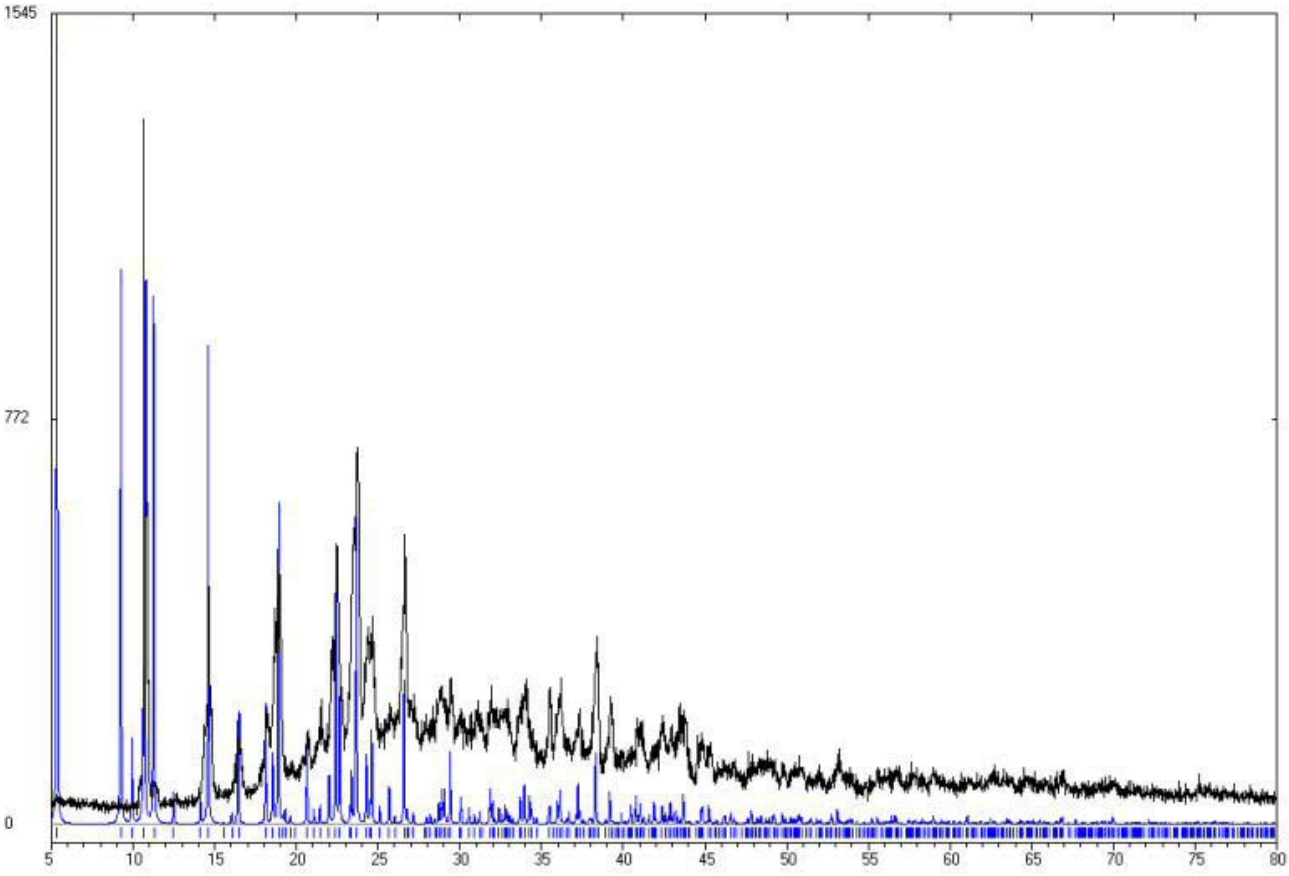
Electronic Supplementary Material for CrystEngComm

A Coordination Polymer Supramolecular Isomer Formed From A Single Building-block: An Unexpected Porphyrin Ribbon constructed from Zinc(tetra(4-pyridyl)porphyrin)

Supplementary Material

David J. Ring, M. Carla Aragoni, Neil R. Champness * and Claire Wilson



Powder X-ray diffraction pattern showing experimental data (black line) from ground sample containing crystals of **1** and calculated powder diffraction pattern for compound **2** (blue line). It can be seen that the crystalline phase is consistent with compound **1** and no additional crystalline material, notably for **1**, is observed. However, the broad base-line absorption indicates a significant level of amorphous material consistent with the degradation of **1** upon solvent loss.

Synthesis

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[Zn(tpyp)] (10.0mg, 1.46mmol) was dissolved in $CHCl_3$ ($2cm^3$) to give a purple solution. MeOH ($2cm^3$) was layered over this solution and then the combined $CHCl_3$/MeOH mixture was left to evaporate. After ca. 4 weeks crystals of both **1** and **2** were formed. (Found: C, 61.73; H, 4.13; N, 14.12. Calc. for $C_{40}H_{24}N_8Zn.0.66(CHCl_3).2.33(CH_3OH)$, i.e. $C_{43}H_{34}Cl_2N_8O_{2.33}Zn$: C, 61.75; H, 4.07; N, 13.40%). The single crystal X-ray structures of both **1** and **2** indicate disordered solvent content in the pores formed within the structures Thus non-specific relative amounts of $CHCl_3$ and MeOH solvent are expected in the CHN analysis of the mixture of products, the values quoted give the best fit for the experimental data. IR (KBr)/cm^{-1}: 2996w, 2359m, 2343m, 1593s, 1540w, 1485w, 1407m, 1342m, 1204m, 1076m, 994s, 891m, 854m, 837w, 794s.