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Electronic Supplementary Information

Supramolecular architectures based on transition metal complexes with 1-(3-pyridyl)-2-(4'-pyrimidyl)ethene

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1. Topologic analysis of the 3D structure of 2.

Four independent sets of nodes can be identified in the 3D structure of **2**: the metal coordination sphere, the two independent organic ligands, and the lattice water molecule. The metal coordination sphere can be regarded as a 7-connecting node: each is connected to five organic molecules (through two M-N coordination bonds and three O-H···N hydrogen bonds) and two lattice water molecules (through O-H···O5 hydrogen bonds). The two independent organic ligands can both be regarded as 3-connecting nodes: one is connected to three metal ions through M-N and O-H···N bonds, and the other is connected to two metal nodes (through M-N and an O-H···N bonds) and a lattice water molecule (through O-H···N). The lattice water molecule (O5) is also a 3-connecting node: each is connected to two metal nodes through O-H(coordinated water)··· O5, and it is also hydrogen bonded to an organic node through O-H···N. Therefore, the 3D structure exhibits an unusual type of tetranodal 3,7-connecting net topology (Fig. S1, omitting the purple links between the metal nodes), which has a long Schläfli symbol: $(4^3)(4^16^2)(6^28)(4^46^78^{10})$.

The perchlorate ion has been omitted for simplicity in the above analysis. If the perchlorate ion hydrogen-bonded to two coordinated water molecules from different metal ions is considered as a linker between the metal nodes, the 3D structure can be regarded as a 3,9-connecting net (Fig. S1). The Schläfli symbol can be derived as $(4^3)(4^1\,6^2)(3^1\,6^2)(3^24^46^78^{23})$.

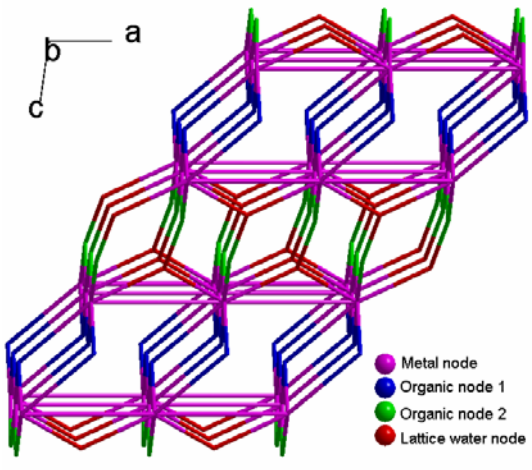

Fig. S1. The 3,9-connecting 3D net in **2**, with four different nodes.

2. Tabulated structural parameters for compounds 1-7.

Table S1. Selected bond lengths (Å) and angles (°) for Compounds **1** and **6**.

Compound	**1** (M = Cd)	**6** (M = Cu)
M1-O1	2.346(2)	2.358(4)
M1-O2	2.307(2)	2.001(4)
M1-N1	2.2843(18)	2.020(4)
O1-M1-O2	90.17(9)	90.21(16)
O1-M1-N1	88.15(8)	90.56(16)
O1-M1-O2a	89.83(9)	89.79(16)
O1-M1-N1a	91.85(8)	89.44(16)
O2-M1-N1	87.46(7)	91.44(16)
O2-M1-N1a	92.54(7)	88.56(16)
O1-M1-O1a	180.0	180.0
O2-M1-O2a	180.0	180.0
N1-M1-N1a	180.0	180.0
Symmetry codes: a = -x+1,-y+2,-z for **1**, and -x,-y+1,-z for **6**.		

Table S2. Selected bond lengths (Å) and angles (°) for Compounds **2**-**5**.

Compound	**2** (M = Mn)	**3** (M = Co)	**4** (M = Ni)	**5** (M = Zn)
M1-O1	2.177(6)	2.108(4)	2.076(5)	2.127(3)
M1-O2	2.178(5)	2.096(4)	2.060(5)	2.108(3)
M1-O3	2.193(6)	2.104(5)	2.088(5)	2.145(3)
M1-O4	2.180(6)	2.090(4)	2.075(5)	2.114(3)
M1-N1	2.261(6)	2.132(5)	2.086(5)	2.131(3)
M1-N4	2.275(6)	2.137(5)	2.100(5)	2.139(3)
O1-M1-O2	176.0(3)	178.43(18)	178.1(2)	178.07(12)
O1-M1-O3	94.4(3)	91.6(2)	90.0(2)	91.21(16)
O1-M1-O4	89.2(3)	90.8(2)	92.4(2)	91.07(16)
O1-M1-N1	87.9(2)	88.45(18)	87.5(2)	87.66(14)
O1-M1-N4	90.1(2)	89.52(18)	90.3(2)	89.84(14)
O2-M1-O3	89.2(2)	89.21(17)	89.5(2)	89.42(14)
O2-M1-O4	87.3(2)	88.42(17)	88.2(2)	88.32(14)
O2-M1-N1	90.4(2)	90.21(17)	90.7(2)	90.54(13)
O2-M1-N4	91.8(2)	91.85(17)	91.5(2)	91.99(13)
O3-M1-O4	176.5(2)	177.59(17)	177.5(2)	177.67(13)
O3-M1-N1	87.8(2)	88.01(18)	87.8(2)	87.54(13)
O3-M1-N4	88.7(2)	89.73(18)	90.7(2)	89.74(13)
O4-M1-N1	92.7(2)	92.46(18)	93.1(2)	93.03(13)
O4-M1-N4	91.0(2)	89.88(18)	88.5(2)	89.79(13)
N1-M1-N4	175.8(2)	176.92(19)	177.3(2)	176.27(13)

Table S3. Selected bond lengths (Å) and angles (°) for Compound **7**.

Cu1-O1	2.0099(17)	Cu2-O4	1.944(3)
Cu1-N1	2.026(2)	Cu2-O5	1.949(3)
Cu1-O2	2.2953(19)	Cu2-N2	2.0874(19)
		Cu2-O3	2.2946(19)
O1-Cu1-O1a	180.00(8)	O3-Cu2-O3b	177.74(11)
O1-Cu1-O2	91.35(8)	O3-Cu2-O4	91.13(5)
O1-Cu1-O2a	88.65(8)	O3-Cu2-O5	88.87(5)
O1-Cu1-N1	88.36(8)	O3-Cu2-N2	91.50(7)
O1-Cu1-N1a	91.64(8)	O3-Cu2-N2b	88.49(7)
N1-Cu1-N1a	180.0	N2-Cu2-N2b	179.62(12)
N1-Cu1-O2	87.37(8)	N2-Cu2-O4	90.19(6)
N1-Cu1-O2a	92.63(8)	N2-Cu2-O5	89.81(6)
O2-Cu1-O2a	180.0	O4-Cu2-O5	180.0

Symmetry codes: a = -x+1,-y+1,-z+1, b = -x,y,-z+1/2.

Table S4. Hydrogen bond lengths (Å) and angles (°) for Compound **3-5**.

D	A [transformation]	d(D-H)	d(H...A)	d(D...A)	<(DHA)
3					
O1	O5	0.85(3)	1.84(3)	2.673(6)	167(7)
O1	O13	0.82(3)	2.41(7)	2.926(7)	122(7)
O2	O5 [x-1,y,z]	0.85(3)	1.90(3)	2.739(7)	167(6)
O2	N3 [-x,-y+1,-z+1]	0.82(3)	2.06(3)	2.860(6)	162(6)
O3	N2 [x,y+1,z]	0.82(3)	2.01(3)	2.797(6)	161(6)
O3	O7	0.85(3)	2.04(4)	2.843(7)	157(5)
O4	N5 [x,y-1,z]	0.84(3)	1.95(3)	2.773(6)	166(5)
O4	O10 [x-1,y,z]	0.83(3)	1.99(4)	2.760(6)	154(6)
O5	O8	0.81(3)	2.00(3)	2.782(7)	162(7)
O5	N6 [-x+1,-y+2,-z]	0.83(3)	1.93(3)	2.753(6)	172(7)
4					
O1	O5	0.86(3)	1.86(4)	2.689(7)	164(8)
O1	O13	0.82(3)	2.16(5)	2.906(10)	152(9)
O2	O5 [x-1,y,z]	0.85(3)	1.91(3)	2.748(7)	170(7)
O2	N3 [-x,-y+1,-z+1]	0.83(3)	2.05(3)	2.860(7)	169(7)
O3	N2 [x,y+1,z]	0.81(3)	2.00(3)	2.803(7)	169(7)
O3	O7	0.82(3)	2.19(6)	2.834(9)	135(7)
O4	N5 [x,y-1,z]	0.85(3)	2.00(4)	2.791(7)	155(7)
O4	O10 [x-1,y,z]	0.84(3)	1.96(4)	2.781(8)	165(8)
O5	O8	0.85(3)	1.99(4)	2.798(9)	159(8)
O5	N6 [-x+1,-y+2,-z]	0.83(3)	1.94(3)	2.763(7)	171(8)
5					

O1	O5	0.84(3)	1.84(3)	2.680(5)	175(8)
O1	O13	0.82(3)	2.09(3)	2.898(7)	166(8)
O2	O5 [x-1,y,z]	0.83(3)	1.92(3)	2.737(5)	167(6)
O2	N3 [-x,-y+1,-z+1]	0.83(3)	2.05(3)	2.852(5)	162(6)
O3	N2 [x,y+1,z]	0.81(3)	2.05(4)	2.809(5)	157(6)
O3	O7	0.85(3)	2.09(4)	2.835(6)	145(5)
O4	N5 [x,y-1,z]	0.86(3)	1.96(3)	2.786(5)	162(6)
O4	O10 [x-1,y,z]	0.83(3)	2.04(4)	2.788(6)	151(6)
O5	O8	0.82(3)	2.03(4)	2.814(6)	159(6)
O5	N6 [-x+1,-y+2,-z]	0.83(3)	1.94(3)	2.759(5)	170(6)

D = donor, A = acceptor.