Electronic Supplementary Information for Dalton Transactions

Synthesis, structure and magnetic properties of polynuclear copper(II) complexes incorporating p-block oxo-anions

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Electronic Supporting Information

Table S1. Parameters of hydrogen bonding interactions within **1**and **2.**

Compound 1:

D-H	d(H..A)	d(D..A)	<DHA
O1-H1O…O11	1.838	2.754(4)	161
O1-H1O…O13	2.509	3.010(5)	112
O2-H2O…O21	2.011	2.822(4)	160
O1W-H1W1…O5W^{i}	1.912	2.768(4)	174
O1W-H1W2…O12	1.792	2.685(4)	170
O2W-H2W1…O2^{ii}	1.902	2.778(3)	165
O2W-H2W2…OW6	2.114	2.729(4)	164
O3W-H3W1…O1	1.818	2.730(3)	153
O3W-H3W2…O13^{iii}	1.968	2.852(3)	141
O4W-H4W1…O23	1.742	2.724(3)	170
O4W-H4W2…O2W^{iv}	1.848	2.813(5)	160
O5W-H5W1…O8W	2.108	2.737(4)	158
O5W-H5W2…O2W	1.841	2.792(3)	170
O6W-H6W1…O7W^{ii}	1.792	2.742(5)	172
O6W-H6W2…O1W	1.839	2.798(3)	172
O7W-H7W1…O1W	1.884	2.826(4)	156
O7W-H7W2…O21	1.743	2.762(4)	158
O8W-H8W1…O11W^{iii}	2.056	2.756(5)	171
O8W-H8W2…O11	1.822	2.741(5)	161
O9W-H9W1…O4W^{v}	1.604	2.731(5)	170
O9W-H9W2…O3W^{vi}	1.704	2.785(4)	172
O10W-H101…O9W^{vii}	2.417	3.116(3)	161
O10W-H102…O9W	1.780	2.825(3)	166
O11W-H111…O10W^{i}	2.172	2.993(4)	166
O11W-H112…O10W^{vii}	1.946	2.867(5)	171

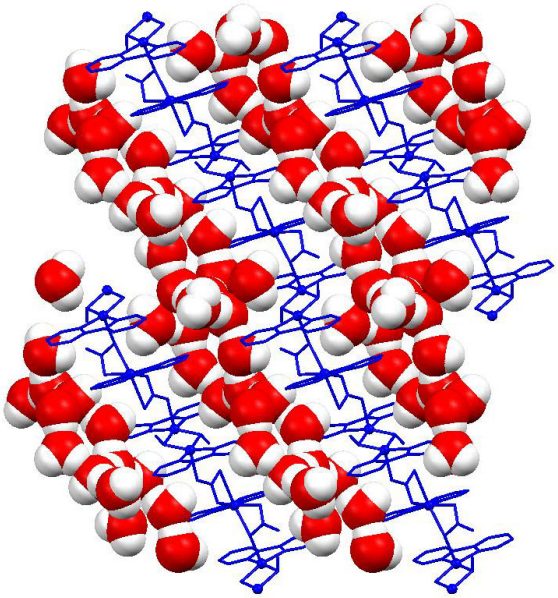
Symmetry codes:- i = x-1,y,z, ii= -x+1,-y+2,-z+1, iii = -x+1,-y+2,-z+2, iv = x-1,y-1,z, v = x+1,y,z, vi = -x+2,-y+2,-z+2, vii = -x+2,-y+1,-z+2

Compound 2:

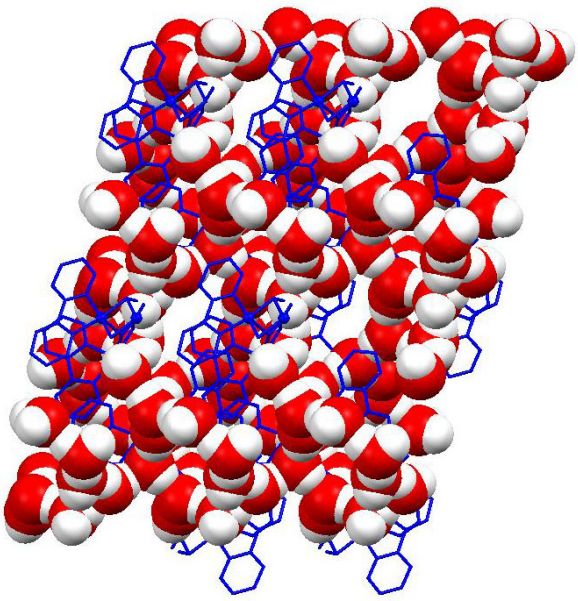
D-H	d(H..A)	d(D..A)	<DHA
O1-H1O…O14	2.19(3)	2.846(3)	163(3)
O2-H2O…O12^{i}	2.04(2)	2.738(2)	171(3)
O1W-H1W1…O14^{i}	1.89(2)	2.702(3)	173(3)
O1W-H1W2…O2W	1.89(3)	2.694(3)	170(3)
O2W-H2W1…O3W	1.99(4)	2.787(3)	172(3)
O2W-H2W2…O4W^{ii}	1.82(2)	2.672(2)	173(3)
O3W-H3W1…O12	1.98(2)	2.839(3)	173(3)
O3W-H3W2…O5W^{iii}	2.16(3)	2.866(3)	174(3)
O4W-H4W1…O13	2.05(4)	2.777(3)	161(3)
O4W-H4W2…O2	1.96(3)	2.744(3)	172(3)
O5W-H5W1…O2W	2.23(4)	2.984(2)	167(3)
O5W-H5W2…O1^{iv}	1.96(3)	2.802(3)	175(3)

Symmetry codes:- i = x,y,z-1, ii = x+1,y,z, iii = x+1,y,z-1, iv = x-1,y,z.

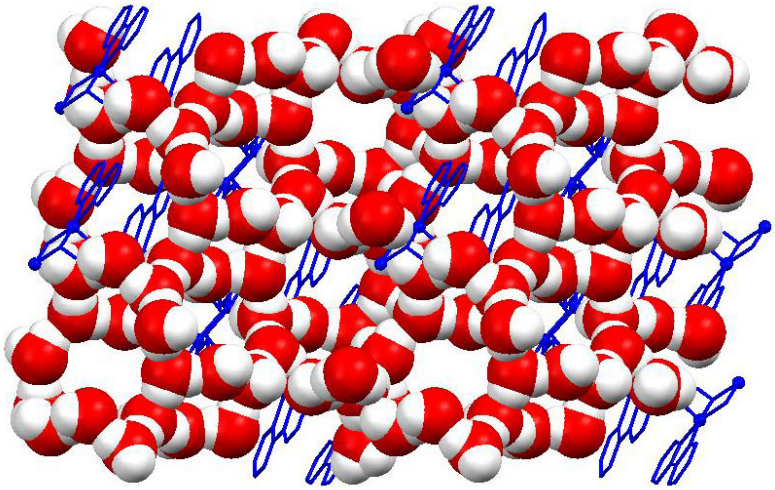
Fig S1. Selected views of the H-bonded water network that encapsulates **1** showing close contacts and π-π interactions. Hydrogen atoms, except those of the water molecules, omitted for clarity.



Viewed down the crystallographic a-axis

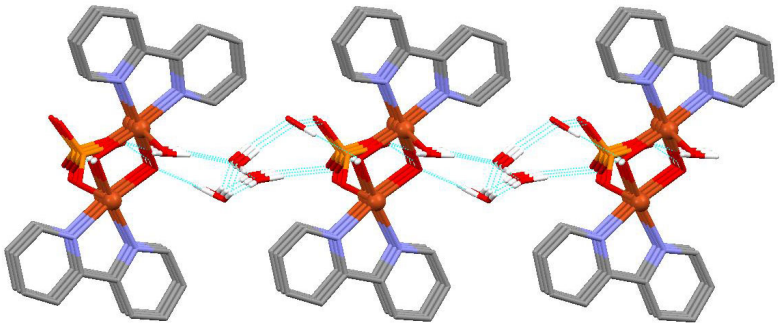


Viewed down the crystallographic c-axis

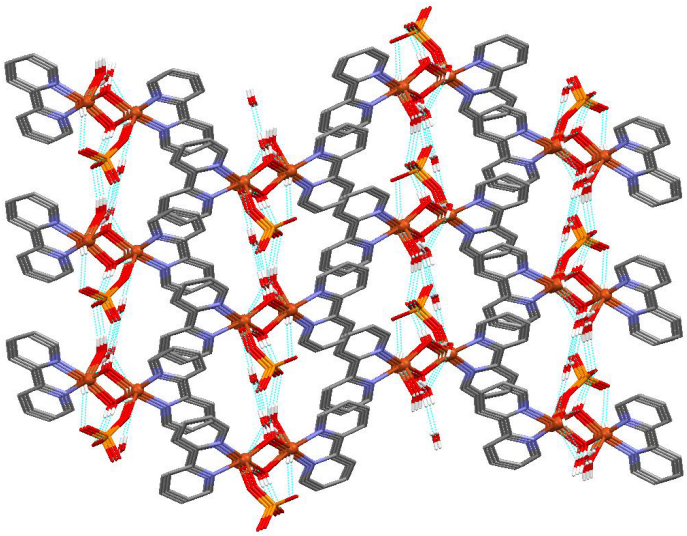


Viewed down the crystallographic b-axis

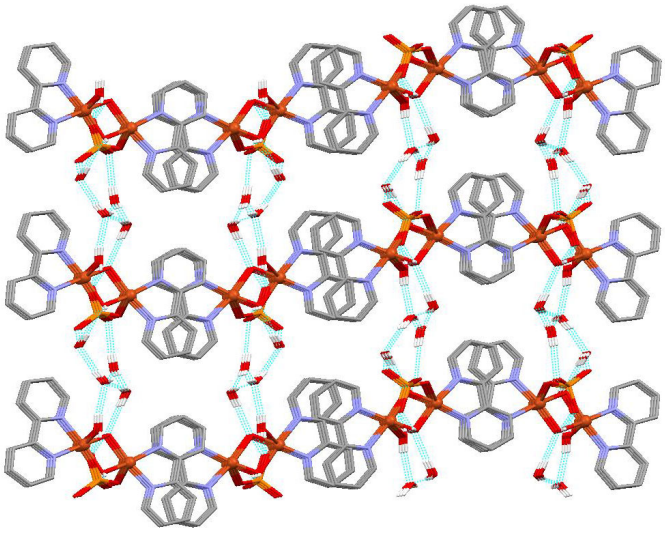
Fig S2. Selected views of the H-bonded chains in **2** showing close contacts and π-π interactions. Hydrogen atoms, except those of the water molecules, omitted for clarity.



Viewed down the crystallographic c-*axis*



Viewed down the crystallographic a-*axis*



Viewed down the crystallographic c-*axis*

Fig S3. Magnetization versus *H* plot for **2** and **4** at 2.0 K: (o) and (Δ) experimental data; (—) the Brillouin function for a magnetically isolated triplet with $g = 2.10$.