

Synthesis, Structure, and Photomagnetic Properties of a Hydrogen-Bonded Lattice of [Fe(bpp)₂]²⁺ Spin-Crossover Complexes and Nicotinate Anions

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Table S1. Enthalpy and entropy values for peaks observed in Differential scanning calorimetry (DSC) curves.

Compound	Curve	T/ K	$\Delta H/ \text{KJ}\cdot\text{mol}^{-1}$	$\Delta S/ \text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$
[Fe(bpp) ₂](nic) ₂ ·4H ₂ O	1	334	147	450
	2	218/262/282	0.54/1.53/2.2	5.50/6.30/8.33
	3	229/264/289	1.0/1.28/3.1	5.50/5.24/10.4

Table S2. Intermolecular hydrogen bonds in the crystal structure of 1·4H₂O.^a

D...A	$d_{D...A}/ \text{\AA}$
N(1)...O(3W)	2.633(3)
N(5)...O(1)#1	2.662(3)
N(6)...O(4W)#2	2.671(3)
N(10)...O(4)	2.635(3)
O(1W)...O(3)#3	2.757(3)
O(1W)...N(11)	2.987(4)
O(2W)...O(2)#4	2.745(3)
O(2W)...N(12)#5	2.900(4)
O(3W)...O(2W)	2.722(3)
O(3W)...O(1)	2.749(3)
O(4W)...O(1W)	2.778(3)
O(4W)...O(4)#6	2.764(3)

^a Symmetry transformations used to generate equivalent atoms:

#1 $x-1, y, z$	#2 $x-1, -y+1, z-1/2$
#3 $x, -y, z+1/2$	#4 $x, y+1, z$
#5 $x, -y+1, z+1/2$	#6 $x+1, -y, z+1/2$

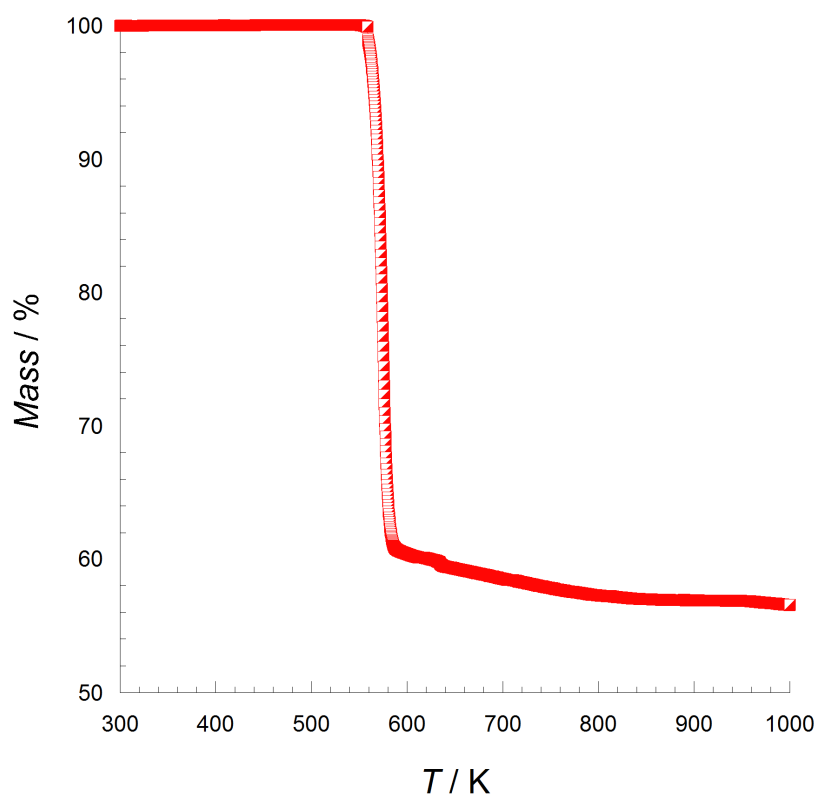


Figure S1. Thermogravimetric analysis of $\text{Ag}(\text{C}_6\text{H}_4\text{NO}_2)$. The plot confirms the anhydrous character of this salt.

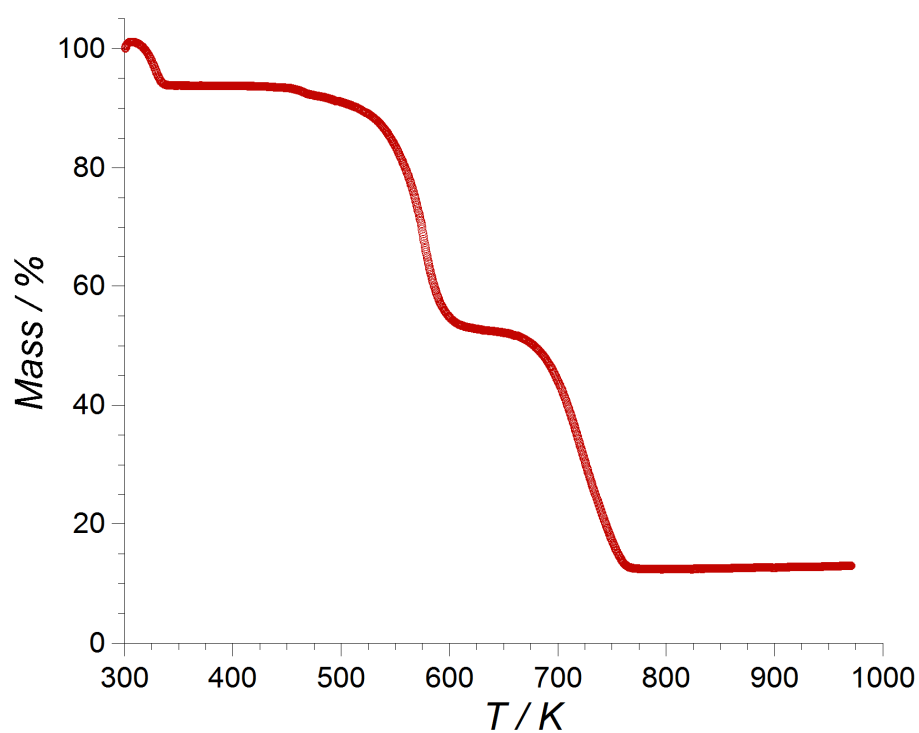


Figure S2. Thermogravimetric analysis of $1 \cdot 4\text{H}_2\text{O}$.

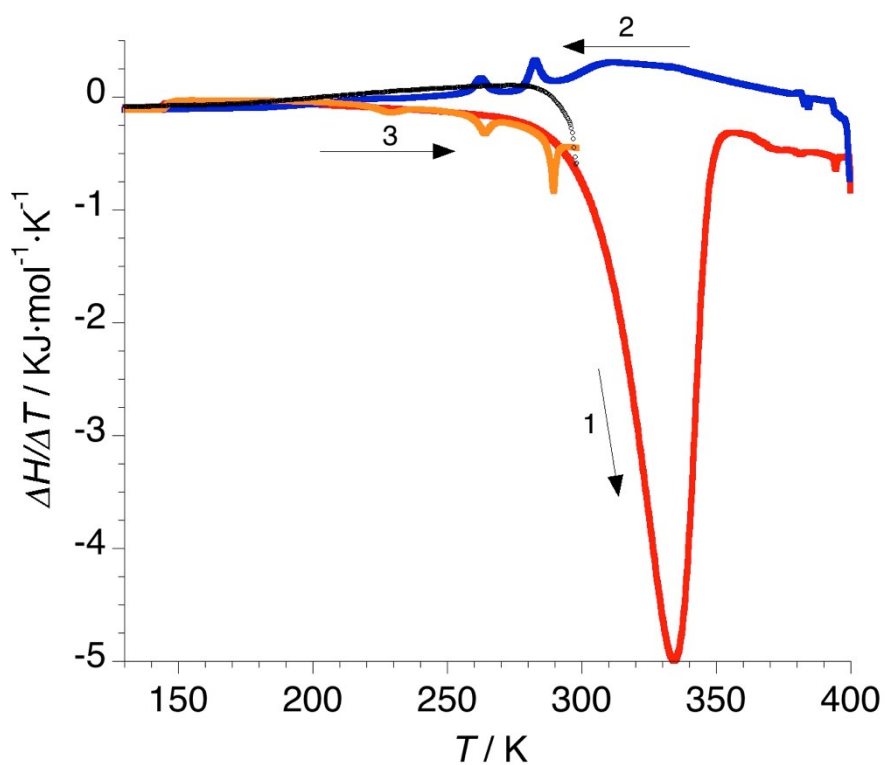


Figure S3. Differential scanning calorimetry of $1\cdot 4\text{H}_2\text{O}$. Black line: cooling down to 133 K. Curve 1: first heating (dehydration process). Curves 2 and 3: first cooling and second heating processes, respectively.

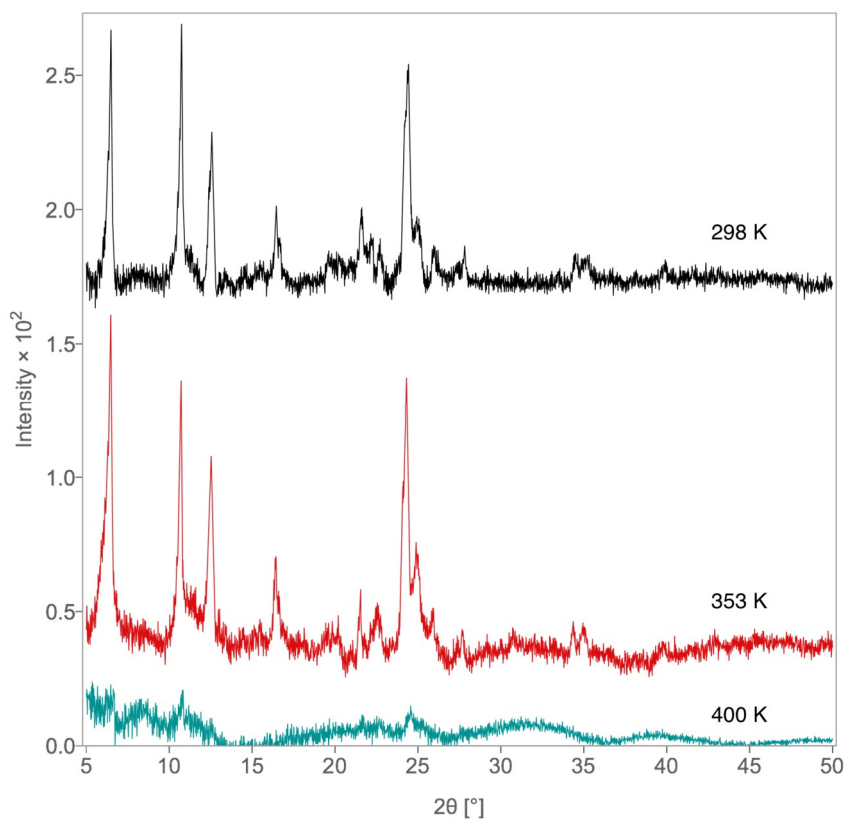


Figure S4. Powder X-ray diffractograms of **1** at different temperatures.

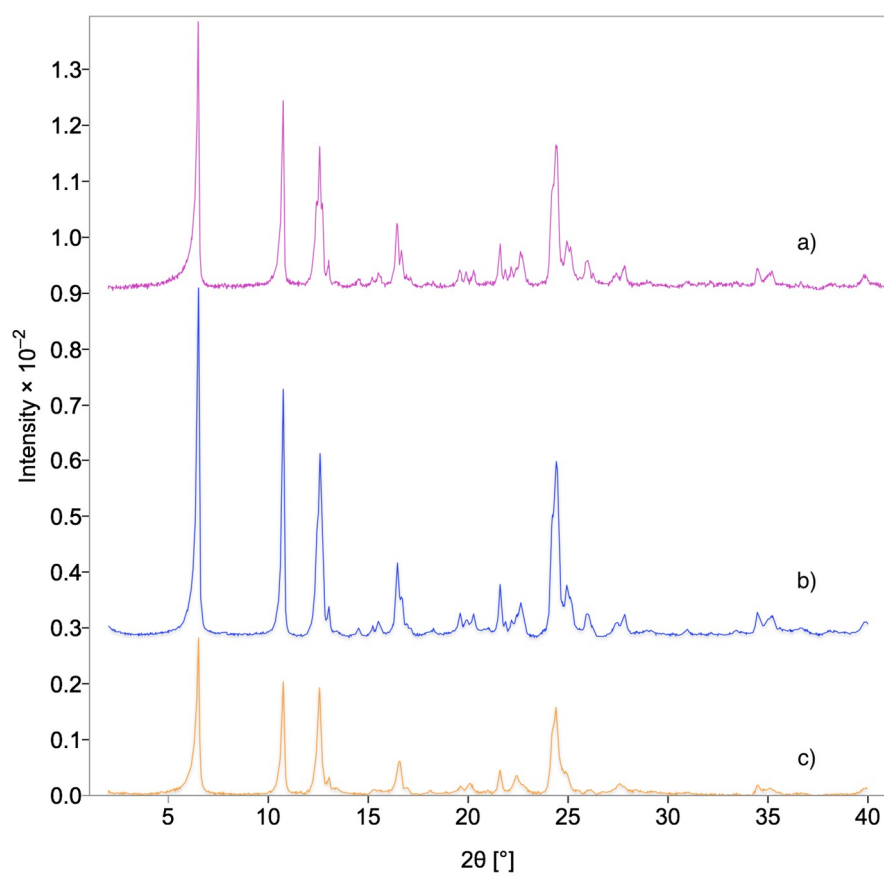


Figure S5. Powder X-ray diffractograms of 1·4H₂O. **a)** original sample; **b)** after dehydration under vacuum at 400 K for 2 h and subsequent rehydration; **c)** after a second dehydration-rehydration cycle.