Supplementary Information

Anion-directed Self-assembly of Cu(II) Coordination Compounds with Tetrazole-1-acetic acid: Syntheses in Ionic Liquid and Crystal Structures

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Table S1. Selected bond lengths (Å) and angles (º) for **1**–**5**

1			
Cu(1)-O(21)#1	1.934(2)	Cu(1)-N(24)	2.025(3)
Cu(1)-O(11)#2	1.945(2)	Cu(1)-O(11)#3	2.425(3)
Cu(1)-N(14)	2.013(3)	O(21)-Cu(1)#5	1.934(2)
N(14)-Cu(1)-N(24)	164.84(15)	Cu(1)#6-O(11)-Cu(1)#7	105.06(10)
O(21)#1-Cu(1)-O(11)#2	171.28(12)	O(21)#1-Cu(1)-O(11)#3	96.64(10)
O(21)#1-Cu(1)-N(14)	91.90(13)	O(11)#2-Cu(1)-O(11)#3	74.94(10)
O(11)#2-Cu(1)-N(14)	89.73(13)	N(14)-Cu(1)-O(11)#3	85.68(12)
O(21)#1-Cu(1)-N(24)	90.14(13)	N(24)-Cu(1)-O(11)#3	109.00(13)
O(11)#2-Cu(1)-N(24)	90.52(13)		
2			
Cu(1)-O(2)#1	1.972(2)	Cu(1)-N(4)#2	2.030(2)
Cu(1)-O(2)	1.972(2)	Cu(1)-N(4)#3	2.030(2)
O(2)#1-Cu(1)-O(2)	180	O(2)#1-Cu(1)-N(4)#3	89.47(10)
O(2)#1-Cu(1)-N(4)#2	90.53(10)	O(2)-Cu(1)-N(4)#3	90.53(10)
O(2)-Cu(1)-N(4)#2	89.47(18)	N(4)#2-Cu(1)-N(4)#3	180
3			
Cu(1)-N(24)	1.997(2)	Cu(1)-Cl(1)	2.2961(8)
Cu(1)-N(14)	2.011(2)	Cu(1)-O(21)#1	2.3949(19)
Cu(1)-O(1W)	2.0300(19)	Cu(1)-Cl(1)#2	2.8204(10)
N(24)-Cu(1)-N(14)	177.18(8)	O(1W)-Cu(1)-O(21)#1	93.10(8)
N(24)-Cu(1)-O(1W)	91.24(8)	Cl(1)-Cu(1)-O(21)#1	90.41(5)
N(14)-Cu(1)-O(1W)	86.05(8)	N(24)-Cu(1)-Cl(1)#2	87.41(7)
N(24)-Cu(1)-Cl(1)	91.23(7)	N(14)-Cu(1)-Cl(1)#2	93.32(7)
N(14)-Cu(1)-Cl(1)	91.52(7)	O(1W)-Cu(1)-Cl(1)#2	88.78(6)
O(1W)-Cu(1)-Cl(1)	175.71(6)	Cl(1)-Cu(1)-Cl(1)#2	87.82(3)
N(24)-Cu(1)-O(21)#1	90.15(8)	O(21)#1-Cu(1)-Cl(1)#2	176.95(5)
N(14)-Cu(1)-O(21)#1	89.20(8)	Cu(1)-Cl(1)-Cu(1)#2	92.18(3)

4			
Cu(1)-N(24)	1.9998(19)	Cu(1)-Cl(1)	2.2955(7)
Cu(1)-O(1W)	2.0014(17)	Cu(1)-Cl(2)	2.7475(7)
Cu(1)-N(14)	2.0062(19)	Cu(1)-Cl(2) #1	2.8796(7)
N(24)-Cu(1)-O(1W)	88.82(7)	N(14)-Cu(1)-Cl(2)	93.17(6)
N(24)-Cu(1)-N(14)	172.84(8)	Cl(1)-Cu(1)-Cl(2)	92.71(2)
O(1W)-Cu(1)-N(14)	88.30(7)	N(24)-Cu(1)-Cl(2) #1	84.45(6)
N(24)-Cu(1)-Cl(1)	90.40(6)	O(1W)-Cu(1)-Cl(2) #1	90.04(5)
O(1W)-Cu(1)-Cl(1)	178.37(5)	N(14)-Cu(1)-Cl(2) #1	90.00(6)
N(14)-Cu(1)-Cl(1)	92.31(6)	Cl(1)-Cu(1)-Cl(2) #1	88.46(2)
N(24)-Cu(1)-Cl(2)	93.33(6)	Cl(2)-Cu(1)-Cl(2) #1	177.50(2)
O(1W)-Cu(1)-Cl(2)	88.77(5)		
5			
Cu(1)-N(14)	1.988(3)	Cu(2)-N(24)	1.998(3)
Cu(1)-Cl(1)	2.2833(15)	Cu(2)-Cl(2)	2.2893(15)
N(14)-Cu(1)-N(24)	179.08(16)	N(14)-Cu(1)-Cl(1)	92.26(10)
N(24)-Cu(1)-Cl(1)	88.49(10)	N(14)-Cu(1)-Cl(2)	88.83(10)
N(24)-Cu(1)-Cl(2)	90.39(11)	Cl(1)-Cu(1)-Cl(2)	176.68(4)

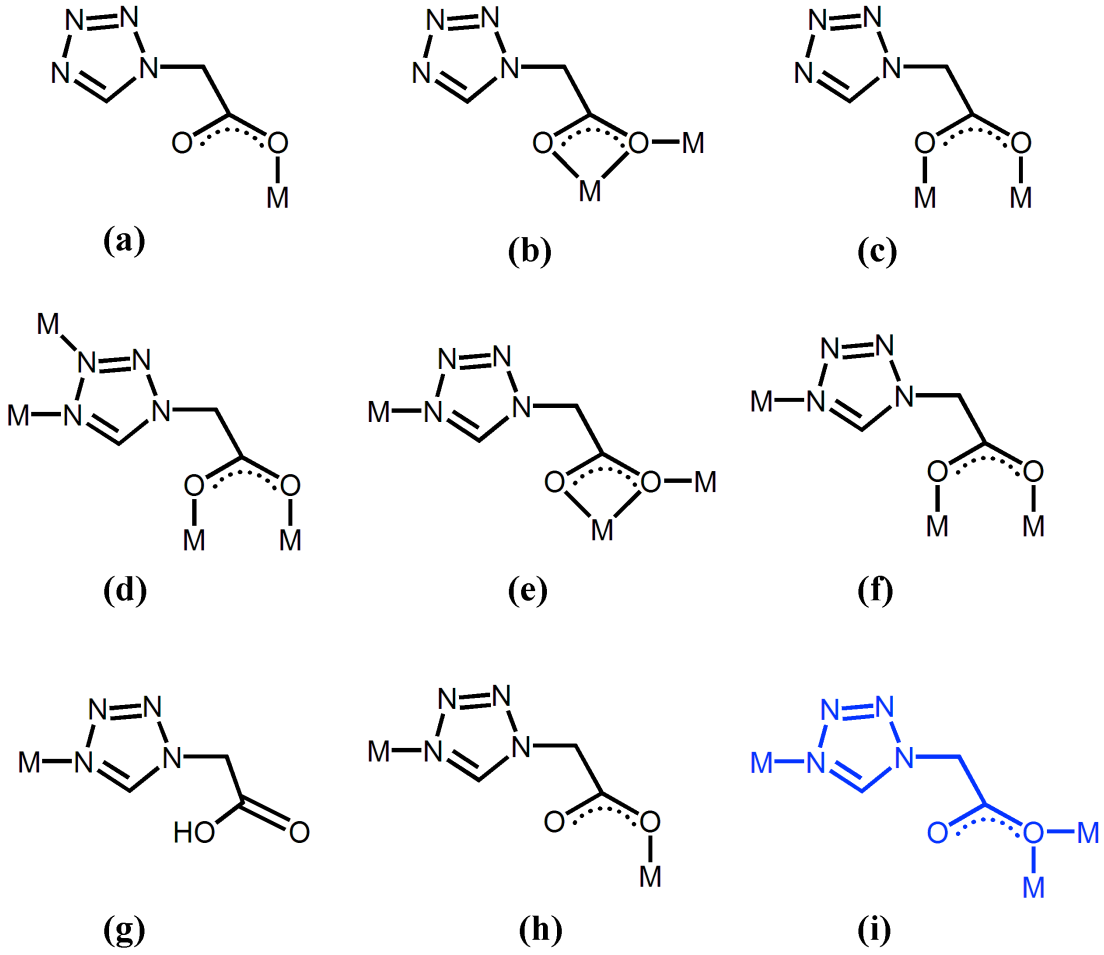
Symmetry codes for **1**: #1 –x + y, –x + 2, z; #2 –x + y, –x + 1, z; #3 x – y + 1, x + 1, –z + 2; #6 –y + 1, x – y + 1, z; #7 y – 1, –x + y, –z + 2; **2**: #1 –x + 1, –y, –z; #2 –y + 1/4, x – 3/4, –z + 1/4; #3 y + 3/4, –x + 3/4, z – 1/4; **3**: #1 –x, –y, –z + 1; #2 –x, –y + 1, –z + 1; **4**: #1 –x, 0.5 + y, 0.5 – z.

Table S2. Hydrogen-bond geometry for compounds **3**–**5**

D-H…A	D-H/Å	H…A/Å	D…A/Å	□ D-H…A/º
3				
O1W-H1WB...O22_$1	0.842(10)	1.996(18)	2.742(3)	147(3)
O1W-H1WA...O11_$2	0.834(10)	2.36(3)	2.984(3)	132(3)
O1W-H1WA...O2W_$2	0.83(2)	2.05(2)	2.835(7)	158(3)
O12-H12C...O22_$3	0.82	1.73	2.539(3)	170.6
4				
O1W-H1WA…Cl1_$1	0.844(7)	2.343(8)	3.1767(18)	170(2)
O1W-H1WB…O2W	0.848(8)	1.824(8)	2.668(3)	173.6(15)
O2W-H2WA…Cl1_$2	0.847(9)	2.466(9)	3.279(2)	161.0(16)
5				
O11-H11B...O1W_$1	0.82	1.99	2.800(6)	170.9
O21-H21B...O12_$2	0.82	1.75	2.569(3)	177.7
O1W-H1WA...O11_$3	0.857(10)	2.04(2)	2.780(4)	144(3)
O1W-H1WB...O12_$4	0.859(10)	2.035(11)	2.894(4)	176(4)

Symmetry codes for **3**: $1 –x + 1, –y, –z + 1; $2 –x – 1, –y, –z; $3 x – 2, y, z – 1; **4**: $1 –x, y – 1/2, –z + 1/2; $2 x + 1, y, z; **5**: $1 x – 1/2, y + 1/2, z; $2 x + 1/2, y + 3/2, z; $3 x + 1/2, –y – 5/2, z + 1/2; $4 x + 1/2, –y – 7/2, z + 1/2.

Scheme S1. Coordination modes of 1-Htza ligands. (a)–(h) are found in literatures, while (i) is first found in this paper.



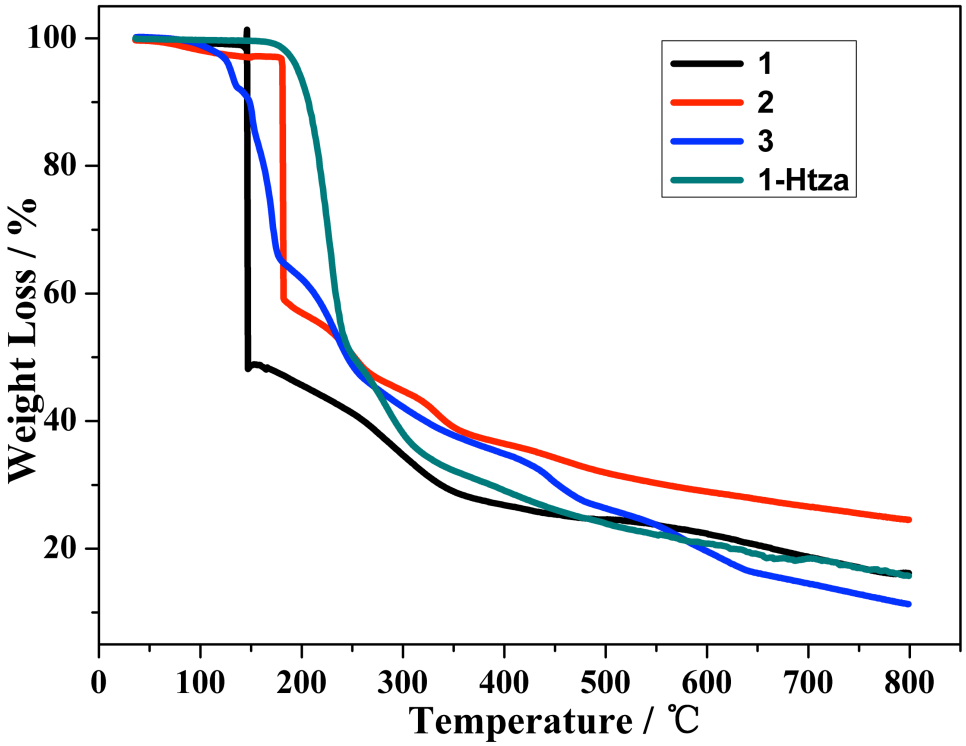


Figure S1. TGA curves for **1**–**3** and 1-Htza.

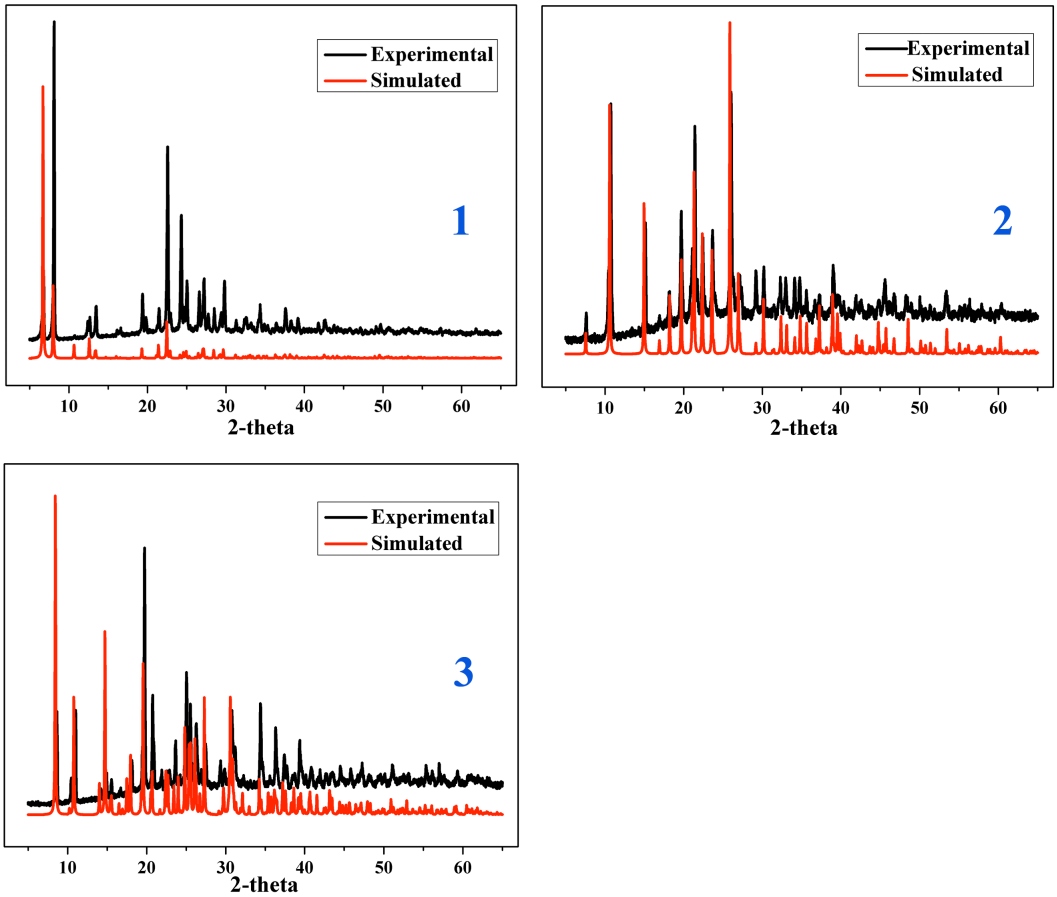


Figure S2. Powdered X-ray diffraction (PXRD) patterns of **1**–**3**.

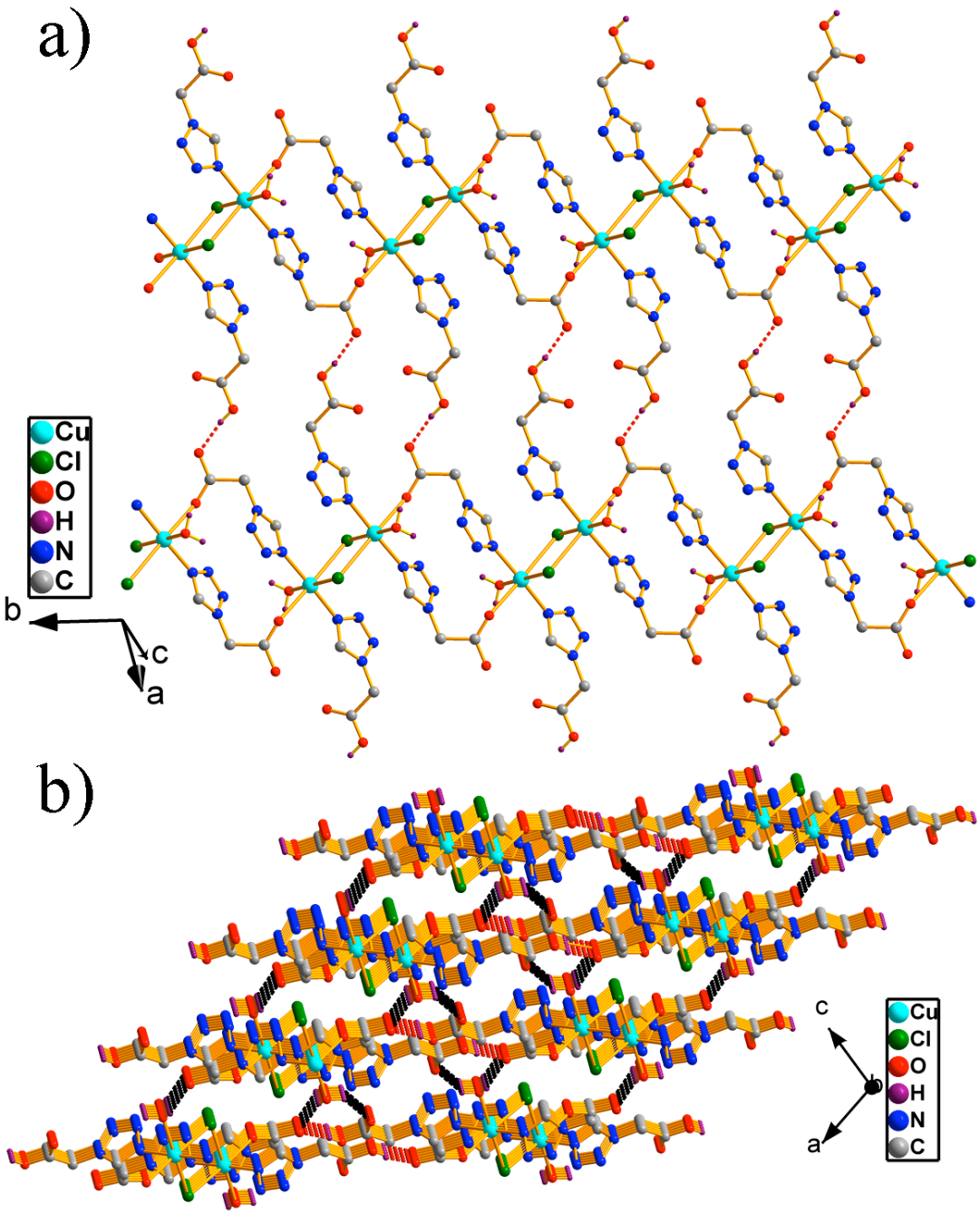


Figure S3. (a) A perspective view of a 2-D supramolecular architecture in **3** via O12–H12C···O22 hydrogen bonds. (b) Schematic representation of 2-D→3-D supramolecular architecture via O1W–H1WB···O11 and O1W–H1WB···O22 hydrogen bonds in **3**.

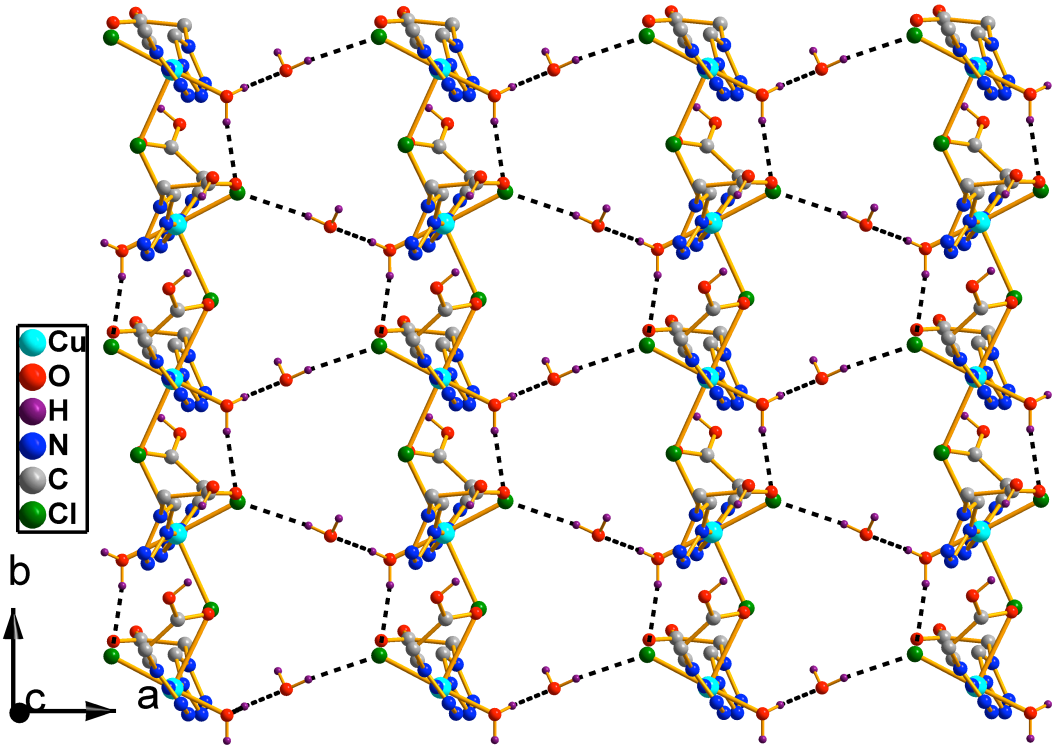


Figure S4. 2-D supramolecular network formed by hydrogen bonds for **4**.

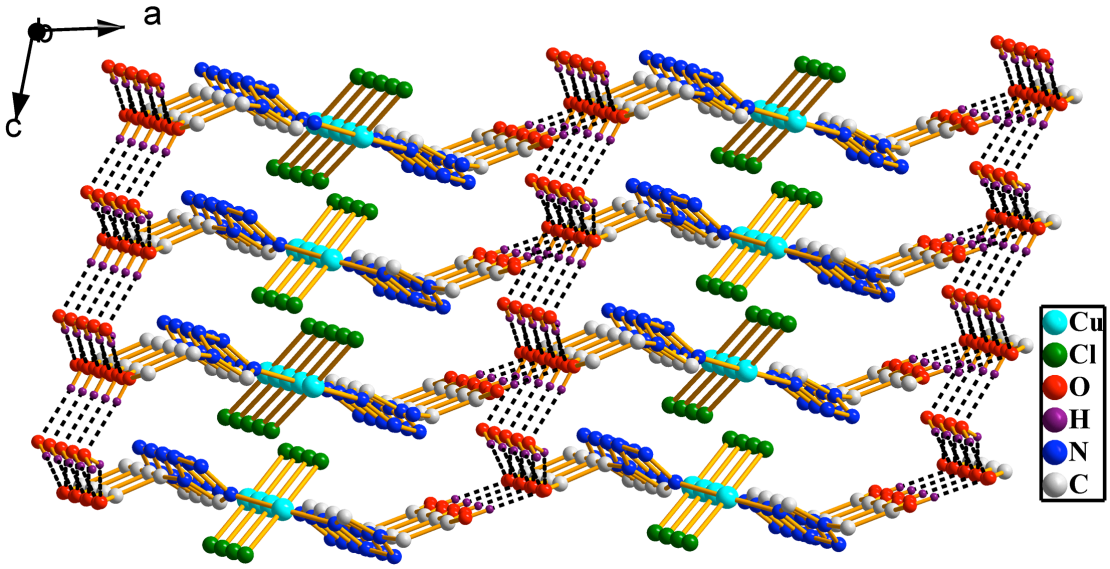


Figure S5. 3-D supramolecular network formed by hydrogen bonds for **5**.

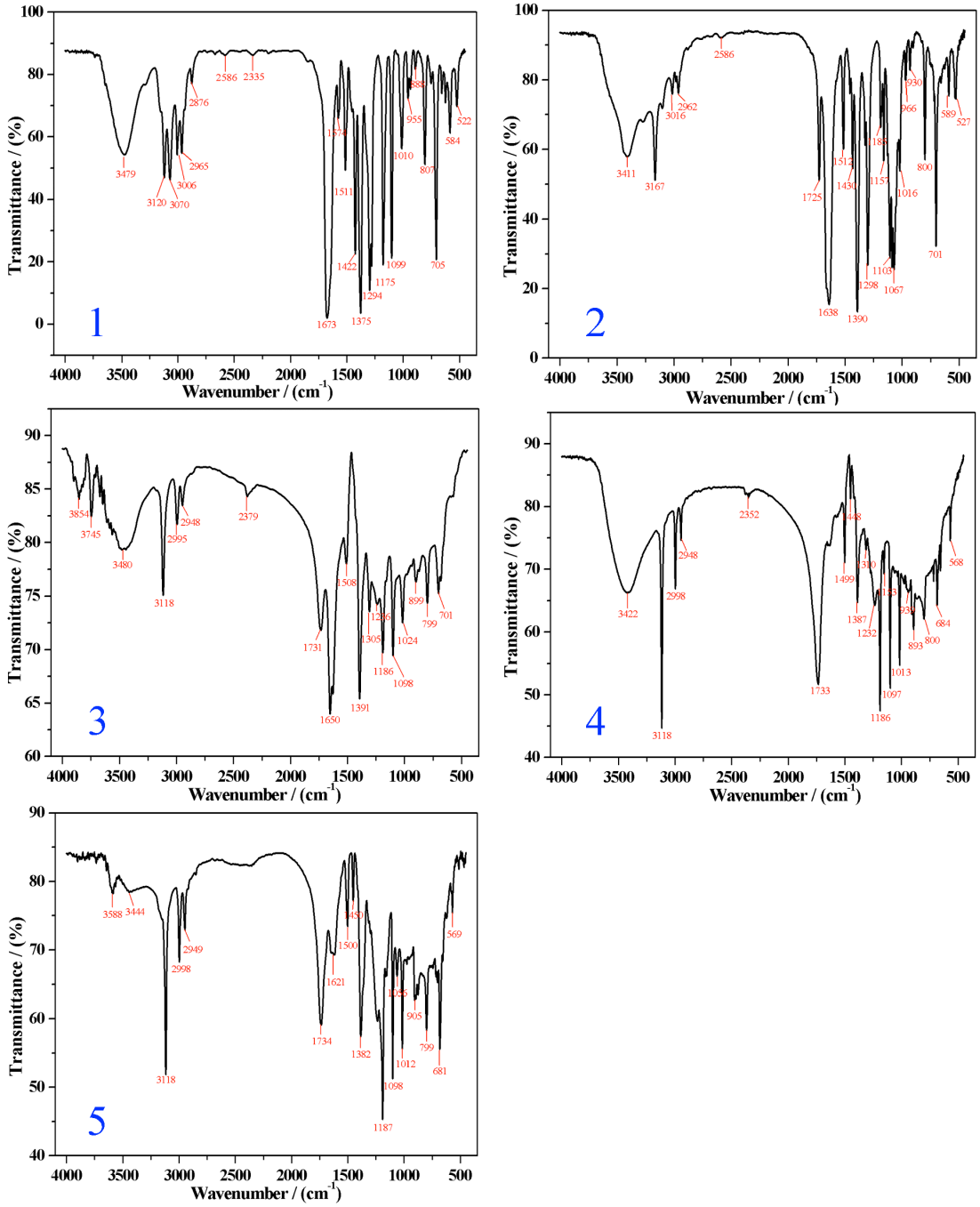


Figure S6. The FT-IR spectra of **1**–**5**.