

Supporting Information for the manuscript

**Reversible Sigma C-C Bond Formation
Between Phenanthroline Ligands Activated
by $(C_5Me_5)_2Yb$**

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1. Magnetism

Figure S1. Temperature dependent magnetic susceptibility data for Cp*₂Yb(phen) (**1**, crystallized) between 2 K and 300 K.

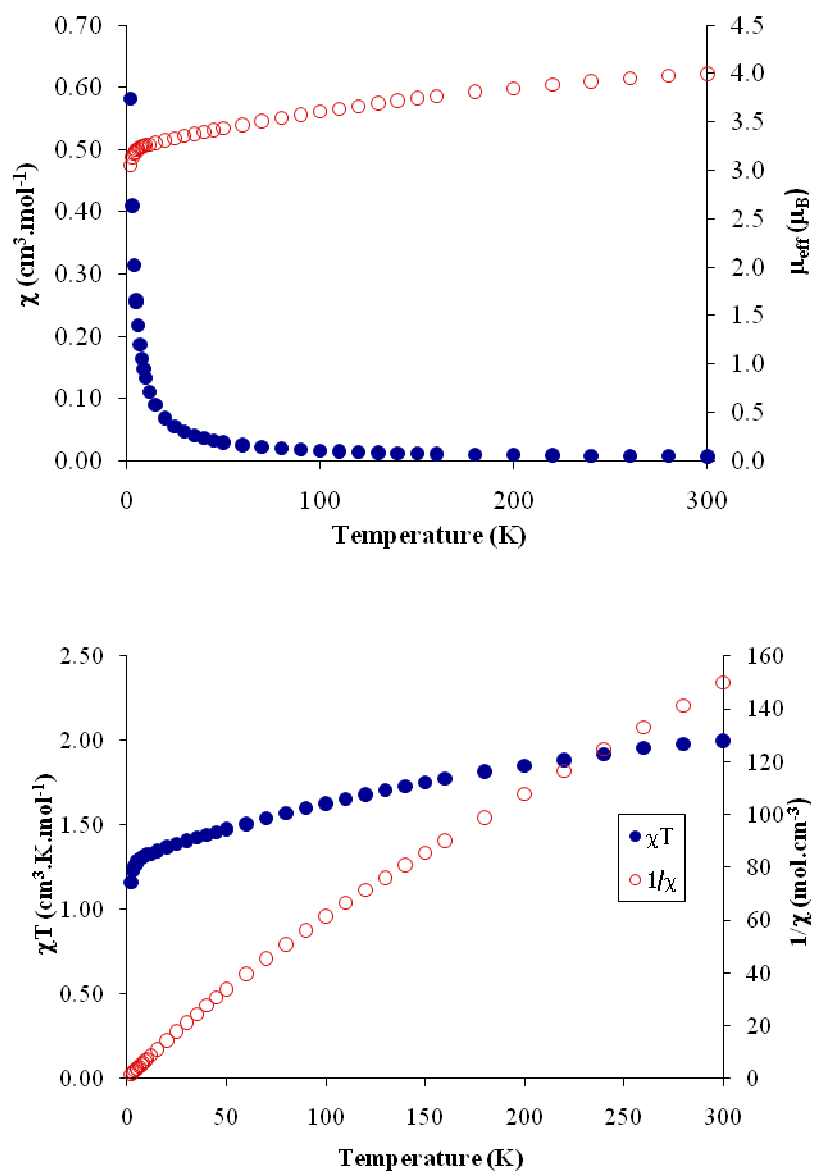


Figure S2. Temperature dependent magnetic susceptibility data for $[\text{Cp}^*_2\text{Yb}(\text{phen})]\text{I}$ (**2**) between 2 K and 300 K.

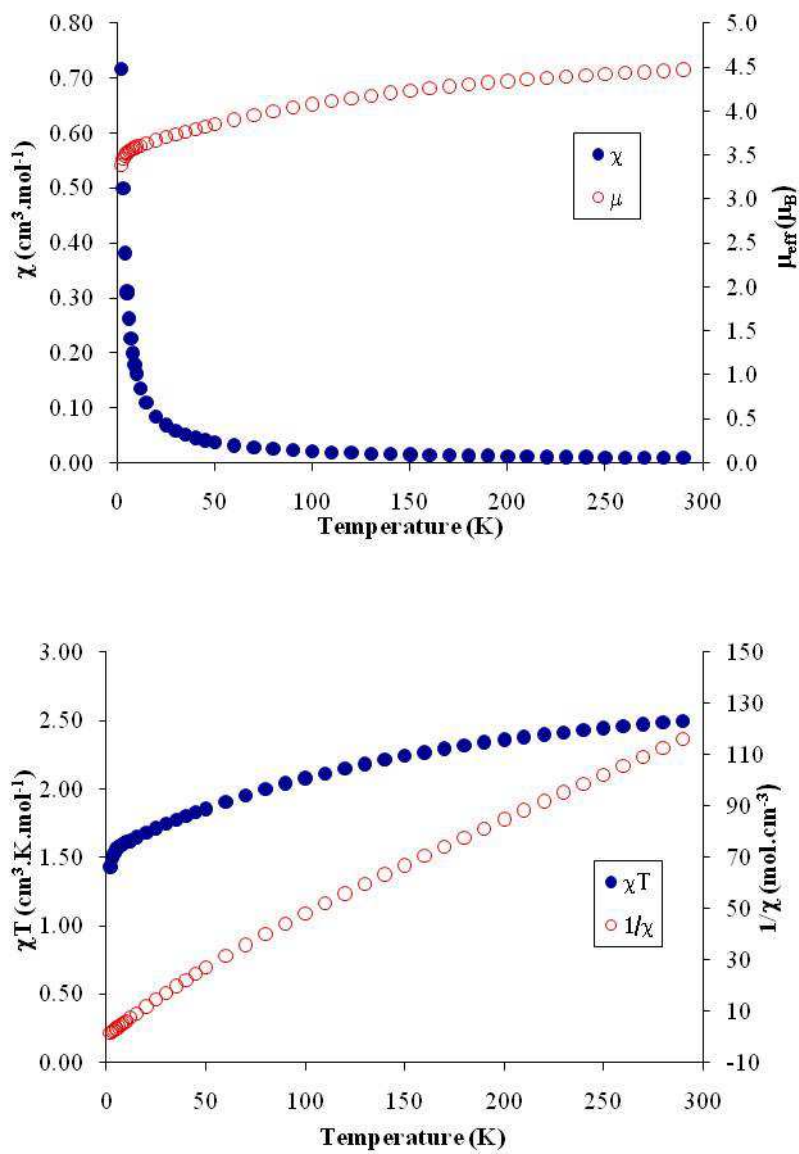


Figure S3. Temperature dependent magnetic susceptibility data for Cp*₂Yb(3,8-Me₂phen) (3) between 2 K and 300 K.

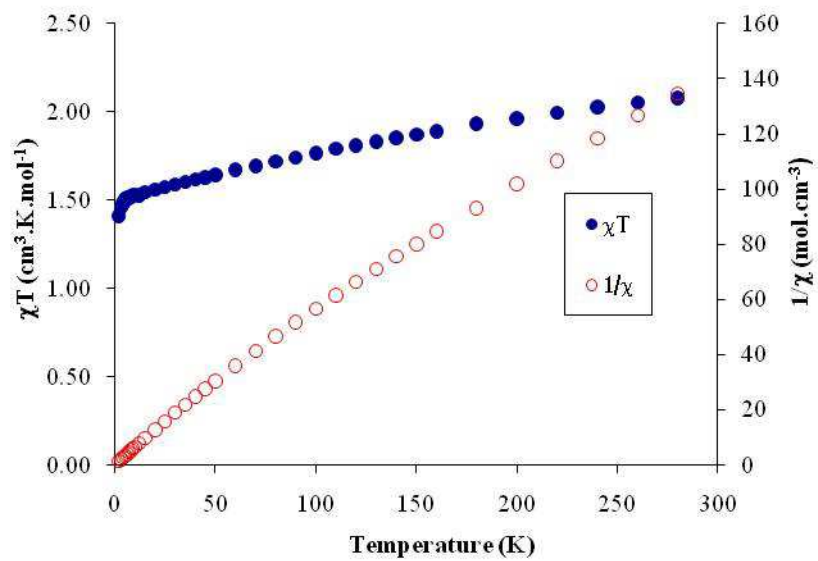
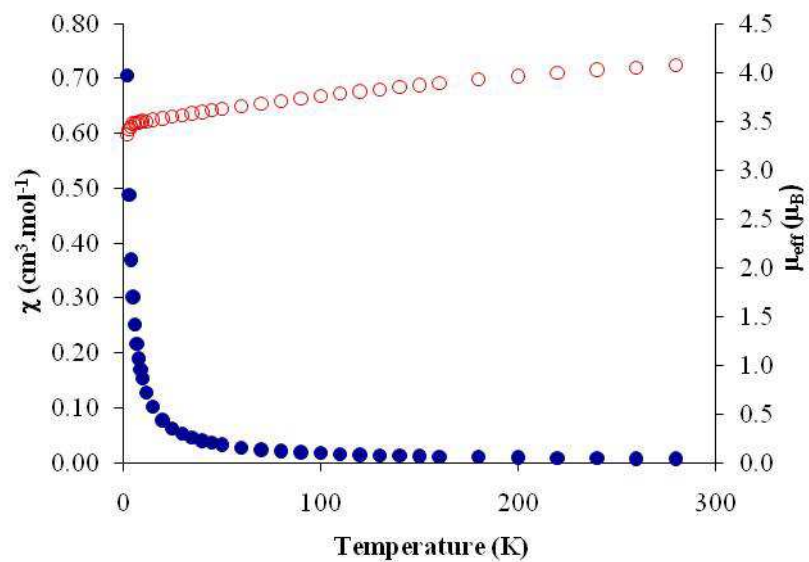


Figure S4. Temperature dependent magnetic susceptibility data for Cp*₂Yb(3-Mephen) (**4**) between 2 K and 300 K.

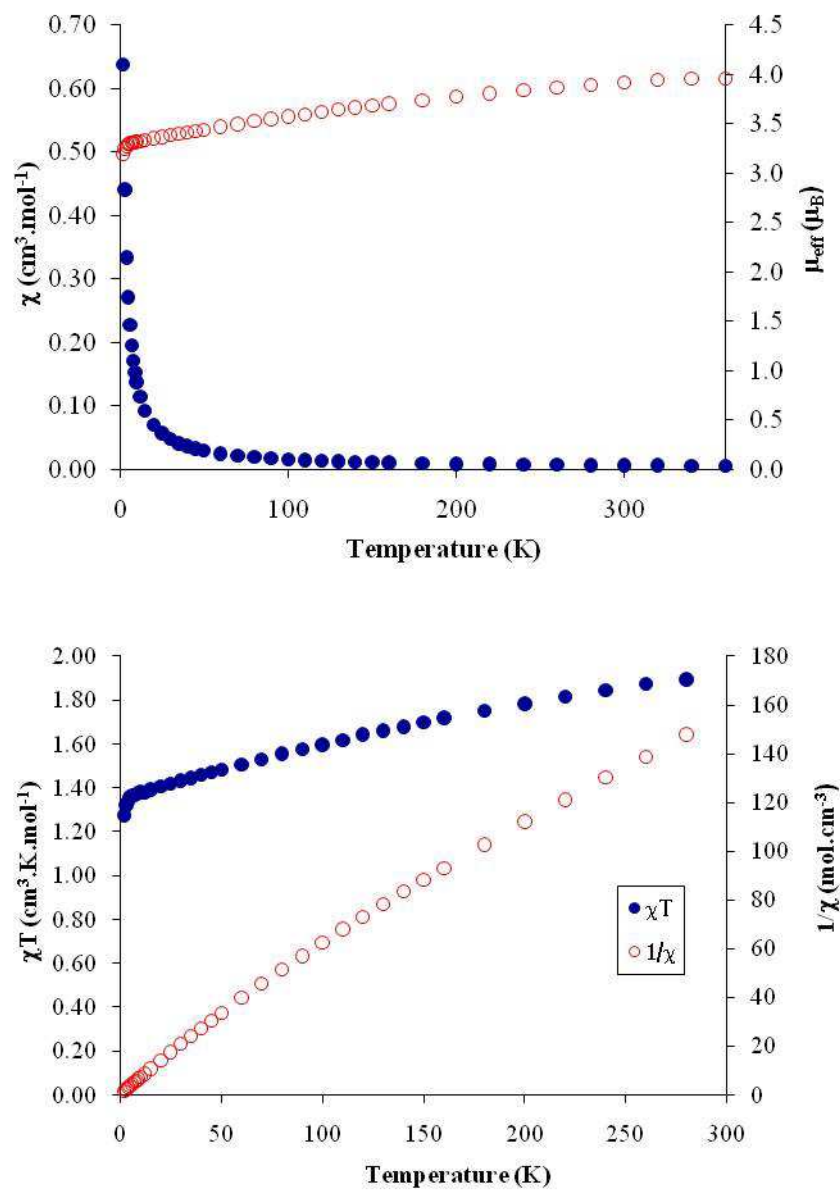


Figure S5. Temperature dependent magnetic susceptibility data for $\text{Cp}^*_2\text{Yb}(4\text{-Mephen})$ (**5**) between 2 K and 300 K.

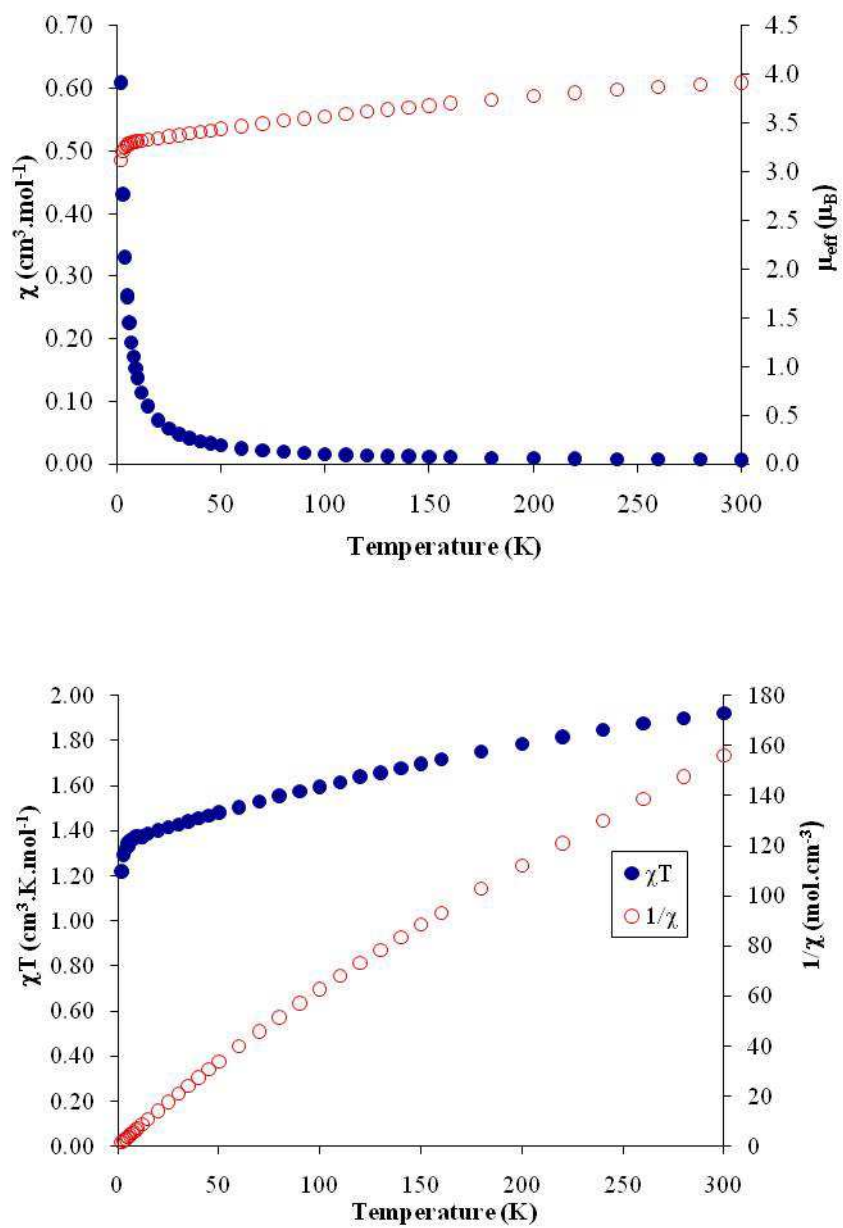


Figure S6. Temperature dependent magnetic susceptibility data for $\text{Cp}^*_2\text{Yb}(5\text{-Mephen})$ (**6**) between 2 K and 300 K.

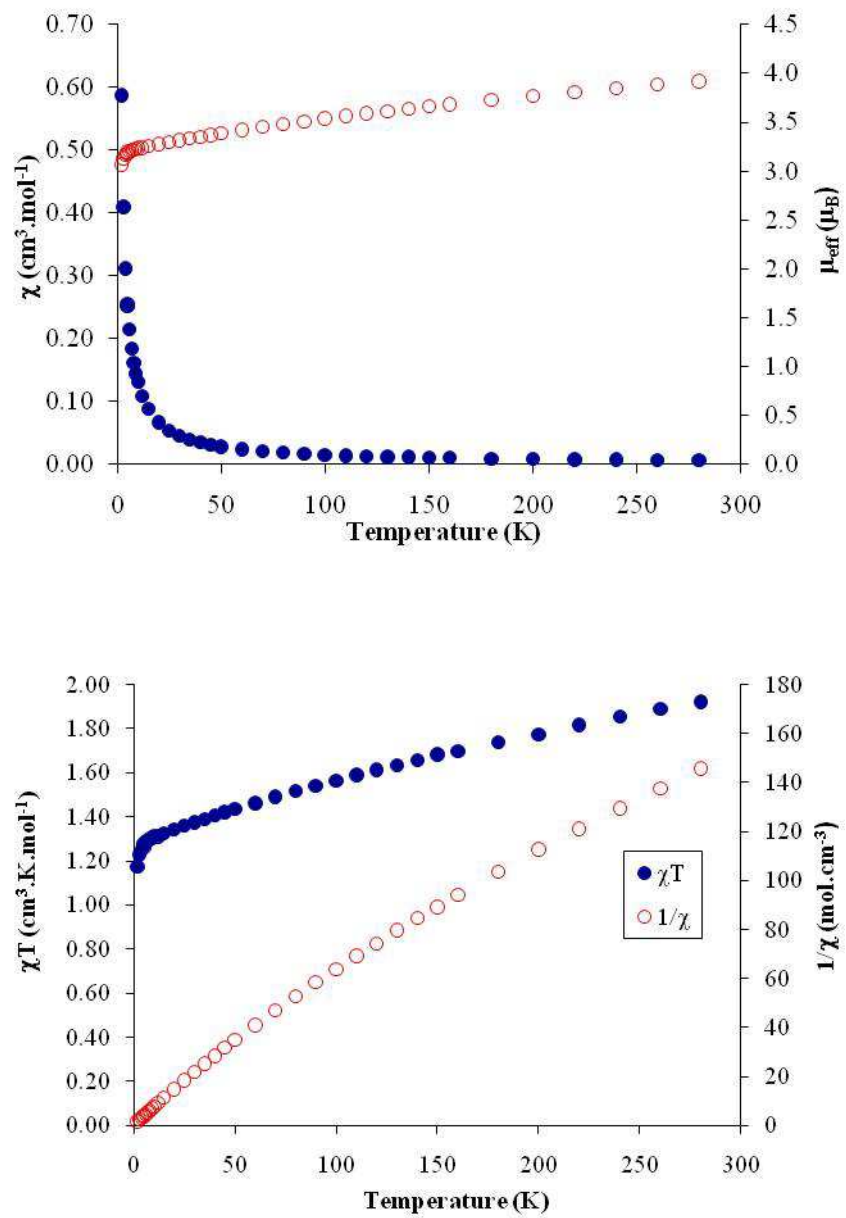


Figure S7. Temperature dependent magnetic susceptibility data for Cp*₂Yb(5,6-Me₂phen) (7) between 2 K and 300 K.

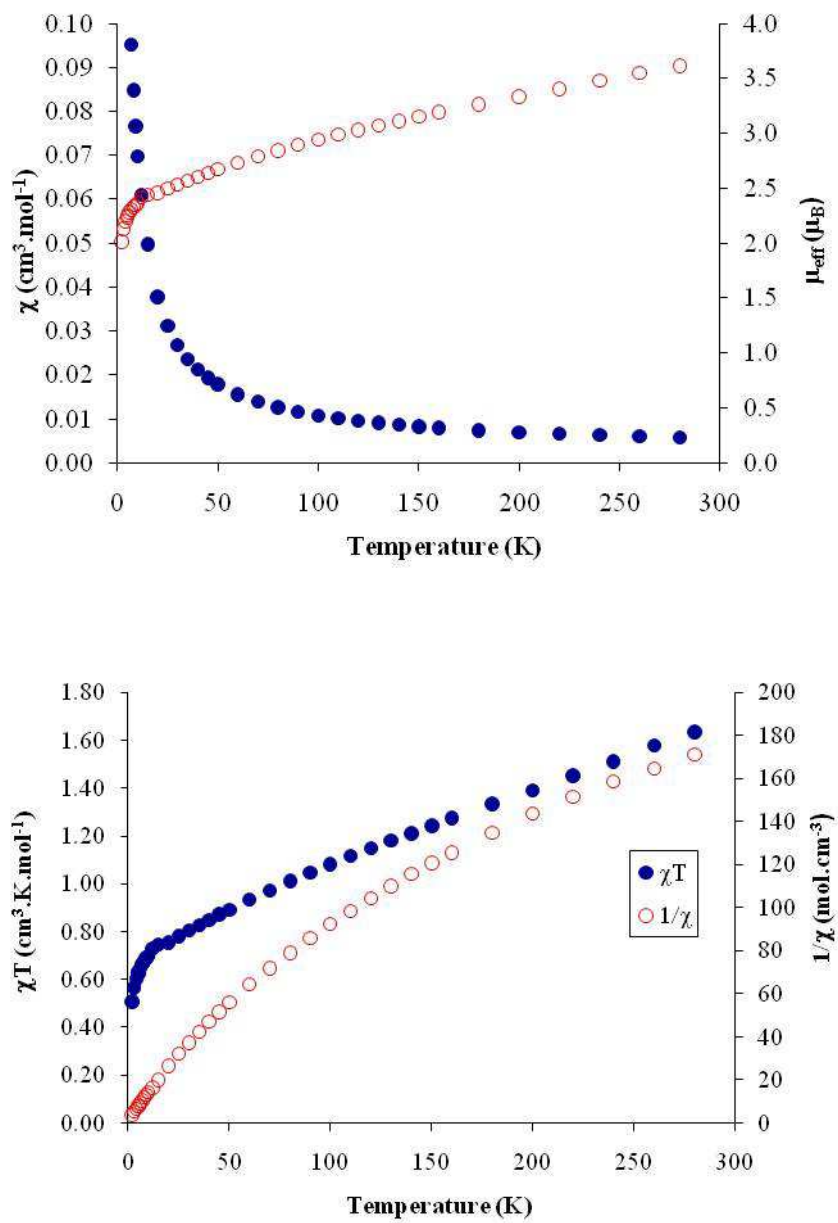
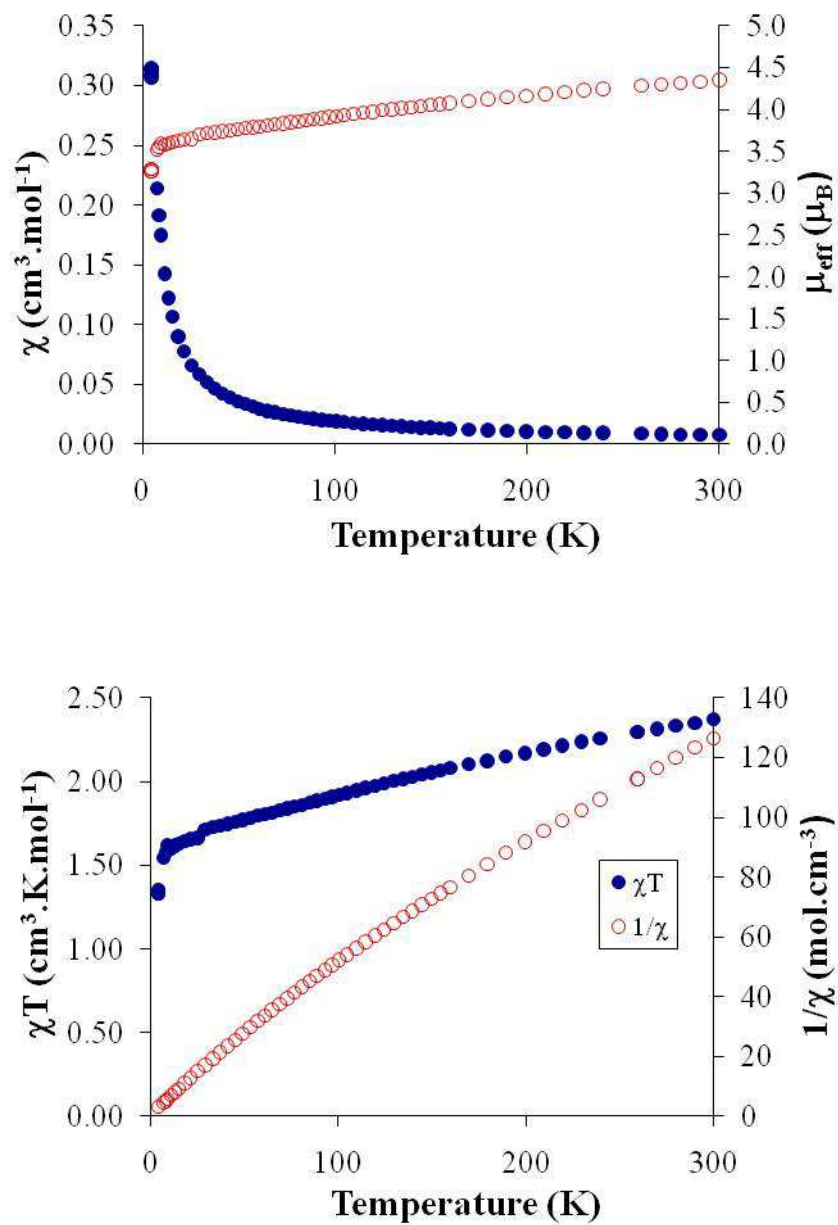


Figure S8. Temperature dependent magnetic susceptibility data for Cp*₂Yb(phen) (**1**, sublimed) between 2 K and 300 K.



2. EPR Studies

Figure S9: EPR spectra recorded in the solid state (powder) at 2 K for $\text{Cp}^*_2\text{Yb}(\text{phen})$ (**1**, **crystallized**) black and simulated spectrum (blue line).

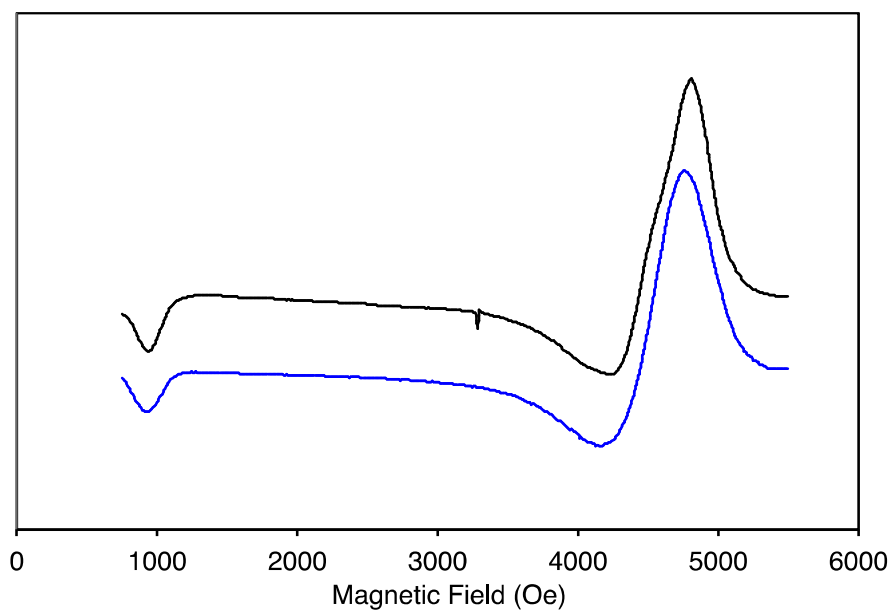


Figure S10: EPR spectra recorded in the solid state (powder) at 2 K for $\text{Cp}^*_2\text{Yb}(3,8\text{-Me}_2\text{phen})$ (**3**) black and simulated spectrum (blue line).

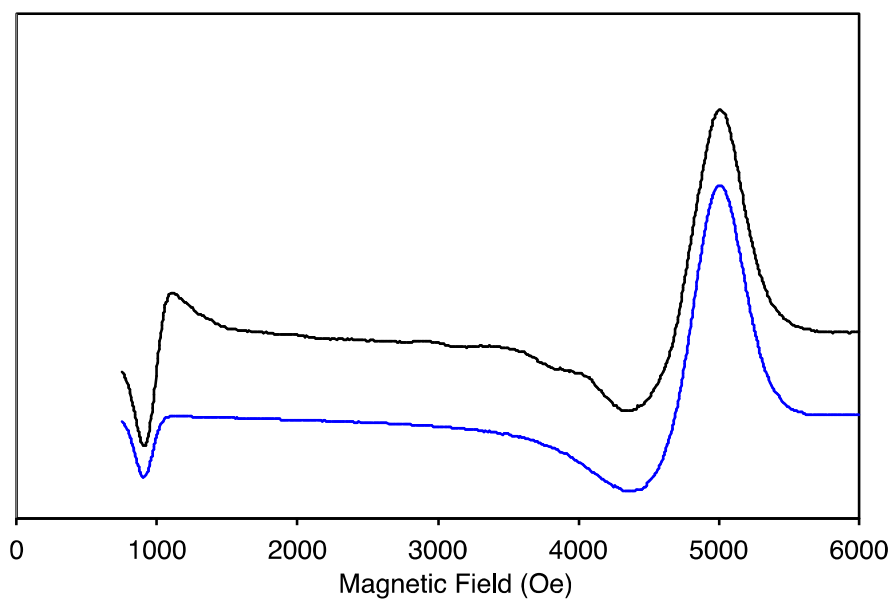


Figure S11: EPR spectra recorded in the solid state (powder) at 2 K for $\text{Cp}^*_2\text{Yb}(\text{3-Mephen})$ (4) and simulated spectrum (blue line).

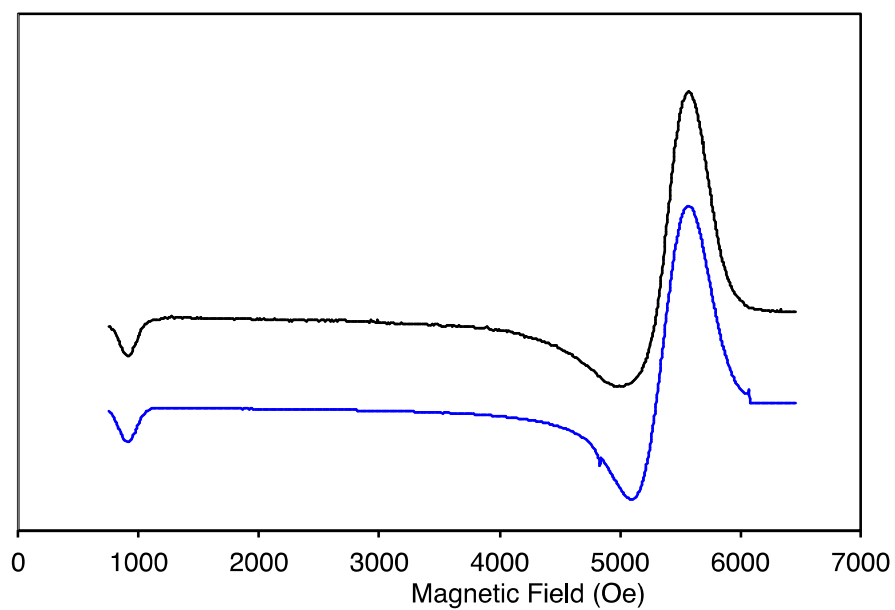


Figure S12: EPR spectra recorded in the solid state (powder) at 2 K for $\text{Cp}^*_2\text{Yb}(\text{4-Mephen})$ (5) and simulated spectrum (blue line).

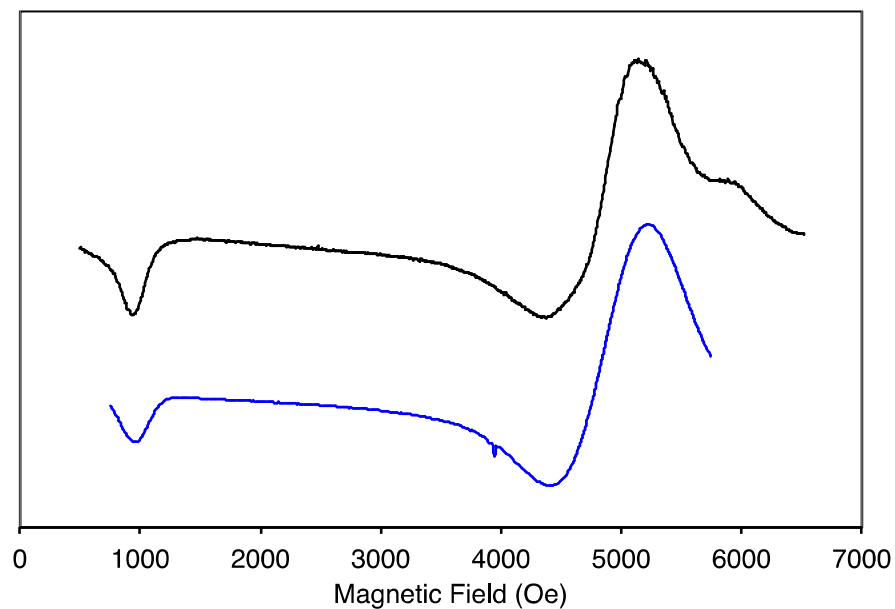
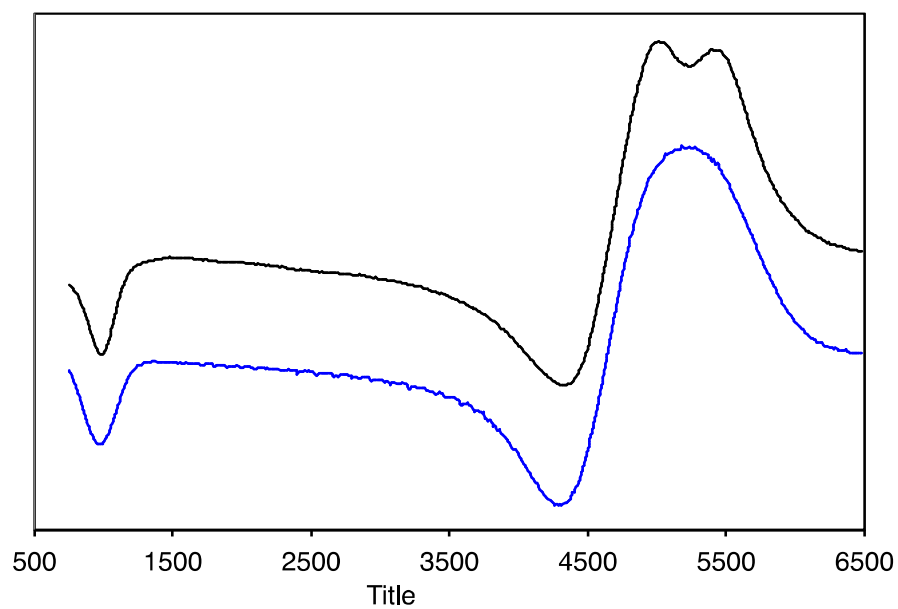


Figure S13: EPR spectra recorded in the solid state (powder) at 2 K for $\text{Cp}^*_2\text{Yb}(\text{5-Mephen})$ (6) and simulated spectrum (blue line).



3. NMR Studies.

Figure S14. Chemical shift (δ) vs. $1/T$ plot of ^1H NMR resonances of $\text{Cp}^*_2\text{Yb}(5\text{-Mephen})$ (**6**) in toluene- d_8 at temperature from 180K to 360K.

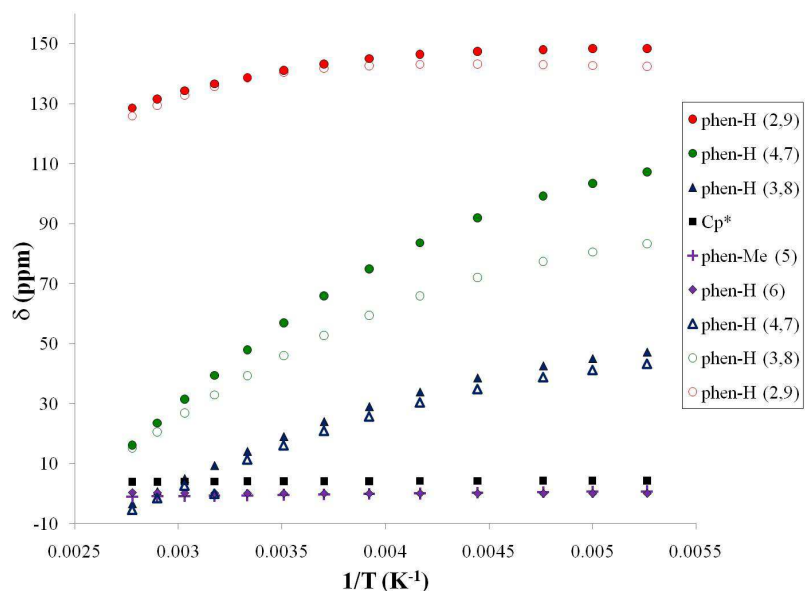
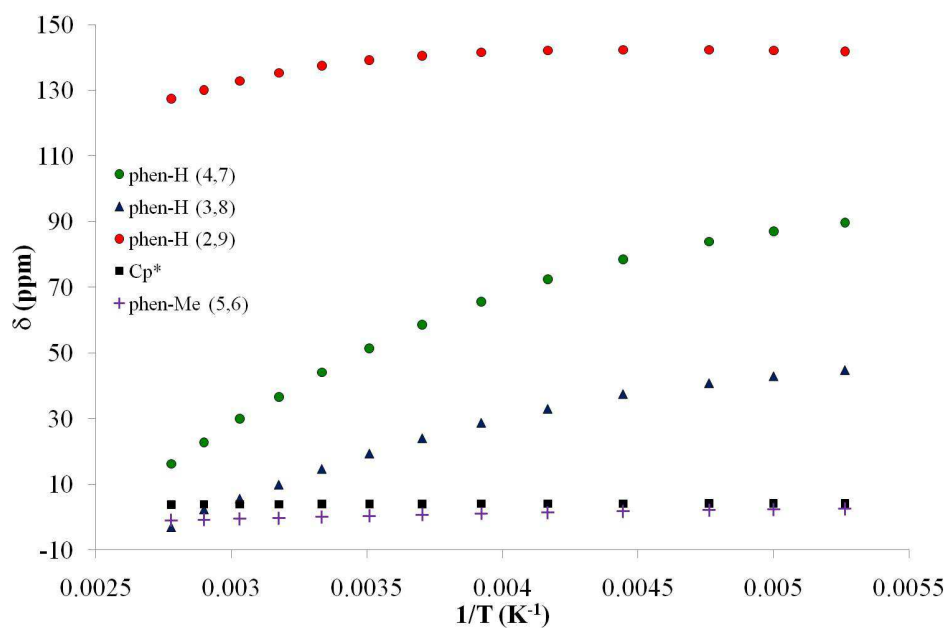


Figure S15. Chemical shift (δ) vs. $1/T$ plot of ^1H NMR resonances of $\text{Cp}^*_2\text{Yb}(5,6\text{-Me}_2\text{phen})$ (**7**) in toluene- d_8 at temperature from 180K to 360K.



4. Visible spectroscopy

Figure S16. Absorption spectrum in the Vis-NIR region for the complex **3** in toluene at room temperature.

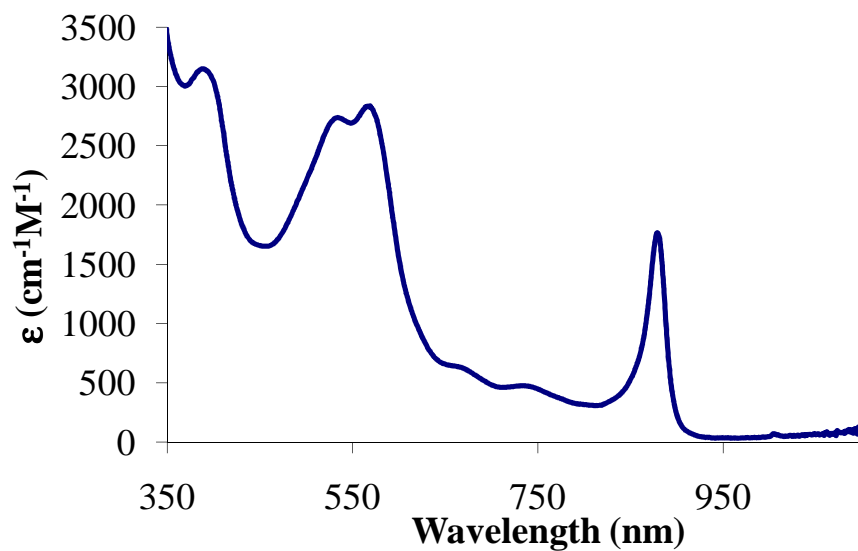


Figure S17. Absorption spectrum in the Vis-NIR region for the complex **5** in toluene at room temperature.

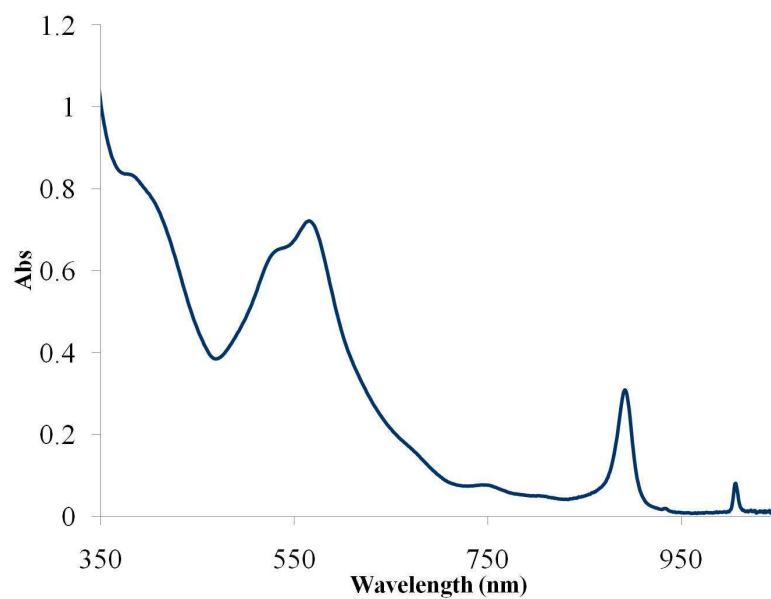


Figure S18. Absorption spectrum in the Vis-NIR region for the complex **6** in toluene at room temperature.

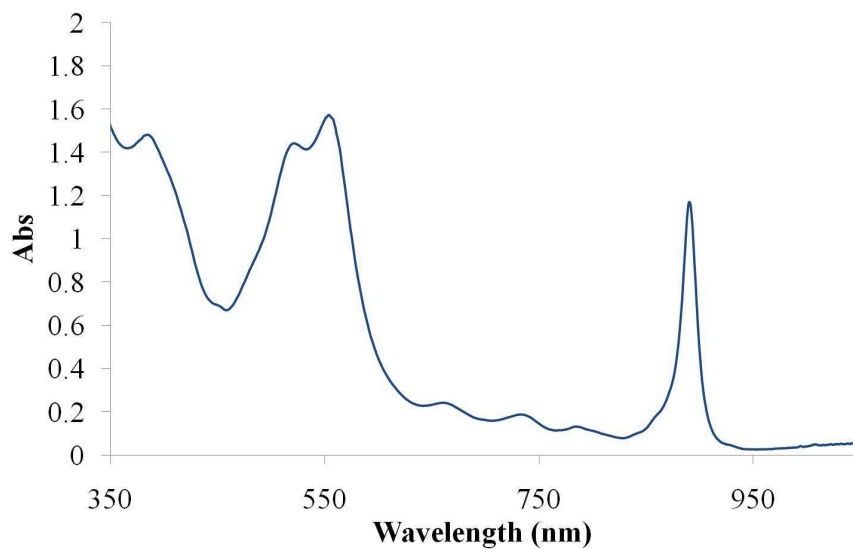
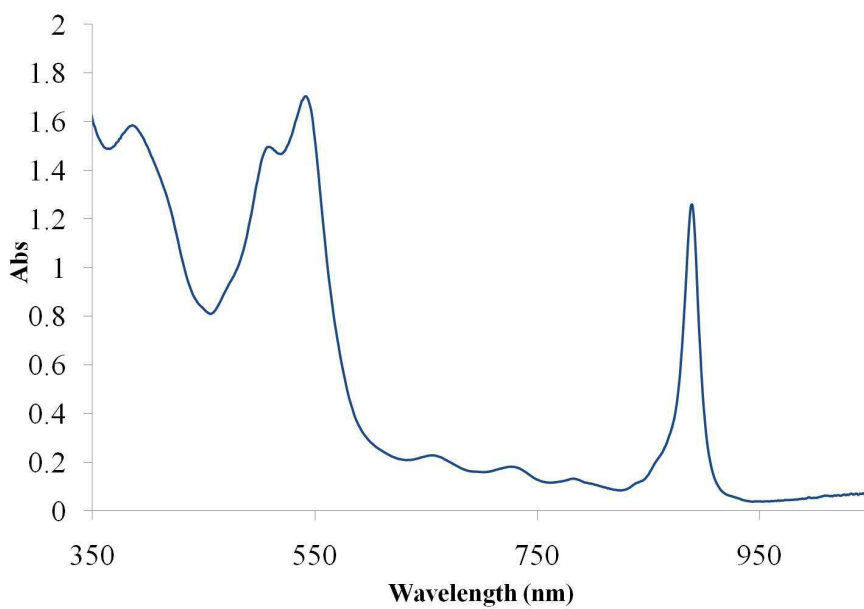


Figure S19. Absorption spectrum in the Vis-NIR region for the complex **7** in toluene at room temperature.



5. X-ray Studies.

5.1. Cp*₂Yb(phen) (1, crystallized)

Data collection

A fragment of a purple block-like crystal of C₆₄H₇₆N₄Yb₂ [Cp*₂Yb(phen)]₂ crystallized from a slow diffusion of a phenanthroline solution in toluene in a toluene solution of the complex Cp*₂YbOEt₂ and having approximate dimension of 0.1 x 0.08 x 0.05 mm was mounted on a Kapton loop using Paratone N hydrocarbon oil. All measurements were made on a Bruker APEX¹ CCD area detector with graphite monochromated Mo-K α radiation.

Cell constants and an orientation matrix, obtained from a least-squared refinement using the measured positions of 9726 reflexions with $I > 10\sigma$ in the range $5.12 < 2\theta < 50.92$ corresponded to a primitive orthorhombic cell with dimensions:

$$\begin{array}{ll} a = 17.9675(15) \text{ \AA} & a = 90^\circ. \\ b = 17.8594(15) \text{ \AA} & b = 90^\circ. \\ c = 16.2715(13) \text{ \AA} & g = 90^\circ. \\ V = 5221.3(7) \text{ \AA}^3 & \end{array}$$

For $Z = 4$ and F.W. = 1247.36, the calculated density is 1.587 g cm^{-3} . Based on a statistical analysis of intensity distribution, and successful solution and refinement of the structure, the space group was determined to be

$$P b c a (\#61)$$

The data were collected at a temperature of $-173(1)^\circ\text{C}$. Exposure time was 20.0s per frame.

Data reduction

Data were integrated by the program SAINT² to a maximum 2θ value of 52.22° . The data were corrected for Lorentz and polarization effects. Data were analyzed for agreement and possible absorption using XPREP.³ A semi-empirical multi-scan absorption correction⁴ was applied using SADABS.⁵ This models the absorption surface using a spherical harmonic series based on differences between equivalent.

Structure solution and refinement

The structure was solved by direct methods.⁶ Non-hydrogen atoms were refined anisotropically and hydrogen atoms were placed in calculated positions and not refined. The final cycle of full matrix least squares refinement was based on 4079 observed reflections and 320 parameters and converged with unweighted and weighted agreement factors of:

$$R = \sum ||F_o| - |F_c|| / \sum |F_o| = 0.0344$$

$$R_w = [(\sum w (|F_o| - |F_c|)^2 / \sum w F_o^2)]^{1/2} = 0.0783$$

The standard deviation of an observation of unit weight was 1.003. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.2 and $-0.799 \text{ e.\AA}^{-3}$, respectively.

The SHELX program uses the neutral atom scattering factors, f' , f'' and absorption coefficients from International Tables for Crystallography, Volume C (1992), Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht: Tables 6.1.1.4(pp. 500-502), 4.2.6.8 (pp.219-222) and 4.2.4.2 (pp. 193-199), respectively. All calculations were performed using the WinGX crystallographic software package.⁷ (“WinGX suite for small molecule single-crystal crystallography”)

Figure S20. ORTEP of $\text{Cp}^*_2\text{Yb}(\text{phen})$ (**1**, crystallized) (50% probability ellipsoids).

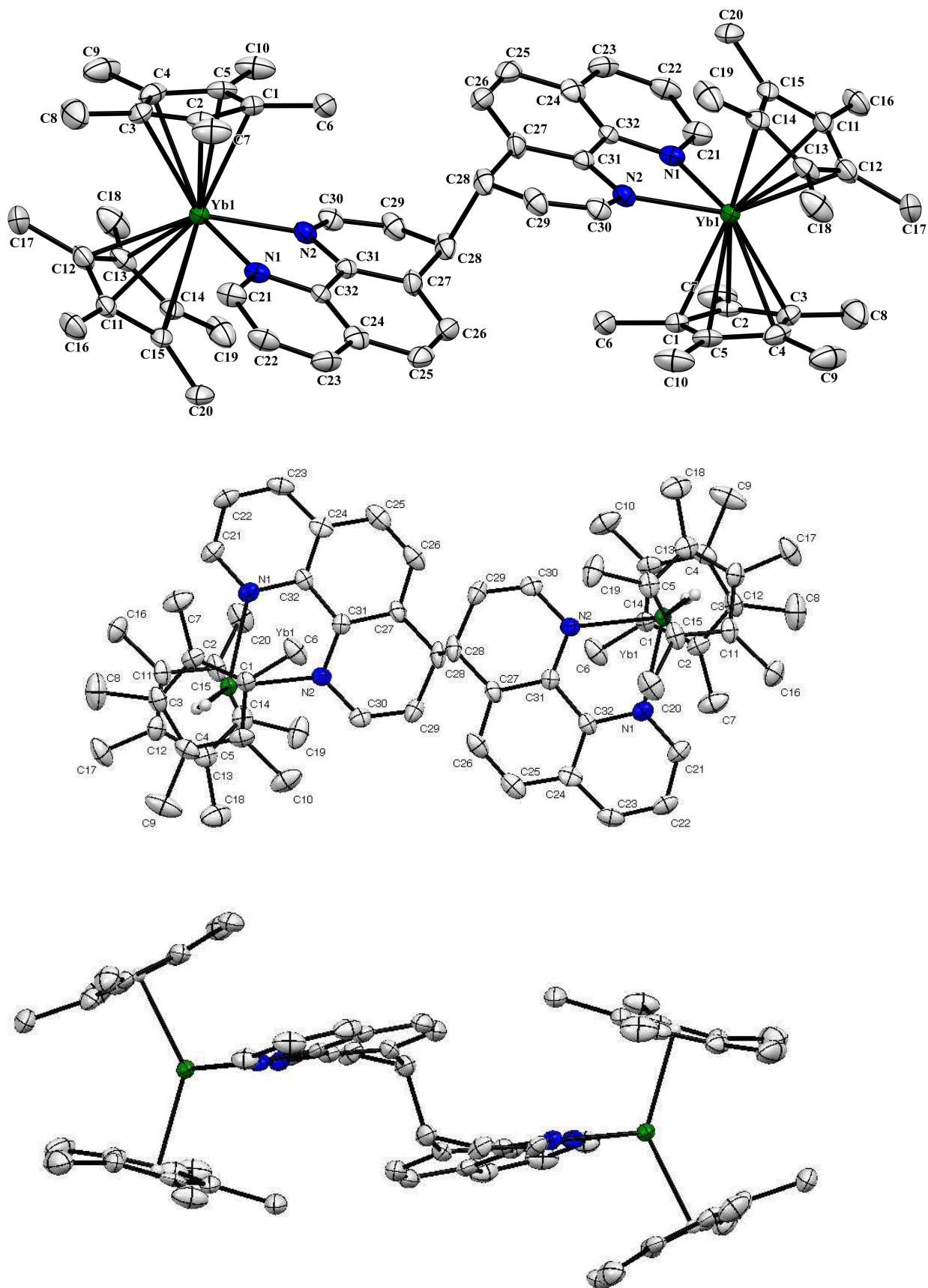


Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cp}^*_2\text{Yb}(\text{phen})$ (**1**, **crystallized**). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(12)	976(4)	1002(3)	5492(3)	29(1)
C(11)	1392(3)	332(3)	5625(3)	26(1)
C(13)	267(4)	912(3)	5826(3)	28(1)
C(5)	1013(3)	2195(3)	7862(3)	26(1)
C(14)	228(4)	190(3)	6175(3)	27(1)
C(3)	1994(4)	2157(3)	6984(3)	29(1)
C(17)	1262(4)	1630(3)	4947(3)	41(2)
C(15)	913(4)	-164(3)	6055(3)	28(1)
C(20)	1083(4)	-963(3)	6286(3)	37(2)
C(4)	1257(4)	2413(3)	7073(3)	29(1)
N(1)	1906(3)	-15(2)	7645(2)	23(1)
C(29)	-552(4)	242(3)	9008(3)	28(1)
N(2)	521(3)	400(2)	8134(2)	23(1)
C(21)	2567(4)	-237(3)	7368(3)	28(1)
C(30)	-207(3)	534(3)	8363(3)	25(1)
C(32)	1560(3)	-459(3)	8239(3)	21(1)
C(27)	524(4)	-585(3)	9183(3)	25(1)
C(31)	854(3)	-198(3)	8520(3)	21(1)
C(28)	-134(4)	-243(3)	9607(3)	27(1)
C(2)	2214(4)	1796(3)	7706(3)	23(1)
C(1)	1601(3)	1821(3)	8262(3)	22(1)
C(16)	2157(4)	153(4)	5288(3)	34(2)
C(26)	853(4)	-1269(3)	9447(3)	32(1)
C(24)	1875(4)	-1119(3)	8524(3)	26(1)
C(6)	1611(4)	1518(3)	9117(3)	36(2)
C(19)	-461(4)	-165(4)	6529(3)	41(2)
C(10)	263(4)	2396(4)	8216(4)	41(2)
C(22)	2917(4)	-896(3)	7614(3)	31(1)
C(23)	2570(4)	-1339(3)	8189(3)	30(1)
C(18)	-373(4)	1438(4)	5753(4)	44(2)
C(7)	2971(4)	1527(4)	7919(4)	41(2)
C(8)	2538(4)	2346(4)	6301(4)	49(2)
C(9)	844(5)	2934(3)	6504(4)	50(2)
C(25)	1488(4)	-1537(3)	9131(3)	32(2)
Yb(1)	1163(1)	943(1)	7080(1)	18(1)
CT01	755	454	5835	10
CT02	1616	2076	7578	10

Table S2. Bond lengths [Å] for Cp^{*}₂Yb(phen) (**1**, crystallized).

C(12)-C(13)	1.395(9)	N(1)-C(32)	1.396(6)
C(12)-C(11)	1.427(8)	N(1)-Yb(1)	2.358(5)
C(12)-C(17)	1.520(8)	C(29)-C(30)	1.326(8)
C(12)-Yb(1)	2.608(5)	C(29)-C(28)	1.504(8)
C(11)-C(15)	1.419(8)	N(2)-C(31)	1.374(7)
C(11)-C(16)	1.515(8)	N(2)-C(30)	1.380(7)
C(11)-Yb(1)	2.639(4)	N(2)-Yb(1)	2.285(4)
C(13)-C(14)	1.411(7)	C(21)-C(22)	1.393(8)
C(13)-C(18)	1.489(9)	C(32)-C(24)	1.387(7)
C(13)-Yb(1)	2.600(5)	C(32)-C(31)	1.428(8)
C(5)-C(1)	1.408(8)	C(27)-C(31)	1.413(7)
C(5)-C(4)	1.412(7)	C(27)-C(26)	1.424(8)
C(5)-C(10)	1.510(9)	C(27)-C(28)	1.500(8)
C(5)-Yb(1)	2.586(5)	C(31)-Yb(1)	3.155(5)
C(14)-C(15)	1.398(9)	C(28)-C(28)#1	1.618(10)
C(14)-C(19)	1.505(8)	C(2)-C(1)	1.425(8)
C(14)-Yb(1)	2.608(5)	C(2)-C(7)	1.484(9)
C(3)-C(2)	1.398(7)	C(2)-Yb(1)	2.631(5)
C(3)-C(4)	1.407(9)	C(1)-C(6)	1.494(7)
C(3)-C(8)	1.518(8)	C(1)-Yb(1)	2.603(5)
C(3)-Yb(1)	2.636(6)	C(26)-C(25)	1.340(9)
C(15)-C(20)	1.506(7)	C(24)-C(23)	1.417(9)
C(15)-Yb(1)	2.626(5)	C(24)-C(25)	1.421(8)
C(4)-C(9)	1.509(8)	C(22)-C(23)	1.375(9)
C(4)-Yb(1)	2.629(5)	Yb(1)-CT01	2.3248(2)
N(1)-C(21)	1.331(7)	Yb(1)-CT02	2.3265(2)

Symmetry transformations used to generate equivalent atoms:

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

Table S3. Bond angles [°] for Cp*₂Yb(phen) (**1**, crystallized)

C(13)-C(12)-C(11)	108.8(5)	C(24)-C(32)-C(31)	122.3(5)
C(11)-C(12)-C(17)	122.0(5)	N(1)-C(32)-C(31)	115.6(4)
C(13)-C(12)-Yb(1)	74.2(3)	C(31)-C(27)-C(26)	118.5(5)
C(11)-C(12)-Yb(1)	75.4(3)	C(31)-C(27)-C(28)	118.8(5)
C(17)-C(12)-Yb(1)	124.3(4)	C(26)-C(27)-C(28)	122.6(5)
C(15)-C(11)-C(12)	106.3(5)	N(2)-C(31)-C(27)	123.2(5)
C(15)-C(11)-C(16)	126.7(5)	N(2)-C(31)-C(32)	119.6(4)
C(12)-C(11)-C(16)	126.6(5)	C(27)-C(31)-C(32)	117.2(5)
C(15)-C(11)-Yb(1)	73.9(3)	N(2)-C(31)-Yb(1)	40.2(2)
C(12)-C(11)-Yb(1)	73.0(3)	C(27)-C(31)-Yb(1)	163.4(4)
C(16)-C(11)-Yb(1)	123.6(4)	C(32)-C(31)-Yb(1)	79.4(3)
C(12)-C(13)-C(14)	107.9(6)	C(27)-C(28)-C(29)	109.3(4)
C(12)-C(13)-C(18)	127.0(6)	C(27)-C(28)-C(28)#1	110.3(6)
C(14)-C(13)-C(18)	124.8(6)	C(29)-C(28)-C(28)#1	110.6(6)
C(12)-C(13)-Yb(1)	74.8(3)	C(3)-C(2)-C(1)	107.4(5)
C(14)-C(13)-Yb(1)	74.6(3)	C(3)-C(2)-C(7)	127.3(6)
C(18)-C(13)-Yb(1)	121.8(3)	C(1)-C(2)-C(7)	124.8(5)
C(1)-C(5)-C(4)	108.5(5)	C(3)-C(2)-Yb(1)	74.8(3)
C(1)-C(5)-C(10)	127.4(5)	C(1)-C(2)-Yb(1)	73.1(3)
C(4)-C(5)-C(10)	124.0(5)	C(7)-C(2)-Yb(1)	124.1(4)
C(1)-C(5)-Yb(1)	74.9(3)	C(5)-C(1)-C(2)	107.6(5)
C(4)-C(5)-Yb(1)	76.0(3)	C(5)-C(1)-C(6)	127.6(5)
C(15)-C(14)-C(13)	108.3(5)	C(2)-C(1)-C(6)	124.8(5)
C(15)-C(14)-C(19)	126.0(5)	C(5)-C(1)-Yb(1)	73.6(3)
C(13)-C(14)-C(19)	125.4(6)	C(2)-C(1)-Yb(1)	75.3(3)
C(15)-C(14)-Yb(1)	75.2(3)	C(6)-C(1)-Yb(1)	118.3(3)
C(13)-C(14)-Yb(1)	74.0(3)	C(25)-C(26)-C(27)	123.0(5)
C(19)-C(14)-Yb(1)	122.1(3)	C(32)-C(24)-C(23)	117.8(5)
C(2)-C(3)-C(4)	109.2(5)	C(32)-C(24)-C(25)	118.6(6)
C(2)-C(3)-C(8)	122.4(6)	C(23)-C(24)-C(25)	123.6(5)
C(4)-C(3)-C(8)	127.5(6)	C(23)-C(22)-C(21)	118.4(6)
C(2)-C(3)-Yb(1)	74.4(3)	C(22)-C(23)-C(24)	120.2(5)
C(4)-C(3)-Yb(1)	74.2(3)	C(26)-C(25)-C(24)	119.7(5)
C(8)-C(3)-Yb(1)	126.2(4)	N(2)-Yb(1)-CT01	109.60(11)
C(14)-C(15)-C(11)	108.7(5)	N(2)-Yb(1)-CT02	106.54(10)
C(14)-C(15)-C(20)	124.9(5)	CT01-Yb(1)-CT02	137.790(8)
C(11)-C(15)-C(20)	126.2(6)	N(2)-Yb(1)-N(1)	71.57(17)
CT01-C(15)-Yb(1)	62.3(2)	CT01-Yb(1)-N(1)	104.24(10)
C(14)-C(15)-Yb(1)	73.8(3)	CT02-Yb(1)-N(1)	107.31(11)
C(11)-C(15)-Yb(1)	74.8(3)	N(2)-Yb(1)-C(5)	86.82(16)
C(20)-C(15)-Yb(1)	121.3(3)	N(1)-Yb(1)-C(5)	119.59(16)
C(3)-C(4)-C(5)	107.2(5)	N(2)-Yb(1)-C(13)	105.50(18)
C(3)-C(4)-C(9)	126.8(6)	N(1)-Yb(1)-C(13)	129.90(16)
C(5)-C(4)-C(9)	125.2(6)	C(5)-Yb(1)-C(13)	109.91(17)
C(3)-C(4)-Yb(1)	74.8(3)	N(2)-Yb(1)-C(1)	81.58(15)
C(5)-C(4)-Yb(1)	72.6(3)	N(1)-Yb(1)-C(1)	88.71(15)
C(9)-C(4)-Yb(1)	125.9(4)	C(5)-Yb(1)-C(1)	31.49(17)
C(21)-N(1)-C(32)	117.6(5)	C(13)-Yb(1)-C(1)	141.27(17)
C(21)-N(1)-Yb(1)	126.1(4)	N(2)-Yb(1)-C(12)	134.11(18)
C(32)-N(1)-Yb(1)	115.5(4)	N(1)-Yb(1)-C(12)	119.27(16)
C(30)-C(29)-C(28)	120.4(6)	C(5)-Yb(1)-C(12)	116.12(17)
C(31)-N(2)-C(30)	115.0(4)	C(13)-Yb(1)-C(12)	31.07(19)
C(31)-N(2)-Yb(1)	117.0(4)	C(1)-Yb(1)-C(12)	138.34(16)
C(30)-N(2)-Yb(1)	127.4(3)	N(2)-Yb(1)-C(14)	83.05(16)
N(1)-C(21)-C(22)	123.9(5)	N(1)-Yb(1)-C(14)	102.15(17)
C(29)-C(30)-N(2)	126.1(5)	C(5)-Yb(1)-C(14)	131.05(19)
C(24)-C(32)-N(1)	122.1(5)	C(13)-Yb(1)-C(14)	31.45(17)

C(1)-Yb(1)-C(14)	157.29(19)	C(4)-Yb(1)-C(2)	51.53(17)
C(12)-Yb(1)-C(14)	51.56(18)	N(2)-Yb(1)-C(3)	132.81(15)
N(2)-Yb(1)-C(15)	94.02(15)	N(1)-Yb(1)-C(3)	107.43(19)
N(1)-Yb(1)-C(15)	78.34(17)	C(5)-Yb(1)-C(3)	51.50(18)
C(5)-Yb(1)-C(15)	161.1(2)	C(13)-Yb(1)-C(3)	108.80(18)
C(13)-Yb(1)-C(15)	51.65(18)	C(1)-Yb(1)-C(3)	51.48(15)
C(1)-Yb(1)-C(15)	167.05(17)	C(12)-Yb(1)-C(3)	88.97(17)
C(12)-Yb(1)-C(15)	51.60(16)	C(14)-Yb(1)-C(3)	139.11(16)
C(14)-Yb(1)-C(15)	30.98(19)	C(15)-Yb(1)-C(3)	132.77(16)
N(2)-Yb(1)-C(4)	117.36(16)	C(4)-Yb(1)-C(3)	30.99(19)
N(1)-Yb(1)-C(4)	133.60(17)	C(2)-Yb(1)-C(3)	30.77(16)
C(5)-Yb(1)-C(4)	31.40(16)	N(2)-Yb(1)-C(11)	125.19(16)
C(13)-Yb(1)-C(4)	93.34(17)	N(1)-Yb(1)-C(11)	87.79(16)
C(1)-Yb(1)-C(4)	51.87(15)	C(5)-Yb(1)-C(11)	144.66(16)
C(12)-Yb(1)-C(4)	87.97(16)	C(13)-Yb(1)-C(11)	51.97(19)
C(14)-Yb(1)-C(4)	123.66(18)	C(1)-Yb(1)-C(11)	149.88(18)
C(15)-Yb(1)-C(4)	139.50(15)	C(12)-Yb(1)-C(11)	31.57(17)
N(2)-Yb(1)-C(2)	108.50(15)	C(14)-Yb(1)-C(11)	51.73(18)
N(1)-Yb(1)-C(2)	82.10(17)	C(15)-Yb(1)-C(11)	31.28(16)
C(5)-Yb(1)-C(2)	51.97(19)	C(4)-Yb(1)-C(11)	113.56(16)
C(13)-Yb(1)-C(2)	139.57(17)	C(2)-Yb(1)-C(11)	118.39(18)
C(1)-Yb(1)-C(2)	31.60(17)	C(3)-Yb(1)-C(11)	101.51(16)
C(12)-Yb(1)-C(2)	116.97(18)		
C(14)-Yb(1)-C(2)	168.45(17)		
C(15)-Yb(1)-C(2)	143.60(19)		

Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z+2

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cp}^*_2\text{Yb}(\text{phen})$ (**1**, crystallized). The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^* 2U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(12)	34(4)	34(3)	19(2)	-6(2)	5(2)	-1(3)
C(11)	33(4)	29(3)	16(2)	-4(2)	2(2)	-8(3)
C(13)	32(4)	34(3)	19(2)	-9(2)	-5(2)	3(3)
C(5)	28(4)	16(2)	35(3)	-8(2)	-4(2)	2(3)
C(14)	33(4)	27(3)	20(2)	-6(2)	-2(2)	-10(3)
C(3)	37(4)	21(2)	27(3)	0(2)	2(2)	-10(3)
C(17)	69(6)	34(3)	19(2)	3(2)	3(3)	-2(3)
C(15)	41(4)	24(3)	18(2)	-3(2)	0(2)	-14(3)
C(20)	58(5)	22(3)	32(3)	-6(2)	-5(3)	-12(3)
C(4)	36(4)	18(2)	33(3)	1(2)	-11(3)	-4(3)
N(1)	23(3)	21(2)	25(2)	-6(2)	-1(2)	0(2)
C(29)	21(4)	40(3)	24(2)	-6(2)	3(2)	-4(3)
N(2)	24(3)	25(2)	19(2)	-3(2)	-2(2)	3(2)
C(21)	21(3)	29(3)	35(3)	-8(2)	2(2)	-1(3)
C(30)	24(4)	28(3)	22(2)	-4(2)	-6(2)	-1(3)
C(32)	28(4)	19(2)	14(2)	-3(2)	-2(2)	-4(3)
C(27)	30(4)	30(3)	15(2)	3(2)	-1(2)	-2(3)
C(31)	22(3)	20(2)	19(2)	-3(2)	0(2)	-4(2)
C(28)	26(4)	36(3)	21(2)	0(2)	3(2)	-15(3)
C(2)	20(3)	17(2)	32(3)	-8(2)	-3(2)	-3(2)
C(1)	25(4)	17(2)	23(2)	-2(2)	0(2)	-2(2)
C(16)	35(4)	42(3)	26(3)	-9(2)	9(2)	1(3)
C(26)	49(5)	22(3)	25(2)	2(2)	-4(3)	-6(3)
C(24)	29(4)	28(3)	22(2)	-4(2)	-11(2)	-2(3)
C(6)	60(5)	26(3)	21(2)	-1(2)	-4(2)	-4(3)
C(19)	34(4)	59(4)	31(3)	-12(3)	5(2)	-18(4)
C(10)	30(4)	33(3)	61(4)	-20(3)	-1(3)	3(3)
C(22)	25(4)	31(3)	36(3)	-12(2)	-1(2)	7(3)
C(23)	36(4)	19(2)	36(3)	-4(2)	-11(3)	4(3)
C(18)	39(5)	58(4)	34(3)	-12(3)	-11(3)	13(4)
C(7)	27(4)	35(3)	60(4)	-13(3)	-7(3)	1(3)
C(8)	60(5)	51(4)	37(3)	-8(3)	14(3)	-25(4)
C(9)	71(6)	26(3)	52(4)	-1(3)	-32(4)	3(4)
C(25)	46(5)	22(3)	27(3)	0(2)	-11(3)	-9(3)
Yb(1)	21(1)	17(1)	17(1)	-1(1)	1(1)	-2(1)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cp}^*_2\text{Yb}(\text{phen})$ (**1**, crystallized).

	x	y	z	U(eq)
H(17A)	1775	1539	4813	61
H(17B)	1220	2098	5233	61
H(17C)	974	1649	4451	61
H(20A)	1588	-1079	6139	56
H(20B)	751	-1293	5999	56
H(20C)	1019	-1026	6868	56
H(29)	-1055	338	9091	34
H(21)	2809	65	6987	34
H(30)	-480	859	8034	30
H(16A)	2360	590	5028	51
H(16B)	2119	-244	4893	51
H(16C)	2478	0	5729	51
H(26)	617	-1543	9858	38
H(6A)	1136	1605	9372	54
H(6B)	1992	1766	9429	54
H(6C)	1710	990	9102	54
H(19A)	-853	199	6552	62
H(19B)	-357	-345	7073	62
H(19C)	-612	-576	6187	62
H(10A)	218	2189	8759	62
H(10B)	-123	2196	7872	62
H(10C)	215	2931	8243	62
H(22)	3376	-1033	7395	37
H(23)	2791	-1783	8358	36
H(18A)	-794	1238	6042	66
H(18B)	-498	1503	5184	66
H(18C)	-239	1913	5986	66
H(7A)	2961	1294	8451	61
H(7B)	3309	1943	7929	61
H(7C)	3133	1170	7516	61
H(8A)	2279	2595	5864	74
H(8B)	2760	1894	6097	74
H(8C)	2920	2669	6512	74
H(9A)	351	3017	6711	74
H(9B)	815	2714	5966	74
H(9C)	1103	3403	6471	74
H(25)	1675	-1996	9308	38
H(28)	-450(30)	-630(30)	9800(30)	19(14)

5.2. Cp*₂Yb(phen), sublimed (1)

Data collection

A fragment of a purple block-like crystal of C₃₂H₃₈N₂Yb (Cp*₂Yb(phen)) crystallized by sublimation at 280°C having approximate dimension of 0.15 x 0.15 x 0.10 mm was mounted on a Kapton loop using Paratone N hydrocarbon oil. All measurements were made on a Bruker APEX¹ CCD area detector with graphite monochromated Mo-K α radiation.

Cell constants and an orientation matrix, obtained from a least-squared refinement using the measured positions of 9920 reflexions with $I > 10\sigma$ in the range $4.79 < 2\theta < 50.79$ corresponded to a primitive monoclinic cell with dimensions:

$$\begin{aligned} a &= 9.656(2) \text{ \AA} & \alpha &= 78.909(4)^\circ \\ b &= 9.741(2) \text{ \AA} & \beta &= 83.300(3)^\circ \\ c &= 14.998(4) \text{ \AA} & \gamma &= 74.702(4)^\circ \\ V &= 1332.1(5) \text{ \AA}^3 \end{aligned}$$

For $Z = 2$ and F.W. = 623.68, the calculated density is 1.555 g cm⁻³. Based on a statistical analysis of intensity distribution, and successful solution and refinement of the structure, the space group was determined to be

$$P - 1 (\#2)$$

The data were collected at a temperature of -173(1) °C. Frames corresponding to an arbitrary hemisphere of data were collected using ω scans of 0.3° counted for a total of 10.0s per frame.

Data reduction

Data were integrated by the program SAINT² to a maximum 2θ value of 50.86°. The data were corrected for Lorentz and polarization effects. Data were analyzed for agreement and possible absorption using XPREP.³ A semi-empirical multi-scan absorption correction⁴ was applied using SADABS.⁵ This models the absorption surface using a spherical harmonic series based on differences between equivalent.

Structure solution and refinement

The structure was solved by Patterson methods.⁶ Non-hydrogen atoms were refined anisotropically and hydrogen atoms were placed in calculated positions and not refined. The final cycle of full matrix least squares refinement was based on 4882 observed reflections ($I > 2.00 \sigma(I)$) and 348 parameters and converged with unweighted and weighted agreement factors of:

$$R = \sum ||F_o| - |F_c|| / \sum |F_o| = 0.0305$$

$$R_w = [(\sum w (|F_o| - |F_c|)^2 / \sum w F_o^2)]^{1/2} = 0.0712$$

The standard deviation of an observation of unit weight was 1.178. The weighting scheme was based on counting statistics and include a factor p to downweight the intense

reflections ($w=1/[\sigma^2F_o^2+(0.0188P)^2+(10.30P)]$ where $P=(\text{Max}(F_o^2,0)+2F_c^2)/3$). Plot of $\Sigma w (|F_o| - |F_c|)^2$ versus $|F_o|$, reflexion order in data collection, $\sin \theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.859 and -1.067 e.A⁻³, respectively.

The SHELX program uses the neutral atom scattering factors, f' , f'' and absorption coefficients from International Tables for Crystallography, Volume C (1992), Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht: Tables 6.1.1.4(pp. 500-502), 4.2.6.8 (pp.219-222) and 4.2.4.2 (pp. 193-199), respectively. All calculations were performed using the WinGX crystallographic software package.⁷ (“WinGX suite for small molecule single-crystal crystallography”)

Figure S21. ORTEP of $\text{Cp}^*_2\text{Yb}(\text{phen})$ (**1**, **sublimed**) (50% probability ellipsoids).

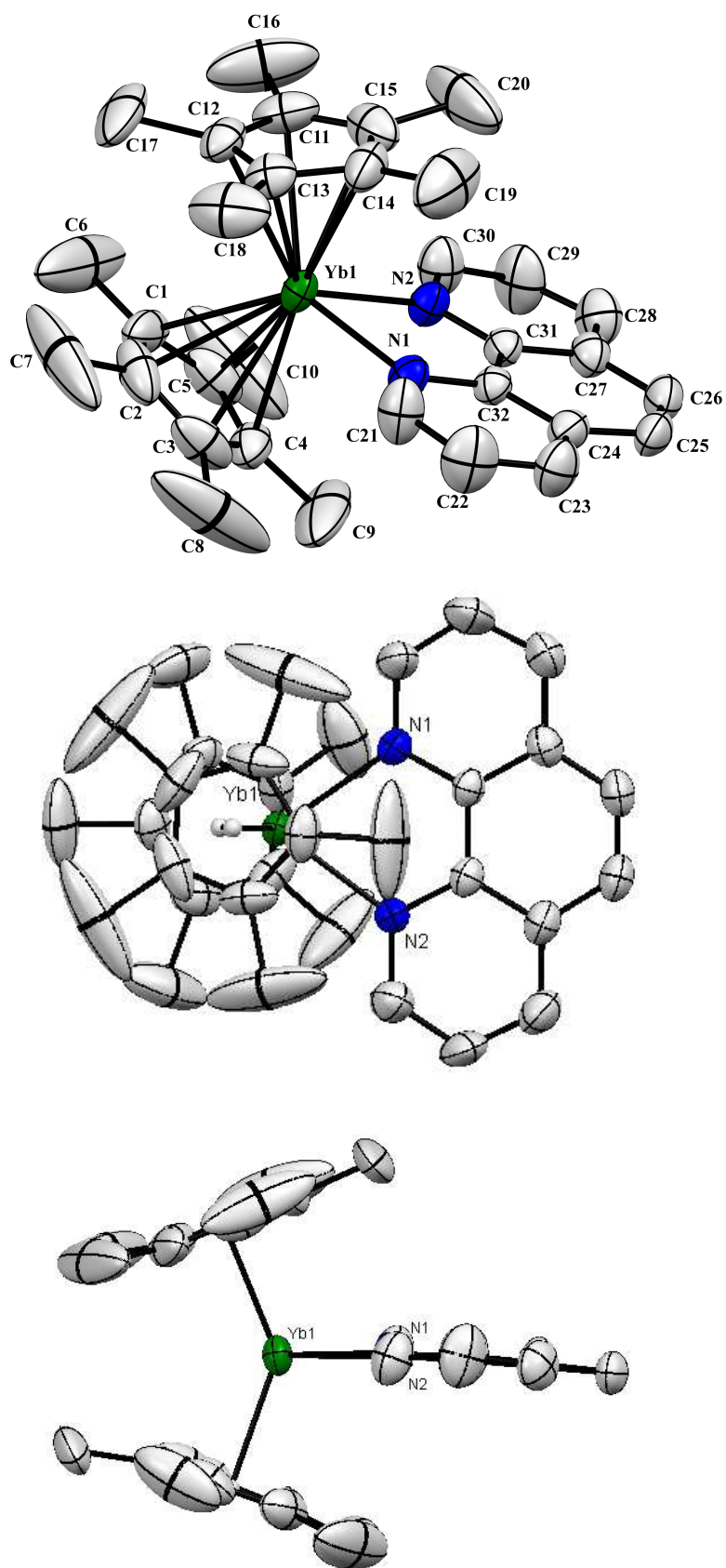


Table S6. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cp}^*\text{Yb}(\text{phen})$ (**1, sublimed**). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Yb(1)	7291(1)	6421(1)	7397(1)	35(1)
N(1)	7445(4)	7608(4)	8559(3)	39(1)
N(2)	9060(4)	7672(4)	6959(3)	40(1)
C(31)	9228(5)	8518(4)	7546(3)	37(1)
C(32)	8373(4)	8487(4)	8393(3)	34(1)
C(13)	4517(5)	7423(6)	7328(4)	48(1)
C(24)	8504(5)	9367(5)	9012(3)	42(1)
C(27)	10201(5)	9430(5)	7341(4)	44(1)
C(5)	9343(7)	4113(6)	7229(4)	61(2)
C(14)	5067(6)	8671(6)	7151(4)	56(1)
C(25)	9457(6)	10276(5)	8773(4)	47(1)
C(12)	4975(5)	6718(5)	6573(4)	51(1)
C(3)	8121(8)	4079(6)	8574(4)	66(2)
C(15)	5885(6)	8660(6)	6310(5)	63(2)
C(4)	9390(6)	4350(5)	8099(5)	55(2)
C(26)	10277(6)	10297(5)	7975(4)	48(1)
C(1)	8105(9)	3726(6)	7156(5)	72(2)
C(2)	7344(6)	3709(6)	7990(6)	73(2)
C(11)	5826(6)	7470(7)	5968(4)	61(2)
C(23)	7616(7)	9331(6)	9868(4)	61(2)
C(30)	9879(7)	7731(6)	6140(4)	60(2)
C(21)	6595(7)	7639(6)	9366(4)	62(2)
C(28)	11084(6)	9418(6)	6494(4)	60(2)
C(29)	10947(7)	8471(7)	5942(5)	72(2)
C(22)	6715(7)	8397(7)	10022(5)	72(2)
C(18)	3535(6)	7010(9)	8121(5)	94(3)
C(17)	4390(8)	5531(7)	6349(7)	108(3)
C(19)	4720(9)	9895(8)	7683(7)	114(3)
C(16)	6485(9)	7112(13)	5038(5)	136(4)
C(20)	6553(9)	9891(9)	5841(8)	144(5)
C(7)	6035(8)	3117(9)	8300(11)	204(8)
C(9)	10572(10)	4728(9)	8479(9)	165(6)
C(10)	10584(11)	4088(9)	6506(7)	187(7)
C(6)	7844(15)	3140(9)	6342(9)	207(8)
C(8)	7769(16)	4032(10)	9582(5)	204(8)

Table S7. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cp}_2^*\text{Yb}(\text{phen})$ (**1**, **sublimed**). The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Yb(1)	33(1)	41(1)	37(1)	-12(1)	1(1)	-16(1)
N(1)	35(2)	46(2)	38(2)	-9(2)	0(2)	-16(2)
N(2)	42(2)	48(2)	35(2)	-12(2)	3(2)	-20(2)
C(31)	32(2)	35(2)	44(3)	-5(2)	-7(2)	-10(2)
C(32)	28(2)	35(2)	40(3)	-7(2)	-5(2)	-8(2)
C(13)	31(2)	62(3)	50(3)	-9(2)	1(2)	-11(2)
C(24)	42(3)	43(2)	43(3)	-10(2)	-9(2)	-10(2)
C(27)	38(2)	40(2)	55(3)	-6(2)	-5(2)	-13(2)
C(5)	65(4)	50(3)	51(4)	1(3)	24(3)	-3(3)
C(14)	47(3)	49(3)	78(4)	-27(3)	-17(3)	-7(2)
C(25)	50(3)	44(3)	55(3)	-17(2)	-14(3)	-15(2)
C(12)	38(3)	52(3)	67(4)	-19(3)	-19(3)	-6(2)
C(3)	93(5)	49(3)	36(3)	-1(2)	18(3)	1(3)
C(15)	42(3)	64(4)	78(4)	17(3)	-9(3)	-23(3)
C(4)	44(3)	43(3)	83(5)	-12(3)	-24(3)	-8(2)
C(26)	47(3)	43(3)	60(4)	-8(2)	-9(3)	-20(2)
C(1)	102(5)	39(3)	81(5)	-21(3)	-53(4)	1(3)
C(2)	40(3)	39(3)	135(7)	4(3)	-3(4)	-15(2)
C(11)	41(3)	98(5)	39(3)	-8(3)	-7(2)	-10(3)
C(23)	69(4)	62(3)	60(4)	-27(3)	0(3)	-24(3)
C(30)	70(4)	60(3)	57(4)	-20(3)	12(3)	-28(3)
C(21)	66(4)	66(3)	63(4)	-30(3)	25(3)	-33(3)
C(28)	52(3)	61(3)	70(4)	-9(3)	6(3)	-27(3)
C(29)	83(4)	84(4)	59(4)	-18(3)	32(4)	-49(4)
C(22)	78(4)	86(4)	59(4)	-35(3)	26(3)	-28(3)
C(18)	40(3)	147(7)	78(5)	18(5)	4(3)	-25(4)
C(17)	75(5)	79(5)	192(10)	-49(5)	-78(6)	-8(4)
C(19)	106(6)	89(5)	153(9)	-74(6)	-44(6)	18(5)
C(16)	81(5)	252(12)	51(5)	-43(6)	-7(4)	15(7)
C(20)	85(5)	112(6)	206(11)	94(7)	-39(6)	-53(5)
C(7)	56(4)	73(5)	430(20)	95(9)	-20(8)	-27(4)
C(9)	127(8)	79(5)	315(16)	-31(7)	-165(10)	-7(5)
C(10)	182(10)	80(5)	193(11)	36(6)	142(9)	44(6)
C(6)	302(16)	87(6)	229(13)	-105(8)	-203(13)	92(8)
C(8)	363(19)	98(6)	45(5)	6(4)	42(8)	92(9)

Table S8. Bond lengths [Å] for Cp^{*}₂Yb(phen) (**1**, sublimed).

Yb(1)-N(1)	2.307(4)	C(24)-C(23)	1.458(8)
Yb(1)-N(2)	2.316(4)	C(27)-C(26)	1.407(7)
Yb(1)-CT02	2.3243(4)	C(27)-C(28)	1.445(8)
Yb(1)-CT01	2.3320(5)	C(5)-C(1)	1.367(9)
Yb(1)-C(11)	2.597(6)	C(5)-C(4)	1.376(9)
Yb(1)-C(12)	2.604(5)	C(5)-C(10)	1.517(8)
Yb(1)-C(13)	2.604(5)	C(14)-C(15)	1.408(9)
Yb(1)-C(3)	2.603(5)	C(14)-C(19)	1.504(8)
Yb(1)-C(4)	2.609(5)	C(25)-C(26)	1.356(8)
Yb(1)-C(5)	2.607(5)	C(12)-C(11)	1.387(8)
Yb(1)-C(2)	2.609(5)	C(12)-C(17)	1.518(8)
Yb(1)-C(15)	2.616(5)	C(3)-C(2)	1.371(10)
Yb(1)-C(1)	2.617(5)	C(3)-C(4)	1.404(9)
Yb(1)-C(14)	2.635(5)	C(3)-C(8)	1.506(9)
N(1)-C(32)	1.367(5)	C(15)-C(20)	1.525(8)
N(1)-C(21)	1.383(6)	C(4)-C(9)	1.489(9)
N(2)-C(31)	1.365(6)	C(1)-C(2)	1.374(11)
N(2)-C(30)	1.381(7)	C(1)-C(6)	1.516(10)
C(31)-C(27)	1.426(6)	C(2)-C(7)	1.513(9)
C(31)-C(32)	1.433(6)	C(11)-C(16)	1.527(9)
C(32)-C(24)	1.414(7)	C(23)-C(22)	1.388(9)
C(13)-C(12)	1.404(8)	C(30)-C(29)	1.382(8)
C(13)-C(14)	1.420(7)	C(21)-C(22)	1.371(9)
C(13)-C(18)	1.493(7)	C(28)-C(29)	1.392(9)
C(24)-C(25)	1.411(7)		

Table S9. Bond angles [deg] for Cp^{*}₂Yb(phen) (**1**, sublimed).

N(1)-Yb(1)-N(2)	71.59(13)	CT01-Yb(1)-C(15)	154.62(17)
N(1)-Yb(1)-CT02	105.45(9)	C(11)-Yb(1)-C(15)	30.5(2)
N(2)-Yb(1)-CT02	106.62(10)	C(12)-Yb(1)-C(15)	50.83(18)
N(1)-Yb(1)-CT01	107.90(9)	C(13)-Yb(1)-C(15)	51.74(16)
N(2)-Yb(1)-CT01	106.97(10)	C(3)-Yb(1)-C(15)	167.1(2)
CT02-Yb(1)-CT01	138.411(9)	C(4)-Yb(1)-C(15)	161.04(19)
N(1)-Yb(1)-C(11)	127.11(18)	C(5)-Yb(1)-C(15)	136.8(2)
N(2)-Yb(1)-C(11)	96.75(17)	C(2)-Yb(1)-C(15)	140.3(2)
CT02-Yb(1)-C(11)	27.06(12)	N(1)-Yb(1)-C(1)	134.35(17)
CT01-Yb(1)-C(11)	124.60(16)	N(2)-Yb(1)-C(1)	113.7(2)
N(1)-Yb(1)-C(12)	125.40(15)	CT02-Yb(1)-C(1)	114.92(14)
N(2)-Yb(1)-C(12)	127.19(16)	CT01-Yb(1)-C(1)	26.57(14)
CT02-Yb(1)-C(12)	26.96(11)	C(11)-Yb(1)-C(1)	98.0(2)
CT01-Yb(1)-C(12)	111.45(11)	C(12)-Yb(1)-C(1)	88.94(18)
C(11)-Yb(1)-C(12)	30.93(18)	C(13)-Yb(1)-C(1)	111.4(2)
N(1)-Yb(1)-C(13)	94.53(15)	C(3)-Yb(1)-C(1)	50.4(2)
N(2)-Yb(1)-C(13)	127.87(15)	C(4)-Yb(1)-C(1)	50.92(18)
CT02-Yb(1)-C(13)	27.56(12)	C(5)-Yb(1)-C(1)	30.3(2)
CT01-Yb(1)-C(13)	124.96(12)	C(2)-Yb(1)-C(1)	30.5(2)
C(11)-Yb(1)-C(13)	51.75(17)	C(15)-Yb(1)-C(1)	128.2(2)
C(12)-Yb(1)-C(13)	31.28(17)	N(1)-Yb(1)-C(14)	78.51(16)
N(1)-Yb(1)-C(3)	84.93(18)	N(2)-Yb(1)-C(14)	96.86(16)
N(2)-Yb(1)-C(3)	112.9(2)	CT02-Yb(1)-C(14)	26.98(13)
CT02-Yb(1)-C(3)	140.37(18)	CT01-Yb(1)-C(14)	156.15(13)
CT01-Yb(1)-C(3)	26.67(12)	C(11)-Yb(1)-C(14)	51.13(19)
C(11)-Yb(1)-C(3)	142.8(2)	C(12)-Yb(1)-C(14)	51.20(16)
C(12)-Yb(1)-C(3)	117.8(2)	C(13)-Yb(1)-C(14)	31.44(16)
C(13)-Yb(1)-C(3)	115.5(2)	C(3)-Yb(1)-C(14)	139.17(19)
N(1)-Yb(1)-C(4)	86.86(16)	C(4)-Yb(1)-C(14)	164.1(2)
N(2)-Yb(1)-C(4)	84.19(16)	C(5)-Yb(1)-C(14)	165.1(2)
CT02-Yb(1)-C(4)	165.56(12)	C(2)-Yb(1)-C(14)	129.42(18)
CT01-Yb(1)-C(4)	27.24(12)	C(15)-Yb(1)-C(14)	31.10(19)
C(11)-Yb(1)-C(4)	144.7(2)	C(1)-Yb(1)-C(14)	139.91(19)
C(12)-Yb(1)-C(4)	138.65(16)	C(32)-N(1)-C(21)	116.4(4)
C(13)-Yb(1)-C(4)	146.63(17)	C(32)-N(1)-Yb(1)	116.5(3)
C(3)-Yb(1)-C(4)	31.26(19)	C(21)-N(1)-Yb(1)	126.7(3)
N(1)-Yb(1)-C(5)	116.04(19)	C(31)-N(2)-C(30)	117.0(4)
N(2)-Yb(1)-C(5)	85.64(17)	C(31)-N(2)-Yb(1)	116.1(3)
CT02-Yb(1)-C(5)	138.47(17)	C(30)-N(2)-Yb(1)	126.6(4)
CT01-Yb(1)-C(5)	26.31(11)	N(2)-C(31)-C(27)	122.6(4)
C(11)-Yb(1)-C(5)	114.1(2)	N(2)-C(31)-C(32)	117.9(4)
C(12)-Yb(1)-C(5)	116.1(2)	C(27)-C(31)-C(32)	119.5(4)
C(13)-Yb(1)-C(5)	141.6(2)	N(2)-C(31)-Yb(1)	41.1(2)
C(3)-Yb(1)-C(5)	50.29(17)	C(27)-C(31)-Yb(1)	163.3(4)
C(4)-Yb(1)-C(5)	30.59(19)	C(32)-C(31)-Yb(1)	76.9(3)
N(1)-Yb(1)-C(2)	112.0(2)	N(1)-C(32)-C(24)	123.0(4)
N(2)-Yb(1)-C(2)	133.70(16)	N(1)-C(32)-C(31)	117.6(4)
CT02-Yb(1)-C(2)	115.71(15)	C(24)-C(32)-C(31)	119.4(4)
CT01-Yb(1)-C(2)	26.73(12)	N(1)-C(32)-Yb(1)	40.7(2)
C(11)-Yb(1)-C(2)	112.3(3)	C(24)-C(32)-Yb(1)	163.3(3)
C(12)-Yb(1)-C(2)	89.8(2)	C(31)-C(32)-Yb(1)	76.9(3)
C(13)-Yb(1)-C(2)	98.34(17)	CT02-C(13)-C(12)	53.1(3)
C(3)-Yb(1)-C(2)	30.5(2)	CT02-C(13)-C(14)	53.4(3)
C(4)-Yb(1)-C(2)	51.22(18)	C(12)-C(13)-C(14)	106.6(5)
C(5)-Yb(1)-C(2)	50.22(18)	CT02-C(13)-C(18)	177.0(5)
N(1)-Yb(1)-C(15)	97.46(19)	C(12)-C(13)-C(18)	126.5(6)
N(2)-Yb(1)-C(15)	79.74(15)	C(14)-C(13)-C(18)	126.7(6)
CT02-Yb(1)-C(15)	26.88(12)	CT02-C(13)-Yb(1)	63.2(2)

C(12)-C(13)-Yb(1)	74.3(3)	CT01-C(4)-C(5)	52.9(4)
C(14)-C(13)-Yb(1)	75.5(3)	CT01-C(4)-C(3)	52.7(4)
C(18)-C(13)-Yb(1)	119.8(4)	C(5)-C(4)-C(3)	105.5(5)
C(25)-C(24)-C(32)	119.2(4)	CT01-C(4)-C(9)	177.5(6)
C(25)-C(24)-C(23)	122.1(5)	C(5)-C(4)-C(9)	127.6(8)
C(32)-C(24)-C(23)	118.7(4)	C(3)-C(4)-C(9)	126.8(8)
C(26)-C(27)-C(31)	118.8(5)	CT01-C(4)-Yb(1)	63.3(2)
C(26)-C(27)-C(28)	122.4(5)	C(5)-C(4)-Yb(1)	74.6(3)
C(31)-C(27)-C(28)	118.8(5)	C(3)-C(4)-Yb(1)	74.1(3)
CT01-C(5)-C(1)	54.5(4)	C(9)-C(4)-Yb(1)	119.1(4)
CT01-C(5)-C(4)	55.5(3)	C(25)-C(26)-C(27)	121.6(5)
C(1)-C(5)-C(4)	110.0(5)	CT01-C(1)-C(5)	53.5(4)
CT01-C(5)-C(10)	173.4(5)	CT01-C(1)-C(2)	54.2(4)
C(1)-C(5)-C(10)	125.4(9)	C(5)-C(1)-C(2)	107.7(6)
C(4)-C(5)-C(10)	124.1(8)	CT01-C(1)-C(6)	170.1(6)
CT01-C(5)-Yb(1)	63.4(2)	C(5)-C(1)-C(6)	123.0(9)
C(1)-C(5)-Yb(1)	75.2(3)	C(2)-C(1)-C(6)	128.1(10)
C(4)-C(5)-Yb(1)	74.8(3)	CT01-C(1)-Yb(1)	63.0(2)
C(10)-C(5)-Yb(1)	123.2(4)	C(5)-C(1)-Yb(1)	74.4(3)
CT02-C(14)-C(15)	53.3(4)	C(2)-C(1)-Yb(1)	74.4(3)
CT02-C(14)-C(13)	54.1(3)	C(6)-C(1)-Yb(1)	126.4(4)
C(15)-C(14)-C(13)	107.3(5)	CT01-C(2)-C(3)	54.0(4)
CT02-C(14)-C(19)	173.5(6)	CT01-C(2)-C(1)	54.0(4)
C(15)-C(14)-C(19)	124.6(6)	C(3)-C(2)-C(1)	108.0(5)
C(13)-C(14)-C(19)	127.7(6)	CT01-C(2)-C(7)	171.0(6)
CT02-C(14)-Yb(1)	61.9(2)	C(3)-C(2)-C(7)	123.2(9)
C(15)-C(14)-Yb(1)	73.7(3)	C(1)-C(2)-C(7)	127.8(10)
C(13)-C(14)-Yb(1)	73.1(3)	CT01-C(2)-Yb(1)	63.3(2)
C(19)-C(14)-Yb(1)	124.3(4)	C(3)-C(2)-Yb(1)	74.5(3)
C(26)-C(25)-C(24)	121.4(5)	C(1)-C(2)-Yb(1)	75.1(3)
CT02-C(12)-C(11)	54.1(4)	C(7)-C(2)-Yb(1)	125.3(4)
CT02-C(12)-C(13)	54.8(3)	CT02-C(11)-C(15)	54.6(4)
C(11)-C(12)-C(13)	108.8(5)	CT02-C(11)-C(12)	54.0(3)
CT02-C(12)-C(17)	169.2(5)	C(15)-C(11)-C(12)	108.6(5)
C(11)-C(12)-C(17)	124.2(6)	CT02-C(11)-C(16)	176.7(6)
C(13)-C(12)-C(17)	125.7(6)	C(15)-C(11)-C(16)	125.3(7)
CT02-C(12)-Yb(1)	63.2(2)	C(12)-C(11)-C(16)	125.9(7)
C(11)-C(12)-Yb(1)	74.3(3)	CT02-C(11)-Yb(1)	63.5(2)
C(13)-C(12)-Yb(1)	74.4(3)	C(15)-C(11)-Yb(1)	75.5(3)
C(17)-C(12)-Yb(1)	127.5(4)	C(12)-C(11)-Yb(1)	74.8(3)
CT01-C(3)-C(2)	54.4(4)	C(16)-C(11)-Yb(1)	119.8(4)
CT01-C(3)-C(4)	54.4(3)	C(22)-C(23)-C(24)	116.7(5)
C(2)-C(3)-C(4)	108.7(5)	C(29)-C(30)-N(2)	123.0(6)
CT01-C(3)-C(8)	174.2(6)	C(22)-C(21)-N(1)	124.0(5)
C(2)-C(3)-C(8)	125.8(9)	C(29)-C(28)-C(27)	116.8(5)
C(4)-C(3)-C(8)	125.1(9)	C(30)-C(29)-C(28)	120.9(6)
CT01-C(3)-Yb(1)	63.6(2)	C(21)-C(22)-C(23)	120.9(6)
C(2)-C(3)-Yb(1)	75.0(3)	C(5)-CT01-C(3)	144.6(6)
C(4)-C(3)-Yb(1)	74.6(3)	C(5)-CT01-C(1)	72.0(5)
C(8)-C(3)-Yb(1)	122.2(4)	C(3)-CT01-C(1)	143.4(6)
CT02-C(15)-C(11)	54.5(3)	C(5)-CT01-C(2)	143.7(6)
CT02-C(15)-C(14)	54.1(3)	C(3)-CT01-C(2)	71.7(5)
C(11)-C(15)-C(14)	108.6(5)	C(1)-CT01-C(2)	71.8(6)
CT02-C(15)-C(20)	174.3(6)	C(5)-CT01-C(4)	71.7(5)
C(11)-C(15)-C(20)	127.6(7)	C(3)-CT01-C(4)	72.9(5)
C(14)-C(15)-C(20)	123.4(7)	C(1)-CT01-C(4)	143.6(5)
CT02-C(15)-Yb(1)	62.7(2)	C(2)-CT01-C(4)	144.6(6)
C(11)-C(15)-Yb(1)	74.0(3)	C(5)-CT01-Yb(1)	90.3(3)
C(14)-C(15)-Yb(1)	75.2(3)	C(3)-CT01-Yb(1)	89.7(3)
C(20)-C(15)-Yb(1)	122.5(4)	C(1)-CT01-Yb(1)	90.4(3)

C(2)-CT01-Yb(1)	89.9(3)	C(12)-CT02-C(13)	72.1(4)
C(4)-CT01-Yb(1)	89.4(2)	C(15)-CT02-C(13)	145.1(4)
C(11)-CT02-C(12)	71.9(4)	C(14)-CT02-C(13)	72.5(4)
C(11)-CT02-C(15)	70.9(5)	C(11)-CT02-Yb(1)	89.4(3)
C(12)-CT02-C(15)	142.8(5)	C(12)-CT02-Yb(1)	89.8(2)
C(11)-CT02-C(14)	143.5(4)	C(15)-CT02-Yb(1)	90.4(3)
C(12)-CT02-C(14)	144.6(4)	C(14)-CT02-Yb(1)	91.1(3)
C(15)-CT02-C(14)	72.6(4)	C(13)-CT02-Yb(1)	89.3(2)
C(11)-CT02-C(13)	144.0(4)		

Table S10. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cp}^*\text{Yb}(\text{phen})$ (**1**, **sublimed**).

	x	y	z	U(eq)
H(18A)	3329	6116	8072	140
H(18B)	2654	7752	8124	140
H(18C)	3990	6896	8676	140
H(17A)	3838	5164	6871	163
H(17B)	5176	4765	6185	163
H(17C)	3787	5915	5848	163
H(19A)	4152	9656	8232	171
H(19B)	4189	10755	7322	171
H(19C)	5598	10055	7834	171
H(16A)	6291	6229	4955	204
H(16B)	7506	7000	5008	204
H(16C)	6072	7880	4568	204
H(20A)	6444	10573	6244	215
H(20B)	6077	10362	5296	215
H(20C)	7557	9511	5688	215
H(7A)	5655	2935	7783	306
H(7B)	5316	3807	8592	306
H(7C)	6305	2233	8723	306
H(9A)	10311	4832	9105	248
H(9B)	10729	5620	8137	248
H(9C)	11438	3975	8442	248
H(10A)	11330	4399	6722	281
H(10B)	10250	4725	5960	281
H(10C)	10958	3124	6380	281
H(6A)	6909	2946	6426	310
H(6B)	8564	2263	6283	310
H(6C)	7894	3838	5800	310
H(8A)	8483	4339	9836	307
H(8B)	7761	3063	9868	307
H(8C)	6840	4664	9687	307
H(28)	11470(50)	8470(50)	5420(40)	41(13)
H(21)	5940(60)	7060(50)	9420(40)	52(15)
H(29)	9820(60)	7090(60)	5800(40)	59(17)
H(27)	11860(60)	9950(50)	6330(40)	53(14)
H(26)	11020(60)	10850(60)	7860(40)	62(16)
H(22)	6100(60)	8350(60)	10600(40)	70(17)
H(23)	7800(70)	9890(70)	10280(50)	90(20)
H(25)	9520(50)	10850(50)	9210(40)	52(15)

5.3. Cp*₂Yb(3,8-Me₂phen) (3)

Data collection

A fragment of a red block-like crystal of C₄₁H₅₀N₂Yb (Cp*₂Yb(3,8-Me₂phen)·C₇H₈) crystallized from toluene having approximate dimension of 0.20 x 0.20 x 0.08 mm was mounted on a Kapton loop using Paratone N hydrocarbon oil. All measurements were made on a Bruker APEX¹ CCD area detector with graphite monochromated Mo-K α radiation.

Cell constants and an orientation matrix, obtained from a least-squared refinement using the measured positions of 9854 reflexions with $I > 10\sigma$ in the range $4.48 < 2\theta < 50.70$ corresponded to a primitive monoclinic cell with dimensions:

$$\begin{aligned} a &= 9.4244(13) \text{ \AA} & \alpha &= 83.002(2)^\circ \\ b &= 13.0969(18) \text{ \AA} & \beta &= 77.287(2)^\circ \\ c &= 14.5221(19) \text{ \AA} & \gamma &= 78.976(2)^\circ \\ V &= 1710.3(4) \text{ \AA}^3 \end{aligned}$$

For $Z = 2$ and F.W. = 743.87, the calculated density is 1.444 g cm^{-3} . Based on a statistical analysis of intensity distribution, and successful solution and refinement of the structure, the space group was determined to be

$$P - 1 (\#2)$$

The data were collected at a temperature of $-173(1)^\circ\text{C}$. Frames corresponding to an arbitrary hemisphere of data were collected using ω scans of 0.3° counted for a total of 10.0s per frame.

Data reduction

Data were integrated by the program SAINT² to a maximum 2θ value of 50.70° . The data were corrected for Lorentz and polarization effects. Data were analyzed for agreement and possible absorption using XPREP.³ A semi-empirical multi-scan absorption correction⁴ was applied using SADABS.⁵ This models the absorption surface using a spherical harmonic series based on differences between equivalent.

Structure solution and refinement

The structure was solved by direct methods.⁶ Non-hydrogen atoms were refined anisotropically and hydrogen atoms were placed in calculated positions and not refined. The final cycle of full matrix least squares refinement was based on 6213 observed reflections ($I > 2.00 \sigma(I)$) and 394 parameters and converged with unweighted and weighted agreement factors of:

$$R = \sum ||F_o| - |F_c|| / \sum |F_o| = 0.0369$$

$$R_w = [(\sum w (|F_o| - |F_c|)^2 / \sum w F_o^2)]^{1/2} = 0.0844$$

The standard deviation of an observation of unit weight was 1.070. The weighting scheme was based on counting statistics and include a factor p to downweight the intense

reflections ($w=1/[\sigma^2F_o^2+(0.0188P)^2+(10.30P)]$ where $P=(\text{Max}(F_o^2,0)+2F_c^2)/3$). Plot of $\Sigma w (|F_o| - |F_c|)^2$ versus $|F_o|$, reflexion order in data collection, $\sin \theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.235 and -1.252 e.A⁻³, respectively.

The SHELX program uses the neutral atom scattering factors, f' , f'' and absorption coefficients from International Tables for Crystallography, Volume C (1992), Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht: Tables 6.1.1.4(pp. 500-502), 4.2.6.8 (pp.219-222) and 4.2.4.2 (pp. 193-199), respectively. All calculations were performed using the WinGX crystallographic software package.⁷ (“WinGX suite for small molecule single-crystal crystallography”).

Figure S22. ORTEP of $\text{Cp}^*_2\text{Yb}(3,8\text{-Me}_2\text{phen})$ (**3**) when C(28) atom is forced to remain in the plane of the phenanthroline (*FLAT N2 C31 C27 C28 C29 C30*) (50% probability ellipsoids).

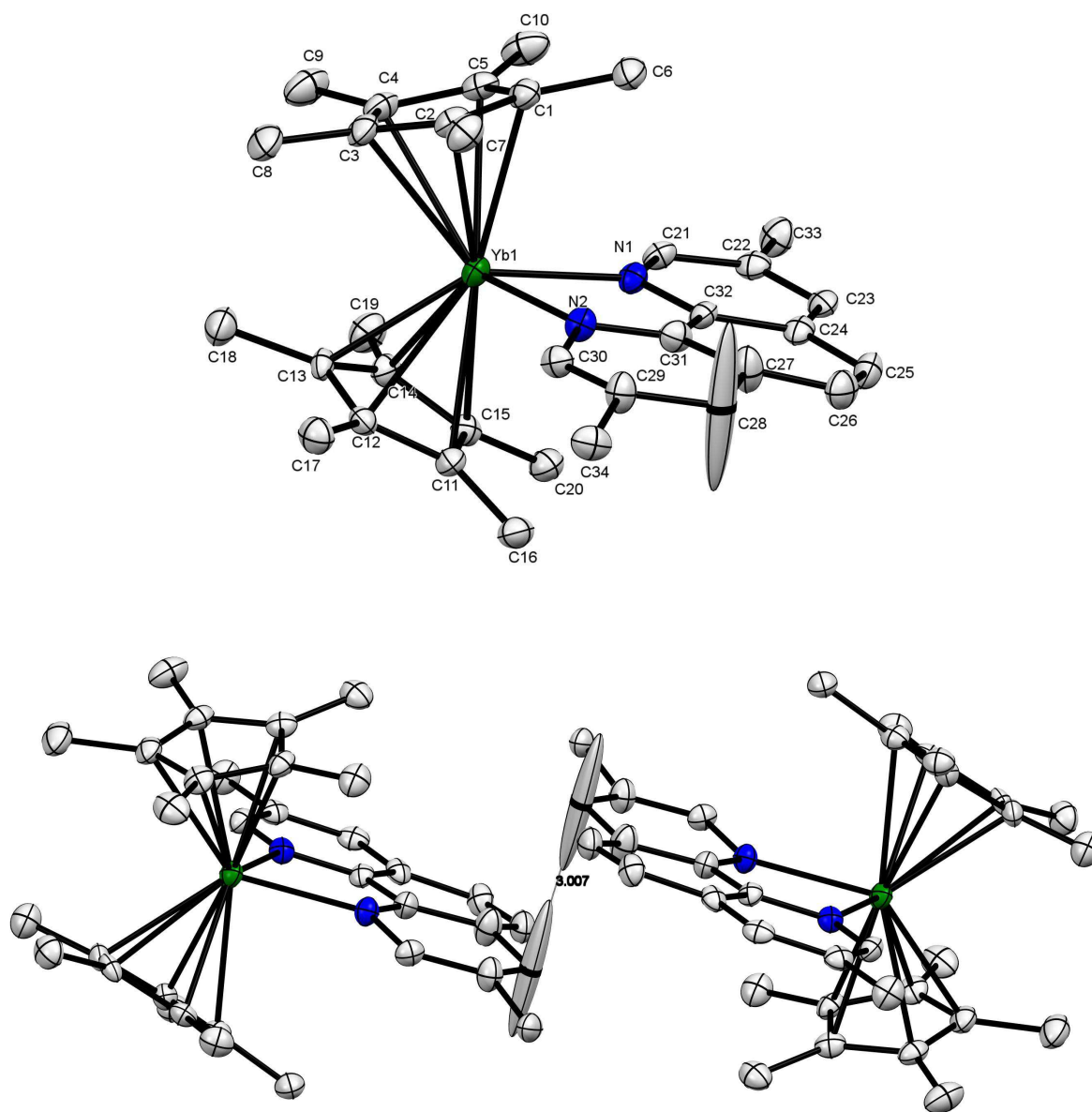


Figure S23. ORTEP of $\text{Cp}^*_2\text{Yb}(3,8\text{-Me}_2\text{phen})$ (**3**) when a position disorder for C(28) is allowed (50% probability ellipsoids).

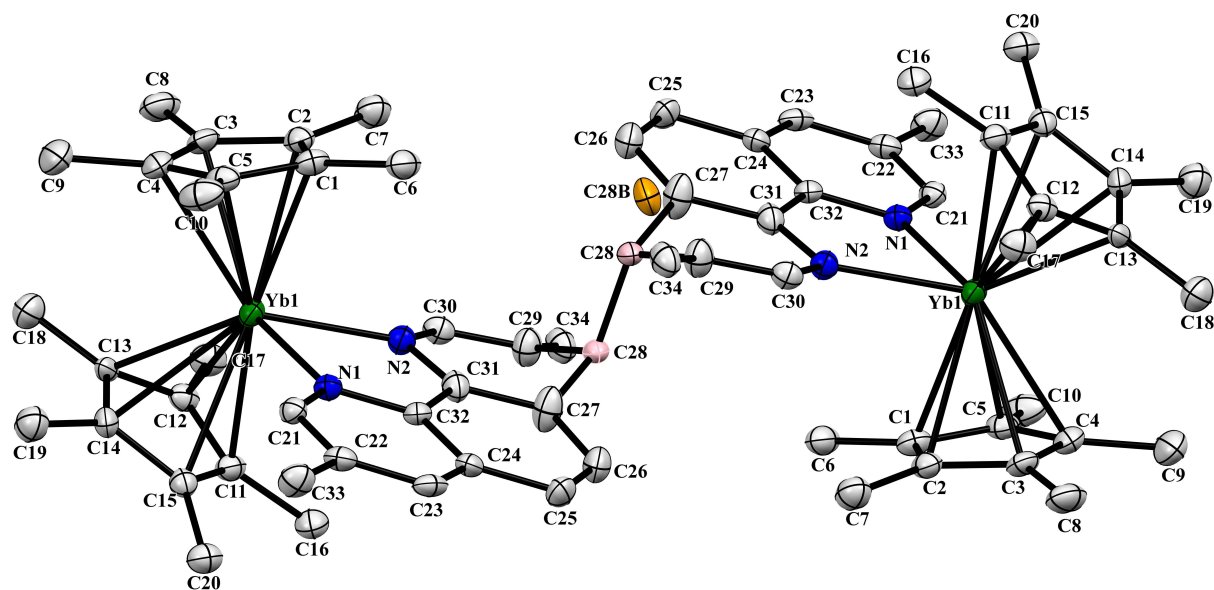


Table S11. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cp}^*_2\text{Yb}(\text{3,8-Me}_2\text{phen})$ (**3**). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Yb(1)	6979(1)	7917(1)	7415(1)	18(1)
N(2)	6359(4)	6841(3)	8765(3)	20(1)
N(1)	4493(4)	8524(3)	8123(3)	18(1)
C(15)	7191(5)	9622(4)	8166(3)	19(1)
C(2)	7290(6)	6211(4)	6560(3)	20(1)
C(11)	8030(5)	8769(4)	8620(3)	20(1)
C(21)	3570(5)	9339(4)	7817(3)	18(1)
C(13)	9165(5)	8943(4)	7051(3)	18(1)
C(32)	3999(5)	7991(4)	8981(3)	17(1)
C(12)	9237(5)	8343(4)	7936(3)	18(1)
C(5)	5937(6)	7683(4)	5939(3)	21(1)
C(14)	7908(6)	9729(4)	7196(3)	21(1)
C(30)	7295(5)	6083(4)	9195(3)	19(1)
C(3)	8294(6)	6812(4)	5957(3)	22(1)
C(16)	7697(6)	8453(4)	9672(3)	25(1)
C(6)	4436(6)	6353(4)	7054(4)	27(1)
C(1)	5831(6)	6745(4)	6545(4)	21(1)
C(20)	5893(6)	10360(4)	8659(4)	25(1)
C(23)	1653(6)	9159(4)	9160(3)	20(1)
C(25)	2126(6)	7751(4)	10415(4)	24(1)
C(24)	2570(5)	8316(4)	9526(3)	19(1)
C(33)	1173(6)	10600(4)	7892(4)	26(1)
C(31)	4962(6)	7102(4)	9293(3)	21(1)
C(7)	7712(6)	5160(4)	7054(4)	28(1)
C(34)	7974(6)	4751(4)	10486(4)	25(1)
C(22)	2132(6)	9691(4)	8294(3)	20(1)
C(17)	10439(6)	7438(4)	8097(4)	26(1)
C(8)	9932(6)	6437(5)	5659(4)	32(1)
C(4)	7447(6)	7712(4)	5576(3)	24(1)
C(18)	10401(6)	8890(4)	6197(4)	29(1)
C(29)	6894(6)	5470(4)	9993(4)	26(1)
C(10)	4692(7)	8433(4)	5626(4)	33(1)
C(27)	4437(6)	6532(4)	10141(4)	30(1)
C(19)	7497(6)	10617(4)	6494(4)	29(1)
C(9)	7990(7)	8468(5)	4765(4)	35(1)
C(26)	3043(6)	6900(4)	10701(4)	27(1)
C(2S)	5421(7)	6475(4)	3702(4)	34(1)
C(7S)	6787(7)	6244(5)	3959(5)	40(2)
C(3S)	5373(9)	6808(5)	2758(4)	44(2)
C(1S)	4037(7)	6351(5)	4405(5)	45(2)
C(6S)	8072(8)	6321(5)	3301(5)	50(2)
C(5S)	8005(11)	6639(5)	2362(6)	66(3)
C(4S)	6626(10)	6884(5)	2102(5)	56(2)
CT02	8307	9080	7794	10
CT01	6959	7032	6115	10
C(28)	5253(8)	5399(6)	10277(5)	18(2)
C(28B)	5470(20)	5863(14)	10611(13)	31(4)

Table S12. Bond lengths [Å] and angles [°] for Cp*₂Yb(3,8-Me₂phen) (**3**).

Yb(1)-N(2)	2.304(4)	C(4)-C(9)	1.509(7)
Yb(1)-CT02	2.3292(3)	C(29)-C(28B)	1.478(18)
Yb(1)-CT01	2.3377(3)	C(29)-C(28)	1.529(9)
Yb(1)-N(1)	2.367(4)	C(27)-C(26)	1.415(8)
Yb(1)-C(12)	2.584(5)	C(27)-C(28B)	1.417(19)
Yb(1)-C(13)	2.596(4)	C(27)-C(28)	1.547(9)
Yb(1)-C(1)	2.614(5)	C(2S)-C(7S)	1.387(9)
Yb(1)-C(5)	2.619(5)	C(2S)-C(3S)	1.394(8)
Yb(1)-C(2)	2.624(5)	C(2S)-C(1S)	1.492(9)
Yb(1)-C(11)	2.636(5)	C(7S)-C(6S)	1.380(9)
Yb(1)-C(14)	2.644(5)	C(3S)-C(4S)	1.355(10)
Yb(1)-C(4)	2.648(5)	C(6S)-C(5S)	1.389(11)
Yb(1)-C(3)	2.651(5)	C(5S)-C(4S)	1.400(12)
Yb(1)-C(15)	2.659(5)	C(28)-C(28)#1	1.592(16)
N(2)-C(31)	1.374(6)		
N(2)-C(30)	1.381(6)	N(2)-Yb(1)-CT02	107.03(10)
N(1)-C(21)	1.339(6)	N(2)-Yb(1)-CT01	107.72(10)
N(1)-C(32)	1.384(6)	CT02-Yb(1)-CT01	138.196(10)
C(15)-CT02	1.208(5)	N(2)-Yb(1)-N(1)	72.13(14)
C(15)-C(11)	1.422(7)	CT02-Yb(1)-N(1)	104.75(9)
C(15)-C(14)	1.425(7)	CT01-Yb(1)-N(1)	107.46(10)
C(15)-C(20)	1.508(7)	N(2)-Yb(1)-C(12)	93.47(15)
C(2)-CT01	1.209(5)	CT02-Yb(1)-C(12)	27.76(11)
C(2)-C(1)	1.422(7)	CT01-Yb(1)-C(12)	127.88(11)
C(2)-C(3)	1.426(7)	N(1)-Yb(1)-C(12)	124.42(14)
C(2)-C(7)	1.498(7)	N(2)-Yb(1)-C(13)	125.49(15)
C(11)-CT02	1.208(5)	CT02-Yb(1)-C(13)	27.70(10)
C(11)-C(12)	1.410(7)	CT01-Yb(1)-C(13)	110.72(11)
C(11)-C(16)	1.512(7)	N(1)-Yb(1)-C(13)	127.43(14)
C(21)-C(22)	1.399(7)	C(12)-Yb(1)-C(13)	32.04(16)
C(13)-CT02	1.207(5)	N(2)-Yb(1)-C(1)	86.88(15)
C(13)-C(14)	1.409(7)	CT02-Yb(1)-C(1)	165.15(11)
C(13)-C(12)	1.430(7)	CT01-Yb(1)-C(1)	27.57(11)
C(13)-C(18)	1.502(7)	N(1)-Yb(1)-C(1)	84.17(14)
C(32)-C(24)	1.419(7)	C(12)-Yb(1)-C(1)	150.05(15)
C(32)-C(31)	1.425(7)	C(13)-Yb(1)-C(1)	138.23(15)
C(12)-CT02	1.205(5)	N(2)-Yb(1)-C(5)	117.12(15)
C(12)-C(17)	1.510(7)	CT02-Yb(1)-C(5)	135.64(11)
C(5)-CT01	1.208(5)	CT01-Yb(1)-C(5)	27.47(11)
C(5)-C(4)	1.410(7)	N(1)-Yb(1)-C(5)	85.58(15)
C(5)-C(1)	1.427(7)	C(12)-Yb(1)-C(5)	143.67(16)
C(5)-C(10)	1.495(7)	C(13)-Yb(1)-C(5)	114.91(16)
C(14)-CT02	1.207(5)	C(1)-Yb(1)-C(5)	31.66(15)
C(14)-C(19)	1.502(7)	N(2)-Yb(1)-C(2)	83.53(14)
C(30)-C(29)	1.352(7)	CT02-Yb(1)-C(2)	142.59(11)
C(3)-CT01	1.213(5)	CT01-Yb(1)-C(2)	27.44(11)
C(3)-C(4)	1.417(7)	N(1)-Yb(1)-C(2)	112.62(15)
C(3)-C(8)	1.510(7)	C(12)-Yb(1)-C(2)	118.75(16)
C(6)-C(1)	1.508(7)	C(13)-Yb(1)-C(2)	118.05(15)
C(1)-CT01	1.210(5)	C(1)-Yb(1)-C(2)	31.50(16)
C(23)-C(22)	1.388(7)	C(5)-Yb(1)-C(2)	52.08(16)
C(23)-C(24)	1.394(7)	N(2)-Yb(1)-C(11)	80.00(15)
C(25)-C(26)	1.355(8)	CT02-Yb(1)-C(11)	27.27(11)
C(25)-C(24)	1.428(7)	CT01-Yb(1)-C(11)	159.20(11)
C(33)-C(22)	1.492(7)	N(1)-Yb(1)-C(11)	93.26(14)
C(31)-C(27)	1.403(7)	C(12)-Yb(1)-C(11)	31.32(15)
C(34)-C(29)	1.491(7)	C(13)-Yb(1)-C(11)	52.11(15)
C(4)-CT01	1.202(5)	C(1)-Yb(1)-C(11)	166.78(15)

C(5)-Yb(1)-C(11)	161.25(16)	CT02-C(15)-Yb(1)	61.09(19)
C(2)-Yb(1)-C(11)	143.19(16)	C(11)-C(15)-Yb(1)	73.5(3)
N(2)-Yb(1)-C(14)	130.34(15)	C(14)-C(15)-Yb(1)	73.8(3)
CT02-Yb(1)-C(14)	27.17(11)	C(20)-C(15)-Yb(1)	124.5(3)
CT01-Yb(1)-C(14)	121.53(11)	CT01-C(2)-C(1)	54.0(3)
N(1)-Yb(1)-C(14)	97.27(14)	CT01-C(2)-C(3)	54.0(3)
C(12)-Yb(1)-C(14)	52.05(16)	C(1)-C(2)-C(3)	108.1(4)
C(13)-Yb(1)-C(14)	31.17(15)	CT01-C(2)-C(7)	176.3(5)
C(1)-Yb(1)-C(14)	141.52(16)	C(1)-C(2)-C(7)	126.4(5)
C(5)-Yb(1)-C(14)	109.89(16)	C(3)-C(2)-C(7)	125.3(5)
C(2)-Yb(1)-C(14)	141.43(15)	CT01-C(2)-Yb(1)	63.0(2)
C(11)-Yb(1)-C(14)	51.64(15)	C(1)-C(2)-Yb(1)	73.9(3)
N(2)-Yb(1)-C(4)	134.47(15)	C(3)-C(2)-Yb(1)	75.3(3)
CT02-Yb(1)-C(4)	113.47(11)	C(7)-C(2)-Yb(1)	120.7(3)
CT01-Yb(1)-C(4)	26.98(11)	CT02-C(11)-C(12)	54.1(3)
N(1)-Yb(1)-C(4)	114.71(16)	CT02-C(11)-C(15)	54.0(3)
C(12)-Yb(1)-C(4)	113.02(16)	C(12)-C(11)-C(15)	108.1(4)
C(13)-Yb(1)-C(4)	87.62(16)	CT02-C(11)-C(16)	176.0(5)
C(1)-Yb(1)-C(4)	51.67(15)	C(12)-C(11)-C(16)	127.7(5)
C(5)-Yb(1)-C(4)	31.06(16)	C(15)-C(11)-C(16)	124.1(4)
C(2)-Yb(1)-C(4)	51.57(15)	CT02-C(11)-Yb(1)	62.1(2)
C(11)-Yb(1)-C(4)	139.73(15)	C(12)-C(11)-Yb(1)	72.3(3)
C(14)-Yb(1)-C(4)	94.54(15)	C(15)-C(11)-Yb(1)	75.3(3)
N(2)-Yb(1)-C(3)	110.93(15)	C(16)-C(11)-Yb(1)	121.5(3)
CT02-Yb(1)-C(3)	116.20(11)	N(1)-C(21)-C(22)	125.0(4)
CT01-Yb(1)-C(3)	27.22(11)	CT02-C(13)-C(14)	54.3(3)
N(1)-Yb(1)-C(3)	134.66(15)	CT02-C(13)-C(12)	53.6(3)
C(12)-Yb(1)-C(3)	100.85(16)	C(14)-C(13)-C(12)	107.9(4)
C(13)-Yb(1)-C(3)	89.01(15)	CT02-C(13)-C(18)	169.3(5)
C(1)-Yb(1)-C(3)	51.92(15)	C(14)-C(13)-C(18)	126.2(5)
C(5)-Yb(1)-C(3)	51.74(16)	C(12)-C(13)-C(18)	124.5(5)
C(2)-Yb(1)-C(3)	31.37(15)	CT02-C(13)-Yb(1)	63.76(19)
C(11)-Yb(1)-C(3)	132.09(16)	C(14)-C(13)-Yb(1)	76.3(3)
C(14)-Yb(1)-C(3)	110.09(15)	C(12)-C(13)-Yb(1)	73.5(3)
C(4)-Yb(1)-C(3)	31.02(16)	C(18)-C(13)-Yb(1)	126.8(3)
N(2)-Yb(1)-C(15)	100.71(14)	N(1)-C(32)-C(24)	120.8(4)
CT02-Yb(1)-C(15)	27.00(11)	N(1)-C(32)-C(31)	117.9(4)
CT01-Yb(1)-C(15)	151.36(10)	C(24)-C(32)-C(31)	121.3(4)
N(1)-Yb(1)-C(15)	77.83(14)	N(1)-C(32)-Yb(1)	42.5(2)
C(12)-Yb(1)-C(15)	51.81(15)	C(24)-C(32)-Yb(1)	162.8(3)
C(13)-Yb(1)-C(15)	51.77(14)	C(31)-C(32)-Yb(1)	75.6(3)
C(1)-Yb(1)-C(15)	157.11(16)	CT02-C(12)-C(11)	54.4(3)
C(5)-Yb(1)-C(15)	131.38(15)	CT02-C(12)-C(13)	53.7(3)
C(2)-Yb(1)-C(15)	169.54(15)	C(11)-C(12)-C(13)	108.1(4)
C(11)-Yb(1)-C(15)	31.14(15)	CT02-C(12)-C(17)	178.3(5)
C(14)-Yb(1)-C(15)	31.17(14)	C(11)-C(12)-C(17)	126.9(5)
C(4)-Yb(1)-C(15)	124.81(15)	C(13)-C(12)-C(17)	125.0(4)
C(3)-Yb(1)-C(15)	139.80(15)	CT02-C(12)-Yb(1)	64.3(2)
C(31)-N(2)-C(30)	115.4(4)	C(11)-C(12)-Yb(1)	76.4(3)
C(31)-N(2)-Yb(1)	116.0(3)	C(13)-C(12)-Yb(1)	74.4(3)
C(30)-N(2)-Yb(1)	127.5(3)	C(17)-C(12)-Yb(1)	117.0(3)
C(21)-N(1)-C(32)	117.8(4)	CT01-C(5)-C(4)	54.0(3)
C(21)-N(1)-Yb(1)	127.8(3)	CT01-C(5)-C(1)	53.9(3)
C(32)-N(1)-Yb(1)	114.2(3)	C(4)-C(5)-C(1)	107.8(4)
CT02-C(15)-C(11)	54.0(3)	CT01-C(5)-C(10)	173.9(5)
CT02-C(15)-C(14)	53.8(3)	C(4)-C(5)-C(10)	124.9(5)
C(11)-C(15)-C(14)	107.8(4)	C(1)-C(5)-C(10)	126.8(5)
CT02-C(15)-C(20)	174.4(5)	CT01-C(5)-Yb(1)	63.2(2)
C(11)-C(15)-C(20)	125.4(4)	C(4)-C(5)-Yb(1)	75.6(3)
C(14)-C(15)-C(20)	126.4(5)	C(1)-C(5)-Yb(1)	74.0(3)

C(10)-C(5)-Yb(1)	122.8(3)	C(30)-C(29)-C(28)	115.8(5)
CT02-C(14)-C(13)	54.3(3)	C(28B)-C(29)-C(28)	34.8(7)
CT02-C(14)-C(15)	53.9(3)	C(34)-C(29)-C(28)	119.9(5)
C(13)-C(14)-C(15)	108.2(4)	C(31)-C(27)-C(26)	119.8(5)
CT02-C(14)-C(19)	173.6(5)	C(31)-C(27)-C(28B)	118.6(8)
C(13)-C(14)-C(19)	126.3(4)	C(26)-C(27)-C(28B)	117.0(8)
C(15)-C(14)-C(19)	125.1(5)	C(31)-C(27)-C(28)	115.9(5)
CT02-C(14)-Yb(1)	61.74(19)	C(26)-C(27)-C(28)	122.5(5)
C(13)-C(14)-Yb(1)	72.5(3)	C(28B)-C(27)-C(28)	35.1(8)
C(15)-C(14)-Yb(1)	75.0(3)	C(25)-C(26)-C(27)	122.3(5)
C(19)-C(14)-Yb(1)	124.6(3)	C(7S)-C(2S)-C(3S)	118.2(6)
C(29)-C(30)-N(2)	125.9(5)	C(7S)-C(2S)-C(1S)	121.3(6)
CT01-C(3)-C(4)	53.7(3)	C(3S)-C(2S)-C(1S)	120.5(6)
CT01-C(3)-C(2)	53.8(3)	C(6S)-C(7S)-C(2S)	121.3(6)
C(4)-C(3)-C(2)	107.5(4)	C(4S)-C(3S)-C(2S)	121.2(7)
CT01-C(3)-C(8)	171.8(5)	C(7S)-C(6S)-C(5S)	119.6(8)
C(4)-C(3)-C(8)	127.1(5)	C(6S)-C(5S)-C(4S)	119.1(7)
C(2)-C(3)-C(8)	124.6(5)	C(3S)-C(4S)-C(5S)	120.5(7)
CT01-C(3)-Yb(1)	61.86(19)	C(12)-CT02-C(13)	72.7(3)
C(4)-C(3)-Yb(1)	74.4(3)	C(12)-CT02-C(14)	144.1(3)
C(2)-C(3)-Yb(1)	73.3(3)	C(13)-CT02-C(14)	71.4(3)
C(8)-C(3)-Yb(1)	126.2(3)	C(12)-CT02-C(15)	143.6(3)
CT01-C(1)-C(2)	54.0(3)	C(13)-CT02-C(15)	143.7(3)
CT01-C(1)-C(5)	53.8(3)	C(14)-CT02-C(15)	72.3(3)
C(2)-C(1)-C(5)	107.8(4)	C(12)-CT02-C(11)	71.5(3)
CT01-C(1)-C(6)	177.7(5)	C(13)-CT02-C(11)	144.2(3)
C(2)-C(1)-C(6)	125.3(5)	C(14)-CT02-C(11)	144.4(3)
C(5)-C(1)-C(6)	126.9(5)	C(15)-CT02-C(11)	72.1(3)
CT01-C(1)-Yb(1)	63.4(2)	C(12)-CT02-Yb(1)	88.0(2)
C(2)-C(1)-Yb(1)	74.6(3)	C(13)-CT02-Yb(1)	88.5(2)
C(5)-C(1)-Yb(1)	74.4(3)	C(14)-CT02-Yb(1)	91.1(2)
C(6)-C(1)-Yb(1)	118.8(3)	C(15)-CT02-Yb(1)	91.9(2)
C(22)-C(23)-C(24)	121.1(5)	C(11)-CT02-Yb(1)	90.7(2)
C(26)-C(25)-C(24)	119.8(5)	C(4)-CT01-C(5)	71.6(4)
C(23)-C(24)-C(32)	118.6(4)	C(4)-CT01-C(2)	144.0(4)
C(23)-C(24)-C(25)	123.0(5)	C(5)-CT01-C(2)	144.3(3)
C(32)-C(24)-C(25)	118.5(5)	C(4)-CT01-C(1)	144.0(4)
N(2)-C(31)-C(27)	122.5(5)	C(5)-CT01-C(1)	72.4(3)
N(2)-C(31)-C(32)	119.5(4)	C(2)-CT01-C(1)	72.0(3)
C(27)-C(31)-C(32)	118.0(5)	C(4)-CT01-C(3)	71.9(4)
N(2)-C(31)-Yb(1)	41.0(2)	C(5)-CT01-C(3)	143.5(3)
C(27)-C(31)-Yb(1)	163.5(4)	C(2)-CT01-C(3)	72.1(3)
C(32)-C(31)-Yb(1)	78.5(3)	C(1)-CT01-C(3)	144.1(3)
C(23)-C(22)-C(21)	116.7(5)	C(4)-CT01-Yb(1)	91.1(2)
C(23)-C(22)-C(33)	122.0(5)	C(5)-CT01-Yb(1)	89.3(2)
C(21)-C(22)-C(33)	121.3(4)	C(2)-CT01-Yb(1)	89.6(2)
CT01-C(4)-C(5)	54.4(3)	C(1)-CT01-Yb(1)	89.0(2)
CT01-C(4)-C(3)	54.4(3)	C(3)-CT01-Yb(1)	90.9(2)
C(5)-C(4)-C(3)	108.8(4)	C(29)-C(28)-C(27)	105.2(5)
CT01-C(4)-C(9)	169.8(5)	C(29)-C(28)-C(28)#1	114.5(7)
C(5)-C(4)-C(9)	123.1(5)	C(27)-C(28)-C(28)#1	113.2(8)
C(3)-C(4)-C(9)	126.9(5)	C(27)-C(28B)-C(29)	115.1(12)
CT01-C(4)-Yb(1)	62.0(2)		
C(5)-C(4)-Yb(1)	73.3(3)		
C(3)-C(4)-Yb(1)	74.6(3)		
C(9)-C(4)-Yb(1)	128.0(3)		
C(30)-C(29)-C(28B)	115.8(8)		
C(30)-C(29)-C(34)	123.4(5)		
C(28B)-C(29)-C(34)	115.0(8)		

Symmetry transformations used to generate

equivalent atoms:

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

Table S13. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cp}^*_2\text{Yb}(3,8\text{-Me}_2\text{phen})$ (**3**). The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Yb(1)	19(1)	20(1)	14(1)	-1(1)	0(1)	-3(1)
N(2)	20(2)	17(2)	19(2)	-1(2)	-1(2)	-1(2)
N(1)	18(2)	16(2)	18(2)	-3(2)	-2(2)	-2(2)
C(15)	20(3)	18(2)	18(2)	0(2)	-5(2)	-5(2)
C(2)	27(3)	18(2)	15(2)	-3(2)	-4(2)	-1(2)
C(11)	19(3)	23(3)	19(2)	-7(2)	-1(2)	-5(2)
C(21)	23(3)	16(2)	14(2)	-1(2)	-4(2)	-2(2)
C(13)	16(2)	15(2)	20(2)	-6(2)	5(2)	-6(2)
C(32)	20(3)	16(2)	14(2)	-5(2)	-2(2)	-4(2)
C(12)	15(2)	19(2)	22(3)	-5(2)	-3(2)	-4(2)
C(5)	27(3)	21(2)	17(2)	-5(2)	-7(2)	-1(2)
C(14)	25(3)	19(2)	18(2)	1(2)	-1(2)	-10(2)
C(30)	18(3)	18(2)	22(3)	-3(2)	-5(2)	-1(2)
C(3)	23(3)	24(3)	17(2)	-9(2)	2(2)	-2(2)
C(16)	30(3)	27(3)	20(3)	-4(2)	-5(2)	-8(2)
C(6)	25(3)	30(3)	26(3)	-11(2)	1(2)	-9(2)
C(1)	20(3)	23(3)	19(2)	-7(2)	-3(2)	0(2)
C(20)	26(3)	26(3)	23(3)	-7(2)	-4(2)	-3(2)
C(23)	18(3)	22(2)	21(3)	-12(2)	-2(2)	-1(2)
C(25)	24(3)	23(3)	21(3)	-4(2)	5(2)	-4(2)
C(24)	23(3)	15(2)	19(2)	-6(2)	0(2)	-6(2)
C(33)	23(3)	25(3)	27(3)	-4(2)	-2(2)	3(2)
C(31)	25(3)	20(2)	19(2)	2(2)	-6(2)	-8(2)
C(7)	32(3)	25(3)	25(3)	-4(2)	-2(2)	0(2)
C(34)	33(3)	21(3)	24(3)	4(2)	-11(2)	-8(2)
C(22)	24(3)	17(2)	21(2)	-7(2)	-5(2)	-2(2)
C(17)	22(3)	27(3)	30(3)	-6(2)	-5(2)	-2(2)
C(8)	29(3)	36(3)	30(3)	-17(3)	4(3)	-5(3)
C(4)	32(3)	25(3)	14(2)	-4(2)	-2(2)	-7(2)
C(18)	28(3)	32(3)	26(3)	-5(2)	2(2)	-8(2)
C(29)	22(3)	28(3)	27(3)	2(2)	0(2)	-5(2)
C(10)	41(4)	32(3)	25(3)	-7(3)	-13(3)	6(3)
C(27)	21(3)	33(3)	29(3)	9(3)	-1(2)	0(2)
C(19)	33(3)	26(3)	25(3)	0(2)	-3(2)	-3(2)
C(9)	52(4)	33(3)	20(3)	-1(2)	-3(3)	-12(3)
C(26)	31(3)	28(3)	21(3)	2(2)	0(2)	-11(2)
C(2S)	46(4)	27(3)	29(3)	-7(3)	-4(3)	-7(3)
C(7S)	56(4)	29(3)	37(3)	-8(3)	-17(3)	-5(3)
C(3S)	74(5)	25(3)	32(3)	-2(3)	-16(3)	3(3)
C(1S)	50(4)	49(4)	37(4)	-9(3)	-6(3)	-14(3)
C(6S)	50(4)	35(3)	63(5)	-18(3)	-3(4)	-3(3)
C(5S)	87(7)	36(4)	64(5)	-22(4)	28(5)	-21(4)
C(4S)	89(6)	34(4)	34(4)	-3(3)	5(4)	-2(4)
C(28)	27(4)	16(4)	13(3)	-3(3)	-2(3)	-7(3)
C(28B)	40(11)	24(9)	31(9)	2(8)	-1(8)	-18(8)

Table S14. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cp}^*_2\text{Yb}(3,8\text{-Me}_2\text{phen})$ (**3**).

	x	y	z	U(eq)
H(21)	3911	9699	7243	22
H(30)	8291	5987	8909	23
H(16A)	6804	8880	9964	38
H(16B)	8497	8545	9947	38
H(16C)	7577	7734	9773	38
H(6A)	3595	6853	6934	40
H(6B)	4417	6258	7722	40
H(6C)	4409	5700	6828	40
H(20A)	5627	10106	9311	37
H(20B)	5072	10405	8356	37
H(20C)	6156	11039	8622	37
H(23)	704	9368	9502	24
H(25)	1211	7965	10796	28
H(33A)	1698	10858	7292	39
H(33B)	907	11142	8318	39
H(33C)	295	10384	7806	39
H(7A)	8768	4982	6952	42
H(7B)	7326	4647	6807	42
H(7C)	7312	5178	7721	42
H(34A)	7451	4393	11034	38
H(34B)	8602	5146	10678	38
H(34C)	8562	4251	10063	38
H(17A)	11121	7310	7509	40
H(17B)	10009	6826	8336	40
H(17C)	10953	7602	8547	40
H(8A)	10216	5808	6036	48
H(8B)	10460	6964	5747	48
H(8C)	10162	6301	5003	48
H(18A)	11120	8276	6275	44
H(18B)	10857	9498	6126	44
H(18C)	10016	8861	5643	44
H(10A)	3770	8255	5975	50
H(10B)	4752	8398	4961	50
H(10C)	4755	9129	5739	50
H(19A)	6591	11041	6771	43
H(19B)	7372	10345	5937	43
H(19C)	8266	11033	6324	43
H(9A)	9050	8355	4633	53
H(9B)	7617	9170	4933	53
H(9C)	7650	8362	4213	53
H(26)	2745	6545	11286	33
H(7S)	6838	6033	4588	48
H(3S)	4466	6980	2575	53
H(1S1)	3209	6540	4098	67
H(1S2)	3917	6796	4905	67
H(1S3)	4095	5638	4665	67
H(6S)	8979	6162	3486	60
H(5S)	8864	6688	1911	79
H(4S)	6569	7102	1476	68
H(28)	5030(60)	5300(50)	11010(40)	32(16)

$\text{Cp}^*_2\text{Yb}(5,6\text{-Me}_2\text{phen})$ (7), Sublimed.

A fragment of a dark-brown block-like crystal of $\text{C}_{34}\text{H}_{42}\text{N}_2\text{Yb}$ sublimed at 195 °C, having approximate dimensions of 0.11 x 0.07 x 0.04 mm was mounted on a Kapton loop using Paratone N hydrocarbon oil. It was transferred to a APEX II QUAZAR diffractometer with CCD area detector,¹ centered in the beam, and the crystal was cooled during data collection by a nitrogen flow low-temperature apparatus previously calibrated by a thermocouple placed at the same position as the crystal ($T = 100 \text{ K}$). Preliminary orientation matrixes and cell constants were determined by collection of 36 10 s frames, followed by spot integration and least-squares refinement. A data collection strategy was computed with COSMO to ensure a redundant and complete data set, and the raw data were integrated using SAINT.² The data were corrected for Lorentz and polarization effects, but no correction for crystal decay was applied. An empirical absorption correction based on comparison of redundant and equivalent reflections was applied using SADABS.⁵ XPREP³ was used to determinate the space group. The structures were solved using SIR-97⁸ and refined on all data by full-matrix least-squares with SHELXL-97.⁶ Thermal parameters for all non-hydrogen atoms were refined anisotropically. Hydrogen atoms were found in the Fourier map and refined isotropically.

Figure S24. ORTEP of $\text{Cp}^*_2\text{Yb}(5,6\text{-Me}_2\text{phen})$ (7), Sublimed (50% probability ellipsoids).

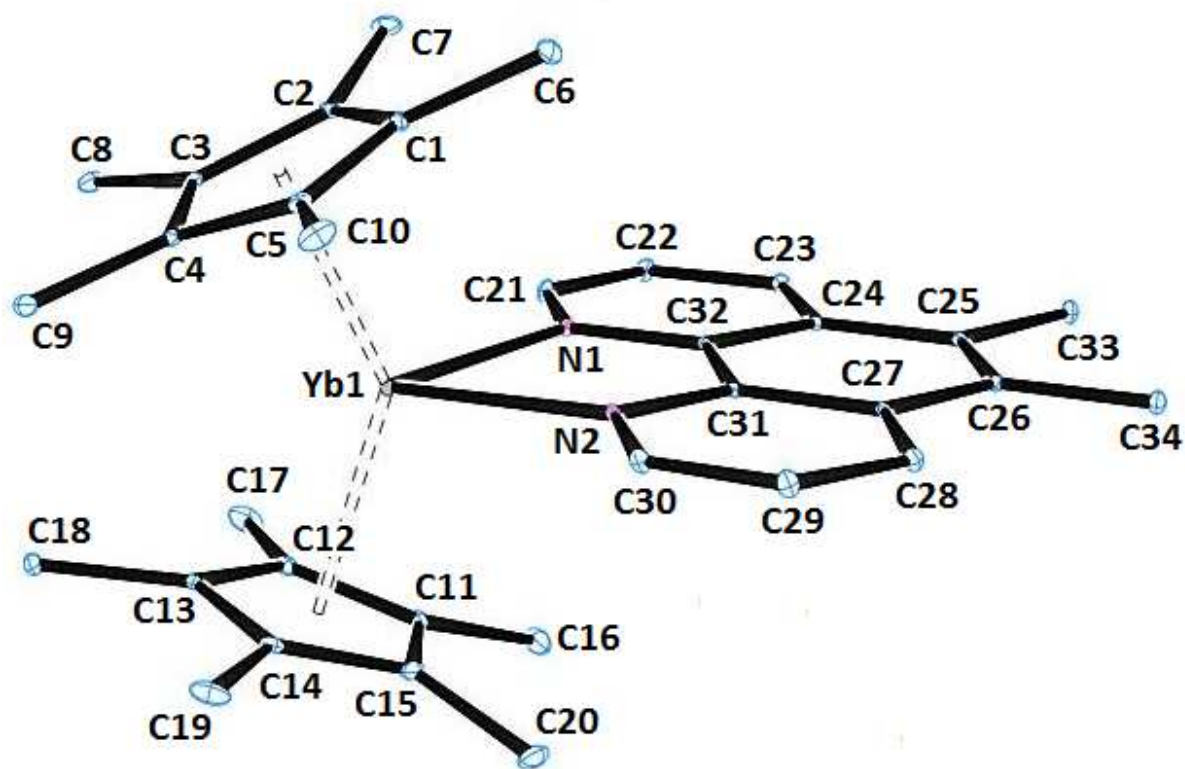


Table S15. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cp}^*_2\text{Yb}(5,6\text{-Me}_2\text{phen})$ (7), Sublimed. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8109(4)	2203(2)	2899(2)	27(1)
C(2)	6861(3)	1843(2)	2582(2)	26(1)
C(3)	7181(3)	1052(2)	2475(2)	22(1)
C(4)	8633(3)	919(2)	2731(2)	22(1)
C(5)	9215(3)	1627(2)	2989(2)	27(1)
C(6)	8202(6)	3037(2)	3136(2)	52(1)
C(7)	5379(4)	2229(2)	2461(2)	45(1)
C(8)	6100(4)	459(2)	2193(2)	37(1)
C(9)	9388(4)	149(2)	2834(2)	38(1)
C(10)	10692(4)	1708(3)	3373(2)	47(1)
C(11)	9495(4)	1649(2)	214(2)	35(1)
C(12)	8616(4)	990(2)	406(2)	29(1)
C(13)	9500(3)	529(2)	863(2)	24(1)
C(14)	10872(4)	908(2)	968(2)	31(1)
C(15)	10861(4)	1583(2)	560(2)	36(1)
C(16)	9076(6)	2249(2)	-344(2)	61(1)
C(17)	7127(4)	772(3)	101(2)	54(1)
C(18)	9135(5)	-292(2)	1068(2)	42(1)
C(19)	12200(4)	611(3)	1400(2)	54(1)
C(20)	12178(5)	2113(3)	437(3)	62(1)
C(21)	6223(3)	2754(2)	805(2)	26(1)
C(22)	5495(3)	3349(2)	476(2)	25(1)
C(23)	6158(3)	4086(2)	441(2)	23(1)
C(24)	7609(3)	4181(2)	757(1)	16(1)
C(25)	8374(3)	4907(2)	754(2)	19(1)
C(26)	9773(3)	4968(2)	1050(2)	19(1)
C(27)	10469(3)	4311(2)	1376(2)	17(1)
C(28)	11910(3)	4339(2)	1694(2)	26(1)
C(29)	12489(3)	3674(2)	2007(2)	30(1)
C(30)	11683(3)	2997(2)	1990(2)	25(1)
C(31)	9712(3)	3590(2)	1392(1)	16(1)
C(32)	8268(3)	3527(2)	1086(1)	16(1)
C(33)	7623(4)	5601(2)	419(2)	27(1)
C(34)	10579(3)	5738(2)	1044(2)	26(1)
N(1)	7587(3)	2811(1)	1118(1)	18(1)
N(2)	10314(3)	2934(1)	1693(1)	19(1)
Yb(1)	8926(1)	1803(1)	1592(1)	16(1)

Table S16. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cp}^*_2\text{Yb}(5,6\text{-Me}_2\text{phen})$ (7), Sublimed. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	46(2)	20(2)	16(2)	-1(1)	7(1)	3(1)
C(2)	25(2)	32(2)	20(2)	6(1)	5(1)	13(1)
C(3)	22(2)	25(2)	19(1)	3(1)	5(1)	0(1)
C(4)	24(2)	23(2)	20(2)	7(1)	6(1)	7(1)
C(5)	27(2)	39(2)	16(1)	4(1)	-2(1)	-2(1)
C(6)	93(3)	31(2)	33(2)	-9(2)	19(2)	-2(2)
C(7)	39(2)	59(3)	38(2)	15(2)	13(2)	27(2)
C(8)	32(2)	49(2)	30(2)	-4(2)	8(1)	-12(2)
C(9)	45(2)	39(2)	30(2)	16(2)	11(2)	21(2)
C(10)	38(2)	79(3)	25(2)	8(2)	-10(2)	-14(2)
C(11)	64(2)	21(2)	20(2)	2(1)	13(2)	9(2)
C(12)	36(2)	30(2)	22(2)	-10(1)	-2(1)	3(1)
C(13)	32(2)	18(2)	21(2)	-3(1)	11(1)	1(1)
C(14)	25(2)	36(2)	30(2)	-12(2)	7(1)	3(1)
C(15)	38(2)	34(2)	35(2)	-12(2)	16(2)	-11(2)
C(16)	108(4)	42(2)	32(2)	12(2)	20(2)	27(2)
C(17)	44(2)	66(3)	51(2)	-30(2)	-14(2)	6(2)
C(18)	68(3)	19(2)	39(2)	-2(2)	22(2)	0(2)
C(19)	33(2)	79(3)	50(2)	-16(2)	-1(2)	23(2)
C(20)	61(3)	60(3)	66(3)	-22(2)	38(2)	-32(2)
C(21)	24(2)	24(2)	31(2)	5(1)	-7(1)	-7(1)
C(22)	17(1)	28(2)	30(2)	5(1)	-10(1)	-3(1)
C(23)	20(2)	25(2)	24(2)	0(1)	-4(1)	2(1)
C(24)	18(1)	18(1)	14(1)	-1(1)	2(1)	1(1)
C(25)	24(2)	17(1)	15(1)	1(1)	2(1)	2(1)
C(26)	24(2)	16(1)	16(1)	0(1)	3(1)	-3(1)
C(27)	14(1)	17(1)	20(1)	-3(1)	2(1)	0(1)
C(28)	20(2)	22(2)	36(2)	-2(1)	-4(1)	-1(1)
C(29)	17(2)	29(2)	44(2)	-3(2)	-10(1)	-1(1)
C(30)	20(2)	23(2)	34(2)	0(1)	-8(1)	5(1)
C(31)	16(1)	15(1)	16(1)	-2(1)	0(1)	2(1)
C(32)	17(1)	16(1)	16(1)	-2(1)	2(1)	2(1)
C(33)	30(2)	19(2)	33(2)	6(1)	-3(1)	0(1)
C(34)	26(2)	19(2)	35(2)	3(1)	-2(1)	-4(1)
N(1)	17(1)	17(1)	19(1)	2(1)	-2(1)	-3(1)
N(2)	17(1)	17(1)	22(1)	-1(1)	-4(1)	3(1)
Yb(1)	20(1)	13(1)	16(1)	1(1)	0(1)	1(1)

Table S17. Bond lengths [\AA] for $\text{Cp}^*_2\text{Yb}(5,6\text{-Me}_2\text{phen})$ (7), Sublimed.

C(1)-C(2)	1.411(5)	C(16)-H(16C)	0.9800
C(1)-C(5)	1.418(5)	C(17)-H(17A)	0.9800
C(1)-C(6)	1.509(5)	C(17)-H(17B)	0.9800
C(1)-Yb(1)	2.624(3)	C(17)-H(17C)	0.9800
C(2)-C(3)	1.412(4)	C(18)-H(18A)	0.9800
C(2)-C(7)	1.509(4)	C(18)-H(18B)	0.9800
C(2)-Yb(1)	2.618(3)	C(18)-H(18C)	0.9800
C(3)-C(4)	1.408(4)	C(19)-H(19A)	0.9800
C(3)-C(8)	1.506(4)	C(19)-H(19B)	0.9800
C(3)-Yb(1)	2.618(3)	C(19)-H(19C)	0.9800
C(4)-C(5)	1.414(5)	C(20)-H(20A)	0.9800
C(4)-C(9)	1.507(4)	C(20)-H(20B)	0.9800
C(4)-Yb(1)	2.618(3)	C(20)-H(20C)	0.9800
C(5)-C(10)	1.512(5)	C(21)-N(1)	1.361(4)
C(5)-Yb(1)	2.617(3)	C(21)-C(22)	1.362(4)
C(6)-H(6A)	0.9800	C(21)-H(21)	0.9500
C(6)-H(6B)	0.9800	C(22)-C(23)	1.408(4)
C(6)-H(6C)	0.9800	C(22)-H(22)	0.9500
C(7)-H(7A)	0.9800	C(23)-C(24)	1.439(4)
C(7)-H(7B)	0.9800	C(23)-H(23)	0.9500
C(7)-H(7C)	0.9800	C(24)-C(32)	1.414(4)
C(8)-H(8A)	0.9800	C(24)-C(25)	1.433(4)
C(8)-H(8B)	0.9800	C(25)-C(26)	1.377(4)
C(8)-H(8C)	0.9800	C(25)-C(33)	1.508(4)
C(9)-H(9A)	0.9800	C(26)-C(27)	1.430(4)
C(9)-H(9B)	0.9800	C(26)-C(34)	1.516(4)
C(9)-H(9C)	0.9800	C(27)-C(31)	1.421(4)
C(10)-H(10A)	0.9800	C(27)-C(28)	1.425(4)
C(10)-H(10B)	0.9800	C(28)-C(29)	1.388(4)
C(10)-H(10C)	0.9800	C(28)-H(28)	0.9500
C(11)-C(15)	1.389(5)	C(29)-C(30)	1.378(4)
C(11)-C(12)	1.433(5)	C(29)-H(29)	0.9500
C(11)-C(16)	1.511(5)	C(30)-N(2)	1.353(4)
C(11)-Yb(1)	2.618(3)	C(30)-H(30)	0.9500
C(12)-C(13)	1.406(5)	C(31)-N(2)	1.374(4)
C(12)-C(17)	1.503(5)	C(31)-C(32)	1.421(4)
C(12)-Yb(1)	2.620(3)	C(32)-N(1)	1.381(4)
C(13)-C(14)	1.412(4)	C(33)-H(33A)	0.9800
C(13)-C(18)	1.506(4)	C(33)-H(33B)	0.9800
C(13)-Yb(1)	2.635(3)	C(33)-H(33C)	0.9800
C(14)-C(15)	1.390(5)	C(34)-H(34A)	0.9800
C(14)-C(19)	1.525(5)	C(34)-H(34B)	0.9800
C(14)-Yb(1)	2.611(3)	C(34)-H(34C)	0.9800
C(15)-C(20)	1.518(5)	N(1)-Yb(1)	2.292(2)
C(15)-Yb(1)	2.619(3)	N(2)-Yb(1)	2.328(2)
C(16)-H(16A)	0.9800	Cp(1)-Yb(1)	2.335(4)
C(16)-H(16B)	0.9800	Cp(2)-Yb(1)	2.337(4)

Table S18. Bond Angles (deg) for Cp^{*}₂Yb(5,6-Me₂phen) (**7**), Sublimed.

C(2)-C(1)-C(5)	107.3(3)	H(10A)-C(10)-H(10B)	109.5
C(2)-C(1)-C(6)	125.9(3)	C(5)-C(10)-H(10C)	109.5
C(5)-C(1)-C(6)	126.7(3)	H(10A)-C(10)-H(10C)	109.5
C(2)-C(1)-Yb(1)	74.17(17)	H(10B)-C(10)-H(10C)	109.5
C(5)-C(1)-Yb(1)	74.03(17)	C(15)-C(11)-C(12)	108.0(3)
C(6)-C(1)-Yb(1)	120.3(2)	C(15)-C(11)-C(16)	126.2(4)
C(1)-C(2)-C(3)	108.8(3)	C(12)-C(11)-C(16)	125.4(4)
C(1)-C(2)-C(7)	124.8(3)	C(15)-C(11)-Yb(1)	74.68(19)
C(3)-C(2)-C(7)	126.0(3)	C(12)-C(11)-Yb(1)	74.21(17)
C(1)-C(2)-Yb(1)	74.61(17)	C(16)-C(11)-Yb(1)	123.1(2)
C(3)-C(2)-Yb(1)	74.34(16)	C(13)-C(12)-C(11)	106.7(3)
C(7)-C(2)-Yb(1)	122.5(2)	C(13)-C(12)-C(17)	125.9(3)
C(4)-C(3)-C(2)	107.5(3)	C(11)-C(12)-C(17)	126.9(3)
C(4)-C(3)-C(8)	127.2(3)	C(13)-C(12)-Yb(1)	75.07(17)
C(2)-C(3)-C(8)	125.1(3)	C(11)-C(12)-Yb(1)	74.04(18)
C(4)-C(3)-Yb(1)	74.39(16)	C(17)-C(12)-Yb(1)	122.8(2)
C(2)-C(3)-Yb(1)	74.36(17)	C(12)-C(13)-C(14)	108.3(3)
C(8)-C(3)-Yb(1)	120.7(2)	C(12)-C(13)-C(18)	124.2(3)
C(3)-C(4)-C(5)	108.4(3)	C(14)-C(13)-C(18)	126.5(3)
C(3)-C(4)-C(9)	127.2(3)	C(12)-C(13)-Yb(1)	73.89(17)
C(5)-C(4)-C(9)	123.7(3)	C(14)-C(13)-Yb(1)	73.47(17)
C(3)-C(4)-Yb(1)	74.41(16)	C(18)-C(13)-Yb(1)	128.0(2)
C(5)-C(4)-Yb(1)	74.29(17)	C(15)-C(14)-C(13)	108.0(3)
C(9)-C(4)-Yb(1)	124.9(2)	C(15)-C(14)-C(19)	124.8(3)
C(4)-C(5)-C(1)	108.0(3)	C(13)-C(14)-C(19)	127.0(3)
C(4)-C(5)-C(10)	124.3(3)	C(15)-C(14)-Yb(1)	74.91(19)
C(1)-C(5)-C(10)	127.4(3)	C(13)-C(14)-Yb(1)	75.31(17)
C(4)-C(5)-Yb(1)	74.37(17)	C(19)-C(14)-Yb(1)	119.7(2)
C(1)-C(5)-Yb(1)	74.58(17)	C(11)-C(15)-C(14)	108.9(3)
C(10)-C(5)-Yb(1)	122.5(2)	C(11)-C(15)-C(20)	124.9(4)
C(1)-C(6)-H(6A)	109.5	C(14)-C(15)-C(20)	125.8(4)
C(1)-C(6)-H(6B)	109.5	C(11)-C(15)-Yb(1)	74.55(19)
H(6A)-C(6)-H(6B)	109.5	C(14)-C(15)-Yb(1)	74.27(18)
C(1)-C(6)-H(6C)	109.5	C(20)-C(15)-Yb(1)	123.0(2)
H(6A)-C(6)-H(6C)	109.5	C(11)-C(16)-H(16A)	109.5
H(6B)-C(6)-H(6C)	109.5	C(11)-C(16)-H(16B)	109.5
C(2)-C(7)-H(7A)	109.5	H(16A)-C(16)-H(16B)	109.5
C(2)-C(7)-H(7B)	109.5	C(11)-C(16)-H(16C)	109.5
H(7A)-C(7)-H(7B)	109.5	H(16A)-C(16)-H(16C)	109.5
C(2)-C(7)-H(7C)	109.5	H(16B)-C(16)-H(16C)	109.5
H(7A)-C(7)-H(7C)	109.5	C(12)-C(17)-H(17A)	109.5
H(7B)-C(7)-H(7C)	109.5	C(12)-C(17)-H(17B)	109.5
C(3)-C(8)-H(8A)	109.5	H(17A)-C(17)-H(17B)	109.5
C(3)-C(8)-H(8B)	109.5	C(12)-C(17)-H(17C)	109.5
H(8A)-C(8)-H(8B)	109.5	H(17A)-C(17)-H(17C)	109.5
C(3)-C(8)-H(8C)	109.5	H(17B)-C(17)-H(17C)	109.5
H(8A)-C(8)-H(8C)	109.5	C(13)-C(18)-H(18A)	109.5
H(8B)-C(8)-H(8C)	109.5	C(13)-C(18)-H(18B)	109.5
C(4)-C(9)-H(9A)	109.5	H(18A)-C(18)-H(18B)	109.5
C(4)-C(9)-H(9B)	109.5	C(13)-C(18)-H(18C)	109.5
H(9A)-C(9)-H(9B)	109.5	H(18A)-C(18)-H(18C)	109.5
C(4)-C(9)-H(9C)	109.5	H(18B)-C(18)-H(18C)	109.5
H(9A)-C(9)-H(9C)	109.5	C(14)-C(19)-H(19A)	109.5
H(9B)-C(9)-H(9C)	109.5	C(14)-C(19)-H(19B)	109.5
C(5)-C(10)-H(10A)	109.5	H(19A)-C(19)-H(19B)	109.5
C(5)-C(10)-H(10B)	109.5	C(14)-C(19)-H(19C)	109.5

H(19A)-C(19)-H(19C)	109.5	C(30)-N(2)-Yb(1)	126.1(2)
H(19B)-C(19)-H(19C)	109.5	C(31)-N(2)-Yb(1)	116.68(17)
C(15)-C(20)-H(20A)	109.5	N(1)-Yb(1)-N(2)	70.97(8)
C(15)-C(20)-H(20B)	109.5	N(1)-Yb(1)-C(14)	129.41(10)
H(20A)-C(20)-H(20B)	109.5	N(2)-Yb(1)-C(14)	99.86(9)
C(15)-C(20)-H(20C)	109.5	N(1)-Yb(1)-C(5)	121.12(9)
H(20A)-C(20)-H(20C)	109.5	N(2)-Yb(1)-C(5)	88.12(9)
H(20B)-C(20)-H(20C)	109.5	C(14)-Yb(1)-C(5)	107.68(10)
N(1)-C(21)-C(22)	124.5(3)	N(1)-Yb(1)-C(11)	79.03(9)
N(1)-C(21)-H(21)	117.7	N(2)-Yb(1)-C(11)	93.23(10)
C(22)-C(21)-H(21)	117.7	C(14)-Yb(1)-C(11)	51.26(11)
C(21)-C(22)-C(23)	120.1(3)	C(5)-Yb(1)-C(11)	158.82(11)
C(21)-C(22)-H(22)	120.0	N(1)-Yb(1)-C(4)	134.21(8)
C(23)-C(22)-H(22)	120.0	N(2)-Yb(1)-C(4)	118.78(9)
C(22)-C(23)-C(24)	117.9(3)	C(14)-Yb(1)-C(4)	94.60(10)
C(22)-C(23)-H(23)	121.0	C(5)-Yb(1)-C(4)	31.34(10)
C(24)-C(23)-H(23)	121.0	C(11)-Yb(1)-C(4)	138.25(10)
C(32)-C(24)-C(25)	120.1(2)	N(1)-Yb(1)-C(3)	107.46(9)
C(32)-C(24)-C(23)	117.6(3)	N(2)-Yb(1)-C(3)	133.67(9)
C(25)-C(24)-C(23)	122.3(3)	C(14)-Yb(1)-C(3)	112.83(10)
C(26)-C(25)-C(24)	120.4(3)	C(5)-Yb(1)-C(3)	51.85(10)
C(26)-C(25)-C(33)	120.8(3)	C(11)-Yb(1)-C(3)	132.74(11)
C(24)-C(25)-C(33)	118.9(3)	C(4)-Yb(1)-C(3)	31.20(9)
C(25)-C(26)-C(27)	120.4(3)	N(1)-Yb(1)-C(2)	82.74(9)
C(25)-C(26)-C(34)	120.2(3)	N(2)-Yb(1)-C(2)	107.76(9)
C(27)-C(26)-C(34)	119.4(3)	C(14)-Yb(1)-C(2)	143.66(10)
C(31)-C(27)-C(28)	117.3(3)	C(5)-Yb(1)-C(2)	51.60(10)
C(31)-C(27)-C(26)	119.7(2)	C(11)-Yb(1)-C(2)	145.87(11)
C(28)-C(27)-C(26)	123.0(3)	C(4)-Yb(1)-C(2)	51.48(9)
C(29)-C(28)-C(27)	119.0(3)	C(3)-Yb(1)-C(2)	31.29(9)
C(29)-C(28)-H(28)	120.5	N(1)-Yb(1)-C(15)	100.52(11)
C(27)-C(28)-H(28)	120.5	N(2)-Yb(1)-C(15)	79.72(9)
C(30)-C(29)-C(28)	119.8(3)	C(14)-Yb(1)-C(15)	30.82(11)
C(30)-C(29)-H(29)	120.1	C(5)-Yb(1)-C(15)	129.81(11)
C(28)-C(29)-H(29)	120.1	C(11)-Yb(1)-C(15)	30.77(12)
N(2)-C(30)-C(29)	123.8(3)	C(4)-Yb(1)-C(15)	124.88(11)
N(2)-C(30)-H(30)	118.1	C(3)-Yb(1)-C(15)	141.85(10)
C(29)-C(30)-H(30)	118.1	C(2)-Yb(1)-C(15)	172.51(11)
N(2)-C(31)-C(27)	122.9(2)	N(1)-Yb(1)-C(12)	91.92(9)
N(2)-C(31)-C(32)	117.2(2)	N(2)-Yb(1)-C(12)	124.95(10)
C(27)-C(31)-C(32)	119.9(2)	C(14)-Yb(1)-C(12)	51.77(10)
N(1)-C(32)-C(24)	123.3(2)	C(5)-Yb(1)-C(12)	140.85(10)
N(1)-C(32)-C(31)	117.2(2)	C(11)-Yb(1)-C(12)	31.75(11)
C(24)-C(32)-C(31)	119.5(3)	C(4)-Yb(1)-C(12)	110.53(10)
C(25)-C(33)-H(33A)	109.5	C(3)-Yb(1)-C(12)	101.24(10)
C(25)-C(33)-H(33B)	109.5	C(2)-Yb(1)-C(12)	121.81(11)
H(33A)-C(33)-H(33B)	109.5	C(15)-Yb(1)-C(12)	51.68(11)
C(25)-C(33)-H(33C)	109.5	N(1)-Yb(1)-C(1)	90.19(9)
H(33A)-C(33)-H(33C)	109.5	N(2)-Yb(1)-C(1)	81.81(9)
H(33B)-C(33)-H(33C)	109.5	C(14)-Yb(1)-C(1)	139.02(10)
C(26)-C(34)-H(34A)	109.5	C(5)-Yb(1)-C(1)	31.39(10)
C(26)-C(34)-H(34B)	109.5	C(11)-Yb(1)-C(1)	169.13(10)
H(34A)-C(34)-H(34B)	109.5	C(4)-Yb(1)-C(1)	51.81(9)
C(26)-C(34)-H(34C)	109.5	C(3)-Yb(1)-C(1)	51.94(10)
H(34A)-C(34)-H(34C)	109.5	C(2)-Yb(1)-C(1)	31.22(10)
H(34B)-C(34)-H(34C)	109.5	C(15)-Yb(1)-C(1)	154.24(11)
C(21)-N(1)-C(32)	116.6(2)	C(12)-Yb(1)-C(1)	152.16(10)
C(21)-N(1)-Yb(1)	125.49(19)	N(1)-Yb(1)-C(13)	122.94(9)
C(32)-N(1)-Yb(1)	117.65(17)	N(2)-Yb(1)-C(13)	129.51(9)
C(30)-N(2)-C(31)	117.2(2)	C(14)-Yb(1)-C(13)	31.23(10)

C(5)-Yb(1)-C(13)	112.96(10)	C(15)-Yb(1)-C(13)	51.12(10)
C(11)-Yb(1)-C(13)	51.40(9)	C(12)-Yb(1)-C(13)	31.04(10)
C(4)-Yb(1)-C(13)	86.86(9)	C(1)-Yb(1)-C(13)	138.46(9)
C(3)-Yb(1)-C(13)	91.42(9)	Cp(1)-Yb(1)-Cp(2)	138.3(1)
C(2)-Yb(1)-C(13)	121.47(10)		

Table S19. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cp}^* \text{Yb}(5,6\text{-Me}_2\text{phen}) (7)$, Sublimed.

	x	y	z	U(eq)
H(6A)	7733	3368	2771	78
H(6B)	9246	3185	3194	78
H(6C)	7688	3099	3598	78
H(7A)	4779	1913	2130	68
H(7B)	5533	2742	2249	68
H(7C)	4863	2281	2923	68
H(8A)	5115	559	2395	55
H(8B)	6431	-59	2335	55
H(8C)	6051	492	1665	55
H(9A)	8710	-267	2691	57
H(9B)	9663	86	3344	57
H(9C)	10283	128	2536	57
H(10A)	10635	1463	3849	71
H(10B)	10931	2257	3430	71
H(10C)	11467	1455	3087	71
H(16A)	9538	2745	-218	91
H(16B)	7995	2309	-355	91
H(16C)	9424	2082	-820	91
H(17A)	7254	371	-268	80
H(17B)	6660	1228	-116	80
H(17C)	6495	573	489	80
H(18A)	8170	-306	1310	63
H(18B)	9902	-491	1395	63
H(18C)	9095	-613	632	63
H(19A)	13107	679	1116	81
H(19B)	12061	61	1509	81
H(19C)	12286	903	1852	81
H(20A)	12781	1911	40	94
H(20B)	12781	2139	878	94
H(20C)	11822	2633	313	94
H(21)	5744	2264	816	32
H(22)	4540	3268	271	30
H(23)	5663	4507	215	27
H(28)	12467	4806	1691	31
H(29)	13438	3686	2232	36
H(30)	12113	2548	2199	30
H(33A)	6773	5753	715	41
H(33B)	7279	5469	-69	41
H(33C)	8329	6031	392	41
H(34A)	10960	5839	558	39
H(34B)	11407	5721	1389	39
H(34C)	9891	6151	1182	39

Cp*₂Yb(5,6-Me₂phen) (7), crystallized.

Data collection

A fragment of a red block-like crystal of C₃₄H₄₂N₂Yb (Cp*₂Yb(5,6-Me₂phen)) (7) crystallized from cyclohexane having approximate dimension of 0.3 x 0.30 x 0.20 mm was mounted on a Kapton loop using Paratone N hydrocarbon oil. All measurements were made on a Bruker SMART 1000¹ CCD area detector with graphite monochromated Mo-K α radiation.

Cell constants and an orientation matrix, obtained from a least-squared refinement corresponded to a primitive monoclinic cell with dimensions:

$$\begin{array}{ll} a = 9.7032(13) & \alpha = 90^\circ \\ b = 31.081(4) & \beta = 99.71^\circ \\ c = 28.751(4) & \gamma = 90^\circ \\ V = 8546(2) \text{ \AA}^3 & \end{array}$$

For $Z = 12$ and F.W. = 651.74, the calculated density is 1.520 g cm⁻³. Based on a statistical analysis of intensity distribution, and successful solution and refinement of the structure, the space group was determined to be

$$P2(1)/n \text{ (#14)}$$

The data were collected at a temperature of -136(2) °C. Frames corresponding to an arbitrary hemisphere of data were collected using ω scans of 0.3° counted for a total of 10.0 s per frame.

Data reduction

Data were integrated by the program SAINT² to a maximum 2θ value of 50.48°. The data were corrected for Lorentz and polarization effects. Data were analyzed for agreement and possible absorption using XPREP.³ A semi-empirical multi-scan absorption correction⁴ was applied using SADABS.⁵ This models the absorption surface using a spherical harmonic series based on differences between equivalent.

Structure solution and refinement

The structure was solved by direct methods.⁶ Non-hydrogen atoms were refined anisotropically and hydrogen atoms were placed in calculated positions and not refined. The final cycle of full matrix least squares refinement was based on 12833 observed reflections ($I > 2.00 \sigma(I)$) and 1000 parameters and converged with unweighted and weighted agreement factors of:

$$R = \sum ||F_o| - |F_c|| / \sum |F_o| = 0.0369$$

$$R_w = [(\sum w (|F_o| - |F_c|)^2 / \sum w F_o^2)]^{1/2} = 0.0653$$

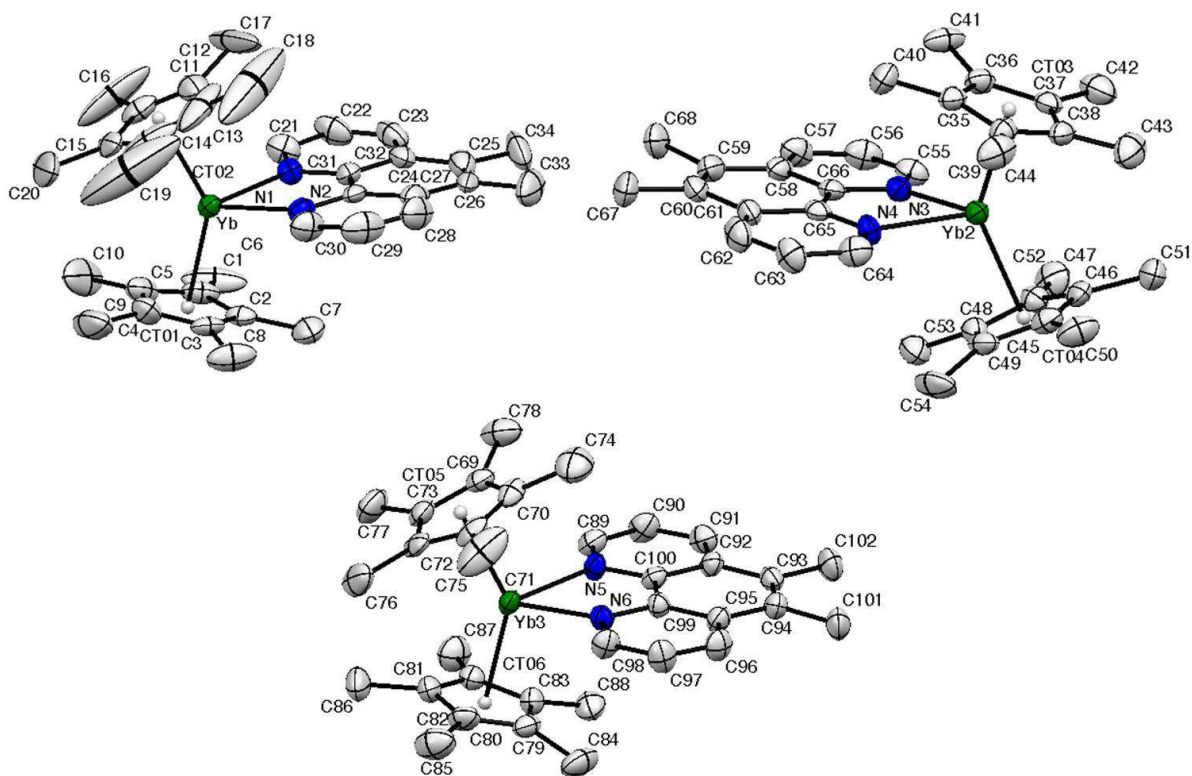
The standard deviation of an observation of unit weight was 0.980. The weighting scheme was based on counting statistics and include a factor p to downweight the intense reflections ($w=1/[\sigma^2 F_o^2+(0.0188P)^2+(10.30P)]$ where $P=(\text{Max}(F_o^2,0)+2F_c^2)/3$). Plot of Σ

w $(|F_o| - |F_c|)^2$ versus $|F_o|$, reflexion order in data collection, $\sin \theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.225 and -0.917 e.A⁻³, respectively.

The SHELX program uses the neutral atom scattering factors, f' , f'' and absorption coefficients from International Tables for Crystallography, Volume C (1992), Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht: Tables 6.1.1.4(pp. 500-502), 4.2.6.8 (pp.219-222) and 4.2.4.2 (pp. 193-199), respectively. All calculations were performed using the WinGX crystallographic software package.⁷ (“WinGX suite for small molecule single-crystal crystallography”)

The carbons C16, C17, C18 and C19 have large thermic ellipsoids. As a result several A-levels alerts are present in the checkcif report. However, it does not alterate the structurals parameters (i.e. distances and bond angles) wheather there are refined isotropically or anisotropically.

Figure S25. ORTEP of $\text{Cp}^*_2\text{Yb}(5,6\text{-Me}_2\text{phen})$ (**7**) (50% probability ellipsoids).



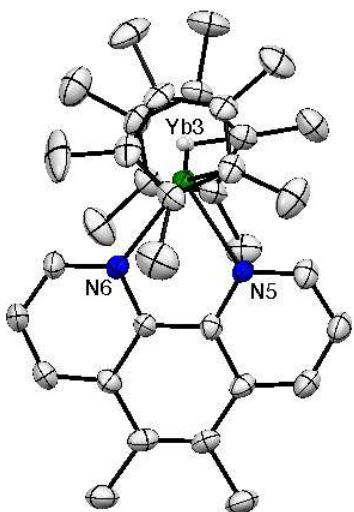
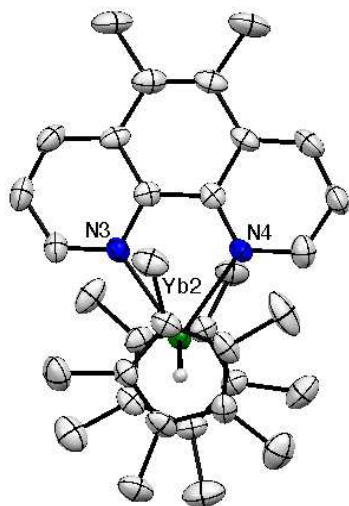
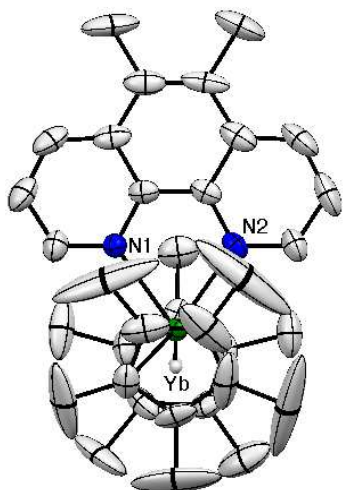


Table S20. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cp}^*_2\text{Yb}(5,6\text{-Me}_2\text{phen})$ (**7**). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
N(6)	2122(4)	9092(1)	3921(1)	29(1)
C(99)	3346(5)	9180(1)	4226(2)	27(1)
N(5)	2853(4)	8550(1)	4649(1)	29(1)
C(100)	3722(5)	8891(1)	4608(2)	28(1)
C(80)	-1531(6)	8960(2)	4155(2)	42(2)
C(83)	39(6)	8955(2)	4838(2)	34(1)
C(92)	4975(5)	8967(1)	4938(2)	31(1)
C(79)	-477(6)	9196(1)	4434(2)	35(1)
C(82)	-701(6)	8563(2)	4811(2)	34(1)
C(85)	-2472(7)	9110(2)	3711(2)	62(2)
C(93)	5808(5)	9339(2)	4876(2)	31(1)
C(102)	7101(6)	9407(2)	5248(2)	47(2)
C(58)	5615(5)	3112(1)	7280(2)	33(1)
C(94)	5440(6)	9617(2)	4519(2)	36(1)
C(26)	6020(6)	2029(2)	8482(3)	59(2)
C(55)	3275(6)	3363(2)	6666(2)	35(1)
C(98)	1760(6)	9367(1)	3554(2)	36(1)
C(72)	-246(6)	8005(1)	3440(2)	38(2)
C(81)	-1686(6)	8567(2)	4397(2)	37(1)
C(89)	3213(6)	8286(1)	5022(2)	36(1)
C(70)	2116(6)	8106(2)	3554(2)	36(1)
C(96)	3758(6)	9807(2)	3784(2)	39(1)
C(91)	5253(6)	8679(2)	5306(2)	39(1)
C(71)	858(7)	8228(2)	3283(2)	43(2)
C(97)	2554(6)	9714(2)	3474(2)	41(2)
C(95)	4190(6)	9544(1)	4169(2)	32(1)
N(3)	3537(4)	3571(1)	7085(1)	30(1)
C(56)	4112(6)	3046(2)	6529(2)	43(2)
C(101)	6264(6)	10021(2)	4446(2)	47(2)
C(43)	-1464(6)	4315(2)	7593(2)	59(2)
C(42)	-1134(7)	3573(2)	6855(2)	54(2)
C(40)	2442(6)	3315(2)	8360(2)	45(2)
C(66)	4749(5)	3454(1)	7384(2)	29(1)
C(69)	1809(6)	7793(1)	3881(2)	35(1)
C(60)	7170(6)	3214(2)	8029(2)	39(1)
Yb	11009(1)	1204(1)	9299(1)	28(1)
C(59)	6837(6)	2998(2)	7622(2)	42(2)
C(41)	1268(7)	2934(1)	7365(2)	46(2)
C(49)	3185(6)	4841(1)	7239(2)	38(2)
C(90)	4382(6)	8332(2)	5351(2)	43(2)
C(50)	1134(7)	5207(2)	7562(2)	56(2)
C(76)	-1774(6)	8009(2)	3208(2)	65(2)
C(54)	4365(7)	5047(2)	7581(2)	64(2)
C(57)	5290(6)	2913(2)	6837(2)	42(2)
C(73)	354(6)	7734(1)	3812(2)	38(1)
C(53)	4740(6)	4461(2)	6729(2)	49(2)
C(84)	-61(7)	9660(2)	4356(2)	57(2)
C(44)	857(7)	4188(2)	8487(2)	52(2)
C(88)	1082(6)	9113(2)	5251(2)	45(2)
C(67)	8415(6)	3111(2)	8399(2)	56(2)
C(74)	3551(7)	8253(2)	3489(2)	68(2)
C(77)	-357(7)	7397(2)	4064(2)	59(2)
C(68)	7688(6)	2607(2)	7506(2)	56(2)

C(32)	8131(6)	1389(2)	8605(2)	35(1)
C(3)	12670(6)	1840(1)	9160(2)	37(1)
C(31)	8202(6)	1725(1)	8930(2)	34(1)
C(2)	12003(6)	1714(2)	8715(2)	35(1)
C(15)	11892(6)	670(2)	9985(2)	54(2)
C(23)	6967(7)	1017(2)	7919(2)	54(2)
C(24)	6994(6)	1368(2)	8219(2)	47(2)
C(11)	10960(8)	437(2)	9656(2)	47(2)
C(8)	12573(8)	2278(2)	9372(2)	68(2)
C(12)	9667(8)	595(3)	9647(3)	69(2)
C(4)	13572(7)	1519(2)	9356(2)	51(2)
C(25)	5968(6)	1708(2)	8159(2)	55(2)
N(1)	9183(4)	1087(1)	8668(1)	32(1)
N(2)	9328(5)	1735(1)	9295(2)	36(1)
C(21)	9089(6)	753(2)	8372(2)	45(2)
C(87)	-602(7)	8231(2)	5198(2)	55(2)
C(22)	7985(7)	708(2)	8002(2)	57(2)
C(7)	11019(7)	1981(2)	8375(2)	59(2)
C(27)	7115(6)	2046(2)	8886(2)	48(2)
C(30)	9358(7)	2047(2)	9620(2)	48(2)
C(78)	2885(7)	7523(2)	4201(2)	60(2)
C(28)	7216(7)	2356(2)	9237(3)	64(2)
C(75)	669(10)	8520(2)	2857(2)	87(3)
C(29)	8333(8)	2354(2)	9605(3)	65(2)
C(86)	-2882(6)	8254(2)	4278(2)	57(2)
C(1)	12495(7)	1300(2)	8627(2)	45(2)
C(5)	13466(7)	1179(2)	9016(3)	55(2)
C(14)	11078(14)	978(2)	10173(2)	95(4)
C(6)	12181(9)	1048(2)	8173(2)	92(3)
C(13)	9740(13)	922(3)	9956(4)	110(4)
C(17)	8326(11)	399(4)	9378(4)	259(11)
C(19)	11710(20)	1267(3)	10576(3)	283(13)
C(18)	8431(17)	1153(4)	10081(6)	299(12)
C(34)	4834(7)	1700(3)	7724(2)	88(3)
C(33)	4938(7)	2380(2)	8430(3)	80(2)
C(20)	13388(9)	564(3)	10165(4)	181(7)
C(10)	14406(7)	782(2)	9030(4)	109(4)
C(16)	11335(14)	62(2)	9383(3)	163(6)
C(9)	14655(8)	1553(2)	9795(3)	94(3)
Yb(2)	2130(1)	4082(1)	7370(1)	27(1)
N(4)	4199(4)	4005(1)	7898(1)	30(1)
C(65)	5062(5)	3684(1)	7816(2)	28(1)
C(45)	1755(6)	4918(1)	7229(2)	37(1)
C(48)	3373(6)	4589(2)	6846(2)	35(1)
C(37)	-196(6)	3649(2)	7319(2)	34(1)
C(61)	6299(5)	3574(2)	8136(2)	34(1)
C(46)	1039(6)	4717(1)	6816(2)	37(1)
C(38)	-304(6)	3994(1)	7642(2)	34(1)
C(62)	6574(6)	3819(2)	8549(2)	46(2)
C(35)	1407(5)	3537(1)	7989(2)	31(1)
C(39)	690(6)	3926(1)	8043(2)	33(1)
C(63)	5702(6)	4151(2)	8622(2)	44(2)
C(47)	2019(6)	4514(2)	6585(2)	32(1)
C(36)	872(6)	3366(1)	7537(2)	36(1)
C(52)	1666(7)	4294(2)	6114(2)	53(2)
C(64)	4528(6)	4232(2)	8303(2)	42(2)
C(51)	-495(6)	4778(2)	6606(2)	47(2)
Yb(3)	773(1)	8527(1)	4126(1)	27(1)
CT01	12841	1510	8975	10
CT02	10667	720	9883	10

CT03	494	3694	7706	10
CT04	2274	4716	6943	10
CT05	978	7973	3594	10
CT06	-871	8848	4527	10

Table S21. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cp}^*_2\text{Yb}(5,6\text{-Me}_2\text{phen})$ (7). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(6)	26(2)	30(2)	29(2)	3(2)	-1(2)	1(2)
C(99)	26(3)	26(2)	30(3)	2(2)	3(2)	-2(2)
N(5)	29(2)	25(2)	30(2)	3(2)	-7(2)	-2(2)
C(100)	33(3)	22(2)	27(3)	1(2)	3(2)	3(2)
C(80)	42(4)	34(3)	44(3)	0(2)	-4(3)	14(3)
C(83)	30(3)	32(3)	41(3)	-2(2)	7(3)	-4(2)
C(92)	30(3)	28(2)	31(3)	-6(2)	-4(3)	1(2)
C(79)	41(3)	25(2)	43(3)	-3(2)	16(3)	3(2)
C(82)	31(3)	32(3)	40(3)	-3(2)	10(3)	1(2)
C(85)	70(5)	56(4)	55(4)	-1(3)	-4(4)	19(3)
C(93)	23(3)	38(3)	32(3)	-7(2)	2(2)	1(2)
C(102)	30(3)	51(3)	55(4)	-4(3)	-8(3)	-5(3)
C(58)	27(3)	27(2)	48(3)	4(2)	15(3)	0(2)
C(94)	29(3)	33(3)	46(3)	-10(2)	2(3)	-3(2)
C(26)	23(3)	63(4)	92(5)	53(4)	17(4)	7(3)
C(55)	38(3)	39(3)	30(3)	-6(2)	9(3)	-10(2)
C(98)	41(3)	30(2)	34(3)	9(2)	-3(3)	0(2)
C(72)	41(4)	27(2)	40(3)	-17(2)	-12(3)	4(2)
C(81)	28(3)	33(3)	52(3)	-6(2)	11(3)	-4(2)
C(89)	46(4)	27(2)	32(3)	-2(2)	1(3)	3(2)
C(70)	49(4)	34(3)	28(3)	-8(2)	16(3)	-9(3)
C(96)	43(4)	32(3)	42(3)	10(2)	6(3)	-6(2)
C(91)	37(3)	42(3)	33(3)	-2(2)	-6(3)	5(3)
C(71)	66(4)	30(3)	28(3)	-10(2)	-3(3)	-3(3)
C(97)	40(4)	39(3)	41(3)	18(2)	0(3)	-3(3)
C(95)	35(3)	25(2)	36(3)	-1(2)	3(3)	-3(2)
N(3)	29(2)	28(2)	31(2)	-1(2)	0(2)	-3(2)
C(56)	54(4)	40(3)	38(3)	-14(2)	14(3)	-9(3)
C(101)	33(3)	41(3)	63(4)	-1(3)	-1(3)	-9(3)
C(43)	48(4)	60(4)	74(5)	19(3)	27(4)	15(3)
C(42)	49(4)	61(4)	50(4)	6(3)	5(3)	-18(3)
C(40)	43(4)	38(3)	51(3)	11(2)	4(3)	9(3)
C(66)	27(3)	23(2)	39(3)	3(2)	9(3)	-6(2)
C(69)	45(4)	25(2)	34(3)	-7(2)	2(3)	5(2)
C(60)	23(3)	43(3)	50(3)	13(3)	5(3)	-2(2)
Yb	31(1)	24(1)	28(1)	2(1)	4(1)	0(1)
C(59)	32(3)	32(3)	64(4)	9(3)	10(3)	1(2)
C(41)	66(4)	24(2)	57(4)	-3(2)	34(3)	-5(3)
C(49)	41(4)	30(3)	37(3)	9(2)	-6(3)	-13(2)
C(90)	50(4)	34(3)	39(3)	6(2)	-9(3)	4(3)
C(50)	78(5)	35(3)	58(4)	0(3)	19(4)	1(3)
C(76)	51(4)	52(3)	78(5)	-25(3)	-28(4)	6(3)
C(54)	68(5)	58(4)	55(4)	9(3)	-19(4)	-39(3)
C(57)	41(4)	32(3)	58(4)	-12(2)	18(3)	0(2)
C(73)	45(4)	24(2)	42(3)	-8(2)	0(3)	-4(2)
C(53)	35(4)	56(3)	57(4)	14(3)	9(3)	-4(3)
C(84)	79(5)	27(3)	69(4)	-1(3)	30(4)	1(3)
C(44)	68(4)	42(3)	53(4)	-1(3)	29(4)	8(3)
C(88)	46(4)	50(3)	42(3)	-16(2)	12(3)	-3(3)
C(67)	35(4)	54(3)	75(4)	23(3)	-2(4)	11(3)
C(74)	76(5)	68(4)	67(5)	-19(3)	31(4)	-6(4)
C(77)	71(5)	30(3)	78(5)	-4(3)	16(4)	-12(3)
C(68)	30(3)	50(3)	89(5)	10(3)	13(4)	12(3)

C(32)	31(3)	34(3)	40(3)	13(2)	4(3)	-3(2)
C(3)	45(4)	25(2)	44(3)	-2(2)	21(3)	-13(2)
C(31)	31(3)	26(2)	48(3)	16(2)	16(3)	0(2)
C(2)	38(3)	38(3)	31(3)	2(2)	14(3)	-12(2)
C(15)	44(4)	60(4)	50(4)	37(3)	-13(3)	-12(3)
C(23)	35(4)	83(4)	40(3)	5(3)	-1(3)	-17(3)
C(24)	27(3)	58(3)	53(4)	22(3)	4(3)	-9(3)
C(11)	81(5)	30(3)	31(3)	7(2)	12(3)	-3(3)
C(8)	102(6)	46(3)	64(4)	-19(3)	43(4)	-25(4)
C(12)	48(5)	87(5)	70(5)	45(4)	3(4)	-12(4)
C(4)	39(4)	51(3)	60(4)	6(3)	-6(3)	-14(3)
C(25)	32(4)	73(4)	61(4)	29(3)	10(3)	2(3)
N(1)	31(3)	34(2)	31(2)	-2(2)	5(2)	1(2)
N(2)	38(3)	25(2)	46(3)	2(2)	14(2)	2(2)
C(21)	48(4)	48(3)	41(3)	-11(2)	11(3)	-6(3)
C(87)	62(4)	43(3)	64(4)	9(3)	20(4)	-7(3)
C(22)	48(4)	73(4)	47(4)	-14(3)	3(3)	-22(3)
C(7)	55(4)	66(4)	56(4)	26(3)	12(4)	-6(3)
C(27)	37(4)	36(3)	78(4)	17(3)	26(3)	3(3)
C(30)	55(4)	34(3)	59(4)	-9(3)	20(3)	1(3)
C(78)	69(5)	54(3)	51(4)	-11(3)	-5(4)	25(3)
C(28)	54(5)	40(3)	105(6)	7(4)	34(4)	18(3)
C(75)	174(9)	55(4)	24(3)	4(3)	-9(5)	-5(5)
C(29)	83(5)	35(3)	91(5)	-16(3)	51(5)	2(3)
C(86)	41(4)	54(3)	79(5)	-16(3)	18(4)	-19(3)
C(1)	52(4)	36(3)	51(4)	-12(3)	25(3)	-18(3)
C(5)	39(4)	31(3)	100(5)	-1(3)	29(4)	0(3)
C(14)	216(11)	41(4)	26(3)	1(3)	18(5)	-24(6)
C(6)	134(7)	87(5)	76(5)	-46(4)	78(5)	-68(5)
C(13)	169(11)	89(7)	97(8)	66(6)	93(8)	70(7)
C(17)	109(9)	347(17)	268(15)	258(14)	-124(11)	-167(11)
C(19)	700(40)	86(6)	36(4)	-8(4)	-13(11)	-138(13)
C(18)	390(20)	249(15)	360(20)	234(16)	343(19)	260(16)
C(34)	28(4)	151(7)	81(5)	57(5)	-3(4)	8(4)
C(33)	55(5)	72(4)	121(7)	42(4)	37(5)	35(4)
C(20)	59(6)	209(11)	250(13)	195(10)	-40(8)	-19(7)
C(10)	60(5)	59(4)	224(11)	23(6)	71(6)	31(4)
C(16)	403(19)	27(3)	79(5)	10(3)	103(9)	36(7)
C(9)	72(6)	106(6)	90(6)	41(5)	-27(5)	-50(5)
Yb(2)	26(1)	25(1)	27(1)	1(1)	1(1)	-1(1)
N(4)	23(2)	37(2)	30(2)	-6(2)	-1(2)	-1(2)
C(65)	27(3)	29(2)	28(3)	6(2)	7(2)	-8(2)
C(45)	49(4)	28(2)	31(3)	3(2)	2(3)	-1(2)
C(48)	29(3)	38(3)	38(3)	10(2)	3(3)	-3(2)
C(37)	29(3)	37(3)	36(3)	9(2)	4(3)	-12(2)
C(61)	22(3)	42(3)	37(3)	9(2)	0(3)	-4(2)
C(46)	37(3)	29(2)	42(3)	14(2)	-6(3)	-1(2)
C(38)	30(3)	27(2)	48(3)	9(2)	14(3)	2(2)
C(62)	35(4)	62(4)	36(3)	6(3)	-8(3)	-2(3)
C(35)	33(3)	26(2)	36(3)	4(2)	10(3)	-2(2)
C(39)	34(3)	31(2)	35(3)	2(2)	9(3)	3(2)
C(63)	40(4)	56(3)	30(3)	-6(2)	-5(3)	-4(3)
C(47)	34(3)	36(3)	27(3)	4(2)	4(3)	-4(2)
C(36)	36(3)	25(2)	48(3)	-2(2)	12(3)	-2(2)
C(52)	64(4)	57(3)	35(3)	1(3)	-5(3)	0(3)
C(64)	53(4)	41(3)	31(3)	-1(2)	5(3)	-5(3)
C(51)	36(4)	43(3)	58(4)	14(3)	-2(3)	3(3)
Yb(3)	30(1)	21(1)	30(1)	-1(1)	-1(1)	-3(1)

Table S22. Bond lengths (Å) for Cp^{*}₂Yb(5,6-Me₂phen) (7).

N(6)-C(98)	1.359(6)	C(70)-Yb(3)	2.616(6)
N(6)-C(99)	1.380(6)	C(96)-C(97)	1.376(6)
N(6)-Yb(3)	2.323(4)	C(96)-C(95)	1.381(6)
C(99)-C(100)	1.418(6)	C(91)-C(90)	1.388(8)
C(99)-C(95)	1.423(7)	C(71)-CT05	1.185(5)
C(99)-Yb(3)	3.192(5)	C(71)-C(75)	1.510(7)
N(5)-C(89)	1.348(5)	C(71)-Yb(3)	2.611(5)
N(5)-C(100)	1.371(6)	N(3)-C(66)	1.384(6)
N(5)-Yb(3)	2.304(3)	N(3)-Yb(2)	2.329(4)
C(100)-C(92)	1.429(6)	C(56)-C(57)	1.385(7)
C(100)-Yb(3)	3.169(5)	C(43)-C(38)	1.493(7)
C(80)-CT06	1.201(5)	C(42)-C(37)	1.499(7)
C(80)-C(79)	1.398(7)	C(40)-C(35)	1.503(6)
C(80)-C(81)	1.425(7)	C(66)-C(65)	1.420(6)
C(80)-C(85)	1.513(7)	C(66)-Yb(2)	3.197(5)
C(80)-Yb(3)	2.623(6)	C(69)-CT05	1.191(5)
C(83)-CT06	1.194(5)	C(69)-C(73)	1.404(8)
C(83)-C(79)	1.402(7)	C(69)-C(78)	1.522(6)
C(83)-C(82)	1.409(7)	C(69)-Yb(3)	2.638(5)
C(83)-C(88)	1.506(6)	C(60)-C(59)	1.340(7)
C(83)-Yb(3)	2.638(6)	C(60)-C(61)	1.466(8)
C(92)-C(91)	1.378(6)	C(60)-C(67)	1.502(7)
C(92)-C(93)	1.438(7)	Yb-N(2)	2.319(4)
C(79)-CT06	1.192(5)	Yb-CT02	2.3203(3)
C(79)-C(84)	1.522(7)	Yb-N(1)	2.341(4)
C(79)-Yb(3)	2.635(5)	Yb-CT01	2.3438(3)
C(82)-CT06	1.196(5)	Yb-C(13)	2.577(10)
C(82)-C(81)	1.395(7)	Yb-C(12)	2.591(7)
C(82)-C(87)	1.510(7)	Yb-C(11)	2.600(5)
C(82)-Yb(3)	2.623(6)	Yb-C(14)	2.600(7)
C(93)-C(94)	1.345(7)	Yb-C(2)	2.608(5)
C(93)-C(102)	1.520(6)	Yb-C(15)	2.610(5)
C(58)-C(57)	1.403(7)	Yb-C(1)	2.615(7)
C(58)-C(66)	1.419(7)	Yb-C(3)	2.624(5)
C(58)-C(59)	1.451(7)	C(59)-C(68)	1.540(8)
C(94)-C(95)	1.458(6)	C(41)-C(36)	1.502(7)
C(94)-C(101)	1.521(7)	C(49)-CT04	1.185(4)
C(26)-C(25)	1.359(9)	C(49)-C(45)	1.403(8)
C(26)-C(27)	1.437(8)	C(49)-C(48)	1.413(8)
C(26)-C(33)	1.504(8)	C(49)-C(54)	1.519(6)
C(55)-N(3)	1.354(6)	C(49)-Yb(2)	2.624(5)
C(55)-C(56)	1.376(8)	C(50)-C(45)	1.509(8)
C(98)-C(97)	1.368(7)	C(73)-CT05	1.200(6)
C(72)-CT05	1.199(5)	C(73)-C(77)	1.507(8)
C(72)-C(73)	1.408(6)	C(73)-Yb(3)	2.634(4)
C(72)-C(71)	1.412(9)	C(53)-C(48)	1.477(8)
C(72)-C(76)	1.519(7)	C(44)-C(39)	1.499(7)
C(72)-Yb(3)	2.618(4)	C(32)-N(1)	1.375(6)
C(81)-CT06	1.196(5)	C(32)-C(31)	1.396(7)
C(81)-C(86)	1.510(7)	C(32)-C(24)	1.429(7)
C(81)-Yb(3)	2.634(6)	C(3)-CT01	1.180(5)
C(89)-C(90)	1.356(6)	C(3)-C(4)	1.385(7)
C(70)-CT05	1.202(6)	C(3)-C(2)	1.389(7)
C(70)-C(71)	1.386(7)	C(3)-C(8)	1.501(7)
C(70)-C(69)	1.418(7)	C(31)-N(2)	1.381(6)
C(70)-C(74)	1.507(9)	C(31)-C(27)	1.442(7)

Table S22. Bond lengths (Å) for Cp*₂Yb(5,6-Me₂phen) (**7**) (Continued).

C(2)-CT01	1.189(5)	Yb(2)-N(4)	2.315(3)
C(2)-C(1)	1.410(7)	Yb(2)-CT03	2.3291(3)
C(2)-C(7)	1.496(7)	Yb(2)-CT04	2.3376(3)
C(15)-CT02	1.186(6)	Yb(2)-C(48)	2.610(5)
C(15)-C(11)	1.395(7)	Yb(2)-C(37)	2.611(5)
C(15)-C(14)	1.407(12)	Yb(2)-C(47)	2.612(5)
C(15)-C(20)	1.492(9)	Yb(2)-C(39)	2.617(6)
C(23)-C(22)	1.369(8)	Yb(2)-C(36)	2.622(5)
C(23)-C(24)	1.388(9)	Yb(2)-C(38)	2.625(6)
C(24)-C(25)	1.440(8)	Yb(2)-C(35)	2.635(5)
C(11)-CT02	1.160(6)	N(4)-C(65)	1.348(6)
C(11)-C(12)	1.344(10)	N(4)-C(64)	1.353(6)
C(11)-C(16)	1.486(9)	C(65)-C(61)	1.425(6)
C(12)-CT02	1.155(7)	C(45)-CT04	1.210(6)
C(12)-C(13)	1.343(12)	C(45)-C(46)	1.416(6)
C(12)-C(17)	1.524(10)	C(48)-CT04	1.212(6)
C(4)-CT01	1.201(5)	C(48)-C(47)	1.417(7)
C(4)-C(5)	1.431(8)	C(37)-CT03	1.206(5)
C(4)-C(9)	1.504(7)	C(37)-C(36)	1.423(7)
C(25)-C(34)	1.520(8)	C(37)-C(38)	1.434(7)
N(1)-C(21)	1.336(6)	C(61)-C(62)	1.397(7)
N(2)-C(30)	1.343(7)	C(46)-CT04	1.193(5)
C(21)-C(22)	1.383(7)	C(46)-C(47)	1.398(8)
C(27)-C(28)	1.387(9)	C(46)-C(51)	1.520(7)
C(30)-C(29)	1.373(8)	C(38)-CT03	1.205(5)
C(28)-C(29)	1.381(8)	C(38)-C(39)	1.390(6)
C(1)-CT01	1.195(5)	C(62)-C(63)	1.373(8)
C(1)-C(5)	1.386(8)	C(35)-CT03	1.200(4)
C(1)-C(6)	1.510(8)	C(35)-C(39)	1.415(7)
C(5)-CT01	1.190(5)	C(35)-C(36)	1.418(7)
C(5)-C(10)	1.532(8)	C(39)-CT03	1.196(5)
C(14)-CT02	1.176(6)	C(63)-C(64)	1.360(7)
C(14)-C(13)	1.354(13)	C(47)-CT04	1.194(5)
C(14)-C(19)	1.512(9)	C(47)-C(52)	1.506(7)
C(13)-CT02	1.144(10)	C(36)-CT03	1.214(5)
C(13)-C(18)	1.555(14)	Yb(3)-CT05	2.3350(3)
		Yb(3)-CT06	2.3431(3)

Table S23. Bond angles [deg] for Cp^{*}₂Yb(5,6-Me₂phen) (7).

C(98)-N(6)-C(99)	116.8(4)	CT06-C(82)-Yb(3)	63.3(3)
C(98)-N(6)-Yb(3)	126.2(3)	C(81)-C(82)-Yb(3)	75.1(3)
C(99)-N(6)-Yb(3)	116.7(3)	C(83)-C(82)-Yb(3)	75.1(3)
N(6)-C(99)-C(100)	116.6(4)	C(87)-C(82)-Yb(3)	123.2(4)
N(6)-C(99)-C(95)	122.3(4)	C(94)-C(93)-C(92)	122.0(4)
C(100)-C(99)-C(95)	121.1(4)	C(94)-C(93)-C(102)	121.9(5)
N(6)-C(99)-Yb(3)	40.5(2)	C(92)-C(93)-C(102)	116.1(4)
C(100)-C(99)-Yb(3)	76.2(3)	C(57)-C(58)-C(66)	118.2(4)
C(95)-C(99)-Yb(3)	162.1(3)	C(57)-C(58)-C(59)	122.7(5)
C(89)-N(5)-C(100)	117.2(4)	C(66)-C(58)-C(59)	119.0(5)
C(89)-N(5)-Yb(3)	125.5(3)	C(93)-C(94)-C(95)	120.6(5)
C(100)-N(5)-Yb(3)	116.8(3)	C(93)-C(94)-C(101)	124.0(4)
N(5)-C(100)-C(99)	118.3(4)	C(95)-C(94)-C(101)	115.5(4)
N(5)-C(100)-C(92)	122.6(4)	C(25)-C(26)-C(27)	121.1(5)
C(99)-C(100)-C(92)	119.1(4)	C(25)-C(26)-C(33)	121.4(6)
N(5)-C(100)-Yb(3)	40.46(19)	C(27)-C(26)-C(33)	117.5(7)
C(99)-C(100)-Yb(3)	78.0(3)	N(3)-C(55)-C(56)	124.4(5)
C(92)-C(100)-Yb(3)	162.4(3)	N(6)-C(98)-C(97)	123.3(4)
CT06-C(80)-C(79)	54.0(3)	CT05-C(72)-C(73)	54.1(3)
CT06-C(80)-C(81)	53.3(3)	CT05-C(72)-C(71)	53.2(3)
C(79)-C(80)-C(81)	107.3(4)	C(73)-C(72)-C(71)	107.3(5)
CT06-C(80)-C(85)	174.7(6)	CT05-C(72)-C(76)	174.0(5)
C(79)-C(80)-C(85)	127.0(5)	C(73)-C(72)-C(76)	125.9(6)
C(81)-C(80)-C(85)	125.2(5)	C(71)-C(72)-C(76)	126.3(5)
CT06-C(80)-Yb(3)	63.3(2)	CT05-C(72)-Yb(3)	63.12(17)
C(79)-C(80)-Yb(3)	75.1(3)	C(73)-C(72)-Yb(3)	75.1(2)
C(81)-C(80)-Yb(3)	74.7(3)	C(71)-C(72)-Yb(3)	74.1(3)
C(85)-C(80)-Yb(3)	121.8(4)	C(76)-C(72)-Yb(3)	122.9(4)
CT06-C(83)-C(79)	54.0(3)	CT06-C(81)-C(82)	54.4(3)
CT06-C(83)-C(82)	54.0(3)	CT06-C(81)-C(80)	53.7(3)
C(79)-C(83)-C(82)	107.9(4)	C(82)-C(81)-C(80)	108.0(4)
CT06-C(83)-C(88)	174.4(5)	CT06-C(81)-C(86)	170.1(6)
C(79)-C(83)-C(88)	125.2(4)	C(82)-C(81)-C(86)	125.3(5)
C(82)-C(83)-C(88)	126.5(5)	C(80)-C(81)-C(86)	125.6(5)
CT06-C(83)-Yb(3)	62.6(2)	CT06-C(81)-Yb(3)	62.8(3)
C(79)-C(83)-Yb(3)	74.5(3)	C(82)-C(81)-Yb(3)	74.2(3)
C(82)-C(83)-Yb(3)	73.9(3)	C(80)-C(81)-Yb(3)	73.8(4)
C(88)-C(83)-Yb(3)	122.9(4)	C(86)-C(81)-Yb(3)	127.1(4)
C(91)-C(92)-C(100)	115.8(5)	N(5)-C(89)-C(90)	124.4(5)
C(91)-C(92)-C(93)	125.2(4)	CT05-C(70)-C(71)	54.0(3)
C(100)-C(92)-C(93)	119.0(4)	CT05-C(70)-C(69)	53.3(3)
CT06-C(79)-C(80)	54.6(3)	C(71)-C(70)-C(69)	107.3(5)
CT06-C(79)-C(83)	54.0(3)	CT05-C(70)-C(74)	177.2(5)
C(80)-C(79)-C(83)	108.6(4)	C(71)-C(70)-C(74)	126.3(5)
CT06-C(79)-C(84)	173.7(6)	C(69)-C(70)-C(74)	126.3(5)
C(80)-C(79)-C(84)	126.8(5)	CT05-C(70)-Yb(3)	63.2(2)
C(83)-C(79)-C(84)	124.2(4)	C(71)-C(70)-Yb(3)	74.4(3)
CT06-C(79)-Yb(3)	62.8(2)	C(69)-C(70)-Yb(3)	75.2(3)
C(80)-C(79)-Yb(3)	74.1(3)	C(74)-C(70)-Yb(3)	119.6(4)
C(83)-C(79)-Yb(3)	74.7(3)	C(97)-C(96)-C(95)	120.3(5)
C(84)-C(79)-Yb(3)	123.3(4)	C(92)-C(91)-C(90)	122.2(4)
CT06-C(82)-C(81)	54.3(3)	CT05-C(71)-C(70)	55.1(3)
CT06-C(82)-C(83)	53.8(3)	CT05-C(71)-C(72)	54.2(3)
C(81)-C(82)-C(83)	108.1(4)	C(70)-C(71)-C(72)	109.2(4)
CT06-C(82)-C(87)	173.5(6)	CT05-C(71)-C(75)	174.9(4)
C(81)-C(82)-C(87)	125.7(5)	C(70)-C(71)-C(75)	126.5(7)
C(83)-C(82)-C(87)	125.6(4)	C(72)-C(71)-C(75)	124.0(6)

Table S23. Bond angles [deg] for Cp*₂Yb(5,6-Me₂phen) (**7**) (continued).

CT05-C(71)-Yb(3)	63.4(2)	C(12)-Yb-C(14)	50.4(2)
C(70)-C(71)-Yb(3)	74.8(3)	C(11)-Yb-C(14)	50.90(19)
C(72)-C(71)-Yb(3)	74.6(3)	N(2)-Yb-C(2)	84.32(17)
C(75)-C(71)-Yb(3)	121.4(4)	CT02-Yb-C(2)	166.72(12)
C(98)-C(97)-C(96)	119.7(4)	N(1)-Yb-C(2)	84.78(15)
C(96)-C(95)-C(99)	117.5(4)	CT01-Yb-C(2)	27.11(11)
C(96)-C(95)-C(94)	124.4(5)	C(13)-Yb-C(2)	162.4(2)
C(99)-C(95)-C(94)	118.2(4)	C(12)-Yb-C(2)	162.9(2)
C(55)-N(3)-C(66)	116.1(4)	C(11)-Yb-C(2)	147.6(2)
C(55)-N(3)-Yb(2)	127.3(3)	C(14)-Yb-C(2)	146.6(2)
C(66)-N(3)-Yb(2)	116.5(3)	N(2)-Yb-C(15)	126.7(2)
C(55)-C(56)-C(57)	119.7(5)	CT02-Yb-C(15)	27.02(15)
N(3)-C(66)-C(58)	122.4(4)	N(1)-Yb-C(15)	126.55(16)
N(3)-C(66)-C(65)	116.5(4)	CT01-Yb-C(15)	112.61(15)
C(58)-C(66)-C(65)	121.0(4)	C(13)-Yb-C(15)	50.7(3)
N(3)-C(66)-Yb(2)	40.7(2)	C(12)-Yb-C(15)	50.66(19)
C(58)-C(66)-Yb(2)	162.2(3)	C(11)-Yb-C(15)	31.06(17)
C(65)-C(66)-Yb(2)	75.9(3)	C(14)-Yb-C(15)	31.3(3)
CT05-C(69)-C(73)	54.3(3)	C(2)-Yb-C(15)	139.71(19)
CT05-C(69)-C(70)	54.0(3)	N(2)-Yb-C(1)	113.00(18)
C(73)-C(69)-C(70)	108.3(4)	CT02-Yb-C(1)	140.56(13)
CT05-C(69)-C(78)	173.2(5)	N(1)-Yb-C(1)	83.37(17)
C(73)-C(69)-C(78)	125.8(5)	CT01-Yb-C(1)	27.18(11)
C(70)-C(69)-C(78)	125.4(6)	C(13)-Yb-C(1)	166.3(2)
CT05-C(69)-Yb(3)	62.2(2)	C(12)-Yb-C(1)	138.0(3)
C(73)-C(69)-Yb(3)	74.4(3)	C(11)-Yb-C(1)	116.4(2)
C(70)-C(69)-Yb(3)	73.5(3)	C(14)-Yb-C(1)	144.8(3)
C(78)-C(69)-Yb(3)	124.6(3)	C(2)-Yb-C(1)	31.32(16)
C(59)-C(60)-C(61)	120.1(4)	C(15)-Yb-C(1)	118.6(2)
C(59)-C(60)-C(67)	123.9(5)	N(2)-Yb-C(3)	84.98(17)
C(61)-C(60)-C(67)	116.0(5)	CT02-Yb-C(3)	139.96(11)
N(2)-Yb-CT02	106.18(12)	N(1)-Yb-C(3)	113.76(15)
N(2)-Yb-N(1)	70.55(14)	CT01-Yb-C(3)	26.74(12)
CT02-Yb-N(1)	106.17(10)	C(13)-Yb-C(3)	138.6(3)
N(2)-Yb-CT01	106.81(11)	C(12)-Yb-C(3)	166.1(2)
CT02-Yb-CT01	139.625(10)	C(11)-Yb-C(3)	143.5(2)
N(1)-Yb-CT01	106.29(11)	C(14)-Yb-C(3)	115.8(2)
N(2)-Yb-C(13)	79.8(2)	C(2)-Yb-C(3)	30.80(15)
CT02-Yb-C(13)	26.36(18)	C(15)-Yb-C(3)	117.60(17)
N(1)-Yb-C(13)	97.0(3)	C(1)-Yb-C(3)	51.13(16)
CT01-Yb-C(13)	156.7(3)	C(60)-C(59)-C(58)	121.3(5)
N(2)-Yb-C(12)	97.0(2)	C(60)-C(59)-C(68)	121.8(5)
CT02-Yb-C(12)	26.46(14)	C(58)-C(59)-C(68)	116.9(5)
N(1)-Yb-C(12)	79.71(18)	CT04-C(49)-C(45)	55.0(3)
CT01-Yb-C(12)	156.1(2)	CT04-C(49)-C(48)	54.8(3)
C(13)-Yb-C(12)	30.1(3)	C(45)-C(49)-C(48)	109.8(4)
N(2)-Yb-C(11)	126.5(2)	CT04-C(49)-C(54)	173.2(5)
CT02-Yb-C(11)	26.50(14)	C(45)-C(49)-C(54)	125.2(6)
N(1)-Yb-C(11)	95.82(16)	C(48)-C(49)-C(54)	124.5(6)
CT01-Yb-C(11)	126.51(17)	CT04-C(49)-Yb(2)	63.0(2)
C(13)-Yb-C(11)	49.9(2)	C(45)-C(49)-Yb(2)	75.4(3)
C(12)-Yb-C(11)	30.0(2)	C(48)-C(49)-Yb(2)	73.8(3)
N(2)-Yb-C(14)	95.8(3)	C(54)-C(49)-Yb(2)	123.8(3)
CT02-Yb-C(14)	26.88(14)	C(89)-C(90)-C(91)	117.9(5)
N(1)-Yb-C(14)	126.9(3)	C(56)-C(57)-C(58)	118.9(5)
CT01-Yb-C(14)	126.6(3)	CT05-C(73)-C(69)	53.8(3)
C(13)-Yb-C(14)	30.3(3)	CT05-C(73)-C(72)	54.1(3)

Table S23. Bond angles [deg] for Cp*₂Yb(5,6-Me₂phen) (**7**) (continued).

C(69)-C(73)-C(72)	107.9(5)	CT02-C(11)-C(16)	177.5(5)
CT05-C(73)-C(77)	174.2(5)	C(12)-C(11)-C(16)	126.1(8)
C(69)-C(73)-C(77)	123.6(5)	C(15)-C(11)-C(16)	125.2(8)
C(72)-C(73)-C(77)	128.2(5)	CT02-C(11)-Yb	63.2(2)
CT05-C(73)-Yb(3)	62.45(18)	C(12)-C(11)-Yb	74.6(3)
C(69)-C(73)-Yb(3)	74.7(3)	C(15)-C(11)-Yb	74.8(3)
C(72)-C(73)-Yb(3)	73.8(2)	C(16)-C(11)-Yb	119.3(4)
C(77)-C(73)-Yb(3)	122.8(4)	CT02-C(12)-C(13)	53.9(6)
N(1)-C(32)-C(31)	118.1(4)	CT02-C(12)-C(11)	54.7(4)
N(1)-C(32)-C(24)	122.0(5)	C(13)-C(12)-C(11)	108.6(7)
C(31)-C(32)-C(24)	119.9(5)	CT02-C(12)-C(17)	173.8(7)
N(1)-C(32)-Yb	41.0(2)	C(13)-C(12)-C(17)	125.7(11)
C(31)-C(32)-Yb	77.1(3)	C(11)-C(12)-C(17)	125.3(10)
C(24)-C(32)-Yb	162.8(4)	CT02-C(12)-Yb	63.6(3)
CT01-C(3)-C(4)	55.2(3)	C(13)-C(12)-Yb	74.4(5)
CT01-C(3)-C(2)	54.4(3)	C(11)-C(12)-Yb	75.4(4)
C(4)-C(3)-C(2)	109.5(5)	C(17)-C(12)-Yb	122.7(5)
CT01-C(3)-C(8)	174.1(6)	CT01-C(4)-C(3)	53.7(3)
C(4)-C(3)-C(8)	124.6(5)	CT01-C(4)-C(5)	52.9(3)
C(2)-C(3)-C(8)	125.5(5)	C(3)-C(4)-C(5)	106.6(5)
CT01-C(3)-Yb	63.3(2)	CT01-C(4)-C(9)	171.5(7)
C(4)-C(3)-Yb	75.9(3)	C(3)-C(4)-C(9)	126.5(6)
C(2)-C(3)-Yb	74.0(3)	C(5)-C(4)-C(9)	125.9(6)
C(8)-C(3)-Yb	122.6(4)	CT01-C(4)-Yb	62.1(3)
N(2)-C(31)-C(32)	117.9(4)	C(3)-C(4)-Yb	73.7(3)
N(2)-C(31)-C(27)	121.6(5)	C(5)-C(4)-Yb	74.1(3)
C(32)-C(31)-C(27)	120.4(5)	C(9)-C(4)-Yb	126.4(5)
N(2)-C(31)-Yb	40.4(2)	C(26)-C(25)-C(24)	120.8(5)
C(32)-C(31)-Yb	77.6(3)	C(26)-C(25)-C(34)	120.8(6)
C(27)-C(31)-Yb	161.9(4)	C(24)-C(25)-C(34)	118.4(6)
CT01-C(2)-C(3)	53.8(3)	C(21)-N(1)-C(32)	118.5(4)
CT01-C(2)-C(1)	53.9(3)	C(21)-N(1)-Yb	125.2(3)
C(3)-C(2)-C(1)	107.7(5)	C(32)-N(1)-Yb	116.3(3)
CT01-C(2)-C(7)	176.5(6)	C(30)-N(2)-C(31)	117.8(4)
C(3)-C(2)-C(7)	126.1(5)	C(30)-N(2)-Yb	125.3(4)
C(1)-C(2)-C(7)	126.0(5)	C(31)-N(2)-Yb	117.0(3)
CT01-C(2)-Yb	64.0(2)	N(1)-C(21)-C(22)	122.0(5)
C(3)-C(2)-Yb	75.2(3)	C(23)-C(22)-C(21)	120.3(6)
C(1)-C(2)-Yb	74.6(3)	C(28)-C(27)-C(26)	124.5(6)
C(7)-C(2)-Yb	119.5(4)	C(28)-C(27)-C(31)	117.1(5)
CT02-C(15)-C(11)	52.7(4)	C(26)-C(27)-C(31)	118.4(6)
CT02-C(15)-C(14)	53.1(5)	N(2)-C(30)-C(29)	123.3(6)
C(11)-C(15)-C(14)	105.8(6)	C(29)-C(28)-C(27)	120.2(6)
CT02-C(15)-C(20)	171.9(6)	C(30)-C(29)-C(28)	119.9(6)
C(11)-C(15)-C(20)	127.1(8)	CT01-C(1)-C(5)	54.3(3)
C(14)-C(15)-C(20)	126.2(9)	CT01-C(1)-C(2)	53.5(3)
CT02-C(15)-Yb	62.7(2)	C(5)-C(1)-C(2)	107.9(5)
C(11)-C(15)-Yb	74.1(3)	CT01-C(1)-C(6)	174.6(6)
C(14)-C(15)-Yb	74.0(3)	C(5)-C(1)-C(6)	124.6(6)
C(20)-C(15)-Yb	125.3(5)	C(2)-C(1)-C(6)	127.1(6)
C(22)-C(23)-C(24)	120.4(5)	CT01-C(1)-Yb	63.7(3)
C(23)-C(24)-C(32)	116.6(5)	C(5)-C(1)-Yb	76.0(4)
C(23)-C(24)-C(25)	124.2(5)	C(2)-C(1)-Yb	74.1(4)
C(32)-C(24)-C(25)	119.2(6)	C(6)-C(1)-Yb	121.7(4)
CT02-C(11)-C(12)	54.3(5)	CT01-C(5)-C(1)	54.6(3)
CT02-C(11)-C(15)	54.3(4)	CT01-C(5)-C(4)	53.6(3)
C(12)-C(11)-C(15)	108.7(6)	C(1)-C(5)-C(4)	108.2(5)

Table S23. Bond angles [deg] for Cp*₂Yb(5,6-Me₂phen) (**7**) (continued).

CT01-C(5)-C(10)	172.2(7)	N(3)-Yb(2)-C(36)	78.75(16)
C(1)-C(5)-C(10)	124.1(7)	CT04-Yb(2)-C(36)	151.97(11)
C(4)-C(5)-C(10)	127.0(6)	C(48)-Yb(2)-C(36)	153.22(17)
CT01-C(5)-Yb	62.3(3)	C(37)-Yb(2)-C(36)	31.56(14)
C(1)-C(5)-Yb	73.5(4)	C(47)-Yb(2)-C(36)	129.97(15)
C(4)-C(5)-Yb	74.5(4)	C(39)-Yb(2)-C(36)	51.95(16)
C(10)-C(5)-Yb	125.4(4)	N(4)-Yb(2)-C(49)	82.54(14)
CT02-C(14)-C(13)	53.2(5)	CT03-Yb(2)-C(49)	146.51(15)
CT02-C(14)-C(15)	53.7(4)	N(3)-Yb(2)-C(49)	107.25(18)
C(13)-C(14)-C(15)	107.0(6)	CT04-Yb(2)-C(49)	26.84(10)
CT02-C(14)-C(19)	173.3(9)	C(48)-Yb(2)-C(49)	31.31(17)
C(13)-C(14)-C(19)	131.5(13)	C(37)-Yb(2)-C(49)	144.06(16)
C(15)-C(14)-C(19)	121.3(12)	C(47)-Yb(2)-C(49)	51.26(14)
CT02-C(14)-Yb	63.2(3)	C(39)-Yb(2)-C(49)	122.84(17)
C(13)-C(14)-Yb	73.9(5)	C(36)-Yb(2)-C(49)	174.00(19)
C(15)-C(14)-Yb	74.7(4)	N(4)-Yb(2)-C(38)	121.20(16)
C(19)-C(14)-Yb	121.4(5)	CT03-Yb(2)-C(38)	27.33(10)
CT02-C(13)-C(12)	54.6(5)	N(3)-Yb(2)-C(38)	130.09(14)
CT02-C(13)-C(14)	55.4(6)	CT04-Yb(2)-C(38)	112.37(10)
C(12)-C(13)-C(14)	110.0(8)	C(48)-Yb(2)-C(38)	139.55(15)
CT02-C(13)-C(18)	174.1(9)	C(37)-Yb(2)-C(38)	31.79(16)
C(12)-C(13)-C(18)	123.3(14)	C(47)-Yb(2)-C(38)	113.76(16)
C(14)-C(13)-C(18)	126.3(13)	C(39)-Yb(2)-C(38)	30.74(14)
CT02-C(13)-Yb	64.2(4)	C(36)-Yb(2)-C(38)	52.17(16)
C(12)-C(13)-Yb	75.5(5)	C(49)-Yb(2)-C(38)	121.89(18)
C(14)-C(13)-Yb	75.8(5)	N(4)-Yb(2)-C(35)	77.99(15)
C(18)-C(13)-Yb	121.4(5)	CT03-Yb(2)-C(35)	27.09(11)
N(4)-Yb(2)-CT03	104.55(11)	N(3)-Yb(2)-C(35)	92.22(15)
N(4)-Yb(2)-N(3)	70.52(13)	CT04-Yb(2)-C(35)	160.38(11)
CT03-Yb(2)-N(3)	105.94(10)	C(48)-Yb(2)-C(35)	168.13(15)
N(4)-Yb(2)-CT04	107.97(10)	C(37)-Yb(2)-C(35)	51.72(14)
CT03-Yb(2)-CT04	139.364(10)	C(47)-Yb(2)-C(35)	159.47(15)
N(3)-Yb(2)-CT04	107.40(10)	C(39)-Yb(2)-C(35)	31.25(15)
N(4)-Yb(2)-C(48)	90.37(15)	C(36)-Yb(2)-C(35)	31.30(15)
CT03-Yb(2)-C(48)	164.78(11)	C(49)-Yb(2)-C(35)	145.98(15)
N(3)-Yb(2)-C(48)	81.57(16)	C(38)-Yb(2)-C(35)	51.40(15)
CT04-Yb(2)-C(48)	27.67(12)	C(65)-N(4)-C(64)	118.2(4)
N(4)-Yb(2)-C(37)	129.03(14)	C(65)-N(4)-Yb(2)	117.2(3)
CT03-Yb(2)-C(37)	27.52(11)	C(64)-N(4)-Yb(2)	124.3(4)
N(3)-Yb(2)-C(37)	100.47(16)	N(4)-C(65)-C(66)	118.5(4)
CT04-Yb(2)-C(37)	122.17(10)	N(4)-C(65)-C(61)	123.1(4)
C(48)-Yb(2)-C(37)	139.26(14)	C(66)-C(65)-C(61)	118.4(5)
N(4)-Yb(2)-C(47)	121.58(16)	N(4)-C(65)-Yb(2)	40.6(2)
CT03-Yb(2)-C(47)	133.84(12)	C(66)-C(65)-Yb(2)	78.3(3)
N(3)-Yb(2)-C(47)	89.31(16)	C(61)-C(65)-Yb(2)	163.0(4)
CT04-Yb(2)-C(47)	27.21(10)	CT04-C(45)-C(49)	53.3(3)
C(48)-Yb(2)-C(47)	31.49(15)	CT04-C(45)-C(46)	53.3(3)
C(37)-Yb(2)-C(47)	107.90(15)	C(49)-C(45)-C(46)	106.6(5)
N(4)-Yb(2)-C(39)	90.45(15)	CT04-C(45)-C(50)	174.7(5)
CT03-Yb(2)-C(39)	27.20(10)	C(49)-C(45)-C(50)	125.9(5)
N(3)-Yb(2)-C(39)	123.46(14)	C(46)-C(45)-C(50)	127.0(5)
CT04-Yb(2)-C(39)	129.13(10)	CT04-C(45)-Yb(2)	62.08(19)
C(48)-Yb(2)-C(39)	153.47(16)	C(49)-C(45)-Yb(2)	73.7(3)
C(37)-Yb(2)-C(39)	51.79(16)	C(46)-C(45)-Yb(2)	74.4(2)
C(47)-Yb(2)-C(39)	141.71(17)	C(50)-C(45)-Yb(2)	123.1(4)
N(4)-Yb(2)-C(36)	99.89(15)	CT04-C(48)-C(49)	53.0(3)
CT03-Yb(2)-C(36)	27.59(13)	CT04-C(48)-C(47)	53.3(3)

Table S23. Bond angles [deg] for Cp^{*}₂Yb(5,6-Me₂phen) (**7**) (continued).

C(49)-C(48)-C(47)	106.3(5)	C(35)-C(39)-C(44)	125.0(4)
CT04-C(48)-C(53)	176.6(5)	CT03-C(39)-Yb(2)	62.9(3)
C(49)-C(48)-C(53)	125.0(5)	C(38)-C(39)-Yb(2)	74.9(3)
C(47)-C(48)-C(53)	128.6(5)	C(35)-C(39)-Yb(2)	75.1(3)
CT04-C(48)-Yb(2)	63.5(2)	C(44)-C(39)-Yb(2)	122.3(4)
C(49)-C(48)-Yb(2)	74.9(3)	C(64)-C(63)-C(62)	120.2(5)
C(47)-C(48)-Yb(2)	74.3(3)	CT04-C(47)-C(46)	54.1(3)
C(53)-C(48)-Yb(2)	119.2(3)	CT04-C(47)-C(48)	54.5(3)
CT03-C(37)-C(36)	54.3(3)	C(46)-C(47)-C(48)	108.6(4)
CT03-C(37)-C(38)	53.5(3)	CT04-C(47)-C(52)	175.3(4)
C(36)-C(37)-C(38)	107.7(4)	C(46)-C(47)-C(52)	124.2(5)
CT03-C(37)-C(42)	175.6(5)	C(48)-C(47)-C(52)	126.9(6)
C(36)-C(37)-C(42)	125.6(5)	CT04-C(47)-Yb(2)	63.5(2)
C(38)-C(37)-C(42)	126.4(5)	C(46)-C(47)-Yb(2)	75.8(3)
CT03-C(37)-Yb(2)	63.1(2)	C(48)-C(47)-Yb(2)	74.2(3)
C(36)-C(37)-Yb(2)	74.7(3)	C(52)-C(47)-Yb(2)	120.9(3)
C(38)-C(37)-Yb(2)	74.6(3)	CT03-C(36)-C(35)	53.6(3)
C(42)-C(37)-Yb(2)	121.3(4)	CT03-C(36)-C(37)	53.7(3)
C(62)-C(61)-C(65)	115.9(5)	C(35)-C(36)-C(37)	107.3(4)
C(62)-C(61)-C(60)	124.0(4)	CT03-C(36)-C(41)	174.0(6)
C(65)-C(61)-C(60)	120.0(4)	C(35)-C(36)-C(41)	124.2(4)
CT04-C(46)-C(47)	54.2(3)	C(37)-C(36)-C(41)	128.0(5)
CT04-C(46)-C(45)	54.4(3)	CT03-C(36)-Yb(2)	62.7(2)
C(47)-C(46)-C(45)	108.6(5)	C(35)-C(36)-Yb(2)	74.9(3)
CT04-C(46)-C(51)	171.1(5)	C(37)-C(36)-Yb(2)	73.8(3)
C(47)-C(46)-C(51)	124.6(5)	C(41)-C(36)-Yb(2)	123.0(4)
C(45)-C(46)-C(51)	125.9(6)	N(4)-C(64)-C(63)	122.2(5)
CT04-C(46)-Yb(2)	62.16(18)	N(5)-Yb(3)-N(6)	70.96(13)
C(47)-C(46)-Yb(2)	73.3(3)	N(5)-Yb(3)-CT05	106.74(10)
C(45)-C(46)-Yb(2)	74.6(2)	N(6)-Yb(3)-CT05	106.06(11)
C(51)-C(46)-Yb(2)	126.7(3)	N(5)-Yb(3)-CT06	105.10(11)
CT03-C(38)-C(39)	54.4(3)	N(6)-Yb(3)-CT06	105.21(11)
CT03-C(38)-C(37)	53.6(3)	CT05-Yb(3)-CT06	140.988(10)
C(39)-C(38)-C(37)	107.9(4)	N(5)-Yb(3)-C(71)	117.07(18)
CT03-C(38)-C(43)	170.2(5)	N(6)-Yb(3)-C(71)	85.74(16)
C(39)-C(38)-C(43)	126.0(5)	CT05-Yb(3)-C(71)	27.00(11)
C(37)-C(38)-C(43)	125.0(5)	CT06-Yb(3)-C(71)	137.64(14)
CT03-C(38)-Yb(2)	62.5(2)	N(5)-Yb(3)-C(70)	87.20(16)
C(39)-C(38)-Yb(2)	74.3(3)	N(6)-Yb(3)-C(70)	81.77(16)
C(37)-C(38)-Yb(2)	73.6(3)	CT05-Yb(3)-C(70)	27.35(11)
C(43)-C(38)-Yb(2)	127.2(4)	CT06-Yb(3)-C(70)	167.24(12)
C(63)-C(62)-C(61)	120.4(5)	C(71)-Yb(3)-C(70)	30.76(16)
CT03-C(35)-C(39)	53.7(3)	N(5)-Yb(3)-C(72)	133.51(15)
CT03-C(35)-C(36)	54.5(3)	N(6)-Yb(3)-C(72)	115.72(17)
C(39)-C(35)-C(36)	108.2(4)	CT05-Yb(3)-C(72)	27.27(12)
CT03-C(35)-C(40)	174.4(5)	CT06-Yb(3)-C(72)	115.67(14)
C(39)-C(35)-C(40)	126.5(4)	C(71)-Yb(3)-C(72)	31.34(19)
C(36)-C(35)-C(40)	125.0(4)	C(70)-Yb(3)-C(72)	51.68(18)
CT03-C(35)-Yb(2)	62.1(2)	N(5)-Yb(3)-C(80)	128.40(15)
C(39)-C(35)-Yb(2)	73.7(3)	N(6)-Yb(3)-C(80)	98.06(16)
C(36)-C(35)-Yb(2)	73.8(3)	CT05-Yb(3)-C(80)	124.49(11)
C(40)-C(35)-Yb(2)	123.5(4)	CT06-Yb(3)-C(80)	27.25(12)
CT03-C(39)-C(38)	54.9(3)	C(71)-Yb(3)-C(80)	111.86(17)
CT03-C(39)-C(35)	53.9(3)	C(70)-Yb(3)-C(80)	142.59(16)
C(38)-C(39)-C(35)	108.9(4)	C(72)-Yb(3)-C(80)	97.26(16)
CT03-C(39)-C(44)	174.8(6)	N(5)-Yb(3)-C(82)	92.19(15)
C(38)-C(39)-C(44)	125.7(5)	N(6)-Yb(3)-C(82)	124.04(15)

Table S23. Bond angles [deg] for Cp^{*}₂Yb(5,6-Me₂phen) (**7**) (continued).

CT05-Yb(3)-C(82)	129.87(10)	C(13)-CT02-C(15)	144.5(7)
CT06-Yb(3)-C(82)	27.14(10)	C(12)-CT02-C(15)	144.0(6)
C(71)-Yb(3)-C(82)	144.93(18)	C(11)-CT02-C(15)	73.0(5)
C(70)-Yb(3)-C(82)	152.36(15)	C(14)-CT02-C(15)	73.2(6)
C(72)-Yb(3)-C(82)	114.07(18)	C(13)-CT02-Yb	89.5(4)
C(80)-Yb(3)-C(82)	51.57(16)	C(12)-CT02-Yb	90.0(3)
N(5)-Yb(3)-C(73)	108.67(14)	C(11)-CT02-Yb	90.3(3)
N(6)-Yb(3)-C(73)	132.89(18)	C(14)-CT02-Yb	90.0(3)
CT05-Yb(3)-C(73)	27.10(14)	C(15)-CT02-Yb	90.2(3)
CT06-Yb(3)-C(73)	119.28(14)	C(39)-CT03-C(35)	72.4(3)
C(71)-Yb(3)-C(73)	51.33(17)	C(39)-CT03-C(38)	70.7(3)
C(70)-Yb(3)-C(73)	51.67(18)	C(35)-CT03-C(38)	143.1(3)
C(72)-Yb(3)-C(73)	31.09(14)	C(39)-CT03-C(37)	143.7(3)
C(80)-Yb(3)-C(73)	114.06(17)	C(35)-CT03-C(37)	144.0(3)
C(82)-Yb(3)-C(73)	103.04(17)	C(38)-CT03-C(37)	73.0(3)
N(5)-Yb(3)-C(81)	122.91(16)	C(39)-CT03-C(36)	144.3(3)
N(6)-Yb(3)-C(81)	128.03(14)	C(35)-CT03-C(36)	72.0(3)
CT05-Yb(3)-C(81)	114.20(10)	C(38)-CT03-C(36)	145.0(3)
CT06-Yb(3)-C(81)	26.99(10)	C(37)-CT03-C(36)	72.0(3)
C(71)-Yb(3)-C(81)	117.56(18)	C(39)-CT03-Yb(2)	89.9(3)
C(70)-Yb(3)-C(81)	141.38(15)	C(35)-CT03-Yb(2)	90.8(3)
C(72)-Yb(3)-C(81)	90.35(18)	C(38)-CT03-Yb(2)	90.1(3)
C(80)-Yb(3)-C(81)	31.45(17)	C(37)-CT03-Yb(2)	89.4(3)
C(82)-Yb(3)-C(81)	30.77(15)	C(36)-CT03-Yb(2)	89.8(3)
C(73)-Yb(3)-C(81)	92.89(17)	C(49)-CT04-C(46)	143.9(4)
N(5)-Yb(3)-C(79)	99.14(14)	C(49)-CT04-C(47)	144.3(4)
N(6)-Yb(3)-C(79)	78.46(17)	C(46)-CT04-C(47)	71.7(4)
CT05-Yb(3)-C(79)	153.81(11)	C(49)-CT04-C(45)	71.7(4)
CT06-Yb(3)-C(79)	26.90(12)	C(46)-CT04-C(45)	72.2(4)
C(71)-Yb(3)-C(79)	132.94(16)	C(47)-CT04-C(45)	143.9(4)
C(70)-Yb(3)-C(79)	155.89(16)	C(49)-CT04-C(48)	72.2(4)
C(72)-Yb(3)-C(79)	127.31(16)	C(46)-CT04-C(48)	143.8(3)
C(80)-Yb(3)-C(79)	30.83(15)	C(47)-CT04-C(48)	72.1(4)
C(82)-Yb(3)-C(79)	51.23(16)	C(45)-CT04-C(48)	143.9(3)
C(73)-Yb(3)-C(79)	143.22(18)	C(49)-CT04-Yb(2)	90.2(2)
C(81)-Yb(3)-C(79)	51.12(16)	C(46)-CT04-Yb(2)	91.0(2)
C(3)-CT01-C(2)	71.8(3)	C(47)-CT04-Yb(2)	89.3(2)
C(3)-CT01-C(5)	144.6(4)	C(45)-CT04-Yb(2)	90.7(2)
C(2)-CT01-C(5)	143.6(4)	C(48)-CT04-Yb(2)	88.8(2)
C(3)-CT01-C(1)	144.3(4)	C(71)-CT05-C(69)	143.7(5)
C(2)-CT01-C(1)	72.5(4)	C(71)-CT05-C(72)	72.6(4)
C(5)-CT01-C(1)	71.1(4)	C(69)-CT05-C(72)	143.7(4)
C(3)-CT01-C(4)	71.1(4)	C(71)-CT05-C(73)	144.4(4)
C(2)-CT01-C(4)	142.9(4)	C(69)-CT05-C(73)	71.9(4)
C(5)-CT01-C(4)	73.5(4)	C(72)-CT05-C(73)	71.8(4)
C(1)-CT01-C(4)	144.6(4)	C(71)-CT05-C(70)	71.0(4)
C(3)-CT01-Yb	90.0(3)	C(69)-CT05-C(70)	72.7(4)
C(2)-CT01-Yb	88.9(3)	C(72)-CT05-C(70)	143.6(4)
C(5)-CT01-Yb	91.0(3)	C(73)-CT05-C(70)	144.6(3)
C(1)-CT01-Yb	89.1(3)	C(71)-CT05-Yb(3)	89.6(2)
C(4)-CT01-Yb	91.0(3)	C(69)-CT05-Yb(3)	90.9(2)
C(13)-CT02-C(12)	71.5(7)	C(72)-CT05-Yb(3)	89.6(2)
C(13)-CT02-C(11)	142.5(8)	C(73)-CT05-Yb(3)	90.5(2)
C(12)-CT02-C(11)	71.0(5)	C(70)-CT05-Yb(3)	89.5(2)
C(13)-CT02-C(14)	71.4(7)	C(79)-CT06-C(83)	72.0(3)
C(12)-CT02-C(14)	142.9(8)	C(79)-CT06-C(81)	144.4(3)
C(11)-CT02-C(14)	146.1(7)	C(83)-CT06-C(81)	143.6(3)

Table S23. Bond angles [deg] for Cp^{*}₂Yb(5,6-Me₂phen) (**7**) (continued).

C(79)-CT06-C(82)	144.2(3)
C(83)-CT06-C(82)	72.3(3)
C(81)-CT06-C(82)	71.3(3)
C(79)-CT06-C(80)	71.5(3)
C(83)-CT06-C(80)	143.4(4)
C(81)-CT06-C(80)	73.0(4)
C(82)-CT06-C(80)	144.3(4)
C(79)-CT06-Yb(3)	90.3(3)
C(83)-CT06-Yb(3)	90.5(3)
C(81)-CT06-Yb(3)	90.2(3)
C(82)-CT06-Yb(3)	89.6(3)
C(80)-CT06-Yb(3)	89.4(3)

Table S24. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cp}^*_2\text{Yb}(5,6\text{-Me}_2\text{phen})$.

	x	y	z	U(eq)
H(85A)	-3101	8882	3591	93
H(85B)	-1912	9187	3478	93
H(85C)	-2999	9356	3782	93
H(10A)	7186	9175	5471	71
H(10B)	7019	9674	5408	71
H(10C)	7915	9415	5099	71
H(55)	2475	3439	6456	42
H(98)	930	9318	3347	44
H(89)	2620	8058	5057	43
H(96)	4285	10047	3735	47
H(91)	6051	8717	5531	47
H(97)	2281	9887	3210	49
H(56)	3889	2921	6232	52
H(10D)	5812	10170	4170	70
H(10E)	7195	9943	4407	70
H(10F)	6306	10206	4716	70
H(43A)	-1997	4299	7280	88
H(43B)	-1081	4598	7648	88
H(43C)	-2061	4253	7819	88
H(42A)	-1764	3812	6786	81
H(42B)	-1659	3314	6873	81
H(42C)	-577	3546	6611	81
H(40A)	2645	3496	8633	67
H(40B)	3287	3260	8238	67
H(40C)	2054	3048	8444	67
H(41A)	2025	2816	7587	70
H(41B)	1556	2966	7063	70
H(41C)	478	2744	7335	70
H(90)	4594	8138	5599	52
H(50A)	133	5203	7480	84
H(50B)	1468	5495	7537	84
H(50C)	1407	5106	7879	84
H(76A)	-2306	7832	3387	97
H(76B)	-1858	7898	2892	97
H(76C)	-2122	8298	3197	97
H(54A)	5246	4944	7517	95
H(54B)	4272	4973	7899	95
H(54C)	4321	5354	7544	95
H(57)	5855	2695	6752	51
H(53A)	4597	4292	6445	74
H(53B)	5242	4293	6983	74
H(53C)	5270	4713	6684	74
H(84A)	-540	9758	4055	85
H(84B)	930	9675	4363	85
H(84C)	-312	9838	4601	85
H(44A)	1611	4074	8712	78
H(44B)	7	4177	8616	78
H(44C)	1059	4481	8416	78
H(88A)	1263	8890	5484	68
H(88B)	710	9361	5387	68
H(88C)	1937	9190	5146	68
H(67A)	8447	3306	8659	84
H(67B)	9254	3140	8266	84

H(67C)	8338	2821	8507	84
H(74A)	4243	8120	3723	102
H(74B)	3614	8560	3523	102
H(74C)	3711	8173	3180	102
H(77A)	-1351	7415	3963	89
H(77B)	-140	7445	4398	89
H(77C)	-35	7117	3992	89
H(68A)	7291	2497	7200	84
H(68B)	7665	2387	7739	84
H(68C)	8638	2692	7505	84
H(23)	6253	991	7661	64
H(8A)	11866	2443	9176	101
H(8B)	13457	2422	9395	101
H(8C)	12334	2249	9681	101
H(21)	9786	545	8416	54
H(87A)	156	8302	5445	83
H(87B)	-440	7952	5072	83
H(87C)	-1461	8226	5322	83
H(22)	7934	467	7808	68
H(7A)	10854	2249	8521	88
H(7B)	10150	1830	8289	88
H(7C)	11423	2034	8098	88
H(30)	10111	2056	9867	58
H(78A)	3806	7628	4185	89
H(78B)	2811	7228	4100	89
H(78C)	2716	7542	4520	89
H(28)	6530	2567	9224	77
H(75A)	-309	8552	2736	131
H(75B)	1130	8397	2618	131
H(75C)	1068	8797	2946	131
H(29)	8391	2560	9842	78
H(86A)	-3406	8322	3973	85
H(86B)	-3481	8274	4511	85
H(86C)	-2520	7967	4274	85
H(6A)	11474	1194	7956	138
H(6B)	11853	766	8236	138
H(6C)	13016	1023	8037	138
H(17A)	8555	176	9173	389
H(17B)	7788	618	9194	389
H(17C)	7789	279	9599	389
H(19A)	12703	1227	10640	424
H(19B)	11321	1196	10853	424
H(19C)	11500	1562	10492	424
H(18A)	8720	1368	10317	448
H(18B)	7840	947	10200	448
H(18C)	7924	1288	9803	448
H(34A)	4956	1452	7537	132
H(34B)	4897	1956	7541	132
H(34C)	3933	1688	7819	132
H(33A)	5147	2577	8690	120
H(33B)	4031	2256	8429	120
H(33C)	4944	2531	8139	120
H(20A)	13782	780	10387	271
H(20B)	13897	556	9906	271
H(20C)	13446	289	10318	271
H(10G)	14993	763	9334	163
H(10H)	14979	805	8790	163
H(10I)	13837	528	8976	163
H(16A)	12326	13	9456	244
H(16B)	11073	118	9051	244

H(16C)	10850	-189	9465	244
H(9A)	15151	1286	9849	141
H(9B)	14204	1616	10060	141
H(9C)	15300	1780	9758	141
H(162)	7351	3757	8775	55
H(63)	5915	4321	8891	52
H(52A)	2500	4174	6028	80
H(52B)	1270	4499	5879	80
H(52C)	1003	4068	6133	80
H(64)	3931	4451	8366	50
H(51A)	-957	4928	6828	70
H(51B)	-927	4501	6539	70
H(51C)	-571	4941	6320	70

6. Theoretical calculations

Table S25. Cartesian Coordinates for Cp*₂Yb(phen) (**1**), monomer

Yb	2.359875575	0.1204872353	1.1009923061
C	-0.0386838467	-0.9006206757	1.7147640568
C	0.7408004219	-1.0136909472	2.9007472828
C	1.7664600375	-1.9730354026	2.6609075501
C	1.6207915382	-2.4558679687	1.3260498552
C	0.5011568143	-1.7909788349	0.7402128824
C	2.732412288	1.0535867088	-1.3736457798
C	3.61984908	1.8106803423	-0.5517796129
C	4.6314345743	0.9318596817	-0.0731996868
C	4.3736301673	-0.3707554786	-0.5960812887
C	3.2102780977	-0.2896867778	-1.4182720147
C	1.6068163713	1.6034836476	-2.2050704673
C	3.5908204981	3.2957292314	-0.3382506592
C	5.8551734921	1.351402229	0.6868472679
C	5.2962823721	-1.5531012082	-0.4956554217
C	2.7464099291	-1.3365283201	-2.3874940286
C	0.4581539501	-0.3291066378	4.2053637928
C	2.7071674833	-2.5273708892	3.691901162
C	2.3533344798	-3.6350375466	0.753261737
C	-0.1634573184	-2.1415626981	-0.560727691
C	-1.3251264969	-0.1395655937	1.5751460299
N	1.3824899395	2.1619575201	1.7827811843
C	1.9619540583	2.7688316438	2.8906404653
C	1.4647528512	4.0159094989	3.3904545933
C	0.394980769	4.6250875348	2.7419582986
C	-0.1713188441	4.0043095595	1.6128136918
C	0.3532295379	2.7969154301	1.1884538888
C	2.099762163	4.5874082796	4.5453581257
C	3.1482577143	3.9742818094	5.1529945547
C	3.6695361154	2.7272569887	4.6672031353
C	3.0519242064	2.1359724348	3.5175141202
N	3.5121585193	0.9295267557	3.0021624839
C	4.5586484425	0.3455308985	3.6160190046
C	5.2001491665	0.8588124644	4.7291260864
C	4.7436333378	2.0763382041	5.2661718388
H	0.0094255368	5.5718449078	3.1101732033
H	5.2204552588	2.5139819443	6.1390035486
H	6.0367495999	0.3247235834	5.1657308436
H	4.896544061	-0.5933882601	3.1820037697
H	-0.0730810138	2.2963121283	0.3217545045
H	1.7190401356	5.5325141709	4.9248849372
H	3.6174668626	4.4210771621	6.0261781883
H	-1.0035127445	4.449872663	1.0791119675
H	-0.2222789779	-0.925983274	4.8276398241
H	1.3702605257	-0.1654032405	4.7862112025
H	-0.0105244471	0.6482181127	4.0572688594
H	-2.1757324048	-0.7465323195	1.9140568541
H	-1.3304833623	0.7802555495	2.1666925108
H	-1.5312865502	0.1351796532	0.5350911236
H	-1.0529905973	-2.7621732698	-0.3871487561
H	-0.5004372938	-1.259528132	-1.1171808459
H	0.4989078838	-2.708210401	-1.2184984617
H	1.8872268729	-4.5769763659	1.0735489226
H	2.349351483	-3.6353951062	-0.3400787298
H	3.3980289936	-3.6744043421	1.0776784179

H	2.2573044096	-3.3848815832	4.2104252532
H	3.6443418952	-2.8845739915	3.2510536928
H	2.962203238	-1.7879875902	4.4562108788
H	1.9308118604	1.7931262291	-3.2373277047
H	0.7544814445	0.9167507308	-2.2651031086
H	1.2377396846	2.5548245587	-1.8109652621
H	4.2369887043	3.8091466142	-1.0629470273
H	2.584757174	3.7085636397	-0.4501262245
H	3.9414528153	3.5716872872	0.6606694299
H	3.2905210664	-1.2438999	-3.3378726347
H	2.9207137378	-2.3527609305	-2.0231413155
H	1.6827789802	-1.2441330933	-2.6217800492
H	6.0662670084	-1.5211576616	-1.2785723013
H	5.8258787057	-1.5878435125	0.4625408019
H	4.7639033072	-2.5014038116	-0.6102432534
H	6.6372881949	1.7035674267	0.000723479
H	5.6456211563	2.1643700005	1.3874060287
H	6.2869953103	0.5291713041	1.264874689

Table S26. Cartesian Coordinates for Cp*₂Yb(3,8-Me₂phen), monomer

Yb	2.276325	0.352780	1.194732
C	2.841926	0.602498	-1.426707
C	3.912725	1.238391	-0.729915
C	4.646984	0.236055	-0.033097
C	4.028100	-1.019476	-0.293518
C	2.913251	-0.797217	-1.155146
C	0.118962	1.426357	2.381829
C	0.191518	0.091424	2.867415
C	-0.072092	-0.789041	1.776247
C	-0.329556	0.005902	0.620197
C	-0.188832	1.377351	0.989104
C	0.171521	2.663289	3.229502
C	0.371846	-0.299532	4.304676
C	-0.245169	-2.279747	1.862457
C	-0.933839	-0.500899	-0.656336
C	-0.531872	2.558699	0.125211
C	4.313444	2.677951	-0.878978
C	5.914628	0.444268	0.741215
C	4.574165	-2.363308	0.092875
C	2.128194	-1.881704	-1.837107
C	1.977280	1.269914	-2.457278
N	3.316868	-0.772784	2.989999
C	3.959953	0.040391	3.910870
C	4.592101	-0.521977	5.064221
C	4.542097	-1.897730	5.258071
C	3.874584	-2.724186	4.326090
C	3.295711	-2.100119	3.232318
C	5.251693	0.368780	5.979689
C	5.277151	1.709858	5.767901
C	4.642851	2.298596	4.620383
C	3.978922	1.431960	3.695721
C	4.649653	3.667267	4.376709
C	4.005325	4.190619	3.233805
C	3.381975	3.282555	2.391681
N	3.346555	1.947055	2.573689
H	5.018244	-2.333263	6.133685
C	3.798086	-4.213128	4.509964
H	5.153048	4.332978	5.074350
C	3.989199	5.664899	2.946603
H	2.777854	-2.704818	2.489503
H	2.870409	3.649835	1.503098
H	5.781296	2.369257	6.470297
H	5.733912	-0.060085	6.854835
H	-0.586266	-0.275453	4.841228
H	0.777905	-1.309330	4.408387
H	1.054346	0.375924	4.829302
H	-0.811375	2.872544	3.673081
H	0.887272	2.571052	4.051113

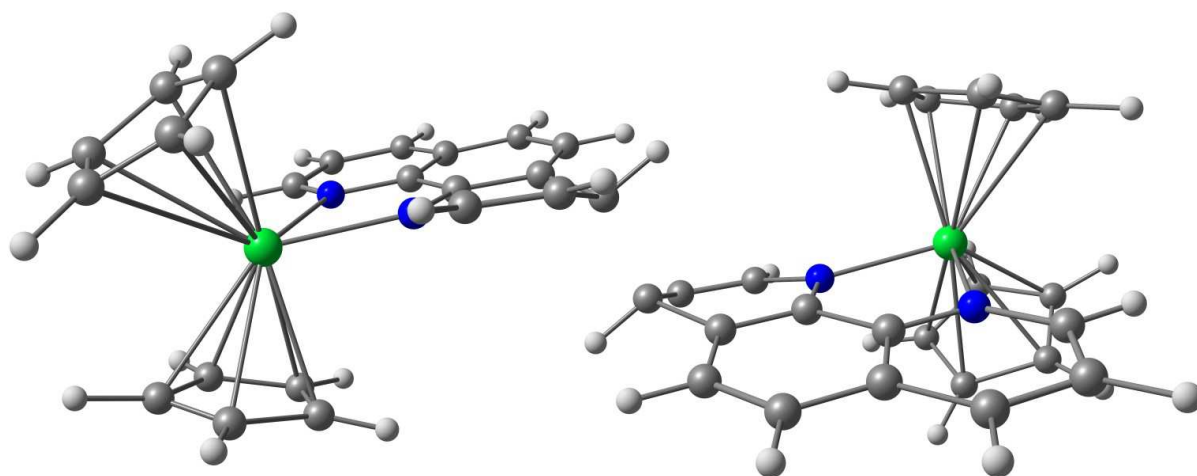
H	0.454323	3.547946	2.651465
H	-1.586115	2.844484	0.242804
H	0.061857	3.444651	0.375592
H	-0.374348	2.348203	-0.936270
H	-2.029652	-0.524952	-0.575219
H	-0.696923	0.133196	-1.514964
H	-0.612797	-1.518333	-0.894297
H	-1.301497	-2.550645	1.994077
H	0.100346	-2.792939	0.957893
H	0.298507	-2.704721	2.711355
H	4.971737	2.812986	-1.748024
H	3.451818	3.336724	-1.034260
H	4.857484	3.046296	-0.004839
H	6.797012	0.311045	0.100703
H	5.971215	1.449933	1.166962
H	6.006487	-0.263441	1.570528
H	2.507536	1.353100	-3.415900
H	1.057596	0.712086	-2.650991
H	1.689773	2.285800	-2.167386
H	2.736259	-2.378760	-2.604898
H	1.794001	-2.664471	-1.146117
H	1.240342	-1.488568	-2.337001
H	5.309900	-2.711316	-0.645053
H	5.076465	-2.342696	1.064183
H	3.792385	-3.128727	0.141010
H	3.296330	-4.477532	5.448955
H	3.245867	-4.689552	3.694378
H	4.796353	-4.666734	4.543226
H	3.461838	5.885459	2.013710
H	3.492857	6.225728	3.748242
H	5.005102	6.068621	2.856147

Table S27. Cartesian Coordinates for Cp*₂Yb(5,6-Me₂phen) (7).

Yb	2.098084	0.232900	0.984480
C	0.462358	-1.157773	2.579816
C	0.578614	0.126708	3.185381
C	1.911234	0.269284	3.673659
C	2.625238	-0.925236	3.355472
C	1.725345	-1.805918	2.683670
C	3.648570	1.187331	-0.987528
C	2.890727	2.302484	-0.534936
C	3.309729	2.615588	0.793250
C	4.346710	1.703006	1.151976
C	4.539213	0.805997	0.059803
N	1.793064	-1.443799	-0.639113
C	0.671300	-1.323914	-1.450832
C	0.400973	-2.263789	-2.495883
C	1.306806	-3.305831	-2.686348
C	2.445864	-3.409327	-1.864759
C	2.634455	-2.467304	-0.873589
C	-0.790442	-2.098802	-3.314652
C	-1.649473	-1.050798	-3.088245
C	-1.376916	-0.093181	-2.027395
C	-0.201602	-0.247680	-1.225280
C	-2.218636	0.982671	-1.750737
C	-1.900236	1.879049	-0.713054
C	-0.742883	1.668669	0.010264
N	0.105329	0.648238	-0.207752
C	-1.003841	-3.127840	-4.394641
C	-2.900910	-0.813892	-3.893945
C	1.954155	3.116557	-1.378144
C	2.893949	3.830969	1.574123
C	5.269302	1.837892	2.327192
C	5.627645	-0.226560	-0.036474
C	3.614159	0.621458	-2.376671
C	2.371382	1.371246	4.583535
C	3.994589	-1.304680	3.845280
C	2.002116	-3.239596	2.336416
C	-0.794519	-1.774856	2.040938
C	-0.549494	1.079936	3.460169
H	1.144919	-4.041258	-3.465731
H	-3.120685	1.138172	-2.330836
H	-2.540235	2.723585	-0.482634
H	3.163582	-4.211418	-1.997114
H	-0.469882	2.352131	0.811953
H	3.502886	-2.529063	-0.220654
H	-3.054532	-1.552048	-4.678801
H	-3.788640	-0.832257	-3.250737
H	-2.873960	0.171291	-4.374203
H	-1.074675	-4.134289	-3.965735
H	-1.907688	-2.959831	-4.976993
H	-0.161176	-3.137046	-5.095921

H	6.579054	0.225092	-0.348787
H	5.814977	-0.724569	0.921284
H	5.391433	-1.001939	-0.771530
H	6.122032	2.481943	2.070525
H	4.780269	2.291590	3.192786
H	5.685183	0.877140	2.643126
H	3.927813	-1.964493	4.720835
H	4.580379	-1.843523	3.091743
H	4.577061	-0.431058	4.146882
H	3.481211	4.711677	1.280165
H	1.841613	4.089327	1.412526
H	3.037572	3.697949	2.650193
H	2.502008	3.892250	-1.930315
H	1.426103	2.503956	-2.114282
H	1.194211	3.627384	-0.779642
H	4.243212	1.212575	-3.055849
H	3.979192	-0.408451	-2.411222
H	2.602289	0.617055	-2.792767
H	1.983098	1.221054	5.600220
H	3.460120	1.412796	4.662362
H	2.026267	2.358206	4.258034
H	-0.998121	0.882566	4.443388
H	-0.218518	2.124555	3.472250
H	-1.351016	0.993847	2.721127
H	-1.313104	-2.355562	2.815860
H	-1.496120	-1.019511	1.676827
H	-0.590917	-2.455598	1.208754
H	1.704979	-3.903307	3.159816
H	1.455317	-3.563484	1.446424
H	3.066090	-3.422709	2.153887

Figure S26. Geometry of the transition state for the dimerization process.



References

- (1) APEX: Area-Detector Software Package; Bruker Analytical X-Ray System, Inc.:Madison, WI (2001-2003)
- (2) SAINT: SAX Area-Detector Integration Program, V7.06; Bruker Analytical X-Ray Systems Inc.: Madison, WI (2005)
- (3) XPREP: (v 6.12) Part of SHELXTL Crystal Structure Determination Package; Bruker Analytical X-Ray Systems, Inc. Madison, WI (2001)
- (4) Blessing, R. H., *Acta Cryst.* **1995**, A51, 33-38.
- (5) SADABS: Bruker-Nonius Area Detector Scaling and Absorption v.2.10; Bruker Analytical X-Ray System, Inc. Madison, WI (2005)
- (6) SHELXL: G. M., *Sheldrick Acta Cryst.* **2008**, A64, 122-122
- (7) Farrugia, L.J, *J. Appl. Cryst.* **1999**, 32, 837-838
- (8) SIR97: Altomare, A., Burla, M. C., Camalli, M., Cascarano, G., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G., & Spagna, R. *J. App. Cryst.*, **1998**.