

Supporting Information for:

**Synthesis and Reactivity of a tris(carbene) Zinc Chloride Complex**

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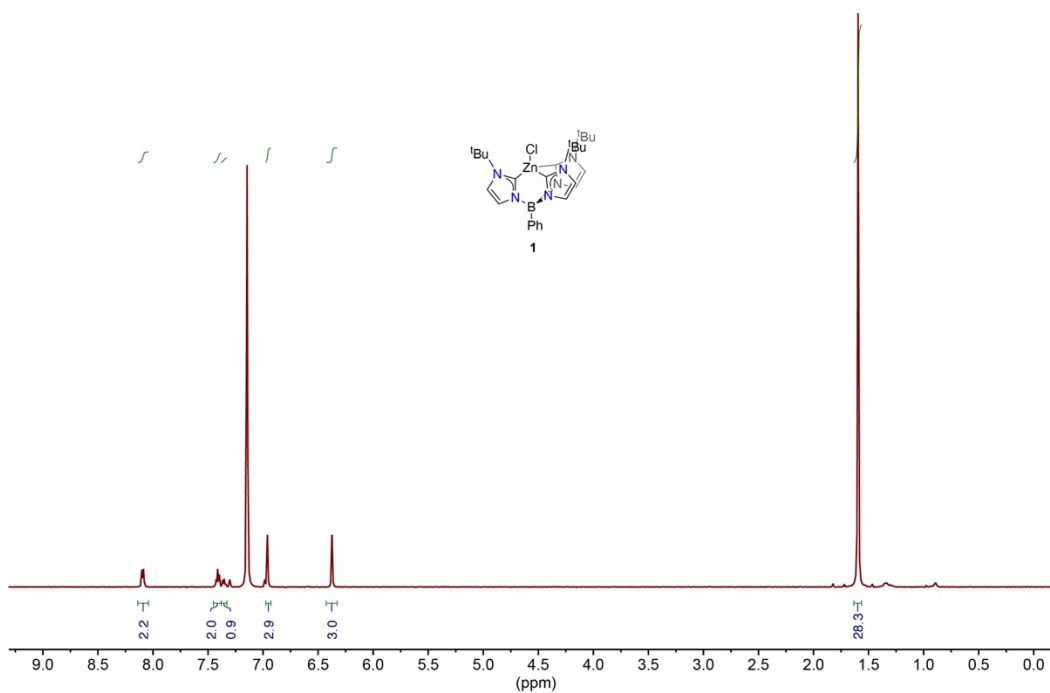
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# 1. X-Ray Crystallographic Data Tables

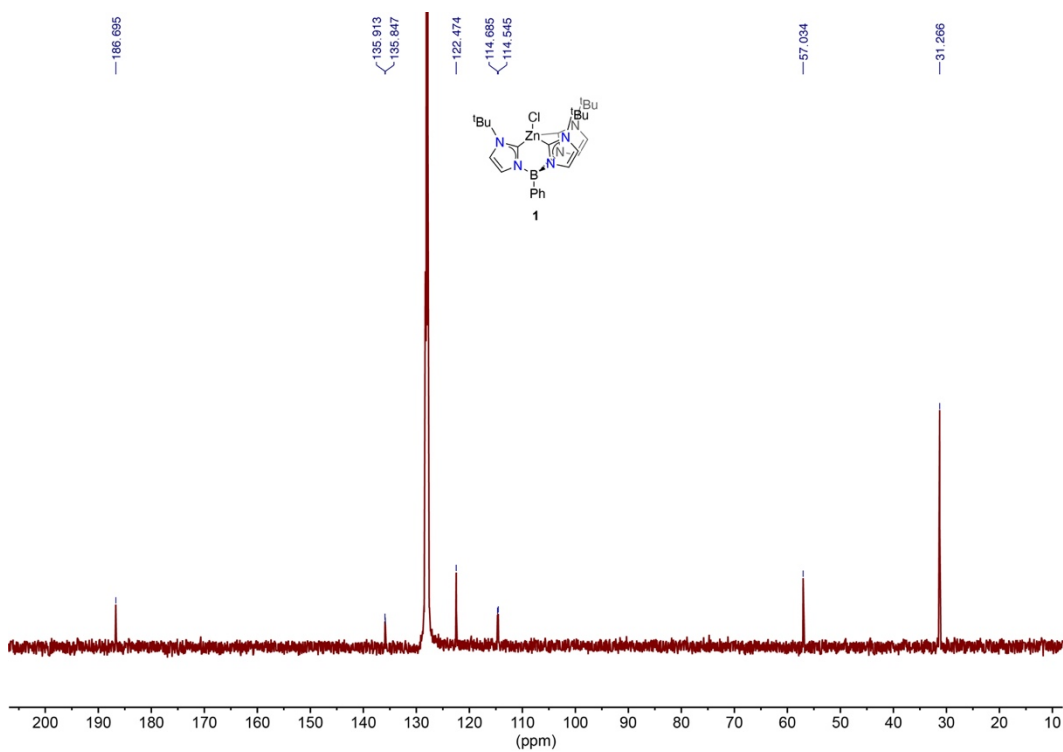
**Table S1.**

	<b>PhB(<sup>t</sup>Bulm)<sub>3</sub>ZnCl</b>	<b>PhB(<sup>t</sup>Bulm)<sub>3</sub>ZnBu</b>	<b>PhB(<sup>t</sup>BulmH)(<sup>t</sup>Bulm)<sub>2</sub>ZnS<sub>4</sub></b>
formula	C <sub>27</sub> H <sub>38</sub> BCIN <sub>6</sub> Zn	C <sub>31</sub> H <sub>47</sub> BN <sub>6</sub> Zn	C <sub>32</sub> H <sub>49</sub> BN <sub>6</sub> O <sub>1.25</sub> S <sub>4</sub> Zn
fw	558.26	579.92	742.19
temperature (K)	173 (2)	213 (2)	173 (2)
crystal syst	Monoclinic	Monoclinic	Orthorhombic
space group	<i>P</i> 21/ <i>n</i>	<i>P</i> 21/ <i>c</i>	<i>P</i> <i>bca</i>
<i>a</i> (Å)	9.6756(3)	10.6870(9)	18.5324(14)
<i>b</i> (Å)	17.8862(5)	16.4527(14)	19.6563(15)
<i>c</i> (Å)	16.4972(5)	18.4919(15)	41.276(3)
$\alpha$ (deg)	90	90	90
$\beta$ (deg)	92.369(2)	105.538(4)	90
$\gamma$ (deg)	90	90	90
<i>V</i> (Å <sup>3</sup> )	2852.56(15)	3132.6(5)	15035.8(19)
<i>Z</i>	4	4	16
$\rho$ (mm <sup>-1</sup> )	1.300	1.230	1.311
F(000)	1176	1240	6272
cryst size (mm <sup>3</sup> )	0.22 × 0.16 × 0.12	0.15 × 0.14 × 0.07	0.02 × 0.01 × 0.01
$\theta$ range (deg)	3.646 – 66.504	3.66– 66.67	2.141 – 49.811
completeness to $\theta$ (%)	96.1	99.2	99.8
total reflns	12099	21092	42179
indep reflns	4843	5512	7645
restraints / param	0 / 325	9 / 365	0 / 740
max, min transmn	0.774, 0.637	0.683, 0.753	0.648, 0.750
R1 (wR2) [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]	0.0362 (0.1006)	0.0363 (0.0980)	0.0759 (0.1827)
R1 (wR2)	0.0429 (0.1059)	0.0404 (0.1014)	0.1304 (0.2145)
GOF ( <i>F</i> <sup>2</sup> )	0.908	1.048	1.023
max, min peaks (e Å <sup>-3</sup> )	0.335, -0.285	1.204, -0.437	0.560, -0.469

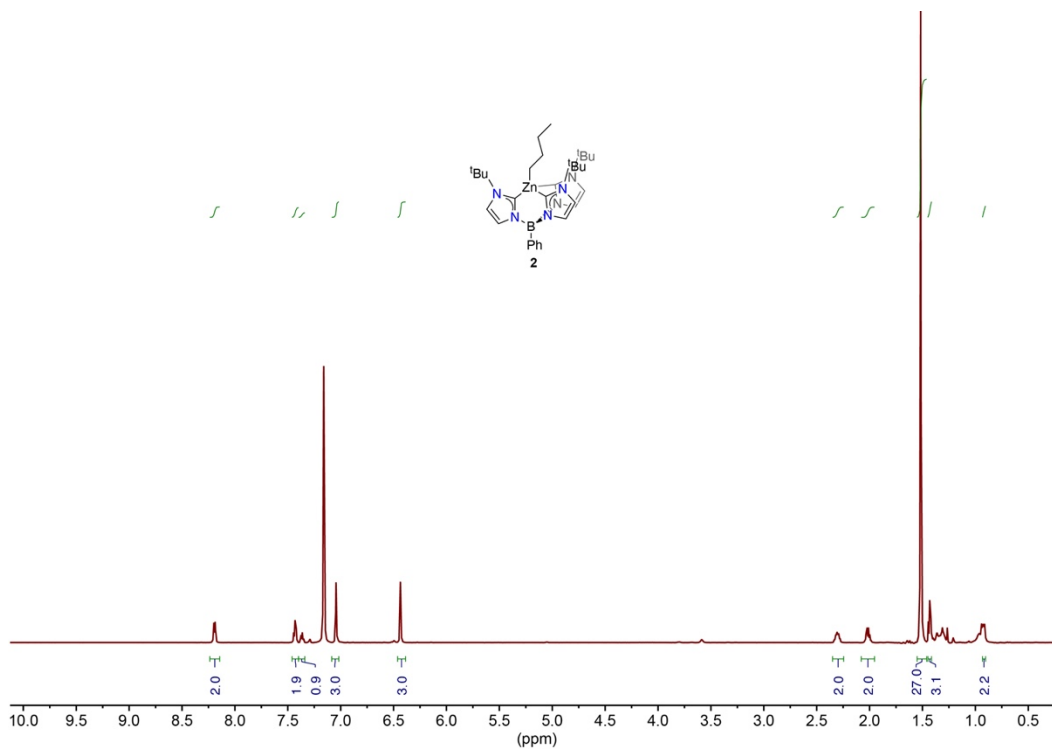
## 2. NMR Spectroscopic Data



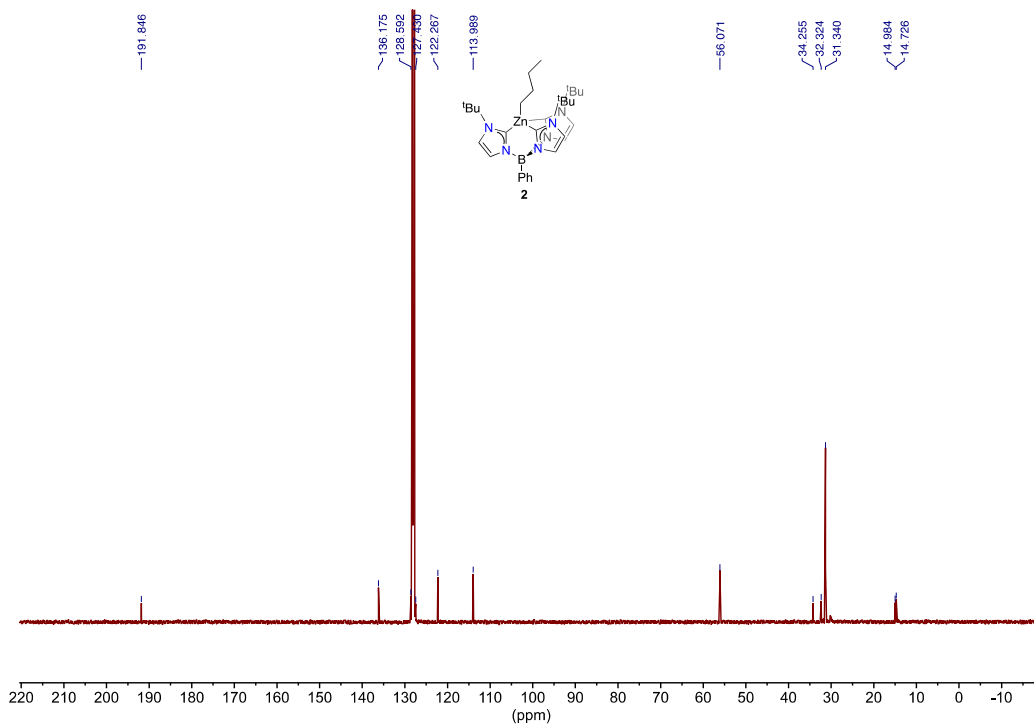
**Figure S1.**  $^1\text{H}$  NMR spectrum of  $\text{PhB}(\text{tBuIm})_3\text{ZnCl}$  (**1**) in  $\text{C}_6\text{D}_6$ .



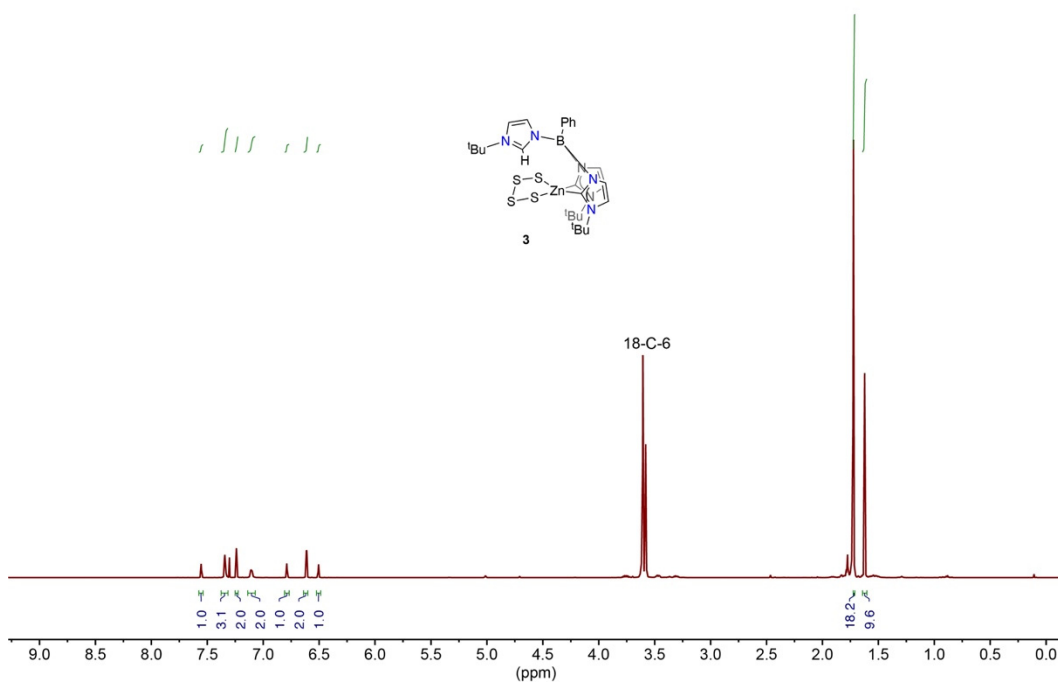
**Figure S2.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of  $\text{PhB}(\text{tBuIm})_3\text{ZnCl}$  (**1**) in  $\text{C}_6\text{D}_6$ .



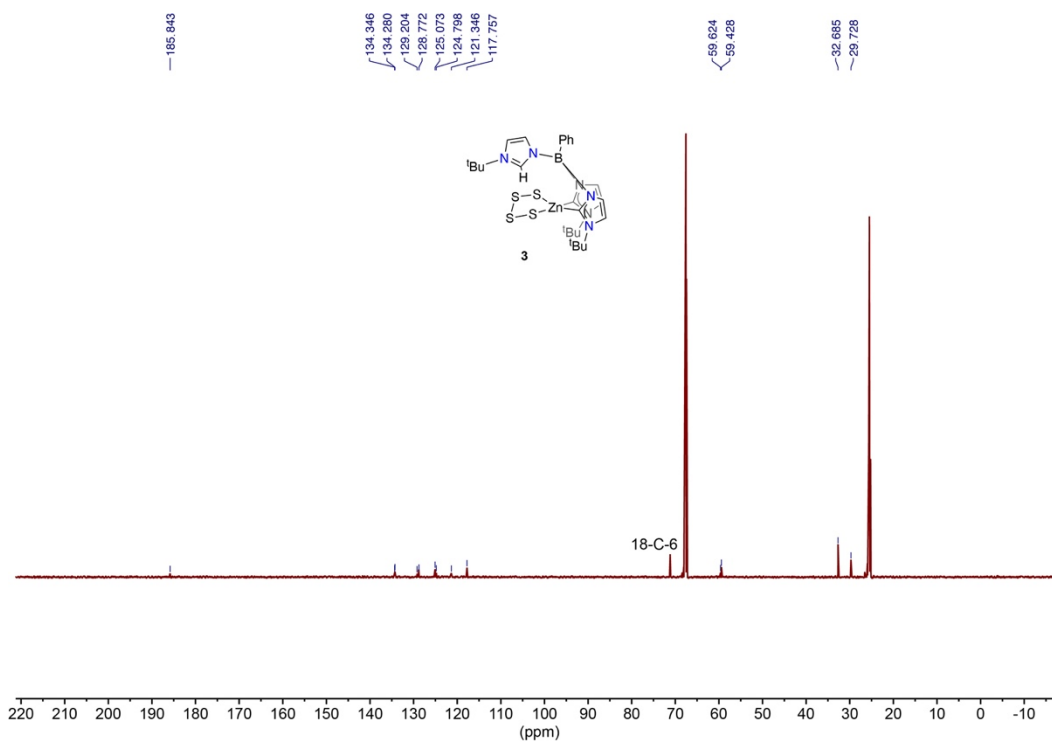
**Figure S3.** <sup>1</sup>H NMR spectrum of PhB(<sup>t</sup>BuIm)<sub>3</sub>ZnBu (**2**) in C<sub>6</sub>D<sub>6</sub>.



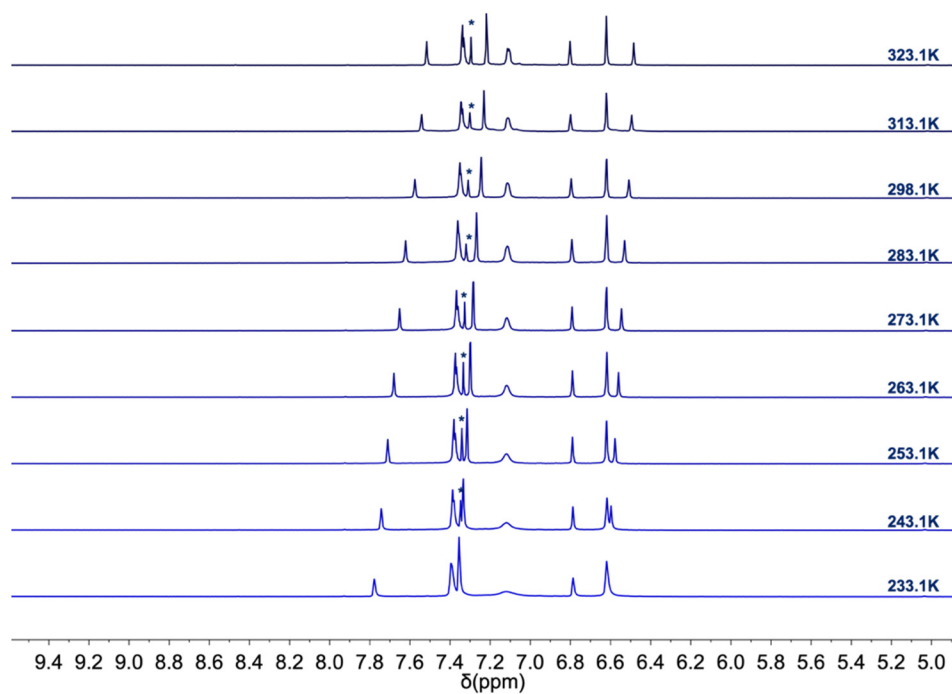
**Figure S4.** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of PhB(<sup>t</sup>BuIm)<sub>3</sub>ZnBu (**2**) in C<sub>6</sub>D<sub>6</sub>.



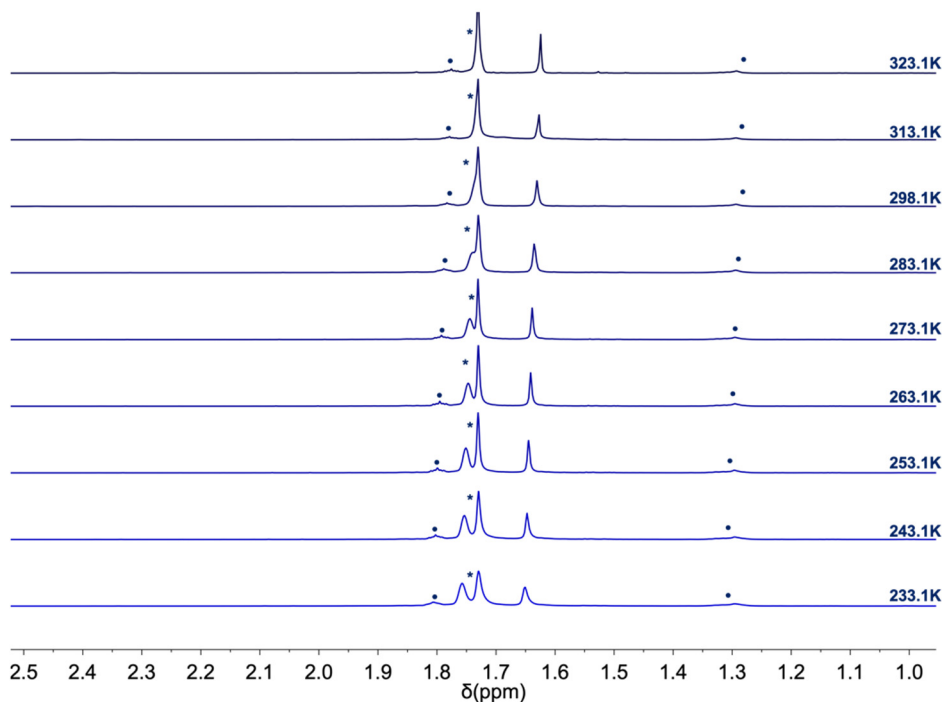
**Figure S5.**  $^1\text{H}$  NMR spectrum of  $\text{PhB}(\text{tBuImH})(\text{tBuIm})_2\text{ZnS}_4$  (**3**) in  $d_8$ -THF.



**Figure S6.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of  $\text{PhB}(\text{tBuImH})(\text{tBuIm})_2\text{ZnS}_4$  (**3**) in  $d_8$ -THF.

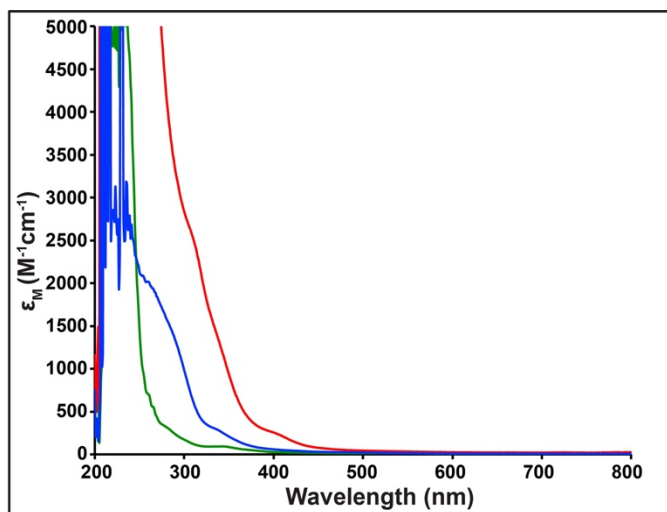


**Figure S7.** Variable temperature  $^1\text{H}$  NMR spectra of the aromatic region of  $\text{PhB}(\text{tBulmH})(\text{tBulm})_2\text{ZnS}_4$  (**3**) in  $\text{d}_8\text{-THF}$ . “\*” denotes residual  $\text{C}_6\text{H}_6$ .



**Figure S8.** Variable temperature  $^1\text{H}$  NMR spectra of the aliphatic region for (**3**) in  $\text{d}_8\text{-THF}$ . “•” denotes solvent signal of  $\text{d}_8\text{-THF}$  and “\*” denotes residual hexanes.

### 3. UV-vis Spectroscopic Data



**Figure S9.** UV-vis spectra of complexes **1** (green), **2** (blue), **3** (red), acquired in THF at 298 K.