

Electronic Supplementary Information for

Copper(II) 5-methoxyisophthalate coordination polymers incorporating dipyridyl co-ligands: Syntheses, crystal structures, and magnetic properties

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

Cu(1)-O(2)	1.972(3)	N(2)-Cu(1)-N(1)#1	176.66(16)
Cu(1)-N(2)	2.017(4)	O(2)-Cu(1)-O(3)#2	149.14(14)
Cu(1)-N(1)#1	2.027(4)	N(2)-Cu(1)-O(3)#2	91.13(15)
Cu(1)-O(3)#2	2.057(3)	N(1)#1-Cu(1)-O(3)#2	89.79(15)
Cu(1)-O(1)#3	2.257(3)	O(2)-Cu(1)-O(1)#3	119.86(13)
O(2)-Cu(1)-N(2)	93.15(15)	N(2)-Cu(1)-O(1)#3	89.08(15)
O(2)-Cu(1)-N(1)#1	87.70(15)	N(1)#1-Cu(1)-O(1)#3	87.70(14)

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

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

Cu(1)-O(2)	1.948(6)	O(10)-Cu(1)-O(6)	157.7(3)
Cu(1)-O(4)#1	1.950(6)	O(2)-Cu(1)-N(1)	91.8(3)
Cu(1)-O(10)	2.002(6)	O(4)#1-Cu(1)-N(1)	97.6(3)
Cu(1)-O(6)	2.010(6)	O(10)-Cu(1)-N(1)	106.0(3)
Cu(1)-N(1)	2.144(8)	O(6)-Cu(1)-N(1)	96.3(3)
Cu(2)-O(9)	1.938(6)	O(9)-Cu(2)-O(7)	176.9(3)
Cu(2)-O(7)	1.947(6)	O(9)-Cu(2)-O(3)#1	90.4(3)
Cu(2)-O(3)#1	1.998(6)	O(7)-Cu(2)-O(3)#1	90.6(3)
Cu(2)-O(1)	2.013(6)	O(9)-Cu(2)-O(1)	89.8(3)
Cu(2)-O(12)	2.191(6)	O(7)-Cu(2)-O(1)	88.4(3)
O(2)-Cu(1)-O(4)#1	170.6(3)	O(3)#1-Cu(2)-O(1)	163.9(3)
O(2)-Cu(1)-O(10)	89.8(3)	O(9)-Cu(2)-O(12)	93.0(3)
O(4)#1-Cu(1)-O(10)	87.3(3)	O(7)-Cu(2)-O(12)	89.6(3)
O(2)-Cu(1)-O(6)	89.8(3)	O(3)#1-Cu(2)-O(12)	101.6(3)

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O(4)#1-Cu(1)-O(6)	89.6(3)	O(1)-Cu(2)-O(12)	94.4(3)
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Symmetry codes: #1 -x+1/2, -y+2, z+1/2.

Table S3. Selected bond lengths (Å) and angles (°) for **3**

Cu(1)-O(3)#1	1.970(2)	O(7)-Cu(1)-O(9)#2	164.65(11)
Cu(1)-O(1)	1.971(2)	O(3)#1-Cu(1)-N(1)	93.95(11)
Cu(1)-O(7)	1.972(2)	O(1)-Cu(1)-N(1)	97.94(11)
Cu(1)-O(9)#2	1.982(2)	O(7)-Cu(1)-N(1)	106.12(11)
Cu(1)-N(1)	2.147(3)	O(9)#2-Cu(1)-N(1)	88.96(11)
Cu(2)-O(4)#1	1.952(2)	O(4)#1-Cu(2)-O(6)	90.02(11)
Cu(2)-O(6)	1.963(2)	O(4)#1-Cu(2)-O(2)	168.04(10)
Cu(2)-O(2)	1.975(2)	O(6)-Cu(2)-O(2)	89.50(11)
Cu(2)-O(8)#2	1.984(2)	O(4)#1-Cu(2)-O(8)#2	88.58(11)
Cu(2)-O(11)	2.197(2)	O(6)-Cu(2)-O(8)#2	170.57(10)
O(3)#1-Cu(1)-O(1)	167.64(11)	O(2)-Cu(2)-O(8)#2	89.95(11)
O(3)#1-Cu(1)-O(7)	91.32(11)	O(4)#1-Cu(2)-O(11)	93.09(10)
O(1)-Cu(1)-O(7)	88.60(11)	O(6)-Cu(2)-O(11)	103.45(10)
O(3)#1-Cu(1)-O(9)#2	90.46(11)	O(2)-Cu(2)-O(11)	98.64(10)
O(1)-Cu(1)-O(9)#2	86.43(11)	O(8)#2-Cu(2)-O(11)	85.94(10)

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

Table S4. Selected bond lengths (Å) and angles (°) for **4**

Cu(1)-O(9)#1	1.958(3)	O(11)-Cu(2)-O(8)#1	87.81(13)
Cu(1)-O(7)	1.971(2)	O(2)-Cu(2)-O(8)#1	88.91(12)
Cu(1)-O(1)	1.978(3)	O(6)-Cu(2)-O(8)#1	164.27(11)
Cu(1)-O(12)	1.989(3)	O(11)-Cu(2)-N(3)	96.36(12)
Cu(1)-N(1)	2.157(3)	O(2)-Cu(2)-N(3)	93.14(12)
Cu(2)-O(11)	1.941(3)	O(6)-Cu(2)-N(3)	98.11(12)
Cu(2)-O(2)	1.955(3)	O(8)#1-Cu(2)-N(3)	97.60(11)
Cu(2)-O(6)	2.002(2)	O(11)-Cu(2)-Cu(1)	87.52(8)
Cu(2)-O(8)#1	2.016(3)	O(2)-Cu(2)-Cu(1)	83.03(8)
Cu(2)-N(3)	2.149(3)	O(6)-Cu(2)-Cu(1)	80.84(8)
Cu(3)-O(13)#2	1.953(3)	O(8)#1-Cu(2)-Cu(1)	83.55(8)
Cu(3)-O(3)	1.966(3)	N(3)-Cu(2)-Cu(1)	175.99(9)
Cu(3)-N(2)#3	2.001(4)	O(13)#2-Cu(3)-O(3)	179.37(13)
Cu(3)-N(4)#4	2.013(3)	O(13)#2-Cu(3)-N(2)#3	91.22(13)
O(9)#1-Cu(1)-O(7)	170.56(12)	O(3)-Cu(3)-N(2)#3	89.41(13)
O(9)#1-Cu(1)-O(1)	89.29(13)	O(13)#2-Cu(3)-N(4)#4	87.52(12)
O(7)-Cu(1)-O(1)	87.70(13)	O(3)-Cu(3)-N(4)#4	91.85(13)
O(9)#1-Cu(1)-O(12)	90.37(12)	N(2)#3-Cu(3)-N(4)#4	178.66(16)
O(7)-Cu(1)-O(12)	90.11(12)	O(1)-Cu(1)-N(1)	99.92(12)
O(1)-Cu(1)-O(12)	164.24(11)	O(12)-Cu(1)-N(1)	95.82(12)
O(9)#1-Cu(1)-N(1)	94.42(12)	O(11)-Cu(2)-O(2)	170.28(11)
O(7)-Cu(1)-N(1)	94.91(12)	O(11)-Cu(2)-O(6)	89.60(12)

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

Table S5. Selected bond lengths (Å) and angles (°) for **5**

Cu(1)-O(9)#1	1.924(3)	O(9)#1-Cu(1)-O(9)	86.83(13)
Cu(1)-O(1)	1.946(3)	O(1)-Cu(1)-O(9)	98.50(13)
Cu(1)-O(3)#2	1.959(4)	O(3)#2-Cu(1)-O(9)	100.61(15)
Cu(1)-O(7)	1.995(4)	O(7)-Cu(1)-O(9)	79.08(15)
Cu(1)-O(9)	2.350(4)	O(9)-Cu(2)-O(4)#3	94.03(14)
Cu(2)-O(9)	1.908(3)	O(9)-Cu(2)-O(2)	90.32(14)
Cu(2)-O(4)#3	1.957(3)	O(4)#3-Cu(2)-O(2)	168.42(15)
Cu(2)-O(2)	1.981(3)	O(9)-Cu(2)-N(1)	175.56(17)
Cu(2)-N(1)	1.998(4)	O(4)#3-Cu(2)-N(1)	87.58(16)
Cu(2)-O(7)	2.400(4)	O(2)-Cu(2)-N(1)	87.34(16)
O(9)#1-Cu(1)-O(1)	174.65(15)	O(9)-Cu(2)-O(7)	79.46(15)
O(9)#1-Cu(1)-O(3)#2	94.60(14)	O(4)#3-Cu(2)-O(7)	89.74(14)
O(1)-Cu(1)-O(3)#2	83.98(15)	O(2)-Cu(2)-O(7)	101.62(14)
O(9)#1-Cu(1)-O(7)	92.13(15)	N(1)-Cu(2)-O(7)	104.71(17)
O(1)-Cu(1)-O(7)	89.38(16)	O(3)#2-Cu(1)-O(7)	173.23(15)

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

Table S6. Hydrogen-bonding geometries of complexes **1-5**

D-H...A	d(D-H)	d(H...A)	d(D...A)	∠(DHA)
1				
O(6)-H(2W)...O(3)#1	0.86	2.12	2.91(2)	152.6
O(6)-H(1W)...O(3)	0.84	2.06	2.88(2)	166.3
2				
O(12)-H(2W)...O(1) #2	0.86	2.27	3.000(10)	143.3
O(12)-H(1W)...O(7) #2	0.85	2.54	3.240(10)	140.9
O(12)-H(1W)...O(1)	0.85	2.61	3.088(9)	117.5
3				
O(11)-H(1W)...O(10) #3	0.82	2.37	3.122(4)	152.3
O(11)-H(2W)...N(2) #4	0.83	1.96	2.767(4)	165.8
O(11)-H(2W)...N(2') #4	0.83	2.02	2.845(14)	171.4
4				
O(16)-H(2W)...O(18)	0.84	2.12	2.840(8)	143.9
O(17)-H(4W)...O(16)	0.87	1.98	2.815(11)	161.2
O(16)-H(1W)...O(8)	0.85	2.41	3.255(6)	179.5
O(16)-H(1W)...O(11)#5	0.85	2.67	3.115(6)	114.5
O(18)-H(5W)...O(1)	0.84	2.33	3.107(7)	155.8
O(18)-H(5W)...O(7)	0.84	2.81	3.125(7)	104.2
5				
O(9)-H(9)...O(5)#6	0.98	1.95	2.848(5)	150.3

#1 -x+1,-y+1,-z+1; #2 -x,-y+2,-z+2; #3 -x+3/2,-y+1,z-1/2; #4 -x+3/2,-y,z-1/2; #5 x,-y,z-1/2; #6 x+1,y,z