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 [Cu$_{12}$] complex highlighting the templating positions of the nitrate anion pair (green dotted line between the two N atoms) at the center of the two [Cu$_3$] motifs.

**Figure S5/ S4.** The crystal packing projected down the c axis.

**Figure S5.** The four unique copper(II) sites (Cu1 to Cu4) with distorted square pyramidal NO$_4$ 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