

## Supporting Information for the manuscript

### Carbon-Hydrogen Bond Breaking and Making in the Open-Shell Singlet Molecule $\text{Cp}^*_2\text{Yb}(4,7\text{-Me}_2\text{phen})$

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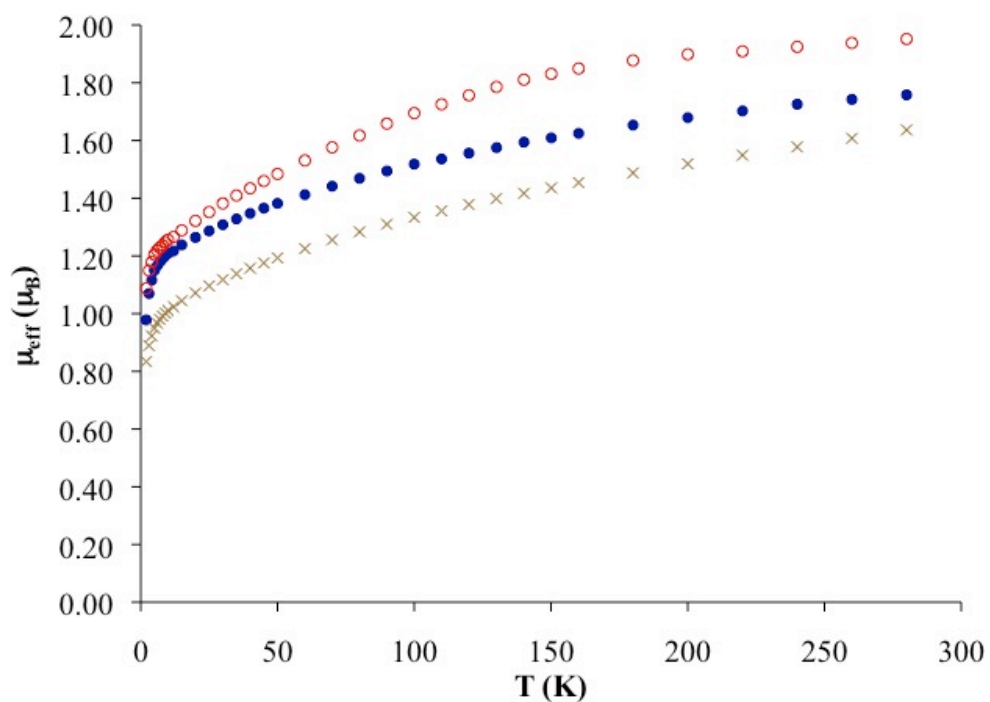
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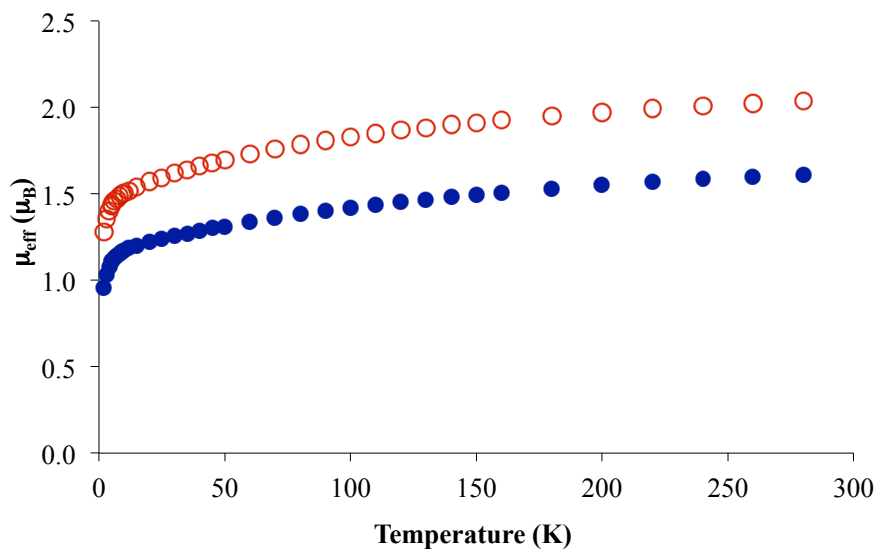
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## 1. Magnetism.

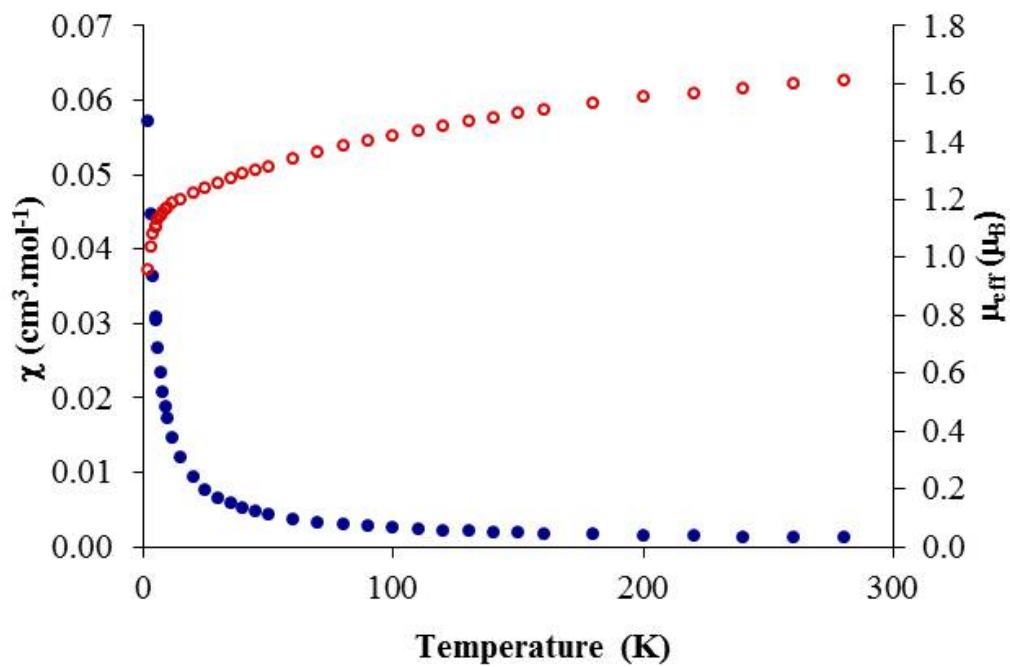
**Figure S1:** Temperature dependent magnetic data. Plot of the effective moment vs. the temperature for  $\text{Cp}^*_2\text{Yb}(4,7\text{-Me}_2\text{phen})$ , **2**, (red unfilled dots),  $\text{Cp}^*_2\text{Yb}(3,4,7,8\text{-Me}_4\text{phen})$ , **3**, (filled blue dots) and  $\text{Cp}^*_2\text{Yb}(3,4,5,6,7,8\text{-Me}_6\text{phen})$ , **4**, (gold yellow crosses).



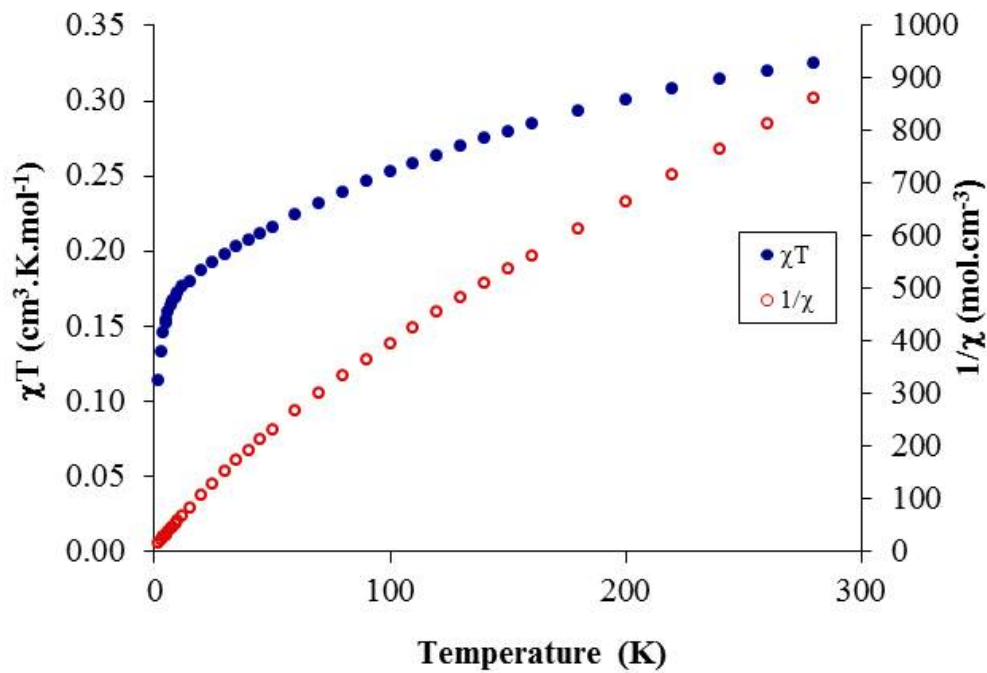
**Figure S2:** Temperature dependent magnetic data. Plot of the effective moment  $\mu_{\text{eff}}$  vs. the temperature for  $\text{Cp}^*_2\text{Yb}(2,9\text{-Me}_2\text{phen})$ , **1**, (filled blue dots),  $\text{Cp}^*_2\text{Yb}(2,9\text{-Me}_2\text{-4,7-Ph}_2\text{phen})$ , **5**, (unfilled red dots).



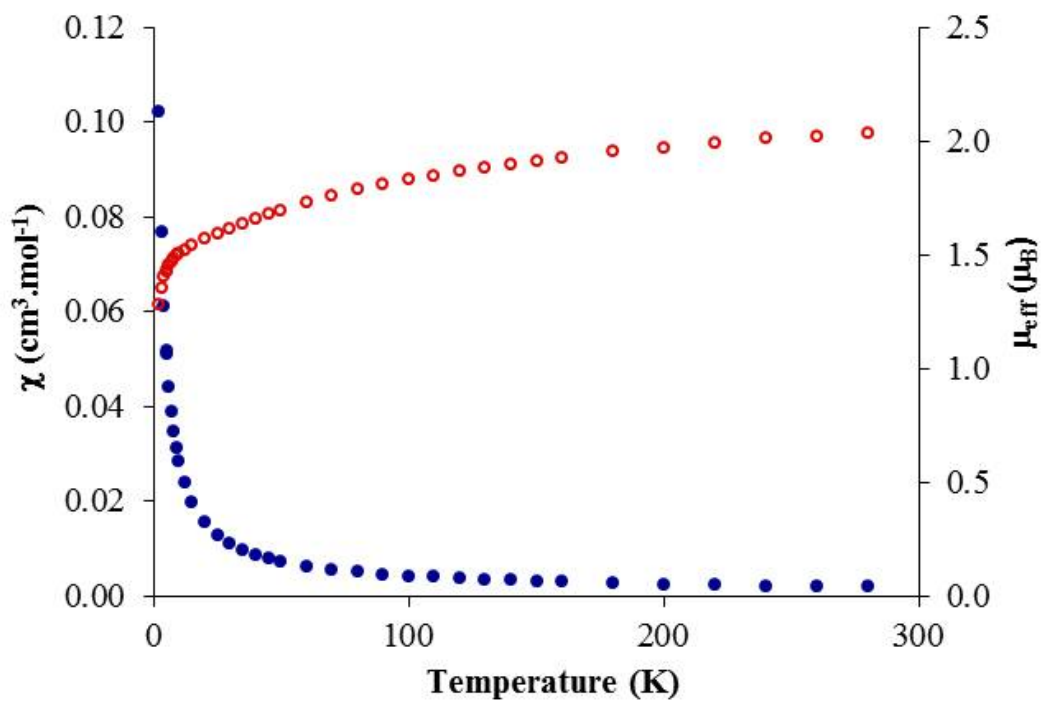
**Figure S3:** Temperature dependent magnetic data. Plot of the effective moment vs. the temperature (unfilled red dots) and the magnetic susceptibility (filled blue dots) for  $\text{Cp}^*_2\text{Yb}(2,9\text{-Me}_2\text{phen})$ , **1**.



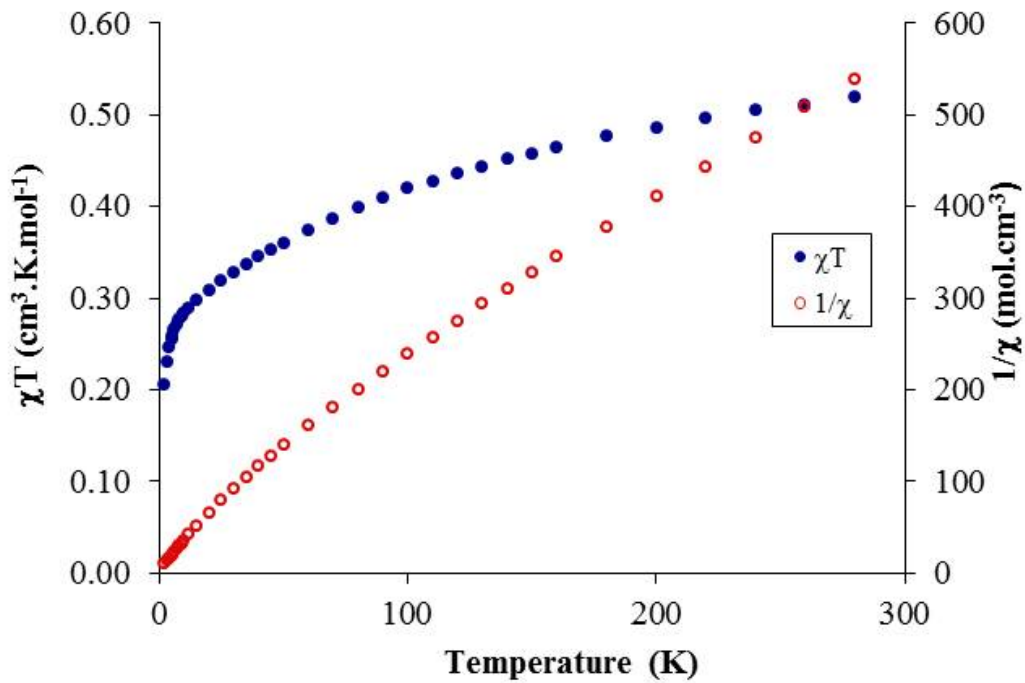
**Figure S4:** Temperature dependent magnetic data. Plot of  $\chi T$  vs. the temperature (filled blue dots) and  $1/\chi$  (unfilled red dots) for  $\text{Cp}^*_2\text{Yb}(2,9\text{-Me}_2\text{phen})$ , **1**.



**Figure S5:** Temperature dependent magnetic data. Plot of the effective moment *vs.* the temperature (unfilled red dots) and the magnetic susceptibility (filled blue dots) for Cp\*<sub>2</sub>Yb(2,9-Me<sub>2</sub>-4,7-Ph<sub>2</sub>phen), **5**.

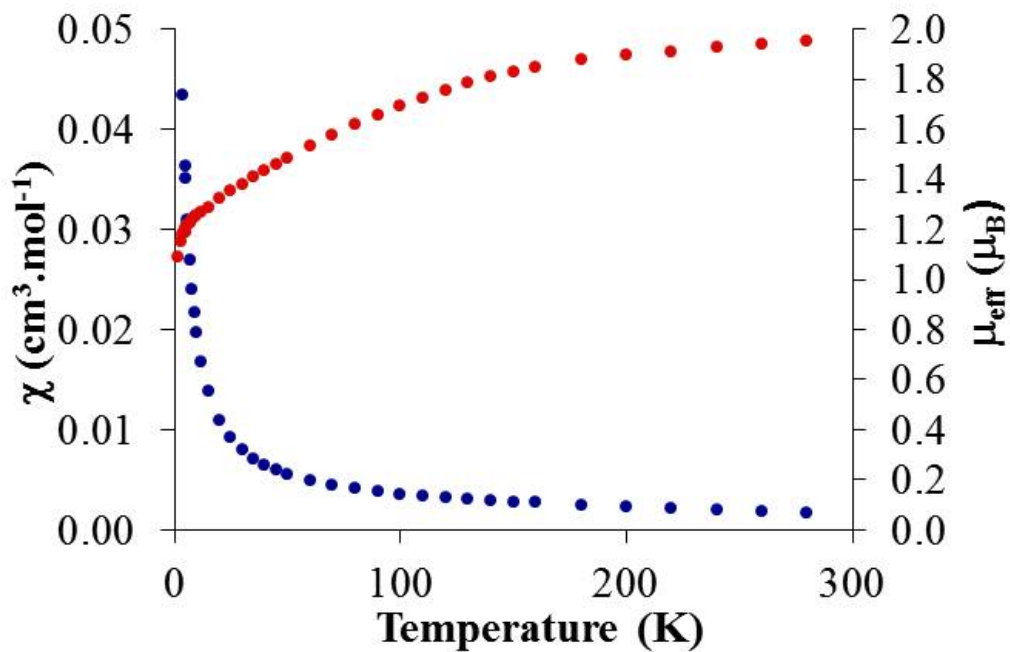


**Figure S6:** Temperature dependent magnetic data. Plot of  $\chi T$  vs. the temperature (filled blue dots) and  $1/\chi$  (unfilled red dots) for  $\text{Cp}^*_2\text{Yb}(2,9\text{-Me}_2\text{-}4,7\text{-Ph}_2\text{phen})$ , **5**.

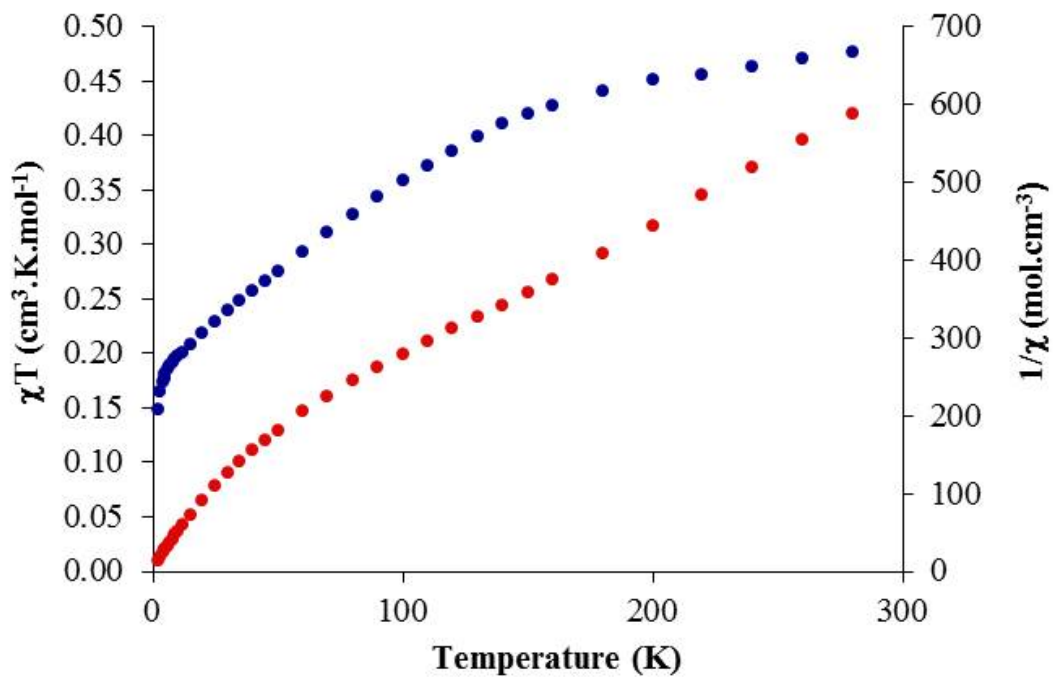




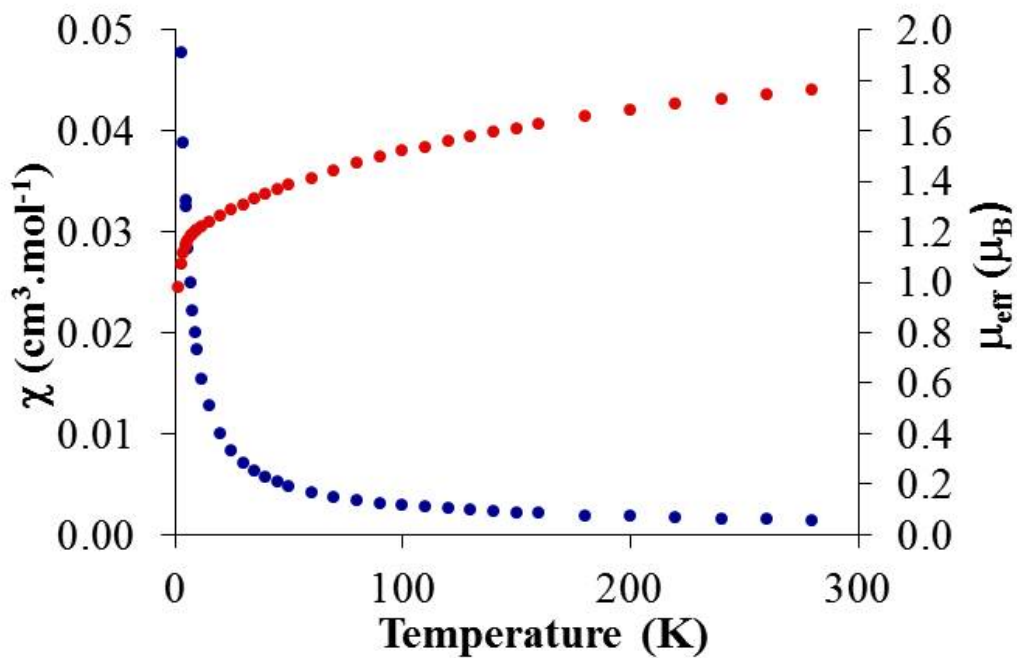
**Figure S7:** Temperature dependent magnetic data. Plot of the effective moment (unfilled red dots) and the magnetic susceptibility (filled blue dots) vs. the temperature for  $\text{Cp}^*_2\text{Yb}(4,7\text{Me}_2\text{phen})_2$ .



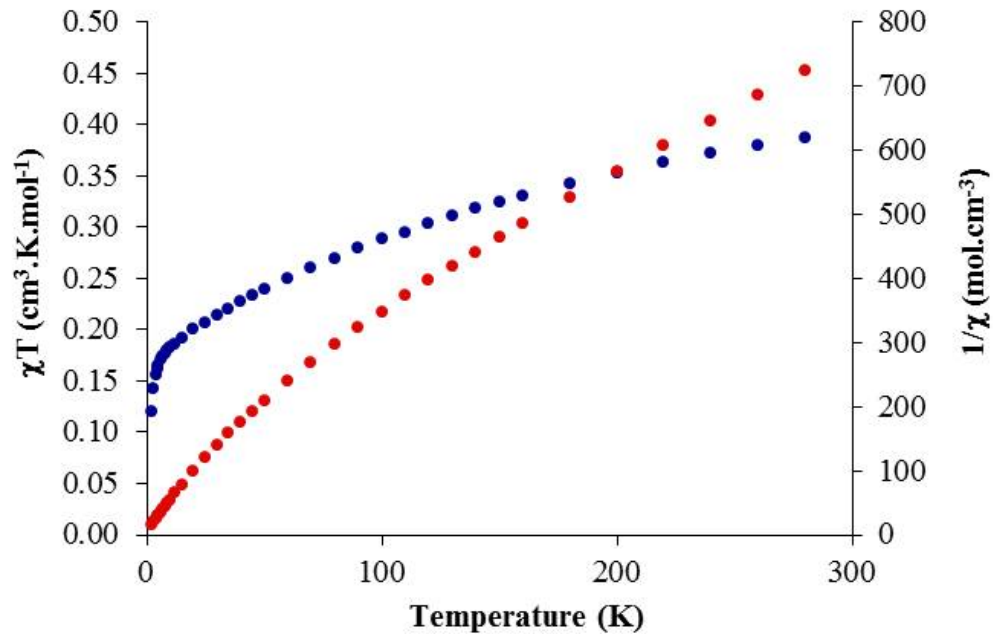
**Figure S8:** Temperature dependent magnetic data. Plot of  $\chi T$  (filled blue dots) and  $1/\chi$  (unfilled red dots) vs. the temperature for  $\text{Cp}^*_2\text{Yb}(4,7\text{-Me}_2\text{phen})$ , **2**.



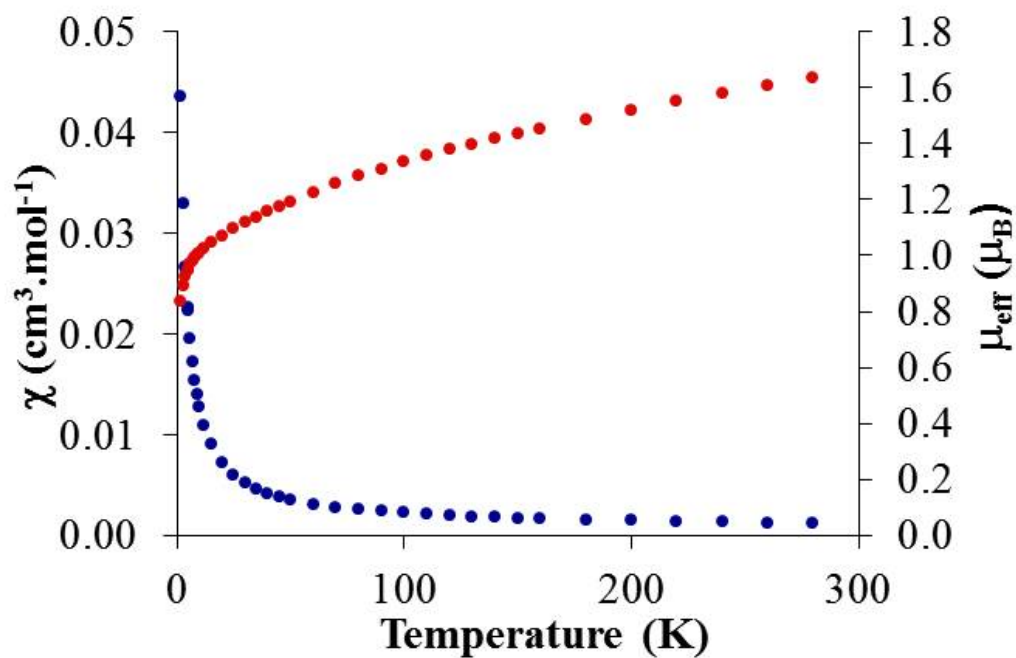
**Figure S9:** Temperature dependent magnetic data. Plot of the effective moment (unfilled red dots) and the magnetic susceptibility (filled blue dots) vs. the temperature for  $\text{Cp}^*_2\text{Yb}(3,4,7,8\text{Me}_4\text{phen}), \mathbf{3}$ .



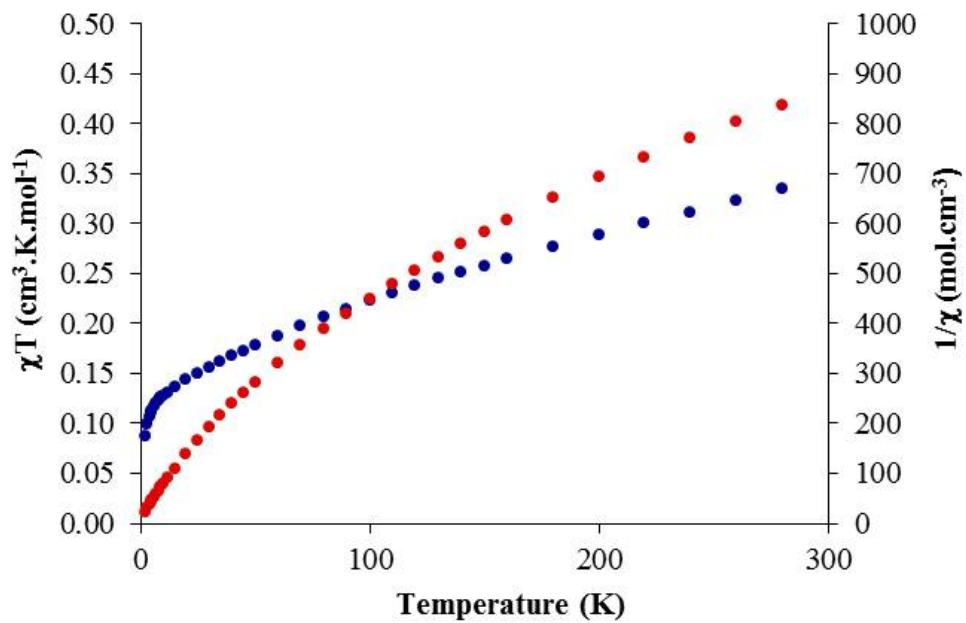
**Figure S10:** Temperature dependent magnetic data. Plot of  $\chi T$  (filled blue dots) and  $1/\chi$  (unfilled red dots) vs. the temperature for  $\text{Cp}^*_2\text{Yb}(\text{3,4,7,8Me}_4\text{phen})$ , **3**.



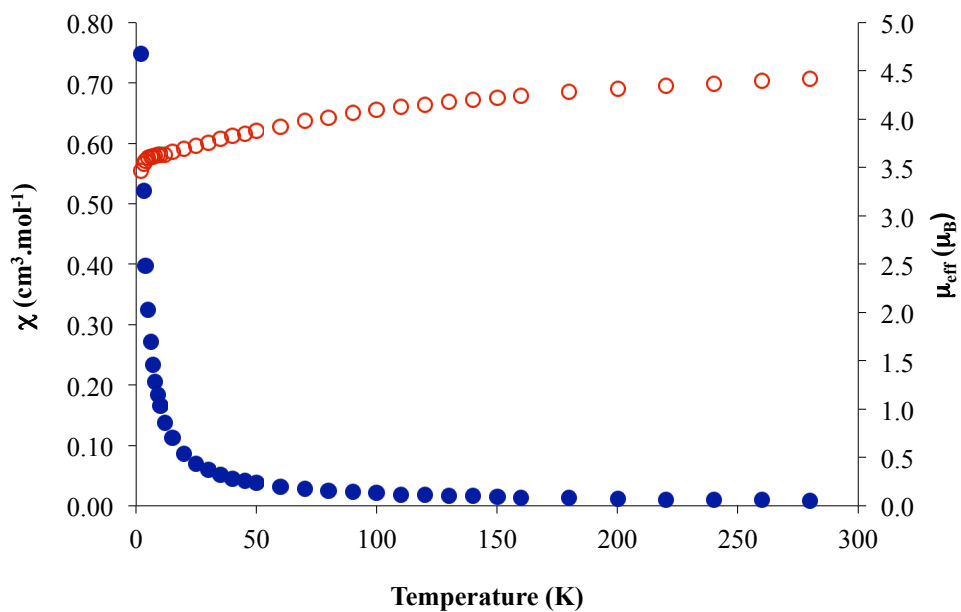
**Figure S11:** Temperature dependent magnetic data. Plot of the effective moment (unfilled red dots) and the magnetic susceptibility (filled blue dots) vs. the temperature for  $\text{Cp}^*_2\text{Yb}(3,4,5,6,7,8\text{Me}_4\text{phen})$ , **4**.



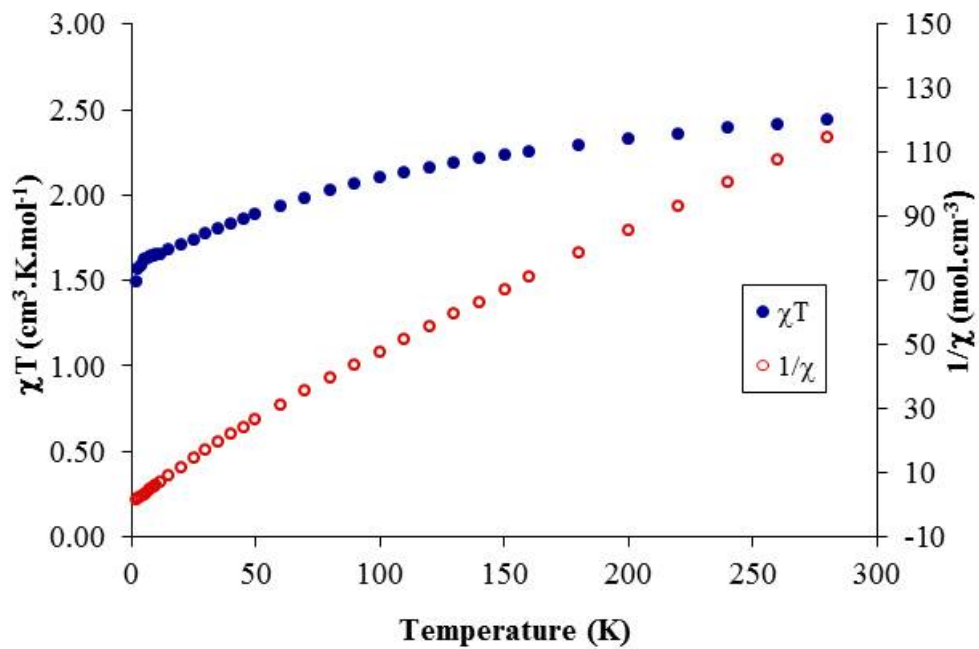
**Figure S12:** Temperature dependent magnetic data. Plot of the effective moment (unfilled red dots) and the magnetic susceptibility (filled blue dots) vs. the temperature for  $\text{Cp}^*_2\text{Yb}(3,4,5,6,7,8\text{Me}_4\text{phen})$ , **4**.



**Figure S13:** Temperature dependent magnetic data. Plot of the effective moment vs. the temperature (unfilled red dots) and the magnetic susceptibility (filled blue dots) for  $[\text{Cp}^*_2\text{Yb}(4,7\text{-Me}_2\text{phen})]\text{I}\cdot\text{CH}_2\text{Cl}_2$ , **6**.



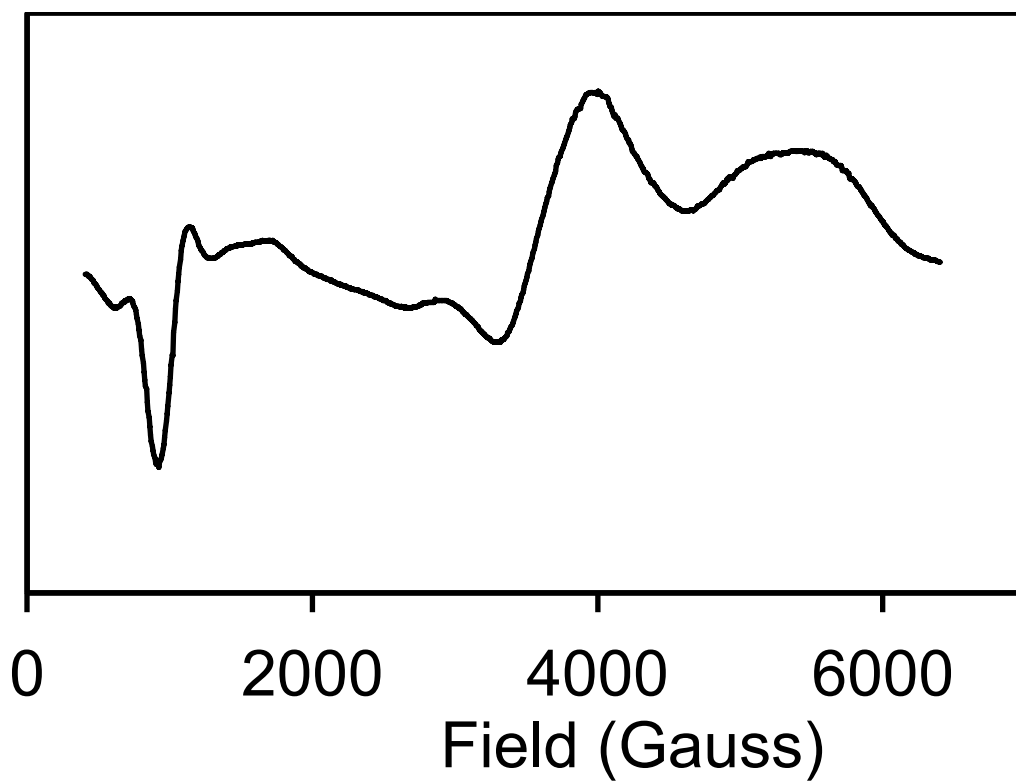
**Figure S14:** Temperature dependent magnetic data. Plot of  $\chi T$  vs. the temperature (filled blue dots) and  $1/\chi$  (unfilled red dots) for  $[\text{Cp}^*_2\text{Yb}(4,7\text{-Me}_2\text{phen})]\text{I}\cdot\text{CH}_2\text{Cl}_2$ , **6**.





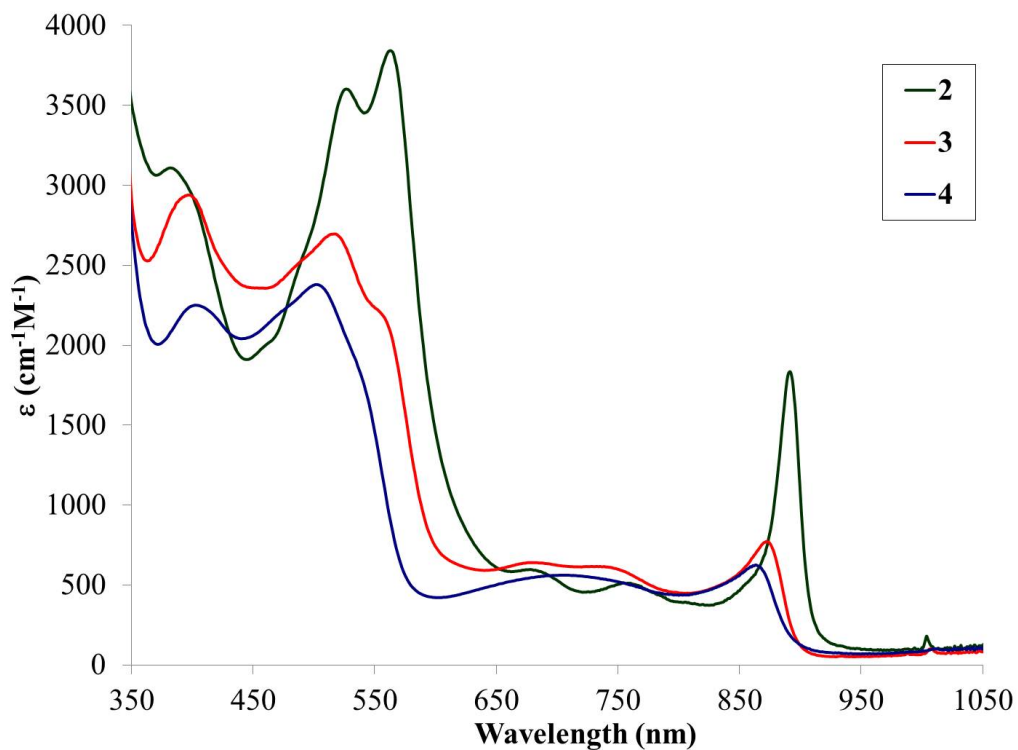
## 2. EPR

**Figure S15:** EPR spectrum of  $[\text{Cp}^*_2\text{Yb}(4,7\text{-Me}_2\text{phen})]\text{I}\cdot\text{CH}_2\text{Cl}_2$ , **6**, in the solid state (powder) recorded at 1.4 K. ( $g_1 = 7.136$ ,  $g_2 = 1.829$ ,  $g_3 = 1.214$ ) ( $\mu_{\text{eff}}(\text{EPR}) = 3.7 \mu_{\text{B}}$ )

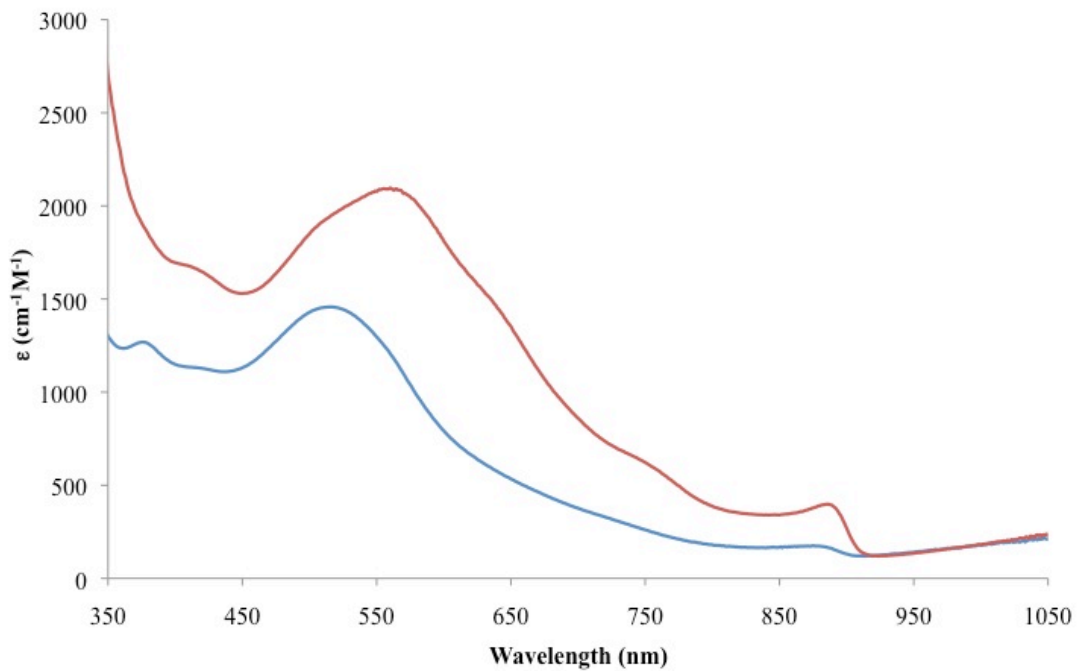


### 3. Visible spectroscopy.

**Figure S16:** Visible-Near IR spectra of  $\text{Cp}^*_2\text{Yb}(4,7\text{-Me}_2\text{phen})$ , **2**, (green),  $\text{Cp}^*_2\text{Yb}(3,4,7,8\text{-Me}_4\text{phen})$ , **3**, (red),  $\text{Cp}^*_2\text{Yb}(3,4,5,6,7,8\text{-Me}_6\text{phen})$ , **4**, (blue).

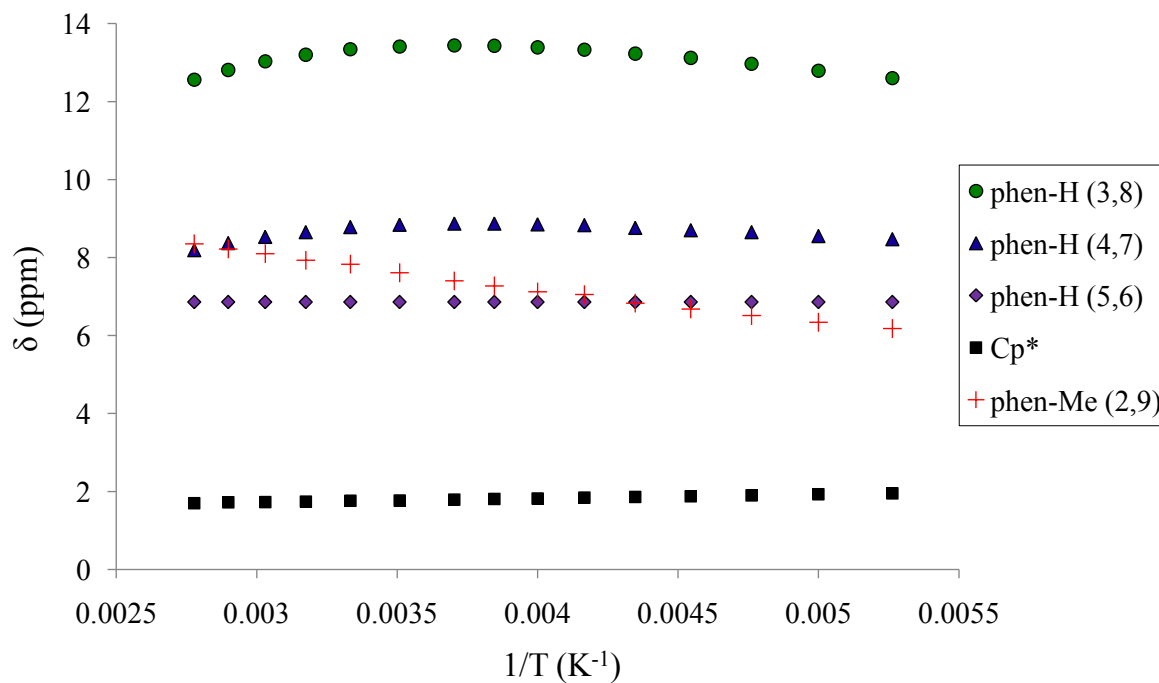


**Figure S17:** Visible-Near IR spectra of  $\text{Cp}^* \text{Yb}(\text{2,9-Me}_2\text{phen})$ , **1**, (blue),  $\text{Cp}^* \text{Yb}(\text{2,9Me}_2\text{-4,7-Ph}_2\text{phen})$ , **5** (red).

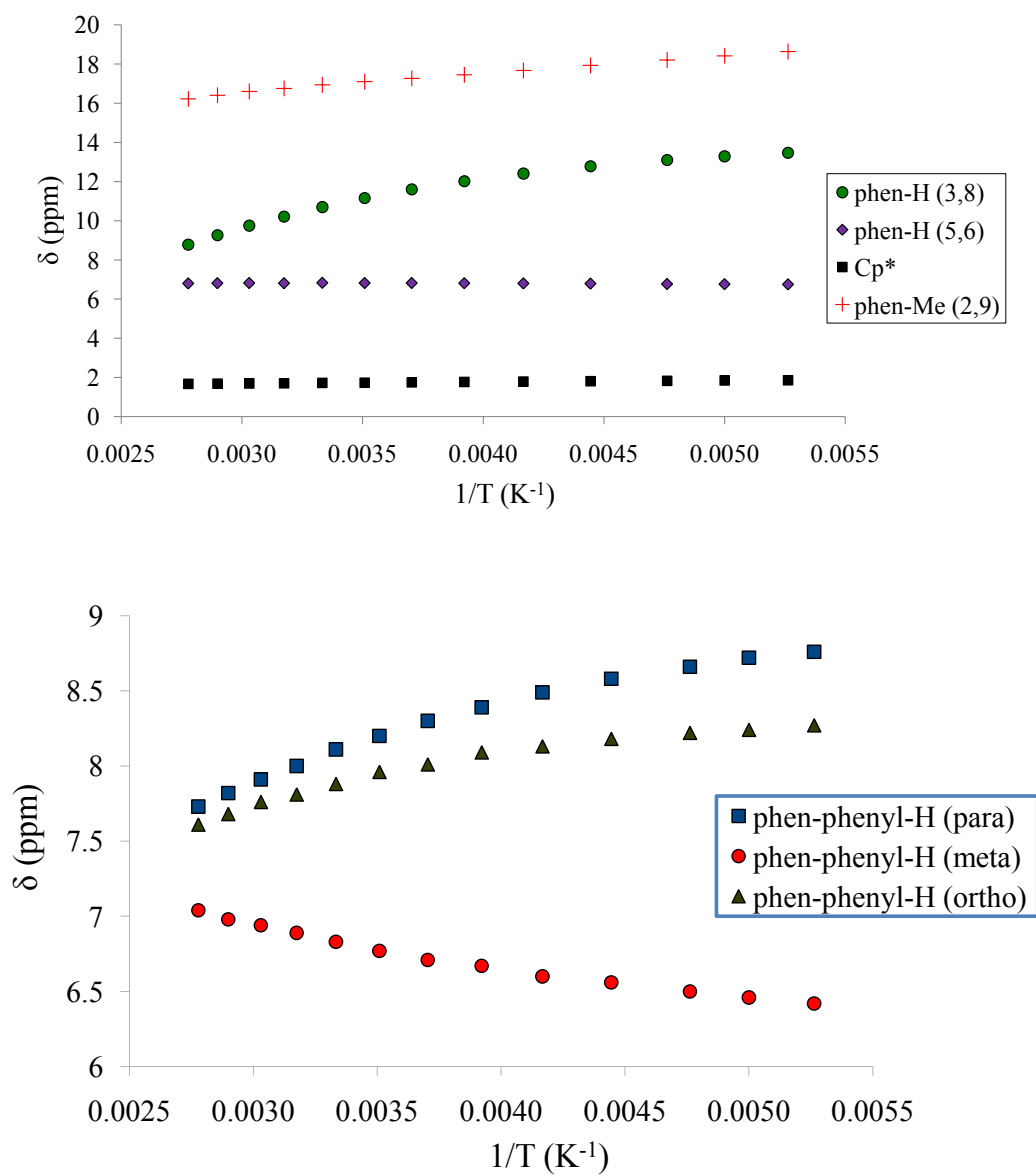


#### 4. Variable Temperature NMR

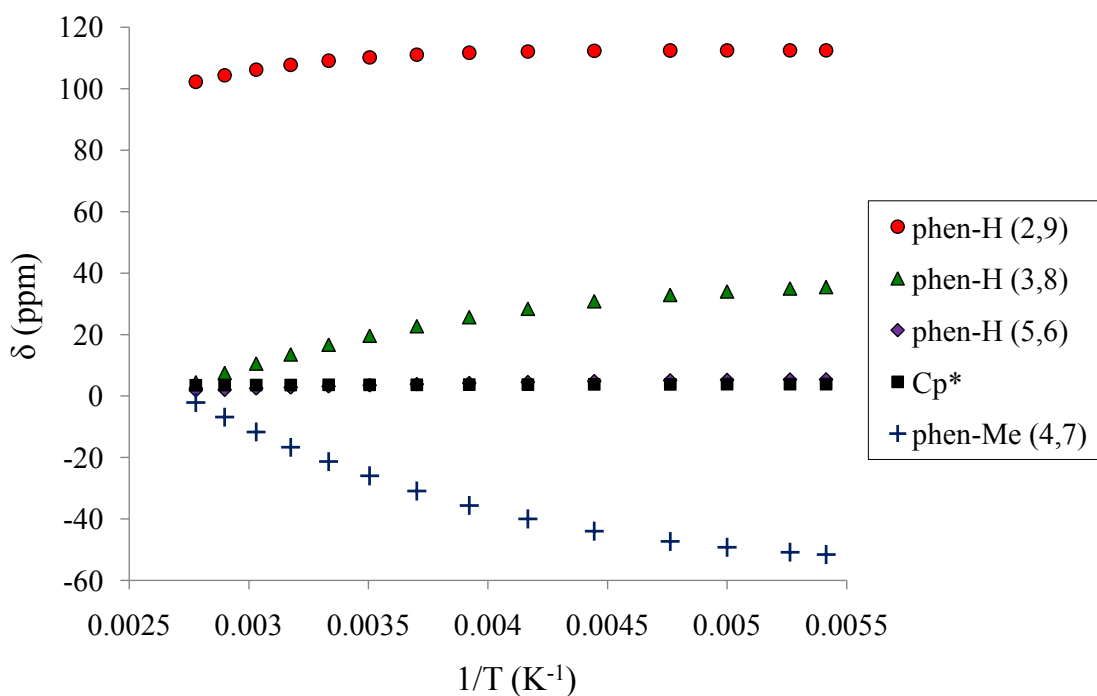
**Figure S18.** Chemical shift ( $\delta$ ) vs.  $1/T$  plot of the proton resonances of  $\text{Cp}^*_2\text{Yb}(\text{2,9-Me}_2\text{-phen})$ , **2**, in toluene- $d_8$ . Temperature range: 180K to 360K.



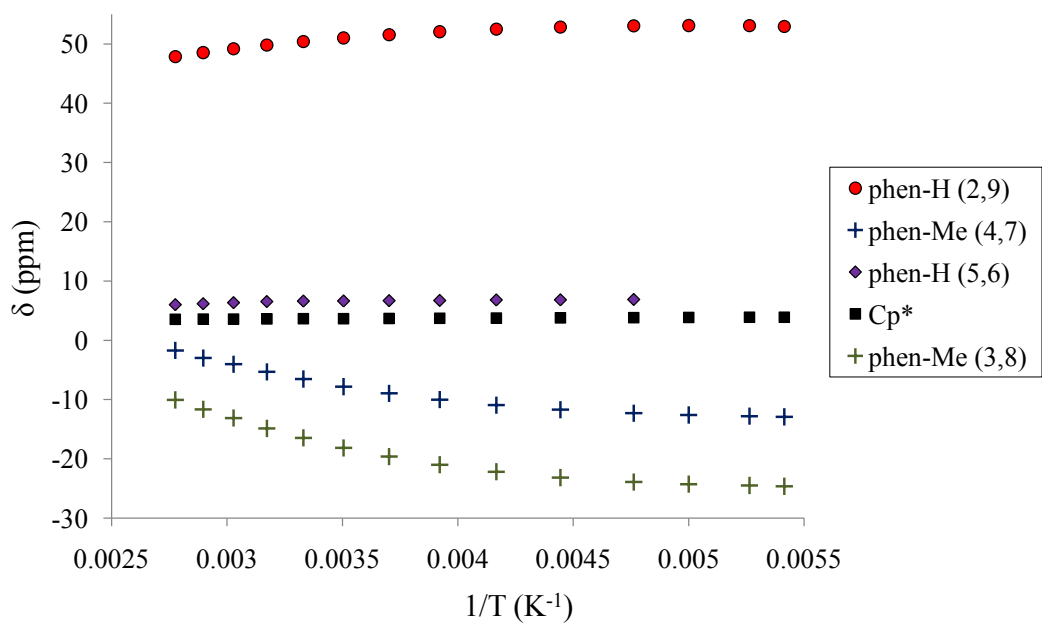
**Figure S19.** Chemical shift ( $\delta$ ) vs.  $1/T$  plot of the proton resonances of  $\text{Cp}^* \text{Yb}(\text{2,9-Me}_2\text{-4,7-Ph}_2\text{-phen})$ , **5**, in toluene- $\text{d}_8$ . Temperature range: 180K to 360K.



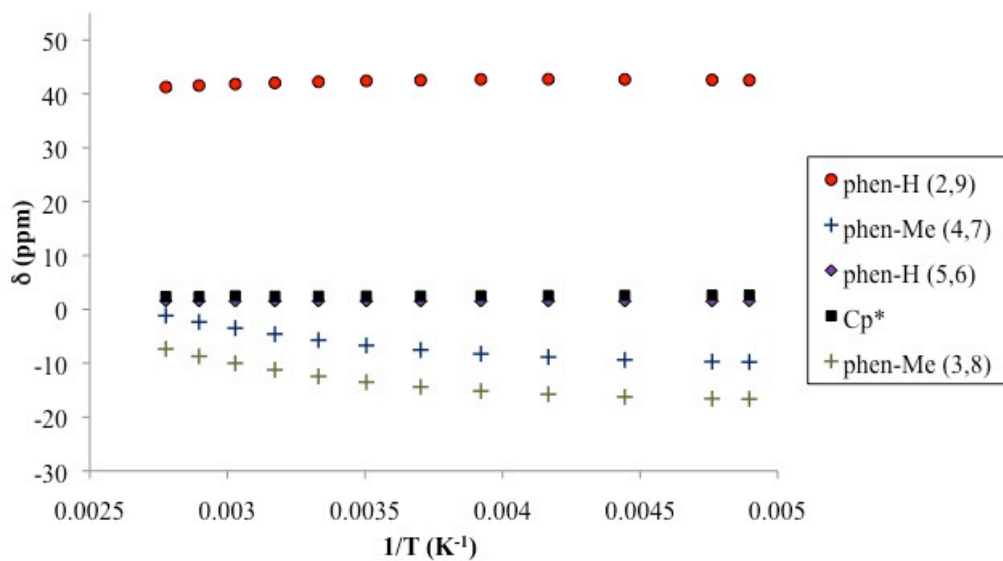
**Figure S20.** Chemical shift ( $\delta$ ) vs.  $1/T$  plot of the proton resonances of  $\text{Cp}^* \text{Yb}(\text{4,7-Me}_2\text{-phen})$ , **2**, in toluene- $d_8$ . Temperature range: 180K to 360K.



**Figure S21.** Chemical shift ( $\delta$ ) vs.  $1/T$  plot of the proton resonances of  $\text{Cp}^* \text{Yb}(\text{3,4,7,8-Me}_4\text{-phen})$ , **3**, in toluene- $d_8$ . Temperature range: 180K to 360K.



**Figure S22.** Chemical shift ( $\delta$ ) vs.  $1/T$  plot of the proton resonances of  $\text{Cp}^*_{2}\text{Yb}(\text{3,4,5,6,7,8-Me}_6\text{-phen})$ , **4**, in toluene- $d_8$ . Temperature range: 180K to 360K.



## 5. X-Ray Crystallography.

**Table S1.** Selected Crystal Data and Data Collection Parameters for Complexes **2**, **5** and **7**

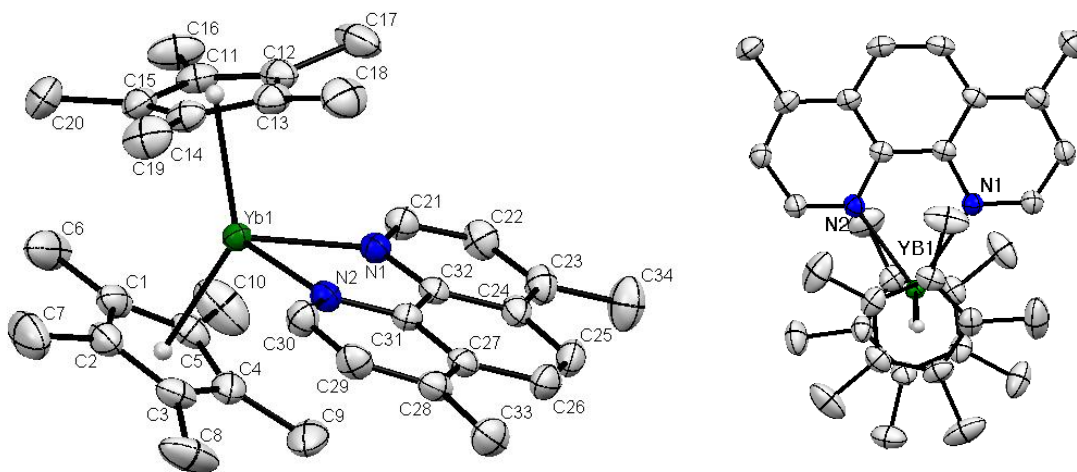
	<b>2</b>	<b>5</b>	<b>7</b>
Formula	2(C <sub>34</sub> H <sub>42</sub> N <sub>2</sub> Yb)·C <sub>7</sub> H <sub>8</sub>	2(C <sub>46</sub> H <sub>50</sub> N <sub>2</sub> Yb) C <sub>7</sub> H <sub>8</sub>	C <sub>34</sub> H <sub>41.56</sub> N <sub>2</sub> Yb
Crystal size (mm)	0.3 x 0.25 x 0.12	0.20 x 0.20 x 0.15	0.20 x 0.15 x 0.10
cryst system	Monoclinic	Triclinic	Monoclinic
space group	<i>P</i> 2(1)/n	<i>P</i> -1	<i>P</i> 2(1)/c
volume (Å <sup>3</sup> )	V = 3172.2(15)	V = 2042.7(14)	V = 3511.1(12)
<i>a</i> (Å)	<i>a</i> = 10.021(3)	<i>a</i> = 12.478(5)	<i>a</i> = 10.682(2)
<i>b</i> (Å)	<i>b</i> = 20.372(5)	<i>b</i> = 12.704(5)	<i>b</i> = 16.132(3)
<i>c</i> (Å)	<i>c</i> = 15.640(4)	<i>c</i> = 14.038(5)	<i>c</i> = 20.460(4)
$\alpha$ (deg)	90	86.974(4)	90
$\beta$ (deg)	96.033(3)	87.632(4)	95.181(3)
$\gamma$ (deg)	90	66.846(4)	90
<i>Z</i>	2	1	4
formula weight (g/mol)	1395.60	1669.97	651.29
density (calcd) (g cm <sup>-3</sup> )	1.450	1.382	1.232
absorption coefficient (mm <sup>-1</sup> )	2.97	2.33	2.68
F(000)	1420	870	1318
temp (K)	150(2)	183(2)	173(1)
diffractometer <sup>a</sup>	SMART APEX	SMART 1000 CCD	SMART APEX
$\theta$ range for data collection (deg)	1.65 to 25.37	2.91 to 25.5	1.6 to 25.40
transmission range	0.414 to 0.700	0.654 to 0.722	0.622 to 0.764
absorption correction	multi scan	multi scan	Multi-scan
total no. reflections	46077	26274	61773
unique reflections [R <sub>int</sub> ]	5786 [0.024]	7442 [0.034]	6427 [0.039]
final R <sup>b</sup> indices [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]	R = 0.019, R <sub>w</sub> = 0.046	R = 0.047, R <sub>w</sub> = 0.130	R = 0.031, R <sub>w</sub> = 0.067
R indices (all data)	R = 0.0218	R = 0.0569	R = 0.0392
largest diff. peak and hole (e.Å <sup>-3</sup> )	0.69 and -0.44	3.06 and -1.23	0.72 and -0.52
Goof	1.08	1.08	1.06

<sup>a</sup> Radiation: graphite monochromated Mo K $\alpha$  ( $\lambda$  = 0.71073 Å).

<sup>b</sup>  $R = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}$ .



**Figure S23.** ORTEP diagram for  $\text{Cp}^* \text{Yb}(\text{4,7-Me}_2\text{phen})$  (**2**). (Thermal ellipsoids are at 50% level). One toluene molecule has been omitted for clarity.



**Table S2:** Bond distances (Å) for Cp\*<sub>2</sub>Yb(4,7-Me<sub>2</sub>phen) (**2**).

Yb1—N1	2.335 (2)	C21—C22	1.369 (4)
Yb1—N2	2.357 (2)	C22—C23	1.401 (4)
Yb1—C1	2.633 (3)	C23—C24	1.419 (4)
Yb1—C11	2.636 (3)	C23—C33	1.482 (4)
Yb1—C2	2.636 (3)	C24—C32	1.415 (3)
Yb1—C12	2.645 (3)	C24—C25	1.431 (4)
Yb1—C14	2.645 (3)	C25—C26	1.352 (4)
Yb1—C13	2.645 (3)	C26—C27	1.430 (4)
Yb1—C4	2.647 (3)	C27—C28	1.408 (4)
Yb1—C3	2.652 (3)	C27—C31	1.420 (3)
Yb1—C15	2.653 (3)	C28—C29	1.385 (4)
N1—C21	1.353 (3)	C28—C34	1.507 (4)
N1—C32	1.381 (3)	C29—C30	1.388 (4)
N2—C30	1.340 (3)	C31—C32	1.430 (3)
N2—C31	1.381 (3)	C37—C38	1.3900
C1—C5	1.409 (4)	C38—C39	1.3900
C1—C2	1.413 (4)	C39—C40	1.3900
C1—C6	1.510 (4)	C40—C41	1.3900
C2—C3	1.418 (4)		
C2—C7	1.505 (4)		
C3—C4	1.409 (4)		
C3—C8	1.507 (4)		
C4—C5	1.408 (4)		
C4—C9	1.508 (4)		
C5—C10	1.507 (4)		
C11—C12	1.416 (4)		
C11—C15	1.417 (4)		
C11—C16	1.509 (4)		
C12—C13	1.413 (4)		
C12—C17	1.505 (4)		
C13—C14	1.413 (4)		
C13—C18	1.511 (4)		
C14—C15	1.416 (4)		
C14—C19	1.508 (4)		
C15—C20	1.510 (4)		

**Table S3:** Bond angles (deg) for Cp<sup>\*</sup><sub>2</sub>Yb(4,7-Me<sub>2</sub>phen) (**2**).

N1—Yb1—N2	69.96 (7)	C12—C11—C15	107.8 (2)
N1—Yb1—C5	87.11 (8)	C12—C11—C16	125.3 (3)
N2—Yb1—C5	118.89 (8)	C15—C11—C16	126.7 (3)
N1—Yb1—C1	117.68 (9)	C12—C11—Yb1	74.80 (15)
N2—Yb1—C1	132.13 (8)	C15—C11—Yb1	75.16 (15)
C5—Yb1—C1	31.06 (9)	C16—C11—Yb1	120.51 (18)
N1—Yb1—C11	102.82 (8)	C13—C12—C11	108.3 (2)
N2—Yb1—C11	131.75 (8)	C13—C12—C17	125.1 (3)
C5—Yb1—C11	107.89 (9)	C11—C12—C17	126.2 (3)
C1—Yb1—C11	94.36 (9)	C13—C12—Yb1	74.52 (15)
N1—Yb1—C2	131.58 (8)	C11—C12—Yb1	74.10 (15)
N2—Yb1—C2	105.87 (8)	C17—C12—Yb1	123.05 (19)
C5—Yb1—C2	51.44 (9)	C12—C13—C14	107.8 (2)
C1—Yb1—C2	31.10 (9)	C12—C13—C18	125.5 (3)
C11—Yb1—C2	112.26 (9)	C14—C13—C18	126.5 (3)
N1—Yb1—C12	80.97 (8)	C12—C13—Yb1	74.49 (15)
N2—Yb1—C12	103.29 (8)	C14—C13—Yb1	74.49 (15)
C5—Yb1—C12	128.74 (9)	C18—C13—Yb1	120.85 (19)
C1—Yb1—C12	124.41 (9)	C13—C14—C15	108.2 (2)
C11—Yb1—C12	31.10 (9)	C13—C14—C19	126.7 (3)
C2—Yb1—C12	142.30 (9)	C15—C14—C19	124.9 (3)
N1—Yb1—C14	123.72 (8)	C13—C14—Yb1	74.51 (15)
N2—Yb1—C14	91.74 (8)	C15—C14—Yb1	74.83 (15)
C5—Yb1—C14	143.75 (9)	C19—C14—Yb1	121.34 (19)
C1—Yb1—C14	113.79 (9)	C14—C15—C11	107.9 (2)
C11—Yb1—C14	51.41 (8)	C14—C15—C20	124.1 (3)
C2—Yb1—C14	104.33 (9)	C11—C15—C20	126.8 (3)
C12—Yb1—C14	51.17 (8)	C14—C15—Yb1	74.16 (15)
N1—Yb1—C13	92.73 (8)	C11—C15—Yb1	73.78 (15)
N2—Yb1—C13	80.67 (8)	C20—C15—Yb1	127.86 (19)
C5—Yb1—C13	158.77 (9)	N1—C21—C22	124.4 (2)
C1—Yb1—C13	140.00 (9)	C21—C22—C23	120.8 (2)
C11—Yb1—C13	51.47 (8)	C22—C23—C24	116.8 (2)
C2—Yb1—C13	135.20 (9)	C22—C23—C33	120.8 (3)
C12—Yb1—C13	30.99 (8)	C24—C23—C33	122.4 (3)

C14—Yb1—C13	31.00 (9)	C32—C24—C23	118.9 (2)
N1—Yb1—C4	80.20 (8)	C32—C24—C25	117.7 (2)
N2—Yb1—C4	88.37 (8)	C23—C24—C25	123.4 (2)
C5—Yb1—C4	30.95 (9)	C26—C25—C24	122.2 (2)
C1—Yb1—C4	51.24 (9)	C25—C26—C27	121.7 (2)
C11—Yb1—C4	138.82 (9)	C28—C27—C31	119.3 (2)
C2—Yb1—C4	51.41 (9)	C28—C27—C26	123.1 (2)
C12—Yb1—C4	152.85 (9)	C31—C27—C26	117.6 (2)
C14—Yb1—C4	154.39 (9)	C29—C28—C27	117.5 (2)
C13—Yb1—C4	168.52 (9)	C29—C28—C34	120.4 (3)
N1—Yb1—C3	105.53 (8)	C27—C28—C34	122.0 (3)
N2—Yb1—C3	80.99 (8)	C28—C29—C30	120.0 (2)
C5—Yb1—C3	51.06 (9)	N2—C30—C29	124.5 (2)
C1—Yb1—C3	51.14 (9)	N2—C31—C27	122.0 (2)
C11—Yb1—C3	142.92 (9)	N2—C31—C32	117.3 (2)
C2—Yb1—C3	31.11 (9)	C27—C31—C32	120.7 (2)
C12—Yb1—C3	173.25 (9)	N1—C32—C24	122.9 (2)
C14—Yb1—C3	124.11 (9)	N1—C32—C31	116.9 (2)
C13—Yb1—C3	147.73 (9)	C24—C32—C31	120.1 (2)
C4—Yb1—C3	30.84 (9)	C37—C36—C35	121.7 (8)
N1—Yb1—C15	131.52 (8)	C41—C36—C35	118.3 (8)
N2—Yb1—C15	122.70 (8)	C5—C1—C2	108.2 (2)
C5—Yb1—C15	114.99 (9)	C5—C1—C6	125.0 (3)
C1—Yb1—C15	88.79 (9)	C2—C1—C6	126.0 (3)
C11—Yb1—C15	31.07 (8)	C5—C1—Yb1	74.34 (15)
C2—Yb1—C15	92.53 (9)	C2—C1—Yb1	74.58 (16)
C12—Yb1—C15	51.17 (8)	C6—C1—Yb1	124.96 (19)
C14—Yb1—C15	31.00 (8)	C1—C2—C3	107.4 (3)
C13—Yb1—C15	51.26 (9)	C1—C2—C7	127.3 (3)
C4—Yb1—C15	139.69 (9)	C3—C2—C7	124.6 (3)
C3—Yb1—C15	122.14 (9)	C1—C2—Yb1	74.32 (15)
C21—N1—C32	116.1 (2)	C3—C2—Yb1	75.05 (15)
C21—N1—Yb1	125.54 (17)	C7—C2—Yb1	124.0 (2)
C32—N1—Yb1	117.99 (16)	C4—C3—C2	108.3 (2)
C30—N2—C31	116.5 (2)	C4—C3—C8	124.8 (3)
C30—N2—Yb1	126.31 (17)	C2—C3—C8	126.4 (3)
C31—N2—Yb1	116.98 (16)	C4—C3—Yb1	74.40 (15)

C2—C3—Yb1	73.84 (15)		
C8—C3—Yb1	123.7 (2)		
C5—C4—C3	107.8 (2)		
C5—C4—C9	125.9 (3)		
C3—C4—C9	126.2 (3)		
C5—C4—Yb1	73.85 (15)		
C3—C4—Yb1	74.76 (15)		
C9—C4—Yb1	120.66 (19)		
C4—C5—C1	108.3 (2)		
C4—C5—C10	127.3 (3)		
C1—C5—C10	124.3 (3)		
C4—C5—Yb1	75.21 (15)		
C1—C5—Yb1	74.60 (16)		
C10—C5—Yb1	118.6 (2)		

**Table S4:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) for  $\text{Cp}^* \text{Yb}(4,7\text{-Me}_2\text{phen})$  (**2**).

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Yb1	0.64386 (2)	0.15199 (2)	0.23319 (2)	0.02264 (4)	
N1	0.5362 (2)	0.05442 (10)	0.26365 (13)	0.0257 (4)	
N2	0.4297 (2)	0.14752 (10)	0.15518 (13)	0.0268 (5)	
C1	0.8874 (3)	0.14352 (15)	0.18518 (18)	0.0371 (7)	
C2	0.8125 (3)	0.17994 (14)	0.11986 (18)	0.0363 (6)	
C3	0.7174 (3)	0.13664 (15)	0.07642 (17)	0.0355 (6)	
C4	0.7326 (3)	0.07445 (14)	0.11566 (18)	0.0347 (6)	
C5	0.8373 (3)	0.07885 (14)	0.18289 (18)	0.0355 (6)	
C6	1.0138 (3)	0.1661 (2)	0.2381 (2)	0.0626 (11)	
H6A	1.0187	0.2141	0.2368	0.094*	
H6B	1.0921	0.1475	0.2142	0.094*	
H6C	1.0125	0.1512	0.2976	0.094*	
C7	0.8405 (4)	0.24843 (17)	0.0905 (3)	0.0655 (11)	
H7A	0.7555	0.2712	0.0741	0.098*	
H7B	0.8926	0.2463	0.0409	0.098*	
H7C	0.8918	0.2724	0.1374	0.098*	
C8	0.6272 (4)	0.1512 (2)	-0.0047 (2)	0.0614 (11)	
H8A	0.6005	0.1975	-0.0050	0.092*	
H8B	0.5471	0.1234	-0.0069	0.092*	
H8C	0.6754	0.1422	-0.0548	0.092*	
C9	0.6573 (4)	0.01286 (18)	0.0869 (2)	0.0598 (10)	
H9A	0.5638	0.0239	0.0676	0.090*	
H9B	0.6602	-0.0181	0.1350	0.090*	
H9C	0.6991	-0.0072	0.0393	0.090*	
C10	0.8937 (4)	0.0243 (2)	0.2410 (3)	0.0656 (11)	
H10A	0.8964	0.0383	0.3011	0.098*	
H10B	0.9847	0.0137	0.2278	0.098*	
H10C	0.8367	-0.0147	0.2318	0.098*	
C11	0.7256 (3)	0.19799 (13)	0.38735 (16)	0.0328 (6)	
C12	0.5905 (3)	0.17902 (13)	0.39145 (17)	0.0340 (6)	
C13	0.5073 (3)	0.22121 (14)	0.33756 (17)	0.0336 (6)	
C14	0.5907 (3)	0.26687 (13)	0.30073 (17)	0.0323 (6)	
C15	0.7255 (3)	0.25310 (13)	0.33211 (17)	0.0327 (6)	

C16	0.8457 (4)	0.16833 (17)	0.4397 (2)	0.0508 (8)	
H16A	0.9244	0.1962	0.4355	0.076*	
H16B	0.8628	0.1244	0.4177	0.076*	
H16C	0.8278	0.1651	0.5000	0.076*	
C17	0.5415 (4)	0.12830 (16)	0.4508 (2)	0.0537 (9)	
H17A	0.6142	0.0974	0.4684	0.081*	
H17B	0.4655	0.1045	0.4209	0.081*	
H17C	0.5130	0.1500	0.5018	0.081*	
C18	0.3557 (3)	0.22070 (19)	0.3276 (2)	0.0534 (9)	
H18A	0.3224	0.2369	0.2703	0.080*	
H18B	0.3227	0.2491	0.3714	0.080*	
H18C	0.3236	0.1758	0.3346	0.080*	
C19	0.5457 (4)	0.32470 (15)	0.2448 (2)	0.0488 (8)	
H19A	0.6069	0.3305	0.2005	0.073*	
H19B	0.5463	0.3644	0.2802	0.073*	
H19C	0.4547	0.3168	0.2174	0.073*	
C20	0.8417 (3)	0.29880 (17)	0.3224 (2)	0.0506 (8)	
H20A	0.8387	0.3131	0.2624	0.076*	
H20B	0.9263	0.2758	0.3390	0.076*	
H20C	0.8353	0.3372	0.3596	0.076*	
C21	0.5876 (3)	0.00713 (13)	0.31828 (16)	0.0302 (6)	
H21	0.6694	0.0162	0.3526	0.036*	
C22	0.5296 (3)	-0.05297 (13)	0.32737 (18)	0.0350 (6)	
H22	0.5716	-0.0837	0.3673	0.042*	
C23	0.4091 (3)	-0.06974 (13)	0.27862 (18)	0.0347 (6)	
C24	0.3507 (3)	-0.02148 (12)	0.22086 (16)	0.0283 (5)	
C25	0.2285 (3)	-0.03147 (14)	0.16638 (18)	0.0347 (6)	
H31	0.1836	-0.0724	0.1685	0.042*	
C26	0.1748 (3)	0.01539 (14)	0.11203 (18)	0.0344 (6)	
H32	0.0933	0.0065	0.0773	0.041*	
C27	0.2376 (2)	0.07795 (13)	0.10554 (15)	0.0273 (5)	
C28	0.1838 (3)	0.12795 (14)	0.05011 (16)	0.0303 (6)	
C29	0.2528 (3)	0.18693 (14)	0.05110 (17)	0.0334 (6)	
H29	0.2178	0.2224	0.0163	0.040*	
C30	0.3731 (3)	0.19417 (13)	0.10294 (17)	0.0320 (6)	
H30	0.4184	0.2350	0.1013	0.038*	
C31	0.3598 (2)	0.08922 (12)	0.15797 (15)	0.0244 (5)	

C32	0.4158 (2)	0.03984 (12)	0.21608 (15)	0.0249 (5)	
C33	0.3473 (3)	-0.13509 (16)	0.2878 (3)	0.0529 (9)	
H34A	0.3378	-0.1574	0.2320	0.079*	
H34B	0.2586	-0.1297	0.3080	0.079*	
H34C	0.4045	-0.1614	0.3294	0.079*	
C34	0.0570 (3)	0.11839 (16)	-0.00947 (19)	0.0406 (7)	
H33A	-0.0168	0.1069	0.0242	0.061*	
H33B	0.0702	0.0830	-0.0501	0.061*	
H33C	0.0351	0.1591	-0.0412	0.061*	
C35	-0.1799 (13)	-0.0250 (7)	0.5575 (8)	0.108 (4)	0.5
H35A	-0.1576	-0.0373	0.6179	0.162*	0.5
H35B	-0.2221	-0.0623	0.5256	0.162*	0.5
H35C	-0.2422	0.0122	0.5539	0.162*	0.5
C36	-0.0578 (7)	-0.0065 (4)	0.5205 (4)	0.080 (2)	0.5
C37	0.0225 (8)	0.0451 (3)	0.5536 (4)	0.094 (4)	0.5
H37	-0.0021	0.0695	0.6013	0.112*	0.5
C38	0.1388 (8)	0.0610 (4)	0.5169 (6)	0.103 (3)	0.5
H38	0.1936	0.0962	0.5395	0.123*	0.5
C39	0.1747 (7)	0.0253 (5)	0.4471 (6)	0.119 (4)	0.5
H39	0.2542	0.0362	0.4220	0.143*	0.5
C40	0.0944 (8)	-0.0262 (4)	0.4140 (4)	0.097 (3)	0.5
H40	0.1190	-0.0506	0.3663	0.117*	0.5
C41	-0.0219 (7)	-0.0422 (3)	0.4507 (4)	0.075 (3)	0.5
H41	-0.0767	-0.0774	0.4280	0.090*	0.5

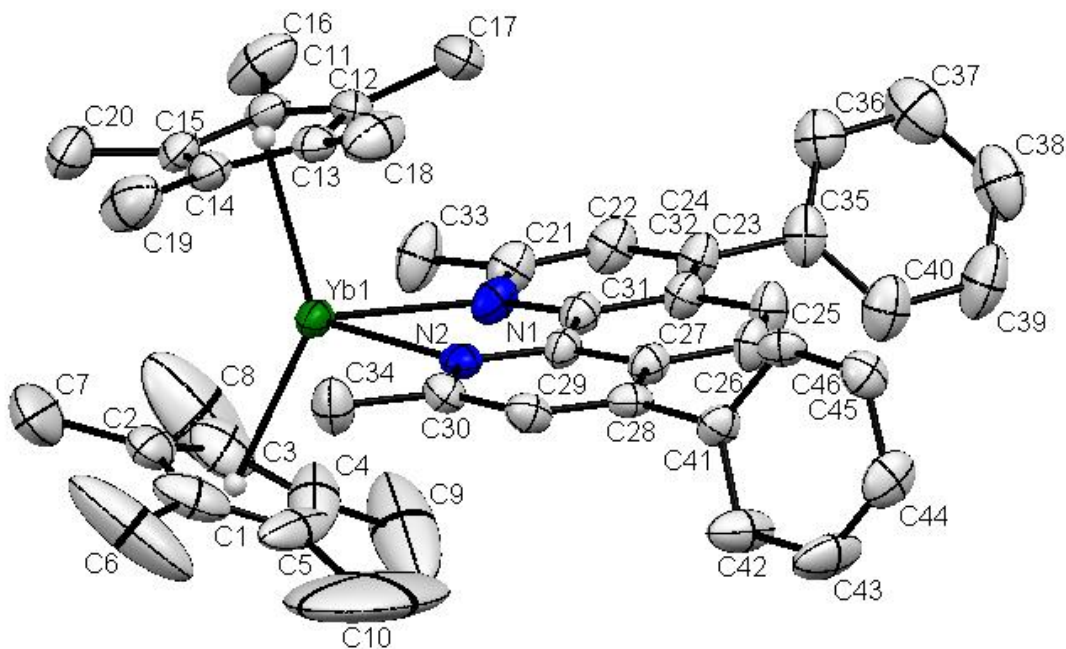


**Table S5:** Atomic displacement parameters ( $\text{\AA}^2$ ) for  $\text{Cp}^*_2\text{Yb}(4,7\text{-Me}_2\text{phen})$  (**2**).

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Yb1	0.02358 (6)	0.02301 (6)	0.02106 (6)	-0.00156 (4)	0.00104 (4)	-0.00035 (4)
N1	0.0268 (11)	0.0264 (11)	0.0241 (10)	-0.0004 (9)	0.0037 (8)	0.0014 (8)
N2	0.0303 (11)	0.0263 (11)	0.0240 (10)	-0.0020 (9)	0.0039 (9)	0.0012 (8)
C1	0.0254 (14)	0.0561 (19)	0.0304 (14)	-0.0037 (12)	0.0063 (11)	-0.0055 (13)
C2	0.0443 (16)	0.0339 (15)	0.0329 (14)	-0.0036 (12)	0.0144 (13)	0.0001 (12)
C3	0.0340 (15)	0.0510 (18)	0.0225 (13)	0.0063 (13)	0.0063 (11)	-0.0014 (12)
C4	0.0368 (15)	0.0336 (15)	0.0356 (14)	-0.0034 (12)	0.0131 (12)	-0.0080 (12)
C5	0.0337 (14)	0.0409 (16)	0.0339 (14)	0.0098 (12)	0.0121 (12)	0.0047 (12)
C6	0.0278 (16)	0.112 (3)	0.048 (2)	-0.0082 (18)	0.0050 (14)	-0.024 (2)
C7	0.092 (3)	0.044 (2)	0.066 (2)	-0.0115 (19)	0.036 (2)	0.0061 (17)
C8	0.058 (2)	0.100 (3)	0.0257 (15)	0.024 (2)	0.0025 (15)	0.0020 (17)
C9	0.065 (2)	0.053 (2)	0.066 (2)	-0.0175 (17)	0.0314 (19)	-0.0337 (18)
C10	0.060 (2)	0.074 (3)	0.066 (2)	0.033 (2)	0.0225 (19)	0.032 (2)
C11	0.0405 (15)	0.0317 (14)	0.0248 (13)	0.0074 (12)	-0.0031 (11)	-0.0064 (11)
C12	0.0483 (17)	0.0275 (14)	0.0273 (13)	0.0004 (12)	0.0095 (12)	-0.0025 (11)
C13	0.0338 (14)	0.0349 (15)	0.0325 (14)	0.0030 (12)	0.0052 (12)	-0.0083 (12)
C14	0.0412 (15)	0.0256 (13)	0.0290 (13)	0.0047 (11)	-0.0011 (12)	-0.0018 (11)
C15	0.0382 (15)	0.0291 (14)	0.0301 (13)	-0.0043 (11)	0.0010 (11)	-0.0063 (11)
C16	0.059 (2)	0.055 (2)	0.0346 (16)	0.0199 (16)	-0.0135 (15)	-0.0072 (14)
C17	0.088 (3)	0.0407 (18)	0.0364 (17)	-0.0005 (17)	0.0273 (18)	0.0010 (14)
C18	0.0354 (17)	0.070 (2)	0.056 (2)	0.0041 (16)	0.0112 (15)	-0.0159 (18)
C19	0.065 (2)	0.0318 (16)	0.0476 (18)	0.0121 (15)	-0.0013 (16)	0.0043 (14)
C20	0.0503 (19)	0.0477 (19)	0.0535 (19)	-0.0185 (15)	0.0033 (15)	-0.0117 (15)
C21	0.0308 (13)	0.0303 (14)	0.0290 (13)	0.0008 (11)	0.0016 (11)	0.0026 (11)
C22	0.0389 (15)	0.0293 (15)	0.0368 (14)	0.0033 (12)	0.0033 (12)	0.0083 (12)
C23	0.0351 (14)	0.0265 (14)	0.0436 (16)	-0.0016 (11)	0.0099 (12)	0.0022 (12)
C24	0.0301 (13)	0.0250 (13)	0.0312 (13)	-0.0025 (10)	0.0106 (11)	-0.0033 (10)
C25	0.0313 (14)	0.0304 (15)	0.0432 (15)	-0.0091 (11)	0.0071 (12)	-0.0052 (12)
C26	0.0262 (13)	0.0415 (16)	0.0355 (14)	-0.0067 (12)	0.0025 (11)	-0.0068 (12)
C27	0.0261 (12)	0.0337 (14)	0.0229 (12)	-0.0008 (10)	0.0070 (10)	-0.0040 (10)
C28	0.0256 (13)	0.0414 (15)	0.0243 (12)	0.0014 (11)	0.0041 (10)	-0.0025 (11)
C29	0.0346 (14)	0.0380 (16)	0.0272 (13)	0.0020 (12)	0.0009 (11)	0.0058 (11)
C30	0.0345 (14)	0.0288 (14)	0.0322 (14)	-0.0029 (11)	0.0017 (11)	0.0038 (11)
C31	0.0252 (12)	0.0257 (13)	0.0229 (12)	-0.0013 (10)	0.0062 (10)	-0.0032 (10)

C32	0.0252 (12)	0.0269 (13)	0.0238 (12)	-0.0009 (10)	0.0084 (10)	-0.0031 (10)
C33	0.0477 (19)	0.0357 (17)	0.074 (2)	-0.0068 (14)	0.0019 (17)	0.0109 (16)
C34	0.0309 (15)	0.0539 (19)	0.0357 (15)	-0.0017 (13)	-0.0025 (12)	-0.0008 (13)
C35	0.083 (7)	0.145 (9)	0.095 (7)	0.021 (7)	0.002 (7)	0.061 (7)
C36	0.082 (5)	0.089 (5)	0.065 (4)	0.026 (4)	-0.016 (4)	0.032 (4)
C37	0.106 (7)	0.081 (6)	0.083 (6)	0.019 (6)	-0.039 (6)	0.024 (6)
C38	0.095 (6)	0.086 (6)	0.113 (6)	-0.003 (5)	-0.057 (5)	0.031 (5)
C39	0.108 (8)	0.127 (8)	0.115 (8)	0.019 (7)	-0.024 (7)	0.047 (7)
C40	0.113 (6)	0.098 (6)	0.076 (5)	0.043 (5)	-0.011 (5)	0.018 (5)
C41	0.106 (6)	0.066 (5)	0.048 (5)	0.038 (5)	-0.020 (5)	-0.005 (5)

**Figure 24.** ORTEP diagram for  $\text{Cp}^*_2\text{Yb}(\text{2,9-Me}_2\text{-4,7-Ph}_2\text{phen})$  (**5**). (Thermal ellipsoids are at 50% level). One toluene molecule has been omitted for clarity.



**Table S6:** Bond distances (Å) for Cp\*<sub>2</sub>Yb(2,9-Me<sub>2</sub>-4,7-Ph<sub>2</sub>phen) (**5**).

Yb1—N1	2.511 (6)	C21—C22	1.390 (10)
Yb1—N2	2.515 (5)	C21—C33	1.508 (10)
Yb1—C5	2.691 (9)	C22—C23	1.352 (10)
Yb1—C14	2.725 (6)	C23—C24	1.446 (9)
Yb1—C13	2.729 (6)	C23—C35	1.509 (9)
Yb1—C15	2.738 (6)	C24—C32	1.411 (9)
Yb1—C12	2.744 (6)	C24—C25	1.425 (9)
Yb1—C3	2.749 (8)	C25—C26	1.365 (9)
Yb1—C1	2.770 (9)	C26—C27	1.432 (9)
Yb1—C2	2.783 (7)	C27—C31	1.409 (8)
N1—C21	1.343 (8)	C27—C28	1.427 (8)
N1—C32	1.368 (8)	C28—C29	1.361 (9)
N2—C30	1.335 (8)	C28—C41	1.499 (9)
N2—C31	1.377 (8)	C29—C30	1.417 (9)
C1—C2	1.368 (14)	C30—C34	1.496 (9)
C1—C5	1.422 (17)	C31—C32	1.455 (8)
C1—C6	1.517 (17)	C35—C36	1.386 (11)
C2—C3	1.378 (15)	C35—C40	1.396 (11)
C2—C7	1.503 (14)	C36—C37	1.407 (12)
C3—C4	1.418 (16)	C37—C38	1.370 (14)
C3—C8	1.565 (16)	C38—C39	1.415 (14)
C4—C5	1.389 (18)	C39—C40	1.406 (11)
C4—C9	1.492 (18)	C41—C46	1.393 (9)
C5—C10	1.502 (15)	C41—C42	1.398 (9)
C11—C15	1.394 (9)	C42—C43	1.397 (11)
C11—C12	1.413 (10)	C43—C44	1.369 (12)
C11—C16	1.538 (11)	C44—C45	1.379 (10)
C12—C13	1.418 (10)	C45—C46	1.389 (9)
C12—C17	1.525 (10)		
C13—C14	1.402 (10)		
C14—C15	1.428 (10)		

**Table S7:** Bond angles (deg) for Cp<sup>\*</sup><sub>2</sub>Yb(2,9-Me<sub>2</sub>-4,7-Ph<sub>2</sub>phen) (**5**).

N1—Yb1—N2	66.18 (17)	C13—C14—C15	107.7 (6)
N1—Yb1—C5	99.6 (3)	C13—C14—C19	128.1 (7)
N2—Yb1—C5	83.1 (2)	C15—C14—C19	123.9 (7)
N1—Yb1—C4	82.6 (3)	C13—C14—Yb1	75.3 (4)
N2—Yb1—C4	98.5 (3)	C15—C14—Yb1	75.4 (4)
C5—Yb1—C4	29.9 (4)	C19—C14—Yb1	120.7 (5)
N1—Yb1—C14	127.05 (19)	C11—C15—C14	107.9 (6)
N2—Yb1—C14	100.46 (19)	C11—C15—C20	125.1 (7)
C5—Yb1—C14	130.8 (4)	C14—C15—C20	126.1 (7)
C4—Yb1—C14	149.5 (3)	C11—C15—Yb1	75.9 (4)
N1—Yb1—C13	99.17 (19)	C14—C15—Yb1	74.3 (4)
N2—Yb1—C13	78.96 (18)	C20—C15—Yb1	124.5 (5)
C5—Yb1—C13	146.0 (3)	N1—C21—C22	122.6 (6)
C4—Yb1—C13	175.9 (4)	N1—C21—C33	118.3 (6)
C14—Yb1—C13	29.8 (2)	C22—C21—C33	119.1 (6)
N1—Yb1—C15	121.16 (19)	C23—C22—C21	121.9 (6)
N2—Yb1—C15	127.99 (18)	C22—C23—C24	117.6 (6)
C5—Yb1—C15	135.3 (3)	C22—C23—C35	119.8 (6)
C4—Yb1—C15	132.6 (3)	C24—C23—C35	122.5 (6)
C14—Yb1—C15	30.3 (2)	C32—C24—C25	120.1 (6)
C13—Yb1—C15	49.4 (2)	C32—C24—C23	117.3 (6)
N1—Yb1—C12	78.61 (18)	C25—C24—C23	122.6 (6)
N2—Yb1—C12	90.43 (19)	C26—C25—C24	120.9 (6)
C5—Yb1—C12	173.4 (2)	C25—C26—C27	121.1 (6)
C4—Yb1—C12	153.9 (4)	C31—C27—C28	118.7 (6)
C14—Yb1—C12	49.4 (2)	C31—C27—C26	119.3 (5)
C13—Yb1—C12	30.0 (2)	C28—C27—C26	122.0 (6)
C15—Yb1—C12	49.18 (19)	C29—C28—C27	117.7 (6)
N1—Yb1—C3	100.2 (3)	C29—C28—C41	121.1 (5)
N2—Yb1—C3	128.1 (3)	C27—C28—C41	121.2 (5)
C5—Yb1—C3	48.6 (3)	C28—C29—C30	121.2 (6)
C4—Yb1—C3	30.2 (3)	N2—C30—C29	121.8 (6)
C14—Yb1—C3	123.8 (3)	N2—C30—C34	118.0 (6)
C13—Yb1—C3	151.6 (3)	C29—C30—C34	120.2 (6)
C15—Yb1—C3	102.5 (3)	N2—C31—C27	122.0 (5)

C12—Yb1—C3	137.9 (3)	N2—C31—C32	118.2 (5)
N1—Yb1—C11	91.78 (18)	C27—C31—C32	119.8 (5)
N2—Yb1—C11	120.21 (19)	N1—C32—C24	123.3 (6)
C5—Yb1—C11	156.7 (3)	N1—C32—C31	117.8 (5)
C4—Yb1—C11	134.7 (4)	C24—C32—C31	118.9 (5)
C14—Yb1—C11	49.2 (2)	C36—C35—C40	119.5 (7)
C13—Yb1—C11	49.2 (2)	C36—C35—C23	118.5 (7)
C15—Yb1—C11	29.4 (2)	C40—C35—C23	121.9 (7)
C12—Yb1—C11	29.8 (2)	C35—C36—C37	121.6 (8)
C3—Yb1—C11	109.5 (3)	C38—C37—C36	119.0 (9)
N1—Yb1—C1	129.2 (3)	C37—C38—C39	120.5 (8)
N2—Yb1—C1	100.4 (2)	C40—C39—C38	119.8 (8)
C5—Yb1—C1	30.1 (4)	C35—C40—C39	119.5 (8)
C4—Yb1—C1	49.8 (4)	C46—C41—C42	118.9 (6)
C14—Yb1—C1	103.0 (3)	C46—C41—C28	122.1 (5)
C13—Yb1—C1	127.2 (3)	C42—C41—C28	118.9 (6)
C15—Yb1—C1	105.8 (3)	C43—C42—C41	119.8 (7)
C12—Yb1—C1	152.1 (3)	C44—C43—C42	120.5 (7)
C3—Yb1—C1	48.3 (3)	C43—C44—C45	120.0 (7)
C11—Yb1—C1	132.4 (3)	C44—C45—C46	120.4 (6)
N1—Yb1—C2	128.4 (3)	C45—C46—C41	120.2 (6)
N2—Yb1—C2	128.1 (2)	C2S—C1S—C7S	115.3 (18)
C5—Yb1—C2	47.8 (3)	C6S—C1S—C7S	124.7 (18)
C4—Yb1—C2	48.7 (3)	C2—C1—C5	105.6 (10)
C14—Yb1—C2	100.9 (3)	C2—C1—C6	127.1 (12)
C13—Yb1—C2	130.6 (3)	C5—C1—C6	126.1 (12)
C15—Yb1—C2	89.6 (2)	C2—C1—Yb1	76.3 (5)
C12—Yb1—C2	137.9 (2)	C5—C1—Yb1	71.8 (5)
C3—Yb1—C2	28.8 (3)	C6—C1—Yb1	126.6 (7)
C11—Yb1—C2	109.5 (2)	C1—C2—C3	110.7 (10)
C1—Yb1—C2	28.5 (3)	C1—C2—C7	122.6 (11)
C21—N1—C32	117.3 (6)	C3—C2—C7	125.9 (10)
C21—N1—Yb1	123.3 (4)	C1—C2—Yb1	75.2 (5)
C32—N1—Yb1	119.0 (4)	C3—C2—Yb1	74.2 (5)
C30—N2—C31	118.4 (5)	C7—C2—Yb1	125.8 (6)
C30—N2—Yb1	123.1 (4)	C2—C3—C4	108.0 (11)
C31—N2—Yb1	118.5 (4)	C2—C3—C8	121.1 (10)

C4—C3—C8	130.5 (12)		
C2—C3—Yb1	77.0 (5)		
C4—C3—Yb1	73.0 (5)		
C8—C3—Yb1	121.6 (7)		
C5—C4—C3	105.7 (11)		
C5—C4—C9	132.4 (14)		
C3—C4—C9	121.1 (15)		
C5—C4—Yb1	74.7 (5)		
C3—C4—Yb1	76.9 (5)		
C9—C4—Yb1	121.2 (8)		
C4—C5—C1	110.0 (9)		
C4—C5—C10	124.6 (13)		
C1—C5—C10	124.9 (14)		
C4—C5—Yb1	75.4 (6)		
C1—C5—Yb1	78.0 (5)		
C10—C5—Yb1	120.2 (6)		
C15—C11—C12	108.8 (6)		
C15—C11—C16	123.1 (7)		
C12—C11—C16	127.2 (7)		
C15—C11—Yb1	74.7 (4)		
C12—C11—Yb1	74.7 (4)		
C16—C11—Yb1	125.7 (5)		
C11—C12—C13	107.4 (6)		
C11—C12—C17	126.8 (7)		
C13—C12—C17	125.2 (7)		
C11—C12—Yb1	75.5 (4)		
C13—C12—Yb1	74.4 (3)		
C17—C12—Yb1	122.9 (5)		
C14—C13—C12	108.3 (6)		
C14—C13—C18	125.6 (7)		
C12—C13—C18	125.4 (7)		
C14—C13—Yb1	74.9 (4)		
C12—C13—Yb1	75.6 (4)		
C18—C13—Yb1	123.2 (5)		

**Table S8:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) for  $\text{Cp}^*_2\text{Yb}(2,9\text{-Me}_2\text{-}4,7\text{-Ph}_2\text{phen})$  (**5**).

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Yb1	-0.13898 (2)	0.82411 (2)	0.26095 (2)	0.03010 (11)	
N1	0.0756 (5)	0.7058 (4)	0.2740 (4)	0.0349 (12)	
N2	-0.0154 (4)	0.9402 (4)	0.2513 (3)	0.0287 (11)	
C1	-0.2706 (11)	0.9090 (10)	0.0992 (6)	0.075 (2)	
C2	-0.2918 (8)	0.8138 (9)	0.1263 (6)	0.0623 (19)	
C3	-0.1921 (10)	0.7159 (10)	0.1166 (7)	0.075 (2)	
C4	-0.1012 (10)	0.7489 (14)	0.0815 (7)	0.095 (3)	
C5	-0.1508 (11)	0.8676 (12)	0.0711 (6)	0.083 (2)	
C6	-0.3603 (14)	1.0299 (12)	0.0818 (10)	0.118 (4)	
H6A	-0.4264	1.0272	0.0482	0.177*	
H6B	-0.3248	1.0745	0.0429	0.177*	
H6C	-0.3875	1.0660	0.1430	0.177*	
C7	-0.4126 (10)	0.8182 (13)	0.1468 (8)	0.095 (3)	
H7A	-0.4584	0.8432	0.0887	0.143*	
H7B	-0.4501	0.8724	0.1970	0.143*	
H7C	-0.4081	0.7419	0.1680	0.143*	
C8	-0.1952 (13)	0.5944 (11)	0.1330 (10)	0.108 (3)	
H8A	-0.2749	0.5997	0.1252	0.162*	
H8B	-0.1696	0.5648	0.1976	0.162*	
H8C	-0.1431	0.5424	0.0864	0.162*	
C9	0.0141 (13)	0.6617 (16)	0.0508 (10)	0.140 (5)	
H9A	0.0578	0.6999	0.0138	0.211*	
H9B	0.0020	0.6062	0.0112	0.211*	
H9C	0.0582	0.6219	0.1071	0.211*	
C10	-0.0912 (14)	0.9396 (15)	0.0242 (8)	0.118 (3)	
H10A	-0.0067	0.8955	0.0227	0.177*	
H10B	-0.1092	1.0086	0.0605	0.177*	
H10C	-0.1187	0.9617	-0.0411	0.177*	
C11	-0.1856 (6)	0.7381 (6)	0.4347 (5)	0.0366 (15)	
C12	-0.1150 (6)	0.7974 (6)	0.4552 (4)	0.0375 (15)	
C13	-0.1814 (6)	0.9158 (6)	0.4368 (4)	0.0350 (14)	
C14	-0.2909 (6)	0.9287 (6)	0.4048 (5)	0.0370 (15)	
C15	-0.2930 (6)	0.8172 (6)	0.4034 (4)	0.0356 (14)	

C16	-0.1619 (9)	0.6116 (8)	0.4596 (7)	0.072 (3)	
H16A	-0.0791	0.5699	0.4735	0.108*	
H16B	-0.1822	0.5778	0.4056	0.108*	
H16C	-0.2093	0.6066	0.5158	0.108*	
C17	0.0034 (7)	0.7473 (9)	0.5025 (6)	0.064 (3)	
H17A	0.0453	0.6679	0.4841	0.096*	
H17B	-0.0079	0.7493	0.5720	0.096*	
H17C	0.0488	0.7926	0.4819	0.096*	
C18	-0.1474 (9)	1.0115 (8)	0.4627 (6)	0.061 (2)	
H18A	-0.2157	1.0841	0.4594	0.092*	
H18B	-0.0867	1.0158	0.4178	0.092*	
H18C	-0.1175	0.9971	0.5276	0.092*	
C19	-0.3958 (8)	1.0389 (7)	0.3854 (7)	0.064 (2)	
H19A	-0.4655	1.0328	0.4157	0.096*	
H19B	-0.4067	1.0520	0.3164	0.096*	
H19C	-0.3832	1.1030	0.4115	0.096*	
C20	-0.3985 (7)	0.7909 (9)	0.3891 (6)	0.062 (2)	
H20A	-0.4534	0.8513	0.3482	0.093*	
H20B	-0.4362	0.7870	0.4511	0.093*	
H20C	-0.3747	0.7171	0.3587	0.093*	
C21	0.1203 (6)	0.5915 (6)	0.2882 (5)	0.0392 (15)	
C22	0.2373 (6)	0.5288 (6)	0.3074 (5)	0.0413 (16)	
H22	0.2636	0.4484	0.3194	0.050*	
C23	0.3146 (6)	0.5790 (5)	0.3094 (5)	0.0376 (15)	
C24	0.2708 (6)	0.7021 (5)	0.2940 (5)	0.0341 (14)	
C25	0.3434 (6)	0.7647 (6)	0.2969 (5)	0.0389 (15)	
H25	0.4239	0.7251	0.3101	0.047*	
C26	0.2990 (6)	0.8807 (6)	0.2810 (5)	0.0363 (14)	
H26	0.3496	0.9204	0.2809	0.044*	
C27	0.1774 (5)	0.9436 (5)	0.2646 (4)	0.0302 (13)	
C28	0.1291 (5)	1.0649 (5)	0.2479 (4)	0.0291 (13)	
C29	0.0121 (6)	1.1175 (6)	0.2354 (4)	0.0328 (13)	
H29	-0.0223	1.1983	0.2249	0.039*	
C30	-0.0593 (6)	1.0540 (5)	0.2376 (4)	0.0324 (13)	
C31	0.1030 (5)	0.8842 (5)	0.2632 (4)	0.0273 (12)	
C32	0.1505 (5)	0.7602 (5)	0.2777 (4)	0.0311 (13)	
C33	0.0405 (7)	0.5289 (7)	0.2804 (7)	0.054 (2)	



H33A	-0.0399	0.5847	0.2734	0.080*	
H33B	0.0458	0.4804	0.3381	0.080*	
H33C	0.0639	0.4811	0.2246	0.080*	
C34	-0.1882 (6)	1.1142 (6)	0.2260 (6)	0.0448 (17)	
H34A	-0.2206	1.0591	0.2088	0.067*	
H34B	-0.2041	1.1743	0.1755	0.067*	
H34C	-0.2244	1.1487	0.2861	0.067*	
C35	0.4409 (6)	0.5071 (6)	0.3297 (6)	0.0435 (17)	
C36	0.4669 (7)	0.4316 (6)	0.4085 (6)	0.0488 (18)	
H36	0.4050	0.4268	0.4477	0.059*	
C37	0.5826 (8)	0.3620 (7)	0.4317 (7)	0.064 (2)	
H37	0.5989	0.3113	0.4864	0.076*	
C38	0.6715 (8)	0.3683 (7)	0.3743 (8)	0.066 (3)	
H38	0.7501	0.3238	0.3906	0.079*	
C39	0.6472 (7)	0.4408 (7)	0.2910 (8)	0.064 (2)	
H39	0.7091	0.4423	0.2501	0.077*	
C40	0.5311 (7)	0.5105 (6)	0.2691 (7)	0.0522 (19)	
H40	0.5142	0.5596	0.2134	0.063*	
C41	0.2051 (6)	1.1319 (5)	0.2421 (4)	0.0307 (13)	
C42	0.2267 (9)	1.1752 (8)	0.1530 (5)	0.057 (2)	
H42	0.1899	1.1660	0.0980	0.069*	
C43	0.3024 (9)	1.2322 (8)	0.1452 (6)	0.064 (2)	
H43	0.3181	1.2604	0.0844	0.076*	
C44	0.3541 (7)	1.2479 (6)	0.2243 (6)	0.0456 (17)	
H44	0.4074	1.2846	0.2181	0.055*	
C45	0.3289 (6)	1.2103 (6)	0.3130 (5)	0.0378 (15)	
H45	0.3606	1.2260	0.3683	0.045*	
C46	0.2572 (6)	1.1497 (5)	0.3220 (4)	0.0313 (13)	
H46	0.2437	1.1204	0.3830	0.038*	
C7S	0.664 (3)	0.331 (2)	-0.022 (2)	0.103 (6)	0.5
H7S1	0.7299	0.3470	-0.0484	0.154*	0.5
H7S2	0.6444	0.2838	-0.0662	0.154*	0.5
H7S3	0.6845	0.2892	0.0396	0.154*	0.5
C1S	0.5633 (12)	0.4382 (11)	-0.0094 (14)	0.080 (4)	0.5
C2S	0.4633 (15)	0.4271 (12)	0.0283 (13)	0.083 (5)	0.5
H2S	0.4639	0.3532	0.0440	0.099*	0.5
C3S	0.3625 (12)	0.5242 (17)	0.0431 (13)	0.091 (5)	0.5

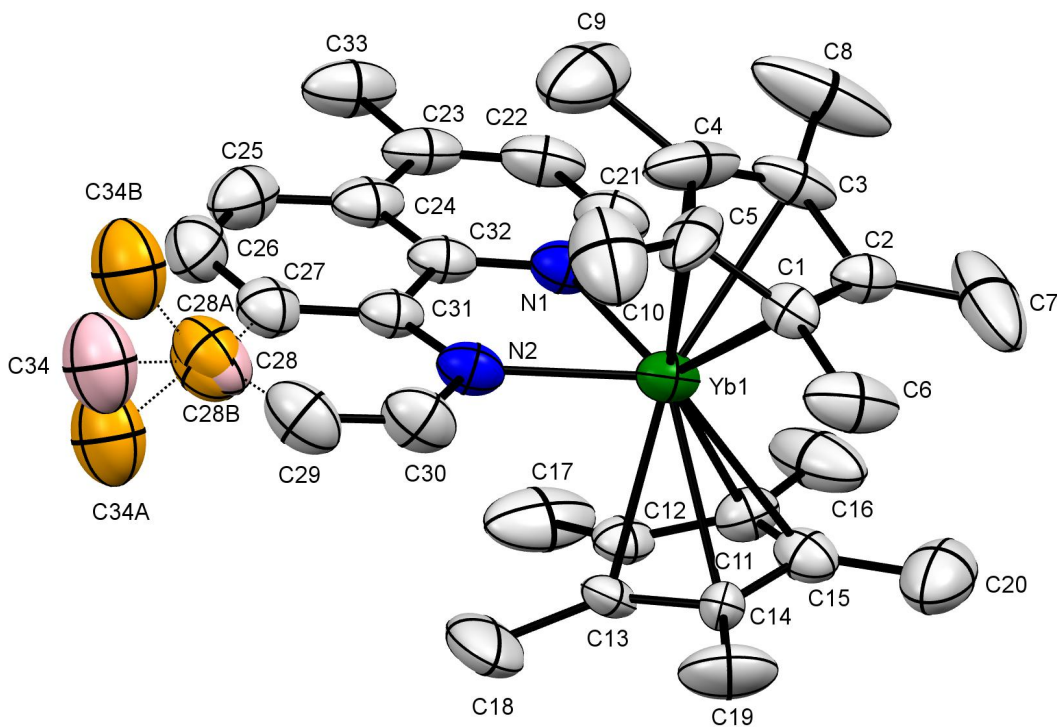
H3S	0.2941	0.5166	0.0689	0.109*	0.5
C4S	0.3616 (13)	0.6323 (13)	0.0201 (15)	0.104 (6)	0.5
H4S	0.2926	0.6986	0.0302	0.125*	0.5
C5S	0.4615 (17)	0.6433 (10)	-0.0176 (13)	0.092 (5)	0.5
H5S	0.4609	0.7172	-0.0333	0.110*	0.5
C6S	0.5624 (13)	0.5463 (14)	-0.0324 (12)	0.075 (4)	0.5
H6S	0.6307	0.5538	-0.0582	0.090*	0.5

**Table S9:** Atomic displacement parameters ( $\text{\AA}^2$ ) for  $\text{Cp}^* \text{Yb}(\text{2,9-Me}_2\text{-4,7-Ph}_2\text{phen})$  (**5**).

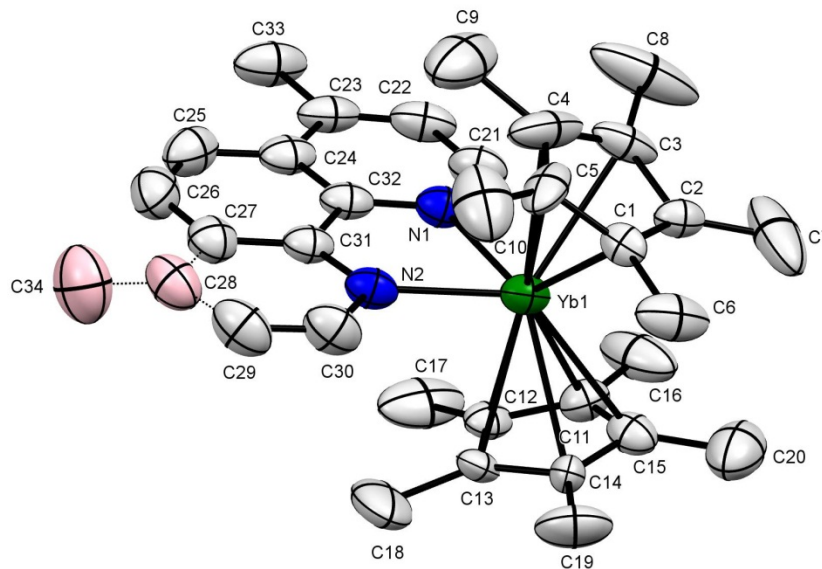
	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Yb1	0.03064 (16)	0.04143 (17)	0.02541 (15)	-0.02181 (12)	0.00232 (10)	-0.00402 (10)
N1	0.042 (3)	0.032 (3)	0.038 (3)	-0.023 (2)	0.008 (2)	-0.007 (2)
N2	0.034 (3)	0.033 (3)	0.021 (2)	-0.015 (2)	-0.001 (2)	-0.004 (2)
C1	0.111 (5)	0.096 (5)	0.040 (4)	-0.062 (4)	-0.026 (4)	-0.002 (4)
C2	0.071 (4)	0.107 (5)	0.035 (3)	-0.061 (4)	-0.013 (3)	-0.002 (4)
C3	0.090 (5)	0.100 (5)	0.060 (4)	-0.061 (4)	-0.013 (4)	-0.024 (4)
C4	0.081 (5)	0.165 (7)	0.052 (4)	-0.056 (5)	0.006 (4)	-0.052 (5)
C5	0.116 (5)	0.156 (6)	0.031 (3)	-0.112 (5)	-0.001 (4)	-0.011 (4)
C6	0.153 (9)	0.105 (7)	0.086 (7)	-0.035 (7)	-0.062 (6)	-0.001 (6)
C7	0.078 (6)	0.160 (8)	0.063 (5)	-0.063 (6)	-0.021 (5)	0.001 (6)
C8	0.131 (8)	0.103 (7)	0.114 (7)	-0.068 (6)	-0.036 (6)	-0.015 (6)
C9	0.100 (8)	0.219 (10)	0.081 (7)	-0.032 (8)	0.008 (6)	-0.075 (7)
C10	0.167 (8)	0.199 (9)	0.050 (5)	-0.140 (7)	0.007 (6)	-0.005 (6)
C11	0.036 (3)	0.038 (4)	0.032 (3)	-0.011 (3)	0.007 (3)	0.004 (3)
C12	0.031 (3)	0.059 (4)	0.021 (3)	-0.016 (3)	-0.001 (2)	0.000 (3)
C13	0.040 (4)	0.046 (4)	0.023 (3)	-0.020 (3)	0.003 (3)	-0.004 (3)
C14	0.034 (3)	0.043 (4)	0.031 (3)	-0.012 (3)	0.004 (3)	0.001 (3)
C15	0.031 (3)	0.050 (4)	0.030 (3)	-0.021 (3)	0.007 (3)	-0.006 (3)
C16	0.078 (6)	0.054 (5)	0.075 (6)	-0.021 (5)	0.026 (5)	0.009 (4)
C17	0.041 (4)	0.109 (8)	0.036 (4)	-0.024 (5)	-0.005 (3)	0.009 (4)
C18	0.084 (6)	0.081 (6)	0.043 (4)	-0.057 (5)	0.011 (4)	-0.017 (4)
C19	0.054 (5)	0.055 (5)	0.066 (6)	-0.006 (4)	0.015 (4)	0.008 (4)
C20	0.051 (5)	0.100 (7)	0.049 (5)	-0.046 (5)	0.007 (4)	-0.005 (4)
C21	0.040 (4)	0.030 (3)	0.050 (4)	-0.016 (3)	0.009 (3)	-0.008 (3)
C22	0.041 (4)	0.030 (3)	0.055 (4)	-0.016 (3)	0.007 (3)	-0.007 (3)
C23	0.029 (3)	0.031 (3)	0.052 (4)	-0.011 (3)	0.008 (3)	-0.005 (3)
C24	0.031 (3)	0.034 (3)	0.040 (4)	-0.015 (3)	0.003 (3)	-0.001 (3)
C25	0.028 (3)	0.036 (3)	0.056 (4)	-0.016 (3)	-0.001 (3)	-0.005 (3)
C26	0.030 (3)	0.039 (4)	0.048 (4)	-0.022 (3)	0.000 (3)	-0.004 (3)
C27	0.034 (3)	0.032 (3)	0.029 (3)	-0.018 (3)	0.002 (2)	-0.002 (2)
C28	0.038 (3)	0.031 (3)	0.021 (3)	-0.016 (3)	0.000 (2)	-0.001 (2)
C29	0.039 (3)	0.034 (3)	0.028 (3)	-0.017 (3)	-0.004 (3)	0.002 (3)
C30	0.033 (3)	0.037 (3)	0.028 (3)	-0.015 (3)	-0.003 (2)	-0.001 (3)
C31	0.025 (3)	0.031 (3)	0.029 (3)	-0.015 (3)	0.003 (2)	-0.003 (2)

C32	0.032 (3)	0.034 (3)	0.033 (3)	-0.018 (3)	0.003 (2)	-0.004 (3)
C33	0.044 (4)	0.040 (4)	0.086 (6)	-0.026 (3)	0.011 (4)	-0.011 (4)
C34	0.033 (4)	0.042 (4)	0.062 (5)	-0.017 (3)	-0.008 (3)	0.006 (3)
C35	0.031 (4)	0.032 (3)	0.067 (5)	-0.011 (3)	-0.001 (3)	-0.008 (3)
C36	0.046 (4)	0.039 (4)	0.059 (5)	-0.014 (3)	-0.003 (3)	-0.005 (3)
C37	0.061 (6)	0.046 (5)	0.071 (6)	-0.005 (4)	-0.015 (5)	-0.006 (4)
C38	0.045 (5)	0.043 (5)	0.098 (7)	-0.003 (4)	-0.016 (5)	-0.014 (5)
C39	0.038 (4)	0.051 (5)	0.101 (7)	-0.015 (4)	0.015 (4)	-0.013 (5)
C40	0.043 (4)	0.037 (4)	0.076 (6)	-0.017 (3)	0.003 (4)	-0.003 (4)
C41	0.035 (3)	0.031 (3)	0.030 (3)	-0.018 (3)	0.002 (2)	0.000 (2)
C42	0.098 (7)	0.073 (5)	0.031 (4)	-0.066 (5)	0.000 (4)	-0.001 (4)
C43	0.102 (7)	0.081 (6)	0.040 (4)	-0.073 (6)	0.016 (4)	-0.005 (4)
C44	0.053 (4)	0.039 (4)	0.057 (5)	-0.031 (3)	0.008 (3)	-0.009 (3)
C45	0.043 (4)	0.034 (3)	0.039 (4)	-0.017 (3)	-0.006 (3)	-0.004 (3)
C46	0.040 (3)	0.023 (3)	0.029 (3)	-0.011 (3)	-0.002 (3)	0.005 (2)
C7S	0.101 (11)	0.094 (11)	0.090 (10)	-0.016 (10)	-0.011 (10)	0.028 (10)
C1S	0.083 (8)	0.079 (8)	0.081 (7)	-0.038 (7)	-0.016 (7)	0.027 (7)
C2S	0.082 (9)	0.092 (10)	0.085 (8)	-0.047 (8)	-0.006 (8)	0.014 (8)
C3S	0.087 (10)	0.098 (10)	0.095 (9)	-0.044 (9)	-0.012 (9)	0.006 (9)
C4S	0.100 (10)	0.096 (11)	0.105 (9)	-0.025 (10)	-0.012 (9)	0.010 (10)
C5S	0.097 (10)	0.080 (9)	0.102 (9)	-0.039 (8)	-0.015 (9)	0.021 (9)
C6S	0.086 (9)	0.070 (9)	0.089 (8)	-0.053 (8)	-0.018 (8)	0.026 (8)

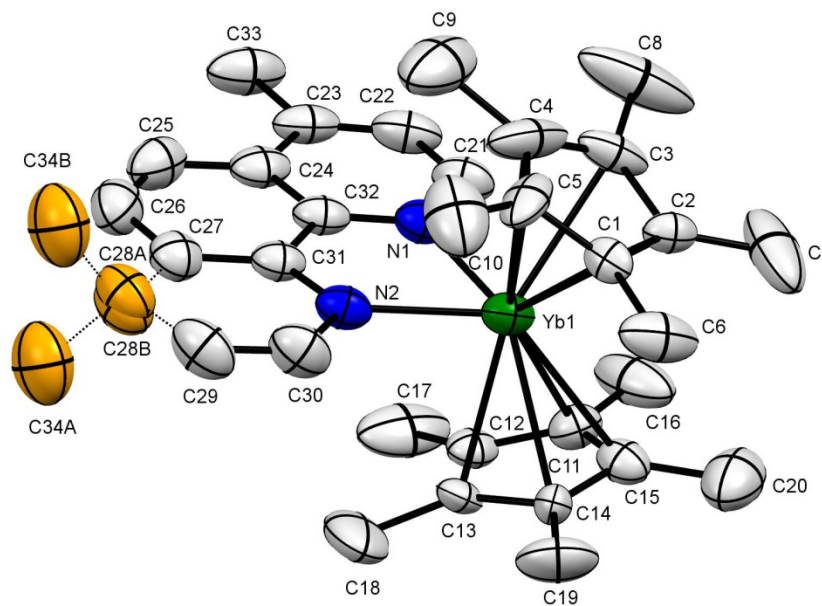
**Figure S25.** ORTEP diagram for 7. (Thermal ellipsoids are at 50% level). One disordered solvent molecule has been SQUEEZED and hydrogen atoms are removed for clarity. The carbon atoms represented in orange are due to a position disorder of a methyl group connected to the phenanthroline ring and the carbon atoms represented in pink is due to a methylene group.



**Figure S26.** ORTEP diagram for **7**. (Thermal ellipsoids are at 50% level). One disordered solvent molecule has been SQUEEZED and hydrogen atoms are removed for clarity. Only the methylene is represented (pink, 72 %).



**Figure S27.** ORTEP diagram for **7**. (Thermal ellipsoids are at 50% level). One disordered solvent molecule has been SQUEEZED and hydrogen atoms are removed for clarity. Only the disorder on the methyl is represented (orange, 28 %).



**Table S10:** Bond distances (Å) for **7**.

Yb1—N2	2.268 (3)	C11A—C12A	1.393 (6)
Yb1—N1	2.362 (3)	C11A—C15A	1.410 (6)
Yb1—C14A	2.584 (11)	C11A—C16A	1.547 (6)
Yb1—C4	2.590 (5)	C12A—C13A	1.401 (6)
Yb1—C1	2.592 (6)	C12A—C17A	1.546 (6)
Yb1—C11	2.59 (2)	C13A—C14A	1.399 (6)
Yb1—C1A	2.600 (5)	C13A—C18A	1.506 (6)
Yb1—C2A	2.600 (7)	C14A—C15A	1.419 (6)
Yb1—C5	2.604 (5)	C14A—C19A	1.525 (6)
Yb1—C13	2.60 (2)	C15A—C20A	1.522 (6)
Yb1—C3	2.608 (6)	C21—C22	1.398 (6)
Yb1—C3A	2.608 (8)	C22—C23	1.357 (6)
N1—C21	1.332 (4)	C23—C24	1.428 (6)
N1—C32	1.368 (5)	C23—C33	1.498 (6)
N2—C31	1.376 (5)	C24—C32	1.407 (5)
N2—C30	1.387 (5)	C24—C25	1.410 (6)
C1—C5	1.364 (3)	C25—C26	1.362 (7)
C1—C2	1.437 (3)	C26—C27	1.404 (6)
C1—C6	1.548 (3)	C27—C31	1.396 (6)
C2—C3	1.457 (3)	C27—C28	1.473 (10)
C2—C7	1.501 (3)	C27—C28A	1.51 (2)
C3—C4	1.373 (3)	C27—C28B	1.51 (2)
C3—C8	1.541 (3)	C29—C30	1.325 (6)
C4—C5	1.330 (3)	C29—C28	1.424 (11)
C4—C9	1.560 (3)	C29—C28A	1.51 (2)
C5—C10	1.579 (3)	C29—C28B	1.51 (2)
C1A—C5A	1.364 (3)	C31—C32	1.447 (5)
C1A—C2A	1.420 (3)	C28—C34	1.336 (12)
C1A—C6A	1.570 (4)	C28A—C34A	1.54 (2)
C2A—C3A	1.434 (3)	C28B—C34B	1.54 (2)
C2A—C7A	1.504 (4)	C5A—C10A	1.475 (3)
C3A—C4A	1.436 (3)	C11—C15	1.386 (10)
C3A—C8A	1.482 (4)	C11—C12	1.417 (10)
C4A—C5A	1.350 (3)	C11—C16	1.512 (11)
C4A—C9A	1.488 (4)	C12—C13	1.393 (10)

C12—C17	1.495 (11)		
C13—C14	1.433 (10)		
C13—C18	1.538 (11)		
C14—C15	1.386 (10)		
C14—C19	1.524 (11)		
C15—C20	1.517 (11)		



**Table S11:** Bond angles (deg) for **7**.

N2—Yb1—N1	70.52 (11)	C14—C15—Yb1	74.5 (6)
N2—Yb1—C14A	95.4 (2)	C11—C15—Yb1	72.9 (6)
N1—Yb1—C14A	125.6 (2)	C20—C15—Yb1	129.9 (6)
N2—Yb1—C4	88.15 (17)	C12A—C11A—Yb1	75.2 (4)
N1—Yb1—C4	81.91 (14)	C15A—C11A—Yb1	73.6 (4)
N2—Yb1—C1	108.29 (14)	C16A—C11A—Yb1	120.2 (4)
C5—Yb1—C3	50.02 (12)	C11A—C12A—Yb1	74.1 (3)
C13—Yb1—C3	161.2 (4)	C13A—C12A—Yb1	74.4 (4)
N2—Yb1—C3A	132.35 (14)	C17A—C12A—Yb1	122.5 (3)
N1—Yb1—C3A	104.73 (16)	C14A—C13A—Yb1	72.3 (3)
C14A—Yb1—C3A	120.9 (2)	C12A—C13A—Yb1	74.8 (4)
C1A—Yb1—C3A	51.86 (15)	C18A—C13A—Yb1	123.0 (3)
C2A—Yb1—C3A	31.96 (10)	C13A—C14A—Yb1	76.6 (4)
C21—N1—C32	117.5 (4)	C15A—C14A—Yb1	75.1 (3)
C21—N1—Yb1	126.0 (3)	C19A—C14A—Yb1	122.7 (4)
C32—N1—Yb1	116.4 (2)	C11A—C15A—Yb1	75.2 (4)
C31—N2—C30	114.7 (4)	C14A—C15A—Yb1	73.2 (4)
C31—N2—Yb1	119.8 (2)	C20A—C15A—Yb1	129.0 (4)
C30—N2—Yb1	125.5 (3)	N1—C21—C22	122.6 (4)
C5—C1—Yb1	75.24 (18)	C23—C22—C21	121.4 (4)
C2—C1—Yb1	75.14 (19)	C22—C23—C24	117.8 (4)
C6—C1—Yb1	121.93 (16)	C22—C23—C33	121.3 (4)
C1—C2—Yb1	72.88 (17)	C24—C23—C33	120.9 (4)
C3—C2—Yb1	73.31 (16)	C32—C24—C25	119.0 (4)
C7—C2—Yb1	126.66 (17)	C32—C24—C23	117.7 (4)
C4—C3—Yb1	73.93 (19)	C25—C24—C23	123.2 (4)
C2—C3—Yb1	74.33 (17)	C26—C25—C24	120.2 (4)
C8—C3—Yb1	122.38 (16)	C25—C26—C27	122.7 (4)
C5—C4—Yb1	75.75 (17)	C31—C27—C26	118.9 (4)
C3—C4—Yb1	75.4 (2)	C31—C27—C28	118.9 (5)
C9—C4—Yb1	118.69 (19)	C26—C27—C28	122.2 (5)
C4—C5—Yb1	74.58 (17)	C31—C27—C28A	122.8 (9)
C1—C5—Yb1	74.33 (19)	C26—C27—C28A	118.2 (9)
C10—C5—Yb1	120.48 (19)	C31—C27—C28B	122.6 (10)
C1—C6—H6B	109.5	C26—C27—C28B	118.3 (9)

C5A—C1A—Yb1	76.72 (19)	C30—C29—C28	123.1 (5)
C2A—C1A—Yb1	74.2 (2)	C30—C29—C28A	125.7 (9)
C6A—C1A—Yb1	120.1 (2)	C30—C29—C28B	125.6 (10)
C1A—C2A—Yb1	74.1 (2)	N2—C31—C27	124.7 (3)
C3A—C2A—Yb1	74.3 (2)	N2—C31—C32	116.2 (3)
C7A—C2A—Yb1	125.51 (18)	C27—C31—C32	119.1 (4)
C2A—C3A—Yb1	73.7 (2)	N2—C31—Yb1	38.16 (18)
C4A—C3A—Yb1	75.97 (19)	C27—C31—Yb1	162.8 (3)
C8A—C3A—Yb1	122.1 (2)	C32—C31—Yb1	78.1 (2)
C5A—C4A—Yb1	74.8 (2)	N1—C32—C24	123.1 (4)
C3A—C4A—Yb1	72.4 (2)	N1—C32—C31	116.9 (3)
C9A—C4A—Yb1	125.37 (19)	C24—C32—C31	120.1 (4)
C4A—C5A—Yb1	75.7 (2)	C34—C28—C29	121.6 (8)
C1A—C5A—Yb1	73.14 (19)	C34—C28—C27	124.5 (8)
C10A—C5A—Yb1	121.7 (2)	C29—C28—C27	113.8 (7)
C15—C11—Yb1	76.4 (6)	C27—C28A—C29	107.0 (16)
C12—C11—Yb1	75.1 (6)	C27—C28A—C34A	107 (3)
C16—C11—Yb1	119.5 (6)	C29—C28A—C34A	114 (4)
C13—C12—Yb1	74.1 (6)	C27—C28B—C29	106.9 (16)
C11—C12—Yb1	73.3 (5)	C27—C28B—C34B	103 (3)
C17—C12—Yb1	122.8 (6)	C29—C28B—C34B	113 (4)
C12—C13—Yb1	75.0 (6)		
C14—C13—Yb1	75.2 (6)		
C18—C13—Yb1	120.8 (5)		
C15—C14—Yb1	75.0 (6)		
C13—C14—Yb1	73.1 (6)		
C19—C14—Yb1	120.2 (6)		

**Table S12:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) for **7**.

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Yb1	0.70603 (2)	0.06198 (2)	0.19024 (2)	0.04303 (7)	
N1	0.7402 (3)	0.1829 (2)	0.25456 (14)	0.0449 (8)	
N2	0.6860 (3)	0.1753 (2)	0.12453 (14)	0.0456 (8)	
C1	0.5096 (5)	-0.0309 (3)	0.1645 (2)	0.035 (2)	0.535 (7)
C2	0.5502 (6)	-0.0474 (4)	0.2322 (3)	0.040 (2)	0.535 (7)
C3	0.5254 (6)	0.0308 (4)	0.2643 (3)	0.056 (4)	0.535 (7)
C4	0.4767 (5)	0.0858 (3)	0.2175 (3)	0.087 (8)	0.535 (7)
C5	0.4651 (4)	0.0483 (3)	0.1594 (3)	0.067 (5)	0.535 (7)
C6	0.5121 (8)	-0.1083 (5)	0.1200 (4)	0.074 (4)	0.535 (7)
H6A	0.4410	-0.1062	0.0862	0.111*	0.535 (7)
H6B	0.5060	-0.1584	0.1465	0.111*	0.535 (7)
H6C	0.5910	-0.1093	0.0989	0.111*	0.535 (7)
C7	0.5843 (9)	-0.1223 (6)	0.2735 (4)	0.116 (7)	0.535 (7)
H7A	0.5092	-0.1434	0.2921	0.174*	0.535 (7)
H7B	0.6478	-0.1071	0.3090	0.174*	0.535 (7)
H7C	0.6183	-0.1653	0.2462	0.174*	0.535 (7)
C8	0.5319 (9)	0.0572 (7)	0.3369 (4)	0.138 (7)	0.535 (7)
H8A	0.5456	0.1172	0.3403	0.207*	0.535 (7)
H8B	0.6015	0.0282	0.3617	0.207*	0.535 (7)
H8C	0.4528	0.0430	0.3550	0.207*	0.535 (7)
C9	0.4253 (7)	0.1762 (4)	0.2179 (6)	0.107 (4)	0.535 (7)
H9A	0.4456	0.2049	0.1780	0.161*	0.535 (7)
H9B	0.4641	0.2057	0.2564	0.161*	0.535 (7)
H9C	0.3339	0.1750	0.2195	0.161*	0.535 (7)
C10	0.4057 (7)	0.0730 (6)	0.0886 (4)	0.096 (3)	0.535 (7)
H10A	0.3162	0.0854	0.0902	0.144*	0.535 (7)
H10B	0.4153	0.0269	0.0583	0.144*	0.535 (7)
H10C	0.4488	0.1220	0.0734	0.144*	0.535 (7)
C1A	0.4816 (5)	0.0159 (4)	0.1450 (2)	0.042 (4)	0.465 (7)
C2A	0.5329 (6)	-0.0517 (4)	0.1829 (3)	0.031 (2)	0.465 (7)
C3A	0.5434 (7)	-0.0239 (4)	0.2498 (3)	0.032 (2)	0.465 (7)
C4A	0.4941 (6)	0.0590 (4)	0.2488 (3)	0.045 (4)	0.465 (7)
C5A	0.4594 (5)	0.0800 (4)	0.1859 (3)	0.051 (5)	0.465 (7)

C6A	0.4464 (9)	0.0095 (7)	0.0690 (4)	0.106 (4)	0.465 (7)
H6A1	0.3586	-0.0081	0.0606	0.160*	0.465 (7)
H6A2	0.5013	-0.0310	0.0503	0.160*	0.465 (7)
H6A3	0.4573	0.0638	0.0488	0.160*	0.465 (7)
C7A	0.5479 (11)	-0.1388 (6)	0.1584 (5)	0.105 (5)	0.465 (7)
H7A1	0.4661	-0.1600	0.1404	0.158*	0.465 (7)
H7A2	0.5813	-0.1742	0.1949	0.158*	0.465 (7)
H7A3	0.6063	-0.1388	0.1241	0.158*	0.465 (7)
C8A	0.5818 (11)	-0.0793 (7)	0.3058 (5)	0.119 (7)	0.465 (7)
H8A1	0.5118	-0.1160	0.3140	0.178*	0.465 (7)
H8A2	0.6049	-0.0458	0.3450	0.178*	0.465 (7)
H8A3	0.6541	-0.1127	0.2955	0.178*	0.465 (7)
C9A	0.4698 (10)	0.1072 (6)	0.3083 (4)	0.120 (7)	0.465 (7)
H9A1	0.4821	0.1664	0.3002	0.180*	0.465 (7)
H9A2	0.5281	0.0893	0.3454	0.180*	0.465 (7)
H9A3	0.3832	0.0977	0.3187	0.180*	0.465 (7)
C10A	0.3962 (8)	0.1560 (5)	0.1601 (5)	0.101 (3)	0.465 (7)
H10D	0.3067	0.1535	0.1671	0.152*	0.465 (7)
H10E	0.4055	0.1608	0.1130	0.152*	0.465 (7)
H10F	0.4344	0.2044	0.1830	0.152*	0.465 (7)
C11	0.9236 (19)	0.0094 (11)	0.2398 (8)	0.045 (5)	0.37 (2)
C12	0.951 (2)	0.0769 (11)	0.1991 (9)	0.041 (4)	0.37 (2)
C13	0.9160 (19)	0.0496 (11)	0.1354 (8)	0.035 (4)	0.37 (2)
C14	0.8690 (16)	-0.0335 (10)	0.1371 (7)	0.031 (4)	0.37 (2)
C15	0.8758 (16)	-0.0570 (9)	0.2024 (8)	0.046 (5)	0.37 (2)
C16	0.948 (3)	-0.0002 (16)	0.3133 (12)	0.092 (6)	0.37 (2)
H16A	0.8683	-0.0022	0.3331	0.137*	0.37 (2)
H16B	0.9980	0.0470	0.3312	0.137*	0.37 (2)
H16C	0.9951	-0.0517	0.3232	0.137*	0.37 (2)
C17	1.018 (3)	0.1530 (17)	0.2253 (13)	0.099 (6)	0.37 (2)
H17A	1.1080	0.1419	0.2322	0.148*	0.37 (2)
H17B	0.9861	0.1687	0.2670	0.148*	0.37 (2)
H17C	1.0025	0.1984	0.1937	0.148*	0.37 (2)
C18	0.942 (3)	0.1058 (16)	0.0776 (13)	0.094 (6)	0.37 (2)
H18A	0.9114	0.1619	0.0852	0.140*	0.37 (2)
H18B	0.8997	0.0836	0.0369	0.140*	0.37 (2)
H18C	1.0332	0.1079	0.0737	0.140*	0.37 (2)

C19	0.832 (3)	-0.0773 (16)	0.0722 (10)	0.079 (5)	0.37 (2)
H19A	0.8991	-0.0706	0.0430	0.118*	0.37 (2)
H19B	0.7540	-0.0531	0.0516	0.118*	0.37 (2)
H19C	0.8191	-0.1364	0.0804	0.118*	0.37 (2)
C20	0.862 (2)	-0.1476 (14)	0.2203 (12)	0.090 (6)	0.37 (2)
H20A	0.8207	-0.1776	0.1826	0.135*	0.37 (2)
H20B	0.8104	-0.1521	0.2575	0.135*	0.37 (2)
H20C	0.9449	-0.1716	0.2324	0.135*	0.37 (2)
C11A	0.9111 (11)	-0.0157 (7)	0.2374 (5)	0.052 (3)	0.63 (2)
C12A	0.9533 (13)	0.0596 (7)	0.2144 (6)	0.049 (3)	0.63 (2)
C13A	0.9306 (12)	0.0633 (6)	0.1460 (5)	0.055 (4)	0.63 (2)
C14A	0.8713 (10)	-0.0107 (6)	0.1254 (4)	0.043 (3)	0.63 (2)
C15A	0.8627 (9)	-0.0608 (6)	0.1818 (5)	0.046 (3)	0.63 (2)
C16A	0.9288 (17)	-0.0403 (12)	0.3108 (7)	0.094 (5)	0.63 (2)
H16D	1.0122	-0.0227	0.3296	0.141*	0.63 (2)
H16E	0.9212	-0.1006	0.3148	0.141*	0.63 (2)
H16F	0.8641	-0.0132	0.3343	0.141*	0.63 (2)
C17A	1.0277 (19)	0.1322 (11)	0.2488 (9)	0.102 (5)	0.63 (2)
H17D	1.0168	0.1313	0.2958	0.153*	0.63 (2)
H17E	0.9963	0.1848	0.2298	0.153*	0.63 (2)
H17F	1.1171	0.1263	0.2424	0.153*	0.63 (2)
C18A	0.9689 (18)	0.1260 (10)	0.0970 (8)	0.092 (5)	0.63 (2)
H18D	1.0527	0.1121	0.0843	0.137*	0.63 (2)
H18E	0.9707	0.1813	0.1167	0.137*	0.63 (2)
H18F	0.9084	0.1252	0.0580	0.137*	0.63 (2)
C19A	0.8400 (16)	-0.0462 (10)	0.0567 (6)	0.075 (4)	0.63 (2)
H19D	0.8337	-0.0010	0.0246	0.112*	0.63 (2)
H19E	0.7598	-0.0759	0.0551	0.112*	0.63 (2)
H19F	0.9066	-0.0846	0.0464	0.112*	0.63 (2)
C20A	0.8393 (13)	-0.1535 (8)	0.1877 (8)	0.081 (4)	0.63 (2)
H20D	0.9145	-0.1840	0.1776	0.122*	0.63 (2)
H20E	0.7681	-0.1696	0.1568	0.122*	0.63 (2)
H20F	0.8203	-0.1664	0.2326	0.122*	0.63 (2)
C21	0.7686 (4)	0.1852 (3)	0.31927 (18)	0.0525 (10)	
H21	0.7709	0.1347	0.3432	0.063*	
C22	0.7949 (4)	0.2592 (3)	0.3534 (2)	0.0564 (12)	
H22	0.8151	0.2575	0.3995	0.068*	

C23	0.7923 (3)	0.3332 (3)	0.3219 (2)	0.0524 (11)	
C24	0.7619 (3)	0.3334 (3)	0.2525 (2)	0.0491 (10)	
C25	0.7557 (4)	0.4062 (3)	0.2142 (3)	0.0616 (12)	
H25	0.7712	0.4585	0.2347	0.074*	
C26	0.7277 (4)	0.4018 (3)	0.1480 (2)	0.0619 (12)	
H26	0.7249	0.4516	0.1233	0.074*	
C27	0.7028 (4)	0.3265 (3)	0.1149 (2)	0.0514 (10)	
C29	0.6499 (4)	0.2407 (3)	0.0189 (2)	0.0675 (13)	
H29	0.6299	0.2334	-0.0269	0.081*	
C30	0.6579 (4)	0.1741 (3)	0.0570 (2)	0.0594 (12)	
H30	0.6432	0.1217	0.0366	0.071*	
C31	0.7075 (3)	0.2530 (2)	0.15098 (18)	0.0417 (9)	
C32	0.7375 (3)	0.2566 (3)	0.22134 (18)	0.0424 (9)	
C33	0.8193 (4)	0.4125 (3)	0.3586 (3)	0.0718 (15)	
H33A	0.8199	0.4586	0.3274	0.108*	0.5
H33B	0.9014	0.4087	0.3839	0.108*	0.5
H33C	0.7540	0.4222	0.3885	0.108*	0.5
H33D	0.8303	0.4010	0.4058	0.108*	0.5
H33E	0.7489	0.4509	0.3493	0.108*	0.5
H33F	0.8962	0.4374	0.3447	0.108*	0.5
C28	0.6699 (18)	0.3227 (6)	0.0435 (4)	0.0643 (16)	0.721 (13)
C34	0.6653 (12)	0.3883 (6)	0.0036 (4)	0.098 (4)	0.721 (13)
H34A	0.6483	0.3810	-0.0424	0.117*	0.721 (13)
H34B	0.6790	0.4424	0.0212	0.117*	0.721 (13)
C28A	0.678 (6)	0.3286 (14)	0.0412 (11)	0.0643 (16)	0.160 (11)
H28A	0.7546	0.3489	0.0215	0.077*	0.160 (11)
C34A	0.569 (5)	0.390 (3)	0.0247 (19)	0.098 (4)	0.160 (11)
H34C	0.5440	0.3883	-0.0226	0.146*	0.160 (11)
H34D	0.5957	0.4457	0.0377	0.146*	0.160 (11)
H34E	0.4970	0.3735	0.0486	0.146*	0.160 (11)
C28B	0.661 (7)	0.3294 (14)	0.0425 (12)	0.0643 (16)	0.119 (11)
H28B	0.5794	0.3594	0.0340	0.077*	0.119 (11)
C34B	0.769 (7)	0.377 (4)	0.013 (2)	0.098 (4)	0.119 (11)
H34F	0.8489	0.3500	0.0269	0.146*	0.119 (11)
H34G	0.7705	0.4343	0.0297	0.146*	0.119 (11)
H34H	0.7544	0.3772	-0.0345	0.146*	0.119 (11)

**Table S13:** Atomic displacement parameters ( $\text{\AA}^2$ ) for 7.

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Yb1	0.03632 (9)	0.04938 (11)	0.04415 (10)	-0.00376 (8)	0.00787 (7)	-0.01107 (8)
N1	0.0420 (17)	0.054 (2)	0.0392 (17)	-0.0038 (15)	0.0057 (14)	-0.0105 (16)
N2	0.0432 (18)	0.058 (2)	0.0364 (17)	-0.0033 (15)	0.0059 (14)	-0.0100 (15)
C1	0.025 (4)	0.054 (7)	0.024 (5)	0.000 (4)	-0.008 (4)	0.004 (4)
C2	0.033 (4)	0.047 (6)	0.041 (6)	-0.005 (4)	0.005 (4)	-0.015 (5)
C3	0.043 (7)	0.087 (10)	0.042 (6)	-0.028 (7)	0.018 (5)	-0.030 (7)
C4	0.055 (9)	0.069 (11)	0.142 (19)	-0.016 (8)	0.045 (11)	-0.061 (13)
C5	0.028 (5)	0.043 (9)	0.130 (15)	0.010 (5)	0.009 (8)	0.012 (8)
C6	0.047 (6)	0.091 (8)	0.087 (8)	-0.027 (5)	0.019 (5)	-0.047 (7)
C7	0.050 (5)	0.163 (14)	0.136 (12)	-0.008 (7)	0.011 (7)	0.095 (11)
C8	0.092 (10)	0.243 (18)	0.086 (9)	-0.092 (10)	0.051 (7)	-0.094 (11)
C9	0.058 (6)	0.082 (7)	0.186 (11)	-0.003 (5)	0.035 (7)	-0.021 (7)
C10	0.056 (5)	0.112 (8)	0.115 (7)	-0.015 (5)	-0.018 (5)	0.037 (6)
C1A	0.022 (5)	0.070 (11)	0.032 (5)	-0.003 (6)	-0.006 (4)	0.010 (6)
C2A	0.027 (5)	0.030 (5)	0.034 (6)	-0.002 (4)	-0.001 (4)	-0.004 (5)
C3A	0.033 (5)	0.027 (6)	0.035 (5)	-0.001 (4)	0.012 (4)	-0.014 (5)
C4A	0.033 (6)	0.059 (9)	0.043 (7)	0.004 (5)	0.011 (5)	0.011 (6)
C5A	0.041 (6)	0.036 (10)	0.077 (11)	0.010 (6)	0.013 (6)	0.012 (8)
C6A	0.074 (7)	0.157 (11)	0.085 (7)	-0.049 (7)	-0.014 (6)	0.005 (8)
C7A	0.070 (8)	0.105 (9)	0.143 (11)	-0.030 (7)	0.022 (8)	-0.053 (9)
C8A	0.043 (5)	0.162 (15)	0.152 (13)	0.008 (8)	0.013 (8)	0.102 (12)
C9A	0.070 (9)	0.211 (18)	0.086 (10)	-0.067 (10)	0.043 (7)	-0.095 (11)
C10A	0.057 (5)	0.099 (7)	0.147 (9)	0.000 (5)	0.011 (6)	0.031 (7)
C11	0.039 (10)	0.046 (10)	0.048 (11)	0.004 (7)	0.001 (7)	-0.008 (7)
C12	0.025 (7)	0.047 (9)	0.051 (10)	-0.003 (6)	0.008 (7)	-0.007 (8)
C13	0.031 (7)	0.043 (10)	0.033 (6)	-0.005 (6)	0.014 (6)	-0.005 (7)
C14	0.034 (7)	0.027 (8)	0.033 (9)	0.001 (5)	0.005 (6)	0.002 (6)
C15	0.033 (8)	0.063 (11)	0.042 (10)	0.001 (8)	0.003 (7)	0.004 (7)
C16	0.052 (9)	0.165 (19)	0.058 (7)	0.031 (12)	0.013 (6)	0.027 (11)
C17	0.039 (7)	0.113 (12)	0.146 (15)	-0.019 (9)	0.018 (10)	-0.063 (11)
C18	0.059 (11)	0.110 (11)	0.119 (12)	0.007 (9)	0.050 (10)	0.032 (10)
C19	0.065 (7)	0.104 (14)	0.067 (10)	0.012 (10)	0.013 (8)	-0.039 (8)
C20	0.058 (9)	0.071 (7)	0.144 (15)	0.005 (7)	0.020 (10)	0.009 (11)
C11A	0.031 (5)	0.083 (9)	0.042 (7)	-0.005 (6)	0.006 (4)	0.008 (5)

C12A	0.039 (5)	0.056 (8)	0.055 (6)	-0.009 (6)	0.009 (5)	-0.016 (6)
C13A	0.040 (6)	0.056 (6)	0.073 (9)	-0.004 (5)	0.019 (6)	-0.011 (6)
C14A	0.043 (5)	0.051 (8)	0.035 (4)	0.011 (5)	0.011 (4)	0.005 (5)
C15A	0.031 (4)	0.057 (6)	0.049 (7)	0.003 (4)	-0.002 (4)	-0.004 (5)
C16A	0.052 (6)	0.171 (17)	0.058 (5)	0.014 (9)	0.003 (4)	0.015 (8)
C17A	0.042 (5)	0.119 (11)	0.145 (12)	-0.022 (7)	0.009 (8)	-0.060 (9)
C18A	0.058 (8)	0.103 (9)	0.119 (11)	0.001 (6)	0.040 (8)	0.032 (8)
C19A	0.069 (5)	0.103 (11)	0.053 (6)	0.010 (7)	0.012 (5)	-0.023 (6)
C20A	0.053 (6)	0.063 (5)	0.128 (12)	0.009 (4)	0.014 (7)	0.009 (7)
C21	0.050 (2)	0.073 (3)	0.035 (2)	0.000 (2)	0.0036 (17)	-0.011 (2)
C22	0.038 (2)	0.088 (4)	0.044 (2)	-0.002 (2)	0.0067 (18)	-0.021 (2)
C23	0.032 (2)	0.066 (3)	0.061 (3)	-0.0063 (19)	0.0121 (19)	-0.031 (2)
C24	0.0291 (19)	0.058 (3)	0.061 (3)	-0.0043 (18)	0.0091 (17)	-0.017 (2)
C25	0.049 (3)	0.048 (3)	0.088 (4)	-0.006 (2)	0.010 (2)	-0.016 (2)
C26	0.054 (3)	0.055 (3)	0.077 (3)	-0.004 (2)	0.010 (2)	0.006 (2)
C27	0.041 (2)	0.056 (3)	0.058 (3)	-0.0055 (19)	0.0079 (19)	-0.001 (2)
C29	0.064 (3)	0.096 (4)	0.042 (2)	-0.012 (3)	0.002 (2)	0.003 (3)
C30	0.064 (3)	0.073 (3)	0.042 (2)	-0.009 (2)	0.006 (2)	-0.011 (2)
C31	0.0303 (19)	0.051 (2)	0.044 (2)	-0.0038 (17)	0.0075 (16)	-0.0098 (18)
C32	0.0285 (18)	0.056 (3)	0.044 (2)	-0.0035 (17)	0.0070 (15)	-0.0131 (19)
C33	0.048 (3)	0.082 (4)	0.086 (3)	-0.014 (2)	0.015 (2)	-0.048 (3)
C28	0.056 (4)	0.084 (4)	0.053 (3)	-0.006 (3)	0.004 (2)	0.012 (3)
C34	0.118 (10)	0.100 (6)	0.072 (5)	-0.011 (7)	-0.007 (6)	0.023 (5)
C28A	0.056 (4)	0.084 (4)	0.053 (3)	-0.006 (3)	0.004 (2)	0.012 (3)
C34A	0.118 (10)	0.100 (6)	0.072 (5)	-0.011 (7)	-0.007 (6)	0.023 (5)
C28B	0.056 (4)	0.084 (4)	0.053 (3)	-0.006 (3)	0.004 (2)	0.012 (3)
C34B	0.118 (10)	0.100 (6)	0.072 (5)	-0.011 (7)	-0.007 (6)	0.023 (5)