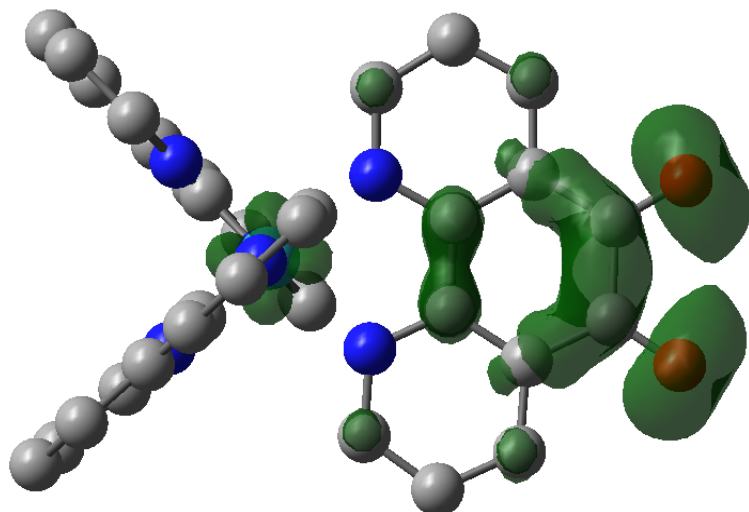


**Supporting Information for:**

**A Little Spin on the Side: Solvent and Temperature Dependent Paramagnetism in  
[Ru<sup>II</sup>(bpy)<sub>2</sub>(phendione)]<sup>2+</sup>**

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Malcolm D. E. Forbes\*

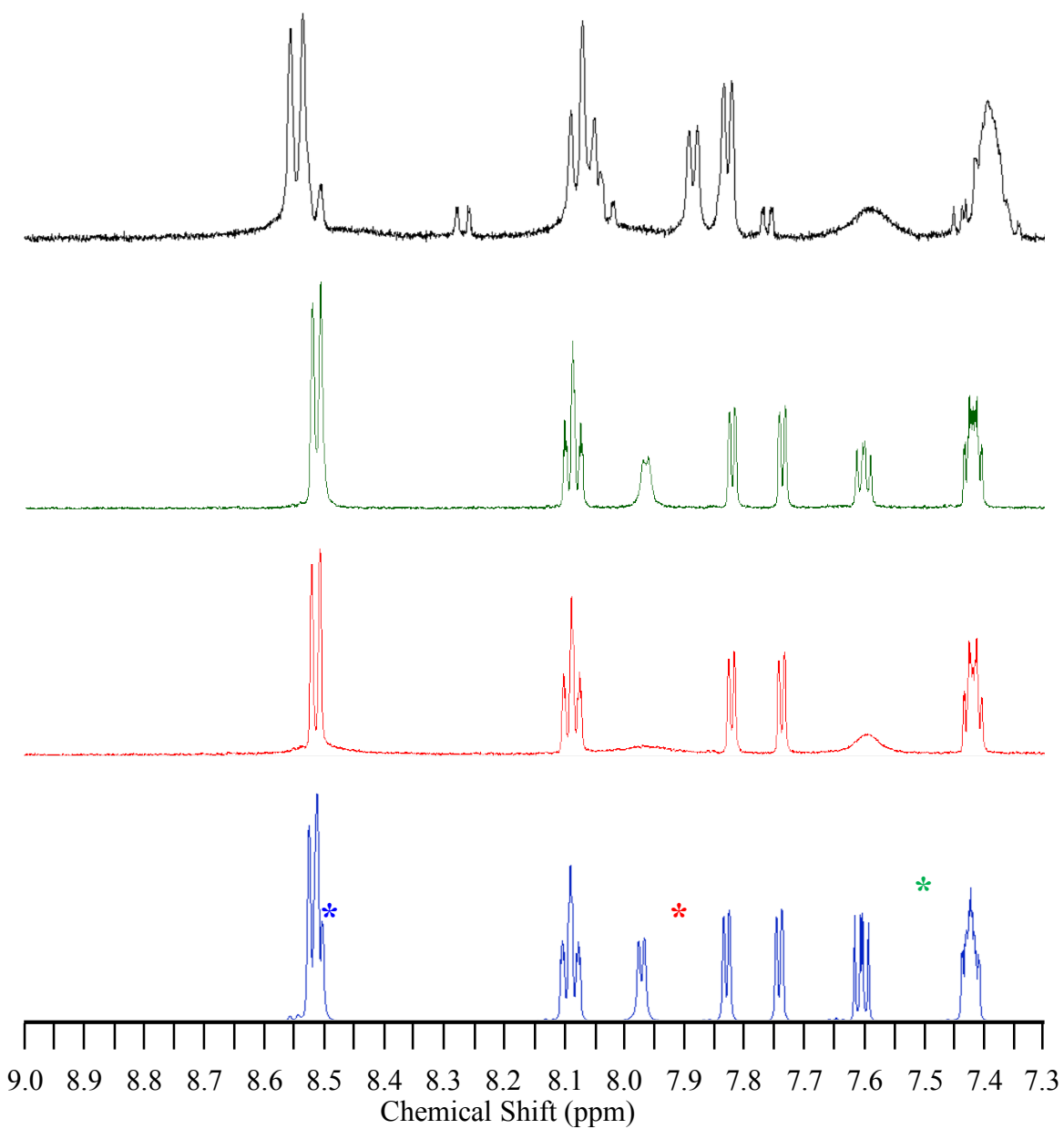
<b>Description</b>	<b>Page</b>
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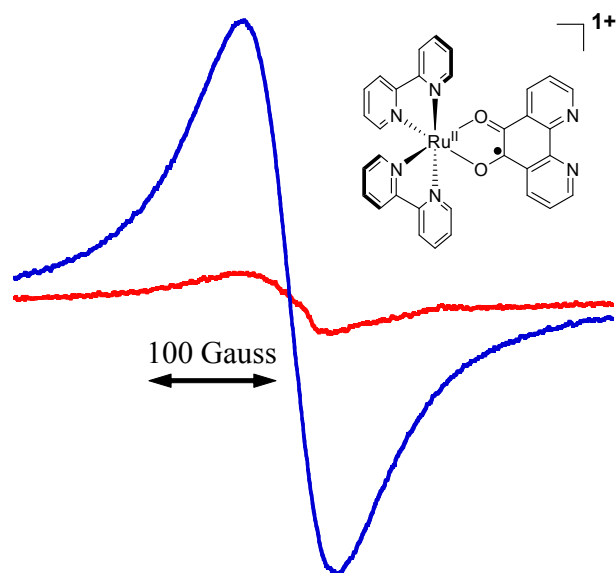
**Figure S1.** Spin density map of the ligand triplet state **3** from DFT calculations.

**Table S1.** Spin densities on dione oxygens and ruthenium highlighting shifts in electron density at the metal and its effect on dione electron density.

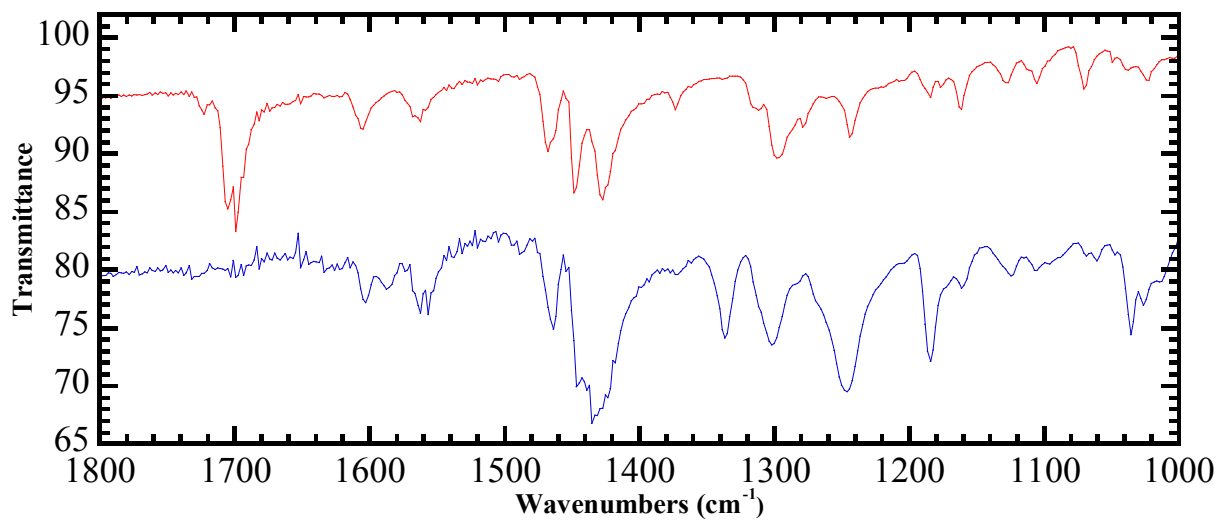
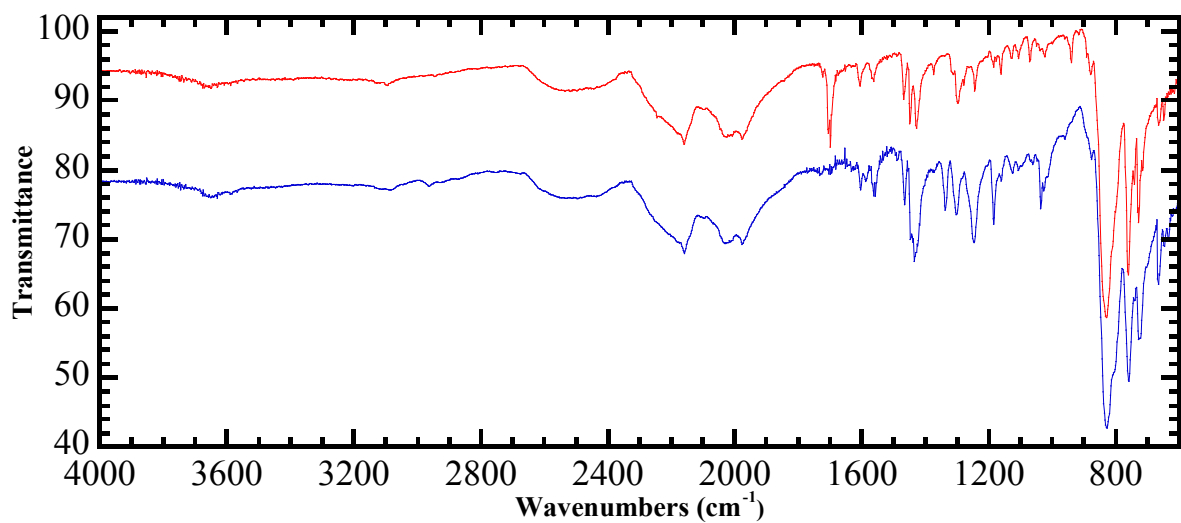
N-N	Triplet Spin Density (Oxygen)	Triplet Spin Density (Ru)
deeb	0.615	0.229
bpy	0.669	0.073
dmeb	0.675	0.054



**Supporting Figure S2.** <sup>1</sup>H-NMR spectra of **1** collected at 10 mM in CD<sub>3</sub>CN (blue), 1 mM in CD<sub>3</sub>CN (red), 1 mM in CD<sub>3</sub>CN/0.25% D<sub>2</sub>O (green), and 1 mM in D<sub>2</sub>O (black). Asterisks correspond to the phendione protons as labeled in Figure 1.



**Supporting Figure S3.** Fluid solution EPR spectra of **5** in anhydrous  $\text{CH}_3\text{CN}$  at 1 mM (red) and 10 mM (blue). Note the *increase* in EPR signal intensity with concentration, expected for a doublet, contrary to the observed *decrease* in intensity observed with **1**.



**Supporting Figure S4.** Infrared spectra for solid samples of **1** (red) and **4** (blue). (Top) Full spectral region, (B) Zoom 1800-1000 cm<sup>-1</sup> region.