Supporting materials

Structural Diversity of the Mixed-Ligand System Mn-cpdba-2,2′-bpy Controlled by Temperature

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Table S1. Selected bond lengths (Å) and angles (deg) for **1**.

Mn(1)-O(4)#1	2.0772(16)	Mn(1)-O(3)#2	2.1131(15)
Mn(1)-O(1)	2.1822(15)	Mn(1)-N(2)	2.2429(18)
Mn(1)-N(1)	2.2755(18)	Mn(1)-O(2)	2.3910(16)
O(4)#1-Mn(1)-O(3)#2	96.79(7)	O(4)#1-Mn(1)-O(1)	90.56(7)
O(3)#2-Mn(1)-O(1)	111.30(6)	O(4)#1-Mn(1)-N(2)	106.08(8)
O(3)#2-Mn(1)-N(2)	90.25(6)	O(1)-Mn(1)-N(2)	151.24(7)
O(4)#1-Mn(1)-N(1)	170.95(8)	O(3)#2-Mn(1)-N(1)	92.15(6)
O(1)-Mn(1)-N(1)	87.46(7)	N(2)-Mn(1)-N(1)	72.40(7)
O(4)#1-Mn(1)-O(2)	80.49(7)	O(3)#2-Mn(1)-O(2)	168.26(6)
O(1)-Mn(1)-O(2)	57.55(6)	N(2)-Mn(1)-O(2)	101.48(6)
N(1)-Mn(1)-O(2)	91.01(6)		

Symmetry codes: #1 x+1,-y+1/2,z+1/2; #2 -x+1,y-1/2,-z+1/2.

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

Mn(1)-O(4)#1	2.150(3)	Mn(1)-O(4)#2	2.150(3)
Mn(1)-O(9)	2.152(3)	Mn(1)-O(9)#3	2.152(3)
Mn(1)-O(1)	2.234(3)	Mn(1)-O(1)#3	2.234(3)
Mn(2)-O(10)#3	2.081(3)	Mn(2)-O(3)#1	2.166(3)
Mn(2)-N(21)	2.221(4)	Mn(2)-O(1)	2.242(3)
Mn(2)-N(4)	2.249(4)	Mn(2)-O(2)	2.423(4)
Mn(3)-O(1W)	2.139(6)	Mn(3)-O(12)	2.268(7)
Mn(3)-O(2W)	2.295(10)	Mn(3)-O(12)#4	2.333(7)
Mn(3)-O(8W)#5	2.359(10)	Mn(3)-O(1W)#4	2.416(6)
O(4)#1-Mn(1)-O(4)#2	180.0(2)	O(4)#1-Mn(1)-O(9)	92.71(15)
O(4)#2-Mn(1)-O(9)	87.29(15)	O(4)#1-Mn(1)-O(9)#3	87.29(15)
O(4)#2-Mn(1)-O(9)#3	92.71(15)	O(9)-Mn(1)-O(9)#3	180.00(18)
O(4)#1-Mn(1)-O(1)	83.48(13)	O(4)#2-Mn(1)-O(1)	96.52(13)

O(9)-Mn(1)-O(1)	89.95(12)	O(9)#3-Mn(1)-O(1)	90.05(12)
O(4)#1-Mn(1)-O(1)#3	96.52(13)	O(4)#2-Mn(1)-O(1)#3	83.48(13)
O(9)-Mn(1)-O(1)#3	90.05(12)	O(9)#3-Mn(1)-O(1)#3	89.95(12)
O(1)-Mn(1)-O(1)#3	180.00(15)	O(10)#3-Mn(2)-O(3)#1	84.82(14)
O(10)#3-Mn(2)-N(21)	102.29(15)	O(3)#1-Mn(2)-N(21)	90.57(15)
O(10)#3-Mn(2)-O(1)	96.21(13)	O(3)#1-Mn(2)-O(1)	118.33(13)
N(21)-Mn(2)-O(1)	147.02(13)	O(10)#3-Mn(2)-N(4)	173.56(15)
O(3)#1-Mn(2)-N(4)	99.80(14)	N(21)-Mn(2)-N(4)	73.33(15)
O(1)-Mn(2)-N(4)	85.59(13)	O(10)#3-Mn(2)-O(2)	90.79(14)
O(3)#1-Mn(2)-O(2)	172.24(14)	N(21)-Mn(2)-O(2)	96.62(14)
O(1)-Mn(2)-O(2)	55.73(12)	N(4)-Mn(2)-O(2)	85.11(15)
O(1W)-Mn(3)-O(12)	81.0(2)	O(1W)-Mn(3)-O(2W)	89.6(3)
O(12)-Mn(3)-O(2W)	136.6(3)	O(1W)-Mn(3)-O(12)#4	80.9(2)
O(12)-Mn(3)-O(12)#4	126.11(18)	O(2W)-Mn(3)-O(12)#4	93.4(3)
O(1W)-Mn(3)-O(8W)#5	134.3(3)	O(12)-Mn(3)-O(8W)#5	88.1(3)
O(2W)-Mn(3)-O(8W)#5	68.6(3)	O(12)#4-Mn(3)-O(8W)#5	137.5(3)
O(1W)-Mn(3)-O(1W)#4	125.92(16)	O(12)-Mn(3)-O(1W)#4	76.6(2)
O(2W)-Mn(3)-O(1W)#4	138.2(3)	O(12)#4-Mn(3)-O(1W)#4	74.2(2)
O(8W)#5-Mn(3)-O(1W)#4	93.6(3)		

Symmetry codes: #1 x-1/2,-y+1/2,z-1/2; #2 -x+3/2,y+1/2,-z+1/2; #3 -x+1,-y+1,-z; #4 -x+1,-y,-z+1; #5 -x+3/2,y-1/2,-z+1/2.

Table S3. Selected bond lengths (Å) and angles (deg) for **4**.

Mn(1)-O(8)#1	2.083(2)	Mn(1)-O(2)	2.110(2)
Mn(1)-O(7)#2	2.208(3)	Mn(1)-O(1)#3	2.232(3)
Mn(1)-N(4)	2.284(3)	Mn(1)-N(5)	2.287(3)
O(1)-Mn(1)#4	2.232(2)	O(8)#1-Mn(1)-O(2)	109.28(9)
O(8)#1-Mn(1)-O(7)#2	88.68(10)	O(2)-Mn(1)-O(7)#2	97.29(10)
O(8)#1-Mn(1)-O(1)#3	101.65(11)	O(2)-Mn(1)-O(1)#3	88.59(10)
O(7)#2-Mn(1)-O(1)#3	165.77(8)	O(8)#1-Mn(1)-N(4)	89.81(11)
O(2)-Mn(1)-N(4)	160.70(10)	O(7)#2-Mn(1)-N(4)	85.66(10)
O(1)#3-Mn(1)-N(4)	84.62(10)	O(8)#1-Mn(1)-N(5)	161.27(10)
O(2)-Mn(1)-N(5)	89.18(10)	O(7)#2-Mn(1)-N(5)	85.75(10)
O(1)#3-Mn(1)-N(5)	81.37(10)	N(4)-Mn(1)-N(5)	71.96(10)

Symmetry codes: #1 x,y+1,z; #2 -x+3/2,y+1,z-1/2; #3 -x+3/2,y,z+1/2.

Table S4. Selected bond lengths (Å) and angles (deg) for **5**.

Mn(1)-O(33)	2.088(2)	Mn(1)-O(3)#1	2.185(2)
Mn(1)-N(5)	2.220(3)	Mn(1)-N(4)	2.253(3)
Mn(1)-O(2)	2.263(2)	Mn(1)-O(1)	2.399(2)
Mn(2)-O(10)	2.152(2)	Mn(2)-O(10)#2	2.152(2)

Mn(2)-O(4)#1	2.163(2)	Mn(2)-O(4)#3	2.163(2)
Mn(2)-O(2)	2.248(2)	Mn(2)-O(2)#2	2.248(2)
Mn(3)-O(17)	2.175(3)	Mn(3)-O(5)	2.202(4)
Mn(3)-O(11)	2.205(3)	Mn(3)-O(9)	2.238(3)
Mn(3)-N(9)	2.288(4)	Mn(3)-N(10)	2.350(4)
Mn(4)-O(27)#4	2.152(2)	Mn(4)-O(27)#5	2.152(2)
Mn(4)-O(19)#6	2.156(2)	Mn(4)-O(19)	2.156(2)
Mn(4)-O(25)	2.230(2)	Mn(4)-O(25)#6	2.230(2)
Mn(5)-O(20)	2.080(3)	Mn(5)-O(28)#4	2.161(2)
Mn(5)-N(15)	2.223(3)	Mn(5)-O(25)#6	2.236(2)
Mn(5)-N(14)	2.251(3)	Mn(5)-O(26)#6	2.471(3)
O(33)-Mn(1)-O(3)#1	84.88(10)	O(33)-Mn(1)-N(5)	103.07(11)
O(3)#1-Mn(1)-N(5)	88.23(10)	O(33)-Mn(1)-N(4)	173.58(11)
O(3)#1-Mn(1)-N(4)	100.33(10)	N(5)-Mn(1)-N(4)	73.55(12)
O(33)-Mn(1)-O(2)	94.25(10)	O(3)#1-Mn(1)-O(2)	121.46(9)
N(5)-Mn(1)-O(2)	147.04(10)	N(4)-Mn(1)-O(2)	86.25(10)
O(33)-Mn(1)-O(1)	91.74(10)	O(3)#1-Mn(1)-O(1)	175.76(10)
N(5)-Mn(1)-O(1)	95.03(10)	N(4)-Mn(1)-O(1)	83.22(10)
O(2)-Mn(1)-O(1)	56.17(8)	O(10)-Mn(2)-O(10)#2	180.00(13)
O(10)-Mn(2)-O(4)#1	86.64(10)	O(10)#2-Mn(2)-O(4)#1	93.36(10)
O(10)-Mn(2)-O(4)#3	93.36(10)	O(10)#2-Mn(2)-O(4)#3	86.64(10)
O(4)#1-Mn(2)-O(4)#3	180.000(1)	O(10)-Mn(2)-O(2)	90.45(9)
O(10)#2-Mn(2)-O(2)	89.55(9)	O(4)#1-Mn(2)-O(2)	82.59(9)
O(4)#3-Mn(2)-O(2)	97.41(9)	O(10)-Mn(2)-O(2)#2	89.55(9)
O(10)#2-Mn(2)-O(2)#2	90.45(9)	O(4)#1-Mn(2)-O(2)#2	97.41(9)
O(4)#3-Mn(2)-O(2)#2	82.59(9)	O(2)-Mn(2)-O(2)#2	180.00(9)
O(17)-Mn(3)-O(5)	84.26(12)	O(17)-Mn(3)-O(11)	141.14(13)
O(5)-Mn(3)-O(11)	80.40(12)	O(17)-Mn(3)-O(9)	81.87(11)
O(5)-Mn(3)-O(9)	135.75(15)	O(11)-Mn(3)-O(9)	84.68(12)
O(17)-Mn(3)-N(9)	126.21(12)	O(5)-Mn(3)-N(9)	137.48(13)
O(11)-Mn(3)-N(9)	87.52(13)	O(9)-Mn(3)-N(9)	82.55(14)
O(17)-Mn(3)-N(10)	80.76(12)	O(5)-Mn(3)-N(10)	90.87(14)
O(11)-Mn(3)-N(10)	134.60(12)	O(9)-Mn(3)-N(10)	127.55(14)
N(9)-Mn(3)-N(10)	69.34(13)	O(27)#4-Mn(4)-O(27)#5	180.00(15)
O(27)#4-Mn(4)-O(19)#6	92.41(10)	O(27)#5-Mn(4)-O(19)#6	87.59(10)
O(27)#4-Mn(4)-O(19)	87.59(10)	O(27)#5-Mn(4)-O(19)	92.41(10)
O(19)#6-Mn(4)-O(19)	180.00(12)	O(27)#4-Mn(4)-O(25)	95.25(9)
O(27)#5-Mn(4)-O(25)	84.75(9)	O(19)#6-Mn(4)-O(25)	89.49(9)
O(19)-Mn(4)-O(25)	90.52(9)	O(27)#4-Mn(4)-O(25)#6	84.75(9)
O(27)#5-Mn(4)-O(25)#6	95.25(9)	O(19)#6-Mn(4)-O(25)#6	90.51(9)
O(19)-Mn(4)-O(25)#6	89.48(9)	O(25)-Mn(4)-O(25)#6	180.00(6)
O(20)-Mn(5)-O(28)#4	84.90(10)	O(20)-Mn(5)-N(15)	101.19(11)
O(28)#4-Mn(5)-N(15)	92.96(10)	O(20)-Mn(5)-O(25)#6	98.19(10)
O(28)#4-Mn(5)-O(25)#6	115.68(9)	N(15)-Mn(5)-O(25)#6	146.65(10)

O(20)-Mn(5)-N(14)	173.06(11)	O(28)#4-Mn(5)-N(14)	99.10(10)
N(15)-Mn(5)-N(14)	73.06(12)	O(25)#6-Mn(5)-N(14)	85.24(10)
O(20)-Mn(5)-O(26)#6	89.46(10)	O(28)#5-Mn(5)-O(26)#6	168.21(10)
N(15)-Mn(5)-O(26)#6	98.29(10)	O(25)#6-Mn(5)-O(26)#6	54.90(9)
N(14)-Mn(5)-O(26)#6	87.60(11)		

Symmetry codes: #1 x, -y+1/2, z-1/2; #2 -x+1, -y+1, -z+1; #3 -x+1, y+1/2, -z+3/2; #4 -x, -y+1/2, -z-1/2; #5 x, -y+5/2, z-1/2; #6 -x, -y+3, -z-1.

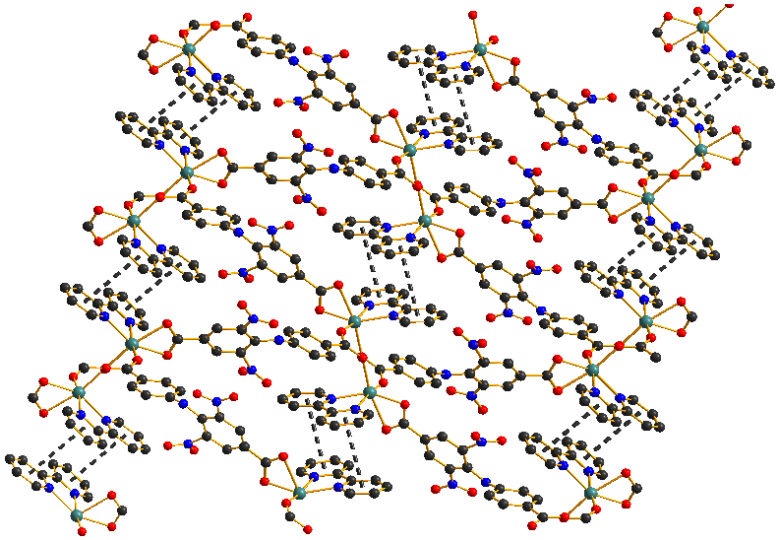

Fig S1. 3D supramolecular architecture of compound **1** with π–π stacking interactions (dashed lines).

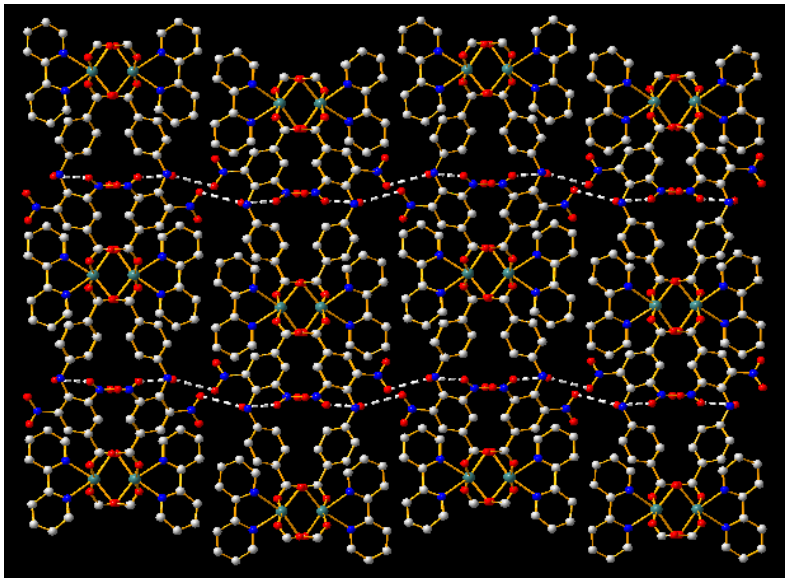

Fig S2. 3D supramolecular architecture of compound **4** with hydrogen bonds (dashed lines).