Pyrophosphate-mediated magnetic interactions in Cu(II) coordination complexes

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Supplementary Information

- **Figure S1.** Crystal packing of **1a** and **1b** along the *a* axis.
- **Figure S1.** Crystal packing of **2** along the *a* axis.
- **Table S1.** Selected bond lengths (Å) and angles (°) for compounds **1a/1b**.
- **Table S2.** Selected bond lengths (Å) and angles (°) for compound **2**.
- **Table S3.** H-bond interactions in compound **2**.
- **Table S4.** Selected bond lengths (Å) and angles (°) for compound **3**.

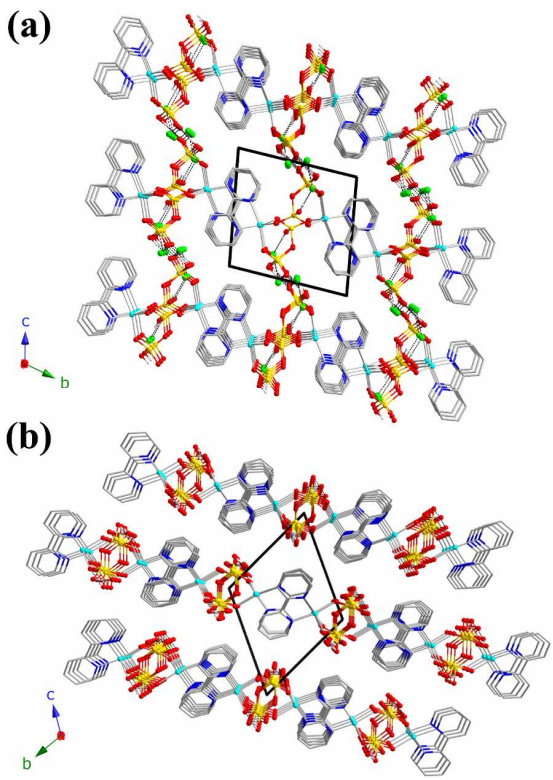

Figure S1. Perspective view of the crystal packing of **1a (a)** and **1b (b)** along the respective crystallographic *a* axis. The hydrogen atoms on the bipy ligands have been omitted for clarity. The water molecules of crystallization in the packing of **1a** have been highlighted as green spheres.

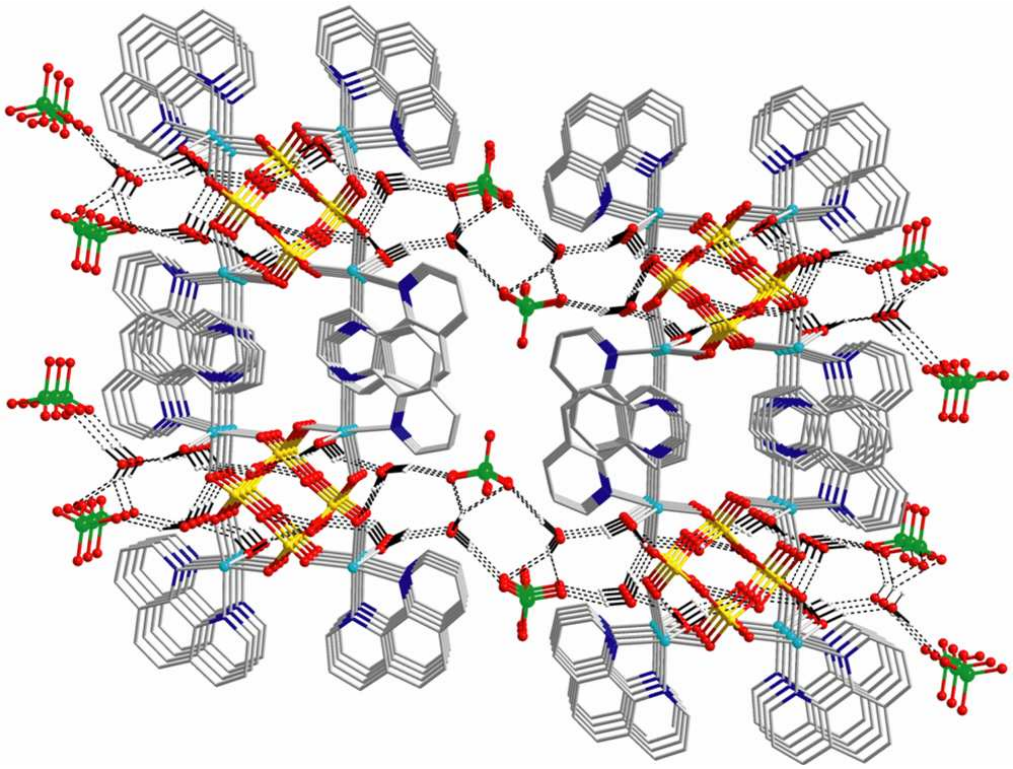

Figure S2. Perspective view of the crystal packing of **2** along the crystallographic *a* axis. The hydrogen atoms on the phen ligands have been omitted for clarity. The hydrogen bonds are depicted as dashes lines.

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

compound 1a		***compound 1b***	
Cu(1)-O(1)	1.922(2)	Cu(1)-O(1)	1.944(2)
Cu(1)-O(5)	1.972(2)	Cu(1)-O(5)	1.951(2)
Cu(1)-N(1)	2.004(2)	Cu(1)-N(1)	1.991(2)
Cu(1)-N(2)	1.997(2)	Cu(1)-N(2)	1.990(2)
Cu(1)-O(2a)	2.172(2)	Cu(1)-O(2a)	2.274(2)
Cu(1)···Cu(1a)	2.172(2)	Cu(1)···Cu(1a)	2.274(2)
O(1)-Cu(1)-O(5)	94.10(7)	O(1)-Cu(1)-O(5)	90.45(8)
O(1)-Cu(1)-N(1)	89.96(8)	O(1)-Cu(1)-N(1)	93.43(9)
O(1)-Cu(1)-N(2)	164.89(8)	O(1)-Cu(1)-N(2)	166.95(9)
O(1)-Cu(1)-O(2a)	99.95(7)	O(5)-Cu(1)-N(1)	164.37(9)
O(5)-Cu(1)-N(1)	164.96(8)	O(5)-Cu(1)-N(2)	91.42(9)
O(5)-Cu(1)-N(2)	91.84(8)	O(5)-Cu(1)-O(2a)	93.72(8)
O(5)-Cu(1)-O(2a)	92.61(7)	N(1)-Cu(1)-N(2)	81.5(1)
N(1)-Cu(1)-N(2)	80.94(8)	O(1)-Cu(1)-O(2a)	94.98(8)
N(1)-Cu(1)-O(2a)	100.96(7)	N(1)-Cu(1)-O(2a)	101.00(8)
N(2)-Cu(1)-O(2a)	93.65(7)	N(2)-Cu(1)-O(2a)	97.78(8)

Table S2. Selected bond lengths (Å) and angles (°) for compound **2**.

Cu(1)-O(1)	1.940(2)	Cu(2)-O(3)	1.932(2)
Cu(1)-O(5)	1.929(2)	Cu(2)-O(6a)	1.934(2)
Cu(1)-N(1)	2.024(2)	Cu(2)-N(3)	2.016(2)
Cu(1)-N(2)	2.016(2)	Cu(2)-N(4)	2.016(2)
Cu(1)-O(1w)	2.238(2)	Cu(2)-O(2w)	2.295(2)
Cu(1)···Cu(1a)	9.6778(8)	Cu(1)···Cu(2a)	6.1446(6)
Cu(1)···Cu(2)	6.0714(6)	Cu(2)···Cu(2a)	7.4552(7)
O(1)-Cu(1)-O(5)	96.52(7)	O(3)-Cu(2)-O(6a)	94.22(7)
O(1)-Cu(1)-N(1)	90.81(8)	O(3)-Cu(2)-N(3)	91.05(8)
O(1)-Cu(1)-N(2)	168.15(8)	O(3)-Cu(2)-N(4)	168.36(8)
O(1)-Cu(1)-O(1w)	96.03(7)	O(3)-Cu(2)-O(2w)	100.68(7)
O(5)-Cu(1)-N(1)	166.78(8)	O(6a)-Cu(2)-N(3)	169.01(7)
O(5)-Cu(1)-N(2)	89.56(8)	O(6a)-Cu(2)-N(4)	91.35(8)
O(5)-Cu(1)-O(1w)	98.97(7)	O(6a)-Cu(2)-O(2w)	94.08(7)
N(1)-Cu(1)-N(2)	81.38(8)	N(3)-Cu(2)-N(4)	81.82(8)
N(1)-Cu(1)-O(1w)	91.15(7)	N(3)-Cu(2)-O(2w)	94.41(7)
N(2)-Cu(1)-O(1w)	93.04(7)	N(4)-Cu(2)-O(2w)	89.09(7)

Table S3. Hydrogen bonding interactions [bond lengths (Å) and angles (°)] in compound **2**.

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(3)-H(3P)···O(7b)	0.82	1.66	2.461(2)	163.7
O(1w)-H(1w)···O(7b)	0.95(1)	1.92(1)	2.822(2)	159(3)
O(1w)-H(2w)···O(3wc)	0.94(1)	2.00(2)	2.871(3)	153(3)
O(2w)-H(3w)···O(4w)	0.94(1)	1.86(1)	2.773(3)	162(3)
O(3w)-H(5w)···O(8d)	0.95(1)	2.06(2)	2.957(3)	157(3)
O(3w)-H(6w)···O(6)	0.94(1)	1.79(1)	2.733(2)	174(3)
O(4w)-H(7w)···O(11c)	0.95(1)	1.97(1)	2.914(5)	173(3)
O(4w)-H(8w)···O(8e)	0.95(1)	2.19(2)	3.016(4)	145(3)

Table S4. Selected bond lengths (Å) and angles (°) for compound **3**.

Cu(1)-O(1)	1.915(4)	Cu(2)-O(2)	1.971(5)
Cu(1)-O(5)	1.933(5)	Cu(2)-O(6)	1.977(5)
Cu(1)-N(1)	1.998(5)	Cu(2)-N(4)	1.995(5)
Cu(1)-N(2)	1.995(6)	Cu(2)-N(5)	2.009(5)
Cu(1)-N(6b)	2.558(5)	Cu(2)-O(6a)	2.202(5)
Cu(1)···Cu(1a)	8.765(3)	Cu(2)···Cu(2a)	3.196(2)
Cu(1)···Cu(2)	4.999(2)		
O(1)-Cu(1)-O(5)	96.9(2)	O(2)-Cu(2)-O(6)	92.5(2)
O(1)-Cu(1)-N(1)	89.8(2)	O(2)-Cu(2)-N(4)	90.0(2)
O(1)-Cu(1)-N(2)	170.3(2)	O(2)-Cu(2)-N(5)	153.8(2)
O(1)-Cu(1)-N(6b)	90.8(2)	O(2)-Cu(2)-O(6a)	98.9(2)
O(5)-Cu(1)-N(1)	169.3(2)	O(6)-Cu(2)-N(4)	172.5(2)
O(5)-Cu(1)-N(2)	90.4(2)	O(6)-Cu(2)-N(5)	92.3(2)
O(5)-Cu(1)-N(6b)	97.3(2)	N(4)-Cu(2)-N(5)	82.4(2)
N(1)-Cu(1)-N(2)	82.1(2)	N(4)-Cu(2)-O(6a)	106.3(2)
N(1)-Cu(1)-N(6b)	91.0(2)	N(5)-Cu(2)-O(6a)	107.3(2)
N(2)-Cu(1)-N(6b)	94.8(2)	O(6)-Cu(2)-O(6a)	80.4(2)