SUPPORTING INFORMATION

Positioning of the HKUST-1 metal–organic framework ($Cu_3(BTC)_2$) through conversion from insoluble Cu-based precursors

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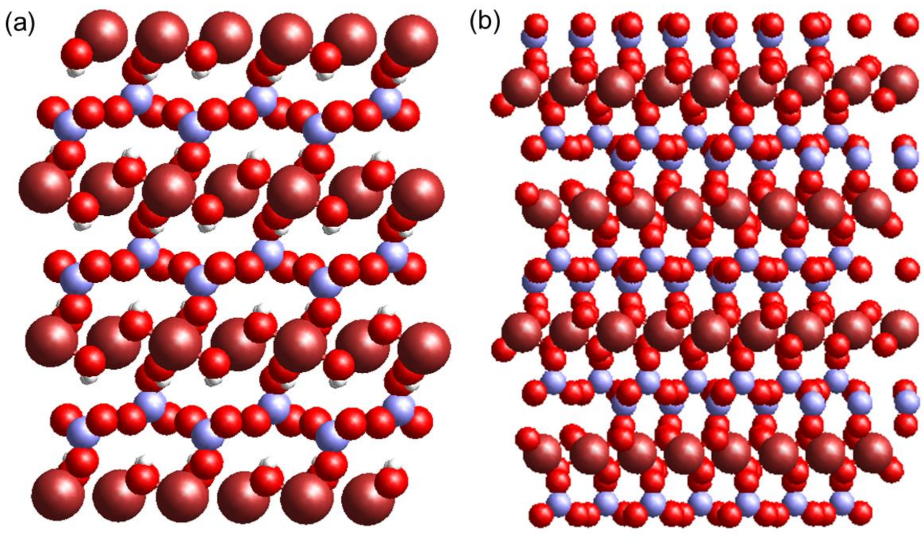

Fig. S1. Crystal structures of the (a) monoclinic Rouaite^{S1} and (b) orthorhombic Gerhardtite^{S2} polymorphous of $Cu_2(OH)_3NO_3$. The main difference lies in the packing of the NO_3 between the Cu layers.

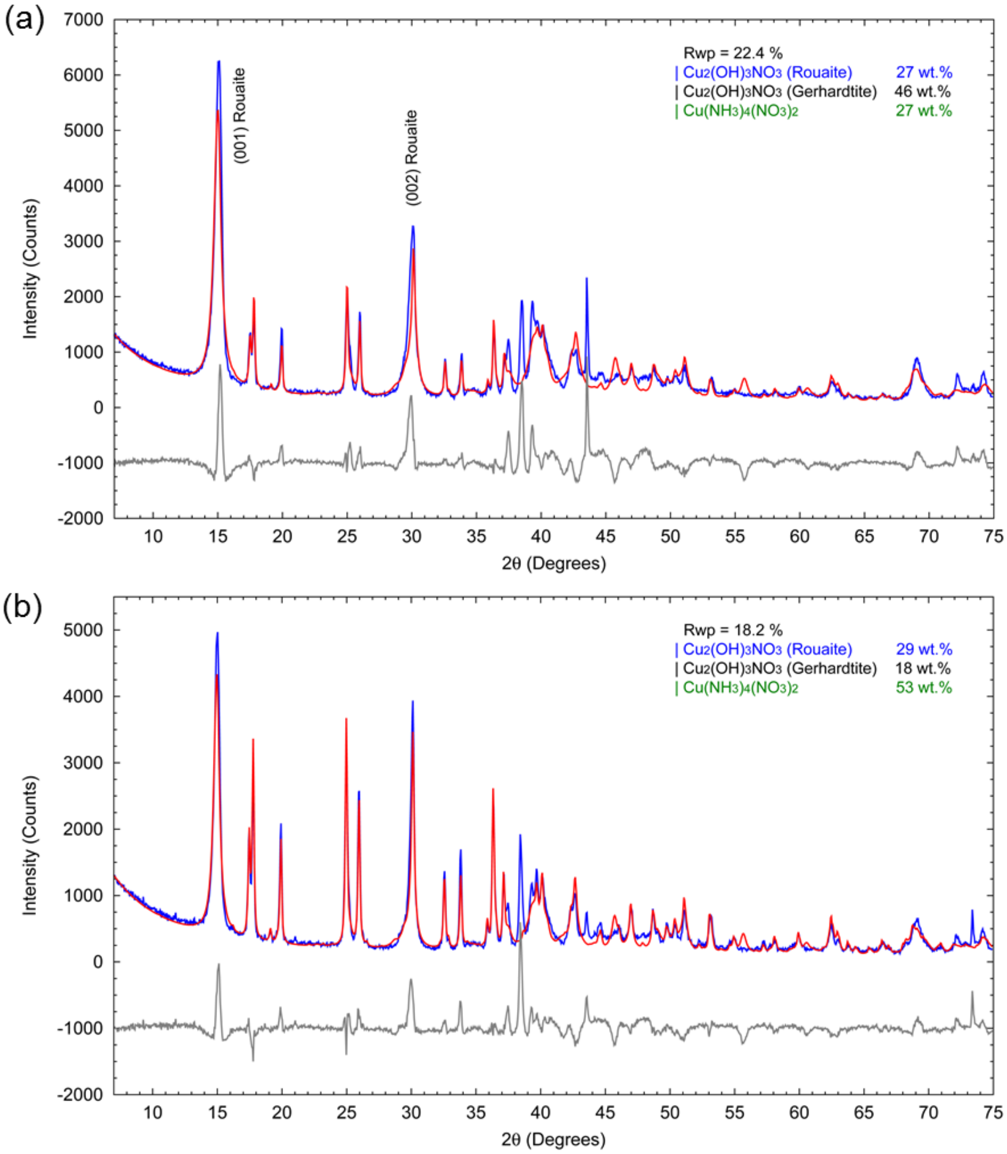

Fig. S2. Observed (blue) and calculated (red) powder diffraction patterns for the Cu-based precursors synthesized using 3 ml (a) and 4 ml (b) of ammonia solution. Difference patterns are shown in grey. The (001) and (002) reflections from the $Cu_2(OH)_3NO_3$ phase (Rouaite), corresponding to the stacking 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

[S1] H. Effenberger, *Zeitschrift fur kristallographie*, 1983, **165**, 127.
[S2] B. Bovio and S. Locchi, *J. Crystallogr. Spectrosc. Res.*, 1982, **12**, 507.