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Accessory Publication

Single-crystal to single-crystal transformations – guest removal and substitution in a robust solvent-templated metallocyclic compound

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Thermal analysis:

Thermal analysis was carried out on approximately 1.5 mg of crushed crystals using a TA Instruments Q500 thermogravimetric analyser with a heating rate of 5 $K.min^{-1}$.

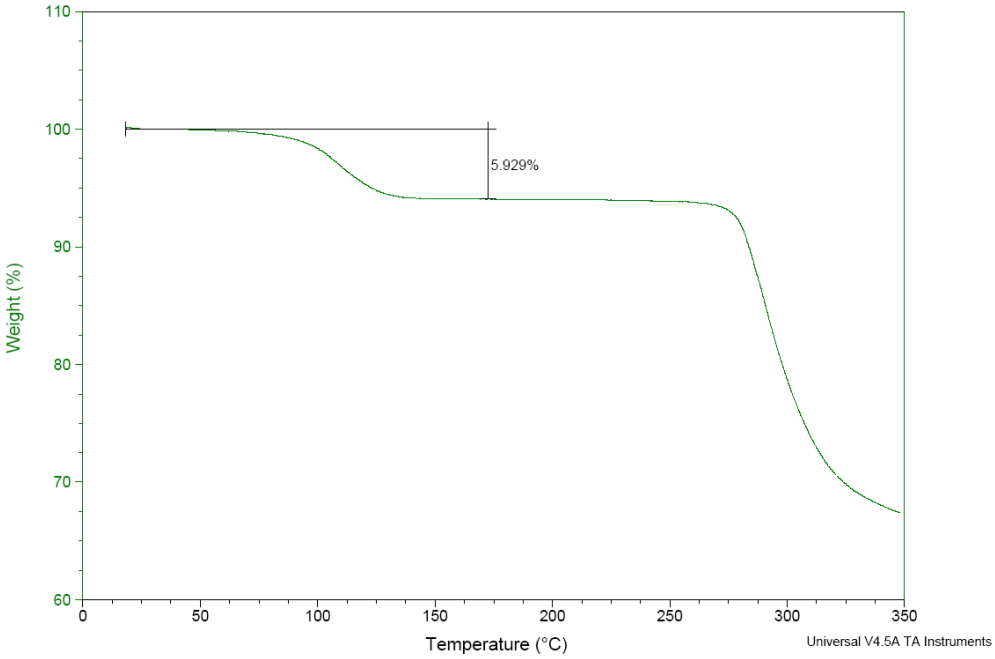

Figure S1: Thermogravimetric analyses of **1**·2CH_3CN.

X-ray Powder Diffraction

The X-ray powder diffraction experiment was carried out on a Bruker D8 Advance instrument using Cu-K_Σ radiation (λ = 1.5418 Å) and a point detector. Intensity data were collected using multiple θ-θ scans. The sample was ground prior to the experiment and rotated at 15 rpm during data collection. The calculated X-ray powder diffractogram below was calculated from the single-crystal X-ray structure using Lazy Pulverix within the X-Seed graphical interface.

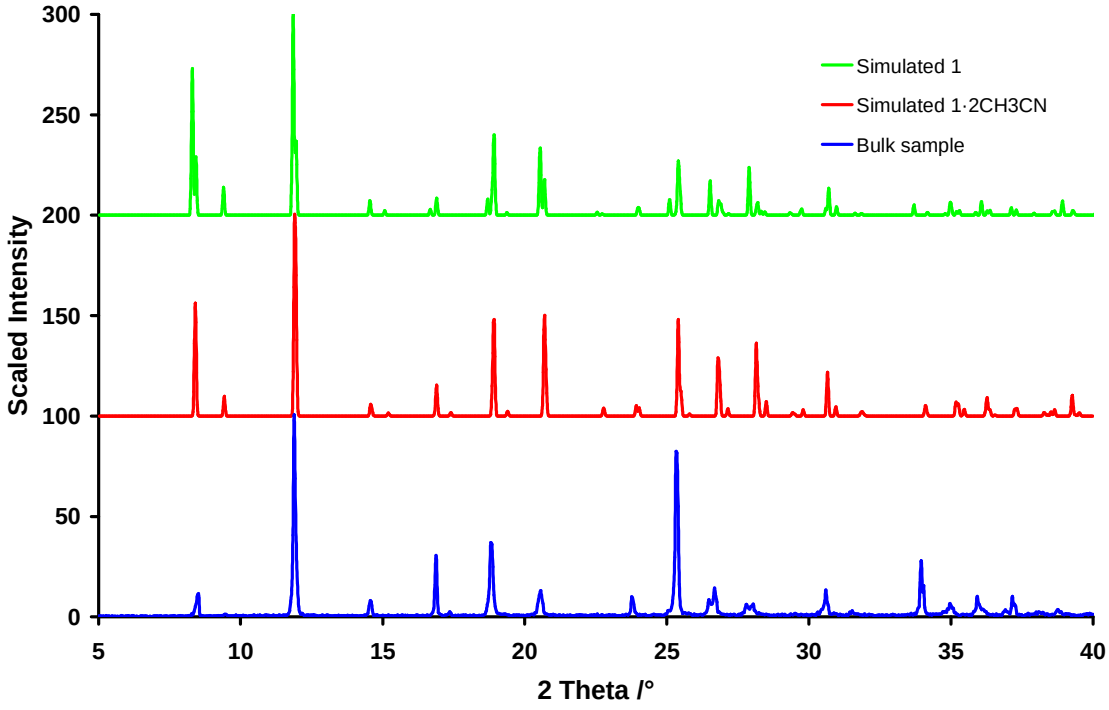

Figure S2: A graph comparing the powder diffraction pattern of the as-synthesised bulk sample **1** (before gas sorption) with the simulated diffractograms of **1**·2CH_3CN and **1** (from single crystal structures collected at 100 K).