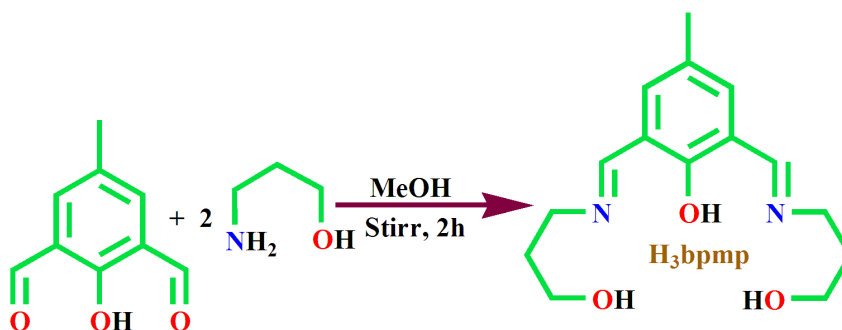


Electronic Supplementary Information

A Dodecanuclear Copper(II) Cage Self-Assembled from Six Dicopper Building Units

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Scheme S1. Scheme of the H₃bpmp ligand synthesis.

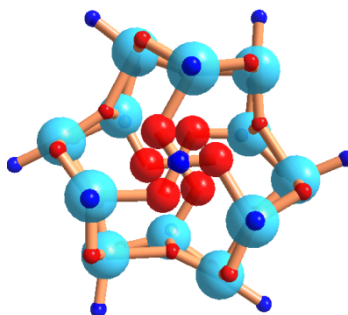


Figure S1. Ball and stick representation of the molecular core of **1**. Most of the ligand and solvent atoms have been omitted for clarity. Atom color code: Cu cyan, N blue, O red.

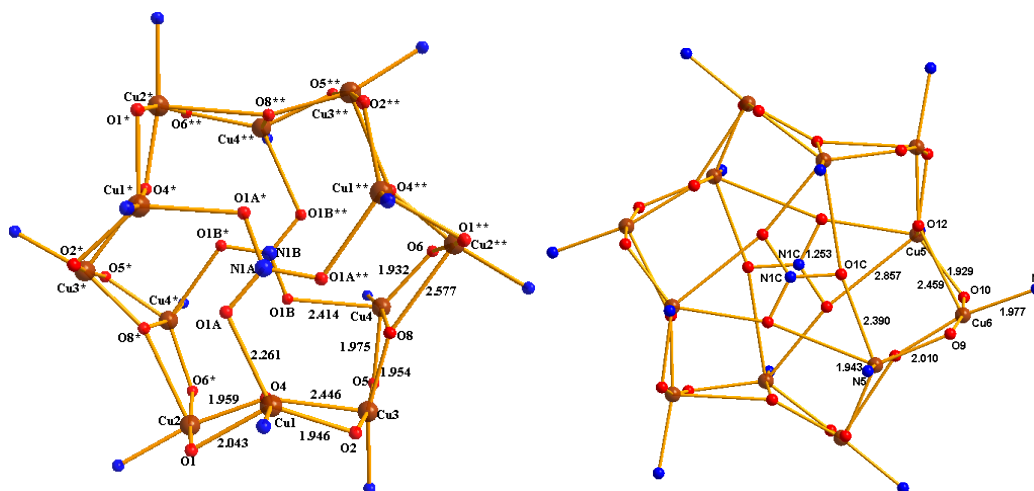


Figure S2. Ball and stick representation of the molecular core of **1** showing the bond lengths around the Cu1, Cu2, Cu3, Cu4, Cu5 and Cu6 sites. Most of the ligand and solvent atoms have been omitted for clarity. Atom color code: Cu brown, N blue, O red.

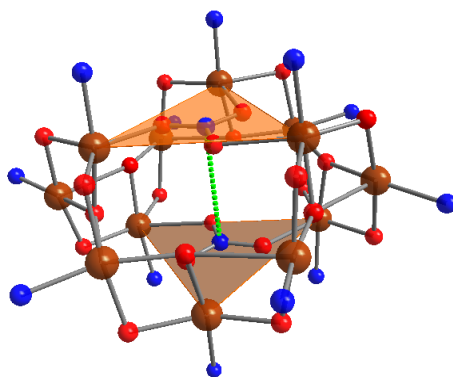
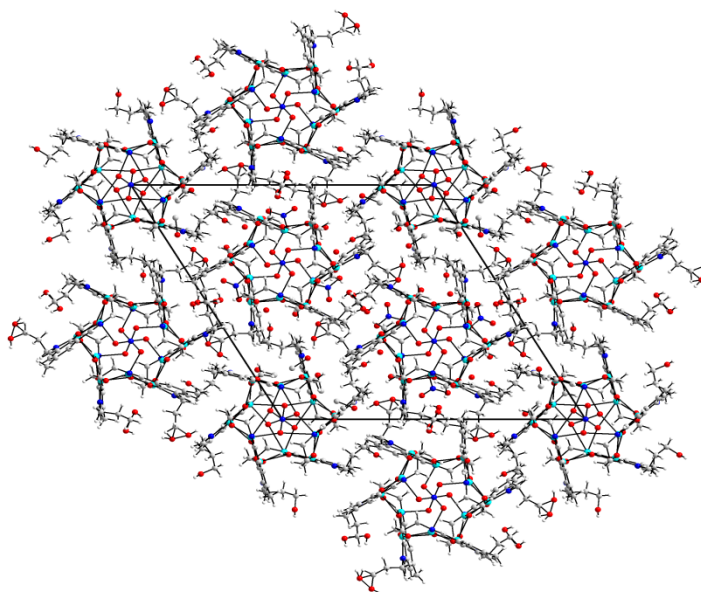


Figure S3. Side view of the [Cu₁₂] complex highlighting the templating positions of the nitrate anion pair (green dotted line between the two N atoms) at the center of the two [Cu₃] motifs.



FigureS5/ S4. The crystal packing projected down the *c* axis.

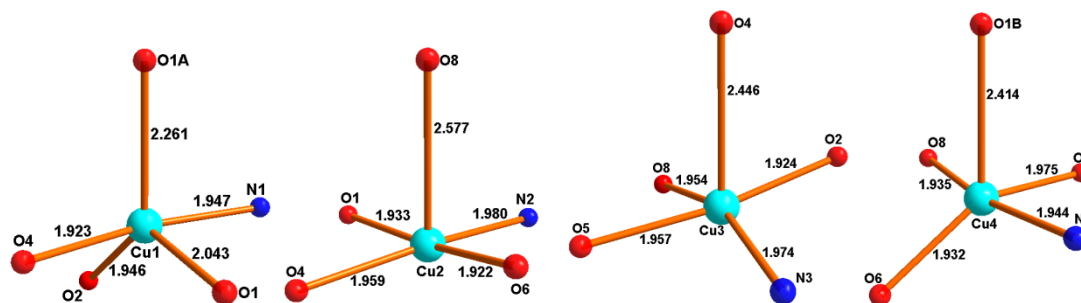


Figure S5. The four unique copper(II) sites (Cu1 to Cu4) with distorted square pyramidal NO₄ coordination geometries ($\tau = 0.639, 0.006, 0.180$ and 0.444).

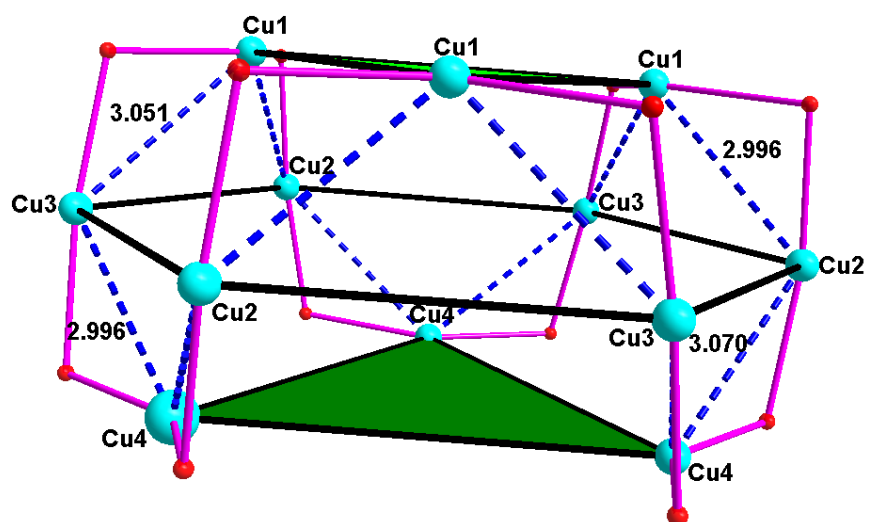


Figure S6. Location of the four unique copper(II) sites in three layers (Cu1, Cu2 and Cu3, and Cu4) within the cuboctahedral cage.

Reference

(1) M. N. Burnett, C. K. Johnson, ORTEP III, Report ORNL-6895, Oak Ridge National Laboratory, Oak Ridge, TN, 1996.