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Supporting Information

Syntheses, structures and properties of five entangled coordination polymers constructed with trigonal N-donor ligands

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Table S1 Selected bond lengths (Å) and angles (°) for **1-5**.

Compound **1**			
Co(1)-O(1)#1	1.9931(15)	O(5)-Co(1)-O(2)#1	96.80(6)
Co(1)-O(2)#1	2.3442(16)	O(5)-Co(1)-N(1)	93.54(7)
Co(1)-O(3)	2.0002(18)	N(1)-Co(1)-O(2)#1	164.83(6)
Co(1)-O(5)	2.0028(15)	O(7)#2-Co(2)-O(7)	180.0
Co(1)-N(1)	2.0484(18)	O(7)#2-Co(2)-N(3)#3	86.62(6)
Co(2)-O(7)#2	2.0965(15)	O(7)#2-Co(2)-N(3)#4	93.38(6)
Co(2)-O(7)	2.0965(15)	O(7)#2-Co(2)-N(6)	92.42(6)
Co(2)-N(3)#3	2.2067(16)	O(7)#2-Co(2)-N(6)#2	87.58(6)
Co(2)-N(3)#4	2.2067(16)	O(7)-Co(2)-N(3)#3	93.38(6)
Co(2)-N(6)	2.1266(17)	O(7)-Co(2)-N(3)#4	86.62(6)
Co(2)-N(6)#2	2.1266(17)	O(7)-Co(2)-N(6)	87.58(6)
O(1)#1-Co(1)-O(2)#1	60.27(6)	O(7)-Co(2)-N(6)#2	92.42(6)
O(1)#1-Co(1)-O(3)	98.25(8)	N(3)#4-Co(2)-N(3)#3	180.00(8)
O(1)#1-Co(1)-O(5)	128.49(7)	N(6)#2-Co(2)-N(3)#3	85.82(6)
O(1)#1-Co(1)-N(1)	104.58(6)	N(6)#2-Co(2)-N(3)#4	94.18(6)
O(3)-Co(1)-O(2)#1	88.04(8)	N(6)-Co(2)-N(3)#3	94.19(6)
O(3)-Co(1)-O(5)	128.47(7)	N(6)-Co(2)-N(3)#4	85.81(6)
O(3)-Co(1)-N(1)	94.19(8)	N(6)-Co(2)-N(6)#2	180.0
Compound **2**			
Ni(1)-O(1)	2.0869(13)	O(5)-Ni(1)-N(5)#2	87.81(6)
Ni(1)-O(5)	2.0933(15)	N(1)-Ni(1)-O(5)	176.86(7)
Ni(1)-O(6)	2.1214(16)	N(1)-Ni(1)-O(6)	89.11(7)
Ni(1)-N(1)	2.0885(15)	N(1)-Ni(1)-N(5)#2	91.50(6)

Ni(1)-N(3)#1	2.0833(15)	N(3)#1-Ni(1)-O(1)	87.78(6)
Ni(1)-N(5)#2	2.0958(15)	N(3)#1-Ni(1)-O(5)	91.26(7)
O(1)-Ni(1)-O(5)	90.60(6)	N(3)#1-Ni(1)-O(6)	172.66(7)
O(1)-Ni(1)-O(6)	84.95(6)	N(3)#1-Ni(1)-N(1)	91.85(6)
O(1)-Ni(1)-N(1)	89.88(6)	N(3)#1-Ni(1)-N(5)#2	96.02(6)
O(1)-Ni(1)-N(5)#2	175.91(6)	N(5)#2-Ni(1)-O(6)	91.22(6)
O(5)-Ni(1)-O(6)	87.84(7)		

Compound **3**

Cu(1)-O(1)	2.0278(13)	O(2)#1-Cu(1)-O(3)#2	149.71(5)
Cu(1)-O(2)#1	1.9548(13)	O(2)#1-Cu(1)-N(1)	87.42(6)
Cu(1)-O(3)#2	2.0251(12)	O(2)#1-Cu(1)-N(2)#3	116.52(6)
Cu(1)-N(1)	2.0418(16)	O(3)#2-Cu(1)-O(1)	92.08(5)
Cu(1)-N(2)#3	2.2738(15)	O(3)#2-Cu(1)-N(1)	86.54(6)
O(1)-Cu(1)-N(1)	176.67(6)	O(3)#2-Cu(1)-N(2)#3	93.50(5)
O(1)-Cu(1)-N(2)#3	89.18(5)	N(1)-Cu(1)-N(2)#3	93.92(6)
O(2)#1-Cu(1)-O(1)	92.28(5)		

Compound **4**

Co(1)-O(1)#1	2.1267(16)	O(2)#1-Co(1)-O(2)	180.00(7)
Co(1)-O(1)	2.1267(16)	O(2)-Co(1)-N(1)#1	88.19(6)
Co(1)-O(2) #1	2.1242(15)	O(2)#1-Co(1)-N(1)#1	91.81(6)
Co(1)-O(2)	2.1242(15)	O(2)-Co(1)-N(1)	91.81(6)
Co(1)-N(1)	2.1960(17)	O(2)#1-Co(1)-N(1)	88.19(6)
Co(1)-N(1)#1	2.1959(17)	N(1)#1-Co(1)-N(1)#1	180.0
Co(2)-O(5)#2	2.0524(15)	O(5)#2-Co(2)-O(5)#3	175.59(10)
Co(2)-O(5)#3	2.0524(15)	O(5)#3-Co(2)-O(6)	84.41(6)
Co(2)-O(6) #4	2.1451(16)	O(5)#2-Co(2)-O(6)#4	84.41(6)
Co(2)-O(6)	2.1451(16)	O(5)#3-Co(2)-O(6)#4	92.43(6)
Co(2)-N(4)#4	2.1603(18)	O(5)#2-Co(2)-O(6)	92.43(6)
Co(2)-N(4)	2.1603(18)	O(5)#2-Co(2)-N(4)#4	90.59(7)
O(1)#1-Co(1)-O(1)	180.0	O(5)#3-Co(2)-N(4)#4	92.52(6)
O(1)-Co(1)-N(1)	89.96(6)	O(5)#2-Co(2)-N(4)	92.52(6)
O(1)#1-Co(1)-N(1)	90.04(6)	O(5)#3-Co(2)-N(4)	90.59(7)
O(1)-Co(1)-N(1)#1	90.03(6)	O(6)#4-Co(2)-O(6)	88.74(10)
O(1)#1-Co(1)-N(1)#1	89.96(6)	O(6)#4-Co(2)-N(4)#4	174.94(7)
O(2)#1-Co(1)-O(1)#1	62.22(6)	O(6)#4 -Co(2)-N(4)	90.67(7)
O(2) -Co(1)-O(1)	62.22(6)	O(6) -Co(2)-N(4)	174.94(7)

O(2)#1-Co(1)-O(1)	117.79(6)	O(6)-Co(2)-N(4)#4	90.67(7)
O(2)-Co(1)-O(1)#1	117.78(6)	N(4)#4-Co(2)-N(4)	90.35(10)

Compound **5**

Ni(1)-O(1)	2.1009(15)	O(2)-Ni(1)-O(2)#1	180.00(5)
Ni(1)-O(1)#1	2.1009(14)	O(2)#1-Ni(1)-N(1)	88.44(6)
Ni(1)-O(2)	2.0855(14)	O(2)-Ni(1)-N(1)	91.56(6)
Ni(1)-O(2)#1	2.0856(14)	O(2)#1-Ni(1)-N(1)#1	91.56(6)
Ni(1)-N(1)#1	2.1474(16)	O(2)-Ni(1)-N(1)#1	88.44(6)
Ni(1)-N(1)	2.1473(16)	N(1)-Ni(1)-N(1)#1	180.00(6)
Ni(2)-O(5)#2	2.0382(14)	O(5)#2-Ni(2)-O(5)#3	176.02(9)
Ni(2)-O(5)#3	2.0382(14)	O(5)#2-Ni(2)-O(6)#4	92.81(6)
Ni(2)-O(6)#4	2.1012(15)	O(5)#3-Ni(2)-O(6)#4	84.32(6)
Ni(2)-O(6)	2.1013(15)	O(5)#2-Ni(2)-O(6)	84.32(6)
Ni(2)-N(4)	2.1061(17)	O(5)#3-Ni(2)-O(6)	92.82(6)
Ni(2)-N(4)#4	2.1061(17)	O(5)#2-Ni(2)-N(4)	91.97(6)
O(1)-Ni(1)-O(1)#1	180.00(6)	O(5)#3-Ni(2)-N(4)	90.83(6)
O(1)-Ni(1)-N(1)#1	89.70(6)	O(5)#3-Ni(2)-N(4)#4	91.97(6)
O(1)#1-Ni(1)-N(1)#1	90.30(6)	O(5)#2-Ni(2)-N(4)#4	90.83(6)
O(1)#1-Ni(1)-N(1)	89.70(6)	O(6)#4-Ni(2)-O(6)	88.03(9)
O(1)-Ni(1)-N(1)	90.30(6)	O(6)#4-Ni(2)-N(4)	174.99(7)
O(2)-Ni(1)-O(1)	63.27(6)	O(6)-Ni(2)-N(4)#4	174.99(7)
O(2)#1-Ni(1)-O(1)#1	63.27(6)	O(6)#4-Ni(2)-N(4)#4	90.97(6)
O(2)-Ni(1)-O(1)#1	116.73(6)	O(6)-Ni(2)-N(4)	90.97(6)
O(2)#1-Ni(1)-O(1)	116.73(6)	N(4)-Ni(2)-N(4)#4	90.43(10)

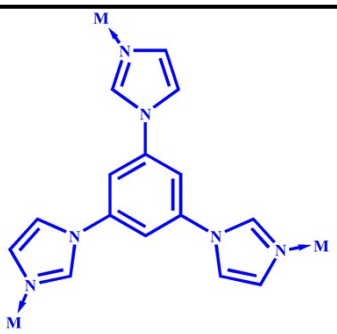
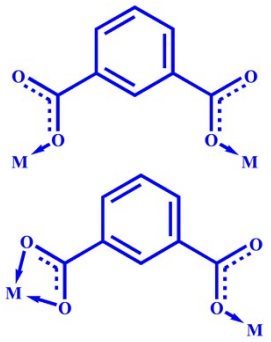
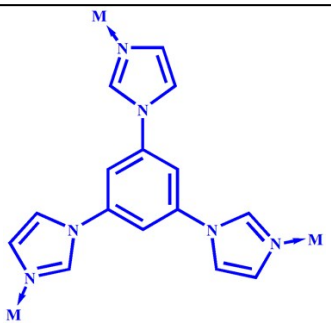
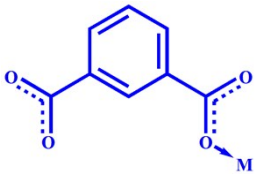
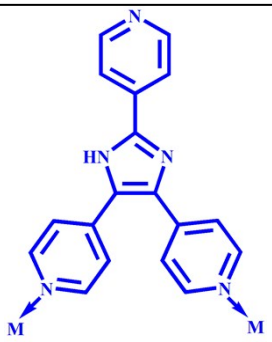
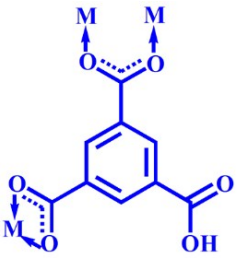
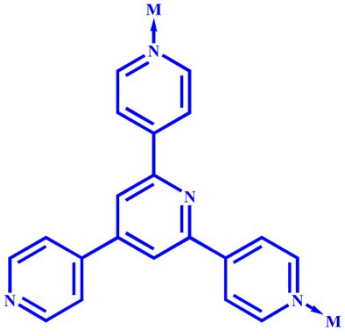
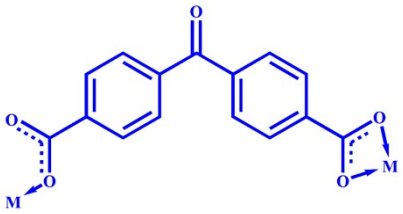
Symmetry transformations used to generate equivalent atoms: for **1**: #1 3/2-x, -1/2+y, 3/2-z. #2 1-x, 1-y, -z. #3 3/2-x, 1/2+y, 1/2-z. #4 -1/2+x, 1/2-y, -1/2+z; for **2**: #1 1/2-x, -1/2+y, +z. #2 +x, 3/2-y, -1/2+z; for **3**: #1 1-x, 1-y, 1-z. #2 1-x, -y, 1-z. #3 3/2-x, 1/2-y, 1-z; for **4**: #1 1-x, 1-y, 1-z. #2 1/2+x, 3/2+y, +z. #3 1/2-x, 3/2+y, 1/2-z. #4 1-x, +y, 1/2-z; for **5**: #1 1/2-x, -1/2-y, 1-z. #2 1/2+x, 3/2+y, +z. #3 1/2-x, 3/2+y, 3/2-z. #4 1-x, +y, 3/2-z.

Table S2 Hydrogen bonds for **1-5** (Å and °).

D-H···A	D···A	D-H	H···A	D-H···A
		Compound **1**		
O(7)-H(7A)···O(5)^{i}	2.7249	0.88	1.97	143
O(7)-H(7B)···O(4)^{ii}	2.6717	0.88	1.89	148
		Compound **2**		
O(6)-H(6B)···O(4)^{i}	2.5994	0.79	1.85	160
O(7)-H(7A)···O(4)^{ii}	2.5942	0.85	1.78	159
O(7)-H(7B)···O(4)^{iii}	2.8795	0.85	2.07	159
		Compound **3**		
N(4)-H(4)···O(4)^{i}	2.7149	0.86	1.91	156
O(6)-H(6)···N(5)^{ii}	2.7610	0.82	1.98	159
		Compound **4**		
O(6)-H(6A)···N(3)^{i}	2.9151	0.87	2.07	162
O(7)-H(7A)···O(4)^{ii}	3.1744	0.85	2.49	139
O(7)-H(7B)···O(6)^{iii}	2.8999	0.76	2.20	153
		Compound **5**		
O(6)-H(6B)···N(3)^{i}	2.9300	0.87	2.08	163
O(7)-H(7A)···O(4)^{ii}	3.1725	0.85	2.46	143
O(7)-H(7B)···O(6)^{ii}	2.8839	0.61	2.35	148

Symmetry transformations used to generate equivalent atoms: for **1**: i -1/2+x, -1/2+y, z. ii -x, -1+y, 1/2-z; for **2**: i 1/2-x, -y, 1/2+z. ii 1/2+x, 1/2-y, -z. iii 1/2-x, 1/2+y, z.; for **3**: i x, -y, 1/2+z. ii x, y, -1+z; for **4**: i 1+x, 1-y, 1/2+z. ii 1/2-x, 1/2+y, 1/2-z. iii -1/2+x, 1/2+y, z; for **5**: i 1/2-x, 1/2-y, 1-z. ii 1/2-x, 1/2+y, 1/2-z.

Table S3 Coordination modes of the ligands in **1-5**.

Compound	Trigonal N-donor ligand coordination mode	Polycarboxylate ligand coordination mode(s)
1	 tib	 1,3-bdc
2	 tib	 1,3-bdc
3	 Htpim	 Hbtc
4&5	 pytpy	 oba

Compound **1**

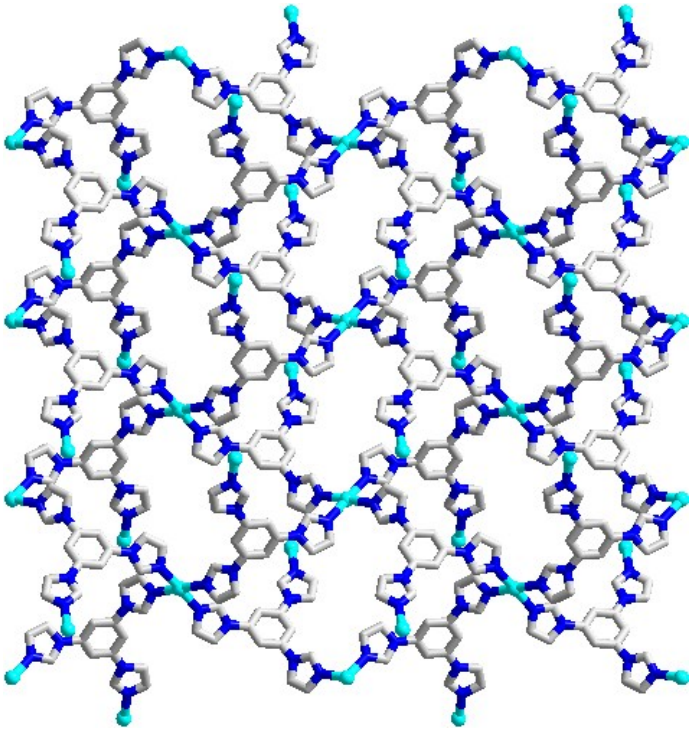


Fig. S1 View of a single 2D layer formed by tib ligands and Co atoms.

Compound **2**

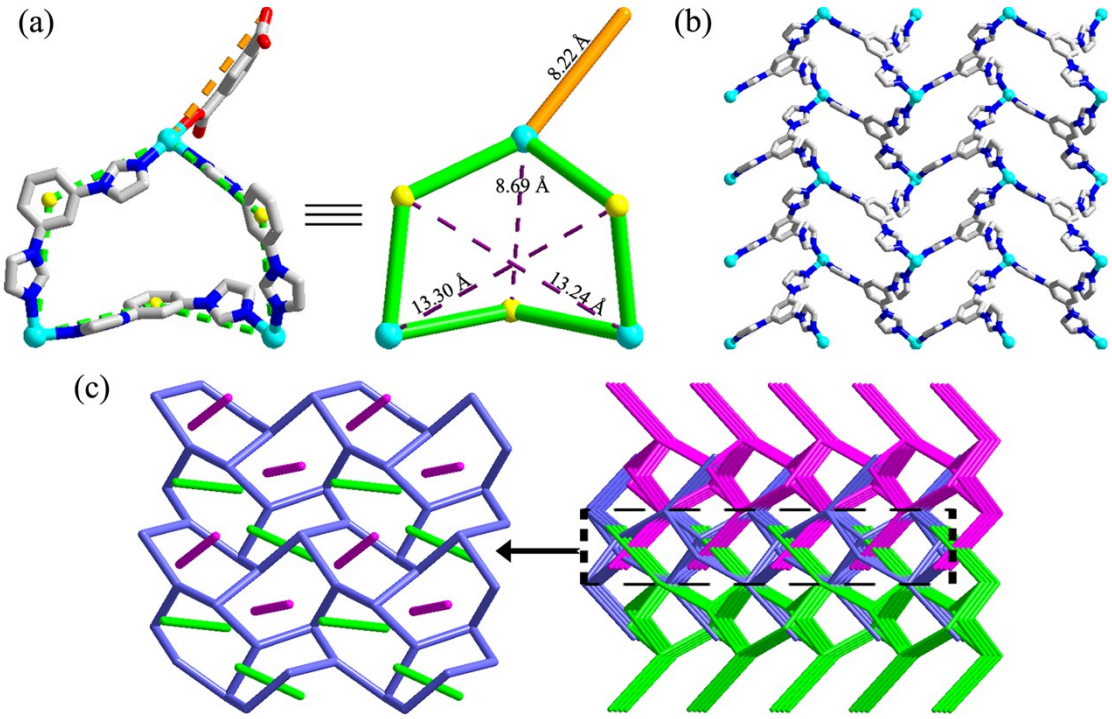


Fig. S2 (a) Perspective and simplified views of a hexagonal window with an orange lateral arm. (b) View of a single 2D layer formed by tib ligands and Ni atoms. (c) Every hexagonal void of each layer is pierced by one arm coming from above or below layers alternately.

Compound **3**

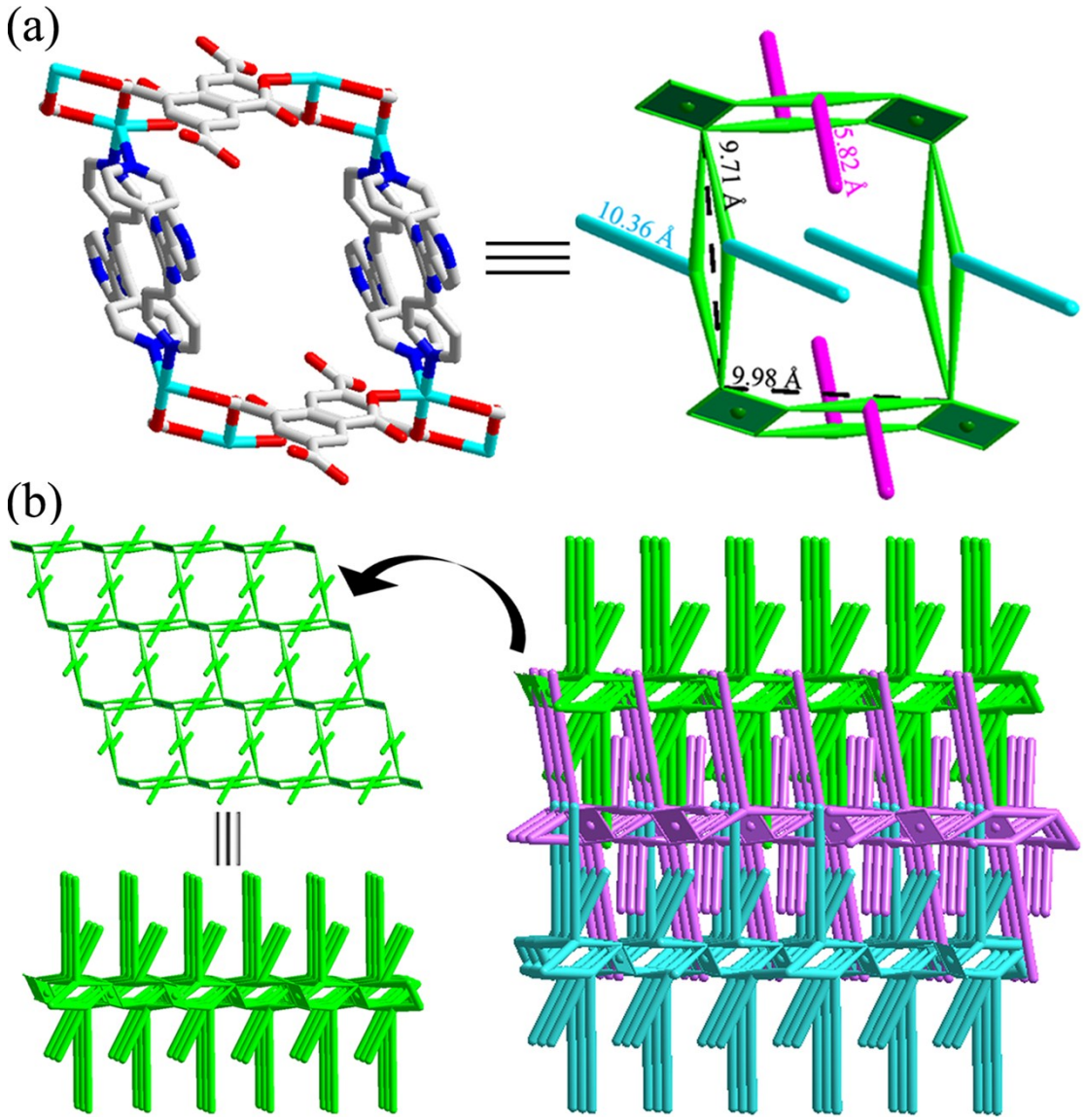


Fig. S3 (a) Perspective and simplified views of a single tetragonal window. The Htpim and Hbtc ligands are highlighted by cerulean and purple lines with effective length respectively. (b) Schematic views of a single double-edged 2D network with two distinct dangling arms (left) and the mutual polythreading and interdigitation of three layers (right).

Compounds **4** & **5**

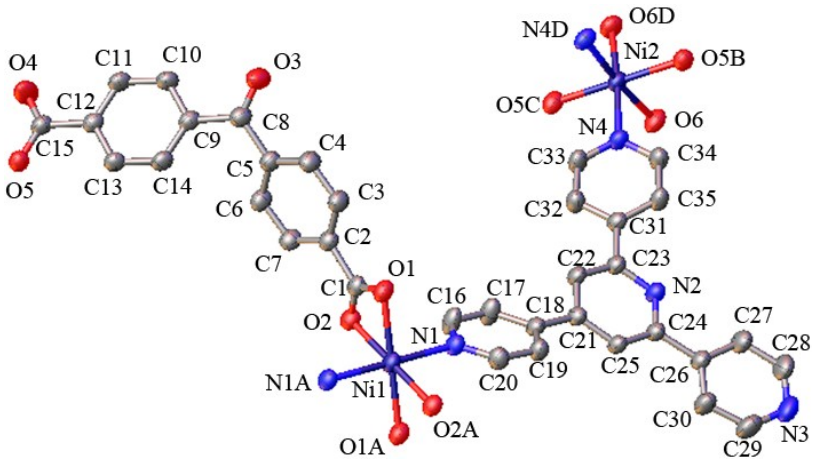


Fig. S4 ORTEP diagram showing the coordination environment for Ni atoms in **5**.

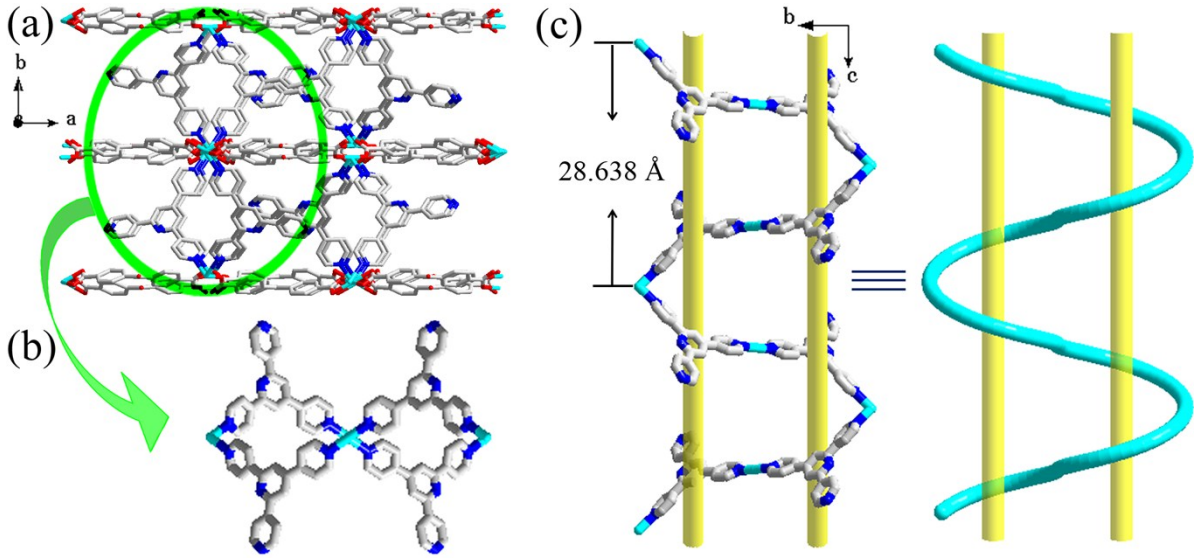


Fig. S5 (a) Perspective view of a single 3D net. (b) Side view of a single-stranded *meso*-helix. (c) Perspective (left) and schematic (right) views of the *meso*-helix.

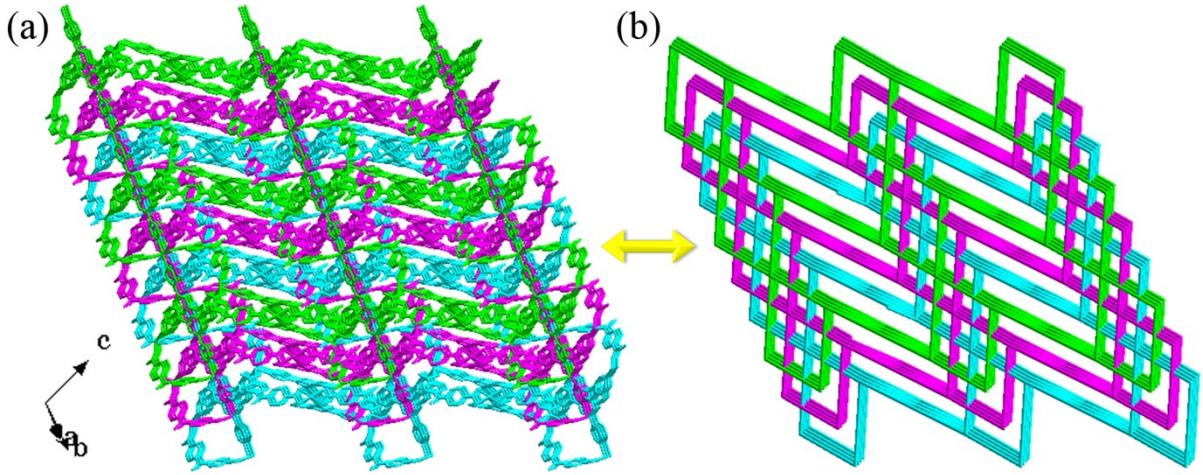


Fig. S6 Perspective (a) and simplified (b) views of 3-fold 3D interpenetrating framework.

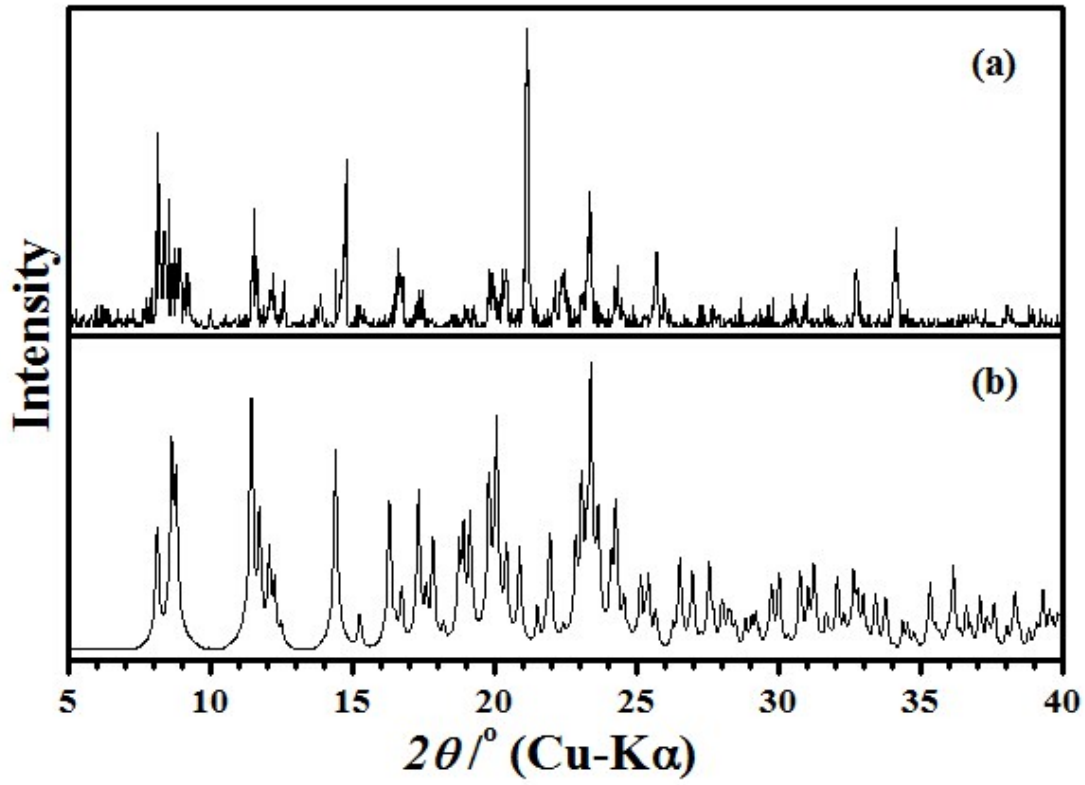


Fig. S7 The XRPD patterns for: (a) as-synthesized samples of **1**, and (b) simulated one based on the single-crystal structure of **1**.

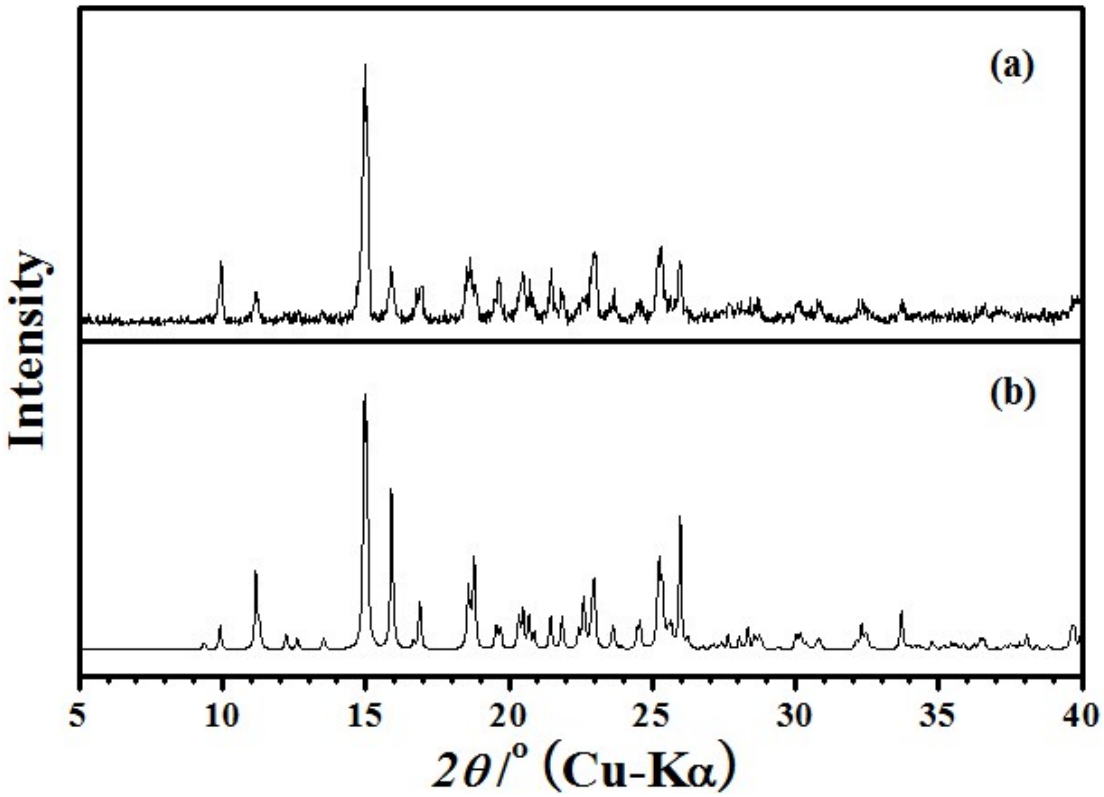


Fig. S8 The XRPD patterns for: (a) as-synthesized samples of **2**, and (b) simulated one based on the single-crystal structure of **2**.

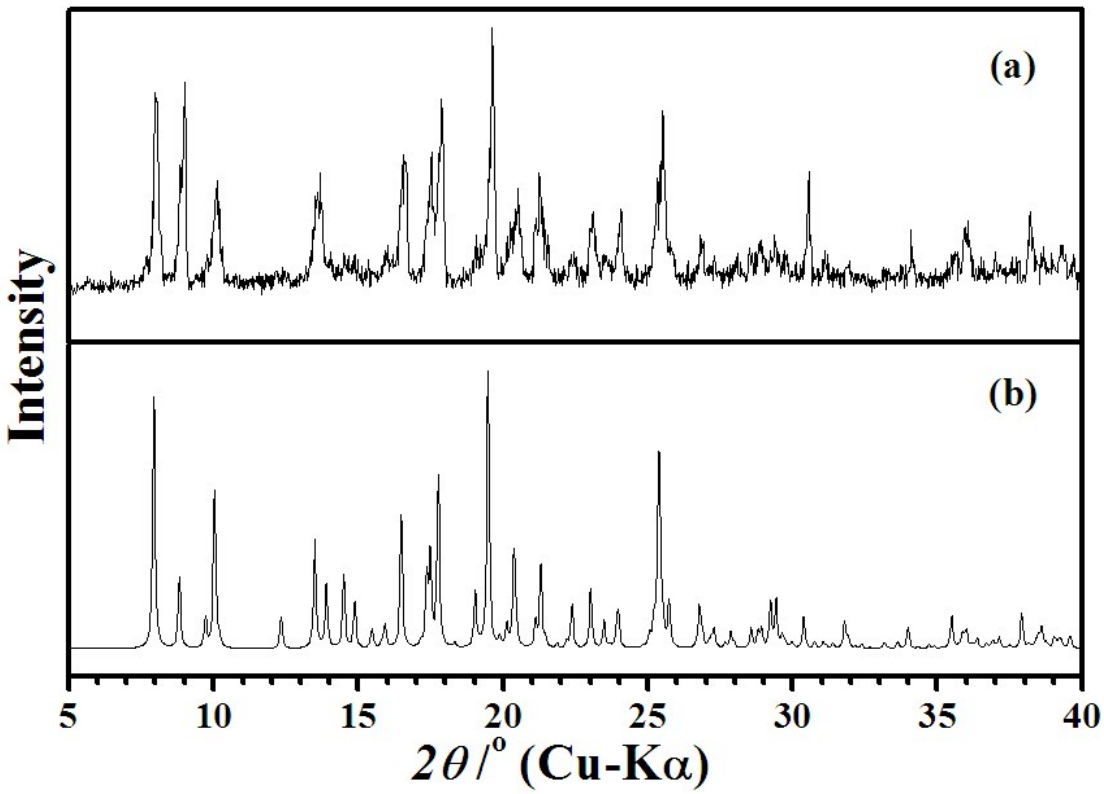


Fig. S9 The XRPD patterns for: (a) as-synthesized samples of **3**, and (b) simulated one based on the single-crystal structure of **3**.

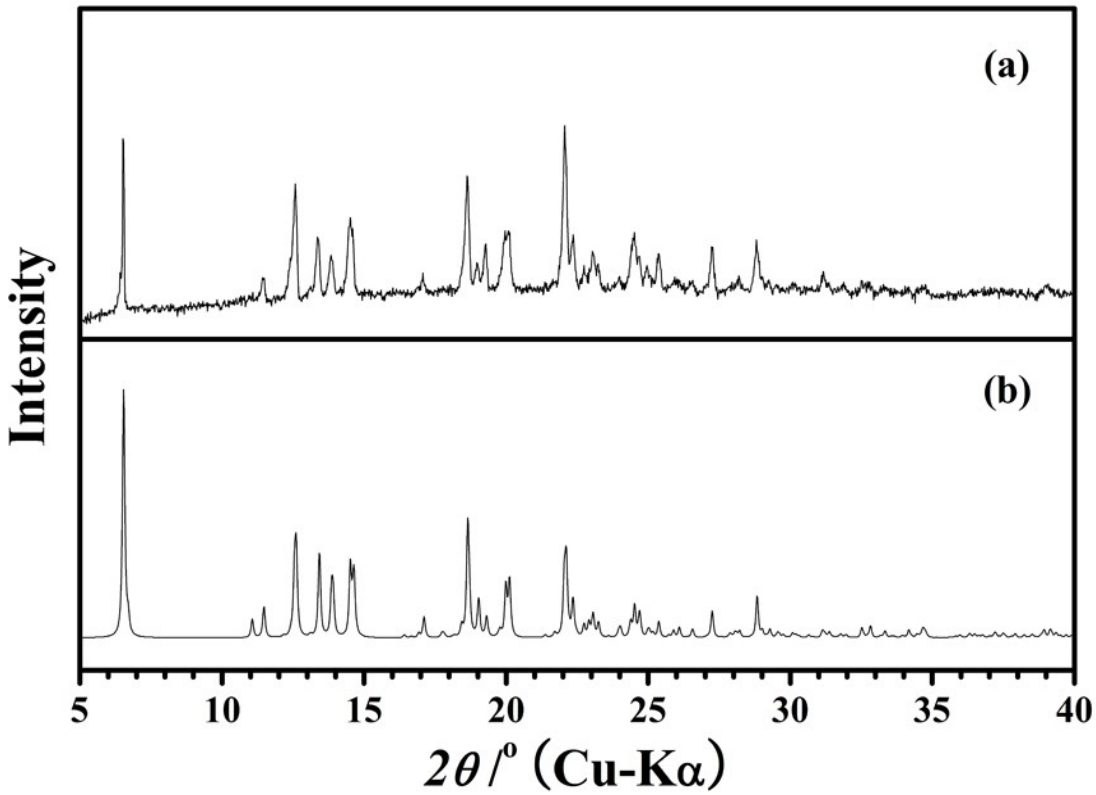


Fig. S10 The XRPD patterns for: (a) as-synthesized samples of **4**, and (b) simulated one based on the single-crystal structure of **4**.

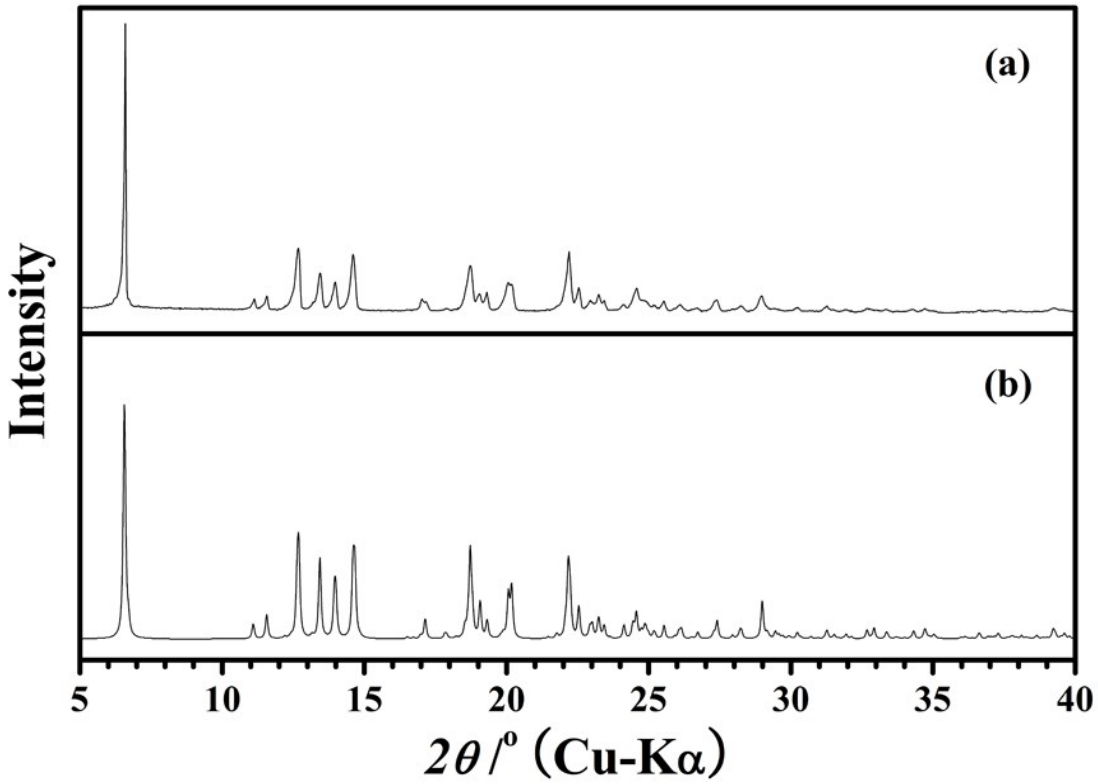


Fig. S11 The XRPD patterns for: (a) as-synthesized samples of **5**, and (b) simulated one based on the single-crystal structure of **5**.

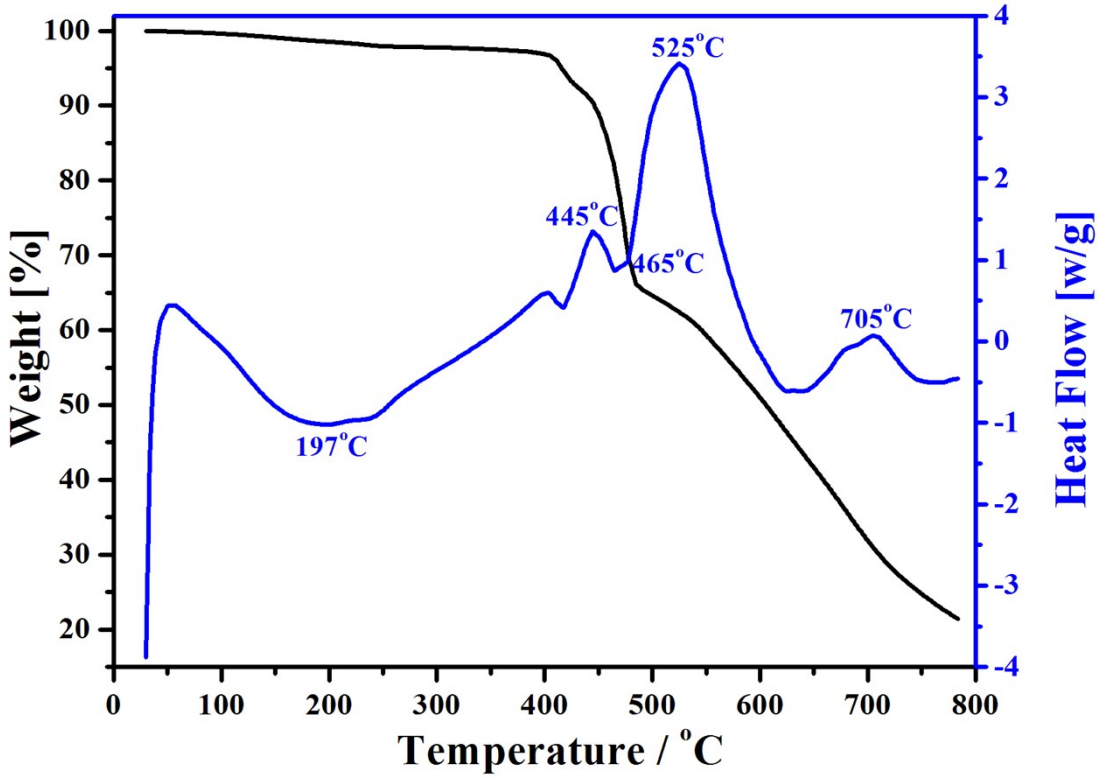


Fig. S12 The TG-DSC curves of compound **1**.

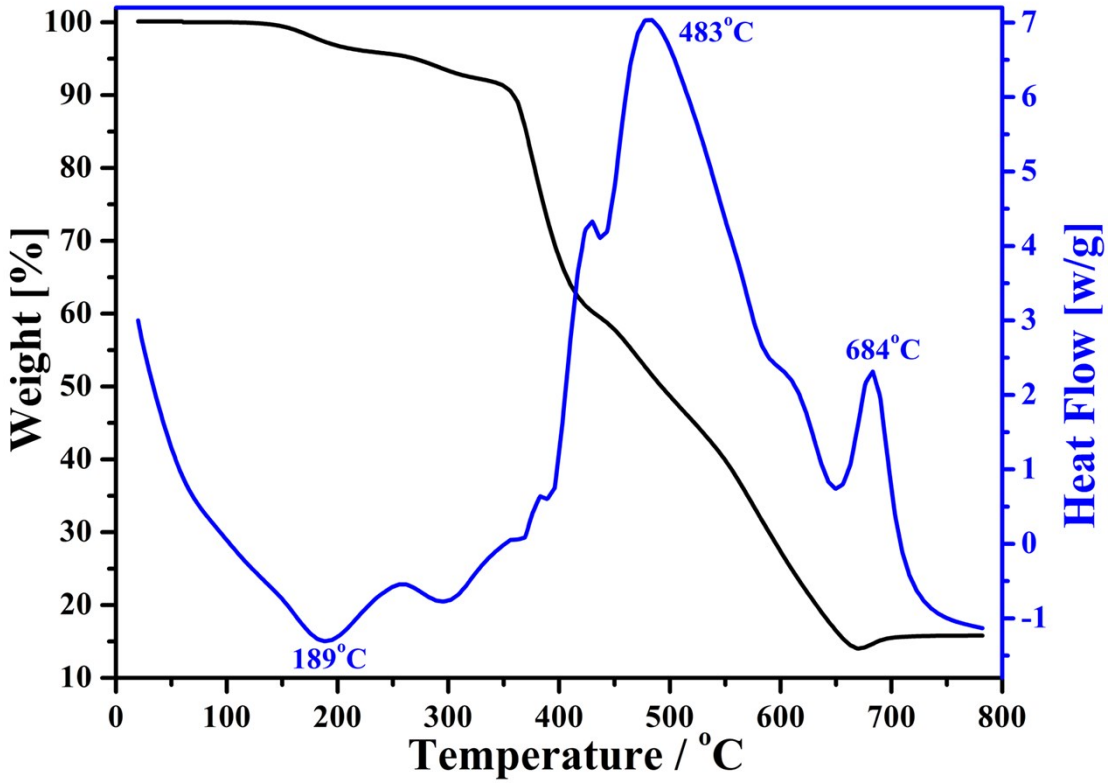


Fig. S13 The TG-DSC curves of compound **2**.

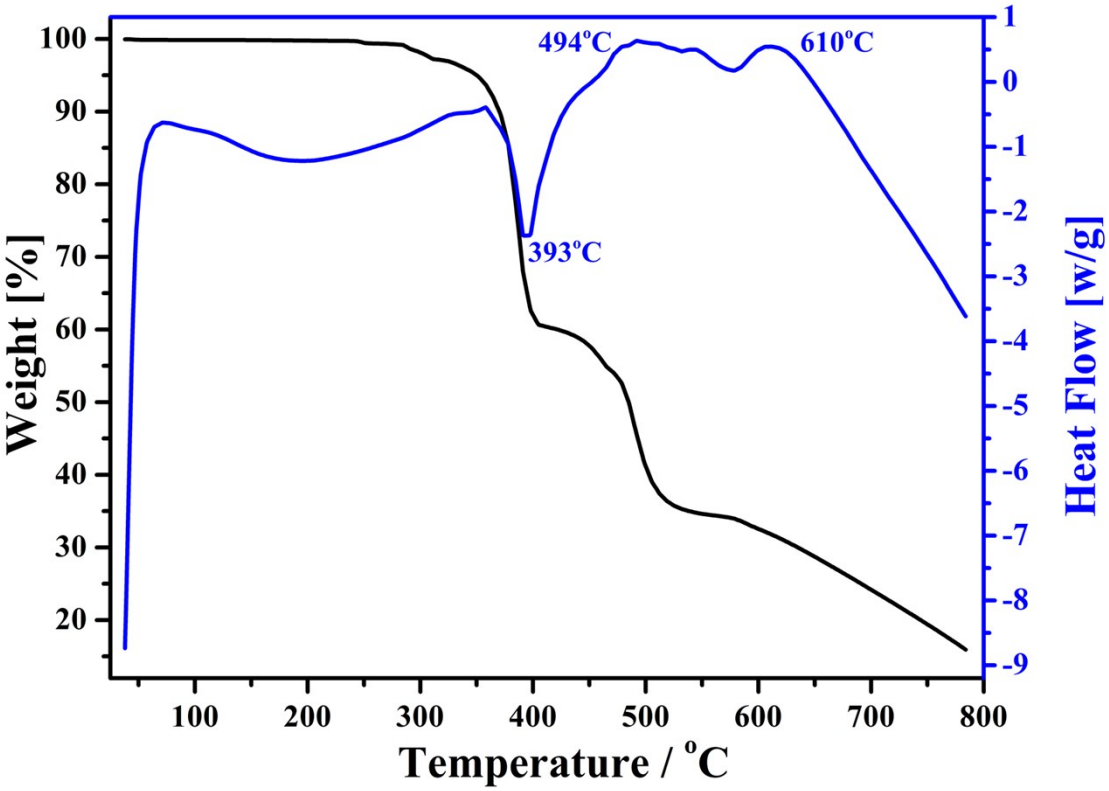


Fig. S14 The TG-DSC curves of compound **3**.

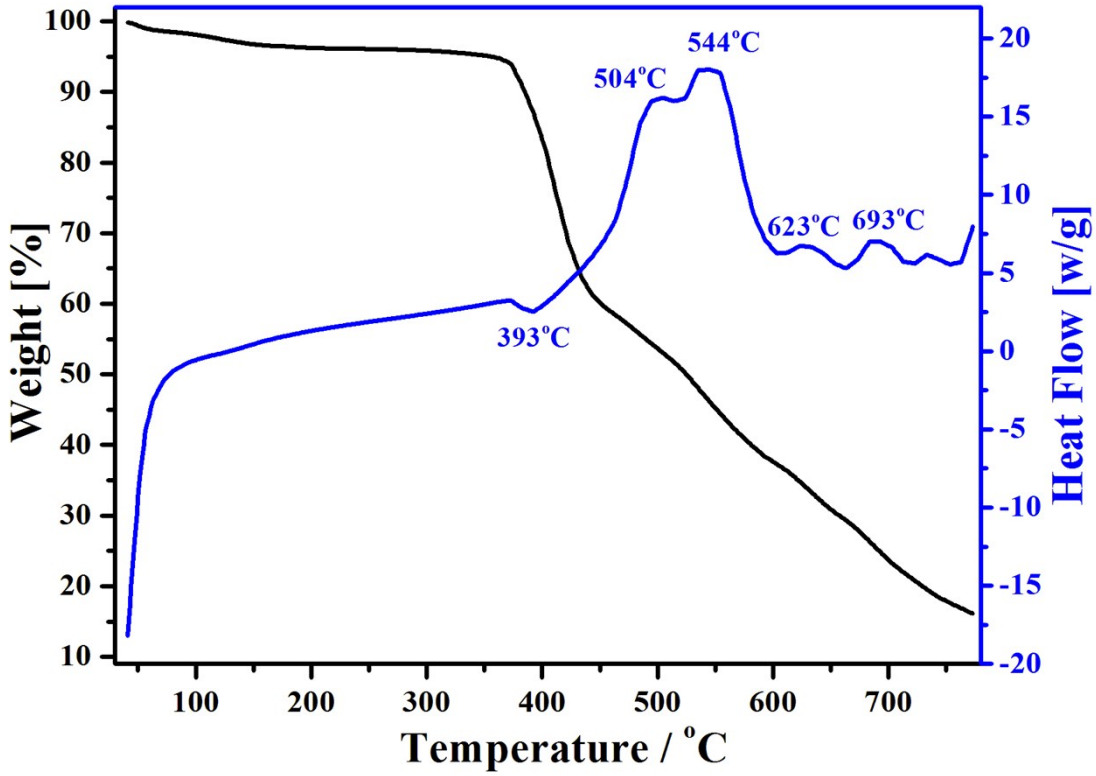


Fig. S15 The TG-DSC curves of compound **4**.

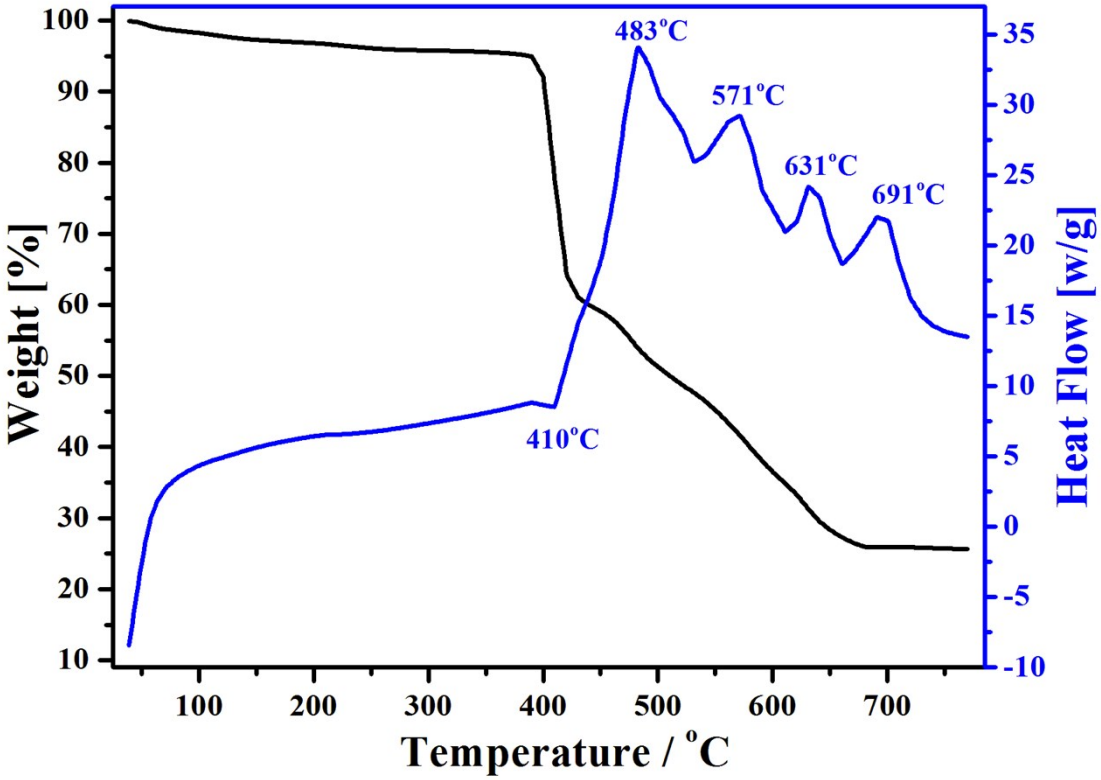


Fig. S16 The TG-DSC curves of compound **5**.

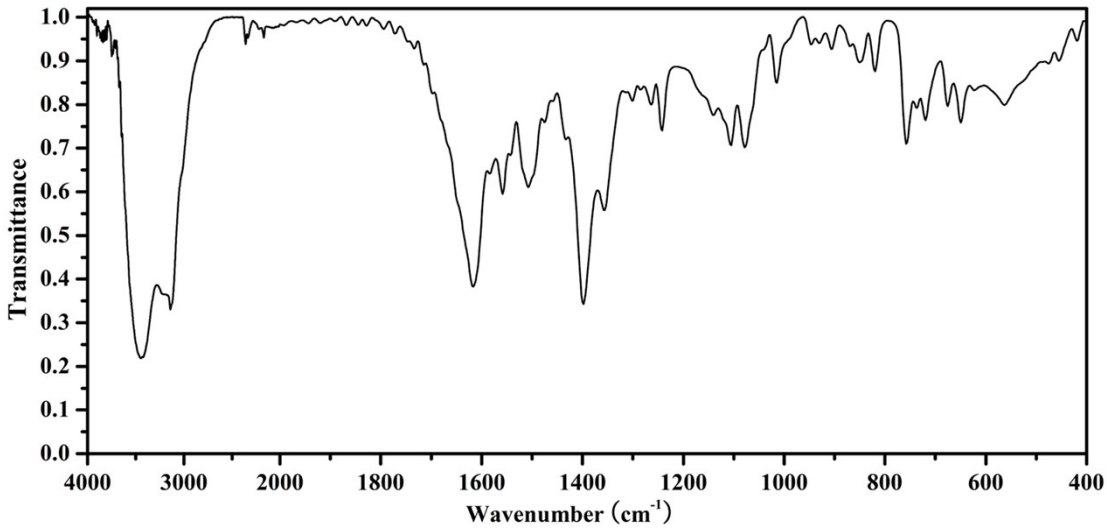


Fig. S17 The IR spectrum of compound **1**.

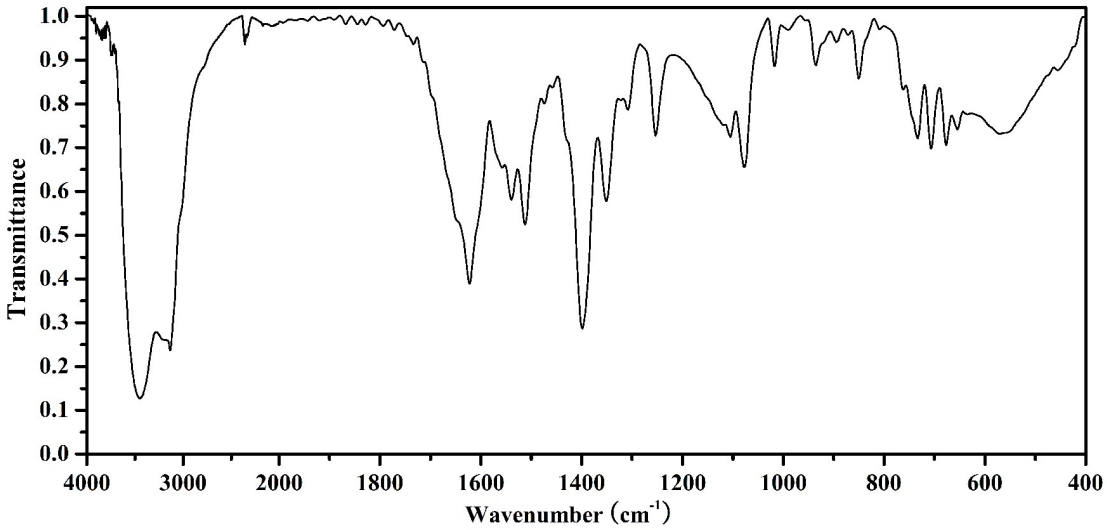


Fig. S18 The IR spectrum of compound **2**.

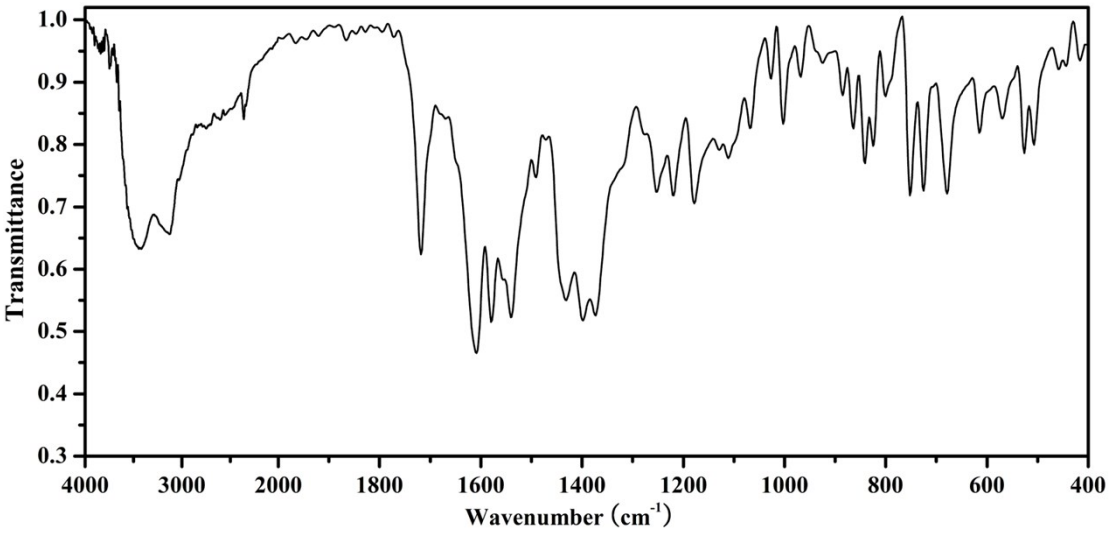


Fig. S19 The IR spectrum of compound **3**.

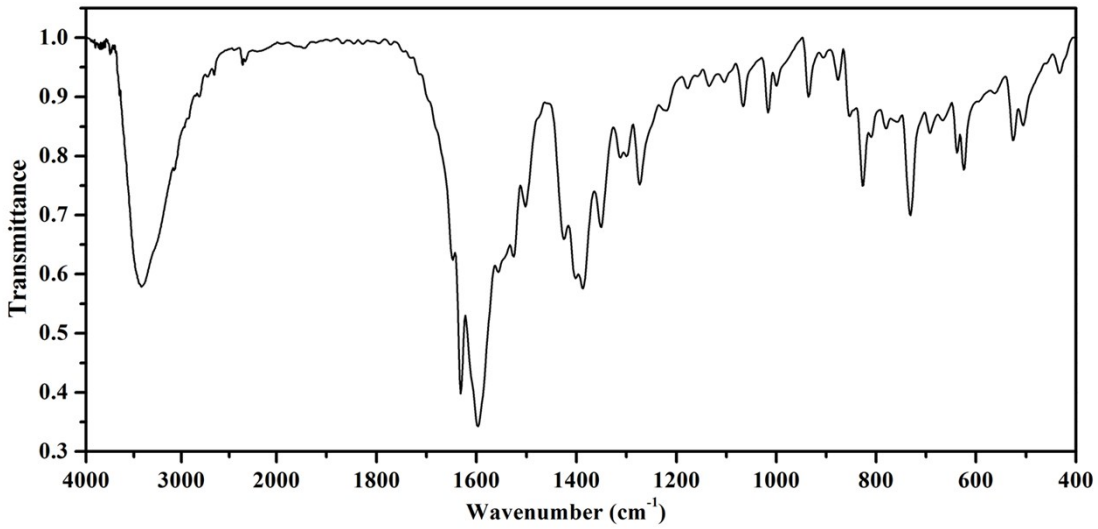


Fig. S20 The IR spectrum of compound **4**.

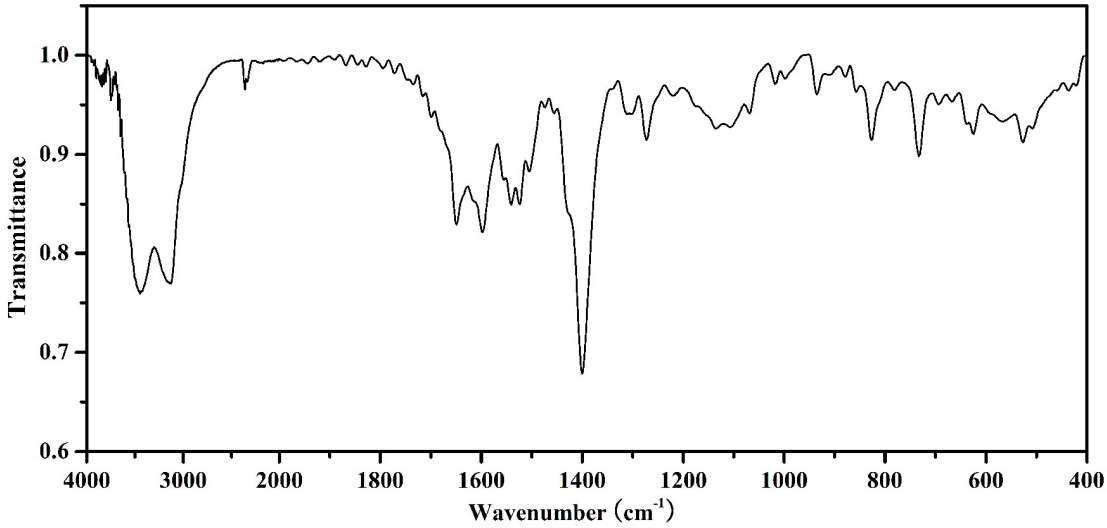


Fig. S21 The IR spectrum of compound **5**.