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Supporting Information

Structure, Magnetic Properties, Polarized Neutron Diffraction and Theoretical Study of a copper(II) cubane.

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Table S1. Selected inter-atomic distances (Å) and angles (deg.) for **[Cu_4]** from X-ray diffraction at 293K.

Cu1 – O1	1.897(5)	Cu2 – O8	1.961(4)	Cu4 – O7	1.917(5)
Cu1 – O2	1.959(4)	Cu2 – O2	2.414(5)	Cu4 – N4	1.934(6)
Cu1 – N1	1.939(6)	Cu3 – O5	1.907(5)	Cu4 – O2	1.944(4)
Cu1 – O6	1.950(4)	Cu3 – O4	1.949(4)	Cu4 – O6	2.456(5)
Cu1 – O4	2.419(5)	Cu3 – N3	1.927(5)	Cu1 ⋯ Cu3	3.109(2)
Cu2 – O3	1.914(3)	Cu3 – O6	1.954(4)	Cu1 ⋯ Cu2	3.297(2)
Cu2 – O4	1.952(4)	Cu3 – O8	2.408(5)	Cu1 ⋯ Cu4	3.130(1)
Cu2 – N2	1.942(5)	Cu4 – O8	1.959(5)	Cu2 ⋯ Cu4	3.150(2)
Cu2 ⋯ Cu3	3.128(2)	Cu3 ⋯ Cu4	3.313(2)		
Cu2 – O8 – Cu4	107.0(2)	Cu4–O8–Cu3	98.20(18)	Cu1–O4–Cu2	97.36(18)
Cu2 – O8 – Cu3	90.88(17)	Cu2–O4–Cu3	106.6(2)	Cu2–O2–Cu1	97.32(18)
Cu4 – O6 – Cu3	96.73(18)	Cu3–O4–Cu1	90.12(16)	Cu3–O6–Cu1	105.60(19)
Cu4 – O6 – Cu1	89.77(17)	Cu1–O2–Cu4	106.6(2)	Cu4–O2–Cu2	91.93(18)

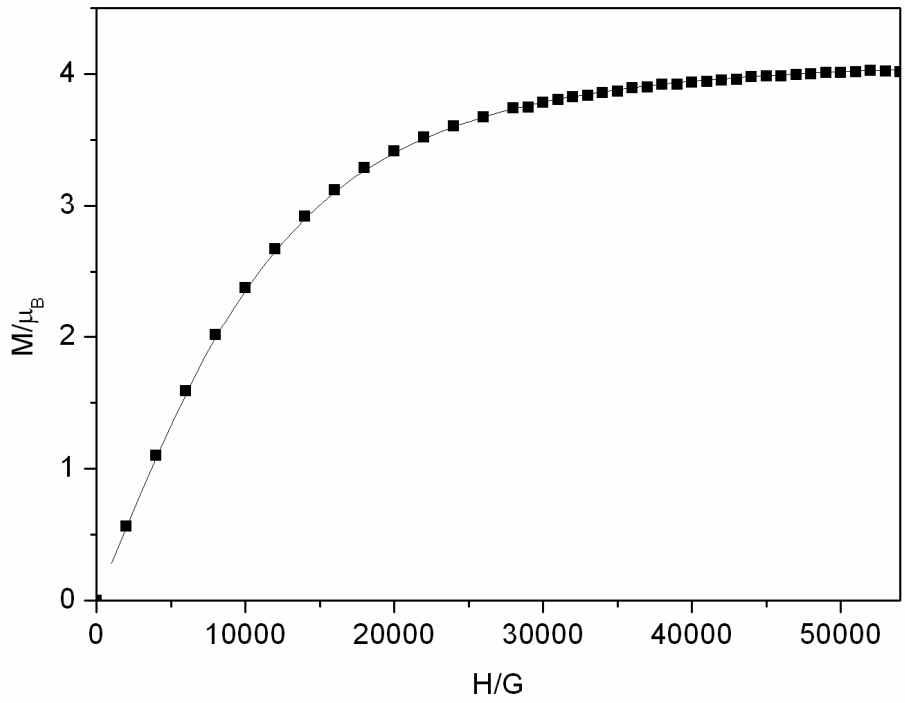

Figure S1. Magnetization at 2 K. The solid lines hold for the best fits of the data as explained in text (g = 2.18, J_1 = + 30.5 cm^{-1}, J_2 = −5.5 cm^{-1} and θ = − 0.10 K).

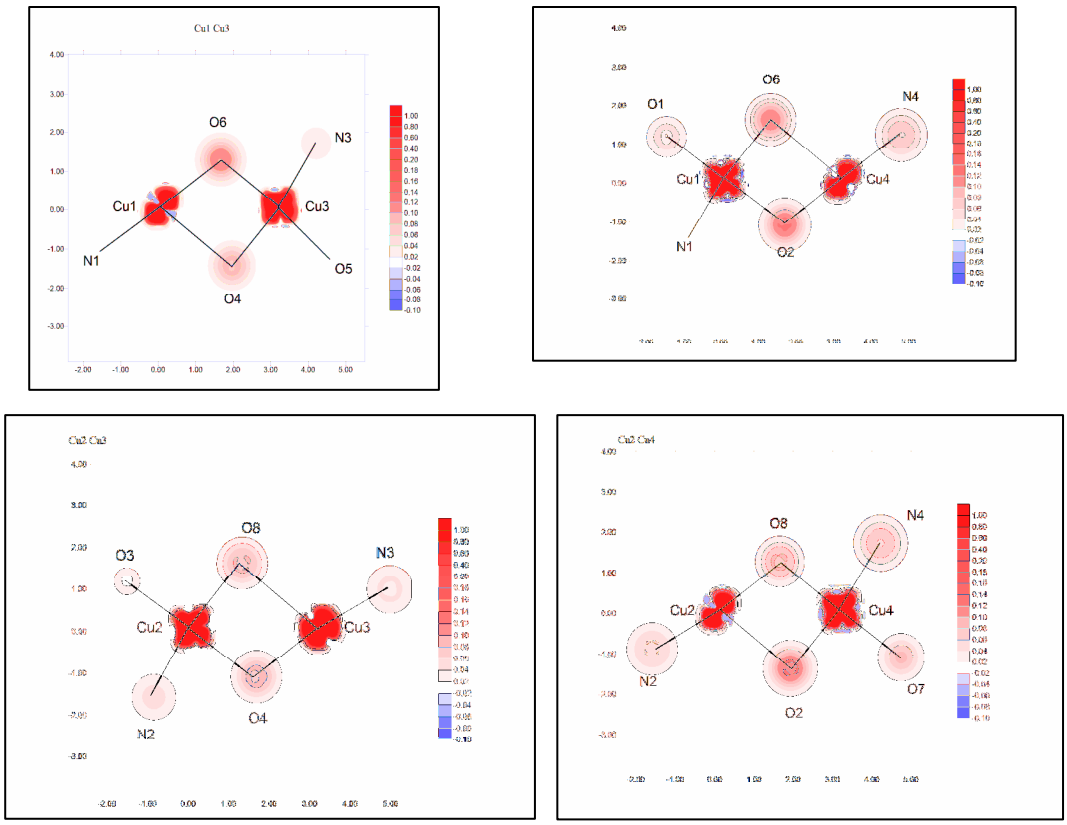

Figure S2: Sections of the reconstructed experimental spin density in the various Cu---Cu dinuclear planes (in $\mu_B/Å^3$) for asymmetrical configurations and the short Cu…Cu distance 3.1 Å.

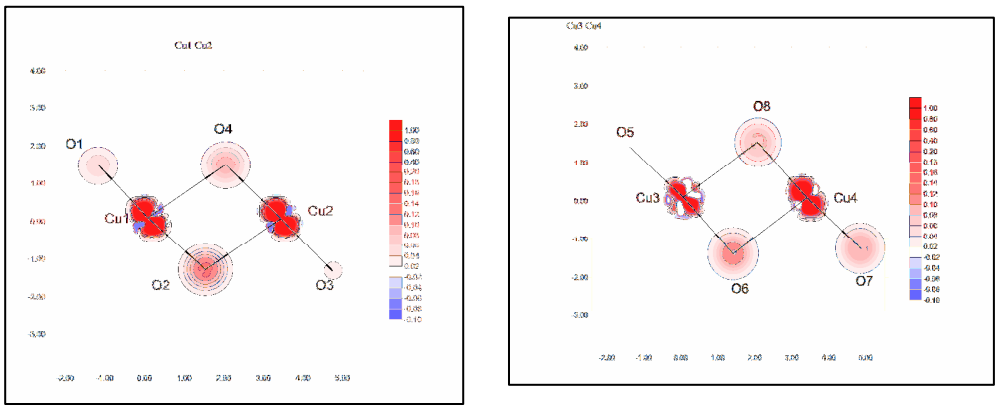

Figure S3: Sections of the reconstructed experimental spin density in the various Cu---Cu dinuclear planes (in $\mu_B/Å^3$) for symmetrical configurations and a long Cu…Cu distance 3.3 Å.