Syntheses and characterizations of six Co(II) and Mn(II) coordination polymers based on amino-substituted 5-aminoisophthalate and flexible bis(imidazolyl) ligands

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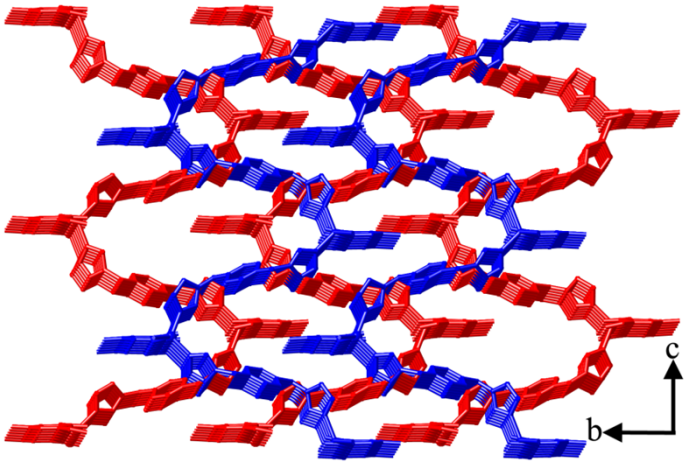


Figure S1 View of 2D→3D interdigitating network along the *a* axis in **1**.

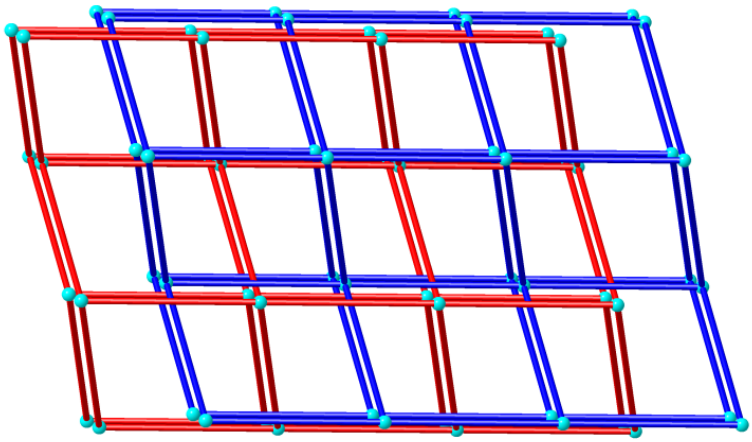
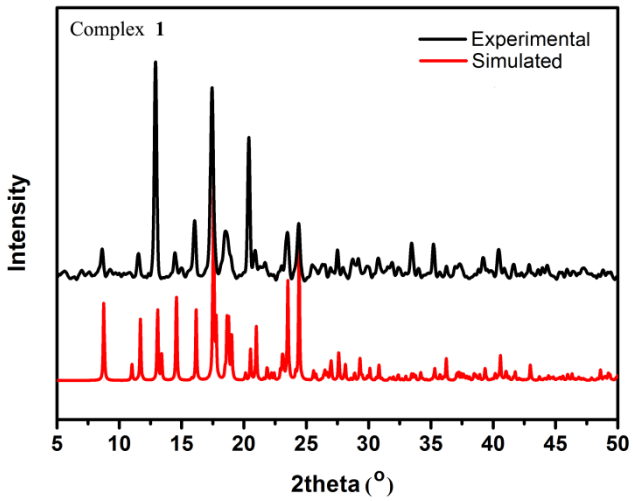


Figure S2 Topological view of ABAB packing of interdigitating 2-D layer along the *b* axis in **1**.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Experimental
Simulated
Intensity
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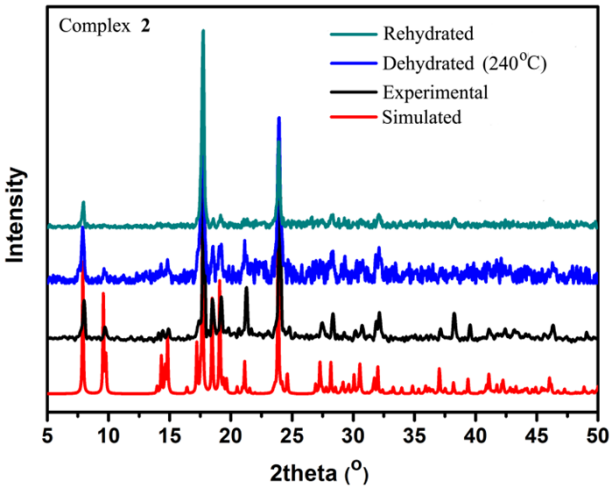
10
15
20
25
30
35
40
45
50
2theta (°)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Rehydrated
Dehydrated (240°C)
Experimental
Simulated
Intensity
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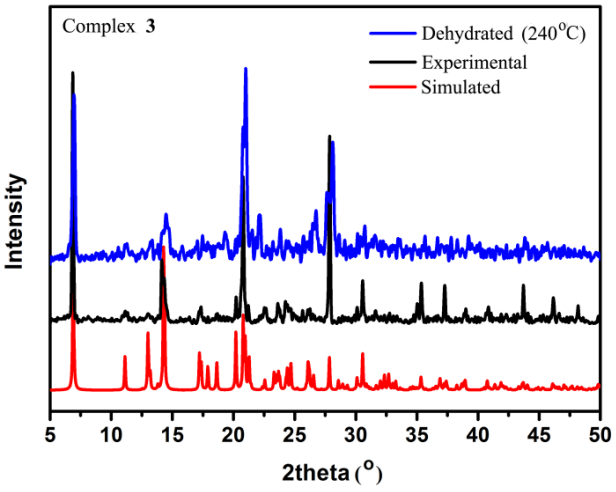
10
15
20
25
30
35
40
45
50
2theta (°)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Dehydrated (240°C)
Experimental
Simulated
Intensity
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35
40
45
50
2theta (°)

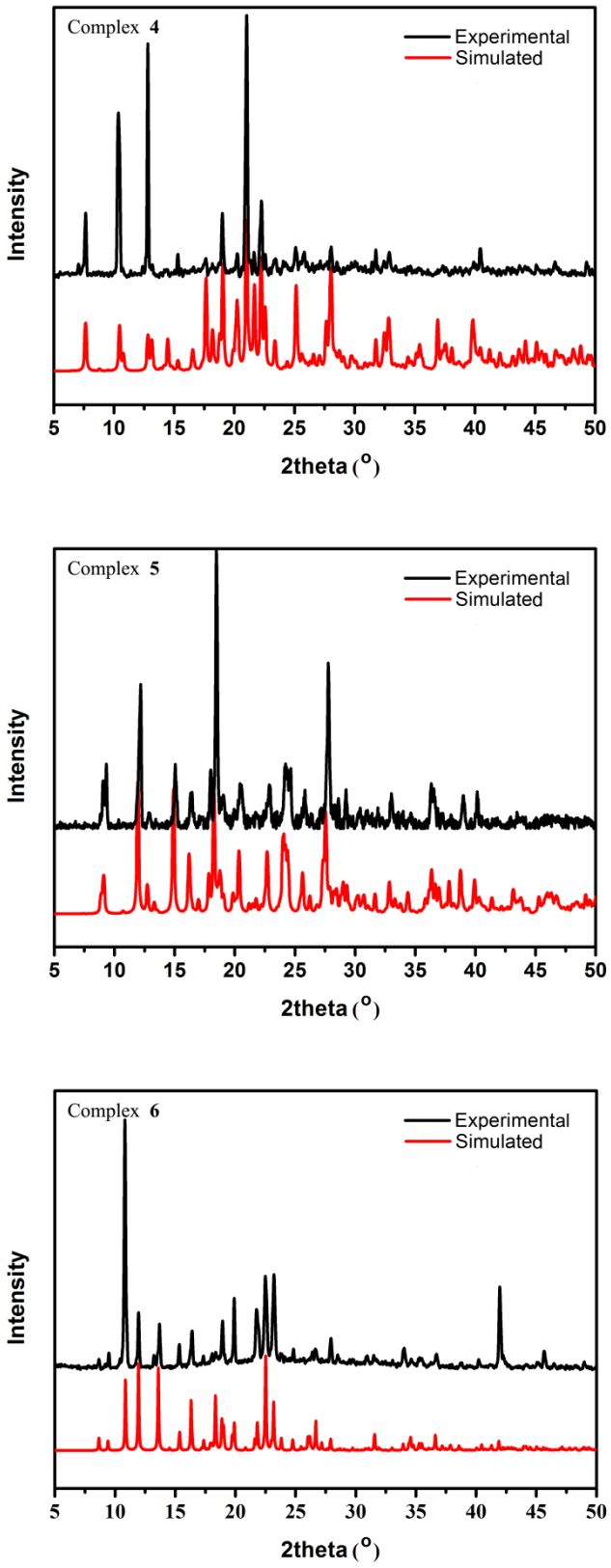

Figure S3 XRD patterns for complexes **1-6**.

Table S1. Crystal data and structure refinement results for **1-6.**

	1	**2**	**3**
Empirical formula	$C_{22}H_{19}N_5O_4Co$	$C_{15}H_{14}N_3O_5Co$	$C_{16}H_{16}N_3O_5Co$
Formula weight	476.35	375.22	389.25
Crystal system	Monoclinic	Triclinic	Monoclinic
Space group	$P2_1/c$	P-1	$P2_1/c$
a (Å)	10.225 (5)	6.630(4)	12.8113(10)
b (Å)	13.530(6)	10.167(5)	7.8747(6)
c (Å)	15.503(8)	12.475(7)	15.8919(17)
α (°)	90	109.11(3)	90
β (°)	102.795(9)	103.70(2)	90.871(8)
γ (°)	90	100.43(3)	90
V(Å^3)	2091.6(17)	740.7(7)	1603.1(2)
Z	4	2	4
F(000)	980	384	800
ρ_{calcd} (g cm^{-3})	1.513	1.682	1.613
$\mu(mm^{-1})$	0.861	1.191	1.104
Reflections collected	17615	5814	12196
Unique reflections	4753	3361	3646
Parameters	289	225	235
R_{int}	0.0531	0.0243	0.0230
S on F^2	1.078	1.050	1.095
$R_1(I>2\sigma(I))$[a]	0.0540	0.0372	0.0332
$wR_2(I>2\sigma(I))$[b]	0.1043	0.0820	0.0845
R_1 (all data)[a]	0.0853	0.0487	0.0362
wR_2 (all data)[b]	0.0853	0.0878	0.0880
$\Delta\rho_{max}$ and $_{min}$ [e·Å^{-3}]	0.394 and -0.404	0.393and -0.554	0.408 and -0.463
	4	**5**	**6**
Empirical formula	$C_{44}H_{38}N_{10}O_8Mn_2$	$C_{27}H_{34}N_6O_7Mn$	$C_{21}H_{17}N_4O_4Mn$
Formula weight	944.72	609.54	444.33
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	P-1	$P2_1/c$	$P2_1/c$
a (Å)	11.6898(19)	9.888(6)	10.4640(19)
b (Å)	12.7428(18)	19.869(12)	15.5072(12)
c (Å)	13.723 (2)	15.809(10)	16.689(2)
α (°)	79.440(4)	90	90
β (°)	82.520(3)	101.072(12)	102.865(8)

γ (°)	84.502(4)	90	90
V(Å^3)	1987.1(5)	2909(3)	1959.1(5)
Z	2	4	4
F(000)	972	1276	912
ρ_{calcd} (g cm^{-3})	1.579	1.392	1.506
$\mu(mm^{-1})$	0.707	0.508	0.711
Reflections collected	16887	22426	14947
Unique reflections	8837	6619	4467
Parameters	577	393	271
R_{int}	0.0221	0.0499	0.0305
S on F^2	0.990	1.179	1.090
$R_1(I>2\sigma(I))$[a]	0.0355	0.0691	0.0393
$wR_2(I>2\sigma(I))$[b]	0.0919	0.1546	0.0924
R_1 (all data)[a]	0.0473	0.1126	0.0472
wR_2 (all data)[b]	0.0986	0.1784	0.0973
$\Delta\rho_{max}$ and $_{min}$ [e·Å^{-3}]	0.377 and -0.271	0.343 and -0.714	0.247 and -0.375

[a]$R_1 = \sum||F_o| - |F_c||/\sum|F_o|$. [b]$wR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$

Table S2 Selected bond lengths (Å) and Angles (°) for **1-6**.

		1	
Co(1)-O(4)#1	1.990(2)	Co(1)-O(1)	1.996(2)
Co(1)-N(2)	2.004(3)	Co(1)-N(5)#2	2.013(3)
O(4)#1-Co(1)-O(1)	100.81(9)	O(4)#1-Co(1)-N(2)	112.22(9)
O(1)-Co(1)-N(2)	111.57(9)	O(4)#1-Co(1)-N(5)#2	106.91(9)
O(1)-Co(1)-N(5)#2	110.64(10)	N(2)-Co(1)-N(5)#2	113.85(11)
		2	
Co(1)-O(4)#1	2.0173(18)	Co(1)-N(1)	2.087(2)
Co(1)-O(2)	2.1264(18)	Co(1)-O(1W)	2.141(2)
Co(1)-N(3)#2	2.198(2)	Co(1)-O(1)	2.2804(19)
O(4)#1-Co(1)-N(1)	94.80(8)	O(4)#1-Co(1)-O(2)	158.51(7)
N(1)-Co(1)-O(2)	88.60(8)	O(4)#1-Co(1)-O(1W)	94.29(8)
N(1)-Co(1)-O(1W)	92.40(8)	O(2)-Co(1)-O(1W)	106.78(7)
O(4)#1-Co(1)-N(3)#2	90.62(8)	N(1)-Co(1)-N(3)#2	172.57(7)
O(2)-Co(1)-N(3)#2	88.20(7)	O(1W)-Co(1)-N(3)#2	82.12(8)
O(4)#1-Co(1)-O(1)	98.89(7)	N(1)-Co(1)-O(1)	92.51(7)
O(2)-Co(1)-O(1)	59.71(6)	O(1W)-Co(1)-O(1)	165.49(7)
N(3)#2-Co(1)-O(1)	91.66(7)		

3

Co(1)-O(4)	1.9566(12)	Co(1)-O(1)#1	2.0204(12)
Co(1)-N(2)	2.0317(16)	Co(1)-N(1)#2	2.0922(14)
O(4)-Co(1)-O(1)#1	104.02(5)	O(4)-Co(1)-N(2)	105.09(6)
O(1)#1-Co(1)-N(2)	109.79(6)	O(4)-Co(1)-N(1)#2	106.04(5)
O(1)#1-Co(1)-N(1)#2	107.14(5)	N(2)-Co(1)-N(1)#2	123.13(6)

4

Mn(1)-O(1)	2.1183(18)	Mn(1)-O(5)	2.1533(19)
Mn(1)-N(7)	2.258(2)	Mn(1)-N(3)	2.260(2)
Mn(1)-O(3)#1	2.2984(19)	Mn(1)-O(4)#1	2.3224(19)
Mn(2)-O(2)	2.1262(19)	Mn(2)-O(6)	2.1285(18)
Mn(2)-N(10)#2	2.236(2)	Mn(2)-N(6)#3	2.246(2)
Mn(2)-O(7)#4	2.2618(19)	Mn(2)-O(8)#4	2.3508(19)
O(1)-Mn(1)-O(5)	112.46(7)	O(1)-Mn(1)-N(7)	94.69(8)
O(5)-Mn(1)-N(7)	90.68(8)	O(1)-Mn(1)-N(3)	88.26(8)
O(5)-Mn(1)-N(3)	86.19(8)	N(7)-Mn(1)-N(3)	176.35(8)
O(1)-Mn(1)-O(3)#1	94.69(7)	O(5)-Mn(1)-O(3)#1	152.85(7)
N(7)-Mn(1)-O(3)#1	87.58(8)	N(3)-Mn(1)-O(3)#1	94.33(8)
O(1)-Mn(1)-O(4)#1	150.82(8)	O(5)-Mn(1)-O(4)#1	96.17(7)
N(7)-Mn(1)-O(4)#1	90.31(8)	N(3)-Mn(1)-O(4)#1	88.15(8)
O(3)#1-Mn(1)-O(4)#1	56.76(6)	O(2)-Mn(2)-O(6)	109.05(7)
O(2)-Mn(2)-N(10)#2	89.51(8)	O(6)-Mn(2)-N(10)#2	85.80(8)
O(2)-Mn(2)-N(6)#3	94.16(9)	O(6)-Mn(2)-N(6)#3	93.70(8)
N(10)#2-Mn(2)-N(6)#3	176.25(8)	O(2)-Mn(2)-O(7)#4	150.00(7)
O(6)-Mn(2)-O(7)#4	100.89(7)	N(10)#2-Mn(2)-O(7)#4	90.84(8)
N(6)#3-Mn(2)-O(7)#4	85.61(8)	O(2)-Mn(2)-O(8)#4	92.93(7)
O(6)-Mn(2)-O(8)#4	157.34(8)	N(10)#2-Mn(2)-O(8)#4	89.04(8)
N(6)#3-Mn(2)-O(8)#4	90.02(8)	O(7)#4-Mn(2)-O(8)#4	57.09(6)

5

Mn(1)-O(1)	2.150(2)	Mn(1)-O(1W)	2.260(3)
Mn(1)-N(1)	2.284(3)	Mn(2)-O(3)	2.164(2)
Mn(2)-O(2W)	2.243(3)	Mn(2)-N(4)	2.259(3)
O(1)-Mn(1)-O(1)#1	179.999(1)	O(1)-Mn(1)-O(1W)#1	90.68(9)
O(1)-Mn(1)-O(1W)	89.32(9)	O(1W)#1-Mn(1)-O(1W)	179.998(1)
O(1)-Mn(1)-N(1)#1	91.58(9)	O(1W)-Mn(1)-N(1)#1	85.65(10)
O(1)-Mn(1)-N(1)	88.43(9)	O(1W)#1-Mn(1)-N(1)	85.65(10)
O(1W)-Mn(1)-N(1)	94.35(10)	N(1)#1-Mn(1)-N(1)	179.999(1)
O(3)#2-Mn(2)-O(3)	180.00(12)	O(3)-Mn(2)-O(2W)#2	92.32(9)
O(3)-Mn(2)-O(2W)	87.68(9)	O(2W)#2-Mn(2)-O(2W)	180.000(1)
O(3)#2-Mn(2)-N(4)	90.99(10)	O(3)-Mn(2)-N(4)	89.01(10)
O(2W)#2-Mn(2)-N(4)	91.71(11)	O(2W)-Mn(2)-N(4)	88.29(11)
N(4)-Mn(2)-N(4)#2	180.00(16)		

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Mn(1)-O(4)#1	2.0714(13)	Mn(1)-N(2)	2.2164(16)
Mn(1)-O(1)#2	2.2180(13)	Mn(1)-O(2)#2	2.2699(13)
Mn(1)-N(4)	2.2920(15)	Mn(1)-N(3)	2.3162(16)
O(4)#1-Mn(1)-N(2)	90.76(6)	O(4)#1-Mn(1)-O(1)#2	114.70(5)
N(2)-Mn(1)-O(1)#2	98.78(6)	O(4)#1-Mn(1)-O(2)#2	172.43(5)
N(2)-Mn(1)-O(2)#2	86.78(6)	O(1)#2-Mn(1)-O(2)#2	58.75(5)
O(4)#1-Mn(1)-N(4)	96.50(6)	N(2)-Mn(1)-N(4)	100.75(6)
O(1)#2-Mn(1)-N(4)	142.73(5)	O(2)#2-Mn(1)-N(4)	90.99(5)
O(4)#1-Mn(1)-N(3)	90.90(6)	N(2)-Mn(1)-N(3)	172.45(6)
O(1)#2-Mn(1)-N(3)	87.21(6)	O(2)#2-Mn(1)-N(3)	92.46(6)
N(4)-Mn(1)-N(3)	71.75(5)		

Symmetry transformation used to generate equivalent atoms: (**1**) #1 *x*+1, *y*, *z*; #2 *x*, -*y*+1/2, *z*+1/2; (**2**) #1 *x*, *y*+1, *z*; #2 -*x*+2, -*y*+1, -*z*+2; (**3**) #1 *x*, -*y*+1/2, *z*-1/2; #2 *x*, -*y*-1/2, *z*-1/2; (**4**) #1 -*x*, -*y*+2, -*z*+1; #2 -*x*+1, -*y*+2, -*z*; (**5**) #1 -*x*+2, -*y*+2, -*z*+1; #2 -*x*+2, -*y*+1, -*z*+1; (**6**) #1 -*x*+1, *y*+1/2, -*z*+1/2; #2 -*x*, *y*+1/2, -*z*+1/2.