Electronic Supplementary Information (ESI) for

Exploring the Structural Diversities and Magnetic Properties of Copper(II) and Manganese(II) Complexes Based on 5-Methoxyisophthalate and Flexible Bis(Imidazole) Ligands

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Table S1 Selected bond lengths (Å) and angles (º) for 1

Cu(1)-O(6)	1.9208(18)□	Cu(1)-O(6)#1	1.9288(17)□
Cu(1)-O(2)	1.9653(17)□	Cu(1)-N(1)	1.987(2)□
Cu(2)-O(4)#2	1.9537(17)□	Cu(2)-O(4)#3	1.9537(17)□
Cu(2)-O(1)	2.0105(17)	Cu(2)-O(1)#4	2.0105(17)□
O(6)-Cu(1)-O(6)#1	80.15(8)□	O(6)-Cu(1)-O(2)	94.47(7)□
O(6)#1-Cu(1)-O(2)	161.74(8)□	O(6)-Cu(1)-N(1)	170.43(9)□
O(6)#1-Cu(1)-N(1)	100.37(8)□	O(2)-Cu(1)-N(1)	87.84(8)□
O(4)#2-Cu(2)-O(4)#3	92.76(11)□	O(4)#2-Cu(2)-O(1)#4	173.99(7)□
O(4)#3-Cu(2)-O(1)#4	87.67(8)□	O(4)#2-Cu(2)-O(1)	87.67(8)□
O(4)#3-Cu(2)-O(1)	173.99(7)□	O(1)#4-Cu(2)-O(1)	92.54(11)

Symmetry transformations used to generate equivalent atoms: #1 –x + 1, –y, –z + 1; #2 –x + 1/2, y – 1/2, z; #3 x + 1/2, y – 1/2, –z + 1/2; #4 –x + 1, y, –z + 1/2.

Table S2 Selected bond lengths (Å) and angles (º) for 2

Cu(1)-N(4)#1	1.979(2)□	Cu(1)-N(1)	1.986(3)□
Cu(1)-O(4)#2	2.004(2)□	Cu(1)-O(1)	2.048(2)□
Cu(1)-O(3)#3	2.273(2)		
N(4)#1-Cu(1)-N(1)	175.10(10)□	N(4)#1-Cu(1)-O(4)#2	95.97(10)□
N(1)-Cu(1)-O(4)#2	87.00(9)□	N(4)#1-Cu(1)-O(1)	89.17(10)□
N(1)-Cu(1)-O(1)	90.15(9)□	O(4)#2-Cu(1)-O(1)	150.44(9)□
N(4)#1-Cu(1)-O(3)#3	90.48(10)□	N(1)-Cu(1)-O(3)#3	84.81(10)□
O(4)#2-Cu(1)-O(3)#3	110.63(8)□	O(1)-Cu(1)-O(3)#3	98.38(9)

Symmetry transformations used to generate equivalent atoms: #1 x + 1, y, z – 1; #2 x – 1, y + 1, z; #3 –x + 2, –y + 1, –z + 1.

Table S3 Selected bond lengths (Å) and angles (º) for 3

Cu(1)-O(1)	1.925(3)□	Cu(1)-O(3)#1	1.933(3)□
Cu(1)-N(4)#2	1.985(4)□	Cu(1)-N(1)	1.994(4)□
Cu(1)-O(6)	2.596(4)		
O(1)-Cu(1)-O(3)#1	148.57(13)□	O(1)-Cu(1)-N(4)#2	93.48(13)□
O(3)#1-Cu(1)-N(4)#2	91.10(13)□	O(1)-Cu(1)-N(1)	92.28(14)□
O(3)#1-Cu(1)-N(1)	88.57(13)□	N(4)#2-Cu(1)-N(1)	169.45(14)□
O(1)-Cu(1)-O(6)	111.57(13)□	O(3)#1-Cu(1)-O(6)	99.85(13)□
N(4)#2-Cu(1)-O(6)	81.25(14)□	N(1)-Cu(1)-O(6)	88.42(14)

Symmetry transformations used to generate equivalent atoms: #1 x + 1, y, z; #2 –x + 1, –y + 1, –z + 2.

Table S4 Selected bond lengths (Å) and angles (º) for 4

Mn(1)-O(6)	2.107(3)□	Mn(1)-O(6)#1	2.107(3)□
Mn(1)-O(4)#2	2.213(3)□	Mn(1)-O(4)#3	2.213(3)□
Mn(1)-O(1)#1	2.217(3)□	Mn(1)-O(1)	2.217(3)□
Mn(2)-O(13)	2.108(3)□	Mn(2)-O(7)	2.128(3)□
Mn(2)-O(25)	2.226(3)□	Mn(2)-O(4)#2	2.315(3)□
Mn(2)-O(2)	2.342(3)□	Mn(2)-O(1)	2.416(3)□
Mn(2)-O(3)#2	2.422(3)□	Mn(3)-O(11)	2.121(3)□
Mn(3)-O(8)	2.159(3)□	Mn(3)-O(18)#2	2.190(3)□
Mn(3)-O(17)	2.203(2)□	Mn(3)-O(26)	2.216(3)□
Mn(4)-O(12)	2.097(3)□	Mn(4)-O(12)#4	2.097(3)□
Mn(4)-O(19)#5	2.177(3)□	Mn(4)-O(19)#2	2.177(3)□
Mn(4)-O(17)	2.220(3)□	Mn(4)-O(17)#4	2.221(3)
O(6)-Mn(1)-O(6)#1	179.998(2)□	O(6)-Mn(1)-O(4)#2	89.22(10)□
O(6)#1-Mn(1)-O(4)#2	90.78(10)□	O(6)-Mn(1)-O(4)#3	90.78(10)□
O(6)#1-Mn(1)-O(4)#3	89.22(10)□	O(4)#2-Mn(1)-O(4)#3	179.998(2)□
O(6)-Mn(1)-O(1)#1	88.52(11)□	O(6)#1-Mn(1)-O(1)#1	91.48(11)□
O(4)#2-Mn(1)-O(1)#1	103.41(10)□	O(4)#3-Mn(1)-O(1)#1	76.59(10)□

O(6)-Mn(1)-O(1)	91.48(11)□	O(6)#1-Mn(1)-O(1)	88.52(11)□
O(4)#2-Mn(1)-O(1)	76.59(10)□	O(4)#3-Mn(1)-O(1)	103.41(10)□
O(1)#1-Mn(1)-O(1)	180.0□	O(13)-Mn(2)-O(7)	88.94(10)□
O(13)-Mn(2)-O(25)	87.87(10)□	O(7)-Mn(2)-O(25)	174.82(10)□
O(13)-Mn(2)-O(4)#2	141.84(10)□	O(7)-Mn(2)-O(4)#2	87.29(10)□
O(25)-Mn(2)-O(4)#2	92.70(10)□	O(13)-Mn(2)-O(2)	92.56(10)□
O(7)-Mn(2)-O(2)	93.33(10)□	O(25)-Mn(2)-O(2)	90.89(10)□
O(4)#2-Mn(2)-O(2)	125.57(9)□	O(13)-Mn(2)-O(1)	147.22(10)□
O(7)-Mn(2)-O(1)	95.62(10)□	O(25)-Mn(2)-O(1)	89.28(10)□
O(4)#2-Mn(2)-O(1)	70.91(10)□	O(2)-Mn(2)-O(1)	54.84(9)□
O(13)-Mn(2)-O(3)#2	86.92(9)□	O(7)-Mn(2)-O(3)#2	89.99(10)□
O(25)-Mn(2)-O(3)#2	85.76(9)□	O(4)#2-Mn(2)-O(3)#2	55.14(9)□
O(2)-Mn(2)-O(3)#2	176.62(9)□	O(1)-Mn(2)-O(3)#2	125.41(9)□
O(11)-Mn(3)-O(8)	84.72(10)□	O(11)-Mn(3)-O(18)#2	98.36(11)□
O(8)-Mn(3)-O(18)#2	91.01(10)□	O(11)-Mn(3)-O(17)	91.71(10)□
O(8)-Mn(3)-O(17)	148.90(9)□	O(18)#2-Mn(3)-O(17)	120.04(11)□
O(11)-Mn(3)-O(26)	169.94(10)□	O(8)-Mn(3)-O(26)	91.48(10)□
O(18)#2-Mn(3)-O(26)	91.00(11)□	O(17)-Mn(3)-O(26)	86.74(10)□
O(12)-Mn(4)-O(12)#4	179.998(1)□	O(12)-Mn(4)-O(19)#5	85.82(11)□
O(12)#4-Mn(4)-O(19)#5	94.18(11)□	O(12)-Mn(4)-O(19)#2	94.18(11)□
O(12)#4-Mn(4)-O(19)#2	85.82(11)□	O(19)#5-Mn(4)-O(19)#2	180.0□
O(12)-Mn(4)-O(17)	88.87(10)□	O(12)#4-Mn(4)-O(17)	91.13(10)□
O(19)#5-Mn(4)-O(17)	97.15(10)□	O(19)#2-Mn(4)-O(17)	82.85(10)□
O(12)-Mn(4)-O(17)#4	91.13(10)□	O(12)#4-Mn(4)-O(17)#4	88.87(10)□
O(19)#5-Mn(4)-O(17)#4	82.85(10)□	O(19)#2-Mn(4)-O(17)#4	97.15(10)□
O(17)-Mn(4)-O(17)#4	179.999(1)		

Symmetry transformations used to generate equivalent atoms: #1 –x + 2, –y + 1, –z + 1; #2 x + 1, y, z; #3 –x + 1, –y + 1, –z + 1; #4 –x + 2, –y + 2, –z; #5 –x + 1, –y + 2, –z.

Table S5 Selected bond lengths (Å) and angles (º) for 5

Mn(1)-O(3)#1	2.1408(16)□	Mn(1)-O(4)#2	2.1433(16)□
Mn(1)-N(1)	2.223(2)□	Mn(1)-N(4)#3	2.228(2)□
Mn(1)-O(1)	2.2610(16)□	Mn(1)-O(2)	2.3510(17)
O(3)#1-Mn(1)-O(4)#2	112.87(6)□	O(3)#1-Mn(1)-N(1)	90.63(7)□
O(4)#2-Mn(1)-N(1)	95.64(7)□	O(3)#1-Mn(1)-N(4)#3	86.61(7)□
O(4)#2-Mn(1)-N(4)#3	85.13(7)□	N(1)-Mn(1)-N(4)#3	177.22(7)□
O(3)#1-Mn(1)-O(1)	97.64(6)□	O(4)#2-Mn(1)-O(1)	149.03(6)□
N(1)-Mn(1)-O(1)	88.97(7)□	N(4)#3-Mn(1)-O(1)	91.73(7)□
O(3)#1-Mn(1)-O(2)	154.44(6)□	O(4)#2-Mn(1)-O(2)	92.26(6)□
N(1)-Mn(1)-O(2)	91.44(7)□	N(4)#3-Mn(1)-O(2)	91.20(7)□
O(1)-Mn(1)-O(2)	56.94(6)		

Symmetry transformations used to generate equivalent atoms: #1 –x, –y + 1, –z + 2; #2 x + 1, y – 1, z; #3 x, y – 1, z + 1.

Table S6 Selected bond lengths (Å) and angles (º) for 6

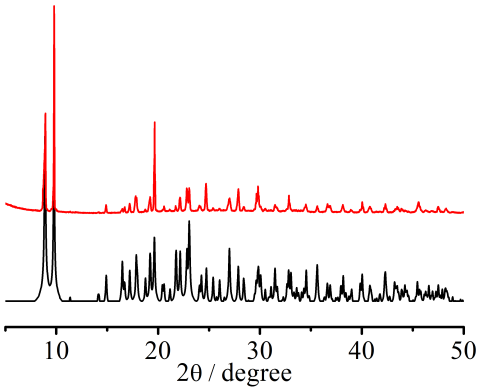
Mn(1)-O(1)#1	2.132(3)□	Mn(1)-O(2)	2.145(3)□
Mn(1)-O(4)#2	2.214(3)□	Mn(1)-N(1)#3	2.235(4)□
Mn(1)-N(3)	2.259(4)□	Mn(1)-O(3)#2	2.347(3)
O(1)#1-Mn(1)-O(2)	118.49(11)□	O(1)#1-Mn(1)-O(4)#2	150.93(11)□
O(2)-Mn(1)-O(4)#2	90.58(11)□	O(1)#1-Mn(1)-N(1)#3	86.46(13)□
O(2)-Mn(1)-N(1)#3	92.32(12)□	O(4)#2-Mn(1)-N(1)#3	92.68(12)□
O(1)#1-Mn(1)-N(3)	85.06(13)□	O(2)-Mn(1)-N(3)	90.80(12)□
O(4)#2-Mn(1)-N(3)	95.24(13)□	N(1)#3-Mn(1)-N(3)	171.45(14)□
O(1)#1-Mn(1)-O(3)#2	93.50(10)□	O(2)-Mn(1)-O(3)#2	147.93(11)□

O(4)#2-Mn(1)-O(3)#2	57.45(10)□	N(1)#3-Mn(1)-O(3)#2	87.22(12)□
N(3)-Mn(1)-O(3)#2	94.35(12)		

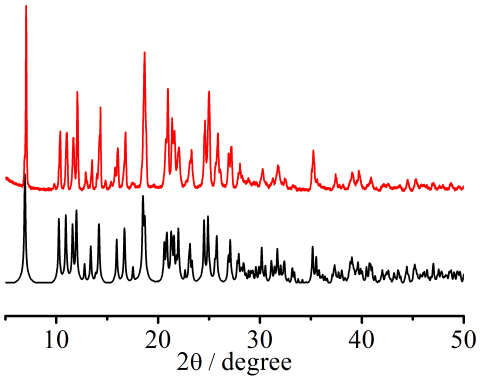
Symmetry transformations used to generate equivalent atoms: #1 –x + 2, y, –z + 1/2; #2 x + 1/2, –y + 1/2, –z + 1; #3 x + 1/2, y + 1/2, –z + 1/2.

Table S7 Hydrogen bonds for 4

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(21)-H(1W)···O(9)#7	0.85	1.95	2.767(4)	159.9
O(21)-H(2W)···O(24)#1	0.85	1.97	2.795(4)	163.7
O(22)-H(3W)···O(3)	0.85	2.10	2.846(4)	146.2
O(22)-H(4W)···O(26)W#8	0.85	2.19	2.820(4)	131.0
O(23)-H(6W)···O(26)W#8	0.85	2.00	2.846(4)	171.6
O(24)-H(7W)···O(25)W	0.85	2.10	2.914(4)	160.0
O(24)-H(8W)···O(16)#9	0.85	2.18	3.025(5)	179.7
O(25)-H(9W)···O(14)	0.85	1.89	2.670(4)	151.1
O(25)-H(10W)···O(23)W	0.85	1.87	2.708(4)	166.8
O(26)-H(11W)···O(9)	0.85	1.95	2.706(4)	147.5
O(26)-H(12W)···O(22)W#10	0.85	1.98	2.820(4)	168.0



(1)



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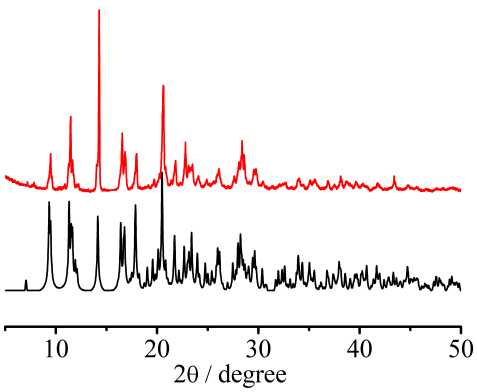

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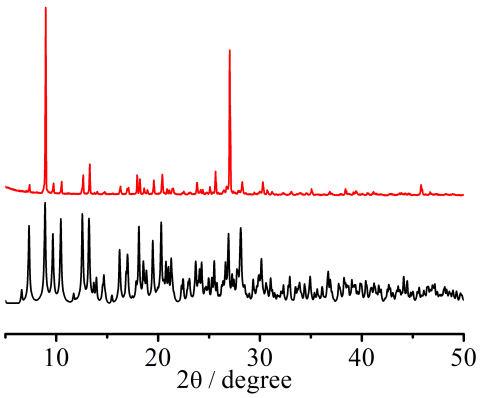

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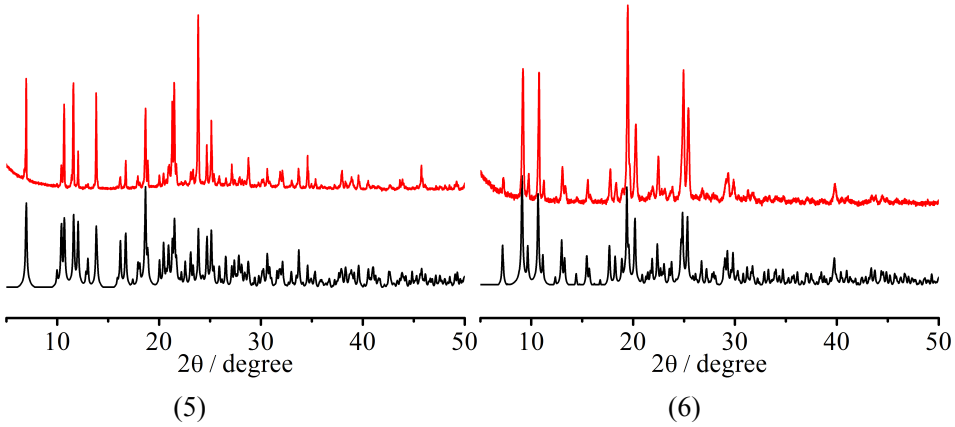
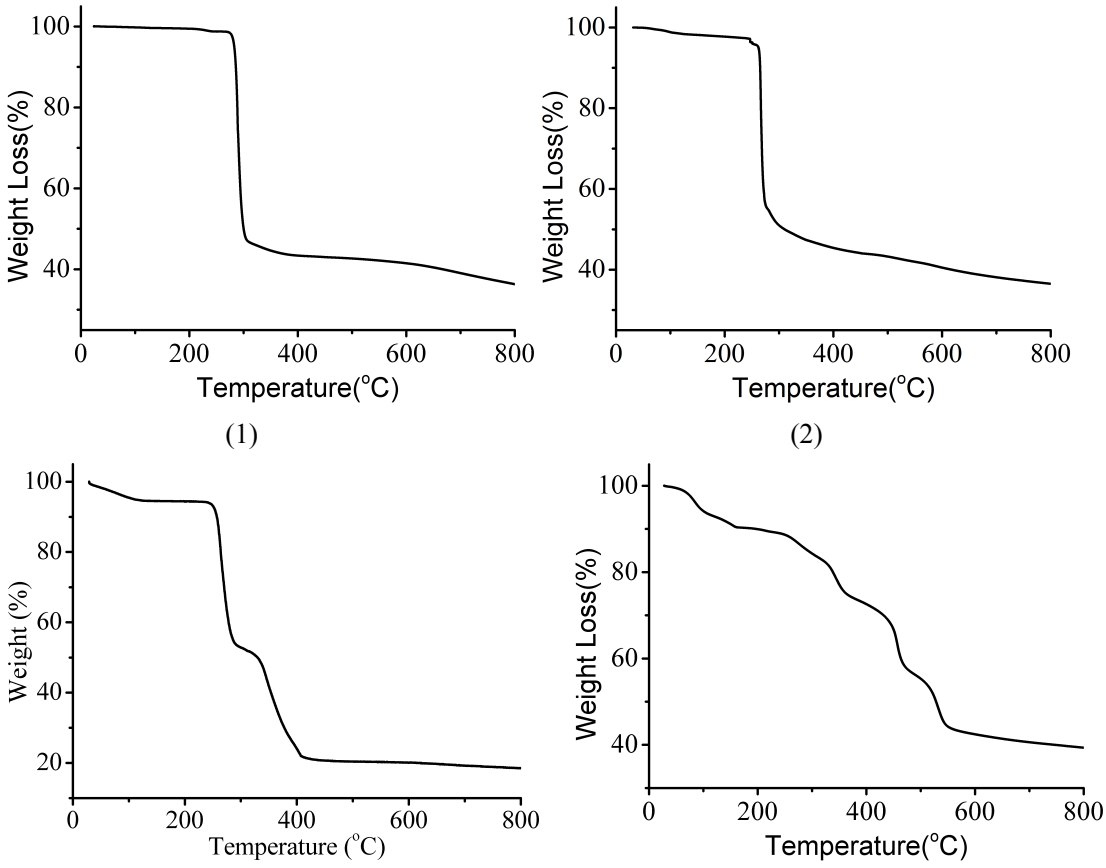
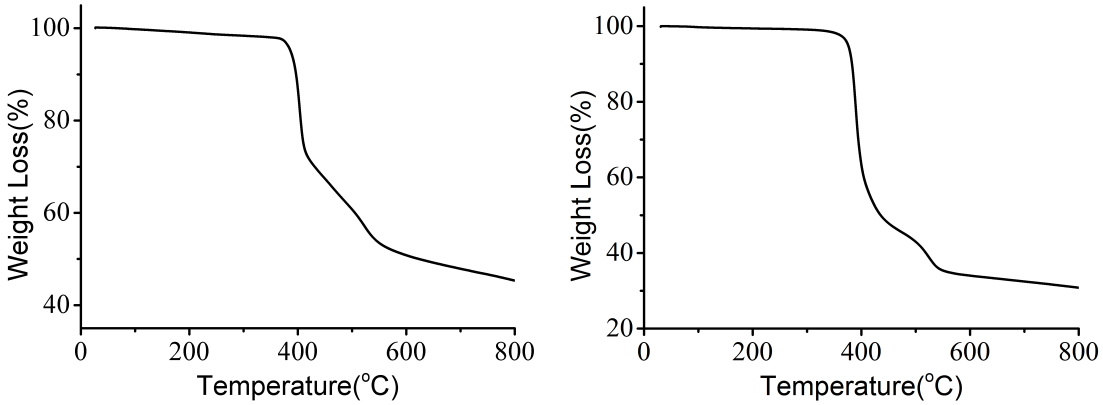


(5) (6)

Figure S1 The XRPD patterns for complexes **1**−**6:** the as-synthesized patterns (red) and the simulated based on X-ray single-crystal data (black).



(1) (2) (3) (4)



(5) (6)

Figure S2. Thermogravimetric curves of complexes **1**−**6**.