

Electronic Supplementary Information (ESI)

Structural Diversity and Luminescent Properties of Coordination Polymers Based on 2,5-Bis(Imidazol-1-yl)Thiophene (Thim₂) and Aromatic Multicarboxylates

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Table S1. Selected bond distances (\AA) and angles($^\circ$) for CPs **1-7**

1				
Zn(1)-O(1)	1.949(4)	Zn(1)-O(3)	1.971(4)	Zn(1)-N(1) 2.014(4)
				Zn(1)-N(4) 2.018(5)
O(1)-Zn(1)-O(3)#1	107.76(16)	O(3)#1-Zn(1)-N(1)	95.51(17)	O(3)#1-Zn(1)-N(4)#2 110.55(18)
O(1)-Zn(1)-N(1)	122.23(17)	O(1)-Zn(1)-N(4)#2	114.47(18)	N(1)-Zn(1)-N(4)#2 104.57(19)
#1= x+1/2,-y+1/2,z+1/2, #2 -x+1/2,y+1/2,-z+5/2				
2				
Co(1)-O(2)	1.966(2)	Co(1)-O(3)#1	2.015(3)	Co(1)-N(1) 2.040(3)
				Co(1)-N(4)#2 2.046(3)
O(2)-Co(1)-O(3)#1	97.68(10)	O(3)#1-Co(1)-N(1)	121.00(12)	O(3)#1-Co(1)-N(4)#2 111.77(11)
O(2)-Co(1)-N(1)	105.75(11)	O(2)-Co(1)-N(4)#2	115.81(11)	N(1)-Co(1)-N(4)#2 105.13(11)
#1 x+1,y,z , #2 -x+3/2,-y+1,z+1/2				
3				
Co(1)-O(1)	1.967(4)	Co(1)-O(5)#1	1.989(4)	Co(1)-N(4)#2 2.011(4)
				Co(1)-N(1) 2.044(5)
O(1)-Co(1)-O(5)#1	107.28(17)	O(5)#1-Co(1)-N(4)#2	116.83(18)	O(5)#1-Co(1)-N(1) 106.90(18)
O(1)-Co(1)-N(4)#2	107.95(18)	O(1)-Co(1)-N(1)	95.17(17)	N(4)#2-Co(1)-N(1) 119.95(19)
#1 x+1/2,-y+1/2,z+1/2 #2 -x+3/2,y-1/2,-z+3/2				
4				
Zn(1)-O(1)	1.959(5)	Zn(1)-O(5)#1	1.976(5)	Zn(1)-N(1) 1.986(5)
				Zn(1)-N(4)#2 2.017(6)
O(1)-Zn(1)-O(5)#1	109.2(2)	O(5)#1-Zn(1)-N(1)	114.9(2)	O(5)#1-Zn(1)-N(4)#2 106.0(2)
O(1)-Zn(1)-N(1)	110.1(2)	O(1)-Zn(1)-N(4)#2	96.2(2)	N(1)-Zn(1)-N(4)#2 118.6(2)
#1 x-1/2,-y+1/2,z+1/2 #2 -x+1/2,y+1/2,-z+1/2				
5				
Co(1)-O(4)#1	1.979(2)	Co(1)-O(1)	1.998(2)	Co(1)-N(4)#2 2.029(3)
				Co(1)-N(1) 2.052(3)
O(4)#1-Co(1)-O(1)	102.13(10)	O(1)-Co(1)-N(4)#2	122.84(11)	O(1)-Co(1)-N(1) 113.38(10)
O(4)#1-Co(1)-N(4)#2	112.22(10)	O(4)#1-Co(1)-N(1)	94.80(10)	N(4)#2-Co(1)-N(1) 107.78(11)
#1 x+1/2,-y+5/2,z+1/2 #2 x,y+1,z				
6				

Zn(1)-O(1)	1.963(3)	Zn(1)-O(4)#1	1.963(2)	Zn(1)-N(1)	2.010(3)
O(1)-Zn(1)-O(4)#1	105.04(11)	O(4)#1-Zn(1)-N(1)	114.84(11)	Zn(1)-N(4)#2	2.041(3)
O(1)-Zn(1)-N(1)	117.06(12)	O(1)-Zn(1)-N(4)#2	115.96(12)	O(4)#1-Zn(1)-N(4)#2	95.01(11)
O(4)-Zn(1)-N(1)		O(4)-Zn(1)-N(4)#2		N(1)-Zn(1)-N(4)#2	107.01(12)
#1 x-1/2,-y+3/2,z-1/2 #2 x,y+1,z					
7					
Mn(1)-O(1)	2.125(3)	Mn(1)-O(7)#2	2.295(3)	Mn(2)-O(6)	2.203(3)
Mn(1)-O(5)	2.135(3)	Mn(1)-O(8)#2	2.350(3)	Mn(2)-O(9W)	2.204(3)
Mn(1)-N(1)	2.238(3)	Mn(2)-O(2)	2.119(3)	Mn(2)-N(5)	2.254(3)
Mn(1)-N(8)#1	2.263(3)	Mn(2)-O(4)#3	2.182(3)	Mn(2)-N(4)#4	2.273(3)
O(1)-Mn(1)-O(5)	114.29(11)	O(1)-Mn(1)-O(8)#2	158.10(10)	O(6)-Mn(2)-O(9W)	102.14(11)
O(1)-Mn(1)-N(1)	89.65(11)	O(5)-Mn(1)-O(8)#2	86.57(10)	O(2)-Mn(2)-N(5)	98.11(11)
O(5)-Mn(1)-N(1)	100.01(11)	N(1)-Mn(1)-O(8)#2	93.28(11)	O(4)#3-Mn(2)-N(5)	98.14(12)
O(1)-Mn(1)-N(8)#1	82.55(11)	N(8)#1-Mn(1)-O(8)#2	88.06(11)	O(6)-Mn(2)-N(5)	90.29(12)
O(5)-Mn(1)-N(8)#1	98.37(11)	O(7)#2-Mn(1)-O(8)#2	56.55(10)	O(9W)-Mn(2)-N(5)	82.86(12)
N(1)-Mn(1)-N(8)#1	161.62(12)	O(2)-Mn(2)-O(4)#3	84.85(11)	O(2)-Mn(2)-N(4)#4	89.14(11)
O(1)-Mn(1)-O(7)#2	102.31(10)	O(2)-Mn(2)-O(6)	89.34(10)	O(4)#3-Mn(2)-N(4)#4	89.95(12)
O(5)-Mn(1)-O(7)#2	143.12(11)	O(4)#3-Mn(2)-O(6)	170.35(10)	O(6)-Mn(2)-N(4)#4	82.25(12)
N(1)-Mn(1)-O(7)#2	84.02(10)	O(2)-Mn(2)-O(9W)	168.48(11)	O(9W)-Mn(2)-N(4)#4	91.55(12)
N(8)#1-Mn(1)-O(7)#2	81.45(11)	O(4)#3-Mn(2)-O(9W)	83.65(11)	N(5)-Mn(2)-N(4)#4	169.56(12)
#1 -x,-y,-z+1, #2 x,y-1,z , #3 -x+1,-y+1,-z , #4 -x+2,-y+1,-z					

Table S2. C–H···O interactions present in **1** and **5–6**

Compound no.	D–H···A	H···A Å	D···A Å	D–H···A (°)
1	C3– H3···O4	2.289(9)	3.203(1)	167.00(2)
	C5– H5···O4	2.596(6)	3.496(7)	163.01(5)
5	C9– H9···O5	2.486(3)	3.247(1)	139.12(1)
6	C3– H3···O5	2.464(2)	3.220(8)	138.51(0)

Table S3. hydrogen bonding interactions present in **3-4**

Compound no.	$D\text{--H}\cdots\text{A}$	$\text{H}\cdots\text{A}$ Å	$D\cdots\text{A}$ Å	$D\text{--H}\cdots\text{A}$ (°)
3	$\text{O}3^-\text{H}3\cdots\text{O}4$	1.83(5)	2.63(5)	173.49(5)
4	$\text{O}4^-\text{H}4\cdots\text{O}3$	1.82(5)	2.62(3)	158.40(5)

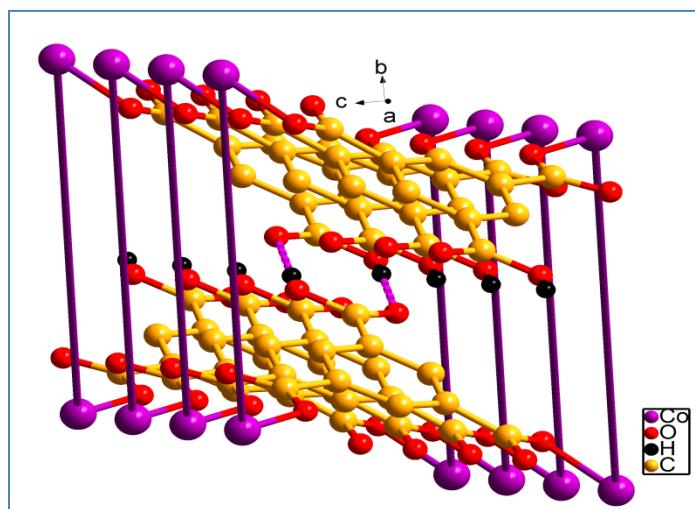


Figure S1. Hydrogen bonding interactions between carboxylate groups (thim₂ ligand has been omitted for clarity)

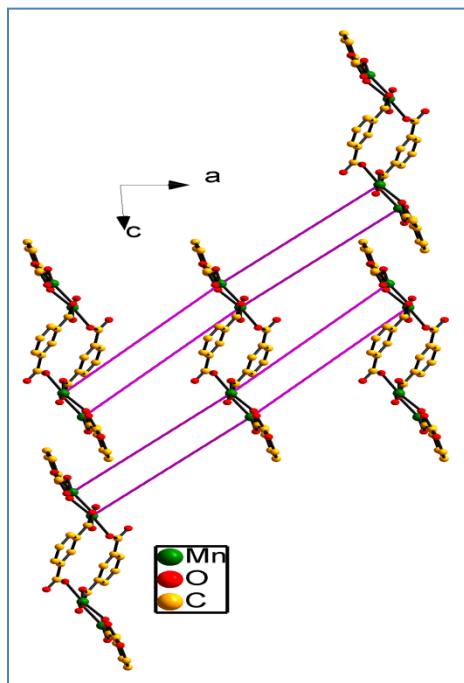


Figure S2. View of Connected neighboring 1D chains (thim₂ ligand has been omitted for clarity)

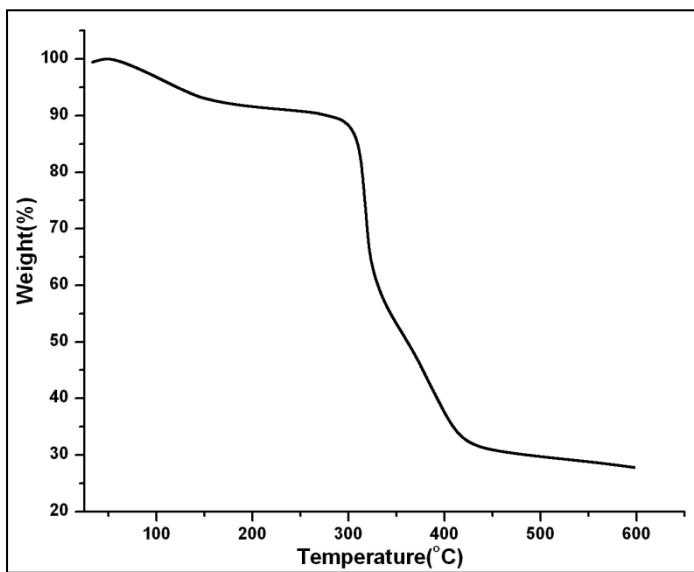


Figure S3. Thermogravimetric analysis of **1**.

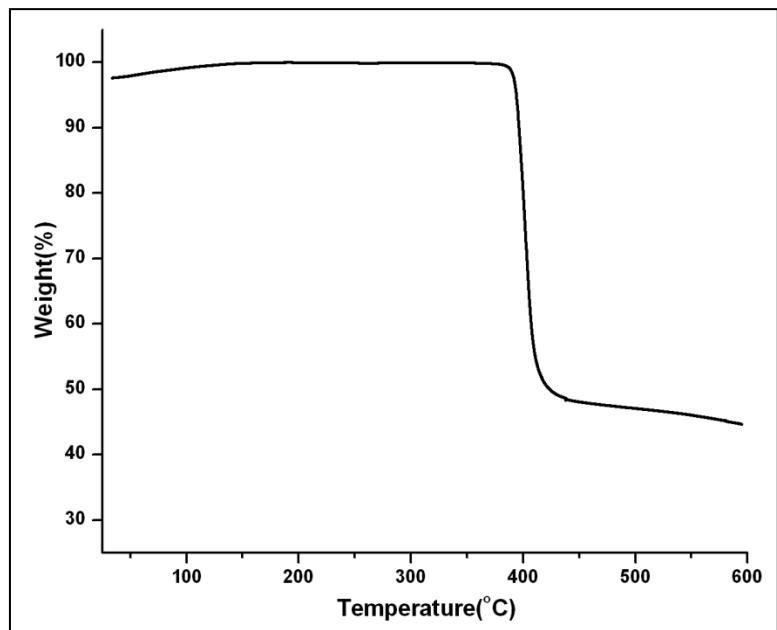


Figure S4. Thermogravimetric analysis of **2**.

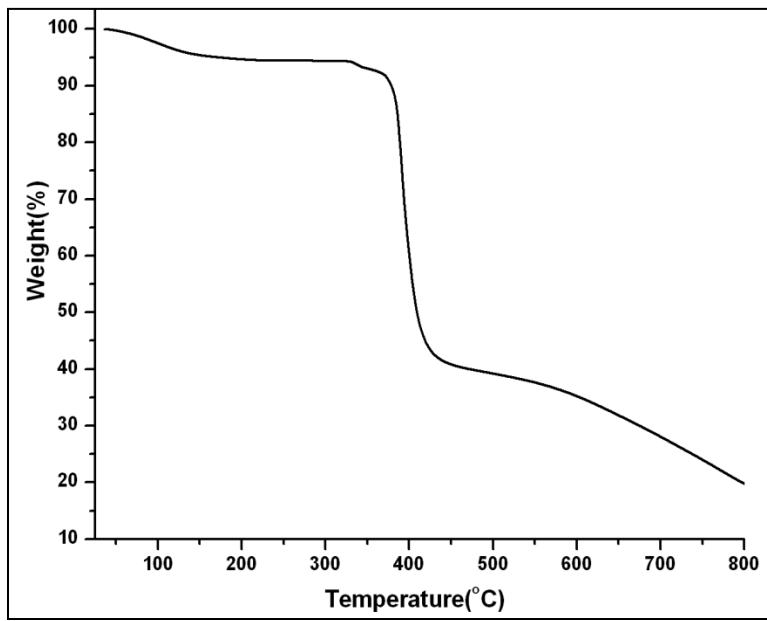


Figure S5. Thermogravimetric analysis of **3**.

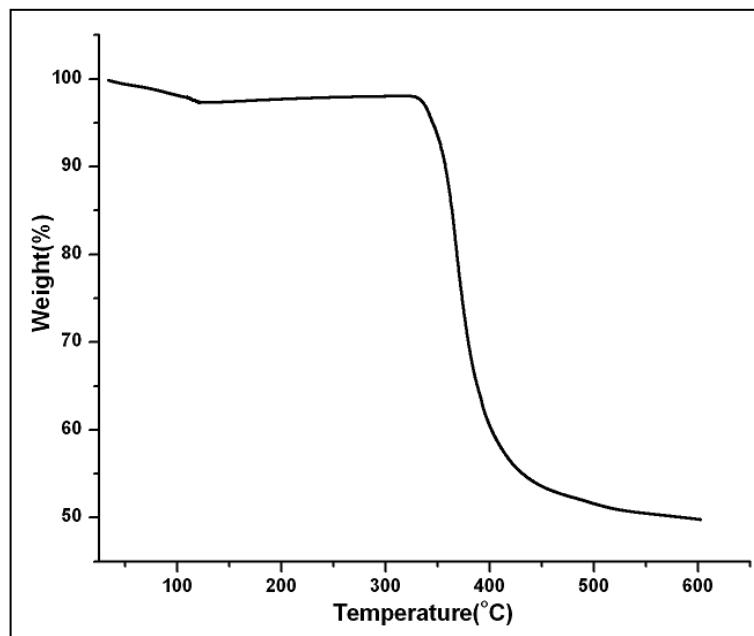


Figure S6. Thermogravimetric analysis of **4**.

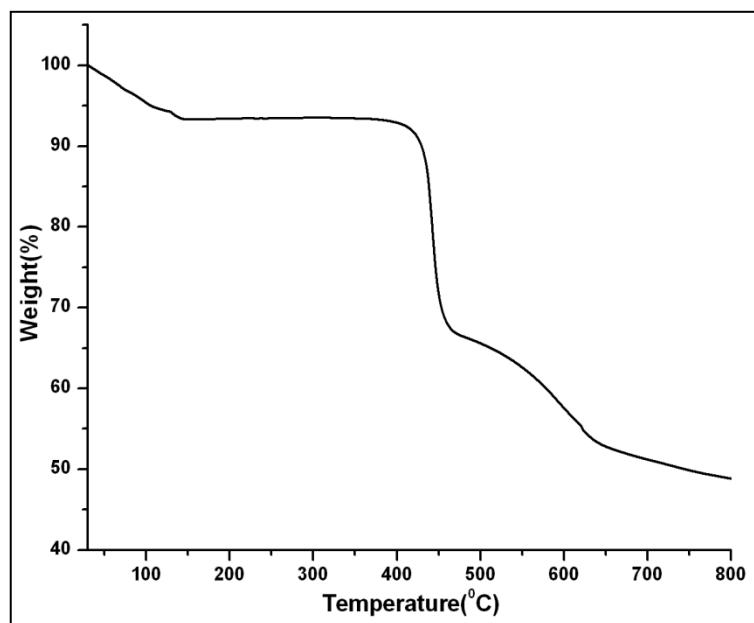


Figure S7. Thermogravimetric analysis of **5**.

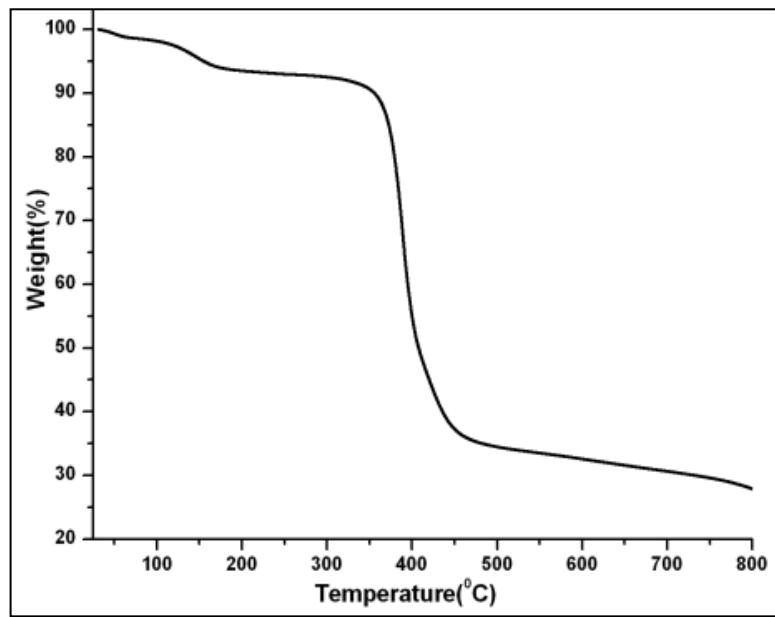


Figure S8. Thermogravimetric analysis of **6**.

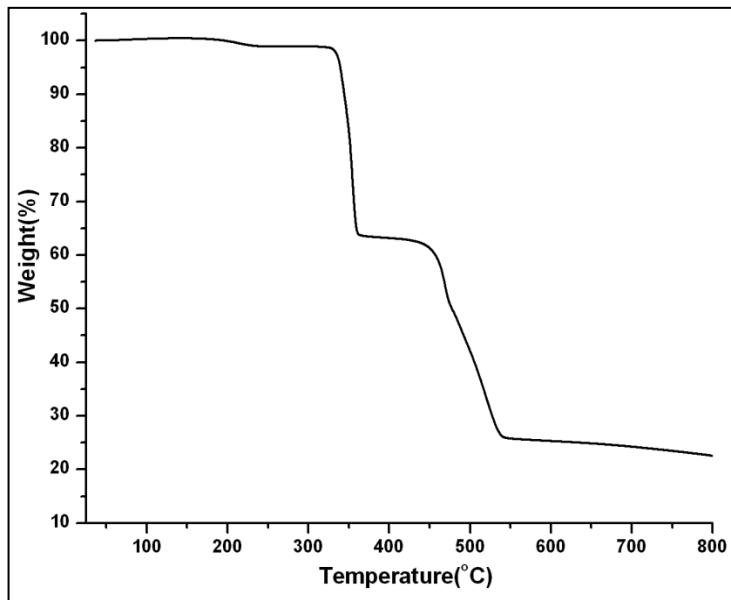


Figure S9. Thermogravimetric analysis of 7.

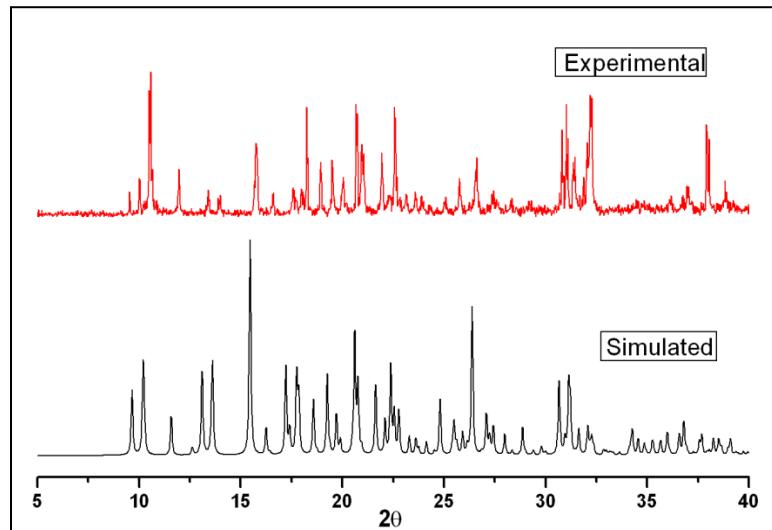


Figure S10. PXRD of complex 1

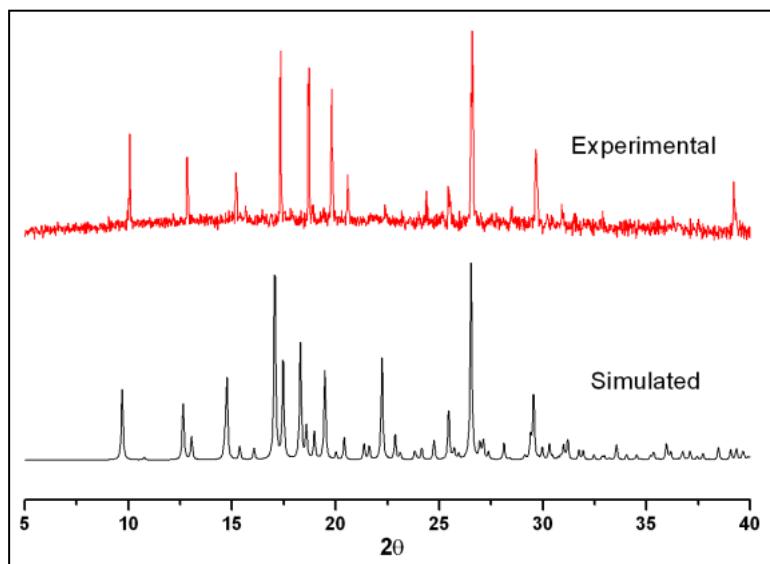


Figure S11. PXRD of complex 2

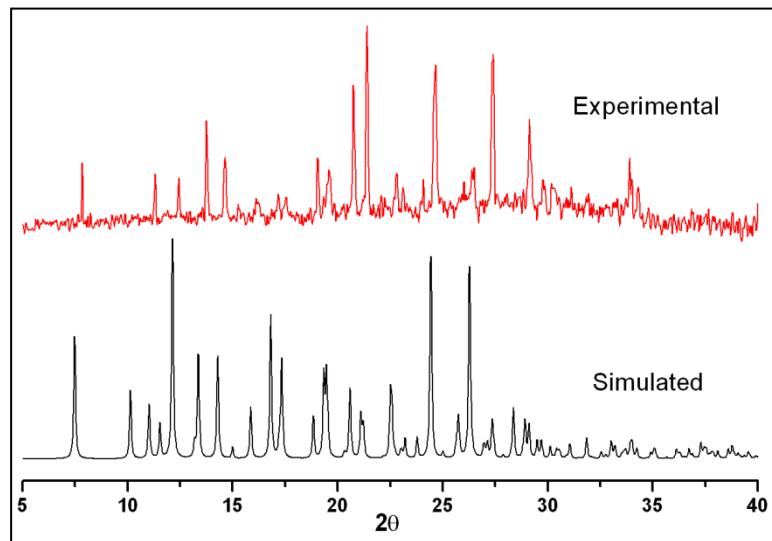


Figure S12. PXRD of complex 3

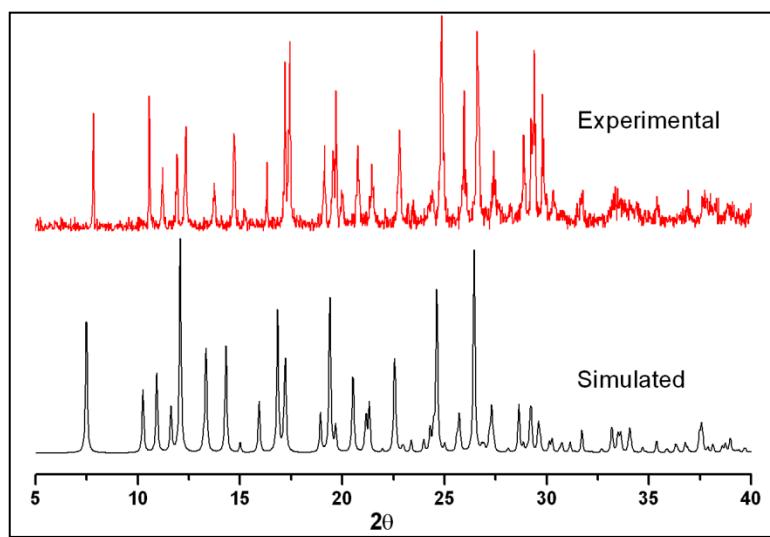


Figure S13. PXRD of complex 4

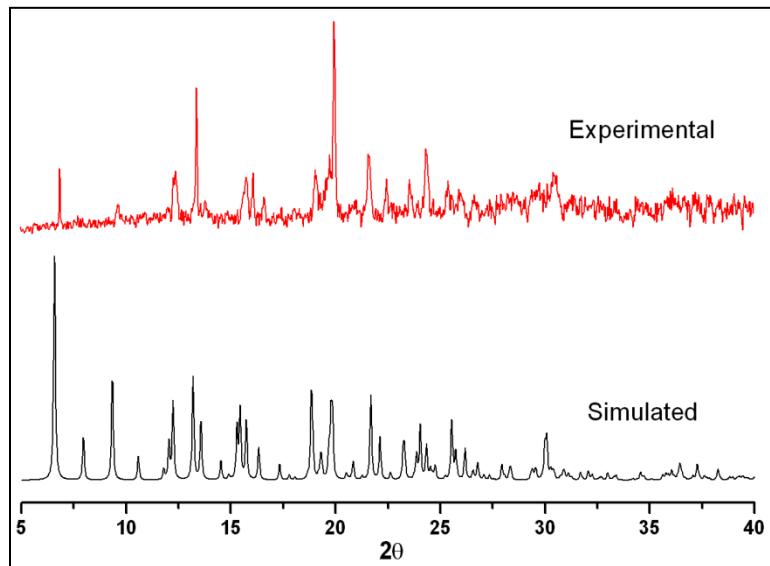


Figure S14. PXRD of complex 5

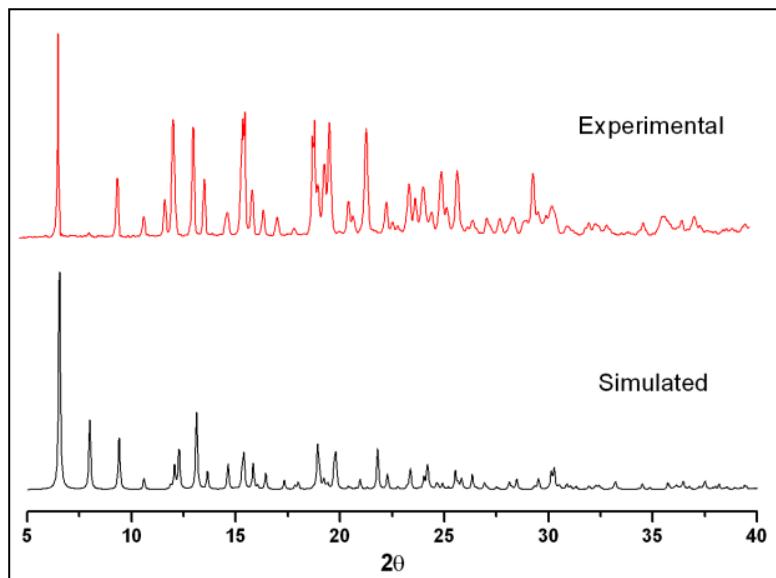


Figure S15. PXRD of complex 6

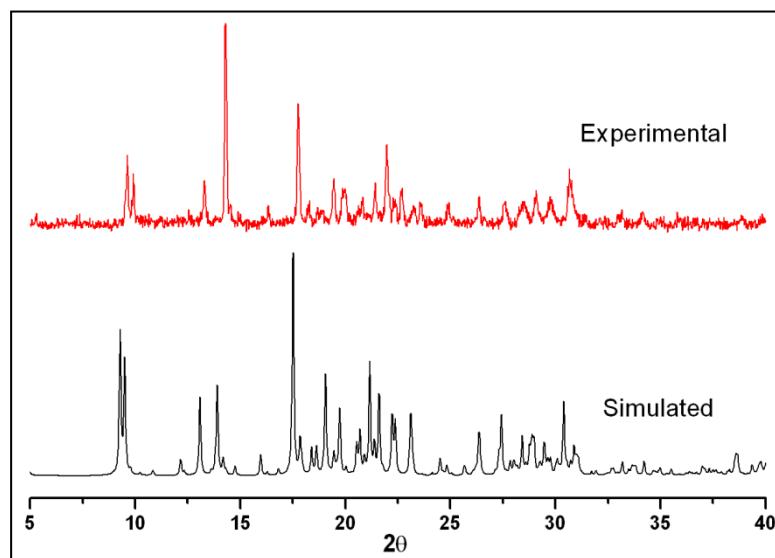


Figure S16. PXRD of complex 7