

Electronic Supplementary Information for

Hexanuclear Copper(II) Cage with $\{\text{Cu}_3\text{O}\cdots\text{H}\cdots\text{OCu}_3\}$ Core Supported by a Dicompartamental Oxime Ligand with *m*-Xylyl Spacer: Synthesis, Molecular Structure and Magnetic Studies

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Table S1. Selected bond lengths (Å) and angles (°) for **1b**

Cu(1)-O(3)	1.917(1)	Cu(2)-O(4)	1.913(1)
Cu(1)-O(1')	1.939(3)	Cu(2)-O(2'')	1.938(3)
Cu(1)-N(1)	1.955(4)	Cu(2)-N(4)	1.968(3)
Cu(1)-N(2)	1.980(4)	Cu(2)-N(3)	1.991(3)
Cu(1)-O(1w)	2.485(7)	Cu(1)-O(2w)	2.534(6)
O(3)...O(4)	2.521(6)	Cu(1)...Cu(2)	3.705(1)
Cu(1)...Cu(1')	3.207(1)	Cu(2)...Cu(2')	3.204(1)
O(3)-Cu(1)-O(1')	91.73(9)	O(4)-Cu(2)-O(2'')	93.27(8)
O(3)-Cu(1)-N(1)	88.03(10)	O(4)-Cu(2)-N(3)	167.73(12)
O(3)-Cu(1)-N(2)	166.88(13)	O(4)-Cu(2)-N(4)	89.10(9)
O(1')-Cu(1)-N(1)	171.15(16)	O(2'')-Cu(2)-N(3)	97.17(13)
O(1')-Cu(1)-N(2)	98.90(14)	O(2'')-Cu(2)-N(4)	177.57(12)
N(1)-Cu(1)-N(2)	80.28(15)	N(4)-Cu(2)-N(3)	80.42(13)
O(3)-Cu(1)-O(1w)	98.9(2)	O(4)-Cu(2)-O(2w)	98.6(2)
O(1')-Cu(1)-O(1w)	89.4(3)	O(2'')-Cu(2)-O(2w)	93.6(2)
N(1)-Cu(1)-O(1w)	99.4(3)	N(3)-Cu(2)-O(2w)	87.17(18)
N(2)-Cu(1)-O(1w)	89.0(2)	N(4)-Cu(2)-O(2w)	86.6(2)
Cu(1)-O(3)-Cu(1')	113.58(11)	Cu(2)-O(4)-Cu(2')	113.70(10)

Symmetry codes: (') y, z, x; (") z, x, y.

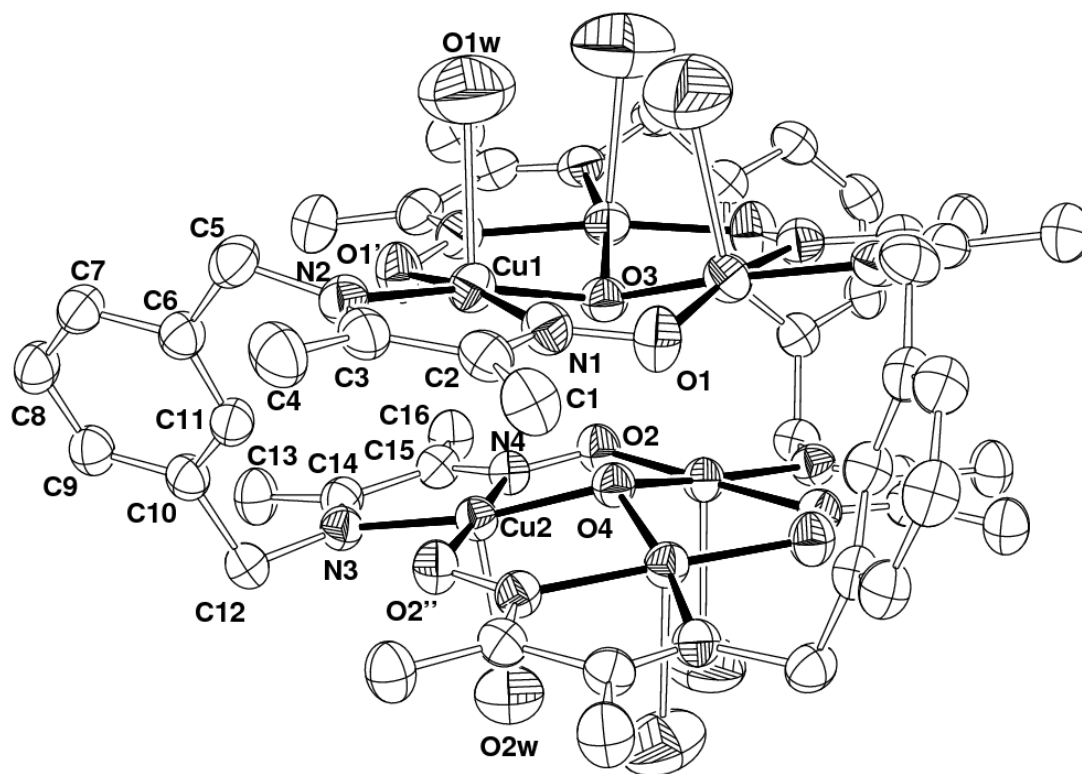


Figure S1 ORTEP drawing (35% probability ellipsoid) of the complex cation **1b** with label scheme of the crystallographic independent part. Symmetry codes (') y, z, x ; (") z, x, y .

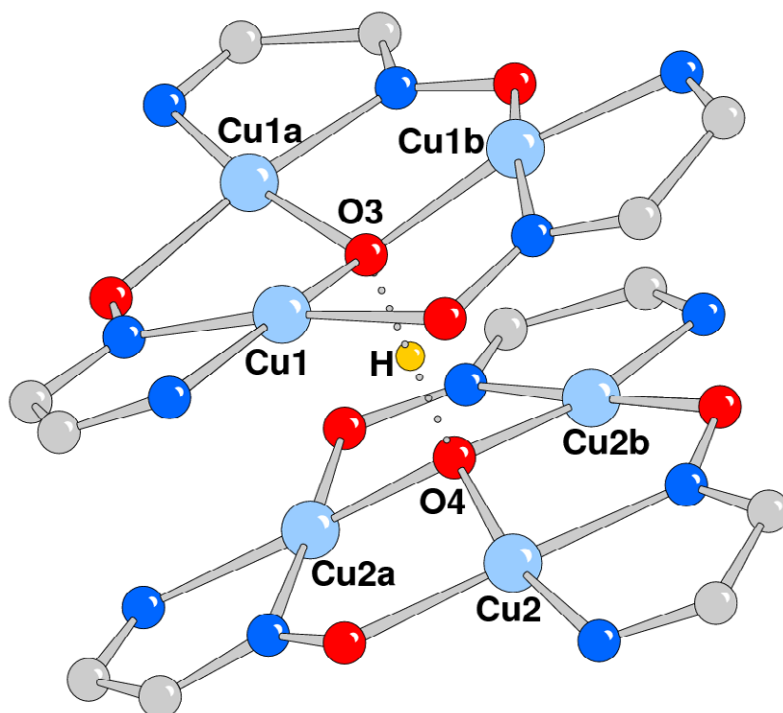


Figure S2 Structure of the hexanuclear core in **1b**.