Electronic Supplementary Material (ESI) for Dalton Transactions

SUPPORTING INFORMATION

Zinc Hydroxide Sulfate and Its Transformation to Crystalline Zinc Oxide

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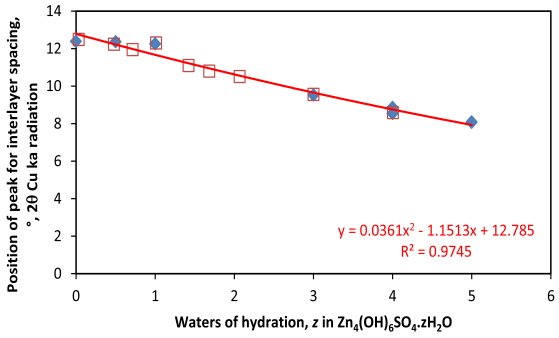

Figure S1. Correlation between waters of hydration, *z,* and peak position in ° (Cu kα scale) in the compounds in the family $Zn_4(OH)_6SO_4.zH_2O$. Data from Bear et al.[1]

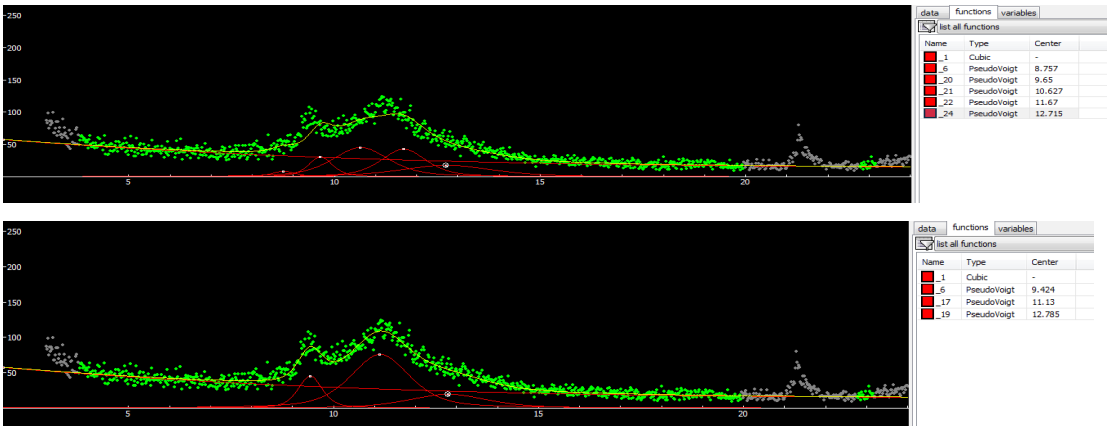

Figure S2. Deconvolution of the XRD pattern of the sample of $Zn_4(OH)_6SO_4.zH_2O$ produced by drying at 60 °C. (a) A scheme based on the 'accepted' waters of hydration of *z*= 4, 3, 1 ½ and 0 H_2O. The problem with this scheme is that it does not provide a match for the observed peaks at ~9.4 ° (z ~3.25) and 11.14° (z ~1.5) (b) an alternate scheme based on waters of hydration of *z*= 3¼, 1½, and 0. Program used was FITYK (www.fityk.nieto.pl).

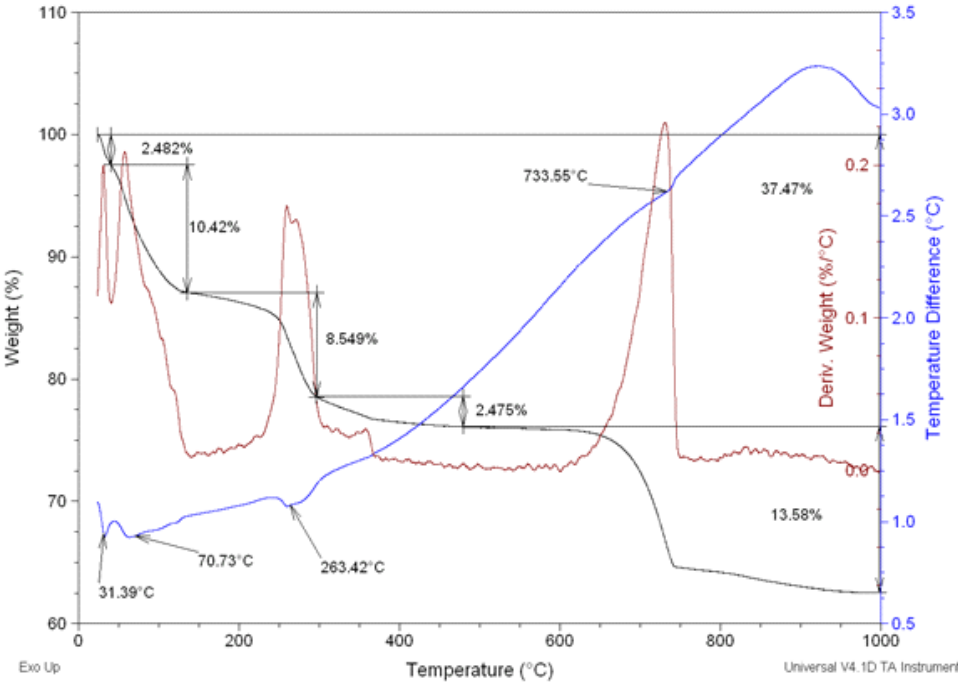

Figure S3. TGA-DTA data for $Zn_4(OH)_6SO_4 \cdot 4H_2O$.

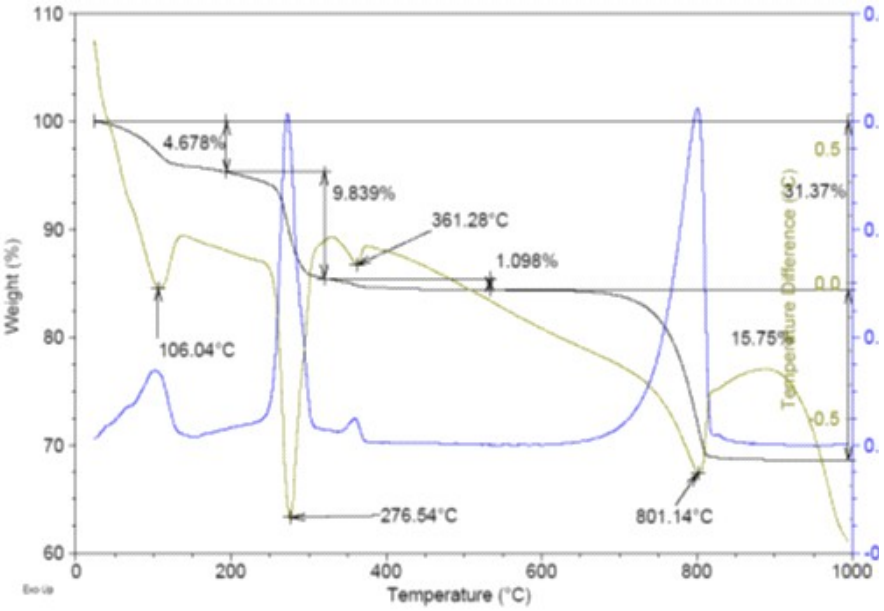

Figure S4. TGA-DTA data $Zn_4(OH)_6SO_4 \cdot H_2O$.

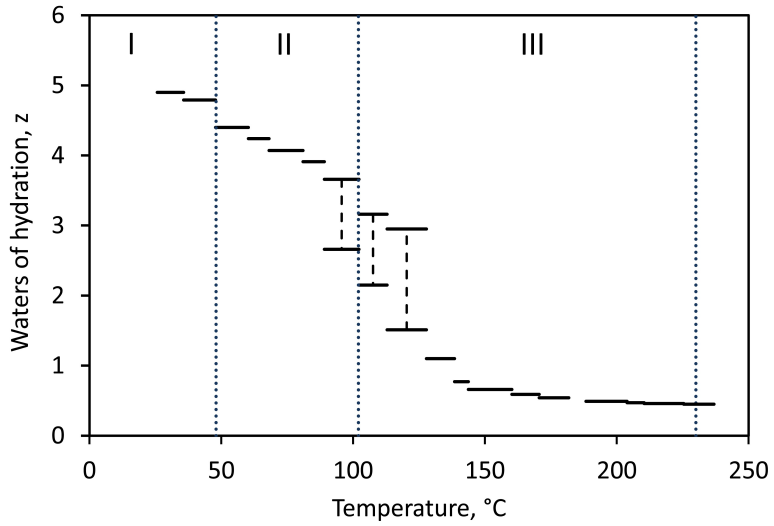

Figure S5. Waters of hydration of sample heated in synchrotron, determined by deconvolving peak due to interlayer spacing and applying the relationship shown in Figure S1. It is clear that the sample consisted of at least two compounds for temperatures between about 100 and 120 °C. However, there is insufficient resolution to identify the various hydrated states with any precision. The 'zones' identified in Figure 6 of the paper are also indicated.

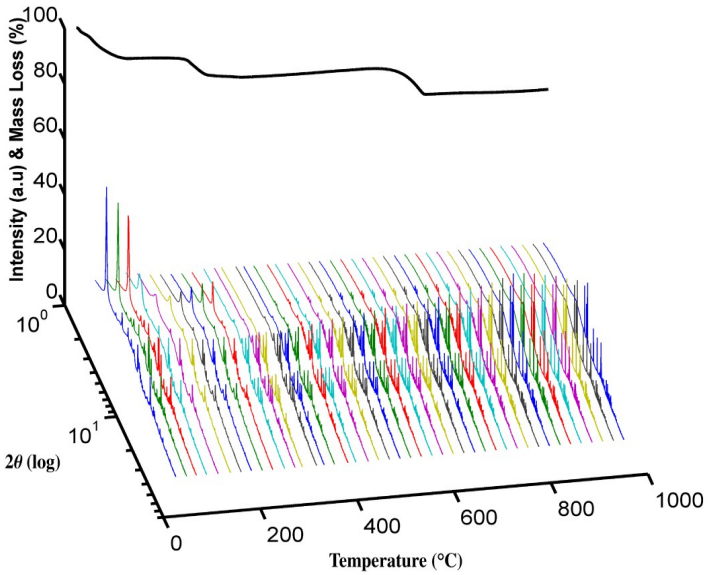

Figure S6. 3D-stacked graph of XRD patterns (synchrotron radiation) plotted with the corresponding TGA data.

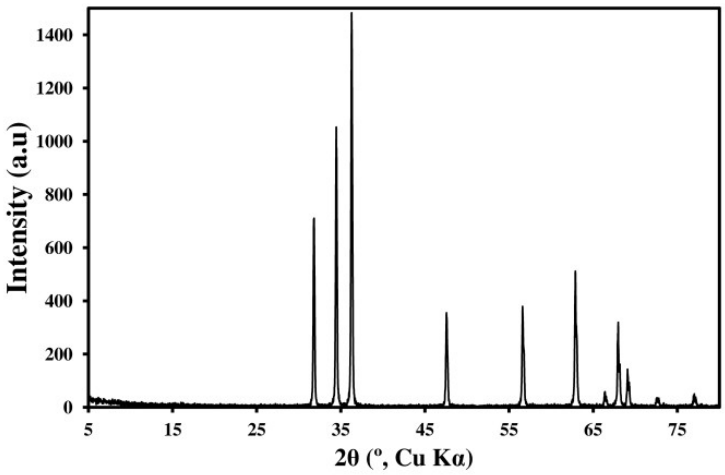

Figure S7. XRD data obtained from the product of calcination of $Zn_4(OH)_6SO_4 \cdot 4H_2O$ at 900 °C. The peaks correspond to ZnO (JC-PDF 01-089-7102).

References

1. I. J. Bear, I. E. Grey, I. E. Newnham and L. J. Rogers, *Australian Journal of Chemistry*, 1987, **40**, 539-556.