Electronic Supplementary Material (ESI) for Journal of Materials Chemistry

The High Pressure Behaviour of the 3D Copper Carbonate Framework $\{[Cu(CO_3)_2](CH_6N_3)_2\}_n$

Elinor C. Spencer, Nancy L. Ross and Ross J. Angel

Supplementary Information

4th Order Birch-Murnaghan Equation of State Fit to the *P–V* data of 1:

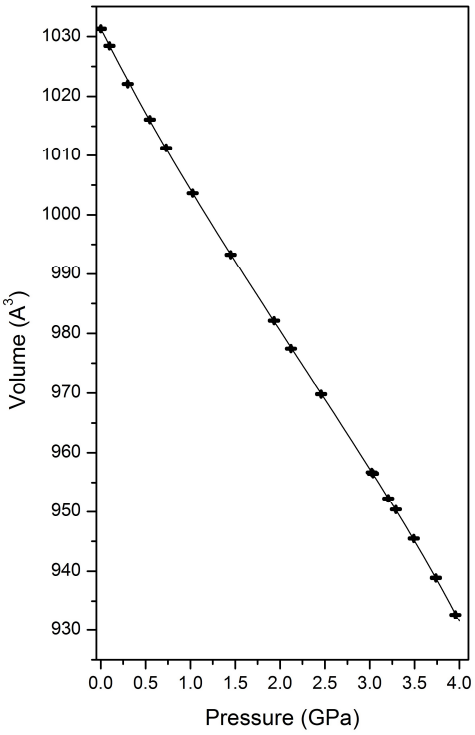

Figure S1. *P–V* data for **1**. Experimental data points are shown, with error bars, as black circles. The solid black curve represents a 4th order BM EoS fit to the data over the 0–4 GPa range ($w\chi^2 = 0.8$).

The 4th order BM EoS to the *P–V* data gave the following values for **1**: $V_0 = 1031.36(7)$ Å^3; $K_0 = 34.3(3)$ GPa; $K' = 8.3(5)$. The V_0 values provided by this fit concurs with both the experimental data and the value obtained from the fit of a 3rd order BM EoS to the data, which means that there is no statistical basis for selecting a 3rd or 4th order fit to the data.

Variable Pressure Unit Cell Data for 1 Recorded with 4:1 Methanol:Ethanol as the Pressure Transmitting Medium:

The crystal of **1** employed in this experiment (denoted crystal II) was 147 × 45 × 48 μm^3 in size and was loaded into a DAC fitted with a gasket that was 300 μm in diameter and 70 μm thick. A 4:1 methanol: ethanol mixture was included in the DAC to act as the pressure medium. A quartz crystal (87 × 84 × 35 μm^3) was included in the cell for pressure calibration measurements. The pressure evolution of the unit cell parameters for crystal II were measured up to ca. 5 GPa with the Huber diffractometer (details for which are in the manuscript associated with this SI). When the pressure in the cell exceeded 5 GPa the quality of the crystal deteriorated to such an extent that further diffraction

measurements were not possible. Figure S2 show the evolution of the unit cell volume of crystal II as a function of pressure. Also shown are the data recorded for the crystal of **1** in isopropanol (denoted crystal I) that have been discussed in detailed in the manuscript associated with this SI.

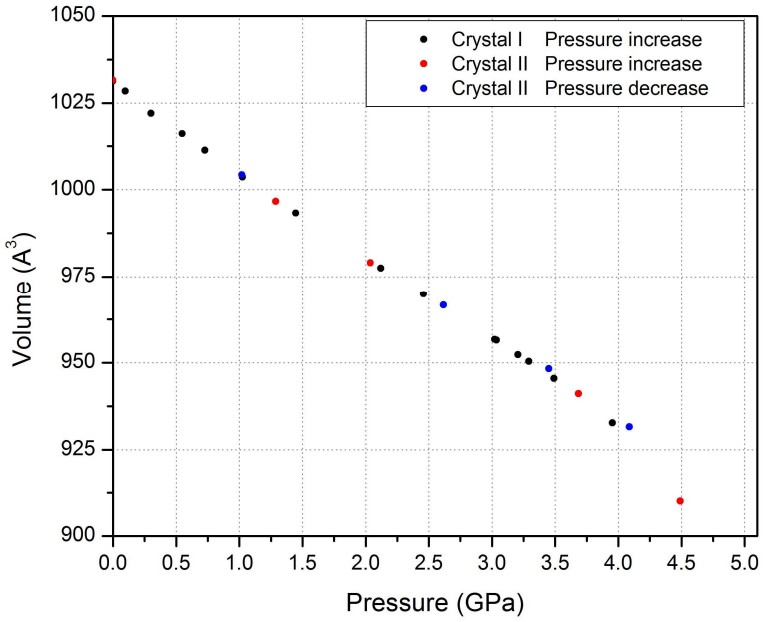

Figure S2. Evolution of the unit cell volume of crystals I and II as a function of pressure. Error bars are smaller than the symbols representing the data points.