SUPPORTING INFORMATION

Positioning of the HKUST-1 metal–organic framework (Cu₃(BTC)₂) through conversion from insoluble Cu-based precursors

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Fig. S1. Crystal structures of the (a) monoclinic Rouaite⁵¹ and (b) orthorhombic Gerhardtite⁵² polymorphs of Cu₂(OH)₃NO₃. The main difference lies in the packing of the NO₃ between the Cu layers.
Fig. S2. Observed (blue) and calculated (red) powder diffraction patterns for the Cu-based precursors synthesized using 3 ml (a) and 4 ml (b) of ammonia solution. Difference patterns are shown in grey. The (001) and (002) reflections from the Cu$_2$(OH)$_3$NO$_3$ phase (Rouaite), corresponding to the stacking direction of the Cu layers, are shown. These Cu layers are also present in the Gerhardtite polymorph, but with a slightly different arrangement in the NO$_3$ packing between layers. Disorder in the way the NO$_3$ ions pack between the layers is thought to be responsible for the discrepancies in the relative peak intensities.

References