

Supplementary Information

Entrapment of [Ru(bpy)₃]²⁺ in the anionic metal-organic framework: Novel photoluminescence behavior exhibiting dual emission at room temperature

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Table S1. Short contacts found in compounds **1** and **2**

Compound 1			
C·····H (Å)	C-H·····C(°)	H·····N(Å)	C-H·····N(°)
2.899	132.32	2.884	128.92
2.872	157.57	2.911	124.43
2.990	104.84		
2.939	134.24		
2.951	107.03		
Compound 2			
C·····H (Å)	C-H·····C(°)	H·····N(Å)	C-H·····N(°)
2.744	156.71	2.879	174.05
2.879	121.19	2.939	122.78
2.660	150.32	2.772	165.18
2.836	117.17	2.782	109.36

2.995	128.64	2.880	140.12
		2.896	150.51
		2.618	138.81

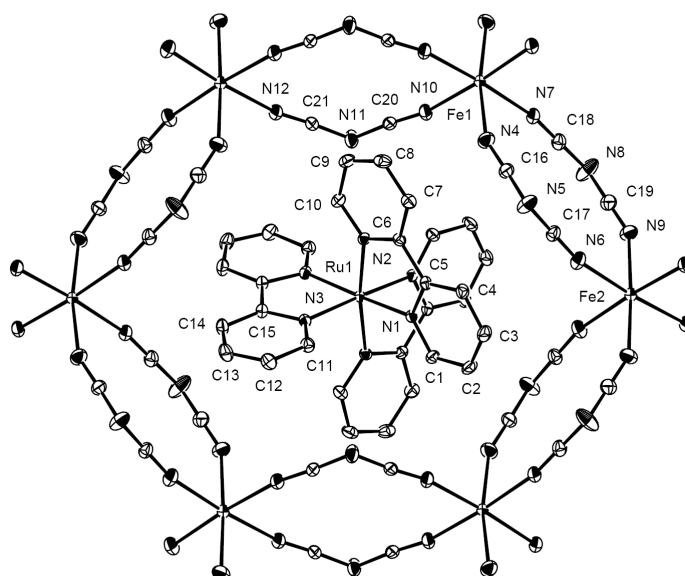


Fig. S1. ORTEP diagram of compound **2** showing atom numbering scheme

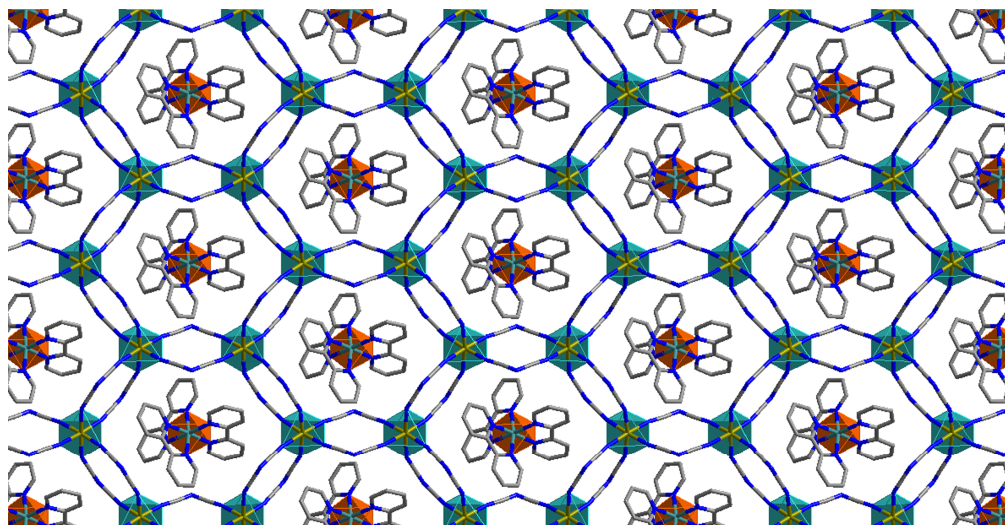


Fig. S2. Diagram showing entrapment of $[\text{Ru}(\text{bpy})_3]^{2+}$ cations in the 2D anionic $[\text{Fe}(\text{dca})_3]^-$ nano cavity in complex **2**. Red polyhedron represents the Ru^{II} sites while green polyhedron represents the Fe^{II} centers.

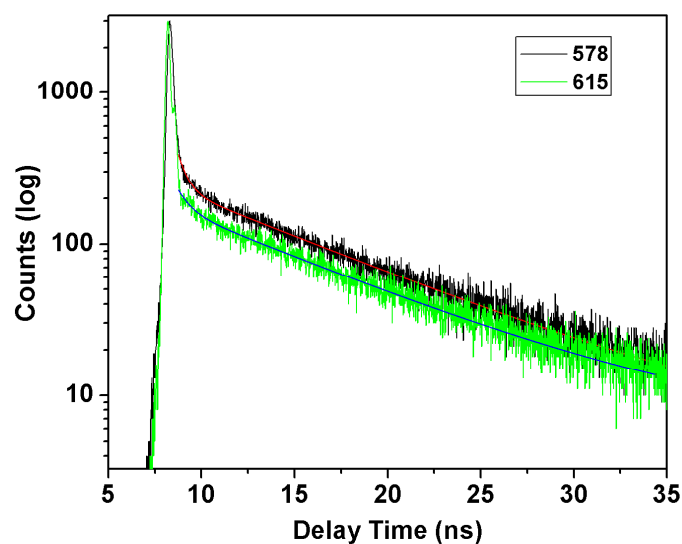


Fig. S3. Diagram showing emission decays of complex **2** monitored at different wavelengths following pulsed excitation ($\lambda_{\text{ex}} = 440 \text{ nm}$) with biexponential fit

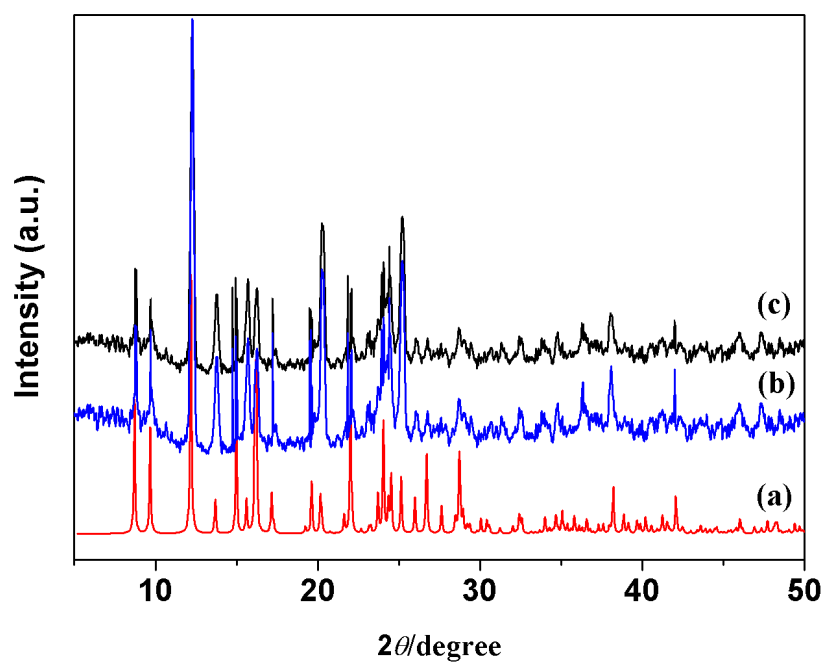


Fig. S4. Powder X-ray diffraction patterns of compound **1**; (—) simulated from single crystal data (a), (—) before irradiation (b) and (—) after irradiation (c).

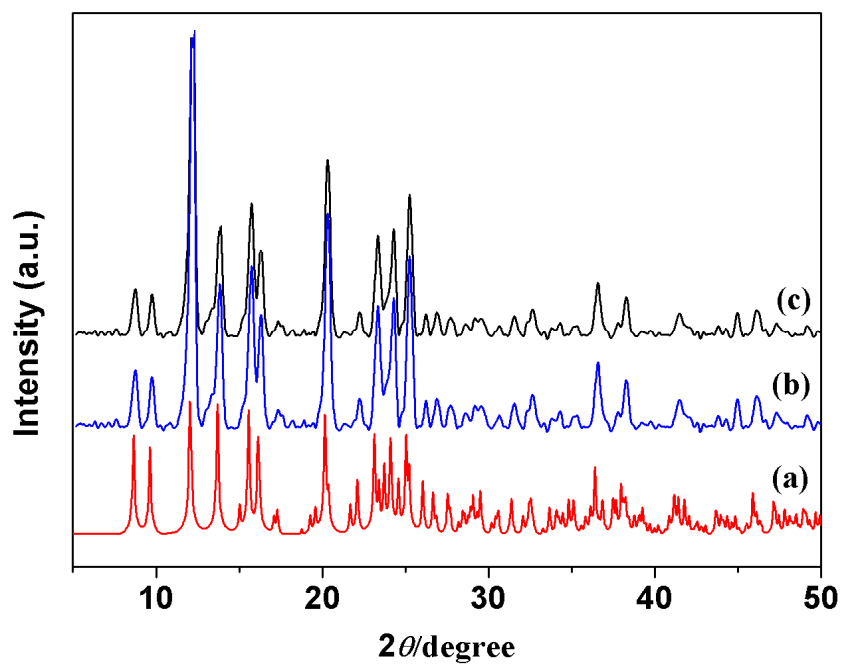


Fig. S5. Powder X-ray diffraction patterns of compound **2**; (—) simulated from single crystal data (a), (—) before irradiation (b) and (—) after irradiation (c).

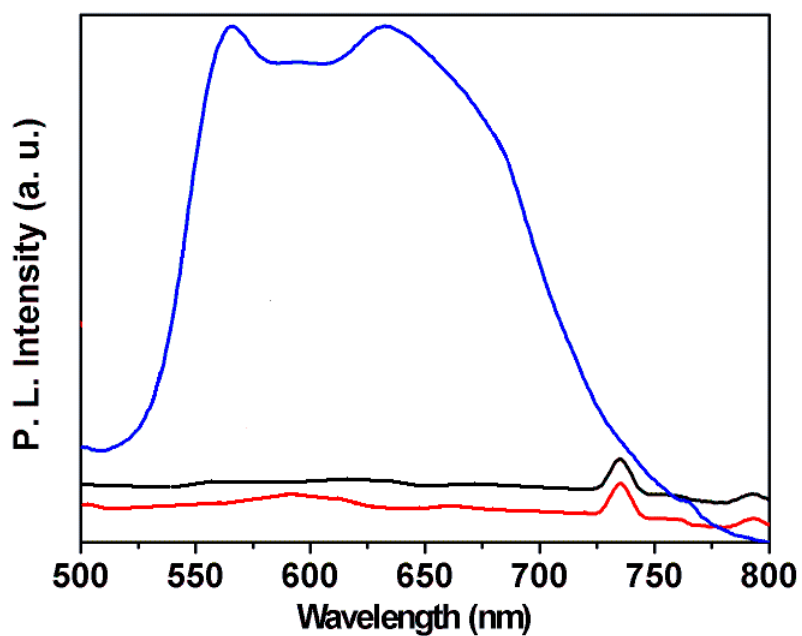


Fig. S6. Diagram showing steady-state emission profile of complex 1(—), (TPA)[Mn(dca)₃] (—) and bipyridine (—) measured at room temperature (excitation wavelength = 440 nm).