(3)	0.022(1)	1
C22	0.5036(6)	0.2234(6)	0.4822(3)	0.035(2)	1
C3	0.1396(6)	0.5123(4)	0.2160(3)	0.020(1)	1
C27	0.3344(5)	0.2120(4)	0.3505(3)	0.019(1)	1
C7	0.3103(5)	0.3959(4)	0.1090(3)	0.019(1)	1
C9	0.3306(5)	0.2369(4)	0.1318(3)	0.019(1)	1
C4	0.0306(6)	0.4689(4)	0.1786(3)	0.020(1)	1
C10	0.4130(5)	0.2856(5)	0.1867(3)	0.020(1)	1
C30	-0.0134(6)	0.1847(4)	0.0962(3)	0.021(1)	1
C14	-0.0432(6)	0.5012(5)	0.1078(3)	0.027(2)	1
C6	0.4004(5)	0.3843(4)	0.1727(3)	0.017(1)	1
C2	0.1690(6)	0.4735(4)	0.2836(3)	0.022(2)	1
C11	0.0715(6)	0.3485(5)	0.3510(3)	0.026(2)	1
C28	0.1708(6)	0.1389(5)	0.2712(3)	0.025(2)	1
C15	-0.1218(6)	0.3470(5)	0.2086(4)	0.028(2)	1
C1	0.0830(5)	0.4035(4)	0.2880(3)	0.019(1)	1
C31	-0.0444(6)	0.0938(5)	0.0688(3)	0.030(2)	1
C8	0.2696(6)	0.3045(5)	0.0846(3)	0.022(1)	1
C5	-0.0044(6)	0.4002(4)	0.2229(3)	0.020(1)	1
C13	0.1937(6)	0.6015(5)	0.1957(3)	0.032(2)	1
C17	0.2802(6)	0.4864(4)	0.0669(3)	0.029(2)	1
C19	0.3221(7)	0.1292(4)	0.1239(4)	0.032(2)	1
C16	0.4810(6)	0.4600(5)	0.2143(4)	0.030(2)	1
C33	-0.0656(6)	0.2609(5)	0.0547(3)	0.025(2)	1
C35	-0.1714(6)	0.1580(5)	-0.0374(3)	0.028(2)	1
C29	0.0825(6)	0.1329(5)	0.2097(3)	0.025(2)	1
C36	-0.2529(7)	0.1443(6)	-0.1095(4)	0.039(2)	1
C20	0.5099(6)	0.2392(5)	0.2415(3)	0.032(2)	1
C18	0.1889(6)	0.2844(5)	0.0133(3)	0.033(2)	1
C32	-0.1214(6)	0.0817(5)	0.0040(3)	0.032(2)	1
C26	0.3891(6)	0.2976(5)	0.3773(4)	0.030(2)	1
C25	0.4666(7)	0.3034(6)	0.4421(4)	0.038(2)	1
C24	0.3719(6)	0.1309(5)	0.3902(3)	0.027(2)	1
C12	0.2644(6)	0.5165(5)	0.3433(3)	0.030(2)	1
C34	-0.1416(6)	0.2487(5)	-0.0100(3)	0.029(2)	1
C23	0.4565(7)	0.1377(6)	0.4549(4)	0.037(2)	1
C21	0.5890(7)	0.2286(8)	0.5534(4)	0.059(3)	1

U_{eq} is defined as one third of the orthogonalized U_{ij} tensor

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Yb1	0.019(1)	0.016(1)	0.011(1)	0.001(1)	0.007(1)	0.000(1)
N1	0.022(3)	0.022(3)	0.013(3)	0.004(2)	0.007(2)	0.003(2)
N2	0.023(3)	0.029(3)	0.015(3)	-0.003(2)	0.007(2)	-0.003(2)
C22	0.021(4)	0.072(6)	0.014(4)	0.005(4)	0.006(3)	0.006(4)
C3	0.029(4)	0.011(3)	0.025(3)	-0.002(3)	0.014(3)	0.002(3)
C27	0.018(3)	0.026(3)	0.018(3)	0.001(3)	0.015(3)	0.001(3)
C7	0.020(3)	0.024(3)	0.015(3)	0.004(3)	0.011(3)	0.000(3)
C9	0.022(4)	0.022(3)	0.018(3)	-0.002(3)	0.013(3)	0.001(3)
C4	0.028(4)	0.018(3)	0.017(3)	0.003(3)	0.012(3)	0.013(3)
C10	0.017(3)	0.028(3)	0.017(3)	0.005(3)	0.011(3)	0.003(3)
C30	0.024(4)	0.023(3)	0.021(3)	-0.002(3)	0.015(3)	-0.006(3)
C14	0.037(4)	0.027(3)	0.019(3)	0.007(3)	0.010(3)	0.009(3)
C6	0.015(3)	0.022(3)	0.017(3)	0.002(3)	0.009(3)	-0.002(3)
C2	0.024(4)	0.027(4)	0.018(3)	-0.007(3)	0.008(3)	0.003(3)
C11	0.027(4)	0.035(4)	0.021(4)	0.002(3)	0.016(3)	0.001(3)
C28	0.034(4)	0.022(3)	0.024(4)	0.006(3)	0.013(3)	-0.001(3)
C15	0.026(4)	0.037(4)	0.024(4)	-0.001(3)	0.011(3)	0.004(3)
C1	0.019(3)	0.026(3)	0.014(3)	0.000(3)	0.010(3)	0.010(3)
C31	0.043(5)	0.022(4)	0.026(4)	-0.003(3)	0.009(3)	-0.006(3)
C8	0.027(4)	0.035(4)	0.009(3)	-0.005(3)	0.013(3)	-0.009(3)
C5	0.020(3)	0.024(3)	0.018(3)	-0.002(3)	0.010(3)	0.001(3)
C13	0.052(5)	0.017(4)	0.038(4)	-0.005(3)	0.030(4)	0.000(3)
C17	0.033(4)	0.029(4)	0.029(4)	0.014(3)	0.017(3)	0.006(3)
C19	0.040(4)	0.019(3)	0.046(5)	-0.011(3)	0.028(4)	0.000(3)
C16	0.026(4)	0.032(4)	0.036(4)	-0.011(3)	0.013(3)	-0.012(3)
C33	0.038(4)	0.022(3)	0.020(3)	-0.002(3)	0.015(3)	-0.003(3)
C35	0.027(4)	0.042(4)	0.018(4)	0.001(3)	0.011(3)	-0.006(3)
C29	0.035(4)	0.020(3)	0.022(4)	0.003(3)	0.009(3)	-0.004(3)
C36	0.030(4)	0.061(5)	0.024(4)	-0.002(4)	0.002(3)	-0.003(4)
C20	0.032(4)	0.046(4)	0.020(4)	0.009(3)	0.010(3)	0.013(3)
C18	0.037(4)	0.049(5)	0.015(3)	-0.005(3)	0.012(3)	-0.006(4)
C32	0.040(4)	0.031(4)	0.028(4)	-0.010(3)	0.012(3)	-0.011(3)
C26	0.025(4)	0.038(4)	0.027(4)	0.015(3)	0.003(3)	0.009(3)
C25	0.035(5)	0.056(5)	0.027(4)	-0.007(4)	0.013(3)	-0.012(4)
C24	0.025(4)	0.034(4)	0.025(4)	0.011(3)	0.014(3)	0.007(3)
C12	0.028(4)	0.030(4)	0.029(4)	-0.010(3)	0.003(3)	0.000(3)
C34	0.032(4)	0.032(4)	0.027(4)	0.003(3)	0.013(3)	0.007(3)
C23	0.028(4)	0.056(5)	0.029(4)	0.024(4)	0.012(3)	0.016(4)
C21	0.028(5)	0.129(9)	0.022(4)	0.008(5)	0.006(3)	-0.001(5)

The general temperature factor expression:

$$\exp(-2\Pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}\,hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Yb1	C100	2.37	Yb1	C101	2.34
Yb1	N2	2.340(5)	Yb1	N1	2.368(5)
Yb1	C6	2.623(6)	Yb1	C10	2.624(6)
Yb1	C9	2.629(6)	Yb1	C7	2.630(6)
Yb1	C5	2.640(6)	Yb1	C1	2.641(6)
Yb1	C8	2.643(6)	Yb1	C4	2.674(6)
Yb1	C3	2.677(6)	Yb1	C2	2.683(6)
N1	C28	1.342(8)	N1	C27	1.404(8)
N2	C29	1.349(8)	N2	C30	1.408(8)
C22	C23	1.376(11)	C22	C25	1.383(10)
C22	C21	1.507(9)	C3	C2	1.411(9)
C3	C4	1.420(9)	C3	C13	1.499(8)
C27	C24	1.392(9)	C27	C26	1.400(9)
C7	C8	1.412(8)	C7	C6	1.429(8)
C7	C17	1.516(8)	C9	C8	1.395(9)
C9	C10	1.426(9)	C9	C19	1.524(9)
C4	C5	1.430(8)	C4	C14	1.518(8)
C10	C6	1.417(9)	C10	C20	1.496(8)
C30	C33	1.394(9)	C30	C31	1.401(8)
C14	H14A	0.9800	C14	H14B	0.9800
C14	H14C	0.9800	C6	C16	1.511(8)
C2	C1	1.408(9)	C2	C12	1.522(9)
C11	C1	1.506(8)	C11	H11A	0.9800
C11	H11B	0.9800	C11	H11C	0.9800
C28	C29	1.380(9)	C28	H28	0.9500
C15	C5	1.499(9)	C15	H15A	0.9800
C15	H15B	0.9800	C15	H15C	0.9800
C1	C5	1.425(8)	C31	C32	1.377(9)
C31	H31	0.9500	C8	C18	1.512(8)
C13	H13A	0.9800	C13	H13B	0.9800
C13	H13C	0.9800	C17	H17A	0.9800
C17	H17B	0.9800	C17	H17C	0.9800
C19	H19A	0.9800	C19	H19B	0.9800
C19	H19C	0.9800	C16	H16A	0.9800
C16	H16B	0.9800	C16	H16C	0.9800
C33	C34	1.371(9)	C33	H33	0.9500
C35	C32	1.387(10)	C35	C34	1.396(9)
C35	C36	1.514(10)	C29	H29	0.9500
C36	H36A	0.9800	C36	H36B	0.9800
C36	H36C	0.9800	C20	H20A	0.9800
C20	H20B	0.9800	C20	H20C	0.9800
C18	H18A	0.9800	C18	H18B	0.9800
C18	H18C	0.9800	C32	H32	0.9500
C26	C25	1.371(10)	C26	H26	0.9500
C25	H25	0.9500	C24	C23	1.407(10)
C24	H24	0.9500	C12	H12A	0.9800
C12	H12B	0.9800	C12	H12C	0.9800
C34	H34	0.9500	C23	H23	0.9500
C21	H21A	0.9800	C21	H21B	0.9800
C21	H21C	0.9800			

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C100	Yb1	C101	137.2	N2	Yb1	N1	73.36(18)
N2	Yb1	C6	132.27(18)	N1	Yb1	C6	106.47(18)
N2	Yb1	C10	107.99(19)	N1	Yb1	C10	80.70(18)
C6	Yb1	C10	31.33(19)	N2	Yb1	C9	80.81(18)
N1	Yb1	C9	87.56(18)	C6	Yb1	C9	51.88(18)
C10	Yb1	C9	31.50(19)	N2	Yb1	C7	115.08(18)
N1	Yb1	C7	132.42(18)	C6	Yb1	C7	31.57(18)
C10	Yb1	C7	51.80(19)	C9	Yb1	C7	51.46(19)
N2	Yb1	C5	81.09(18)	N1	Yb1	C5	101.07(18)
C6	Yb1	C5	141.52(19)	C10	Yb1	C5	170.8(2)
C9	Yb1	C5	156.74(19)	C7	Yb1	C5	126.21(19)
N2	Yb1	C1	98.52(19)	N1	Yb1	C1	81.46(17)
C6	Yb1	C1	129.05(19)	C10	Yb1	C1	142.01(19)
C9	Yb1	C1	168.68(19)	C7	Yb1	C1	136.7(2)
C5	Yb1	C1	31.30(18)	N2	Yb1	C8	85.23(18)
N1	Yb1	C8	117.71(19)	C6	Yb1	C8	51.64(19)
C10	Yb1	C8	51.4(2)	C9	Yb1	C8	30.69(19)
C7	Yb1	C8	31.06(18)	C5	Yb1	C8	132.8(2)
C1	Yb1	C8	160.6(2)	N2	Yb1	C4	98.8(2)
N1	Yb1	C4	130.99(17)	C6	Yb1	C4	112.94(18)
C10	Yb1	C4	144.00(19)	C9	Yb1	C4	140.05(18)
C7	Yb1	C4	95.30(18)	C5	Yb1	C4	31.22(18)
C1	Yb1	C4	51.27(18)	C8	Yb1	C4	109.40(19)
N2	Yb1	C3	129.09(19)	N1	Yb1	C3	126.83(17)
C6	Yb1	C3	90.29(18)	C10	Yb1	C3	120.39(19)
C9	Yb1	C3	137.08(18)	C7	Yb1	C3	85.86(18)
C5	Yb1	C3	51.42(19)	C1	Yb1	C3	51.13(18)
C8	Yb1	C3	112.23(19)	C4	Yb1	C3	30.77(19)
N2	Yb1	C2	128.64(19)	N1	Yb1	C2	96.34(18)
C6	Yb1	C2	99.06(19)	C10	Yb1	C2	119.99(19)
C9	Yb1	C2	150.20(19)	C7	Yb1	C2	108.61(19)
C5	Yb1	C2	50.97(19)	C1	Yb1	C2	30.66(19)
C8	Yb1	C2	139.0(2)	C4	Yb1	C2	50.48(19)
C3	Yb1	C2	30.53(18)	C28	N1	C27	118.4(5)
C28	N1	Yb1	110.4(4)	C27	N1	Yb1	131.1(4)
C29	N2	C30	118.1(5)	C29	N2	Yb1	111.6(4)
C30	N2	Yb1	130.3(4)	C23	C22	C25	116.9(6)
C23	C22	C21	120.7(7)	C25	C22	C21	122.4(8)
C2	C3	C4	107.6(5)	C2	C3	C13	124.4(6)
C4	C3	C13	125.8(6)	C2	C3	Yb1	75.0(3)
C4	C3	Yb1	74.5(3)	C13	C3	Yb1	129.6(4)
C24	C27	C26	116.4(6)	C24	C27	N1	124.6(6)
C26	C27	N1	119.0(5)	C8	C7	C6	107.7(5)
C8	C7	C17	124.4(6)	C6	C7	C17	126.8(6)
C8	C7	Yb1	75.0(3)	C6	C7	Yb1	74.0(3)
C17	C7	Yb1	126.0(4)	C8	C9	C10	108.1(5)
C8	C9	C19	126.9(6)	C10	C9	C19	124.7(6)
C8	C9	Yb1	75.2(3)	C10	C9	Yb1	74.1(3)
C19	C9	Yb1	121.4(4)	C3	C4	C5	108.1(5)
C3	C4	C14	124.6(6)	C5	C4	C14	126.7(6)

C3	C4	Yb1	74.7(3)	C5	C4	Yb1	73.1(3)
C14	C4	Yb1	124.7(4)	C6	C10	C9	107.8(5)
C6	C10	C20	126.2(6)	C9	C10	C20	125.1(6)
C6	C10	Yb1	74.3(3)	C9	C10	Yb1	74.4(3)
C20	C10	Yb1	125.4(4)	C33	C30	C31	116.3(6)
C33	C30	N2	120.0(6)	C31	C30	N2	123.7(6)
C4	C14	H14A	109.5	C4	C14	H14B	109.5
H14A	C14	H14B	109.5	C4	C14	H14C	109.5
H14A	C14	H14C	109.5	H14B	C14	H14C	109.5
C10	C6	C7	107.5(5)	C10	C6	C16	124.4(5)
C7	C6	C16	127.6(6)	C10	C6	Yb1	74.4(3)
C7	C6	Yb1	74.5(3)	C16	C6	Yb1	122.9(4)
C1	C2	C3	109.0(5)	C1	C2	C12	127.1(6)
C3	C2	C12	122.9(6)	C1	C2	Yb1	73.0(3)
C3	C2	Yb1	74.5(3)	C12	C2	Yb1	127.8(4)
C1	C11	H11A	109.5	C1	C11	H11B	109.5
H11A	C11	H11B	109.5	C1	C11	H11C	109.5
H11A	C11	H11C	109.5	H11B	C11	H11C	109.5
N1	C28	C29	122.7(6)	N1	C28	Yb1	45.7(3)
C29	C28	Yb1	77.1(4)	N1	C28	H28	118.6
C29	C28	H28	118.6	Yb1	C28	H28	164.0
C5	C15	H15A	109.5	C5	C15	H15B	109.5
H15A	C15	H15B	109.5	C5	C15	H15C	109.5
H15A	C15	H15C	109.5	H15B	C15	H15C	109.5
C2	C1	C5	107.9(5)	C2	C1	C11	128.2(6)
C5	C1	C11	123.5(6)	C2	C1	Yb1	76.3(3)
C5	C1	Yb1	74.3(3)	C11	C1	Yb1	121.0(4)
C32	C31	C30	121.1(6)	C32	C31	H31	119.4
C30	C31	H31	119.4	C9	C8	C7	108.9(5)
C9	C8	C18	126.0(6)	C7	C8	C18	124.4(6)
C9	C8	Yb1	74.1(3)	C7	C8	Yb1	74.0(3)
C18	C8	Yb1	125.8(4)	C1	C5	C4	107.3(5)
C1	C5	C15	125.5(6)	C4	C5	C15	126.4(6)
C1	C5	Yb1	74.4(3)	C4	C5	Yb1	75.7(3)
C15	C5	Yb1	123.8(4)	C3	C13	H13A	109.5
C3	C13	H13B	109.5	H13A	C13	H13B	109.5
C3	C13	H13C	109.5	H13A	C13	H13C	109.5
H13B	C13	H13C	109.5	C7	C17	H17A	109.5
C7	C17	H17B	109.5	H17A	C17	H17B	109.5
C7	C17	H17C	109.5	H17A	C17	H17C	109.5
H17B	C17	H17C	109.5	C9	C19	H19A	109.5
C9	C19	H19B	109.5	H19A	C19	H19B	109.5
C9	C19	H19C	109.5	H19A	C19	H19C	109.5
H19B	C19	H19C	109.5	C6	C16	H16A	109.5
C6	C16	H16B	109.5	H16A	C16	H16B	109.5
C6	C16	H16C	109.5	H16A	C16	H16C	109.5
H16B	C16	H16C	109.5	C34	C33	C30	122.4(6)
C34	C33	H33	118.8	C30	C33	H33	118.8
C32	C35	C34	116.8(6)	C32	C35	C36	121.9(6)
C34	C35	C36	121.3(7)	N2	C29	C28	121.6(6)
N2	C29	Yb1	44.6(3)	C28	C29	Yb1	77.2(4)
N2	C29	H29	119.2	C28	C29	H29	119.2
Yb1	C29	H29	163.3	C35	C36	H36A	109.5
C35	C36	H36B	109.5	H36A	C36	H36B	109.5
C35	C36	H36C	109.5	H36A	C36	H36C	109.5
H36B	C36	H36C	109.5	C10	C20	H20A	109.5
C10	C20	H20B	109.5	H20A	C20	H20B	109.5

C10	C20	H20C	109.5	H20A	C20	H20C	109.5
H20B	C20	H20C	109.5	C8	C18	H18A	109.5
C8	C18	H18B	109.5	H18A	C18	H18B	109.5
C8	C18	H18C	109.5	H18A	C18	H18C	109.5
H18B	C18	H18C	109.5	C31	C32	C35	122.2(7)
C31	C32	H32	118.9	C35	C32	H32	118.9
C25	C26	C27	122.1(7)	C25	C26	H26	119.0
C27	C26	H26	119.0	C26	C25	C22	121.8(7)
C26	C25	H25	119.1	C22	C25	H25	119.1
C27	C24	C23	120.4(7)	C27	C24	H24	119.8
C23	C24	H24	119.8	C2	C12	H12A	109.5
C2	C12	H12B	109.5	H12A	C12	H12B	109.5
C2	C12	H12C	109.5	H12A	C12	H12C	109.5
H12B	C12	H12C	109.5	C33	C34	C35	121.2(6)
C33	C34	H34	119.4	C35	C34	H34	119.4
C22	C23	C24	122.2(7)	C22	C23	H23	118.9
C24	C23	H23	118.9	C22	C21	H21A	109.5
C22	C21	H21B	109.5	H21A	C21	H21B	109.5
C22	C21	H21C	109.5	H21A	C21	H21C	109.5
H21B	C21	H21C	109.5				

Table 5. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
N2	Yb1	N1	C28	-4.8(4)	C6	Yb1	N1	C28	-134.9(4)
C10	Yb1	N1	C28	-116.9(4)	C9	Yb1	N1	C28	-85.9(4)
C7	Yb1	N1	C28	-113.9(4)	C5	Yb1	N1	C28	72.3(4)
C1	Yb1	N1	C28	96.8(4)	C8	Yb1	N1	C28	-80.0(4)
C4	Yb1	N1	C28	82.4(5)	C3	Yb1	N1	C28	121.9(4)
C2	Yb1	N1	C28	123.7(4)	N2	Yb1	N1	C27	179.5(5)
C6	Yb1	N1	C27	49.5(5)	C10	Yb1	N1	C27	67.5(5)
C9	Yb1	N1	C27	98.4(5)	C7	Yb1	N1	C27	70.5(5)
C5	Yb1	N1	C27	-103.4(5)	C1	Yb1	N1	C27	-78.8(5)
C8	Yb1	N1	C27	104.3(5)	C4	Yb1	N1	C27	-93.2(5)
C3	Yb1	N1	C27	-53.7(5)	C2	Yb1	N1	C27	-52.0(5)
N1	Yb1	N2	C29	5.1(4)	C6	Yb1	N2	C29	102.5(5)
C10	Yb1	N2	C29	79.2(5)	C9	Yb1	N2	C29	95.3(4)
C7	Yb1	N2	C29	134.7(4)	C5	Yb1	N2	C29	-99.4(4)
C1	Yb1	N2	C29	-73.3(4)	C8	Yb1	N2	C29	125.9(5)
C4	Yb1	N2	C29	-125.2(4)	C3	Yb1	N2	C29	-119.2(4)
C2	Yb1	N2	C29	-79.7(5)	N1	Yb1	N2	C30	-171.8(6)
C6	Yb1	N2	C30	-74.4(6)	C10	Yb1	N2	C30	-97.7(5)
C9	Yb1	N2	C30	-81.6(5)	C7	Yb1	N2	C30	-42.2(6)
C5	Yb1	N2	C30	83.8(5)	C1	Yb1	N2	C30	109.9(5)
C8	Yb1	N2	C30	-51.0(5)	C4	Yb1	N2	C30	58.0(5)
C3	Yb1	N2	C30	64.0(6)	C2	Yb1	N2	C30	103.5(5)
N2	Yb1	C3	C2	101.9(4)	N1	Yb1	C3	C2	3.4(5)
C6	Yb1	C3	C2	-107.6(4)	C10	Yb1	C3	C2	-98.4(4)
C9	Yb1	C3	C2	-133.2(4)	C7	Yb1	C3	C2	-138.8(4)
C5	Yb1	C3	C2	76.5(4)	C1	Yb1	C3	C2	36.1(3)
C8	Yb1	C3	C2	-155.6(4)	C4	Yb1	C3	C2	113.5(5)
N2	Yb1	C3	C4	-11.6(4)	N1	Yb1	C3	C4	-110.1(4)
C6	Yb1	C3	C4	138.9(3)	C10	Yb1	C3	C4	148.0(3)
C9	Yb1	C3	C4	113.2(4)	C7	Yb1	C3	C4	107.6(4)
C5	Yb1	C3	C4	-37.0(3)	C1	Yb1	C3	C4	-77.5(4)
C8	Yb1	C3	C4	90.8(4)	C2	Yb1	C3	C4	-113.5(5)
N2	Yb1	C3	C13	-135.6(5)	N1	Yb1	C3	C13	125.9(5)
C6	Yb1	C3	C13	14.9(6)	C10	Yb1	C3	C13	24.0(6)
C9	Yb1	C3	C13	-10.8(7)	C7	Yb1	C3	C13	-16.4(6)
C5	Yb1	C3	C13	-161.0(7)	C1	Yb1	C3	C13	158.5(7)
C8	Yb1	C3	C13	-33.2(6)	C4	Yb1	C3	C13	-124.0(7)
C2	Yb1	C3	C13	122.5(7)	C28	N1	C27	C24	19.1(8)
Yb1	N1	C27	C24	-165.6(4)	C28	N1	C27	C26	-160.8(6)
Yb1	N1	C27	C26	14.5(8)	N2	Yb1	C7	C8	-17.2(4)
N1	Yb1	C7	C8	72.8(4)	C6	Yb1	C7	C8	113.9(5)
C10	Yb1	C7	C8	76.6(4)	C9	Yb1	C7	C8	36.1(4)
C5	Yb1	C7	C8	-114.7(4)	C1	Yb1	C7	C8	-154.6(4)
C4	Yb1	C7	C8	-119.5(4)	C3	Yb1	C7	C8	-148.8(4)
C2	Yb1	C7	C8	-169.5(4)	N2	Yb1	C7	C6	-131.1(3)
N1	Yb1	C7	C6	-41.1(4)	C10	Yb1	C7	C6	-37.3(3)
C9	Yb1	C7	C6	-77.8(4)	C5	Yb1	C7	C6	131.4(3)
C1	Yb1	C7	C6	91.5(4)	C8	Yb1	C7	C6	-113.9(5)
C4	Yb1	C7	C6	126.6(3)	C3	Yb1	C7	C6	97.3(4)
C2	Yb1	C7	C6	76.7(4)	N2	Yb1	C7	C17	104.7(5)
N1	Yb1	C7	C17	-165.3(5)	C6	Yb1	C7	C17	-124.2(7)

C10	Yb1	C7	C17	-161.5(6)	C9	Yb1	C7	C17	158.0(6)
C5	Yb1	C7	C17	7.2(6)	C1	Yb1	C7	C17	-32.7(6)
C8	Yb1	C7	C17	121.9(7)	C4	Yb1	C7	C17	2.4(5)
C3	Yb1	C7	C17	-26.9(5)	C2	Yb1	C7	C17	-47.6(6)
N2	Yb1	C9	C8	96.2(4)	N1	Yb1	C9	C8	169.7(4)
C6	Yb1	C9	C8	-77.1(4)	C10	Yb1	C9	C8	-114.2(5)
C7	Yb1	C9	C8	-36.5(3)	C5	Yb1	C9	C8	56.9(6)
C1	Yb1	C9	C8	-176.3(8)	C4	Yb1	C9	C8	3.4(5)
C3	Yb1	C9	C8	-43.7(5)	C2	Yb1	C9	C8	-91.8(5)
N2	Yb1	C9	C10	-149.6(4)	N1	Yb1	C9	C10	-76.1(4)
C6	Yb1	C9	C10	37.1(3)	C7	Yb1	C9	C10	77.7(4)
C5	Yb1	C9	C10	171.1(4)	C1	Yb1	C9	C10	-62.1(11)
C8	Yb1	C9	C10	114.2(5)	C4	Yb1	C9	C10	117.6(4)
C3	Yb1	C9	C10	70.5(4)	C2	Yb1	C9	C10	22.4(6)
N2	Yb1	C9	C19	-28.3(5)	N1	Yb1	C9	C19	45.2(5)
C6	Yb1	C9	C19	158.4(6)	C10	Yb1	C9	C19	121.3(6)
C7	Yb1	C9	C19	-161.0(6)	C5	Yb1	C9	C19	-67.6(7)
C1	Yb1	C9	C19	59.2(11)	C8	Yb1	C9	C19	-124.5(7)
C4	Yb1	C9	C19	-121.1(5)	C3	Yb1	C9	C19	-168.2(4)
C2	Yb1	C9	C19	143.7(5)	C2	C3	C4	C5	-2.2(7)
C13	C3	C4	C5	-166.0(6)	Yb1	C3	C4	C5	66.0(4)
C2	C3	C4	C14	169.8(5)	C13	C3	C4	C14	6.1(9)
Yb1	C3	C4	C14	-121.9(6)	C2	C3	C4	Yb1	-68.3(4)
C13	C3	C4	Yb1	128.0(6)	N2	Yb1	C4	C3	170.9(3)
N1	Yb1	C4	C3	95.3(4)	C6	Yb1	C4	C3	-45.5(4)
C10	Yb1	C4	C3	-51.0(5)	C9	Yb1	C4	C3	-103.0(4)
C7	Yb1	C4	C3	-72.7(4)	C5	Yb1	C4	C3	114.8(5)
C1	Yb1	C4	C3	77.0(4)	C8	Yb1	C4	C3	-101.1(4)
C2	Yb1	C4	C3	37.1(3)	N2	Yb1	C4	C5	56.1(4)
N1	Yb1	C4	C5	-19.5(5)	C6	Yb1	C4	C5	-160.3(3)
C10	Yb1	C4	C5	-165.8(4)	C9	Yb1	C4	C5	142.3(4)
C7	Yb1	C4	C5	172.5(4)	C1	Yb1	C4	C5	-37.8(3)
C8	Yb1	C4	C5	144.1(4)	C3	Yb1	C4	C5	-114.8(5)
C2	Yb1	C4	C5	-77.7(4)	N2	Yb1	C4	C14	-67.3(5)
N1	Yb1	C4	C14	-142.8(5)	C6	Yb1	C4	C14	76.3(5)
C10	Yb1	C4	C14	70.9(6)	C9	Yb1	C4	C14	18.9(7)
C7	Yb1	C4	C14	49.2(5)	C5	Yb1	C4	C14	-123.4(7)
C1	Yb1	C4	C14	-161.2(6)	C8	Yb1	C4	C14	20.7(6)
C3	Yb1	C4	C14	121.9(7)	C2	Yb1	C4	C14	159.0(6)
C8	C9	C10	C6	0.7(6)	C19	C9	C10	C6	175.2(5)
Yb1	C9	C10	C6	-67.4(4)	C8	C9	C10	C20	-169.3(6)
C19	C9	C10	C20	5.2(9)	Yb1	C9	C10	C20	122.6(6)
C8	C9	C10	Yb1	68.1(4)	C19	C9	C10	Yb1	-117.5(5)
N2	Yb1	C10	C6	145.8(3)	N1	Yb1	C10	C6	-145.2(4)
C9	Yb1	C10	C6	114.1(5)	C7	Yb1	C10	C6	37.6(3)
C5	Yb1	C10	C6	-43.3(13)	C1	Yb1	C10	C6	-82.3(4)
C8	Yb1	C10	C6	77.6(4)	C4	Yb1	C10	C6	9.6(5)
C3	Yb1	C10	C6	-17.8(4)	C2	Yb1	C10	C6	-53.2(4)
N2	Yb1	C10	C9	31.6(4)	N1	Yb1	C10	C9	100.6(4)
C6	Yb1	C10	C9	-114.1(5)	C7	Yb1	C10	C9	-76.5(4)
C5	Yb1	C10	C9	-157.5(10)	C1	Yb1	C10	C9	163.6(3)
C8	Yb1	C10	C9	-36.6(3)	C4	Yb1	C10	C9	-104.5(4)
C3	Yb1	C10	C9	-131.9(3)	C2	Yb1	C10	C9	-167.4(3)
N2	Yb1	C10	C20	-90.6(6)	N1	Yb1	C10	C20	-21.6(6)
C6	Yb1	C10	C20	123.6(7)	C9	Yb1	C10	C20	-122.3(7)
C7	Yb1	C10	C20	161.2(7)	C5	Yb1	C10	C20	80.3(13)
C1	Yb1	C10	C20	41.3(7)	C8	Yb1	C10	C20	-158.9(7)

C4	Yb1	C10	C20	133.2(5)	C3	Yb1	C10	C20	105.8(6)
C2	Yb1	C10	C20	70.4(6)	C29	N2	C30	C33	156.1(6)
Yb1	N2	C30	C33	-27.3(8)	C29	N2	C30	C31	-25.7(9)
Yb1	N2	C30	C31	151.0(5)	C9	C10	C6	C7	-0.2(6)
C20	C10	C6	C7	169.6(6)	Yb1	C10	C6	C7	-67.7(4)
C9	C10	C6	C16	-173.1(6)	C20	C10	C6	C16	-3.2(9)
Yb1	C10	C6	C16	119.5(6)	C9	C10	C6	Yb1	67.5(4)
C20	C10	C6	Yb1	-122.7(6)	C8	C7	C6	C10	-0.4(6)
C17	C7	C6	C10	-169.1(6)	Yb1	C7	C6	C10	67.6(4)
C8	C7	C6	C16	172.2(6)	C17	C7	C6	C16	3.4(10)
Yb1	C7	C6	C16	-119.8(6)	C8	C7	C6	Yb1	-68.0(4)
C17	C7	C6	Yb1	123.2(6)	N2	Yb1	C6	C10	-46.3(4)
N1	Yb1	C6	C10	35.9(4)	C9	Yb1	C6	C10	-37.3(3)
C7	Yb1	C6	C10	-113.7(5)	C5	Yb1	C6	C10	169.9(3)
C1	Yb1	C6	C10	128.2(3)	C8	Yb1	C6	C10	-76.7(4)
C4	Yb1	C6	C10	-173.9(3)	C3	Yb1	C6	C10	164.7(3)
C2	Yb1	C6	C10	135.4(3)	N2	Yb1	C6	C7	67.4(4)
N1	Yb1	C6	C7	149.6(3)	C10	Yb1	C6	C7	113.7(5)
C9	Yb1	C6	C7	76.4(4)	C5	Yb1	C6	C7	-76.5(4)
C1	Yb1	C6	C7	-118.1(4)	C8	Yb1	C6	C7	37.0(3)
C4	Yb1	C6	C7	-60.2(4)	C3	Yb1	C6	C7	-81.6(4)
C2	Yb1	C6	C7	-111.0(3)	N2	Yb1	C6	C16	-167.5(5)
N1	Yb1	C6	C16	-85.3(5)	C10	Yb1	C6	C16	-121.2(6)
C9	Yb1	C6	C16	-158.5(6)	C7	Yb1	C6	C16	125.1(7)
C5	Yb1	C6	C16	48.6(6)	C1	Yb1	C6	C16	7.0(6)
C8	Yb1	C6	C16	162.1(6)	C4	Yb1	C6	C16	64.9(5)
C3	Yb1	C6	C16	43.5(5)	C2	Yb1	C6	C16	14.1(5)
C4	C3	C2	C1	2.6(7)	C13	C3	C2	C1	166.6(6)
Yb1	C3	C2	C1	-65.4(4)	C4	C3	C2	C12	-166.8(5)
C13	C3	C2	C12	-2.8(10)	Yb1	C3	C2	C12	125.3(6)
C4	C3	C2	Yb1	67.9(4)	C13	C3	C2	Yb1	-128.0(6)
N2	Yb1	C2	C1	12.5(4)	N1	Yb1	C2	C1	-61.3(4)
C6	Yb1	C2	C1	-169.1(4)	C10	Yb1	C2	C1	-144.2(3)
C9	Yb1	C2	C1	-157.5(4)	C7	Yb1	C2	C1	159.8(3)
C5	Yb1	C2	C1	37.9(3)	C8	Yb1	C2	C1	151.6(4)
C4	Yb1	C2	C1	78.5(4)	C3	Yb1	C2	C1	116.0(5)
N2	Yb1	C2	C3	-103.5(4)	N1	Yb1	C2	C3	-177.3(4)
C6	Yb1	C2	C3	74.9(4)	C10	Yb1	C2	C3	99.9(4)
C9	Yb1	C2	C3	86.6(5)	C7	Yb1	C2	C3	43.8(4)
C5	Yb1	C2	C3	-78.1(4)	C1	Yb1	C2	C3	-116.0(5)
C8	Yb1	C2	C3	35.6(5)	C4	Yb1	C2	C3	-37.4(4)
N2	Yb1	C2	C12	136.6(5)	N1	Yb1	C2	C12	62.9(5)
C6	Yb1	C2	C12	-45.0(6)	C10	Yb1	C2	C12	-20.0(6)
C9	Yb1	C2	C12	-33.3(7)	C7	Yb1	C2	C12	-76.0(6)
C5	Yb1	C2	C12	162.0(6)	C1	Yb1	C2	C12	124.2(7)
C8	Yb1	C2	C12	-84.3(6)	C4	Yb1	C2	C12	-157.3(6)
C3	Yb1	C2	C12	-119.9(7)	C27	N1	C28	C29	-179.4(6)
Yb1	N1	C28	C29	4.3(8)	C27	N1	C28	Yb1	176.3(7)
N2	Yb1	C28	N1	173.9(5)	C6	Yb1	C28	N1	53.5(5)
C10	Yb1	C28	N1	61.7(4)	C9	Yb1	C28	N1	92.7(4)
C7	Yb1	C28	N1	90.1(5)	C5	Yb1	C28	N1	-110.6(4)
C1	Yb1	C28	N1	-80.3(4)	C8	Yb1	C28	N1	110.7(4)
C4	Yb1	C28	N1	-115.5(4)	C3	Yb1	C28	N1	-78.0(5)
C2	Yb1	C28	N1	-61.0(4)	N2	Yb1	C28	C29	-2.4(4)
N1	Yb1	C28	C29	-176.3(7)	C6	Yb1	C28	C29	-122.8(4)
C10	Yb1	C28	C29	-114.6(4)	C9	Yb1	C28	C29	-83.6(4)
C7	Yb1	C28	C29	-86.2(5)	C5	Yb1	C28	C29	73.1(4)

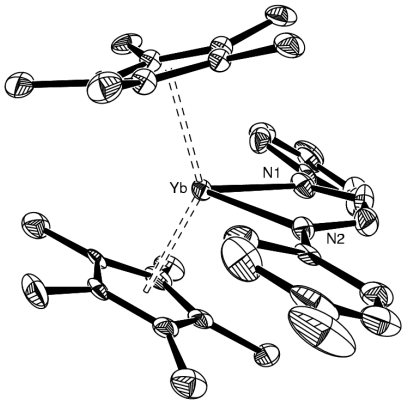
C1	Yb1	C28	C29	103.4(4)	C8	Yb1	C28	C29	-65.6(4)
C4	Yb1	C28	C29	68.2(4)	C3	Yb1	C28	C29	105.7(4)
C2	Yb1	C28	C29	122.7(4)	C3	C2	C1	C5	-1.9(7)
C12	C2	C1	C5	166.9(6)	Yb1	C2	C1	C5	-68.2(4)
C3	C2	C1	C11	-174.8(6)	C12	C2	C1	C11	-6.0(10)
Yb1	C2	C1	C11	118.9(6)	C3	C2	C1	Yb1	66.4(4)
C12	C2	C1	Yb1	-124.9(6)	N2	Yb1	C1	C2	-170.2(4)
N1	Yb1	C1	C2	118.2(4)	C6	Yb1	C1	C2	13.9(4)
C10	Yb1	C1	C2	55.4(5)	C9	Yb1	C1	C2	104.1(10)
C7	Yb1	C1	C2	-28.5(5)	C5	Yb1	C1	C2	-113.4(5)
C8	Yb1	C1	C2	-70.3(7)	C4	Yb1	C1	C2	-75.7(4)
C3	Yb1	C1	C2	-35.9(3)	N2	Yb1	C1	C5	-56.8(4)
N1	Yb1	C1	C5	-128.4(4)	C6	Yb1	C1	C5	127.3(4)
C10	Yb1	C1	C5	168.9(3)	C9	Yb1	C1	C5	-142.5(9)
C7	Yb1	C1	C5	84.9(4)	C8	Yb1	C1	C5	43.2(8)
C4	Yb1	C1	C5	37.7(3)	C3	Yb1	C1	C5	77.5(4)
C2	Yb1	C1	C5	113.4(5)	N2	Yb1	C1	C11	63.2(5)
N1	Yb1	C1	C11	-8.4(5)	C6	Yb1	C1	C11	-112.7(5)
C10	Yb1	C1	C11	-71.1(6)	C9	Yb1	C1	C11	-22.5(13)
C7	Yb1	C1	C11	-155.1(5)	C5	Yb1	C1	C11	120.0(7)
C8	Yb1	C1	C11	163.2(5)	C4	Yb1	C1	C11	157.7(6)
C3	Yb1	C1	C11	-162.5(6)	C2	Yb1	C1	C11	-126.6(7)
C33	C30	C31	C32	0.7(10)	N2	C30	C31	C32	-177.6(6)
C10	C9	C8	C7	-1.0(7)	C19	C9	C8	C7	-175.3(5)
Yb1	C9	C8	C7	66.4(4)	C10	C9	C8	C18	169.7(6)
C19	C9	C8	C18	-4.6(10)	Yb1	C9	C8	C18	-123.0(6)
C10	C9	C8	Yb1	-67.3(4)	C19	C9	C8	Yb1	118.4(6)
C6	C7	C8	C9	0.8(7)	C17	C7	C8	C9	169.9(5)
Yb1	C7	C8	C9	-66.5(4)	C6	C7	C8	C18	-170.0(6)
C17	C7	C8	C18	-0.9(10)	Yb1	C7	C8	C18	122.7(6)
C6	C7	C8	Yb1	67.3(4)	C17	C7	C8	Yb1	-123.6(6)
N2	Yb1	C8	C9	-80.0(4)	N1	Yb1	C8	C9	-11.6(4)
C6	Yb1	C8	C9	77.9(4)	C10	Yb1	C8	C9	37.6(4)
C7	Yb1	C8	C9	115.6(5)	C5	Yb1	C8	C9	-153.2(3)
C1	Yb1	C8	C9	177.8(5)	C4	Yb1	C8	C9	-177.7(4)
C3	Yb1	C8	C9	149.5(4)	C2	Yb1	C8	C9	130.9(4)
N2	Yb1	C8	C7	164.4(4)	N1	Yb1	C8	C7	-127.2(4)
C6	Yb1	C8	C7	-37.6(3)	C10	Yb1	C8	C7	-78.0(4)
C9	Yb1	C8	C7	-115.6(5)	C5	Yb1	C8	C7	91.2(4)
C1	Yb1	C8	C7	62.3(7)	C4	Yb1	C8	C7	66.7(4)
C3	Yb1	C8	C7	33.9(4)	C2	Yb1	C8	C7	15.3(5)
N2	Yb1	C8	C18	43.3(6)	N1	Yb1	C8	C18	111.7(5)
C6	Yb1	C8	C18	-158.8(7)	C10	Yb1	C8	C18	160.9(6)
C9	Yb1	C8	C18	123.3(7)	C7	Yb1	C8	C18	-121.1(7)
C5	Yb1	C8	C18	-29.9(7)	C1	Yb1	C8	C18	-58.9(9)
C4	Yb1	C8	C18	-54.4(6)	C3	Yb1	C8	C18	-87.2(6)
C2	Yb1	C8	C18	-105.8(6)	C2	C1	C5	C4	0.5(7)
C11	C1	C5	C4	173.8(6)	Yb1	C1	C5	C4	-69.1(4)
C2	C1	C5	C15	-169.7(6)	C11	C1	C5	C15	3.6(9)
Yb1	C1	C5	C15	120.7(6)	C2	C1	C5	Yb1	69.6(4)
C11	C1	C5	Yb1	-117.1(6)	C3	C4	C5	C1	1.1(6)
C14	C4	C5	C1	-170.7(5)	Yb1	C4	C5	C1	68.2(4)
C3	C4	C5	C15	171.2(6)	C14	C4	C5	C15	-0.7(10)
Yb1	C4	C5	C15	-121.7(6)	C3	C4	C5	Yb1	-67.1(4)
C14	C4	C5	Yb1	121.0(6)	N2	Yb1	C5	C1	123.1(4)
N1	Yb1	C5	C1	52.2(4)	C6	Yb1	C5	C1	-83.1(4)
C10	Yb1	C5	C1	-48.1(13)	C9	Yb1	C5	C1	162.4(4)

C7	Yb1	C5	C1	-122.2(4)	C8	Yb1	C5	C1	-161.9(3)
C4	Yb1	C5	C1	-113.0(5)	C3	Yb1	C5	C1	-76.5(4)
C2	Yb1	C5	C1	-37.0(3)	N2	Yb1	C5	C4	-123.9(4)
N1	Yb1	C5	C4	165.1(4)	C6	Yb1	C5	C4	29.9(5)
C10	Yb1	C5	C4	64.9(12)	C9	Yb1	C5	C4	-84.6(6)
C7	Yb1	C5	C4	-9.2(5)	C1	Yb1	C5	C4	113.0(5)
C8	Yb1	C5	C4	-49.0(5)	C3	Yb1	C5	C4	36.4(3)
C2	Yb1	C5	C4	75.9(4)	N2	Yb1	C5	C15	0.6(5)
N1	Yb1	C5	C15	-70.4(5)	C6	Yb1	C5	C15	154.4(5)
C10	Yb1	C5	C15	-170.6(10)	C9	Yb1	C5	C15	39.8(8)
C7	Yb1	C5	C15	115.2(5)	C1	Yb1	C5	C15	-122.5(7)
C8	Yb1	C5	C15	75.5(6)	C4	Yb1	C5	C15	124.5(7)
C3	Yb1	C5	C15	160.9(6)	C2	Yb1	C5	C15	-159.6(6)
C31	C30	C33	C34	-1.2(10)	N2	C30	C33	C34	177.2(6)
C30	N2	C29	C28	172.2(6)	Yb1	N2	C29	C28	-5.1(8)
C30	N2	C29	Yb1	177.3(7)	N1	C28	C29	N2	0.5(10)
Yb1	C28	C29	N2	3.7(6)	N1	C28	C29	Yb1	-3.1(6)
N1	Yb1	C29	N2	-173.6(5)	C6	Yb1	C29	N2	-99.9(5)
C10	Yb1	C29	N2	-107.1(4)	C9	Yb1	C29	N2	-81.4(4)
C7	Yb1	C29	N2	-57.4(5)	C5	Yb1	C29	N2	77.9(4)
C1	Yb1	C29	N2	108.7(4)	C8	Yb1	C29	N2	-54.9(5)
C4	Yb1	C29	N2	60.4(5)	C3	Yb1	C29	N2	82.4(5)
C2	Yb1	C29	N2	116.4(4)	N2	Yb1	C29	C28	175.5(7)
N1	Yb1	C29	C28	2.0(4)	C6	Yb1	C29	C28	75.7(4)
C10	Yb1	C29	C28	68.4(4)	C9	Yb1	C29	C28	94.1(4)
C7	Yb1	C29	C28	118.1(4)	C5	Yb1	C29	C28	-106.6(4)
C1	Yb1	C29	C28	-75.8(4)	C8	Yb1	C29	C28	120.7(4)
C4	Yb1	C29	C28	-124.0(4)	C3	Yb1	C29	C28	-102.1(4)
C2	Yb1	C29	C28	-68.1(4)	C30	C31	C32	C35	0.4(11)
C34	C35	C32	C31	-1.0(11)	C36	C35	C32	C31	178.0(7)
C24	C27	C26	C25	-6.2(10)	N1	C27	C26	C25	173.7(6)
C27	C26	C25	C22	5.9(11)	C23	C22	C25	C26	-1.6(10)
C21	C22	C25	C26	179.8(7)	C26	C27	C24	C23	2.6(9)
N1	C27	C24	C23	-177.3(6)	C30	C33	C34	C35	0.6(10)
C32	C35	C34	C33	0.5(10)	C36	C35	C34	C33	-178.5(6)
C25	C22	C23	C24	-1.9(10)	C21	C22	C23	C24	176.7(6)
C27	C24	C23	C22	1.3(10)					

Symmetry Operators:

x, y, z	-x, y+1/2, -z+1/2	-x, -y, -z	x, -y-1/2, z-1/2

Table 5. Least-squares planes (x,y,z in crystal coordinates) and deviations from them
(* indicates atom used to define plane)



- 7.3104 (0.0266) x + 9.8542 (0.0307) y + 9.2401 (0.0527) z = 6.0372 (0.0153)

* -0.0067 (0.0037) C1
* 0.0128 (0.0037) C2
* -0.0139 (0.0037) C3
* 0.0097 (0.0036) C4
* -0.0020 (0.0036) C5
-2.3733 (0.0025) Yb1
0.1173 (0.0111) C11
0.2910 (0.0108) C12
0.2823 (0.0107) C13
0.2137 (0.0106) C14
0.2003 (0.0112) C15

Rms deviation of fitted atoms = 0.0100

9.8387 (0.0182) x - 0.7357 (0.0400) y - 13.9777 (0.0443) z = 1.2417 (0.0182)

Angle to previous plane (with approximate esd) = 41.62 (0.27)

* 0.0004 (0.0034) C6
* -0.0035 (0.0036) C7
* 0.0053 (0.0037) C8
* -0.0050 (0.0036) C9
* 0.0028 (0.0034) C10
-2.3377 (0.0027) Yb1
0.1572 (0.0109) C16
0.2217 (0.0105) C17
0.2213 (0.0112) C18
0.1001 (0.0102) C19
0.2242 (0.0109) C20

Rms deviation of fitted atoms = 0.0038

- 9.2217 (0.0164) x + 5.4080 (0.0248) y + 12.6025 (0.0367) z = 2.4882 (0.0132)

Angle to previous plane (with approximate esd) = 19.65 (0.29)

* 0.0000 (0.0000) Yb1
* 0.0000 (0.0000) N1
* 0.0000 (0.0000) N2
    0.1056 (0.0088) C28
    0.1116 (0.0092) C29

Rms deviation of fitted atoms = 0.0000

- 8.8426 (0.0265) x + 6.6208 (0.0653) y + 11.9701 (0.0518) z = 2.6576 (0.0122)

Angle to previous plane (with approximate esd) = 5.47 (0.45)

* 0.0010 (0.0020) N1
* -0.0010 (0.0020) N2
* -0.0021 (0.0040) C28
* 0.0020 (0.0040) C29
    0.1801 (0.0125) Yb1

Rms deviation of fitted atoms = 0.0016

- 10.1698 (0.0133) x + 1.8242 (0.0402) y + 12.7922 (0.0394) z = 1.4459 (0.0227)

Angle to previous plane (with approximate esd) = 20.76 (0.34)

* 0.0091 (0.0047) C22
* -0.0185 (0.0047) C23
* 0.0020 (0.0044) C24
* 0.0175 (0.0050) C25
* -0.0338 (0.0049) C26
* 0.0236 (0.0042) C27
    0.0599 (0.0114) C21
    0.0997 (0.0089) N1

Rms deviation of fitted atoms = 0.0201

- 10.4212 (0.0126) x - 0.2499 (0.0364) y + 12.3709 (0.0422) z = 1.2894 (0.0070)

Angle to previous plane (with approximate esd) = 8.69 (0.26)

* -0.0064 (0.0047) C30
* 0.0009 (0.0047) C31
* 0.0052 (0.0049) C32
* 0.0057 (0.0046) C33
* 0.0004 (0.0047) C34
* -0.0059 (0.0049) C35
   -0.0450 (0.0116) C36
   -0.0601 (0.0094) N2

Rms deviation of fitted atoms = 0.0048

2. Crystal Structure Data of $(C_5Me_5)_2Yb(dad(H)\text{-}p\text{-}anisyl)$

2.1 Labeling Diagram

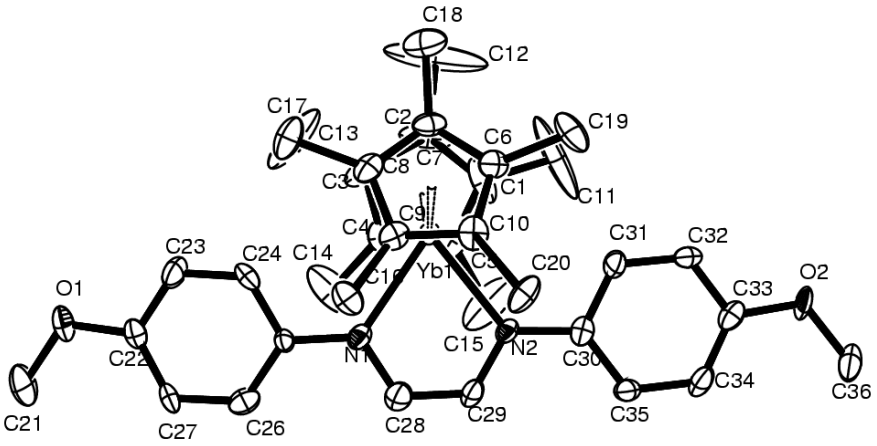


Figure S2. ORTEP diagram of $(C_5Me_5)_2Yb(dad(H)\text{-}p\text{-}anisyl)$ (50% probability ellipsoids).

2.2 Experimental Details

Data Collection

A fragment of a dark green block-like crystal of $C_{36}H_{46}N_2O_2Yb$ having approximate dimensions of 0.19 x 0.13 x 0.04 mm was mounted on a glass fiber using Paratone N hydrocarbon oil. All measurements were made on a Bruker SMART CCD 1k [10] CCD area detector with graphite monochromated MoK_α radiation.

Cell constants and an orientation matrix, obtained from a least-squares refinement using the measured positions of 2640 centered reflections with $I > 10\sigma(I)$ in the range $2.4 < \theta < 23.1^o$ corresponded to a primitive monoclinic cell with dimensions:

a = 9.990(1) Å	$\alpha = 90^o$
b = 30.731(3) Å	$\beta = 97.978(1)^o$
c = 10.457(1) Å	$\gamma = 90^o$
V = 3179.2(5)Å^3	

For Z = 4 and F.W. = 711.79, the calculated density is 1.487 g/cm^3.

Analysis of the systematic absences allowed the space group to be uniquely determined to be:

$P2_1/a$

The data were collected at a temperature of 144(2) K. Frames corresponding to an arbitrary hemisphere of data were collected using ω scans of 0.3^o counted for a total of 10 seconds per frame.

Data Reduction

Data were integrated by the program SAINT[11] to a maximum θ value of 24.73^o. The data were

corrected for Lorentz and polarization effects. Data were analyzed for agreement and possible absorption using XPREP[12]. An empirical absorption correction based on comparison of redundant and equivalent reflections was applied using SADABS[13]. (Tmax = 0.8903, Tmin = 0.6018). Of the 14042 reflections that were collected, 5234 were unique (R_{int} = 0.0886); equivalent reflections were merged. No decay correction was applied.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in calculated positions using a riding model, but not refined. The final cycle of full-matrix least-squares refinement[3] was based on 5234 reflections (all data) and 382 variable parameters and converged (largest parameter shift was 0.000 times its esd) with conventional unweighted and weighted agreement factors of:

$$R_1 = \Sigma||Fo| - |Fc|| / \Sigma|Fo| = 0.0542 \text{ for 3484 data with } I > 2\sigma(I)$$

$$wR_2 = [(\Sigma w (|Fo|^2 - |Fc|^2)^2 / \Sigma w |Fo|^2)]^{1/2} = 0.1108$$

The standard deviation of an observation of unit weight[4] was 0.988. The weighting scheme was based on counting statistics and included a factor (q = 0.0528) to downweight the intense reflections. The maximum and minimum peaks on the final difference Fourier map corresponded to 2.121 and -2.269 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the SHELXTL[9] crystallographic software package of Bruker Analytical X-ray Systems Inc.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{36}H_{46}N_2O_2Yb$
Formula Weight	711.79
Crystal Color, Habit	dark green, block
Crystal Dimensions	0.19 x 0.13 x 0.04 mm
Crystal System	monoclinic
Lattice Type	primitive
Lattice Parameters	a = 9.990(1) Å b = 30.731(3) Å c = 10.457(1) Å α= 90 ^{o} β= 97.978(1) ^{o} γ = 90^o V = 3179.2(5) Å^3
Space Group	$P2_1/a$
Z value	4
D_{calc}	1.487 g/cm^3
F_{000}	1448
μ(MoK)	2.97 cm^{-1}

B. Intensity Measurements

Diffractometer	Bruker SMART CCD 1k
Radiation	MoK$_\alpha$(λ = 0.71069 Å) graphite monochromated
Detector Position	60.00 mm
Exposure Time	10 seconds per frame.
Scan Type	ω (0.3 degrees per frame)
θ_{max}	24.73^o
No. of Reflections Measured	Total: 14042 Unique: 5234 (R_{int} = 0.0886)
Corrections	Lorentz-polarization Absorption (Tmax = 0.8903, Tmin = 0.6018)

C. Structure Solution and Refinement

Structure Solution	direct (SHELXS-97 (Sheldrick, 1997))
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\|F_o\|^2 - \|F_c\|^2)^2$
Least Squares Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (qP)^2 + 0.000P]$ where $P = [F_o^2 + 2F_c^2]/3$
q-factor	0.0528
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>2.00σ(I))	3484
No. Variables	382
Reflection/Parameter Ratio	9.12
Residuals: R; wR_2; Rall	0.0542; 0.1108; 0.1000
Goodness of Fit Indicator	0.988
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	2.121 $e^-/Å^3$
Minimum peak in Final Diff. Map	-2.269 $e^-/Å^3$

2.3 Tables

Table 1. Atomic coordinates and U_{iso}/U_{eq} and occupancy

atom	x	y	z	U_{eq}	Occupancy
C1	0.0659(13)	0.0478(4)	0.6174(9)	0.042(3)	1
C2	0.1927(14)	0.0376(3)	0.5856(12)	0.056(4)	1
C3	0.2258(10)	0.0666(4)	0.4902(11)	0.036(3)	1
C4	0.1162(11)	0.0942(3)	0.4633(9)	0.030(3)	1
C5	0.0182(10)	0.0836(3)	0.5406(9)	0.030(3)	1
C6	0.3438(10)	0.0904(3)	0.9347(8)	0.026(2)	1
C7	0.4313(10)	0.0771(3)	0.8490(9)	0.027(2)	1
C8	0.4824(9)	0.1146(3)	0.7964(8)	0.026(2)	1
C9	0.4256(10)	0.1508(3)	0.8475(8)	0.024(2)	1
C10	0.3391(9)	0.1356(3)	0.9349(8)	0.024(2)	1
C11	-0.017(2)	0.0187(5)	0.6946(11)	0.129(9)	1
C12	0.2696(19)	-0.0046(4)	0.6250(17)	0.156(10)	1
C13	0.3430(13)	0.0626(5)	0.4157(14)	0.094(6)	1
C14	0.0933(14)	0.1279(4)	0.3558(10)	0.070(5)	1
C15	-0.1185(12)	0.1049(4)	0.5335(13)	0.079(5)	1
C16	0.4627(10)	0.1978(3)	0.8292(9)	0.030(3)	1
C17	0.6007(10)	0.1135(4)	0.7157(9)	0.040(3)	1
C18	0.4929(11)	0.0324(3)	0.8430(11)	0.046(3)	1
C19	0.2836(11)	0.0602(3)	1.0282(9)	0.043(3)	1
C20	0.2698(10)	0.1653(3)	1.0219(8)	0.033(3)	1
C21	0.5236(12)	0.2624(3)	0.1583(9)	0.045(3)	1
C22	0.4617(9)	0.2180(3)	0.3279(8)	0.022(2)	1
C23	0.4829(10)	0.1800(3)	0.4000(9)	0.033(3)	1
C24	0.4025(10)	0.1705(3)	0.4923(9)	0.029(2)	1
C25	0.2967(9)	0.1973(3)	0.5161(8)	0.018(2)	1
C26	0.2800(9)	0.2357(3)	0.4471(9)	0.029(2)	1
C27	0.3612(10)	0.2461(3)	0.3514(9)	0.032(3)	1
C28	0.1149(10)	0.2069(3)	0.6383(9)	0.033(3)	1
C29	0.0316(10)	0.1918(3)	0.7237(9)	0.028(2)	1
C30	-0.0372(9)	0.1391(3)	0.8662(8)	0.021(2)	1
C31	-0.0245(10)	0.0957(3)	0.9070(9)	0.030(2)	1
C32	-0.1030(10)	0.0788(3)	0.9936(10)	0.034(3)	1
C33	-0.1963(9)	0.1040(3)	1.0427(9)	0.024(2)	1
C34	-0.2088(10)	0.1466(3)	1.0058(9)	0.029(2)	1
C35	-0.1311(9)	0.1647(3)	0.9186(8)	0.024(2)	1
C36	-0.3684(10)	0.1094(3)	1.1788(9)	0.038(3)	1
N1	0.2149(7)	0.1821(2)	0.6062(7)	0.022(2)	1
N2	0.0474(7)	0.1521(2)	0.7764(7)	0.020(2)	1
O1	0.5450(7)	0.2240(2)	0.2342(6)	0.032(2)	1
O2	-0.2709(6)	0.0840(2)	1.1264(6)	0.034(2)	1
Yb1	0.2226(1)	0.1133(1)	0.7020(1)	0.017(1)	1

U_{eq} is defined as one third of the orthogonalized U_{ij} tensor

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C1	0.074(10)	0.044(7)	0.007(5)	-0.002(5)	-0.001(6)	-0.036(7)
C2	0.081(11)	0.018(6)	0.056(9)	-0.028(6)	-0.038(8)	0.014(6)
C3	0.019(6)	0.047(7)	0.039(7)	-0.029(6)	-0.010(5)	0.006(5)
C4	0.033(7)	0.035(6)	0.020(6)	-0.003(5)	0.001(5)	-0.008(5)
C5	0.018(6)	0.049(7)	0.022(6)	-0.007(5)	-0.004(5)	0.000(5)
C6	0.034(7)	0.028(6)	0.016(5)	-0.003(4)	0.000(5)	0.003(5)
C7	0.030(6)	0.026(6)	0.023(6)	-0.002(5)	-0.004(5)	0.010(5)
C8	0.017(5)	0.038(6)	0.021(5)	-0.002(5)	-0.002(4)	0.005(5)
C9	0.027(6)	0.029(6)	0.014(5)	-0.007(4)	-0.002(4)	0.002(4)
C10	0.019(6)	0.038(6)	0.011(5)	-0.006(4)	-0.011(4)	-0.008(5)
C11	0.25(2)	0.113(13)	0.019(7)	0.002(8)	0.001(10)	-0.152(15)
C12	0.21(2)	0.023(8)	0.179(18)	-0.049(10)	-0.160(16)	0.039(10)
C13	0.042(9)	0.137(14)	0.107(12)	-0.110(11)	0.026(8)	-0.015(9)
C14	0.111(12)	0.060(9)	0.027(7)	0.013(6)	-0.038(7)	-0.037(8)
C15	0.030(8)	0.135(14)	0.069(9)	-0.061(9)	-0.009(7)	0.004(8)
C16	0.034(7)	0.027(6)	0.027(6)	0.000(4)	-0.002(5)	-0.011(5)
C17	0.031(6)	0.061(7)	0.029(6)	-0.017(6)	0.012(5)	-0.006(6)
C18	0.034(7)	0.039(7)	0.062(8)	-0.005(6)	-0.003(6)	0.012(5)
C19	0.052(8)	0.046(7)	0.029(6)	0.019(5)	-0.006(6)	-0.010(6)
C20	0.025(6)	0.053(7)	0.020(5)	-0.017(5)	0.003(4)	0.003(5)
C21	0.060(9)	0.054(8)	0.022(6)	0.009(5)	0.013(6)	-0.012(6)
C22	0.027(6)	0.022(5)	0.016(5)	-0.004(4)	0.003(4)	-0.011(4)
C23	0.033(7)	0.038(7)	0.031(6)	-0.004(5)	0.018(5)	0.002(5)
C24	0.037(7)	0.021(6)	0.030(6)	0.012(4)	0.010(5)	-0.001(5)
C25	0.022(6)	0.017(5)	0.016(5)	0.001(4)	0.006(4)	-0.001(4)
C26	0.019(6)	0.033(6)	0.032(6)	-0.002(5)	-0.002(5)	0.006(4)
C27	0.038(7)	0.026(6)	0.034(6)	0.011(5)	0.018(5)	-0.005(5)
C28	0.034(7)	0.035(6)	0.030(6)	0.004(5)	0.010(5)	0.007(5)
C29	0.029(6)	0.033(6)	0.025(6)	0.000(5)	0.013(5)	0.006(5)
C30	0.015(5)	0.032(6)	0.016(5)	-0.002(4)	-0.001(4)	-0.003(4)
C31	0.022(6)	0.037(6)	0.033(6)	0.011(5)	0.012(5)	0.007(5)
C32	0.034(7)	0.020(6)	0.051(7)	0.007(5)	0.019(5)	0.009(5)
C33	0.015(5)	0.036(7)	0.021(5)	-0.006(4)	0.000(4)	0.001(4)
C34	0.027(6)	0.032(6)	0.031(6)	-0.011(5)	0.015(5)	-0.002(4)
C35	0.022(6)	0.019(5)	0.031(6)	0.001(4)	0.005(4)	0.004(4)
C36	0.027(6)	0.064(8)	0.025(6)	0.010(6)	0.011(5)	0.006(6)
N1	0.017(5)	0.027(5)	0.023(4)	0.000(4)	0.005(4)	0.003(3)
N2	0.014(4)	0.025(5)	0.021(4)	0.000(3)	0.004(3)	0.003(3)
O1	0.037(4)	0.036(4)	0.023(4)	0.003(3)	0.011(3)	-0.013(3)
O2	0.025(4)	0.048(5)	0.034(4)	0.007(3)	0.022(3)	0.004(3)
Yb1	0.018(1)	0.019(1)	0.014(1)	-0.001(1)	0.004(1)	0.001(1)

The general temperature factor expression:

$\exp(-2\Pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}\,hl + 2b^*c^*U_{23}kl))$

Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
C100	Yb1	2.35	C101	Yb1	2.37
C1	C2	1.390(17)	C1	C5	1.404(14)
C1	C11	1.523(15)	C1	Yb1	2.625(10)
C2	C3	1.412(16)	C2	C12	1.534(15)
C2	Yb1	2.622(10)	C3	C4	1.382(14)
C3	C13	1.499(15)	C3	Yb1	2.642(10)
C4	C5	1.392(14)	C4	C14	1.522(14)
C4	Yb1	2.640(9)	C5	C15	1.507(14)
C5	Yb1	2.625(9)	C6	C10	1.390(12)
C6	C7	1.397(13)	C6	C19	1.532(13)
C6	Yb1	2.657(9)	C7	C8	1.402(13)
C7	C18	1.511(12)	C7	Yb1	2.656(9)
C8	C9	1.390(12)	C8	C17	1.544(13)
C8	Yb1	2.646(9)	C9	C10	1.421(13)
C9	C16	1.507(12)	C9	Yb1	2.628(9)
C10	C20	1.521(12)	C10	Yb1	2.640(8)
C11	H11A	0.9800	C11	H11B	0.9800
C11	H11C	0.9800	C12	H12A	0.9800
C12	H12B	0.9800	C12	H12C	0.9800
C13	H13A	0.9800	C13	H13B	0.9800
C13	H13C	0.9800	C14	H14A	0.9800
C14	H14B	0.9800	C14	H14C	0.9800
C15	H15A	0.9800	C15	H15B	0.9800
C15	H15C	0.9800	C16	H16A	0.9800
C16	H16B	0.9800	C16	H16C	0.9800
C17	H17A	0.9800	C17	H17B	0.9800
C17	H17C	0.9800	C18	H18A	0.9800
C18	H18B	0.9800	C18	H18C	0.9800
C19	H19A	0.9800	C19	H19B	0.9800
C19	H19C	0.9800	C20	H20A	0.9800
C20	H20B	0.9800	C20	H20C	0.9800
C21	O1	1.422(11)	C21	H21A	0.9800
C21	H21B	0.9800	C21	H21C	0.9800
C22	C27	1.370(13)	C22	O1	1.384(10)
C22	C23	1.390(12)	C23	C24	1.370(12)
C23	H23	0.9500	C24	C25	1.388(12)
C24	H24	0.9500	C25	C26	1.381(12)
C25	N1	1.410(11)	C26	C27	1.411(13)
C26	H26	0.9500	C27	H27	0.9500
C28	N1	1.335(11)	C28	C29	1.382(13)
C28	Yb1	3.111(10)	C28	H28	0.9500
C29	N2	1.339(11)	C29	Yb1	3.105(10)
C29	H29	0.9500	C30	C35	1.392(12)
C30	C31	1.402(12)	C30	N2	1.406(11)
C31	C32	1.379(13)	C31	H31	0.9500
C32	C33	1.366(12)	C32	H32	0.9500
C33	C34	1.367(12)	C33	O2	1.371(11)
C34	C35	1.392(12)	C34	H34	0.9500
C35	H35	0.9500	C36	O2	1.417(11)
C36	H36A	0.9800	C36	H36B	0.9800
C36	H36C	0.9800	N1	Yb1	2.337(7)

N2	Yb1	2.339(7)

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C100	Yb1	C101	142.5	C2	C1	C5	106.8(10)
C2	C1	C11	124.9(14)	C5	C1	C11	126.7(14)
C2	C1	Yb1	74.5(6)	C5	C1	Yb1	74.5(6)
C11	C1	Yb1	127.8(7)	C1	C2	C3	109.7(10)
C1	C2	C12	124.6(15)	C3	C2	C12	124.5(15)
C1	C2	Yb1	74.7(6)	C3	C2	Yb1	75.2(6)
C12	C2	Yb1	127.2(8)	C4	C3	C2	105.9(10)
C4	C3	C13	126.8(12)	C2	C3	C13	126.2(12)
C4	C3	Yb1	74.7(6)	C2	C3	Yb1	73.7(6)
C13	C3	Yb1	125.6(7)	C3	C4	C5	109.8(9)
C3	C4	C14	126.9(11)	C5	C4	C14	122.9(10)
C3	C4	Yb1	74.9(6)	C5	C4	Yb1	74.1(5)
C14	C4	Yb1	123.2(7)	C4	C5	C1	107.8(10)
C4	C5	C15	125.1(10)	C1	C5	C15	126.9(11)
C4	C5	Yb1	75.2(6)	C1	C5	Yb1	74.5(6)
C15	C5	Yb1	120.0(7)	C10	C6	C7	108.5(9)
C10	C6	C19	126.1(9)	C7	C6	C19	124.6(9)
C10	C6	Yb1	74.1(5)	C7	C6	Yb1	74.7(5)
C19	C6	Yb1	125.1(6)	C6	C7	C8	107.8(8)
C6	C7	C18	126.0(9)	C8	C7	C18	123.9(10)
C6	C7	Yb1	74.8(6)	C8	C7	Yb1	74.3(5)
C18	C7	Yb1	130.4(7)	C9	C8	C7	108.5(8)
C9	C8	C17	127.7(9)	C7	C8	C17	122.9(9)
C9	C8	Yb1	74.0(5)	C7	C8	Yb1	75.0(5)
C17	C8	Yb1	125.5(6)	C8	C9	C10	107.5(8)
C8	C9	C16	126.7(9)	C10	C9	C16	125.3(8)
C8	C9	Yb1	75.5(5)	C10	C9	Yb1	74.8(5)
C16	C9	Yb1	122.0(6)	C6	C10	C9	107.7(9)
C6	C10	C20	128.1(9)	C9	C10	C20	123.8(9)
C6	C10	Yb1	75.5(5)	C9	C10	Yb1	73.9(5)
C20	C10	Yb1	121.9(6)	C1	C11	H11A	109.5
C1	C11	H11B	109.5	H11A	C11	H11B	109.5
C1	C11	H11C	109.5	H11A	C11	H11C	109.5
H11B	C11	H11C	109.5	C2	C12	H12A	109.5
C2	C12	H12B	109.5	H12A	C12	H12B	109.5
C2	C12	H12C	109.5	H12A	C12	H12C	109.5
H12B	C12	H12C	109.5	C3	C13	H13A	109.5
C3	C13	H13B	109.5	H13A	C13	H13B	109.5
C3	C13	H13C	109.5	H13A	C13	H13C	109.5
H13B	C13	H13C	109.5	C4	C14	H14A	109.5
C4	C14	H14B	109.5	H14A	C14	H14B	109.5
C4	C14	H14C	109.5	H14A	C14	H14C	109.5
H14B	C14	H14C	109.5	C5	C15	H15A	109.5
C5	C15	H15B	109.5	H15A	C15	H15B	109.5
C5	C15	H15C	109.5	H15A	C15	H15C	109.5
H15B	C15	H15C	109.5	C9	C16	H16A	109.5
C9	C16	H16B	109.5	H16A	C16	H16B	109.5
C9	C16	H16C	109.5	H16A	C16	H16C	109.5
H16B	C16	H16C	109.5	C8	C17	H17A	109.5
C8	C17	H17B	109.5	H17A	C17	H17B	109.5
C8	C17	H17C	109.5	H17A	C17	H17C	109.5

H17B	C17	H17C	109.5	C7	C18	H18A	109.5
C7	C18	H18B	109.5	H18A	C18	H18B	109.5
C7	C18	H18C	109.5	H18A	C18	H18C	109.5
H18B	C18	H18C	109.5	C6	C19	H19A	109.5
C6	C19	H19B	109.5	H19A	C19	H19B	109.5
C6	C19	H19C	109.5	H19A	C19	H19C	109.5
H19B	C19	H19C	109.5	C10	C20	H20A	109.5
C10	C20	H20B	109.5	H20A	C20	H20B	109.5
C10	C20	H20C	109.5	H20A	C20	H20C	109.5
H20B	C20	H20C	109.5	O1	C21	H21A	109.5
O1	C21	H21B	109.5	H21A	C21	H21B	109.5
O1	C21	H21C	109.5	H21A	C21	H21C	109.5
H21B	C21	H21C	109.5	C27	C22	O1	124.8(8)
C27	C22	C23	119.5(9)	O1	C22	C23	115.7(8)
C24	C23	C22	120.1(9)	C24	C23	H23	120.0
C22	C23	H23	120.0	C23	C24	C25	122.4(9)
C23	C24	H24	118.8	C25	C24	H24	118.8
C26	C25	C24	116.9(8)	C26	C25	N1	126.4(8)
C24	C25	N1	116.8(8)	C25	C26	C27	121.7(9)
C25	C26	H26	119.2	C27	C26	H26	119.2
C22	C27	C26	119.5(9)	C22	C27	H27	120.3
C26	C27	H27	120.3	N1	C28	C29	120.6(9)
N1	C28	Yb1	43.8(5)	C29	C28	Yb1	76.9(6)
N1	C28	H28	119.7	C29	C28	H28	119.7
Yb1	C28	H28	163.4	N2	C29	C28	121.6(9)
N2	C29	Yb1	44.2(4)	C28	C29	Yb1	77.4(6)
N2	C29	H29	119.2	C28	C29	H29	119.2
Yb1	C29	H29	163.4	C35	C30	C31	117.1(8)
C35	C30	N2	127.0(9)	C31	C30	N2	115.9(8)
C32	C31	C30	121.5(9)	C32	C31	H31	119.2
C30	C31	H31	119.2	C33	C32	C31	120.9(9)
C33	C32	H32	119.6	C31	C32	H32	119.6
C32	C33	C34	118.6(9)	C32	C33	O2	116.4(8)
C34	C33	O2	125.1(8)	C33	C34	C35	121.9(9)
C33	C34	H34	119.0	C35	C34	H34	119.0
C30	C35	C34	120.0(9)	C30	C35	H35	120.0
C34	C35	H35	120.0	O2	C36	H36A	109.5
O2	C36	H36B	109.5	H36A	C36	H36B	109.5
O2	C36	H36C	109.5	H36A	C36	H36C	109.5
H36B	C36	H36C	109.5	C28	N1	C25	120.1(8)
C28	N1	Yb1	113.0(6)	C25	N1	Yb1	126.8(6)
C29	N2	C30	119.1(7)	C29	N2	Yb1	112.3(6)
C30	N2	Yb1	128.6(6)	C22	O1	C21	116.5(8)
C33	O2	C36	117.6(7)	N1	Yb1	N2	72.5(2)
N1	Yb1	C2	127.5(3)	N2	Yb1	C2	124.4(4)
N1	Yb1	C1	124.5(3)	N2	Yb1	C1	93.7(4)
C2	Yb1	C1	30.7(4)	N1	Yb1	C5	93.6(3)
N2	Yb1	C5	80.8(3)	C2	Yb1	C5	50.6(3)
C1	Yb1	C5	31.0(3)	N1	Yb1	C9	80.0(3)
N2	Yb1	C9	97.8(3)	C2	Yb1	C9	133.4(3)
C1	Yb1	C9	155.2(3)	C5	Yb1	C9	173.6(3)
N1	Yb1	C4	79.1(3)	N2	Yb1	C4	101.9(3)
C2	Yb1	C4	50.2(3)	C1	Yb1	C4	50.8(3)
C5	Yb1	C4	30.6(3)	C9	Yb1	C4	145.3(3)
N1	Yb1	C10	98.2(3)	N2	Yb1	C10	79.3(3)
C2	Yb1	C10	131.8(3)	C1	Yb1	C10	132.6(3)
C5	Yb1	C10	152.6(3)	C9	Yb1	C10	31.3(3)

C4	Yb1	C10	176.5(3)	N1	Yb1	C3	97.8(3)
N2	Yb1	C3	130.7(3)	C2	Yb1	C3	31.1(4)
C1	Yb1	C3	51.6(3)	C5	Yb1	C3	51.0(3)
C9	Yb1	C3	128.7(3)	C4	Yb1	C3	30.3(3)
C10	Yb1	C3	149.3(3)	N1	Yb1	C8	96.8(3)
N2	Yb1	C8	127.5(3)	C2	Yb1	C8	103.3(4)
C1	Yb1	C8	130.2(4)	C5	Yb1	C8	151.7(3)
C9	Yb1	C8	30.6(3)	C4	Yb1	C8	127.0(3)
C10	Yb1	C8	50.8(3)	C3	Yb1	C8	101.3(3)
N1	Yb1	C7	127.1(3)	N2	Yb1	C7	125.8(3)
C2	Yb1	C7	85.9(3)	C1	Yb1	C7	105.0(3)
C5	Yb1	C7	134.8(3)	C9	Yb1	C7	50.8(3)
C4	Yb1	C7	129.4(3)	C10	Yb1	C7	50.6(3)
C3	Yb1	C7	99.1(3)	C8	Yb1	C7	30.7(3)
N1	Yb1	C6	127.9(3)	N2	Yb1	C6	95.6(3)
C2	Yb1	C6	101.5(3)	C1	Yb1	C6	106.3(3)
C5	Yb1	C6	135.4(3)	C9	Yb1	C6	50.9(3)
C4	Yb1	C6	151.6(3)	C10	Yb1	C6	30.4(3)
C3	Yb1	C6	124.6(3)	C8	Yb1	C6	50.5(3)
C7	Yb1	C6	30.5(3)				

Table 5. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C5	C1	C2	C3	0.4(12)	C11	C1	C2	C3	166.6(9)
Yb1	C1	C2	C3	-67.8(7)	C5	C1	C2	C12	-166.9(10)
C11	C1	C2	C12	-0.7(17)	Yb1	C1	C2	C12	125.0(11)
C5	C1	C2	Yb1	68.1(7)	C11	C1	C2	Yb1	-125.7(10)
C1	C2	C3	C4	-0.9(12)	C12	C2	C3	C4	166.4(10)
Yb1	C2	C3	C4	-68.3(7)	C1	C2	C3	C13	-170.1(10)
C12	C2	C3	C13	-2.8(17)	Yb1	C2	C3	C13	122.5(10)
C1	C2	C3	Yb1	67.5(7)	C12	C2	C3	Yb1	-125.3(11)
C2	C3	C4	C5	1.1(12)	C13	C3	C4	C5	170.2(10)
Yb1	C3	C4	C5	-66.5(7)	C2	C3	C4	C14	-172.0(10)
C13	C3	C4	C14	-2.9(17)	Yb1	C3	C4	C14	120.4(10)
C2	C3	C4	Yb1	67.6(7)	C13	C3	C4	Yb1	-123.3(11)
C3	C4	C5	C1	-0.9(12)	C14	C4	C5	C1	172.5(9)
Yb1	C4	C5	C1	-67.9(7)	C3	C4	C5	C15	-176.5(10)
C14	C4	C5	C15	-3.0(16)	Yb1	C4	C5	C15	116.5(10)
C3	C4	C5	Yb1	67.0(7)	C14	C4	C5	Yb1	-119.5(9)
C2	C1	C5	C4	0.3(11)	C11	C1	C5	C4	-165.5(10)
Yb1	C1	C5	C4	68.5(7)	C2	C1	C5	C15	175.8(10)
C11	C1	C5	C15	9.9(17)	Yb1	C1	C5	C15	-116.1(10)
C2	C1	C5	Yb1	-68.2(7)	C11	C1	C5	Yb1	126.0(11)
C10	C6	C7	C8	0.6(11)	C19	C6	C7	C8	-170.0(8)
Yb1	C6	C7	C8	67.6(7)	C10	C6	C7	C18	163.8(9)
C19	C6	C7	C18	-6.8(16)	Yb1	C6	C7	C18	-129.2(10)
C10	C6	C7	Yb1	-67.0(7)	C19	C6	C7	Yb1	122.4(9)
C6	C7	C8	C9	-0.9(10)	C18	C7	C8	C9	-164.5(9)
Yb1	C7	C8	C9	67.0(6)	C6	C7	C8	C17	169.2(8)
C18	C7	C8	C17	5.6(14)	Yb1	C7	C8	C17	-122.9(8)
C6	C7	C8	Yb1	-67.9(7)	C18	C7	C8	Yb1	128.5(9)
C7	C8	C9	C10	0.9(10)	C17	C8	C9	C10	-168.6(8)
Yb1	C8	C9	C10	68.6(6)	C7	C8	C9	C16	172.9(9)
C17	C8	C9	C16	3.4(15)	Yb1	C8	C9	C16	-119.4(9)
C7	C8	C9	Yb1	-67.7(6)	C17	C8	C9	Yb1	122.8(9)
C7	C6	C10	C9	0.0(11)	C19	C6	C10	C9	170.4(9)
Yb1	C6	C10	C9	-67.4(6)	C7	C6	C10	C20	-173.2(8)
C19	C6	C10	C20	-2.8(16)	Yb1	C6	C10	C20	119.4(9)
C7	C6	C10	Yb1	67.4(7)	C19	C6	C10	Yb1	-122.2(10)
C8	C9	C10	C6	-0.5(10)	C16	C9	C10	C6	-172.7(8)
Yb1	C9	C10	C6	68.5(6)	C8	C9	C10	C20	173.0(8)
C16	C9	C10	C20	0.9(14)	Yb1	C9	C10	C20	-118.0(8)
C8	C9	C10	Yb1	-69.0(6)	C16	C9	C10	Yb1	118.8(9)
C27	C22	C23	C24	0.9(15)	O1	C22	C23	C24	-177.9(8)
C22	C23	C24	C25	1.3(15)	C23	C24	C25	C26	-3.6(15)
C23	C24	C25	N1	175.0(9)	C24	C25	C26	C27	3.7(14)
N1	C25	C26	C27	-174.7(9)	O1	C22	C27	C26	177.9(8)
C23	C22	C27	C26	-0.8(15)	C25	C26	C27	C22	-1.7(15)
N1	C28	C29	N2	-0.4(15)	Yb1	C28	C29	N2	1.2(8)
N1	C28	C29	Yb1	-1.6(8)	C35	C30	C31	C32	1.0(14)
N2	C30	C31	C32	-179.2(9)	C30	C31	C32	C33	0.1(16)
C31	C32	C33	C34	-1.1(16)	C31	C32	C33	O2	178.9(9)
C32	C33	C34	C35	1.1(14)	O2	C33	C34	C35	-178.9(9)
C31	C30	C35	C34	-1.0(13)	N2	C30	C35	C34	179.2(8)

C33	C34	C35	C30	-0.1(14)	C29	C28	N1	C25	178.1(9)
Yb1	C28	N1	C25	175.9(11)	C29	C28	N1	Yb1	2.2(12)
C26	C25	N1	C28	-4.5(14)	C24	C25	N1	C28	177.0(9)
C26	C25	N1	Yb1	170.8(7)	C24	C25	N1	Yb1	-7.7(12)
C28	C29	N2	C30	177.7(9)	Yb1	C29	N2	C30	179.4(10)
C28	C29	N2	Yb1	-1.7(12)	C35	C30	N2	C29	-6.6(14)
C31	C30	N2	C29	173.5(8)	C35	C30	N2	Yb1	172.7(7)
C31	C30	N2	Yb1	-7.2(11)	C27	C22	O1	C21	0.4(13)
C23	C22	O1	C21	179.2(8)	C32	C33	O2	C36	180.0(9)
C34	C33	O2	C36	0.0(13)	C28	N1	Yb1	N2	-2.2(6)
C25	N1	Yb1	N2	-177.7(8)	C28	N1	Yb1	C2	118.1(7)
C25	N1	Yb1	C2	-57.5(9)	C28	N1	Yb1	C1	80.0(7)
C25	N1	Yb1	C1	-95.5(8)	C28	N1	Yb1	C5	77.0(7)
C25	N1	Yb1	C5	-98.5(7)	C28	N1	Yb1	C9	-103.8(7)
C25	N1	Yb1	C9	80.7(7)	C28	N1	Yb1	C4	104.1(7)
C25	N1	Yb1	C4	-71.4(7)	C28	N1	Yb1	C10	-78.2(7)
C25	N1	Yb1	C10	106.3(7)	C28	N1	Yb1	C3	128.1(7)
C25	N1	Yb1	C3	-47.4(7)	C28	N1	Yb1	C8	-129.4(7)
C25	N1	Yb1	C8	55.0(7)	C28	N1	Yb1	C7	-124.2(7)
C25	N1	Yb1	C7	60.3(8)	C28	N1	Yb1	C6	-85.5(7)
C25	N1	Yb1	C6	99.0(7)	C29	N2	Yb1	N1	2.0(6)
C30	N2	Yb1	N1	-177.3(8)	C29	N2	Yb1	C2	-121.9(7)
C30	N2	Yb1	C2	58.8(8)	C29	N2	Yb1	C1	-123.1(6)
C30	N2	Yb1	C1	57.6(7)	C29	N2	Yb1	C5	-94.8(6)
C30	N2	Yb1	C5	85.9(7)	C29	N2	Yb1	C9	78.9(6)
C30	N2	Yb1	C9	-100.4(7)	C29	N2	Yb1	C4	-72.4(6)
C30	N2	Yb1	C4	108.3(7)	C29	N2	Yb1	C10	104.3(6)
C30	N2	Yb1	C10	-75.1(7)	C29	N2	Yb1	C3	-83.2(7)
C30	N2	Yb1	C3	97.5(8)	C29	N2	Yb1	C8	87.0(7)
C30	N2	Yb1	C8	-92.3(8)	C29	N2	Yb1	C7	125.5(6)
C30	N2	Yb1	C7	-53.9(8)	C29	N2	Yb1	C6	130.1(6)
C30	N2	Yb1	C6	-49.3(7)	C1	C2	Yb1	N1	-96.1(8)
C3	C2	Yb1	N1	19.6(9)	C12	C2	Yb1	N1	141.9(15)
C1	C2	Yb1	N2	-2.3(9)	C3	C2	Yb1	N2	113.3(7)
C12	C2	Yb1	N2	-124.4(15)	C3	C2	Yb1	C1	115.6(9)
C12	C2	Yb1	C1	-122.1(19)	C1	C2	Yb1	C5	-38.0(6)
C3	C2	Yb1	C5	77.7(7)	C12	C2	Yb1	C5	-160.0(18)
C1	C2	Yb1	C9	148.7(6)	C3	C2	Yb1	C9	-95.7(7)
C12	C2	Yb1	C9	26.6(18)	C1	C2	Yb1	C4	-78.1(7)
C3	C2	Yb1	C4	37.5(6)	C12	C2	Yb1	C4	159.8(18)
C1	C2	Yb1	C10	105.8(7)	C3	C2	Yb1	C10	-138.6(6)
C12	C2	Yb1	C10	-16.3(18)	C1	C2	Yb1	C3	-115.6(9)
C12	C2	Yb1	C3	122.3(19)	C1	C2	Yb1	C8	154.4(7)
C3	C2	Yb1	C8	-89.9(7)	C12	C2	Yb1	C8	32.4(17)
C1	C2	Yb1	C7	129.0(7)	C3	C2	Yb1	C7	-115.3(7)
C12	C2	Yb1	C7	7.0(16)	C1	C2	Yb1	C6	102.7(7)
C3	C2	Yb1	C6	-141.7(7)	C12	C2	Yb1	C6	-19.4(16)
C2	C1	Yb1	N1	106.9(8)	C5	C1	Yb1	N1	-5.9(8)
C11	C1	Yb1	N1	-130.7(13)	C2	C1	Yb1	N2	178.1(7)
C5	C1	Yb1	N2	65.3(6)	C11	C1	Yb1	N2	-59.5(14)
C5	C1	Yb1	C2	-112.8(9)	C11	C1	Yb1	C2	122.4(17)
C2	C1	Yb1	C5	112.8(9)	C11	C1	Yb1	C5	-124.8(17)
C2	C1	Yb1	C9	-64.2(10)	C5	C1	Yb1	C9	-177.0(6)
C11	C1	Yb1	C9	58.2(18)	C2	C1	Yb1	C4	75.7(7)
C5	C1	Yb1	C4	-37.0(6)	C11	C1	Yb1	C4	-161.8(16)
C2	C1	Yb1	C10	-103.0(7)	C5	C1	Yb1	C10	144.2(6)
C11	C1	Yb1	C10	19.4(16)	C2	C1	Yb1	C3	36.5(6)

C5	C1	Yb1	C3	-76.3(6)	C11	C1	Yb1	C3	159.0(16)
C2	C1	Yb1	C8	-33.4(8)	C5	C1	Yb1	C8	-146.1(6)
C11	C1	Yb1	C8	89.1(15)	C2	C1	Yb1	C7	-53.3(7)
C5	C1	Yb1	C7	-166.1(6)	C11	C1	Yb1	C7	69.1(14)
C2	C1	Yb1	C6	-85.0(7)	C5	C1	Yb1	C6	162.2(6)
C11	C1	Yb1	C6	37.4(15)	C4	C5	Yb1	N1	61.5(6)
C1	C5	Yb1	N1	175.1(7)	C15	C5	Yb1	N1	-60.9(9)
C4	C5	Yb1	N2	133.1(6)	C1	C5	Yb1	N2	-113.3(7)
C15	C5	Yb1	N2	10.7(9)	C4	C5	Yb1	C2	-76.1(7)
C1	C5	Yb1	C2	37.6(7)	C15	C5	Yb1	C2	161.5(11)
C4	C5	Yb1	C1	-113.7(9)	C15	C5	Yb1	C1	124.0(13)
C4	C5	Yb1	C9	55(3)	C1	C5	Yb1	C9	169(2)
C15	C5	Yb1	C9	-67(3)	C1	C5	Yb1	C4	113.7(9)
C15	C5	Yb1	C4	-122.4(12)	C4	C5	Yb1	C10	177.1(6)
C1	C5	Yb1	C10	-69.2(10)	C15	C5	Yb1	C10	54.7(13)
C4	C5	Yb1	C3	-35.6(6)	C1	C5	Yb1	C3	78.0(7)
C15	C5	Yb1	C3	-158.0(11)	C4	C5	Yb1	C8	-50.0(10)
C1	C5	Yb1	C8	63.7(10)	C15	C5	Yb1	C8	-172.3(9)
C4	C5	Yb1	C7	-94.6(7)	C1	C5	Yb1	C7	19.1(9)
C15	C5	Yb1	C7	143.1(9)	C4	C5	Yb1	C6	-138.3(6)
C1	C5	Yb1	C6	-24.6(8)	C15	C5	Yb1	C6	99.3(10)
C8	C9	Yb1	N1	-122.2(6)	C10	C9	Yb1	N1	124.7(6)
C16	C9	Yb1	N1	2.2(7)	C8	C9	Yb1	N2	167.2(6)
C10	C9	Yb1	N2	54.1(6)	C16	C9	Yb1	N2	-68.3(7)
C8	C9	Yb1	C2	11.0(8)	C10	C9	Yb1	C2	-102.1(7)
C16	C9	Yb1	C2	135.5(8)	C8	C9	Yb1	C1	50.3(11)
C10	C9	Yb1	C1	-62.8(10)	C16	C9	Yb1	C1	174.8(8)
C8	C9	Yb1	C5	-116(3)	C10	C9	Yb1	C5	131(2)
C16	C9	Yb1	C5	9(3)	C8	C9	Yb1	C4	-68.4(8)
C10	C9	Yb1	C4	178.5(6)	C16	C9	Yb1	C4	56.0(10)
C8	C9	Yb1	C10	113.1(8)	C16	C9	Yb1	C10	-122.5(10)
C8	C9	Yb1	C3	-30.2(7)	C10	C9	Yb1	C3	-143.3(6)
C16	C9	Yb1	C3	94.2(8)	C10	C9	Yb1	C8	-113.1(8)
C16	C9	Yb1	C8	124.4(10)	C8	C9	Yb1	C7	36.7(5)
C10	C9	Yb1	C7	-76.4(6)	C16	C9	Yb1	C7	161.2(9)
C8	C9	Yb1	C6	76.4(6)	C10	C9	Yb1	C6	-36.7(5)
C16	C9	Yb1	C6	-159.2(9)	C3	C4	Yb1	N1	127.0(7)
C5	C4	Yb1	N1	-116.8(6)	C14	C4	Yb1	N1	2.5(9)
C3	C4	Yb1	N2	-163.7(7)	C5	C4	Yb1	N2	-47.5(6)
C14	C4	Yb1	N2	71.7(10)	C3	C4	Yb1	C2	-38.6(7)
C5	C4	Yb1	C2	77.7(7)	C14	C4	Yb1	C2	-163.1(12)
C3	C4	Yb1	C1	-78.7(7)	C5	C4	Yb1	C1	37.5(6)
C14	C4	Yb1	C1	156.7(12)	C3	C4	Yb1	C5	-116.2(9)
C14	C4	Yb1	C5	119.2(12)	C3	C4	Yb1	C9	73.0(9)
C5	C4	Yb1	C9	-170.8(6)	C14	C4	Yb1	C9	-51.5(12)
C3	C4	Yb1	C10	86(5)	C5	C4	Yb1	C10	-158(5)
C14	C4	Yb1	C10	-38(5)	C5	C4	Yb1	C3	116.2(9)
C14	C4	Yb1	C3	-124.5(13)	C3	C4	Yb1	C8	36.7(8)
C5	C4	Yb1	C8	152.9(6)	C14	C4	Yb1	C8	-87.8(10)
C3	C4	Yb1	C7	-2.5(8)	C5	C4	Yb1	C7	113.7(6)
C14	C4	Yb1	C7	-127.1(9)	C3	C4	Yb1	C6	-36.9(11)
C5	C4	Yb1	C6	79.3(9)	C14	C4	Yb1	C6	-161.5(9)
C6	C10	Yb1	N1	-168.6(6)	C9	C10	Yb1	N1	-54.9(6)
C20	C10	Yb1	N1	65.2(8)	C6	C10	Yb1	N2	121.1(6)
C9	C10	Yb1	N2	-125.2(6)	C20	C10	Yb1	N2	-5.1(7)
C6	C10	Yb1	C2	-5.9(9)	C9	C10	Yb1	C2	107.8(7)
C20	C10	Yb1	C2	-132.1(8)	C6	C10	Yb1	C1	35.9(8)

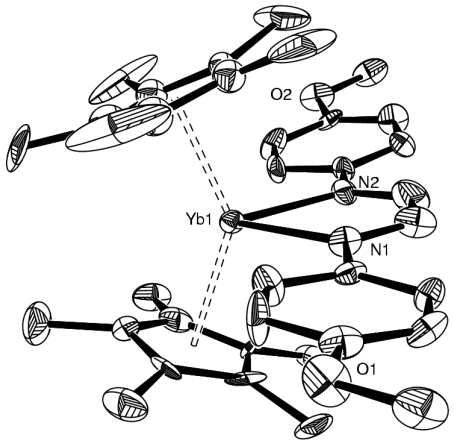
C9	C10	Yb1	C1	149.6(6)	C20	C10	Yb1	C1	-90.2(9)
C6	C10	Yb1	C5	76.8(9)	C9	C10	Yb1	C5	-169.5(6)
C20	C10	Yb1	C5	-49.4(12)	C6	C10	Yb1	C9	-113.7(9)
C20	C10	Yb1	C9	120.1(11)	C6	C10	Yb1	C4	-128(5)
C9	C10	Yb1	C4	-14(5)	C20	C10	Yb1	C4	106(5)
C6	C10	Yb1	C3	-47.9(10)	C9	C10	Yb1	C3	65.8(9)
C20	C10	Yb1	C3	-174.1(7)	C6	C10	Yb1	C8	-76.6(6)
C9	C10	Yb1	C8	37.1(5)	C20	C10	Yb1	C8	157.3(9)
C6	C10	Yb1	C7	-36.6(6)	C9	C10	Yb1	C7	77.1(6)
C20	C10	Yb1	C7	-162.8(9)	C9	C10	Yb1	C6	113.7(9)
C20	C10	Yb1	C6	-126.2(11)	C4	C3	Yb1	N1	-52.3(7)
C2	C3	Yb1	N1	-164.4(7)	C13	C3	Yb1	N1	72.3(12)
C4	C3	Yb1	N2	21.2(9)	C2	C3	Yb1	N2	-90.9(8)
C13	C3	Yb1	N2	145.9(10)	C4	C3	Yb1	C2	112.1(10)
C13	C3	Yb1	C2	-123.2(15)	C4	C3	Yb1	C1	76.1(7)
C2	C3	Yb1	C1	-36.0(7)	C13	C3	Yb1	C1	-159.2(14)
C4	C3	Yb1	C5	36.0(6)	C2	C3	Yb1	C5	-76.1(7)
C13	C3	Yb1	C5	160.7(13)	C4	C3	Yb1	C9	-135.8(6)
C2	C3	Yb1	C9	112.1(7)	C13	C3	Yb1	C9	-11.1(13)
C2	C3	Yb1	C4	-112.1(10)	C13	C3	Yb1	C4	124.7(15)
C4	C3	Yb1	C10	-173.1(6)	C2	C3	Yb1	C10	74.7(9)
C13	C3	Yb1	C10	-48.5(15)	C4	C3	Yb1	C8	-150.9(6)
C2	C3	Yb1	C8	97.0(7)	C13	C3	Yb1	C8	-26.2(12)
C4	C3	Yb1	C7	178.0(7)	C2	C3	Yb1	C7	65.9(7)
C13	C3	Yb1	C7	-57.3(12)	C4	C3	Yb1	C6	159.7(6)
C2	C3	Yb1	C6	47.6(8)	C13	C3	Yb1	C6	-75.6(12)
C9	C8	Yb1	N1	57.1(6)	C7	C8	Yb1	N1	171.8(5)
C17	C8	Yb1	N1	-68.2(8)	C9	C8	Yb1	N2	-16.0(7)
C7	C8	Yb1	N2	98.7(6)	C17	C8	Yb1	N2	-141.3(7)
C9	C8	Yb1	C2	-171.8(6)	C7	C8	Yb1	C2	-57.1(6)
C17	C8	Yb1	C2	63.0(9)	C9	C8	Yb1	C1	-155.0(5)
C7	C8	Yb1	C1	-40.3(7)	C17	C8	Yb1	C1	79.7(9)
C9	C8	Yb1	C5	167.7(6)	C7	C8	Yb1	C5	-77.6(8)
C17	C8	Yb1	C5	42.5(12)	C7	C8	Yb1	C9	114.7(8)
C17	C8	Yb1	C9	-125.2(11)	C9	C8	Yb1	C4	138.5(5)
C7	C8	Yb1	C4	-106.8(6)	C17	C8	Yb1	C4	13.2(10)
C9	C8	Yb1	C10	-38.1(5)	C7	C8	Yb1	C10	76.6(6)
C17	C8	Yb1	C10	-163.3(10)	C9	C8	Yb1	C3	156.4(6)
C7	C8	Yb1	C3	-88.9(6)	C17	C8	Yb1	C3	31.2(9)
C9	C8	Yb1	C7	-114.7(8)	C17	C8	Yb1	C7	120.1(11)
C9	C8	Yb1	C6	-77.7(6)	C7	C8	Yb1	C6	37.0(5)
C17	C8	Yb1	C6	157.0(10)	C6	C7	Yb1	N1	103.6(6)
C8	C7	Yb1	N1	-10.3(7)	C18	C7	Yb1	N1	-131.7(9)
C6	C7	Yb1	N2	9.1(7)	C8	C7	Yb1	N2	-104.8(6)
C18	C7	Yb1	N2	133.7(9)	C6	C7	Yb1	C2	-121.1(7)
C8	C7	Yb1	C2	125.0(7)	C18	C7	Yb1	C2	3.5(10)
C6	C7	Yb1	C1	-96.8(6)	C8	C7	Yb1	C1	149.3(6)
C18	C7	Yb1	C1	27.8(10)	C6	C7	Yb1	C5	-106.9(6)
C8	C7	Yb1	C5	139.2(5)	C18	C7	Yb1	C5	17.7(12)
C6	C7	Yb1	C9	77.3(6)	C8	C7	Yb1	C9	-36.6(5)
C18	C7	Yb1	C9	-158.1(11)	C6	C7	Yb1	C4	-148.0(6)
C8	C7	Yb1	C4	98.1(6)	C18	C7	Yb1	C4	-23.4(11)
C6	C7	Yb1	C10	36.5(5)	C8	C7	Yb1	C10	-77.4(6)
C18	C7	Yb1	C10	161.1(11)	C6	C7	Yb1	C3	-149.3(6)
C8	C7	Yb1	C3	96.8(6)	C18	C7	Yb1	C3	-24.7(10)
C6	C7	Yb1	C8	113.9(8)	C18	C7	Yb1	C8	-121.5(12)
C8	C7	Yb1	C6	-113.9(8)	C18	C7	Yb1	C6	124.6(12)

C10	C6	Yb1	N1	14.4(7)	C7	C6	Yb1	N1	-100.5(6)
C19	C6	Yb1	N1	137.6(8)	C10	C6	Yb1	N2	-57.7(6)
C7	C6	Yb1	N2	-172.6(6)	C19	C6	Yb1	N2	65.5(8)
C10	C6	Yb1	C2	175.5(7)	C7	C6	Yb1	C2	60.6(7)
C19	C6	Yb1	C2	-61.2(9)	C10	C6	Yb1	C1	-153.2(6)
C7	C6	Yb1	C1	91.9(6)	C19	C6	Yb1	C1	-29.9(9)
C10	C6	Yb1	C5	-140.3(6)	C7	C6	Yb1	C5	104.9(6)
C19	C6	Yb1	C5	-17.0(10)	C10	C6	Yb1	C9	37.8(6)
C7	C6	Yb1	C9	-77.0(6)	C19	C6	Yb1	C9	161.1(10)
C10	C6	Yb1	C4	174.2(6)	C7	C6	Yb1	C4	59.3(10)
C19	C6	Yb1	C4	-62.5(11)	C7	C6	Yb1	C10	-114.9(9)
C19	C6	Yb1	C10	123.3(11)	C10	C6	Yb1	C3	152.6(6)
C7	C6	Yb1	C3	37.7(7)	C19	C6	Yb1	C3	-84.2(9)
C10	C6	Yb1	C8	77.7(6)	C7	C6	Yb1	C8	-37.2(5)
C19	C6	Yb1	C8	-159.1(10)	C10	C6	Yb1	C7	114.9(9)
C19	C6	Yb1	C7	-121.9(11)					

Symmetry Operators:

x, y, z	-x+1/2, y+1/2, -z	-x, -y, -z	x-1/2, -y-1/2, z

Table 6. Least-squares planes (x,y,z in crystal coordinates) and deviations from them
(* indicates atom used to define plane)



3.2499 (0.0465) x + 19.2155 (0.1192) y + 6.8738 (0.0376) z = 5.3775 (0.0128)

* 0.0002 (0.0063) C1
* -0.0036 (0.0064) C2
* 0.0057 (0.0063) C3
* -0.0057 (0.0063) C4
* 0.0034 (0.0062) C5
2.3476 (0.0039) Yb1
-0.2976 (0.0177) C11
-0.2939 (0.0189) C12
-0.2032 (0.0180) C13
-0.1717 (0.0182) C14
-0.0805 (0.0186) C15

Rms deviation of fitted atoms = 0.0042

6.6516 (0.0333) x + 0.6587 (0.1427) y + 6.7568 (0.0357) z = 8.6604 (0.0235)

Angle to previous plane (with approximate esd) = 40.62 (0.46)

* 0.0017 (0.0061) C6
* -0.0043 (0.0059) C7
* 0.0052 (0.0056) C8
* -0.0041 (0.0056) C9
* 0.0014 (0.0059) C10
-2.3620 (0.0037) Yb1
0.1501 (0.0160) C16
0.2457 (0.0163) C17
0.3356 (0.0171) C18
0.2131 (0.0164) C19
0.1479 (0.0155) C20

Rms deviation of fitted atoms = 0.0037

3. Packing diagram for $(C_5Me_5)_2Yb(dad(H)\text{-}p\text{-}tolyl)$

View along b-axis: View along a-axis:

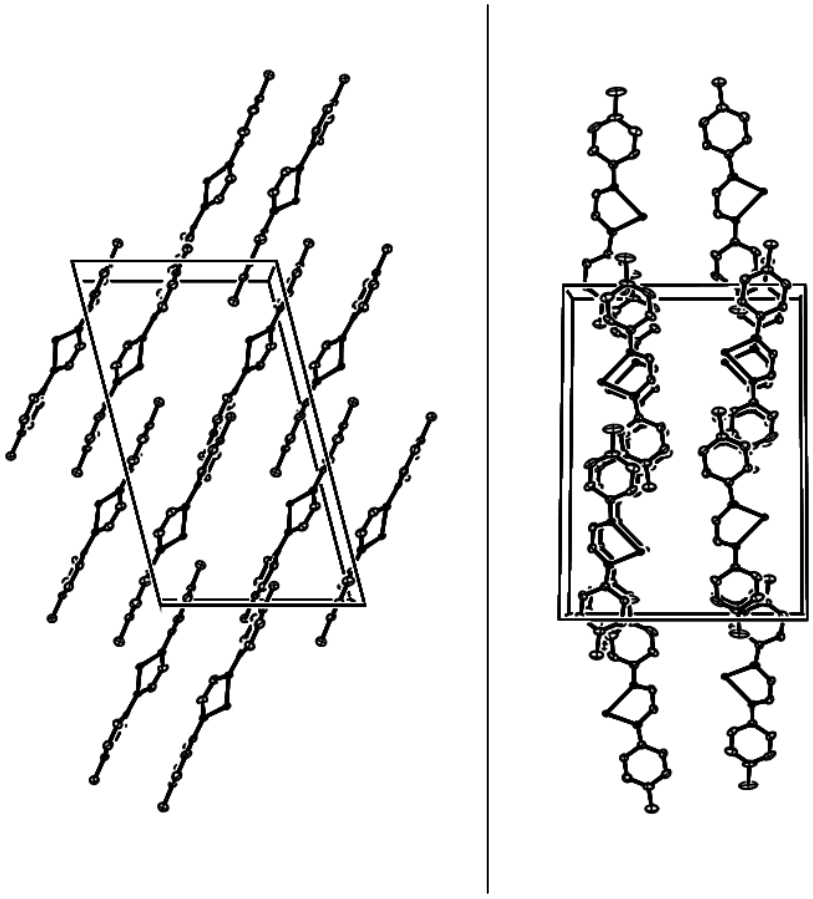


Figure S3. Packing diagram for $(C_5Me_5)_2Yb(dad(H)\text{-}p\text{-}tolyl)$ (ellipsoids at the 50 % probability level). C_5Me_5 rings and hydrogen atoms have been omitted for clarity. Shortest inter-molecular contact between dad-units (C(aromatic)$\underline{C}H_3 \cdots \underline{C}$(aromatic)) is 3.67 Å.

4. Packing diagram for $(C_5Me_5)_2Yb(dad(H)\text{-}p\text{-}anisyl)$

View along a-axis:

View along b-axis:

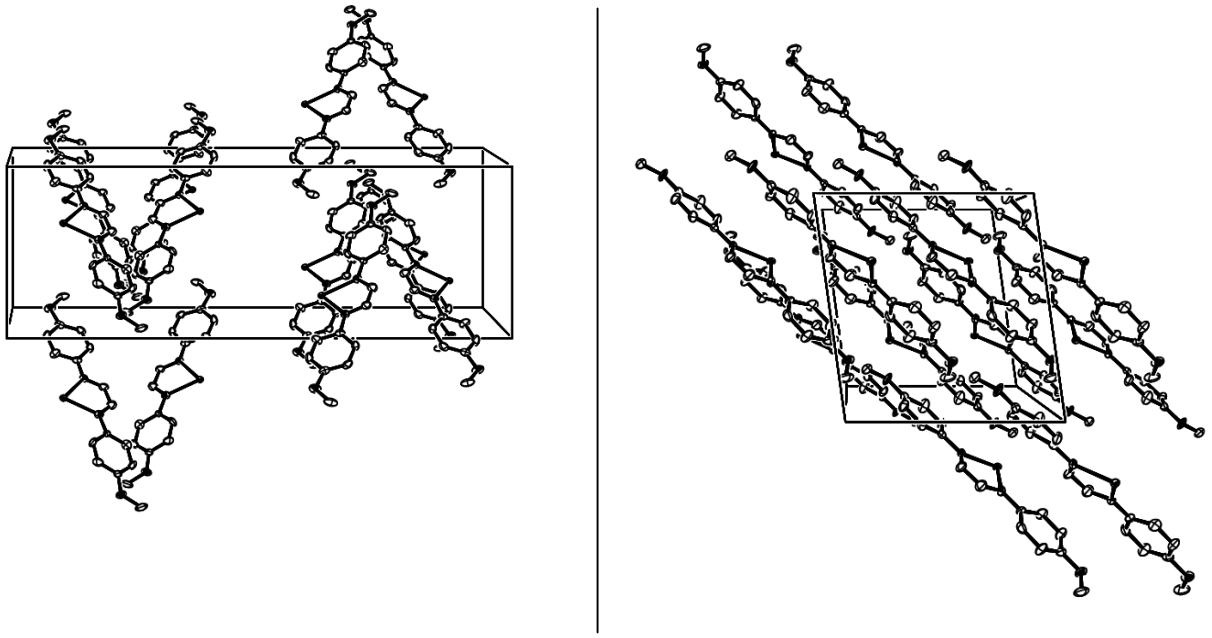
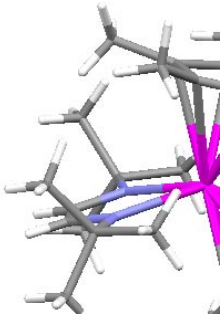
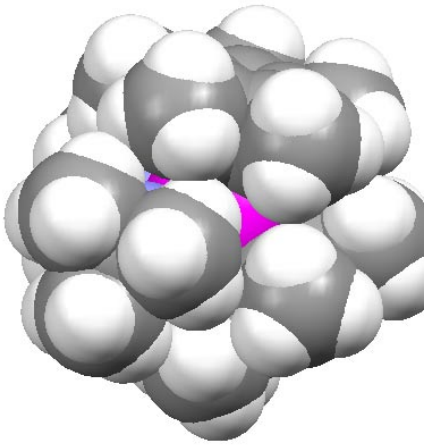


Figure S4. Packing diagram for $(C_5Me_5)_2Yb(dad(H)\text{-}p\text{-}anisyl)$ (ellipsoids at the 50 % probability level). C_5Me_5 rings and hydrogen atoms have been omitted for clarity. Shortest inter-molecular contacts between dad-units are (C(aromatic)O<u>C</u>H_3 ··· <u>C</u>(aromatic)) of 3.64 Å and (<u>C</u>(aromatic)OMe ··· <u>C</u>(aromatic)) of 3.55 Å.

5. Van der Waals Sphere Representation of $(C_5Me_5)_2Yb(dad(H)\text{-}t\text{-}Bu)$





6. Solid State Magnetism

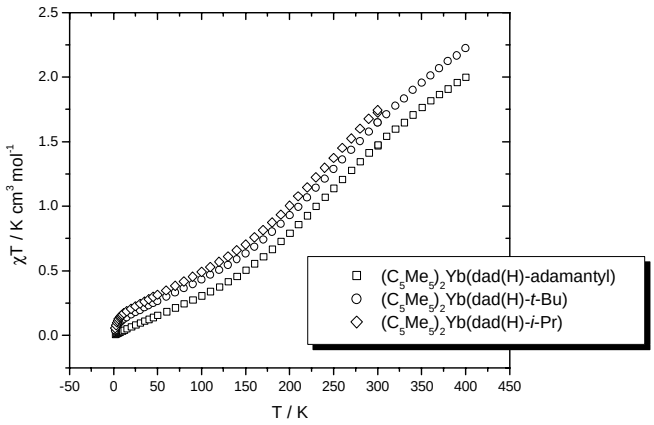


Figure S5a. χT vs. T plot of $(C_5Me_5)_2Yb(dad(H)\text{-alkyl})$ compounds

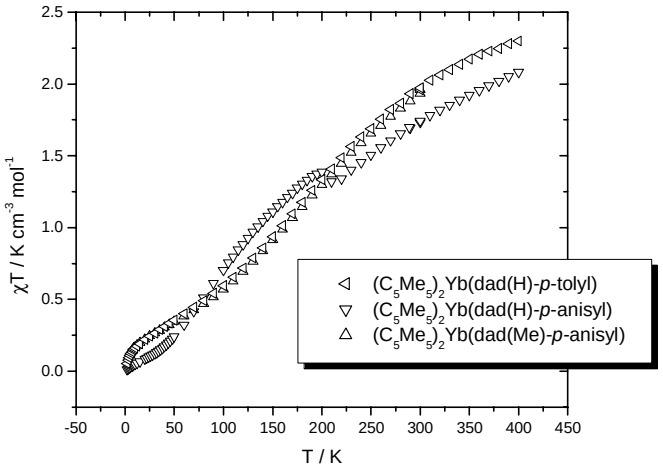


Figure S5b. χT vs. T plot of $(C_5Me_5)_2$Yb(dad(R')-aryl) compounds

7. Variable temperature ^{1}H NMR spectra

7.1 Chemical Shift (δ) vs. T^{-1} plots

Solvent peaks served as internal references for the experimentally observed chemical shifts, δ, at the measuring temperature T.

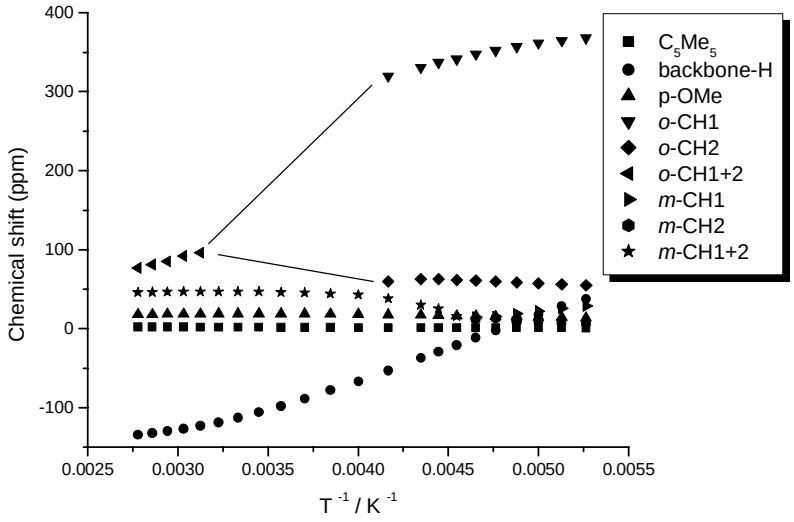


Figure S6a. Chemical shift (δ) vs. T^{-1} plot of the ^{1}H NMR resonances of $(C_5Me_5)_2$Yb(dad(H)-*p*-anisyl) in toluene-d_8 at temperatures from -70 °C to + 90 °C.

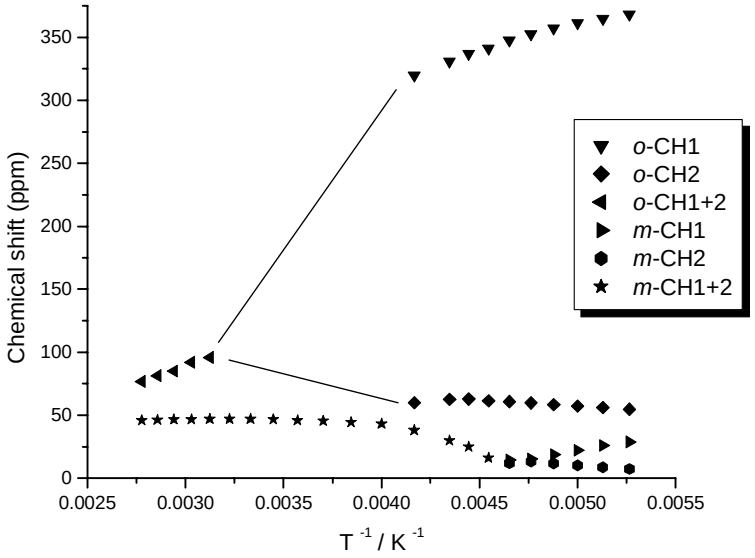


Figure S6b. Chemical shift (δ) vs. T^{-1} plot of the aryl-CH resonances of $(C_5Me_5)_2Yb(dad(H)$-*p*-anisyl) in toluene-d_8 at temperatures from -70 °C to + 90 °C.

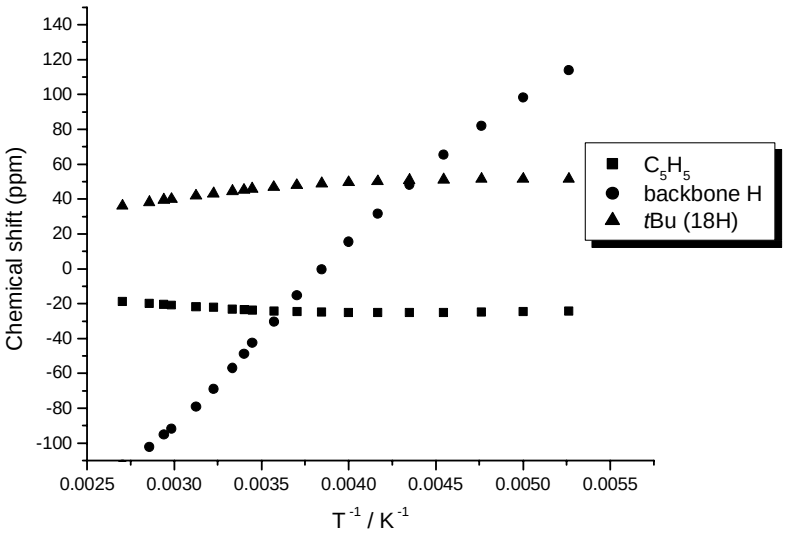


Figure S7. Chemical shift (δ) vs. T^{-1} plot of ^1H NMR resonances of $(C_5H_5)_2Yb(dad(H)$-*t*-Bu) in toluene-d_8 at temperatures from -80 °C to + 95 °C.

7.2 Reduced Observed Chemical Shift (ϑ_{298}) vs. T plots

The observed chemical shifts were reduced to 298 K to give the reduced observed chemical shifts, $\vartheta_{298} = \frac{\delta\, T}{298K}$.

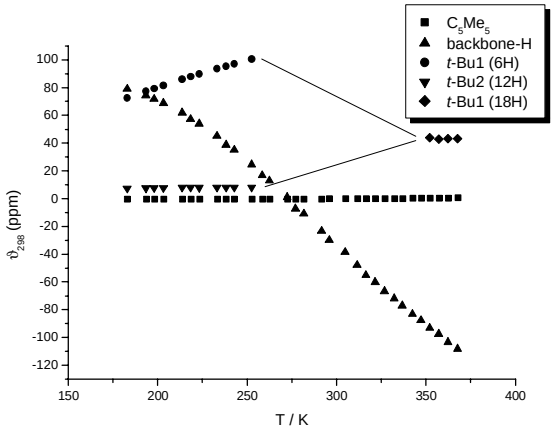


Figure S8. Reduced observed chemical shift (ϑ_{298}) vs. T plot of the ^{1}H NMR resonances of $(C_5Me_5)_2$Yb(dad(H)-*t*-Bu) in toluene-d_8 at temperatures from -70 °C to + 90 °C.

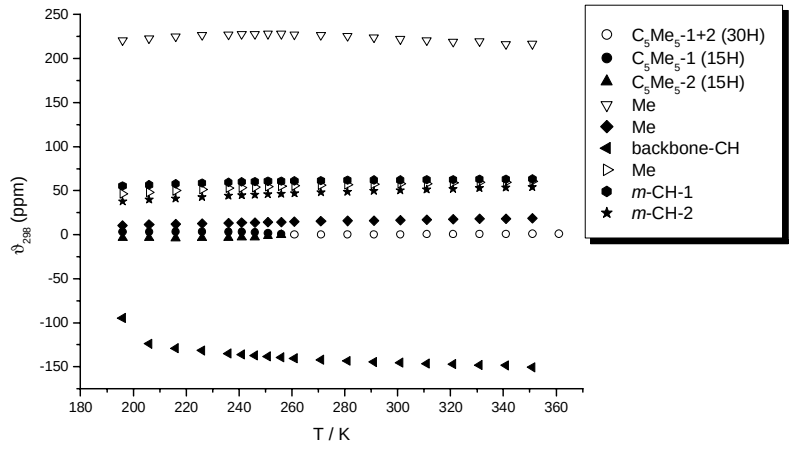


Figure S9. Reduced observed chemical shift (ϑ_{298}) vs. T plot of the ^{1}H NMR resonances of $(C_5Me_5)_2$Yb(dad(H)-mesityl) in toluene-d_8 at temperatures from -65 °C to + 80 °C.

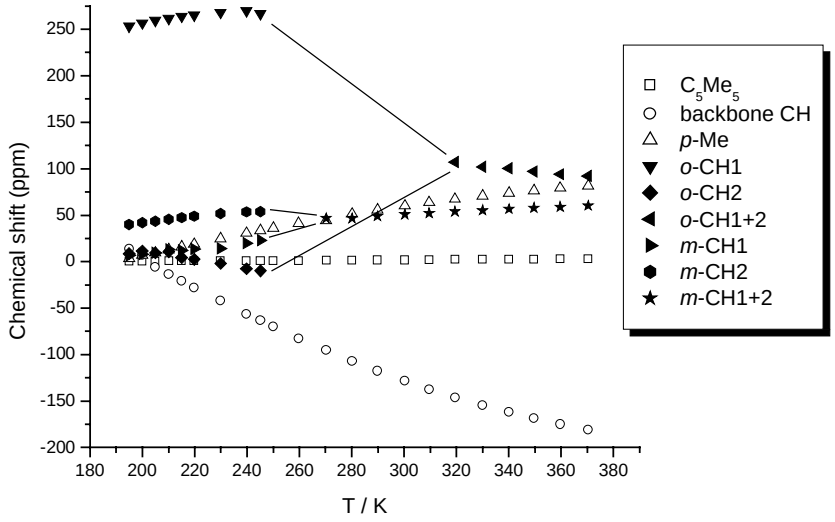


Figure 10. Reduced observed chemical shift (ϑ_{298}) vs. T plot of the ^{1}H NMR resonances of $(C_5Me_5)_2Yb$(dad(H)-*p*-tolyl) in toluene-d_8 at temperatures from -70 to +90°C.

7.3 Reduced Isotropic Chemical Shift (ϑ_{298}^{iso}) vs. T plots

In an attempt to determine isotropic chemical shifts (δ^{iso}) the data were calculated relative to the shifts of the corresponding ligand nuclei of $(C_5Me_5)_2Yb(py)_2$ and the free 1,4-diazabutadiene ligands leading to the paramagnetic chemical shifts (δ^{iso}), where $\delta^{iso} = \delta^{obs} - \delta^{dia}$ (Tables 6.1 and 6.2). The isotropic chemical shifts were then reduced to 298 K to give the reduced isotropic chemical shifts, $\vartheta_{298}^{iso} = \frac{\delta^{iso} T}{298K}$.

The chemical shift of a ligand depends on whether it is free or bound in a diamagnetic complex. They also change depending on the complex. We are unaware of a complete appropriate data set of diamagnetic 1,4-diazabutadiene adducts of the type $[(C_5Me_5)_2M$(dad(R')-R)]. However, systematic errors introduced by non-ideal reference compounds are small for ^{1}H NMR data.

Table 7.1 Diamagnetic Chemical ^{1}H NMR Shifts (δ^{dia})

Compound	Chemical Shift (δ) / ppm (20 °C, C_6D_6)
$(C_5Me_5)_2Yb(py)_2$	2.00 (C_5Me_5)
dad(H)-*t*-Bu	8.13 (backbone-CH), 1.15 (*t*-Bu)
dad(H)-*i*-Pr [a]	8.00 (backbone-CH), 3.55 (C<u>H</u>Me_2), 1.20 (CH<u>Me_2</u>)
dad(H)-*p*-tolyl	8.44 (backbone-CH), 7.13 (*o*-CH), 6.91 (*m*-CH), 2.06 (*p*-CH_3)
dad(H)-*p*-anisyl	8.50 (backbone-CH), 7.21 (*o*-CH), 6.68 (*m*-CH), 3.21 (*p*-OCH_3)

dad(Me)-*p*-anisyl	2.24 (backbone-CMe), 6.73 (*o,m*-CH), 6.72 (o,*m*-CH), 3.30 (*p*-OCH_3)
dad(H)-mesityl	8.00 (backbone-CH), 2.05 (*o*-CH_3), 6.81 (*m*-CH), 2.19 (*p*-CH_3)

[a] recorded in $CDCl_3$ at 20 °C

Table 7.2 Isotropic ^1H NMR Data (δ^{iso}) for $(C_5Me_5)_2Yb$(dad(R')-R) Complexes

Compound	Cp'	R'	R	
$(C_5Me_5)_2Yb$(dad(H)-*p*-tolyl)	-0.26 (35)	-131.8 (320)	*o*-CH	[a)]
			m-CH	43.3 (700)
			p-Me	56.2 (90)
$(C_5Me_5)_2Yb$(dad(H)-*p*-anisyl)	-0.24 (13)	-117.8 (270)	*o*-CH	[a)]
			m-CH	40.2 (350)
			p-OMe	15.7 (4)
$(C_5Me_5)_2Yb$(dad(Me)-*p*-anisyl)	-0.49 (23)	+123.8 (360)	*o*-CH	96.6 (800)
			m-CH	43.4 (34)
			p-OMe	15.2 (8)
$(C_5Me_5)_2Yb$(dad(H)-mesityl)	-1.71 (90)	-154.8 (240)	*o*-CH_3	222.9 (120)
			o-CH_3	56.2 (64)
			m-CH	55.7 (32)
			m-CH	43.6 (24)
			p-Me	56.0 (64)
$(C_5Me_5)_2Yb$(dad(H)-*t*-Bu)	-1.85 (8)	-34.7 (200)	*t*-Bu	[a)]
$(C_5Me_5)_2Yb$(dad(H)-*i*-Pr)	-1.17 (9)	-36.3 (170)	CH	105.4 (260)
			Me	31.1 (12)

Recorded in benzene-d_6 at 20 °C. Isotropic chemical shifts are given in ppm. Line widths, full width at half height (Hz) are given in parentheses. [a] These resonances are not observed at room temperature.

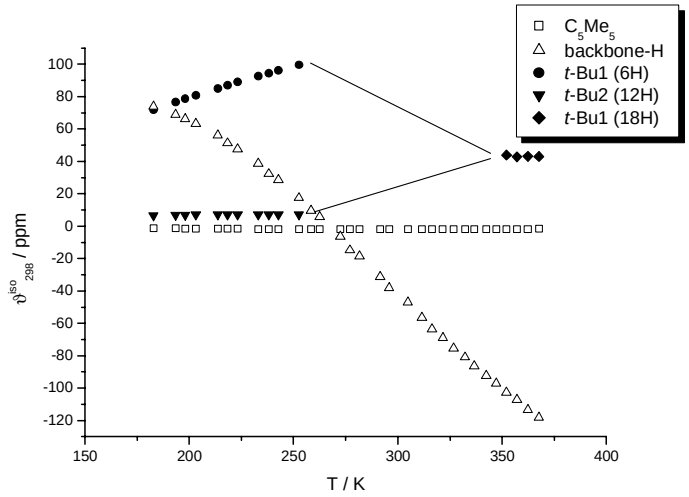


Figure S11. Reduced isotropic chemical shift (ϑ_{298}^{iso}) vs. T plot of ^{1}H NMR resonances of $(C_5Me_5)_2$Yb(dad(H)-*t*-Bu) in toluene-d_8 at temperatures from -80 °C to + 95 °C.

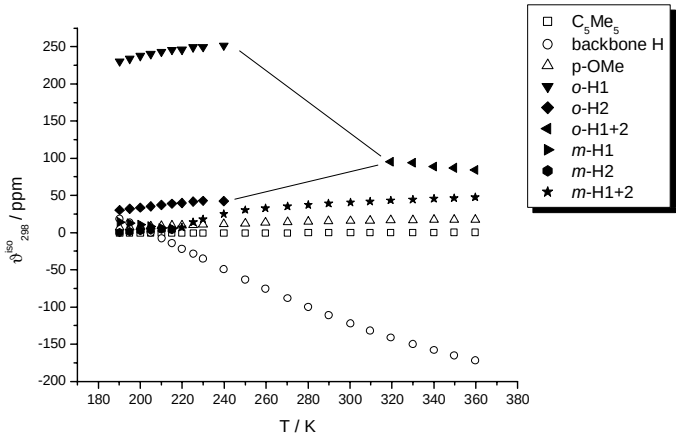


Figure S12. Reduced isotropic chemical shift (ϑ_{298}^{iso}) vs. T plot of ^{1}H NMR resonances of $(C_5Me_5)_2$Yb(dad(H)-*p*-anisyl) in toluene-d_8 at temperatures from -80 °C to + 90 °C.

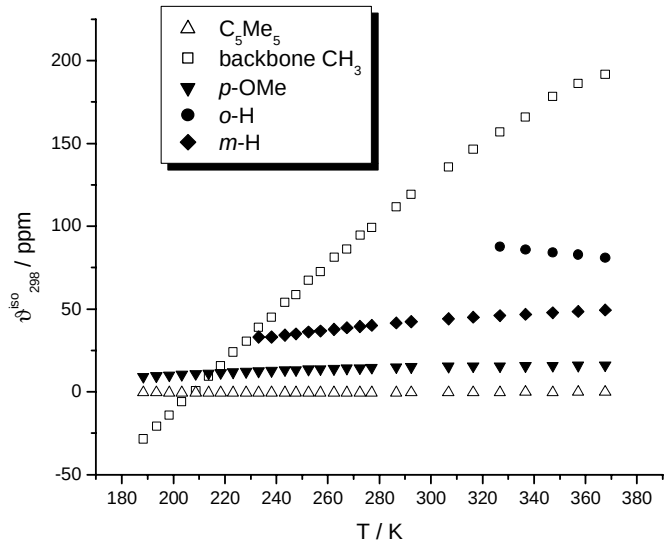


Figure S13. Reduced isotropic chemical shift (ϑ_{298}^{iso}) vs. T plot of ^{1}H NMR resonances of $(C_5Me_5)_2$Yb(dad(Me)-*p*-anisyl) in toluene-d_8 at temperatures from -80 °C to + 100 °C.

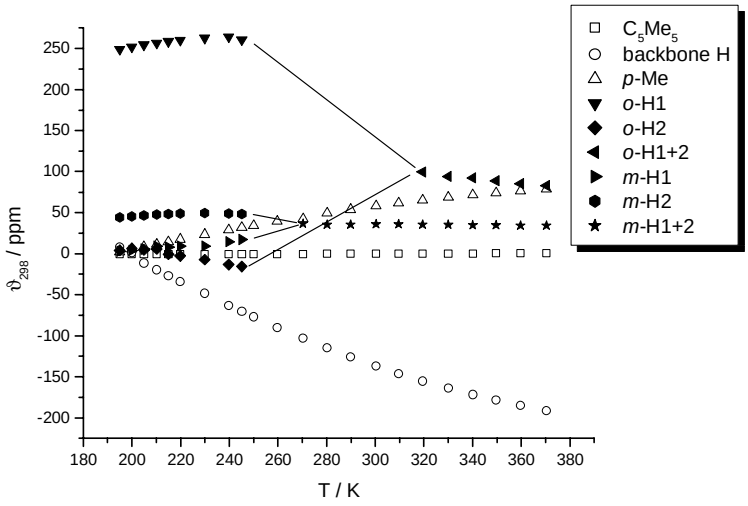


Figure S14. Reduced isotropic chemical shift (ϑ_{298}^{iso}) vs. T plot of ^{1}H NMR resonances of $(C_5Me_5)_2$Yb(dad(H)-*p*-anisyl) in toluene-d_8 at temperatures from -80 °C to + 100 °C.

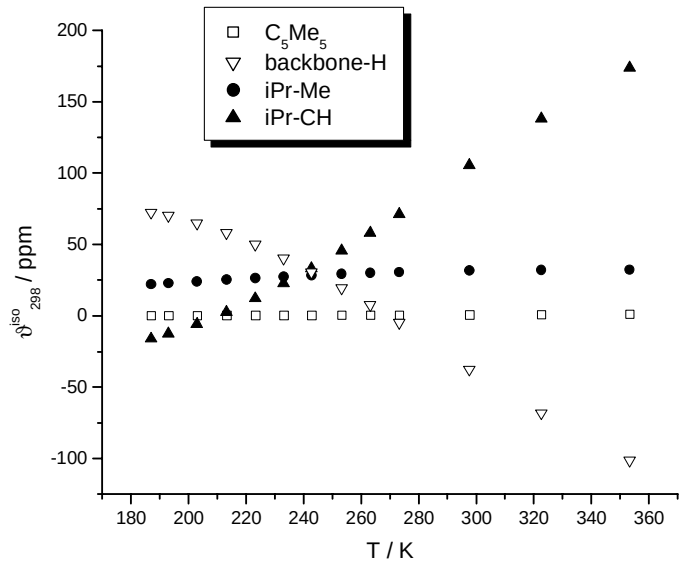


Figure S15. Reduced isotropic chemical shift (ϑ_{298}^{iso}) vs. T plot of ^{1}H NMR resonances of $(C_5Me_5)_2$Yb(dad(H)-*i*-Pr) in toluene-d_8 at temperatures from -80 °C to + 85 °C.

7.4 Comparison between reduced isotropic chemical shifts (ϑ_{298}^{iso}) and solid state magnetic susceptibility (χT) at different temperature plots for the backbone CH/CMe resonances

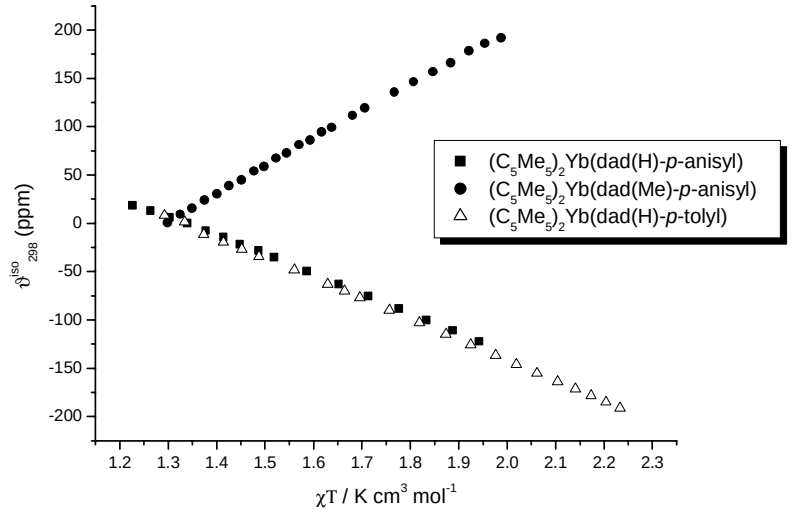


Figure S16. Reduced isotropic chemical shift (ϑ_{298}^{iso}) vs. χT plot of ^{1}H NMR resonances of backbone-R' in

$(C_5Me_5)_2Yb$(dad(R')-aryl) systems in toluene-d_8 at temperatures from -70 °C to + 90 °C.

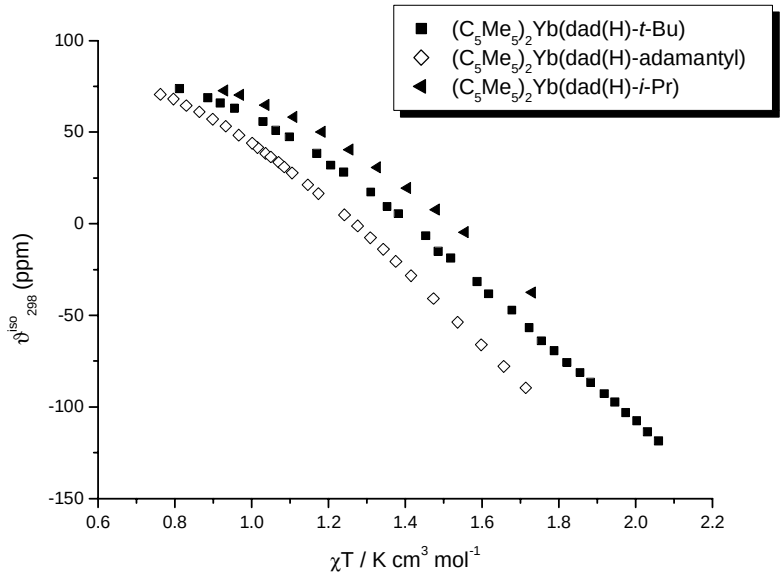


Figure S17. Reduced isotropic chemical shift (ϑ_{298}^{iso}) vs. χT plot of ^{1}H NMR resonances of backbone-H in $(C_5Me_5)_2Yb$(dad(H)-alkyl) systems in toluene-d_8 at temperatures from -70 °C to + 90 °C.

8. References

(1) XS: Program for the Solution of X-ray Crystal Structures, Part of the SHELXTL Crystal Structure Determination Package, Bruker Analytical X-ray Systems Inc.: Madison, WI, (1995-99)

(2) XL: Program for the Refinement of X-ray Crystal Structures, Part of the SHELXTL Crystal Structure Determination Package, Bruker Analytical X-ray Systems Inc.: Madison, WI, (1995-99)

(3) Least-Squares:

Function minimized: $\Sigma w\ (|Fo|^2 - |Fc|^2)^2$

(4) Standard deviation of an observation of unit weight:

$[\Sigma w(|Fo|^2 - |Fc|^2)^2/(N_o - N_v)]^{1/2}$
where: N_o = number of observations
N_v = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) XP: Molecular Graphics program. Part of the SHELXTL Structure Determination Package. Bruker Analytical X-ray Systems Inc.: Madison, WI, (1995-99)

(10) SMART: Area-Detector Software Package, Bruker Analytical X-ray Systems, Inc.: Madison, WI, (1995-99)

(11) SAINT: SAX Area-Dectector Integration Program, V5.04; Siemens Industrial Automation, Inc.: Madison, WI, (1995)

(12) XPREP:(v 5.03) Part of the SHELXTL Crystal Structure Determination Package, Siemens Industrial Automation, Inc.: Madison, WI, (1995)

(13) SADABS: Siemens Area Detector ABSorption correction program, George Sheldrick, (1996). Advance copy, private communication.