Electronic supplementary information

Synthesis, Crystal Structures and Magnetic Properties of bis(μ-dialkoxo)-bridged Linear Trinuclear Copper(II) Complexes with Aminoalcohol Ligands: A Theoretical/Experimental Magneto-Structural Study.

Petri Seppälä[*,a], Enrique Colacio[b], Antonio J. Mota[b] and Reijo Sillanpää[a]

[a] *Department of Chemistry, University of Jyväskylä, P.O. Box 35, FIN-40014 University of Jyväskylä, Jyväskylä, Finland*

[b] *Departamento de Química Inorgánica, Facultad de Ciencias, Universidad de Granada, Avda. de Fuentenueva s/n, 18071, Granada, Spain*

[*] To whom correspondence should be addressed. Email: petri.seppala@jyu.fi.

Table S1 Main hydrogen bond parameters (Å, °) for **1**–**4**

Complex	D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠(D–H···A)
1[a]	N1–H1NB···O11^{i}	0.85(4)	2.35(4)	3.130(4)	152(3)
	N1–H1NA···O6A^{ii}	0.84(4)	2.12(4)	2.959(8)	171(4)
	N1–H1NA···O6B^{ii}	0.84(4)	2.34(5)	3.170(11)	171(4)
	N2–H2NA···O8B^{ii}	0.79(4)	2.12(5)	2.870(9)	158(4)
	N2–H2NA···O8A^{ii}	0.79(4)	2.43(4)	3.099(5)	142(4)
	N2–H2NB···O12^{i}	0.84(4)	2.28(4)	3.020(4)	149(4)
	N3–H3NA···O10^{iii}	0.88(4)	2.30(4)	3.062(4)	145(3)
	N3–H3NB···O2^{iv}	0.86(4)	2.10(4)	2.964(3)	177(3)
	N4–H4NB···O1^{iv}	0.77(4)	2.55(4)	3.193(3)	143(3)
	N4–H4NA···O11^{iii}	0.87(4)	2.16(5)	3.023(4)	171(4)
	O13–H13O···O5	0.79(4)	2.11(4)	2.850(3)	155(4)
2[b]	N1–H1NA···O8^{i}	0.86(4)	2.23(4)	3.059(3)	162(4)
	N1–H1NA···O10^{i}	0.86(4)	2.50(4)	3.244(4)	144(3)
	N2–H2NA···O5^{i}	0.85(4)	2.20(4)	2.926(3)	143(3)
	N2–H2NB···O9^{ii}	0.84(4)	2.31(4)	3.048(3)	147(3)
	N2–H2NB···O8^{i}	0.84(4)	2.59(4)	3.074(3)	118(3)
	N3–H3NA···O6^{iii}	0.91(4)	2.37(4)	3.118(3)	139(3)
	N3–H3NB···O10^{iv}	0.84(4)	2.40(4)	3.121(4)	145(3)
	N4–H4NA···O9	0.83(4)	2.34(4)	3.025(3)	140(3)
	N4–H4NB···O1^{v}	0.91(4)	2.29(4)	3.131(3)	154(3)
	N4–H4NB···O7^{iii}	0.91(4)	2.54(4)	3.061(3)	117(3)
3[c]	N1–H1NA···O2^{i}	0.77(5)	2.53(5)	3.118(4)	134(4)
	N1–H1NA···Br1^{i}	0.77(5)	2.94(5)	3.514(4)	133(5)
	N1–H1NB···Br1^{ii}	0.79(6)	2.65(6)	3.434(4)	172(4)
	N2–H2NA···Br1^{ii}	0.84(5)	2.62(5)	3.457(4)	172(4)
	N2–H2NB···O1^{i}	0.82(5)	2.47(5)	3.148(4)	141(4)
	N2–H2NB···Br1^{i}	0.82(5)	3.01(5)	3.528(4)	123(4)
4[d]	N1–H1NA···O5^{i}	0.90(4)	2.15(4)	2.992(3)	156(3)
	N1–H1NB···O2^{ii}	0.79(4)	2.21(4)	2.971(3)	162(3)
	N2–H2NA···O4	0.87(4)	2.47(4)	2.970(3)	117(3)
	N2–H2NB···O5^{iii}	0.78(3)	2.35(3)	3.111(3)	168(3)
	N2–H2NB···O3^{iii}	0.78(3)	2.32(3)	2.923(3)	135(3)

[a] Symmetry codes for **1**: (i) $x, y, z-1$; (ii) $-x+1, -y+2, -z$; (iii) $-x, -y+1, -z+2$; (iv) $-x, -y+1, -z+1$.
[b] Symmetry codes for **2**: (i) $-x+3/2, y-1/2, -z+1/2$; (ii) $x+1/2, -y+1/2, z+1/2$; (iii) $x-1/2, -y+1/2, z-1/2$; (iv) $-x+1, -y+1, -z$; (v) $-x+1, -y, -z$.
[c] Symmetry codes for **3**: (i) $-x, y+1/2, -z+1/2$; (ii) $x, y+1, z$.
[d] Symmetry codes for **4**: (i) $-x+1/2, y+1/2, -z+1/2$; (ii) $-x+1/2, y-1/2, -z+1/2$; (iii) $x+1/2, -y-1/2, z+1/2$.

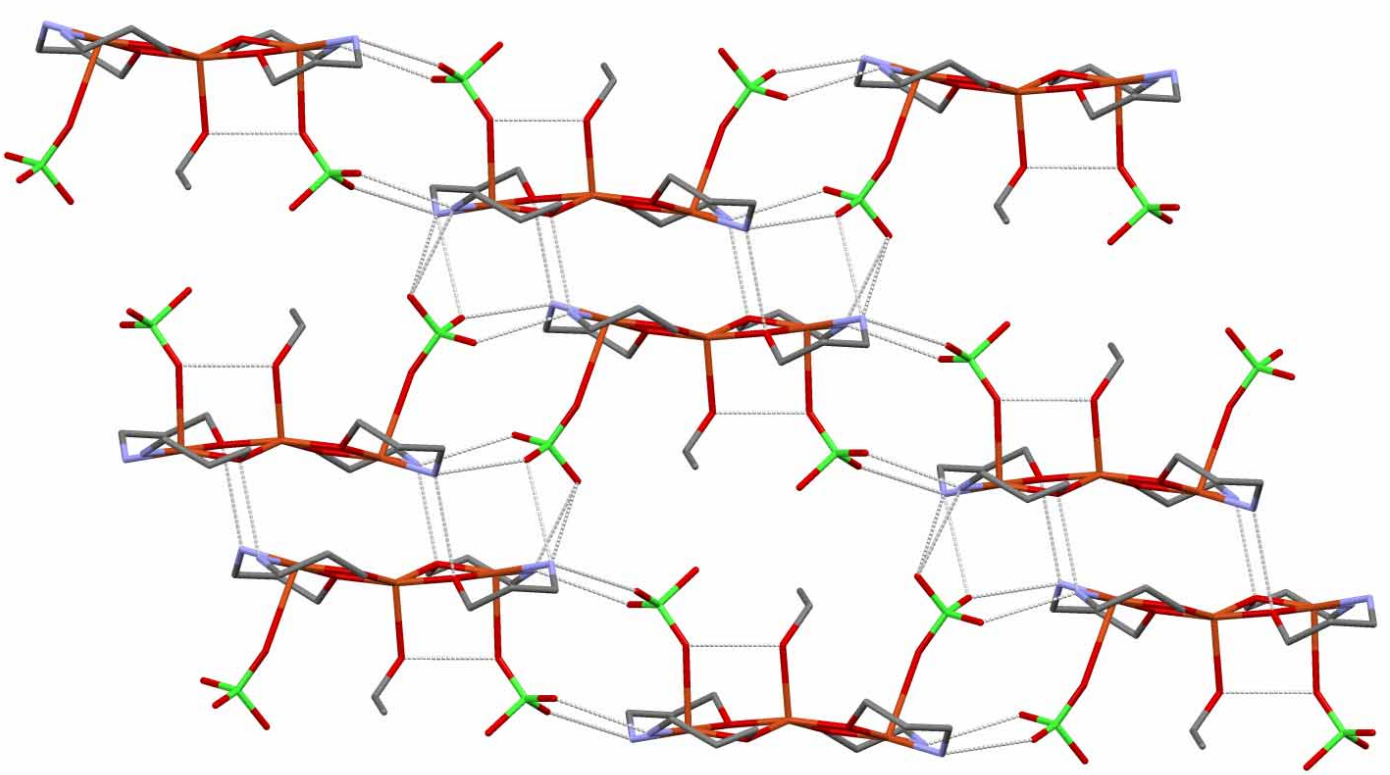

Fig. S1 The partial crystal packing diagram of **1** showing the 2D hydrogen bonding network (grey dashed lines). Hydrogen atoms and minor-occupancy oxygen atoms (O6B, O7B and O8B) of the disordered perchlorate anion are omitted for clarity.

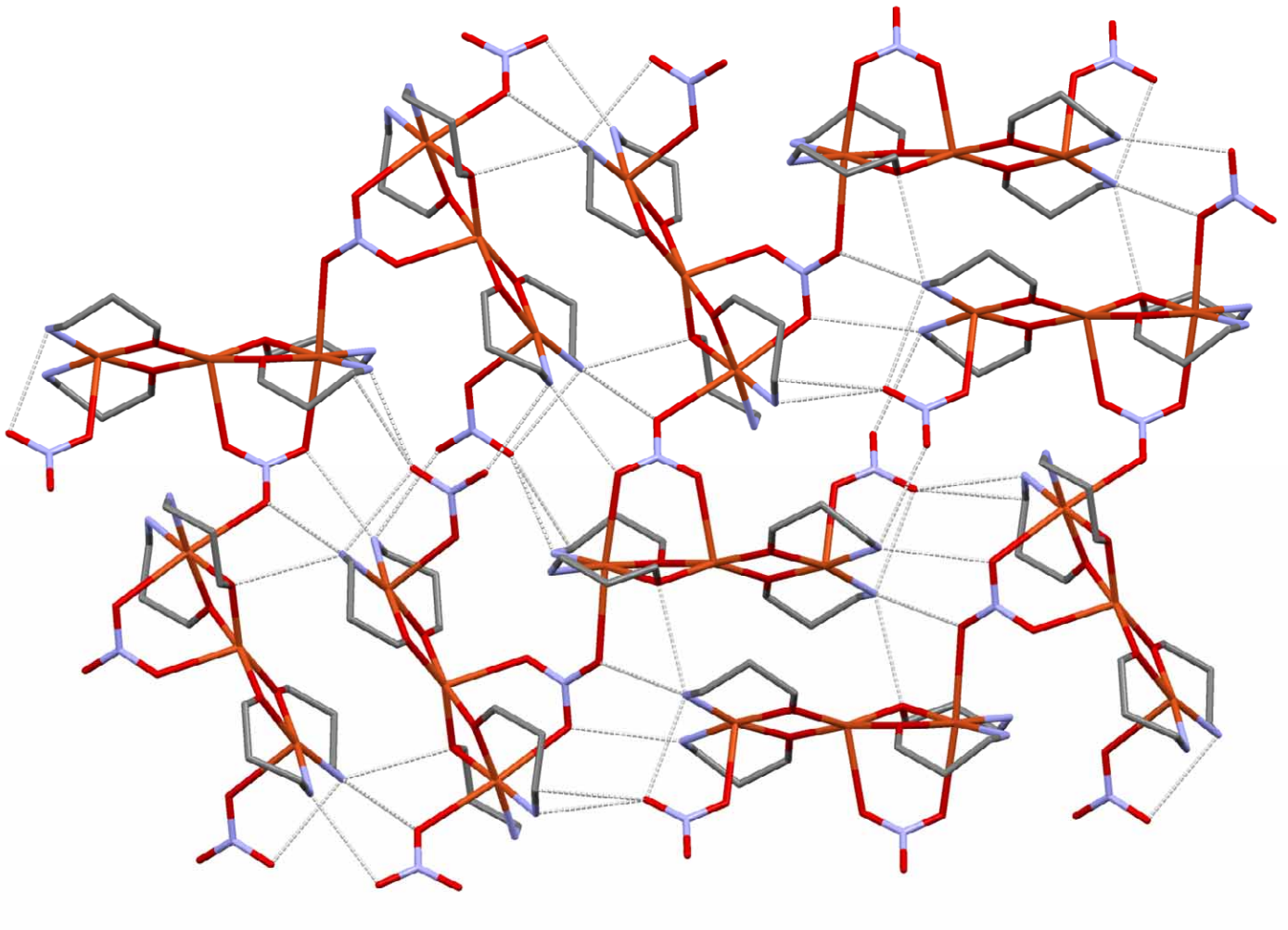

Fig. S2 The partial crystal packing diagram of **2** showing 1D polymeric chains and the extended 2D hydrogen bonding network (grey dashed lines). Hydrogen atoms are omitted for clarity.

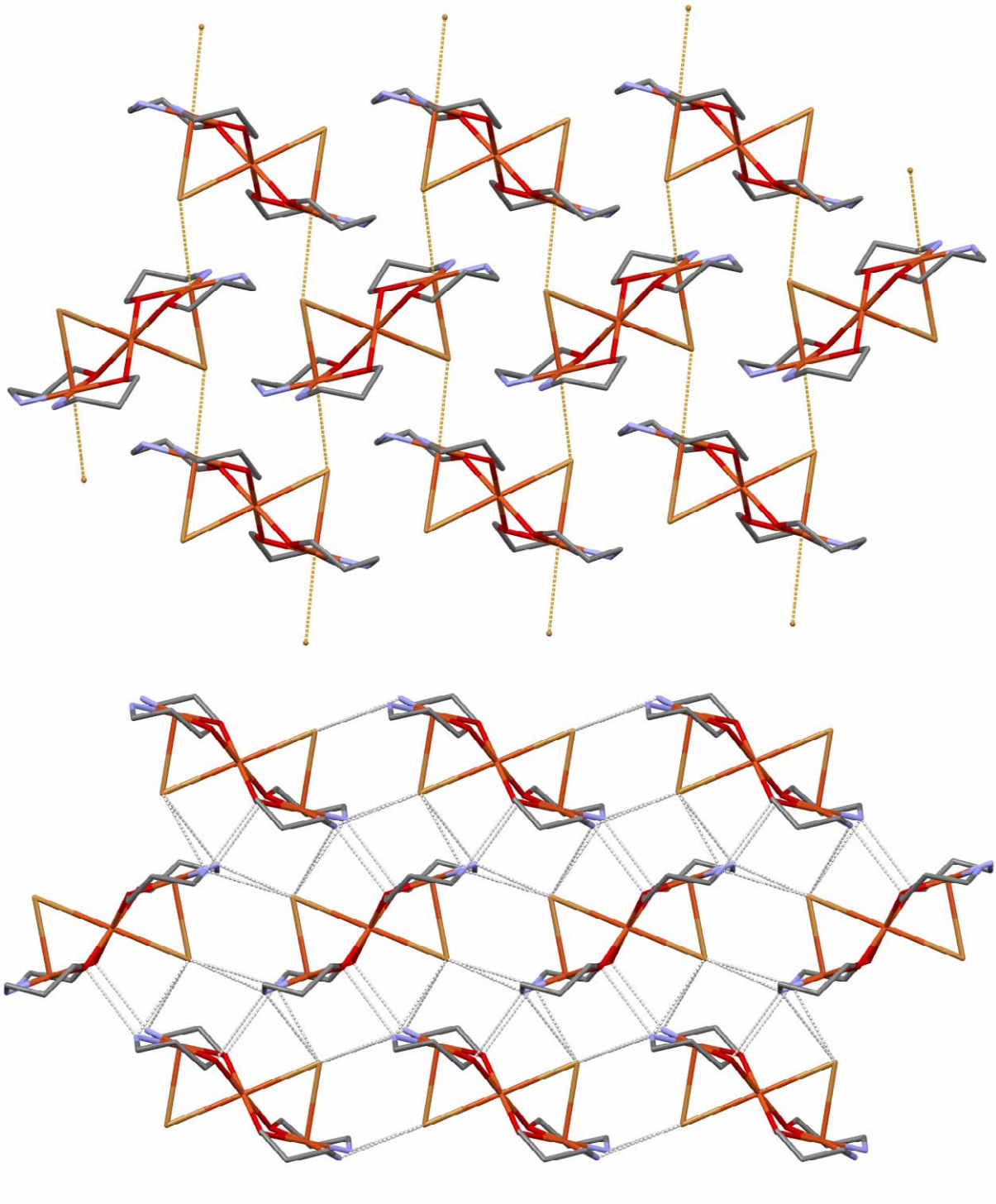

Fig. S3 The partial crystal packing diagram of **3** showing weak Cu···Br interactions (yellow dashed lines) forming the 2D layer (top) and the 2D hydrogen bonding network (bottom, grey dashed lines). Hydrogen atoms are omitted for clarity.

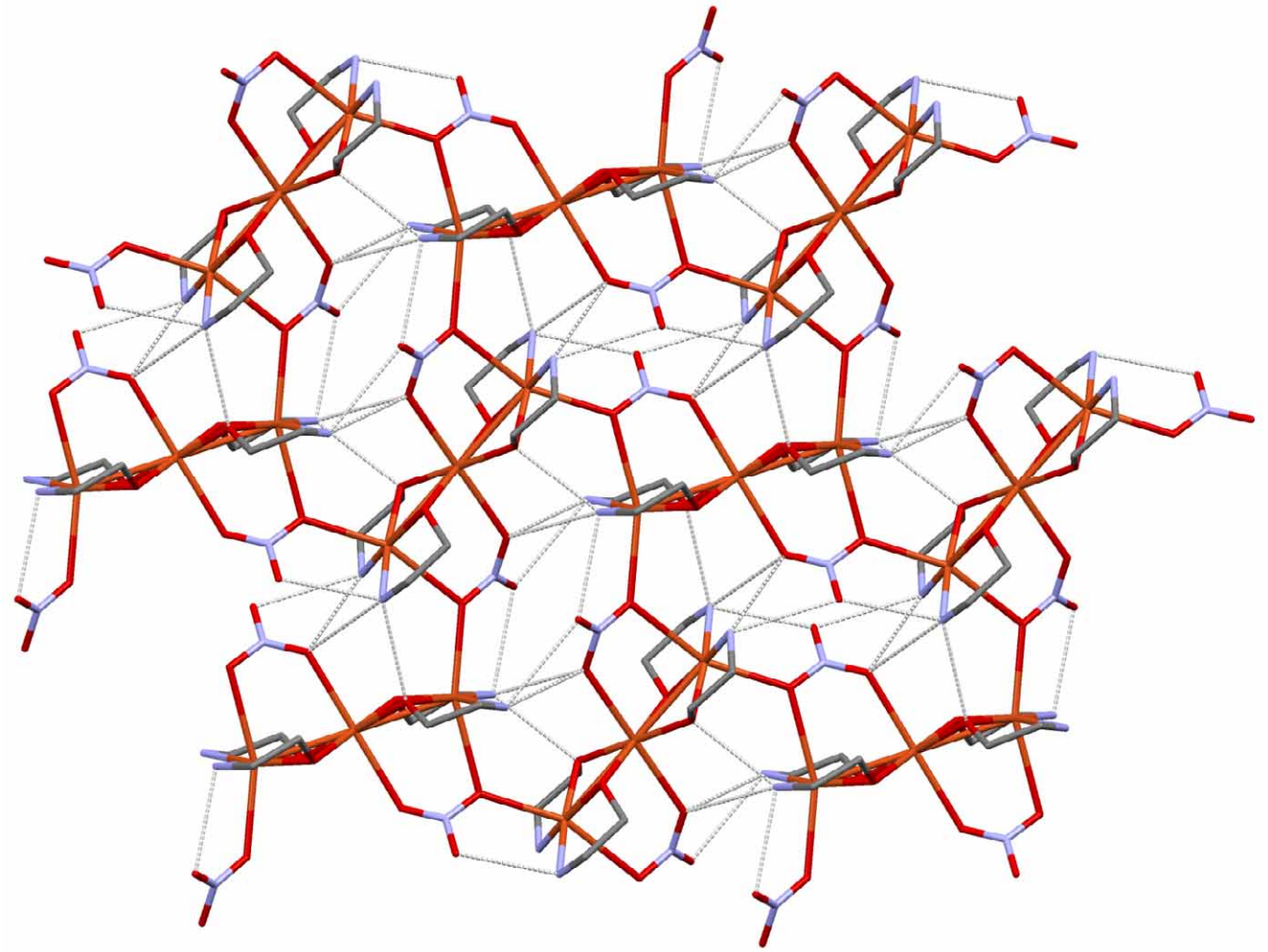

Fig. S4 The partial crystal packing diagram of **4** showing the 2D layer and the 2D hydrogen bonding network (grey dashed lines). Hydrogen atoms are omitted for clarity.