Six new coordination polymers based on a tritopic pyridyldicarboxylate ligand: Structures, Magnetic, and Sorption Properties

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Table S1. Selected Bond Lengths (Å) and Bond Angles (°) for Complex **1**

Co(1)-O(2)#1	2.033(4)	Co(1)-O(5)	2.191(5)
Co(1)-O(1)#2	2.082(4)	Co(1)-O(3)#3	2.142(4)
Co(1)-N(1)	2.139(4)	Co(1)-O(4)#3	2.236(4)
O(2)#1-Co(1)-O(1)#2	98.28(16)	O(1)#2-Co(1)-O(3)#3	92.65(16)
O(2)#1-Co(1)-N(1)	105.77(15)	N(1)-Co(1)-O(4)#3	153.71(13)
O(1)#2-Co(1)-N(1)	91.09(15)	O(3)#3-Co(1)-O(4)#3	60.49(14)
O(2)#1-Co(1)-O(3)#3	157.75(14)	O(5)-Co(1)-O(4)#3	90.25(19)
N(1)-Co(1)-O(3)#3	93.26(14)	O(3)#3-Co(1)-O(5)	86.31(19)
O(2)#1-Co(1)-O(5)	82.60(19)	O(2)#1-Co(1)-O(4)#3	100.22(15)
O(1)#2-Co(1)-O(5)	178.91(16)	O(1)#2-Co(1)-O(4)#3	88.97(16)
N(1)-Co(1)-O(5)	89.27(19)		

Symmetry code: #1 x-1,y+1,z #2 -x+1,-y,-z+1 #3 x+1,y,z-1

Table S2. Selected Bond Lengths (Å) and Bond Angles (º) for Complex **2**

Co(1)-O(2)	2.032(19)	Co(2)-O(5)	2.032(19)
Co(1)-O(6)	2.063(2)	Co(2)-O(1)	2.060(2)
Co(1)-O(2W)	2.125(2)	Co(2)-O(3)#3	2.136(18)
Co(1)-O(7)#1	2.138(18)	Co(2)-O(1W)	2.139(2)
Co(1)-N(2)#2	2.162(2)	Co(2)-N(1)#4	2.158(2)
Co(1)-O(8)#1	2.255(2)	Co(2)-O(4)#3	2.253(2)
O(2)-Co(1)-O(6)	99.18(8)	O(5)-Co(2)-O(1)	100.23(8)
O(2)-Co(1)-O(2W)	83.41(8)	O(5)-Co(2)-O(3)#3	151.27(8)
O(6)-Co(1)-O(2W)	177.32(7)	O(1)-Co(2)-O(3)#3	92.62(8)
O(2)-Co(1)-O(7)#1	152.12(8)	O(5)-Co(2)-O(1W)	83.18(8)
O(6)-Co(1)-O(7)#1	93.31(8)	O(1)-Co(2)-O(1W)	176.53(7)
O(2W)-Co(1)-O(7)#1	84.06(8)	O(3)#3-Co(2)-O(1W)	84.58(8)
O(2)-Co(1)-N(2)#2	107.42(9)	O(5)-Co(2)-N(1)#4	108.09(9)
O(6)-Co(1)-N(2)#2	90.00(8)	O(1)-Co(2)-N(1)#4	89.84(8)
O(2W)-Co(1)-N(2)#2	89.87(8)	O(3)#3-Co(2)-N(1)#4	97.44(8)
O(7)#1-Co(1)-N(2)#2	97.34(8)	O(1W)-Co(2)-N(1)#4	88.49(8)
O(2)-Co(1)-O(8)#1	95.93(8)	O(5)-Co(2)-O(4)#3	95.42(8)
O(6)-Co(1)-O(8)#1	87.89(8)	O(1)-Co(2)-O(4)#3	86.67(8)
O(2W)-Co(1)-O(8)#1	91.17(8)	O(3)#3-Co(2)-O(4)#3	59.55(8)
O(7)#1-Co(1)-O(8)#1	59.54(8)	O(1W)-Co(2)-O(4)#3	93.66(8)
N(2)#2-Co(1)-O(8)#1	156.59(8)	N(1)#4-Co(2)-O(4)#3	156.47(8)

Symmetry code: #1 -x+2,-y+1,-z+1 #2 -x+2,-y+2,-z+1 #3 -x+1,-y+3,-z+2 #4 -x+1,-y+2,-z+2

Table S3. Selected Bond Lengths (Å) and Bond Angles (º) for Complex **3**

Co(1)-O(3)#1	2.030(14)	Co(1)-O(1)#2	2.216(13)
Co(1)-O(5)	2.068(14)	Co(2)-O(4)#3	2.040(13)
Co(1)-N(1)	2.094(13)	Co(2)-O(1)#2	2.095(12)
Co(1)-O (1w)	2.127(16)	Co(2)-O(6)	2.142 (14)
Co(1)-O(2)#2	2.153(14)	O(4)#1-Co(2)-O(4)#3	180.00(6)
O(3)#1-Co(1)-O(5)	91.91(7)	O(4)#1-Co(2)-O(1)#2	87.21(5)
O(3)#1-Co(1)-N(1)	95.44(6)	O(4)#3-Co(2)-O(1)#2	92.79(5)
O(5)-Co(1)-N(1)	90.29(6)	O(4)#1-Co(2)-O(1)#4	92.79(5)
O(3)#1-Co(1)-O(1w)	89.54(7)	O(4)#3-Co(2)-O(1)#4	87.21(5)
O(5)-Co(1)-O(1w)	178.47(8)	O(2)#2-Co(1)-O(1)#2	59.80(5)
N(1)-Co(1)-O(1w)	89.91(6)	O(4)#1-Co(2)-O(6)#5	85.29(6)
O(3)#1-Co(1)-O(2)#2	169.03(5)	O(4)#3-Co(2)-O(6)#5	94.71(6)
O(5)-Co(1)-O(2)#2	89.53(7)	O(1)#2-Co(2)-O(6)#5	86.50(5)
N(1)-Co(1)-O(2)#2	95.42(5)	O(1)#4-Co(2)-O(6)#5	93.50(5)

O(7)-Co(1)-O(2)#2	88.98(7)	O(4)#1-Co(2)-O(6)	94.71(6)
O(3)#1-Co(1)-O(1)#2	109.23(5)	O(4)#3-Co(2)-O(6)	85.29(6)
O(5)-Co(1)-O(1)#2	96.55(5)	O(1)#2-Co(2)-O(6)	93.50(5)
N(1)-Co(1)-O(1)#2	154.07(5)	O(1)#4-Co(2)-O(6)	86.50(5)
O(7)-Co(1)-O(1)#2	82.64(5)	O(1)#2-Co(2)-O(1)#4	180.00

Symmetry code: #1 x,-y,z-1/2 #2 x-1/2,y-1/2,z #3 -x+1,y-1,-z+1/2
#4 -x+3/2,-y-1/2,-z #5 -x+1,-y-1,-z

Table S4. Selected Bond Lengths (Å) and Bond Angles (°) for Complex **4**

Co(1)-O(3)#1	2.020(4)	Co(3)-N(3)	2.183(5)
Co(1)-O(1W)	2.050(4)	Co(3)-O(8)#6	2.202(4)
Co(1)-O(3W)	2.063(4)	Co(3)-O(10)#2	2.263(4)
Co(1)-O(9)#2	2.078(4)	Co(4)-O(1W)	2.040(4)
Co(1)-O(16)#3	2.154(4)	Co(4)-O(14)	2.073(4)
Co(1)-O(2W)	2.269(4)	Co(4)-O(15)#3	2.086(4)
Co(2)-O(2)#4	2.043(4)	Co(4)-O(6)	2.087(4)
Co(2)-O(3W)	2.080(4)	Co(4)-N(1)	2.155(5)
Co(2)-O(12)#5	2.084(4)	Co(4)-O(2W)	2.277(4)
Co(2)-O(10)#2	2.181(4)	Co(5)-O(3W)	2.070(4)
Co(2)-N(2)#2	2.224(5)	Co(5)-O(1)#4	2.095(4)
Co(2)-O(8)#6	2.270(4)	Co(5)-O(4)#1	2.105(4)
Co(3)-O(1W)	2.029(4)	Co(5)-O(11)#5	2.147(4)
Co(3)-O(13)	2.062(4)	Co(5)-N(4)#4	2.164(5)
Co(3)-O(5)	2.087(4)	Co(5)-O(4W)	2.209(4)
O(3)#1-Co(1)-O(1W)	169.87(16)	O(5)-Co(3)-O(8)#6	172.09(16)
O(3)#1-Co(1)-O(3W)	98.31(16)	N(3)-Co(3)-O(8)#6	87.75(16)
O(1W)-Co(1)-O(3W)	91.08(14)	O(1W)-Co(3)-O(10)#2	85.86(14)
O(3)#1-Co(1)-O(9)#2	89.90(17)	O(13)-Co(3)-O(10)#2	175.19(15)
O(1W)-Co(1)-O(9)#2	93.06(15)	O(5)-Co(3)-O(10)#2	89.91(15)
O(3W)-Co(1)-O(9)#2	94.96(15)	N(3)-Co(3)-O(10)#2	92.58(16)
O(3)#1-Co(1)-O(16)#3	88.33(17)	O(8)#6-Co(3)-O(10)#2	83.91(14)
O(1W)-Co(1)-O(16)#3	87.14(15)	O(1W)-Co(4)-O(14)	90.99(15)
O(3W)-Co(1)-O(16)#3	94.67(15)	O(1W)-Co(4)-O(15)#3	88.07(16)
O(9)#2-Co(1)-O(16)#3	170.37(16)	O(14)-Co(4)-O(15)#3	94.45(18)
O(3)#1-Co(1)-O(2W)	87.61(16)	O(1W)-Co(4)-O(6)	96.46(16)
O(1W)-Co(1)-O(2W)	83.01(14)	O(14)-Co(4)-O(6)	100.19(18)
O(3W)-Co(1)-O(2W)	174.08(15)	O(15)#3-Co(4)-O(6)	164.58(18)
O(9)#2-Co(1)-O(2W)	84.92(16)	O(1W)-Co(4)-N(1)	175.78(18)
O(16)#3-Co(1)-O(2W)	85.55(15)	O(14)-Co(4)-N(1)	90.67(17)

O(2)#4-Co(2)-O(3W)	97.62(16)	O(15)#3-Co(4)-N(1)	87.89(18)
O(2)#4-Co(2)-O(12)#5	97.65(17)	O(6)-Co(4)-N(1)	87.11(18)
O(3W)-Co(2)-O(12)#5	90.53(15)	O(1W)-Co(4)-O(2W)	83.02(14)
O(2)#4-Co(2)-O(10)#2	88.28(15)	O(14)-Co(4)-O(2W)	173.94(16)
O(3W)-Co(2)-O(10)#2	95.96(14)	O(15)#3-Co(4)-O(2W)	86.28(17)
O(12)#5-Co(2)-O(10)#2	170.58(15)	O(6)-Co(4)-O(2W)	79.63(16)
O(2)#4-Co(2)-N(2)#2	84.57(17)	N(1)-Co(4)-O(2W)	95.37(16)
O(3W)-Co(2)-N(2)#2	175.79(15)	O(3W)-Co(5)-O(1)#4	97.83(15)
O(12)#5-Co(2)-N(2)#2	85.61(16)	O(3W)-Co(5)-O(4)#1	101.08(16)
O(10)#2-Co(2)-N(2)#2	87.68(16)	O(1)#4-Co(5)-O(4)#1	84.59(19)
O(2)#4-Co(2)-O(8)#6	171.33(15)	O(3W)-Co(5)-O(11)#5	86.65(15)
O(3W)-Co(2)-O(8)#6	87.53(14)	O(1)#4-Co(5)-O(11)#5	96.17(17)
O(12)#5-Co(2)-O(8)#6	89.24(15)	O(4)#1-Co(5)-O(11)#5	172.07(17)
O(10)#2-Co(2)-O(8)#6	84.24(14)	O(3W)-Co(5)-N(4)#4	169.96(16)
N(2)#2-Co(2)-O(8)#6	90.74(16)	O(1)#4-Co(5)-N(4)#4	88.87(17)
O(1W)-Co(3)-O(13)	92.42(16)	O(4)#1-Co(5)-N(4)#4	86.92(19)
O(1W)-Co(3)-O(5)	96.55(15)	O(11)#5-Co(5)-N(4)#4	85.20(18)
O(13)-Co(3)-O(5)	94.75(17)	O(3W)-Co(5)-O(4W)	86.00(15)
O(1W)-Co(3)-N(3)	175.55(16)	O(1)#4-Co(5)-O(4W)	172.88(19)
O(13)-Co(3)-N(3)	88.80(17)	O(4)#1-Co(5)-O(4W)	88.80(19)
O(5)-Co(3)-N(3)	87.60(16)	O(11)#5-Co(5)-O(4W)	90.02(18)
O(1W)-Co(3)-O(8)#6	87.94(14)	N(4)#4-Co(5)-O(4W)	88.80(17)
O(13)-Co(3)-O(8)#6	91.55(15)		

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

Table S5. Selected Bond Lengths (Å) and Bond Angles (º) for Complex **5**

Mn(1)-O(3)#5	2.291(2)	Mn(1)-O(1)#3	2.160(3)
Mn(1)-O(4)#5	2.283(3)	Mn(1)-O(1W)	2.201(3)
Mn(1)-O(2)#4	2.121(2)	Mn(1)-N(1)	2.317(3)
O(2)#4-Mn(1)-O(1)#3	102.39(10)		
O(2)#4-Mn(1)-O(1W)	83.34(11)	O(1)#3-Mn(1)-N(1)	86.65(10)
O(1)#3-Mn(1)-O(1W)	170.74(9)	O(1W)-Mn(1)-N(1)	84.23(10)
O(2)#4-Mn(1)-O(4)#5	93.02(11)	O(4)#5-Mn(1)-N(1)	149.28(9)
O(1)#3-Mn(1)-O(4)#5	89.24(11)	O(3)#5-Mn(1)-N(1)	92.75(9)
O(1W)-Mn(1)-O(4)#5	97.77(11)	O(1W)-Mn(1)-O(3)#5	84.56(10)
O(2)#4-Mn(1)-O(3)#5	145.81(11)	O(4)#5-Mn(1)-O(3)#5	57.21(9)
O(1)#3-Mn(1)-O(3)#5	94.28(10)	O(2)#4-Mn(1)-N(1)	117.59(10)

Symmetry code: #1 x,y,z+1 #2 x-1,y+1,z #3 -x+2,-y+2,-z+1
#4 x+1,y-1,z #5 x,y,z-1

Table S6. Selected Bond Lengths (Å) and Bond Angles (°) for Complex **6**

Zn(1)-O(2)#1	1.965(2)	Zn(1)-O(1)	2.310(3)
Zn(1)-O(2)#2	1.965(2)	Zn(1)-O(1)#4	2.310(3)
Zn(1)-N(1)#3	2.067(4)	N(1)#3-Zn(1)-O(1)	86.83(5)
O(2)#1-Zn(1)-O(2)#2	109.22(16)	O(2)#1-Zn(1)-O(1)#4	98.97(12)
O(2)#1-Zn(1)-N(1)#3	125.39(8)	O(2)#2-Zn(1)-O(1)#4	84.73(12)
O(2)#2-Zn(1)-N(1)#3	125.39(8)	N(1)#3-Zn(1)-O(1)#4	86.83(5)
O(2)#1-Zn(1)-O(1)	84.73(12)	O(1)-Zn(1)-O(1)#4	173.67(10)
O(2)#2-Zn(1)-O(1)	98.97(12)		

Symmetry code: #1 x,-y,z-1/2 #2 -x+1,-y,-z+2 #3 -x+1/2,-y+1/2,-z+1
#4 -x+1,y,-z+3/2

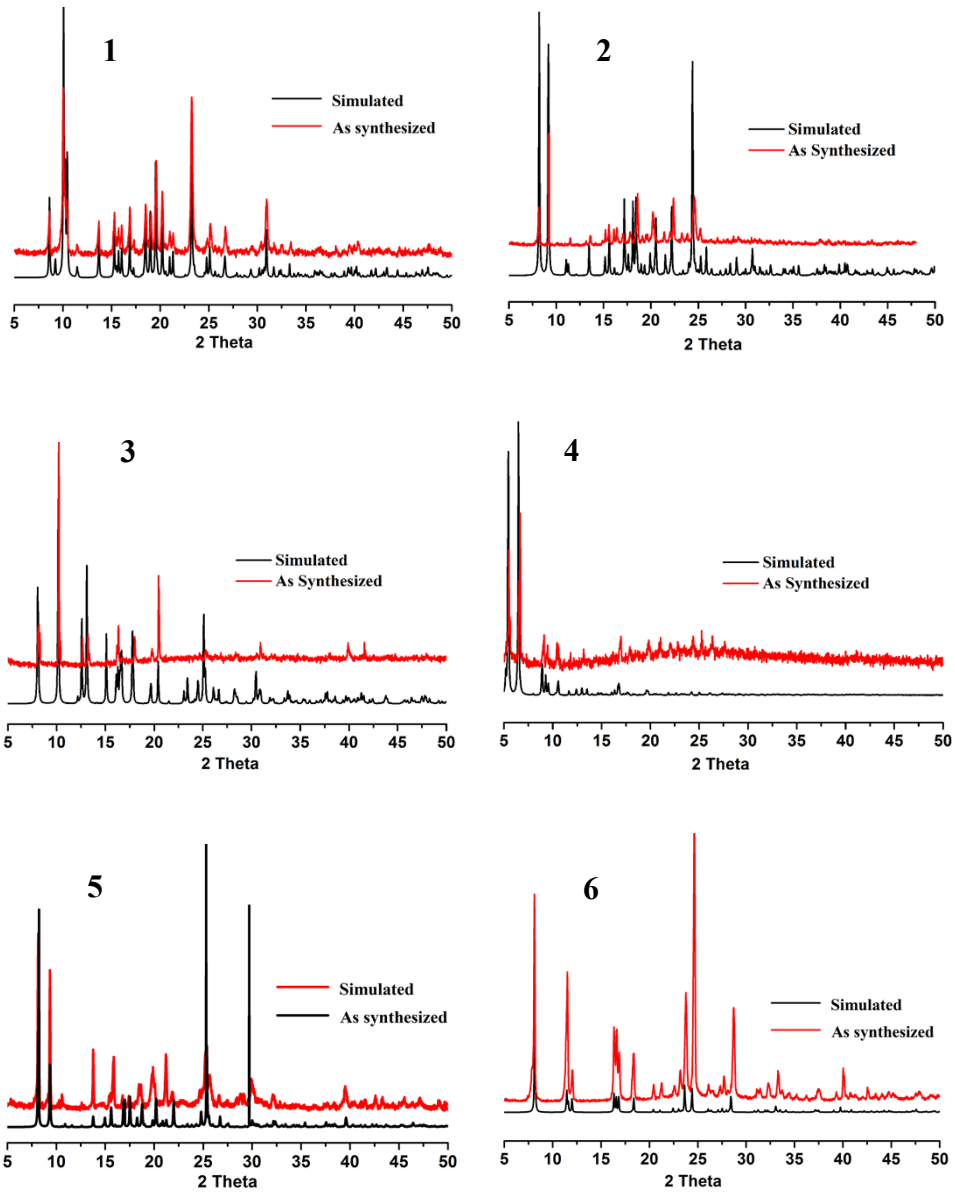

Figure S1. PXRD simulated as-synthesized patterns for complexes **1**−**6**.

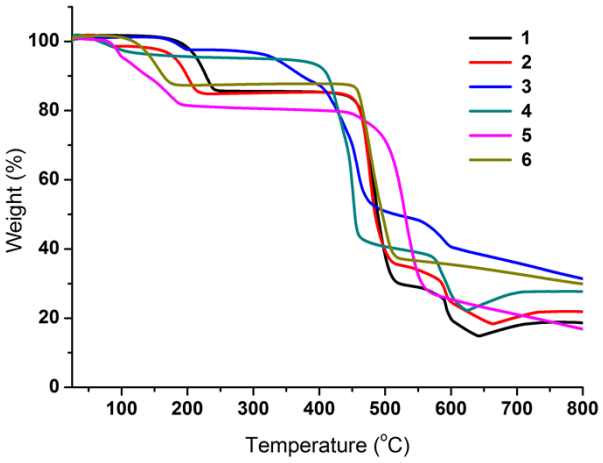

Figure S2. The TG curves of complexes **1**−**6**.