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Synthesis, Crystal Structures and Properties of Transition Metal Coordination Polymers Based on a Rigid Triazole Dicarboxylic Acid

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Table S1. Selected bond lengths [Å] and angles [°] for **1**

Mn(1)-O(15)#1	2.115(2)	Mn(3)-O(14)	2.088(3)
Mn(1)-O(15)	2.115(2)	Mn(3)-O(13)	2.095(3)
Mn(1)-O(8)#1	2.130(3)	Mn(3)-O(3)	2.226(3)
Mn(1)-O(8)	2.130(3)	Mn(3)-N(6)	2.237(4)
Mn(1)-O(6)	2.251(2)	Mn(3)-N(7)	2.257(4)
Mn(1)-O(6)#1	2.251(2)	Mn(3)-O(4)	2.457(3)
Mn(2)-O(9)	2.072(3)	Mn(4)-O(2)#2	2.107(3)
Mn(2)-O(1)	2.147(3)	Mn(4)-O(2)	2.107(3)
Mn(2)-N(4)	2.243(3)	Mn(4)-O(10)	2.158(3)
Mn(2)-N(5)	2.284(3)	Mn(4)-O(10)#2	2.158(3)
Mn(2)-O(6)	2.244(2)	Mn(4)-O(3)#2	2.266(2)
Mn(2)-O(7)	2.342(3)	Mn(4)-O(3)	2.266(2)
O(15)#1-Mn(1)-O(15)	180.000(1)	O(14)-Mn(3)-O(13)	93.84(12)
O(15)#1-Mn(1)-O(8)#1	89.22(10)	O(14)-Mn(3)-O(3)	103.90(12)
O(15)-Mn(1)-O(8)#1	90.78(10)	O(13)-Mn(3)-O(3)	103.70(10)
O(15)#1-Mn(1)-O(8)	90.78(10)	O(14)-Mn(3)-N(6)	102.22(13)
O(15)-Mn(1)-O(8)	89.22(10)	O(13)-Mn(3)-N(6)	89.96(14)

O(8)#1-Mn(1)-O(8)	180.00(11)	O(3)-Mn(3)-N(6)	149.47(12)
O(15)#1-Mn(1)-O(6)	87.74(9)	O(14)-Mn(3)-N(7)	93.69(14)
O(15)-Mn(1)-O(6)	92.26(9)	O(13)-Mn(3)-N(7)	162.60(14)
O(8)#1-Mn(1)-O(6)	90.83(10)	O(3)-Mn(3)-N(7)	89.66(13)
O(8)-Mn(1)-O(6)	89.17(10)	N(6)-Mn(3)-N(7)	73.11(15)
O(15)#1-Mn(1)-O(6)#1	92.26(9)	O(14)-Mn(3)-O(4)	158.50(11)
O(15)-Mn(1)-O(6)#1	87.74(9)	O(13)-Mn(3)-O(4)	98.36(11)
O(8)#1-Mn(1)-O(6)#1	89.17(10)	O(3)-Mn(3)-O(4)	56.01(9)
O(8)-Mn(1)-O(6)#1	90.83(10)	N(6)-Mn(3)-O(4)	95.46(11)
O(6)-Mn(1)-O(6)#1	180.000(1)	N(7)-Mn(3)-O(4)	79.73(12)
O(9)-Mn(2)-O(1)	94.12(11)	O(2)#2-Mn(4)-O(2)	180.000(1)
O(9)-Mn(2)-N(4)	100.61(11)	O(2)#2-Mn(4)-O(10)	88.83(11)
O(1)-Mn(2)-N(4)	87.32(12)	O(2)-Mn(4)-O(10)	91.17(11)
O(9)-Mn(2)-O(6)	97.41(10)	O(2)#2-Mn(4)-O(10)#2	91.17(11)
O(1)-Mn(2)-O(6)	108.86(10)	O(2)-Mn(4)-O(10)#2	88.83(11)
N(4)-Mn(2)-O(6)	154.81(11)	O(10)-Mn(4)-O(10)#2	180.000(1)
O(9)-Mn(2)-N(5)	98.06(12)	O(2)#2-Mn(4)-O(3)#2	90.96(9)
O(1)-Mn(2)-N(5)	158.53(12)	O(2)-Mn(4)-O(3)#2	89.04(9)
N(4)-Mn(2)-N(5)	73.13(13)	O(10)-Mn(4)-O(3)#2	89.36(10)
O(6)-Mn(2)-N(5)	87.08(10)	O(10)#2-Mn(4)-O(3)#2	90.64(10)
O(9)-Mn(2)-O(7)	154.30(10)	O(2)#2-Mn(4)-O(3)	89.04(9)
O(1)-Mn(2)-O(7)	92.41(10)	O(2)-Mn(4)-O(3)	90.96(9)
N(4)-Mn(2)-O(7)	104.51(12)	O(10)-Mn(4)-O(3)	90.64(10)
O(6)-Mn(2)-O(7)	57.02(9)	O(10)#2-Mn(4)-O(3)	89.36(10)
N(5)-Mn(2)-O(7)	84.22(11)	O(3)#2-Mn(4)-O(3)	180.00(11)

[a]Symmetry codes:#1 -x+2,-y+1,-z+2 #2 -x+2,-y-1,-z+1

Table S2. Selected bond lengths [Å] and angles [°] for **2**

Zn(1)-O(6)#1	1.907(17)	Zn(3)-O(9)	1.931(14)
Zn(1)-O(3)	1.947(16)	Zn(3)-O(14)#1	1.975(18)
Zn(1)-O(1)	1.953(15)	Zn(3)-N(5)#4	2.027(18)
Zn(1)-N(2)#2	2.072(19)	Zn(3)-O(10)	2.19(2)
Zn(2)-O(4)	1.898(16)	Zn(3)-O(11)	2.229(18)
Zn(2)-O(6)	1.940(16)	Zn(4)-O(13)	1.935(16)
Zn(2)-O(7)	2.032(14)	Zn(4)-O(15)	1.991(18)
Zn(2)-N(1)#3	2.057(19)	Zn(4)-O(14)	2.012(18)
Zn(4)-N(4)#5	2.033(17)		
O(6)#1-Zn(1)-O(3)	107.2(8)	O(14)#1-Zn(3)-O(11)	96.0(7)
O(6)#1-Zn(1)-O(1)	125.7(7)	N(5)#4-Zn(3)-O(11)	89.1(7)
O(3)-Zn(1)-O(1)	97.2(7)	O(10)-Zn(3)-O(11)	171.0(8)
O(6)#1-Zn(1)-N(2)#2	97.5(7)	O(9)-Zn(3)-Zn(4)#1	165.7(5)
O(3)-Zn(1)-N(2)#2	100.8(7)	O(14)#1-Zn(3)-Zn(4)#1	38.5(5)
O(1)-Zn(1)-N(2)#2	124.9(7)	N(5)#4-Zn(3)-Zn(4)#1	65.7(5)
O(4)-Zn(2)-O(6)	124.3(7)	O(10)-Zn(3)-Zn(4)#1	87.0(6)
O(4)-Zn(2)-O(7)	98.2(7)	O(11)-Zn(3)-Zn(4)#1	97.2(5)
O(6)-Zn(2)-O(7)	107.6(7)	O(13)-Zn(4)-O(15)	98.3(7)
O(4)-Zn(2)-N(1)#3	124.6(7)	O(13)-Zn(4)-O(14)	113.2(7)
O(6)-Zn(2)-N(1)#3	96.1(7)	O(15)-Zn(4)-O(14)	111.3(7)
O(7)-Zn(2)-N(1)#3	104.0(7)	O(13)-Zn(4)-N(4)#5	128.5(7)
O(9)-Zn(3)-O(14)#1	128.2(7)	O(15)-Zn(4)-N(4)#5	104.2(7)
O(9)-Zn(3)-N(5)#4	127.5(7)	O(14)-Zn(4)-N(4)#5	100.8(7)
O(14)#1-Zn(3)-N(5)#4	104.2(7)	O(13)-Zn(4)-Zn(3)#6	143.2(5)
O(9)-Zn(3)-O(10)	88.6(7)	O(15)-Zn(4)-Zn(3)#6	112.6(5)
O(14)#1-Zn(3)-O(10)	92.2(8)	O(14)-Zn(4)-Zn(3)#6	37.7(5)

N(5)#4-Zn(3)-O(10)	85.4(8)	N(4)#5-Zn(4)-Zn(3)#6	63.7(5)

[a]Symmetry codes: #1 x+1,y,z #2 x+1/2,y+1/2,z #3 x-1/2,y+1/2,z #4 x+1/2,y-1/2,z #5 x-1/2,y-1/2,z #6 x-1,y,z

Table S3. Selected bond lengths [Å] and angles [°] for **3**

Cd(1)-O(4)#1	2.253(2)	Cd(1)-O(11)	2.392(3)
Cd(1)-O(2)	2.326(2)	Cd(1)-O(6)	2.407(2)
Cd(1)-O(9)	2.340(3)	Cd(1)-O(3)#1	2.535(3)
Cd(1)-O(6)#2	2.381(2)		
O(4)#1-Cd(1)-O(2)	135.89(9)	O(2)-Cd(1)-O(6)	55.25(8)
O(4)#1-Cd(1)-O(9)	97.82(9)	O(9)-Cd(1)-O(6)	84.79(9)
O(2)-Cd(1)-O(9)	95.19(9)	O(6)#2-Cd(1)-O(6)	76.06(9)
O(4)#1-Cd(1)-O(6)#2	92.71(9)	O(11)-Cd(1)-O(6)	78.64(9)
O(2)-Cd(1)-O(6)#2	131.29(9)	O(4)#1-Cd(1)-O(3)#1	53.97(8)
O(9)-Cd(1)-O(6)#2	77.56(9)	O(2)-Cd(1)-O(3)#1	87.44(8)
O(4)#1-Cd(1)-O(11)	95.85(9)	O(9)-Cd(1)-O(3)#1	80.29(9)
O(2)-Cd(1)-O(11)	85.85(9)	O(6)#2-Cd(1)-O(3)#1	136.50(8)
O(9)-Cd(1)-O(11)	159.08(10)	O(11)-Cd(1)-O(3)#1	120.62(9)
O(6)#2-Cd(1)-O(11)	86.06(9)	O(6)-Cd(1)-O(3)#1	138.23(8)
O(4)#1-Cd(1)-O(6)	167.71(8)		

[a]Symmetry codes: #1 x-1,y-1,z+1 #2 -x,-y+2,-z+2

Table S4. Selected bond lengths [Å] and angles [°] for **4**

Cu(1)-O(2)	1.9433(17)	Cu(1)-N(5)	2.022(2)
Cu(1)-O(3)	1.9502(17)	Cu(1)-O(6)	2.393(2)
Cu(1)-N(4)	2.009(2)		
O(2)-Cu(1)-O(3)	94.07(8)	N(4)-Cu(1)-N(5)	81.64(9)
O(2)-Cu(1)-N(4)	91.09(8)	O(2)-Cu(1)-O(6)	96.62(8)
O(3)-Cu(1)-N(4)	166.45(8)	O(3)-Cu(1)-O(6)	93.58(8)
O(2)-Cu(1)-N(5)	172.73(8)	N(4)-Cu(1)-O(6)	98.26(8)
O(3)-Cu(1)-N(5)	93.03(9)	N(5)-Cu(1)-O(6)	84.51(9)

Table S5. Geometrical Parameters of Hydrogen Bonds (Å, °) for complex **2**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)	Symmetry codes
O(16)-H(16B)...O(7)#1	0.85	2.10	2.79(2)	138.1	x+1,y,z
O(15)-H(15B)...O(17)#7	0.85	1.97	2.81(2)	171.2	x-1,y,z
O(11)-H(11B)...O(6)#9	0.85	2.64	3.12(2)	116.8	x+1,-y+1,z+1/2
O(11)-H(11B)...O(5)#9	0.85	2.29	2.95(2)	133.7	x+1,-y+1,z+1/2
O(17)-H(17B)...O(10)#5	0.85	2.15	2.92(3)	150.4	x, y, z
O(15)-H(15A)...O(5)#5	0.85	1.85	2.70(2)	178.7	x, y, z
O(10)-H(10A)...O(2)#5	0.85	1.88	2.73(2)	175.0	x, y, z
O(7)-H(7A)...O(12)#5	0.85	1.75	2.58(2)	168.4	x, y, z
O(3)-H(3A)...O(16)#5	0.85	1.99	2.82(2)	164.8	x, y, z

Table S6. Geometrical Parameters of Hydrogen Bonds (Å, °) for complex **3**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)	Symmetry codes
O(17)-H(10)...N#5	0.83(8)	2.02(8)	2.832(4)	164(7)	-x+1,-y+1,-z+1
O(16)-H(8)...O(17)#4	0.83(4)	1.98(5)	2.790(4)	167(4)	x, y, z
N(2)-H(6)...O(17)#6	1.08(8)	1.72(8)	2.793(4)	170(6)	x+1, y, z
O(16)-H(2)...N(1)#7	0.88(6)	2.08(6)	2.946(4)	172(5)	-x+1,-y+2,-z+1
O(9)-H(1)...O(11)#2	0.81(6)	2.10(6)	2.913(4)	173(5)	-x,-y+2,-z+2
O(17)-H(17B)...O(4)#8	0.84	1.90	2.726(4)	166.8	x-1,y-1,z
O(13)-H(13B)...O(11)#9	0.80	2.17	2.814(4)	138.4	x, y, z-1

Table S7. Geometrical Parameters of Hydrogen Bonds (Å, °) for complex **4**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)	Symmetry codes
O(4)-H(4B)...O(1)#4	0.842(10)	2.61(3)	3.004(3)	110(2)	-x,-y,-z+1
O(4)-H(4B)...O(3)#4	0.842(10)	2.537(13)	3.347(3)	162(3)	-x,-y,-z+1
O(4)-H(4A)...O(1)#5	0.841(10)	2.214(13)	3.010(3)	158(3)	x,y,z+1
O(6)-H(6B)...O(1)#1	0.80(4)	1.98(4)	2.719(3)	152(4)	x, y, z
O(6)-H(6A)...N(3)#6	0.81(3)	2.18(3)	2.968(3)	165(3)	-x,y+1/2,-z+1/2
N(2)-H(2)...O(7)	0.90(3)	2.00(3)	2.870(3)	163(3)	x-1,y,z