

Spin Crossover Behaviour in Two New Supramolecular Isomers

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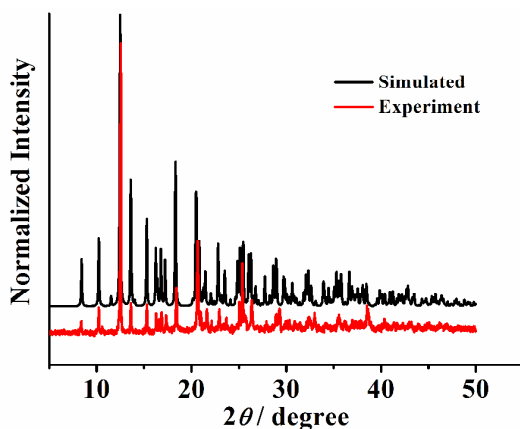


Figure S1. X-ray powder diffraction patterns for **1**. Black: calculated from X-ray single-crystal data; red: as-synthesized data.

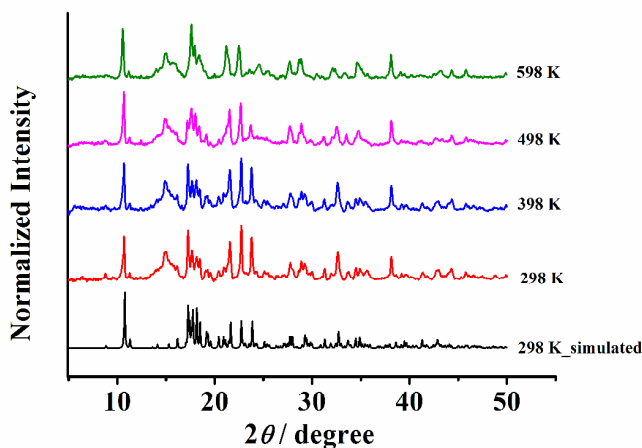


Figure S2. Variable-temperature PXRD patterns for **2**·H₂O.

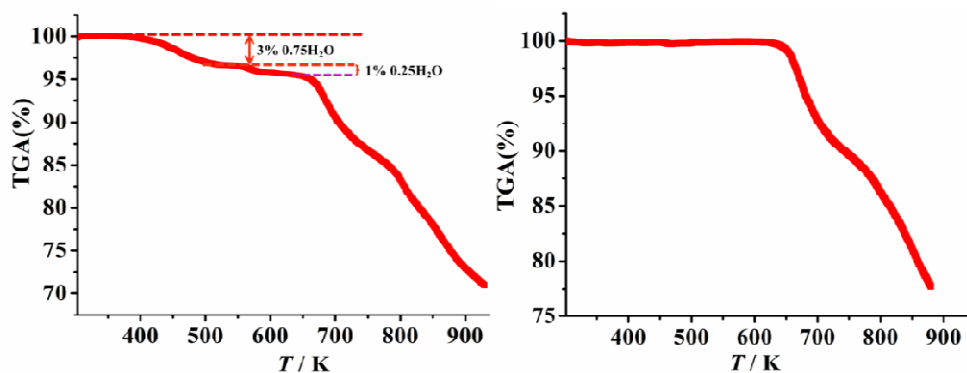


Figure S3. TG curves for $2 \cdot \text{H}_2\text{O}$ (left) and 2 (right, obtained by heating $2 \cdot \text{H}_2\text{O}$ at 593 K for 30 min) under N_2 atmosphere (10 K min^{-1}).

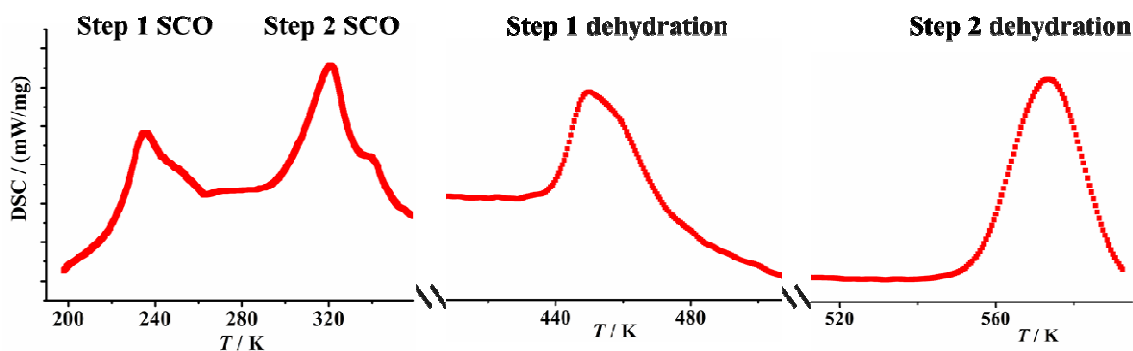


Figure S4. DSC curves for $2 \cdot \text{H}_2\text{O}$ recorded in the SCO and the structural transformation range from $2 \cdot \text{H}_2\text{O}$ to 2 . The traces are measured in heating modes with 5 K min^{-1} .

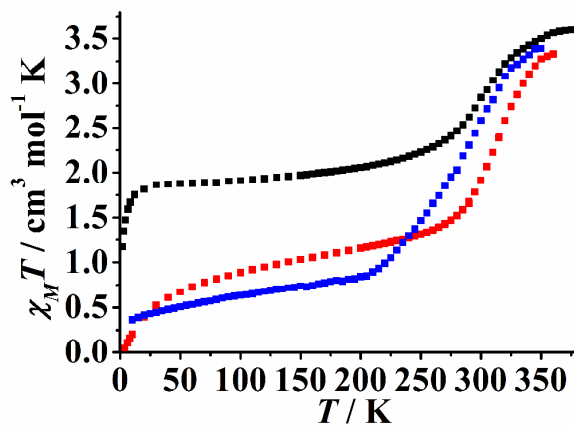


Figure S5. $\chi_m T$ vs T of 1 (■), $2 \cdot \text{H}_2\text{O}$ (■) and 2 (■).

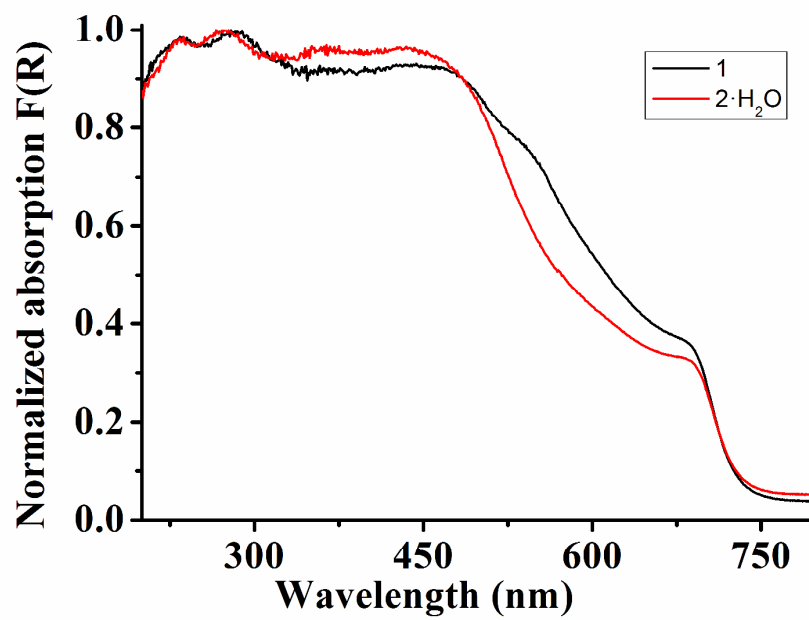


Figure S6. UV-vis spectra at 298 K of **1** and **2·H₂O**.