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Construction of Coordination Polymers based on Methylenebis(3,5-dimethylpyrazole) and Varied Aromatic Carboxlylic Acids

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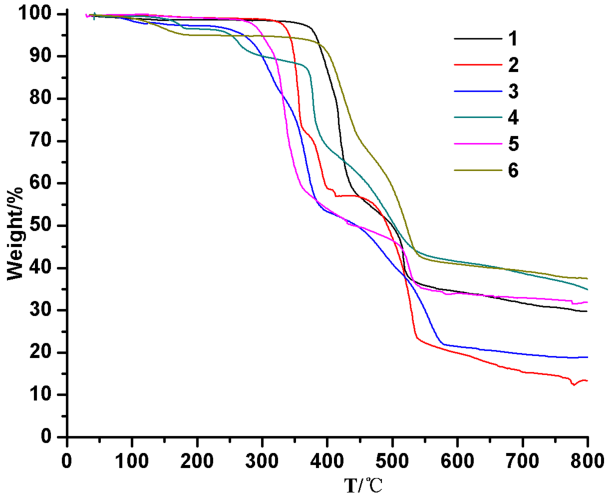

Fig. S1. TGA curves for complexes **1**-**6**.

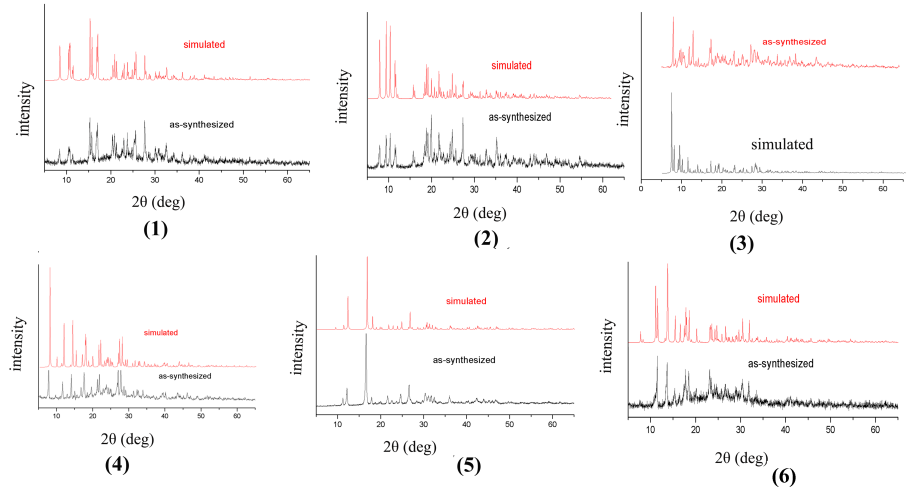

Fig. S2. PXRD patterns of complexes **1**-**6**.

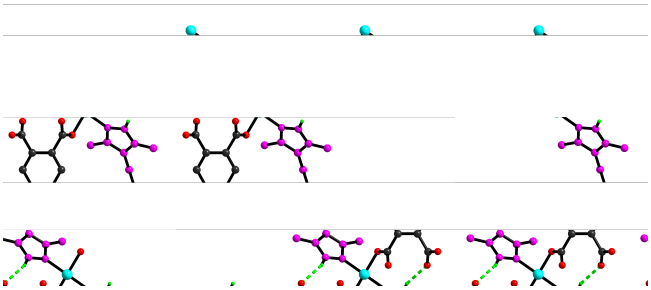

Fig. S3. Perspective view of a selected (4, 4) single layer in **5**. The H_2MDP ligands and Cu(II) ions on another single layer are omitted for the clarity.

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

Bond	Dist	Bond	Dist
Co(1)-O(4)	1.925(3)	Co(1)-N(4)#1	1.992(3)
Co(1)-O(1)	1.930(3)	Co(1)-N(3)	2.004(3)
Angle	(°)	Angle	(°)
O(4)-Co(1)-O(1)	99.57(16)	O(1)-Co(1)-N(3)	114.84(14)
O(4)-Co(1)-N(4)#1	111.21(13)	N(4)#1-Co(1)-N(3)	106.54(13)
O(1)-Co(1)-N(4)#1	116.31(14)	C(1)-N(4)-Co(1)#2	134.0(3)
O(4)-Co(1)-N(3)	108.06(14)	N(1)-N(4)-Co(1)#2	120.0(2)

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

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

Bond	Dist	Bond	Dist
Cd(1)-O(3)	2.186(5)	Cd(1)-O(2)	2.375(7)
Cd(1)-N(4)	2.286(7)	Cd(1)-O(1)	2.384(8)
Cd(1)-N(3)#1	2.288(7)		
Angle	(°)	Angle	(°)
O(3)-Cd(1)-N(4)	137.0(3)	N(4)-Cd(1)-O(2)	90.4(3)
O(3)-Cd(1)-N(3)#1	98.9(2)	N(3)#1-Cd(1)-O(2)	143.0(3)
N(4)-Cd(1)-N(3)#1	99.3(2)	O(3)-Cd(1)-O(1)	98.9(3)
O(3)-Cd(1)-O(2)	97.8(3)	N(4)-Cd(1)-O(1)	119.3(3)
N(3)#1-Cd(1)-O(1)	90.8(2)	O(2)-Cd(1)-O(1)	54.0(3)

Symmetry codes: #1) $-x+1, -y, -z$.

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

Bond	Dist	Bond	Dist
Cd(1)-O(3)#1	2.314(3)	Cd(2)-N(4)	2.318(3)
Cd(1)-O(3)	2.314(3)	Cd(2)-N(4)#4	2.318(3)
Cd(1)-N(7)#2	2.345(3)	Cd(2)-N(3)#3	2.340(3)
Cd(1)-N(7)#3	2.345(3)	Cd(2)-N(3)#5	2.340(3)
Cd(1)-N(5)	2.405(3)	Cd(2)-O(4)#4	2.405(3)
Cd(1)-N(5)#1	2.405(3)	Cd(2)-O(4)	2.405(3)
Angle	(°)	Angle	(°)
O(3)#1-Cd(1)-O(3)	168.19(14)	O(3)-Cd(1)-N(5)#1	87.73(11)
O(3)#1-Cd(1)-N(7)#2	94.82(12)	N(7)#2-Cd(1)-N(5)#1	88.18(12)
O(3)-Cd(1)-N(7)#2	93.67(11)	N(7)#3-Cd(1)-N(5)#1	75.47(12)
O(3)#1-Cd(1)-N(7)#3	93.67(11)	N(5)-Cd(1)-N(5)#1	95.81(16)
O(3)-Cd(1)-N(7)#3	94.82(12)	N(4)-Cd(2)-N(4)#4	87.91(16)

N(7)#2-Cd(1)-N(7)#3	87.92(16)	N(4)-Cd(2)-N(3)#3	95.70(12)
O(3)#1-Cd(1)-N(5)	87.73(11)	N(4)#4-Cd(2)-N(3)#3	66.72(12)
O(3)-Cd(1)-N(5)	84.36(11)	N(4)-Cd(2)-N(3)#5	66.72(12)
N(7)#2-Cd(1)-N(5)	175.47(12)	N(4)#4-Cd(2)-N(3)#5	95.70(12)
N(7)#3-Cd(1)-N(5)	88.18(12)	N(3)#3-Cd(2)-N(3)#5	83.68(17)
O(3)#1-Cd(1)-N(5)#1	84.36(11)	N(4)-Cd(2)-O(4)#4	91.39(10)
N(4)#4-Cd(2)-O(4)#4	87.03(10)	N(4)#4-Cd(2)-O(4)	91.39(10
N(3)#3-Cd(2)-O(4)#4	80.12(11)	N(3)#3-Cd(2)-O(4)	101.54(11
N(3)#5-Cd(2)-O(4)#4	101.54(11)	N(3)#5-Cd(2)-O(4)	80.12(11
N(4)-Cd(2)-O(4)	87.03(10)	O(4)#4-Cd(2)-O(4)	177.81(13

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

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

Bond	Dist	Bond	Dist
Mn(1)-O(6)#1	2.132(2)	Mn(1)-O(1)	2.226(2)
Mn(1)-N(2)	2.207(2)	Mn(1)-O(1W)	2.273(2)
Mn(1)-N(4)#2	2.213(2)	Mn(1)-O(2)	2.343(2)
Angle	(°)	Angle	(°)
O(6)#1-Mn(1)-N(2)	113.35(9)	N(4)#2-Mn(1)-O(1W)	176.41(9)
O(6)#1-Mn(1)-N(4)#2	87.48(9)	O(1)-Mn(1)-O(1W)	84.62(8)
N(2)-Mn(1)-N(4)#2	92.42(9)	O(6)#1-Mn(1)-O(2)	145.54(8)
O(6)#1-Mn(1)-O(1)	88.03(8)	N(2)-Mn(1)-O(2)	100.49(8)
N(2)-Mn(1)-O(1)	156.44(8)	N(4)#2-Mn(1)-O(2)	97.76(9)
N(4)#2-Mn(1)-O(1)	98.55(9)	O(1)-Mn(1)-O(2)	57.52(7)
O(6)#1-Mn(1)-O(1W)	90.96(8)	O(1W)-Mn(1)-O(2)	85.35(7)
N(2)-Mn(1)-O(1W)	85.22(8)		

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

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

Bond	Dist	Bond	Dist
Cu(1)-O(2)#1	1.9208(18)	Cu(1)-N(1)	2.024(2)
Cu(1)-O(2)	1.9208(18)	Cu(1)-N(1)#1	2.024(2)
Angle	(°)	Angle	(°)
O(2)#1-Cu(1)-O(2)	158.09(12)	O(2)#1-Cu(1)-N(1)#1	97.63(8)
O(2)#1-Cu(1)-N(1)	89.26(8)	O(2)-Cu(1)-N(1)#1	89.26(8)
O(2)-Cu(1)-N(1)	97.63(8)	N(1)-Cu(1)-N(1)#1	143.25(12)

Symmetry code: #1) $-x+3/4, \quad -y+3/4, z$.

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

Bond	Dist	Bond	Dist
Co(1)-O(4)#1	1.921(2)	Co(1)-N(4)#2	2.017(3)
Co(1)-O(3)	1.999(2)	Co(1)-N(2)	2.044(2)

Angle	(°)	Angle	(°)
O(4)#1-Co(1)-O(3)	118.00(10)	O(4)#1-Co(1)-N(2)	94.26(9)
O(4)#1-Co(1)-N(4)#2	121.34(10)	O(3)-Co(1)-N(2)	106.56(9)
O(3)-Co(1)-N(4)#2	107.81(10)	N(4)#2-Co(1)-N(2)	106.17(10)
Symmetry codes: #1) *x*, *y*+1, *z*; #2) −*x*+2, *y*, −*z*+5/2.			

D–H/A	d(H…A)/ Å	D(D…A)/ Å	∠DHA/
For complex **1**			
O1W-H1WA…O2	2.02	2.863(9)	175
N1-H1A…O3#1	1.94	2.730(5)	152
O1W-H1WB…O2#2	2.02	2.863(9)	175
N2-H2A…O2	2.16	2.873(7)	140
Symmetry transformations to generate equivalent atoms: #1) 3/2-*x*,-1/2+*y*, 1/2-*z*; #2) 1-*x*, *y*, 1/2-*z*.			

Table S7. Hydrogen bond distance and angle data for 1.

Table S8. Hydrogen bond distance and angle data for **2**

D–H/A	d(H…A)/ Å	D(D…A)/ Å	∠DHA/
For complex **2**			
N2-H2A…O4#1	2.01	2.761(9)	145.6
N1-H1A…O3#2	2.07	2.882(9)	156.8
Symmetry transformations to generate equivalent atoms: #1) -*x*,-*y*,-*z*+1; #2) -*x*-1,-*y*,-*z*+2.			

Table S9. Hydrogen bond distance and angle data for **3**

D–H/A	H…A	D…A	<(DHA)
For complex **3**			
O5-H5D…O1W	1.83	2.651(5)	174.8
N1-H1D…O2	1.93	2.749(4)	159.9
N8-H8C…O1#1	1.89	2.742(4)	173.1
N6-H6A…O1#2	2.23	3.007(4)	149.9
O1W-H1W…O2#3	1.82(7)	2.766(5)	170(5)
Symmetry transformations to generate equivalent atoms：#1）-*x*+1, *y*+1, -*z*+1/2；#2）*x*, -*y*+1, *z*+1/2；#3）*x*, -*y*+1, *z*-1/2.			

Table S10. Hydrogen bond distance and angle data for **5**

D–H/A	H…A	D…A	<(DHA)
For complex **5**			
N2-H2D…O1#1	2.05	2.815(3)	147.1
Symmetry transformations to generate equivalent atoms：#1) -*x*+5/4, *y*, -*z*+5/4.			

Table S11. Hydrogen bond distance and angle data for **6**

D–H/A	H…A	D…A	<(DHA)
For complex **6**			
O1W-H1WD…O3	1.97	2.789(3)	161.5
N1-H1A…O1W#1	2.11	2.928(4)	159.0
N3-H3A…O2#2	2.04	2.867(3)	162.1
Symmetry transformations to generate equivalent atoms：#1) *x*, *y*+1, *z*; #2) -*x*, *y*, -*z*+1/2.			