Syntheses, Structures, and Properties of A Series of 2D and 3D Coordination Polymers Based on Trifunctional Pyridine-dicarboxylate and Different (Bis)imidazole Bridging Ligands

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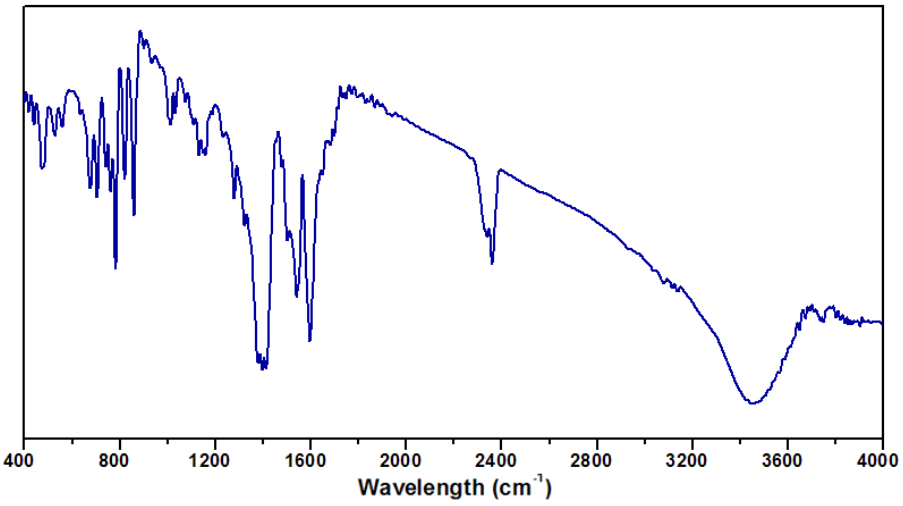
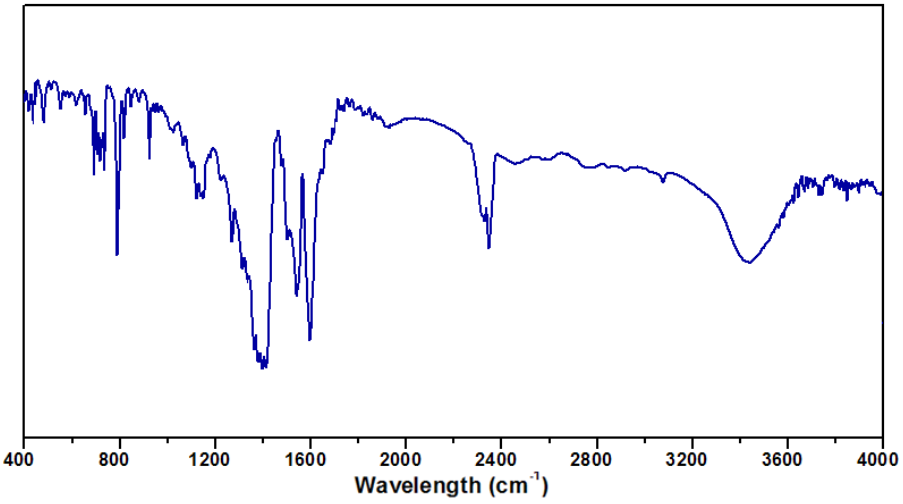
Table S1 Selected bond lengths (Å) and angles (°) for **1 – 10**.

Complex **1**							
Co(1)-O(1)	1.971(3)	Co(1)-N(2)	2.037(4)	Co(1)-N(3)$^{\#3}$	2.076(3)	Co(1)-O(3)$^{\#4}$	2.110(3)
Co(1)-O(4)$^{\#4}$	2.159(3)	O(1)-Co(1)-N(2)	104.93(13)	O(1)-Co(1)-N(3)$^{\#3}$	103.37(13)	O(3)$^{\#4}$-Co(1)-O(4)$^{\#4}$	59.51(13)
O(1)-Co(1)-O(4)$^{\#4}$	94.62(13)	N(2)-Co(1)-O(4)$^{\#4}$	105.49(14)	N(2)-Co(1)-N(3)$^{\#3}$	94.02(12)	N(3)$^{\#3}$-Co(1)-O(4)$^{\#4}$	149.09(14)
N(2)-Co(1)-O(3)$^{\#4}$	99.47(14)	O(1)-Co(1)-O(3)$^{\#4}$	148.59(15)				
Symmetry codes: #1 *x*-1/2, -*y*-1/2, *z*-1/2. #2 -*x*+2, *y*, -*z*+3/2. #3 *x*+1/2, *y*+1/2, *z*. #4 *x*+1/2, -*y*-1/2, *z*+1/2. #5 *x*-1/2, *y*-1/2, *z*.							
Complex **2**							
Cu(1)-O(4)$^{\#3}$	1.942(3)	Cu(1)-N(1)	2.028(3)	Cu(1)-O(2)$^{\#4}$	2.034(3)	Cu(1)-O(1)$^{\#4}$	2.093(3)
Cu(1)-N(2)	2.156(4)	O(4)$^{\#3}$-Cu(1)-N(1)	98.84(13)	N(1)-Cu(1)-O(2)$^{\#4}$	153.58(14)	O(4)$^{\#3}$-Cu(1)-O(1)$^{\#4}$	148.46(14)
O(1)$^{\#4}$-Cu(1)-N(2)	98.64(14)	N(1)-Cu(1)-O(1)$^{\#4}$	95.35(13)	O(4)$^{\#3}$-Cu(1)-N(2)	108.74(14)	O(4)$^{\#3}$-Cu(1)-O(2)$^{\#4}$	93.52(13)
N(1)-Cu(1)-N(2)	92.22(14)	O(2)$^{\#4}$-Cu(1)-N(2)	105.82(14)	O(1)$^{\#4}$-Cu(1)-N(2)	98.64(14)	O(2)$^{\#4}$-Cu(1)-O(1)$^{\#4}$	63.44(12)
Symmetry codes: #1 *x*, -*y*+1, *z*+1/2. #2 -*x*+1, *y*, -*z*+3/2. #3 *x*+1/2, *y*-1/2, *z*. #4 *x*, -*y*+1, *z*-1/2. #5 *x*-1/2, *y*+1/2, *z*.							
Complex **3**							
N(1)-Ni(1)	2.070(3)	N(2)-Ni(1)	2.047(3)	Ni(1)-O(4)$^{\#4}$	2.022(2)	Ni(1)-O(1)$^{\#5}$	2.061(3)
Ni(1)-O(2)$^{\#5}$	2.138(3)	Ni(1)-O(3)$^{\#4}$	2.342(3)	O(4)$^{\#4}$-Ni(1)-N(2)	98.92(11)	O(4)$^{\#4}$-Ni(1)-O(1)$^{\#5}$	155.41(11)
N(2)-Ni(1)-O(1)$^{\#5}$	99.18(12)	N(2)-Ni(1)-O(3)$^{\#4}$	158.92(11)	N(2)-Ni(1)-N(1)	91.64(12)	O(4)$^{\#4}$-Ni(1)-O(2)$^{\#5}$	97.58(11)
O(1)$^{\#5}$-Ni(1)-N(1)	96.12(11)	N(2)-Ni(1)-O(2)$^{\#5}$	101.65(12)	N(1)-Ni(1)-O(2)$^{\#5}$	156.13(11)	O(1)$^{\#5}$-Ni(1)-O(2)$^{\#5}$	62.46(10)
O(4)$^{\#4}$-Ni(1)-N(1)	99.85(12)	O(1)$^{\#5}$-Ni(1)-O(3)$^{\#4}$	101.50(10)	N(1)-Ni(1)-O(3)$^{\#4}$	90.16(11)	O(2)$^{\#5}$-Ni(1)-O(3)$^{\#4}$	84.50(10)
Symmetry codes: #1 *x*, -*y*+1, *z*+1/2. #2 *x*-1/2, *y*+1/2, *z*. #3 -*x*, *y*, -*z*+1/2. #4 *x*+1/2, *y*-1/2, *z*. #5 *x*, -*y*+1, *z*-1/2.							
Complex **4**							
Co(1)-O(4)$^{\#2}$	2.066(7)	Co(1)-O(2)	2.067(6)	Co(1)-N(2)	2.089(7)	Co(1)-O(5)	2.098(7)
Co(1)-N(1)$^{\#3}$	2.145(8)	Co(1)-O(6)	2.1495(13)	O(4)$^{\#2}$-Co(1)-O(2)	86.9(3)	O(4)$^{\#2}$-Co(1)-N(2)	91.4(3)
O(2)-Co(1)-N(2)	173.8(3)	O(4)$^{\#2}$-Co(1)-O(5)	174.6(3)	O(2)-Co(1)-O(5)	87.6(3)	N(2)-Co(1)-O(5)	94.1(3)
O(4)$^{\#2}$-Co(1)-N(1)$^{\#3}$	87.3(4)	O(2)-Co(1)-N(1)$^{\#3}$	90.5(3)	N(2)-Co(1)-N(1)$^{\#3}$	95.4(3)	O(5)-Co(1)-N(1)$^{\#3}$	92.3(4)
O(4)$^{\#2}$-Co(1)-O(6)	94.4(3)	O(2)-Co(1)-O(6)	85.1(2)	N(2)-Co(1)-O(6)	89.2(2)	O(5)-Co(1)-O(6)	85.5(3)
N(1)$^{\#3}$-Co(1)-O(6)	175.1(3)						
Symmetry code: #1-*x*-1/2, -*y*+3/2, -*z*-1. #2 –*x*+1/2, -*y*+3/2, -*z*+1. #3 –*x*+1/2, *y*+1/2, -*z*+1/2. #4 –*x*+1/2, *y*-1/2, -*z*+1/2. #5 –*x*, –*y*+1, -*z*.							
Complex **5**							
Cu(1)-O(1)$^{\#2}$	1.938(4)	Cu(1)-N(1)	2.320(5)	Cu(1)-O(5)	1.968(4)	Cu(1)-N(2)	1.988(5)
Cu(1)-O(4)$^{\#3}$	1.975(4)	O(1)$^{\#2}$-Cu(1)-N(1)	91.27(18)	O(1)$^{\#2}$-Cu(1)-O(5)	90.61(17)	O(4)$^{\#3}$-Cu(1)-O(5)	174.43(19)
O(1)$^{\#2}$-Cu(1)-N(2)	173.97(2)	O(4)$^{\#3}$-Cu(1)-N(2)	90.26(18)	O(5)-Cu(1)-N(2)	91.08(19)	O(1)$^{\#2}$-Cu(1)-O(4)$^{\#3}$	87.52(17)
O(4)$^{\#3}$-Cu(1)-N(1)	86.92(18)	O(5)-Cu(1)-N(1)	98.36(19)	N(2)-Cu(1)-N(1)	94.21(19)		
Symmetry code: #1 -*x*-1/2, -*y*+3/2, -*z*. #2 -*x*+1/2, *y*-1/2, -*z*+3/2. #3 *x*, -*y*+2, *z*+1/2. #4 -*x*+1/2, *y*+1/2, -*z*+3/2. #5 *x*, -*y*+2, *z*-1/2.							
Complex **6**							
Ni(1)-N(4)$^{\#1}$	2.062(6)	Ni(1)-O(1)	2.069(4)	Ni(1)-O(1W)	2.082(4)	Ni(1)-O(3)$^{\#2}$	2.088(4)
Ni(1)-N(1)	2.093(6)	Ni(1)-N(5)$^{\#3}$	2.113(5)	O(3)-Ni(1)$^{\#4}$	2.088(3)	N(5)-Ni(1)$^{\#3}$	2.113(5)
N(4)-Ni(1)$^{\#5}$	2.062(6)	N(4)$^{\#1}$-Ni(1)-O(1)	90.0(2)	O(1)-Ni(1)-O(3)$^{\#2}$	178.48(17)	O(1)-Ni(1)-O(1W)	86.88(16)
N(4)$^{\#1}$-Ni(1)-N(1)	176.9(2)	O(1)-Ni(1)-N(1)	90.3(2)	O(3)$^{\#2}$-Ni(1)-N(1)	90.85(19)	N(4)$^{\#1}$-Ni(1)-O(1W)	90.4(2)
O(1W)-Ni(1)-N(1)	92.7(2)	O(1)-Ni(1)-N(5)$^{\#3}$	90.17(17)	N(1)-Ni(1)-N(5)$^{\#3}$	89.9(2)	O(1W)-Ni(1)-O(3)$^{\#2}$	92.05(16)
Symmetry code: #1 -*x*+1/2, *y*-1/2, -*z*-1/2. #2 *x*-1/2, -*y*+3/2, *z*-1/2. #3 -*x*+1, -*y*+1, -*z*. #4 *x*+1/2, -*y*+3/2, *z*+1/2. #5 -*x*+1/2, *y*+1/2, -*z*-1/2.							
Complex **7**							
Co(1)-O(1)$^{\#3}$	2.018(2)	Co(1)-N(5)	2.142(2)	Co(1)-N(1)	2.147(3)	Co(1)-O(3)$^{\#4}$	2.150(2)
Co(1)-N(3)	2.163(3)	Co(1)-O(4)$^{\#4}$	2.268(2)	O(1)-Co(1)$^{\#5}$	2.018(2)	O(3)-Co(1)$^{\#6}$	2.150(2)
O(4)-Co(1)$^{\#6}$	2.268(2)	O(1)$^{\#3}$-Co(1)-N(5)	113.70(10)	O(1)$^{\#3}$-Co(1)-N(1)	87.49(10)	O(1)$^{\#3}$-Co(1)-O(3)$^{\#4}$	154.87(10)
N(3)-Co(1)-O(4)$^{\#4}$	87.87(10)	N(5)-Co(1)-O(3)$^{\#4}$	91.26(9)	N(1)-Co(1)-O(3)$^{\#4}$	91.06(10)	O(1)$^{\#3}$-Co(1)-N(3)	94.69(10)
N(5)-Co(1)-N(3)	96.06(11)	N(1)-Co(1)-N(3)	174.95(10)	O(3)$^{\#4}$-Co(1)-N(3)	85.03(10)	O(1)$^{\#3}$-Co(1)-O(4)$^{\#4}$	95.48(9)
N(5)-Co(1)-O(4)$^{\#4}$	150.02(9)	N(1)-Co(1)-O(4)$^{\#4}$	87.39(9)	N(5)-Co(1)-N(1)	87.19(10)	O(3)$^{\#4}$-Co(1)-O(4)$^{\#4}$	59.39(8)
Symmetry code: #1 -*x*+2, -*y*+2, -*z*. #2 -*x*+1, -*y*, -*z*+2. #3 *x*+1, *y*, *z*. #4 *x*, *y*-1, *z*. #5 *x*-1, *y*, *z*. #6 *x*, *y*+1, *z*.							
Complex **8**							
Mn(1)-O(5)	2.182(3)	Mn(1)-O(2)	2.186(3)	Mn(1)-O(1W)	2.223(2)	Mn(1)-N(1)$^{\#1}$	2.245(3)
Mn(1)-O(4)$^{\#2}$	2.244(3)	Mn(1)-O(3)$^{\#2}$	2.374(3)	N(1)-Mn(1)$^{\#3}$	2.245(3)	O(2)-Mn(1)-O(3)$^{\#2}$	136.90(10)
O(5)-Mn(1)-O(4)$^{\#2}$	90.47(12)	O(5)-Mn(1)-O(1W)	173.78(10)	O(5)-Mn(1)-O(2)	94.19(12)	O(2)-Mn(1)-N(1)$^{\#1}$	137.05(10)
O(5)-Mn(1)-N(1)$^{\#1}$	87.23(12)	O(2)-Mn(1)-O(1W)	85.19(10)	O(2)-Mn(1)-O(4)	81.72(11)	O(1W)-Mn(1)-N(1)$^{\#1}$	89.01(9)
Symmetry code: #1 *x*+1/2, *y*+1/2, *z*. #2 *x*, *y*+1, *z*. #3 *x*-1/2, *y*-1/2, *z*. #4 *x*, *y*-1, *z*.							
Complex **9**							
N(1)-Ni(1)$^{\#3}$	2.068(4)	N(2)-Ni(1)	2.078(4)	Ni(1)-O(1)	2.013(3)	Ni(1)-N(1)$^{\#4}$	2.068(4)
Ni(1)-O(5)	2.077(4)	Ni(1)-O(3)$^{\#5}$	2.104(3)	Ni(1)-O(4)$^{\#5}$	2.195(3)	O(3)-Ni(1)$^{\#1}$	2.104(3)
O(4)-Ni(1)$^{\#1}$	2.195(3)	O(1)-Ni(1)-N(1)$^{\#4}$	98.64(16)	O(1)-Ni(1)-N(2)	83.85(15)	N(1)$^{\#4}$-Ni(1)-N(2)	91.38(16)
O(1)-Ni(1)-O(5)	90.47(14)	N(1)$^{\#4}$-Ni(1)-O(5)	91.16(15)	N(2)-Ni(1)-O(5)	174.07(15)	O(3)$^{\#5}$-Ni(1)-O(4)$^{\#5}$	61.33(12)
N(2)-Ni(1)-O(3)$^{\#5}$	97.81(15)	O(5)-Ni(1)-O(3)$^{\#5}$	87.09(14)	O(1)-Ni(1)-O(4)$^{\#5}$	101.13(14)	N(1)$^{\#4}$-Ni(1)-O(3)$^{\#5}$	98.92(14)
N(2)-Ni(1)-O(4)$^{\#5}$	90.79(15)	O(1)-Ni(1)-O(3)$^{\#5}$	162.32(14)	O(5)-Ni(1)-O(4)$^{\#5}$	88.63(14)	N(1)$^{\#4}$-Ni(1)-O(4)$^{\#5}$	160.23(14)
Symmetry codes: #1 *x*+1/2, -*y*+1/2, *z*+1/2. #2 -*x*, -*y*+1, -*z*+1. #3 *x*, -*y*+1, *z*+1/2. #4 *x*, -*y*+1, *z*-1/2. #5 *x*-1/2, -*y*+1/2, *z*-1/2.							
Complex **10**							
N(4)-Cu(1)$^{\#1}$	1.996(5)	Cu(1)-O(4)	1.961(3)	Cu(1)-O(1)$^{\#2}$	1.968(3)	Cu(1)-N(1)	1.989(5)
Cu(1)-N(4)$^{\#3}$	1.996(5)	Cu(1)-N(5)$^{\#4}$	2.340(4)	N(5)-Cu(1)$^{\#4}$	2.340(4)	N(4)$^{\#3}$-Cu(1)-N(5)$^{\#4}$	103.51(19)
O(4)-Cu(1)-N(1)	89.03(17)	O(4)-Cu(1)-O(1)$^{\#2}$	176.11(15)	O(1)$^{\#2}$-Cu(1)-N(1)	93.42(17)	O(1)$^{\#2}$-Cu(1)-N(5)$^{\#4}$	88.61(15)
O(4)-Cu(1)-N(4)$^{\#3}$	89.79(18)	N(1)-Cu(1)-N(4)$^{\#3}$	158.2(2)	O(4)-Cu(1)-N(5)$^{\#4}$	88.05(15)	O(1)$^{\#2}$-Cu(1)-N(4)$^{\#3}$	89.05(17)
Symmetry codes: #1 *x*-1/2, -*y*+3/2, -*z*. #2 -*x*+1, *y*-1/2, -*z*+1/2. #3 *x*+1/2, -*y*+3/2, -*z*. #4 -*x*+1, -*y*+2, -*z*+1. #5 -*x*+1, *y*+1/2, -*z*+1/2.							



(a)



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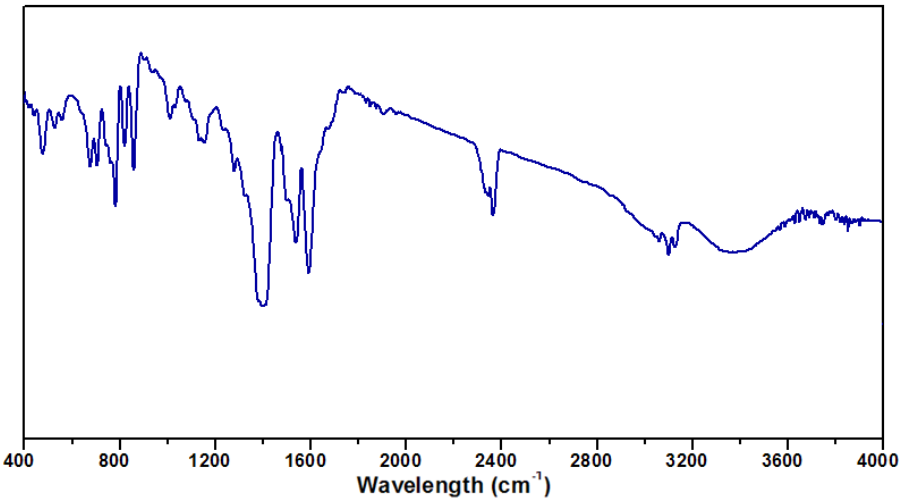

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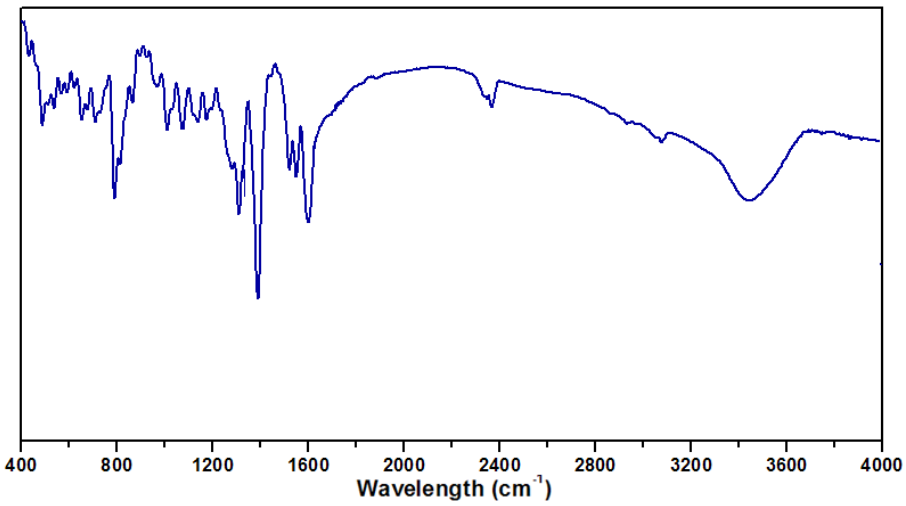

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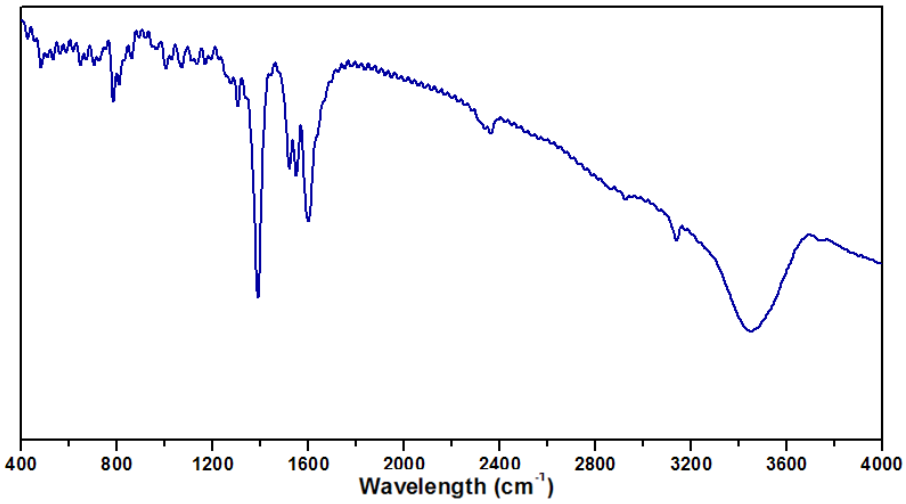

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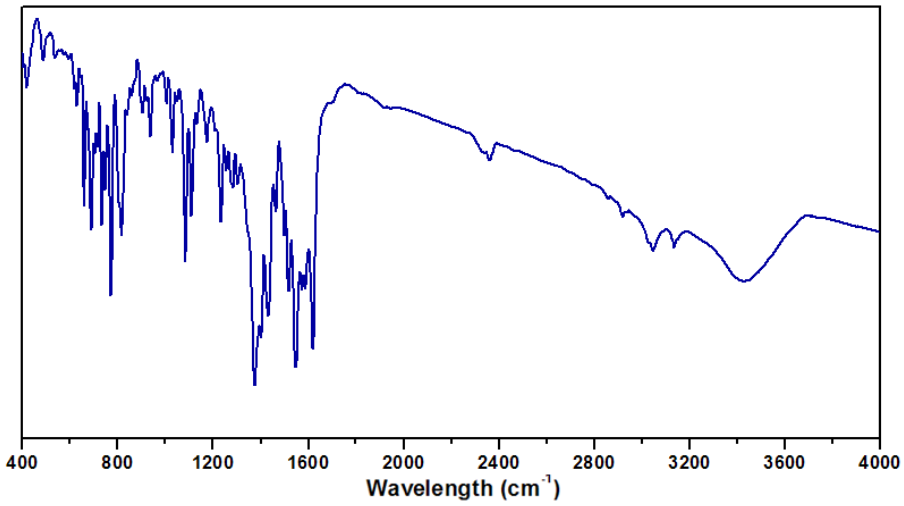
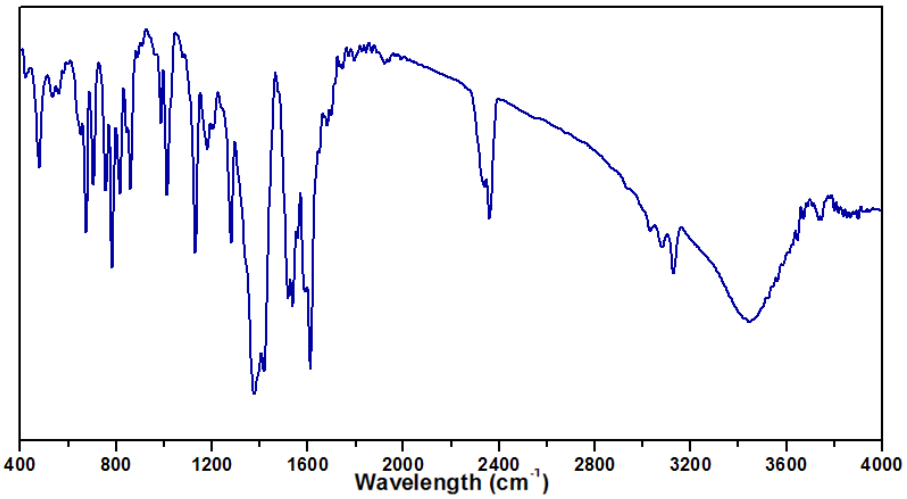
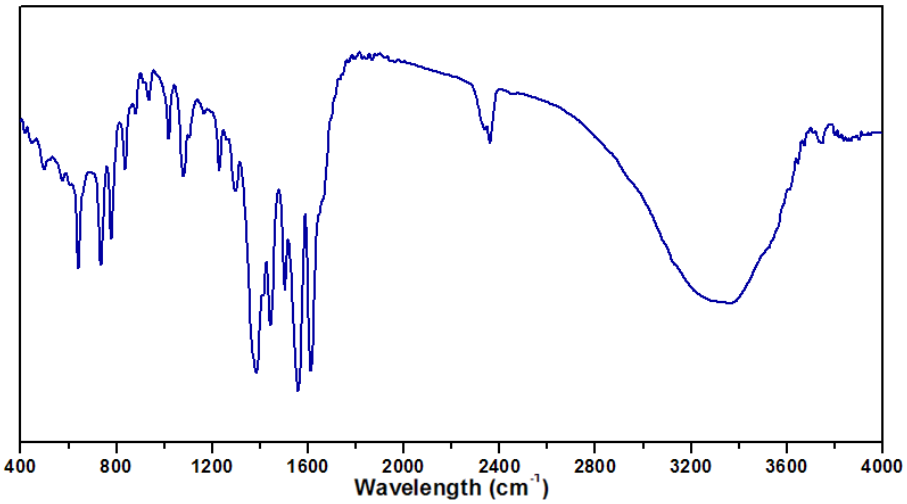


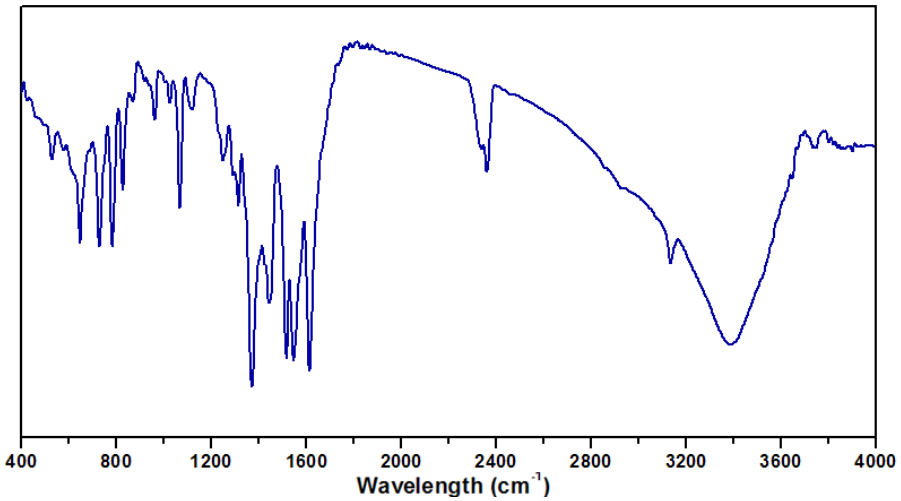
(f)



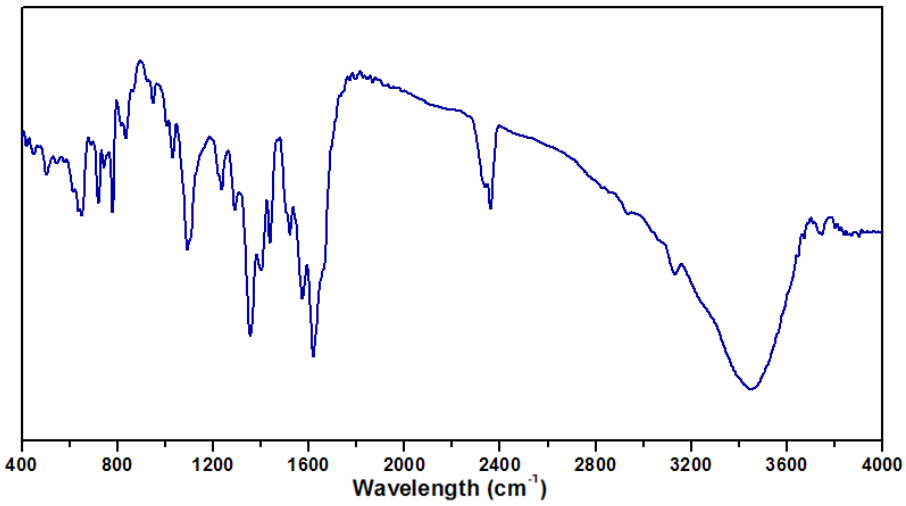
(g)



(h)



(i)



(j)

Figure S1. The IR spectras of (a) **1**, (b) **2**, (c) **3**, (d) **4**, (e) **5**, (f) **6** , (g) **7**, (h) **8**, (i) **9**, and (j) **10**.

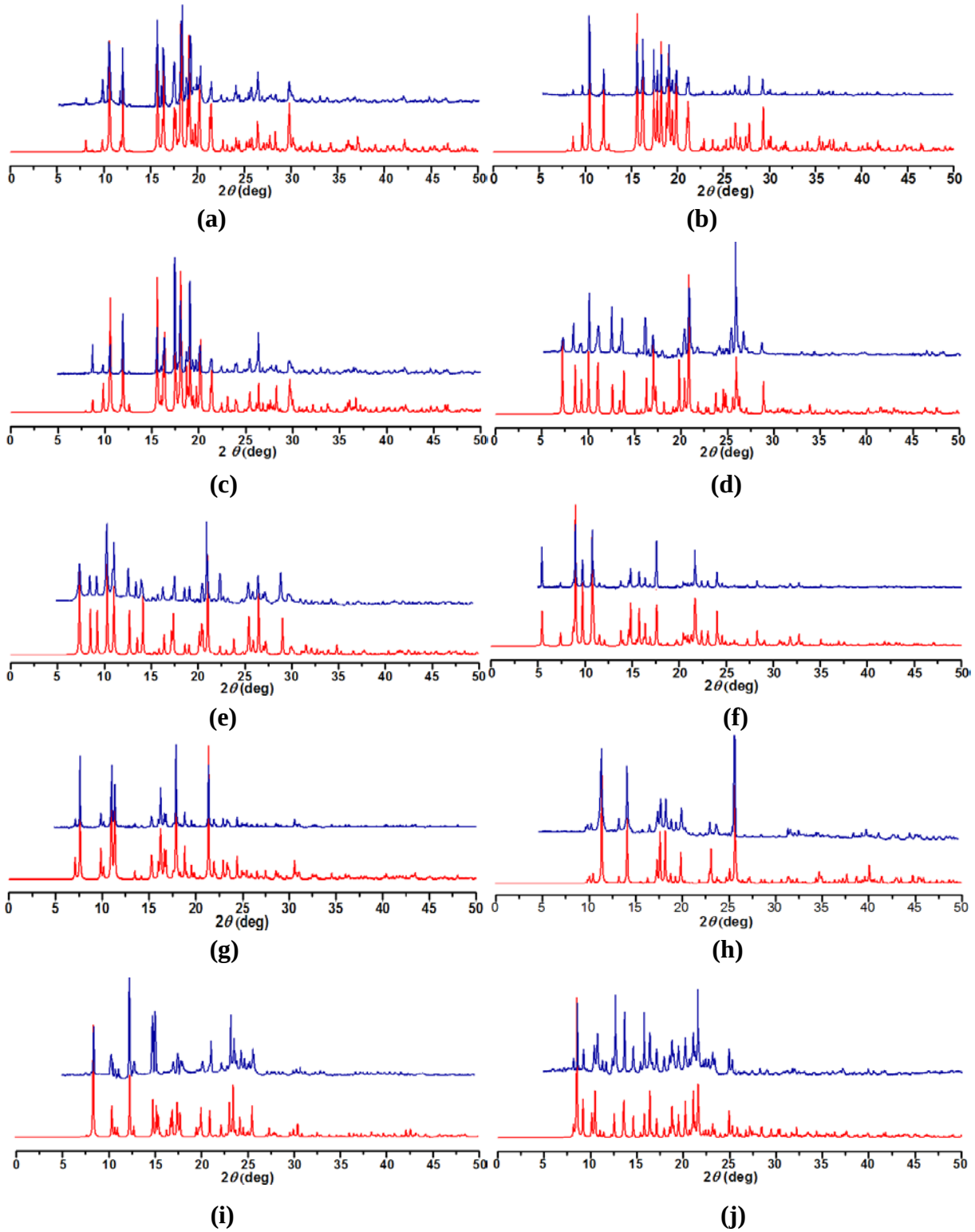


Figure S2. PXRD patterns of (a) **1**, (b) **2**, (c) **3**, (d) **4**, (e) **5**, (f) **6** , (g) **7**, (h) **8**, (i) **9**, and (j) **10**. Red: calculated from the X-ray single-crystal data; Dark blue: observed for the as-synthesized solids.

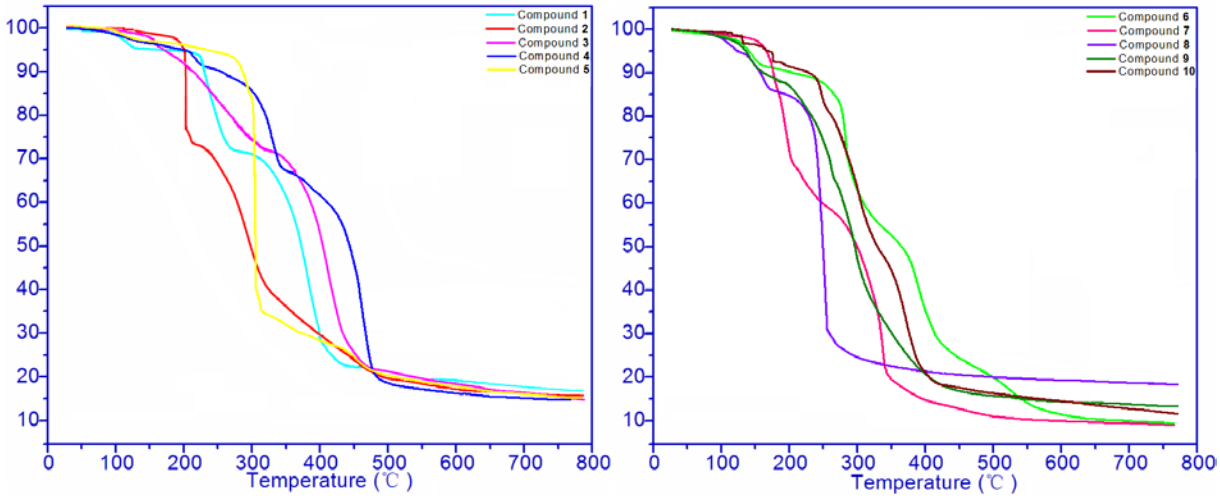


Figure S3. TG curves for complexes **1**-**10**.

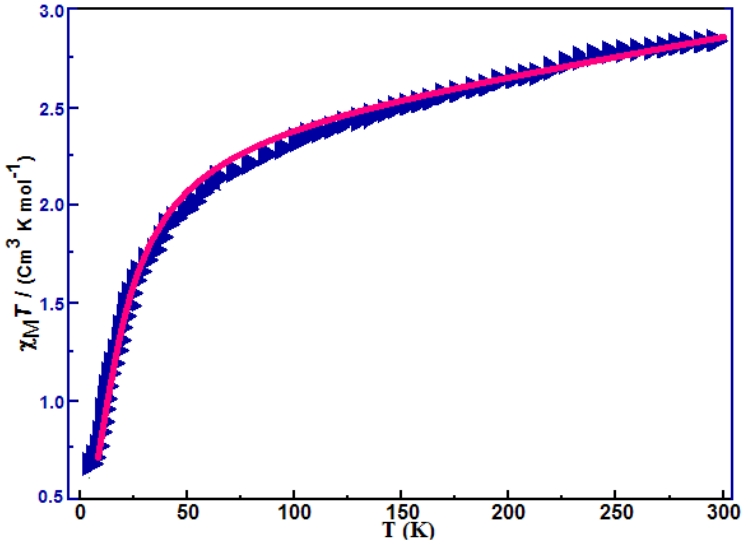


Figure S4. Temperature dependence of $\chi_M T$ in complex **4**. Solid lines represent the best theoretical fits.