Supplementary Material (ESI) for Chemical Communications

SUPPLEMENTARY INFORMATION

Transformation of a 1D to 3D coordination polymer mediated by low temperature lattice solvent loss

Anthony S.R. Chesman, David R. Turner, Glen B. Deacon and Stuart R. Batten

A. S. R. Chesman, Dr. D. R. Turner, Prof. G. B. Deacon, Assoc. Prof. S. R. Batten
School of Chemistry
Monash University
Wellington Rd, Clayton, VIC 3800, Australia
Fax: (+61) 03 9905 4597
E-mail: stuart.batten@sci.monash.edu.au
Homepage: www.chem.monash.edu.au/staff/sbatten/index

X-ray Powder Diffraction Patterns of Complexes 1 and 2.

For all X-ray powder diffraction pattern comparisons contained within Supporting Information the positive blue spectrum represents the collected X-ray powder pattern data, the negative pink spectrum represents the calculated X-ray powder pattern data. All calculated powder pattern spectra were generated using the Mercury v. 1.4.1 software package.[1]

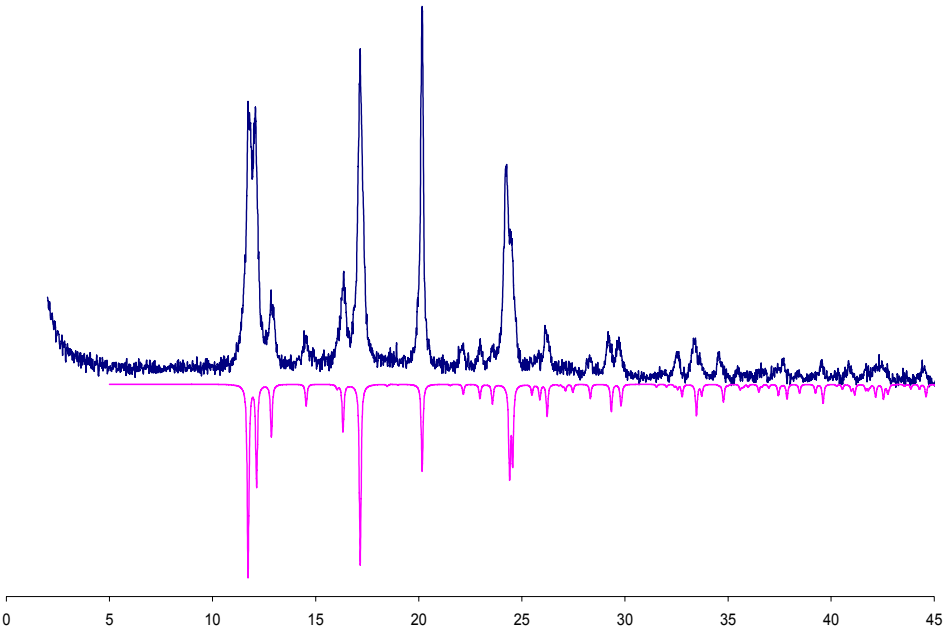

Figure S1. X-ray powder diffraction pattern of ground crystals of complex **1**, demonstrating the conversion to complex **2**.

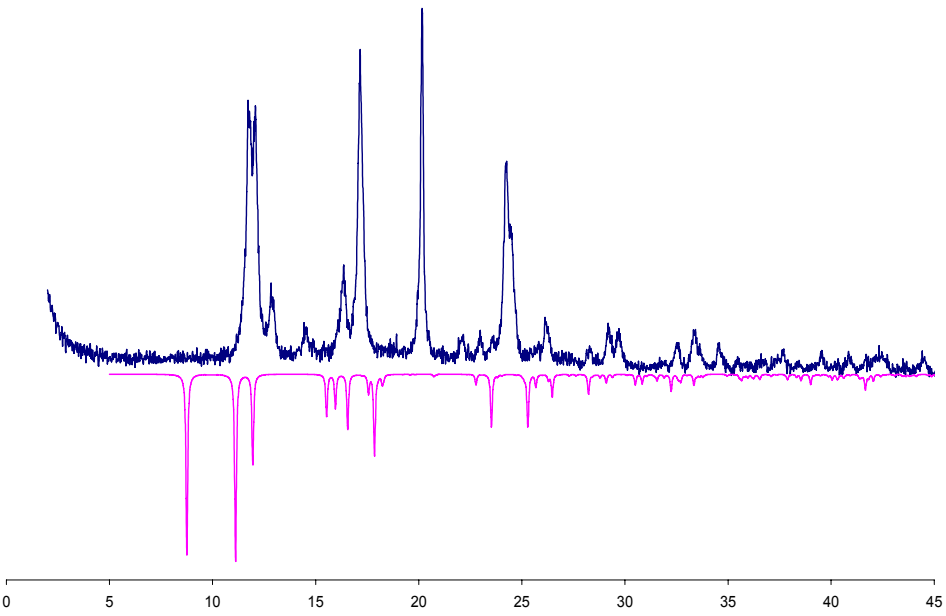

Figure S2. X-ray powder diffraction pattern of ground crystals of complex **1**, against calculated pattern of **1** showing no correlation.

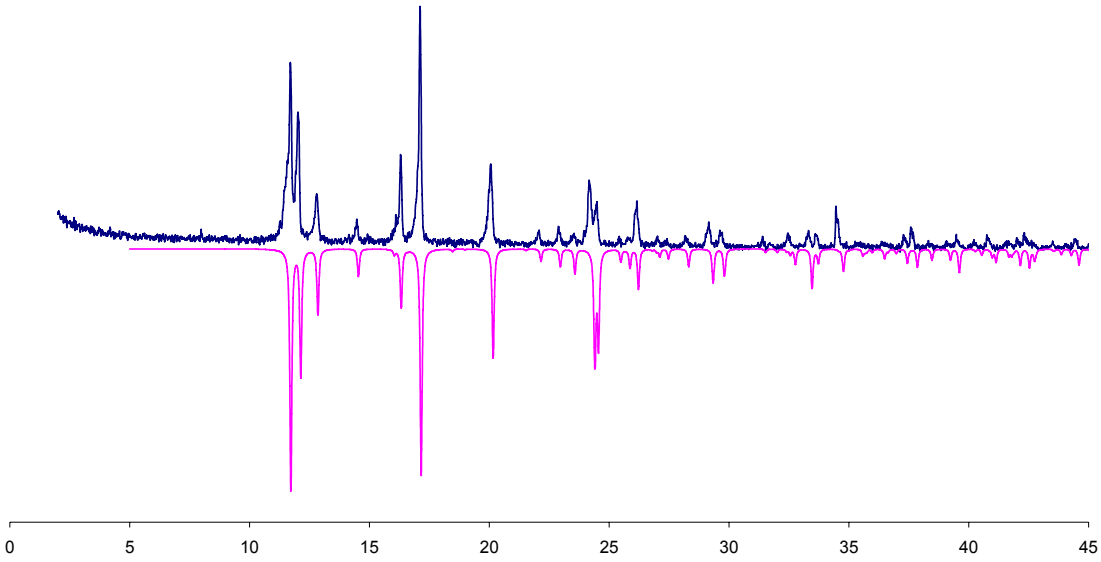

Figure S3. Complex **2** X-ray powder diffraction pattern.

Crystallography

Crystals were mounted on fine glass fibres using viscous hydrocarbon oil. Data were collected using a Bruker X8 Apex II CCD (**1, 2**) equipped with graphite monochromated Mo-Kα radiation (λ = 0.71073 Å). Data collection temperatures were maintained at 123 K using an open-flow N_2 cryostream. Data were initially processed using the SAINT program suite and data were corrected for Lorentz-polarization effects and for absorption.[2] Structures were solved by direct methods using SHELXS-97 [3] and refined using conventional least-squares methods using SHELXL-97 [3] and the program X-Seed as a graphical interface.[4] Hydrogen atoms attached to carbon were placed in idealised positions and refined using a riding model to the atom to which they are attached. Where possible hydrogen atoms attached to nitrogen or oxygen were located from the Fourier difference map and allowed to refine freely.

CCDC 720117 (**1**) and 720116 (**2**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

References

1. C. F. Macrae, P. R. Edgington, P. McCabe, E. Pidcock, G. P. Shields, R. Taylor, M. Towler, J. van de Streek, *J. Appl. Crystallogr.*, 2006, **39**, 453.

2. ApexII, V2.1.0, Bruker AXS Ltd., 2005, Madison, Wisconsin.

3. G. M. Sheldrick, *Acta Crystallogr.*, *Sect. A*, 2008, **64**, 112.

4. L.J. Barbour, *J. Supramol. Chem.*, 2001, **1**, 189.