

# Table 3S

Magnetic moment, electronic spectra and ligand field parameters of metal complexes of H<sub>2</sub>BT

Compound	M <sub>eff</sub> (BM)	Band position (cm <sup>-1</sup> )	Dq (cm <sup>-1</sup> )	B (cm <sup>-1</sup> )	β	ν <sub>2</sub> / ν <sub>1</sub>	Transition
<b>2</b>	2.03	16129	-	-	-	-	<sup>2</sup> B <sub>1g</sub> → <sup>2</sup> E <sub>g</sub>
		14388					<sup>2</sup> B <sub>1g</sub> → <sup>2</sup> A <sub>1g</sub>
<b>3</b>	5.12	14815	793.16	933.129	0.961	2.155	<sup>4</sup> T <sub>1g</sub> → <sup>4</sup> A <sub>2g</sub> (F)
		19802					<sup>4</sup> T <sub>1g</sub> → <sup>4</sup> T <sub>1g</sub> (P)
<b>4</b>	3.12	17241	1104.64	736.43	0.758	1.553	<sup>3</sup> A <sub>2g</sub> → <sup>3</sup> T <sub>1g</sub> (F)
		27027					<sup>3</sup> A <sub>2g</sub> → <sup>3</sup> T <sub>1g</sub> (P)