

Supplementary Material

Two novel topological structure of [Cu(CN)] coordination polymers modified by flexible triazole ligands

Hui Xu,^a Bo-Yu Zhou,^b Kai Yu,^a Zhan-Hua Su,^{*a} Zhi-Feng Zhao,^c Wen-Long Sun,^d and Bai-Bin Zhou,^{*a}

1. Key Laboratory of synthesis of functional materials and green catalysis, Colleges of Heilongjiang Province, Harbin Normal University, Harbin, 150025, People's Republic of China;

2. Institute of Nuclear Physics and Chemistry, China Academy of Engineering Physics, Mianyang 621900, Sichuan, China;

3. College of Materials Science and Engineering, Heilongjiang University of Science & Technology, Harbin 150022, PR China;

4. Harbin University of Science and Technology, Harbin, 150025, People's Republic of China

1. Structural figures

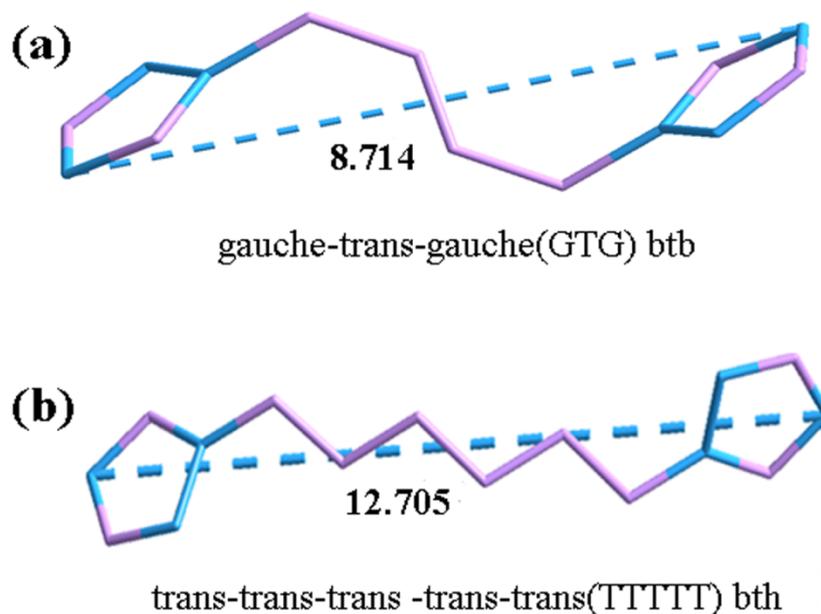


Fig. S1 The coordination modes of the auxiliary flexible ligands btb and bth

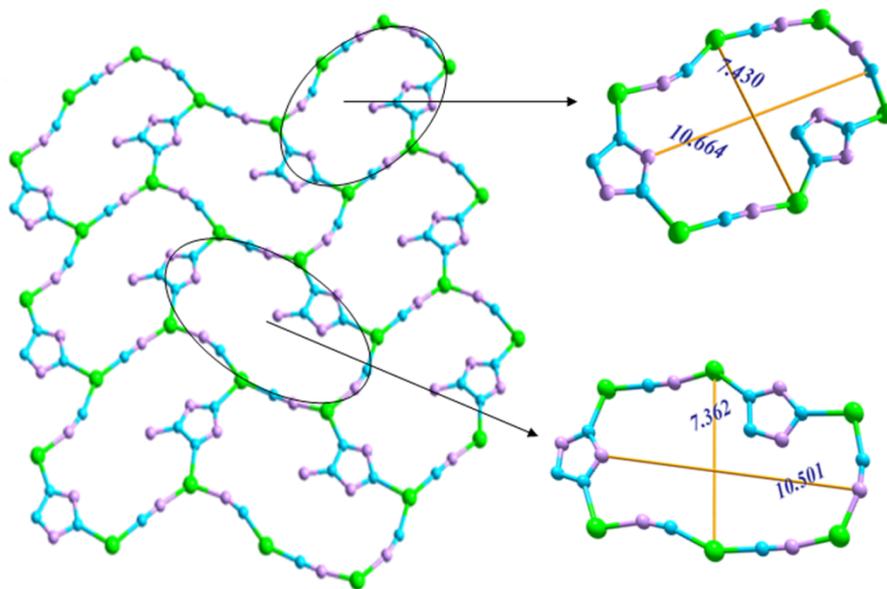


Fig. S2 The layer structure with rings A and B of the polymer 1.

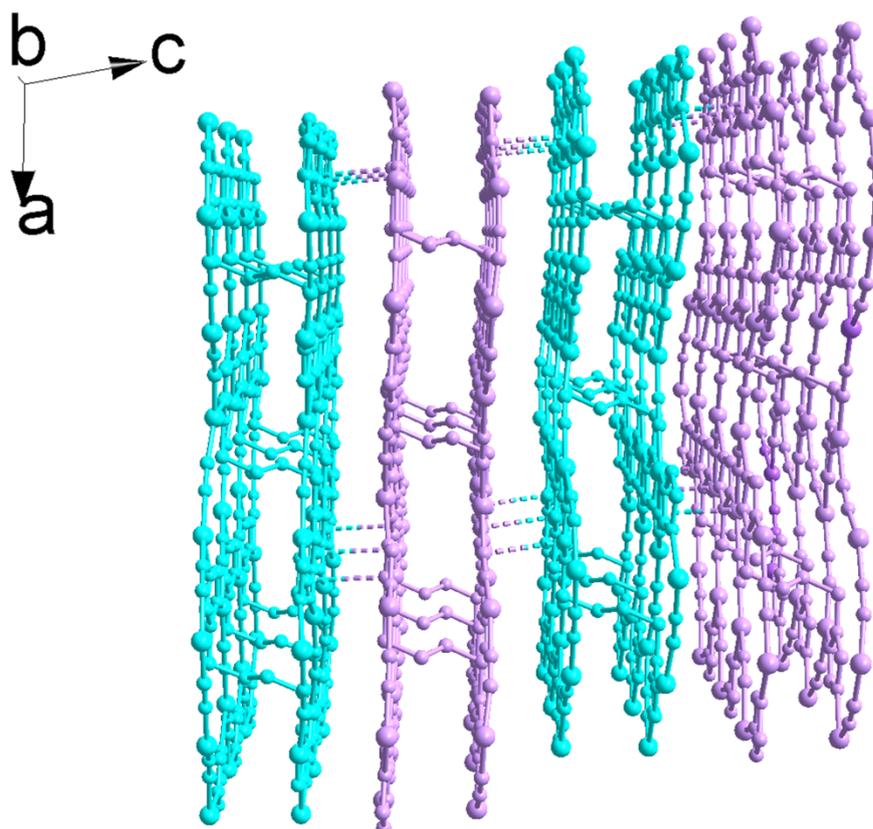


Fig. S3 3-D supramolecular structure of the polymer 1.

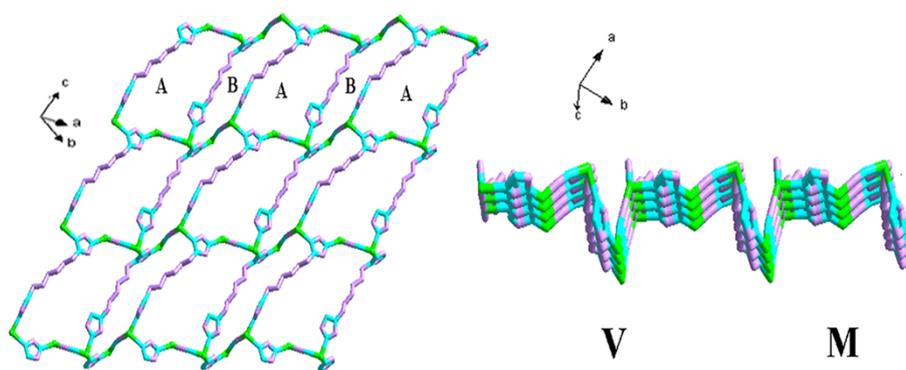


Fig. S4 Five-membered metal ring units in the polymer 2.

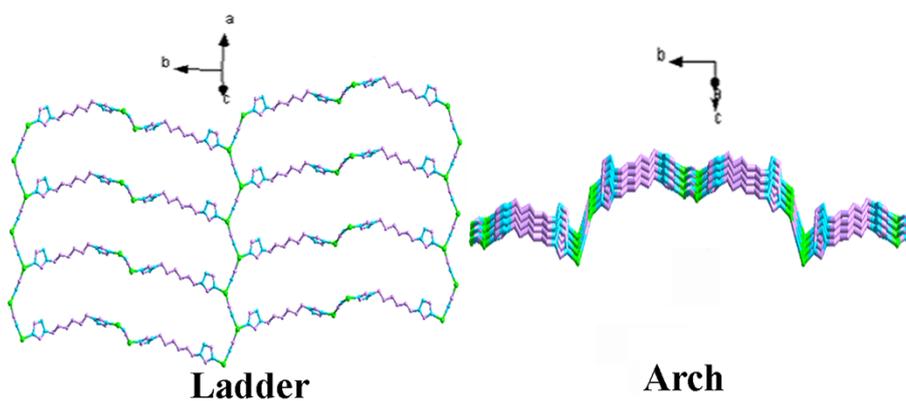


Fig. S5 Ten-membered metal ring units in the polymer 2.

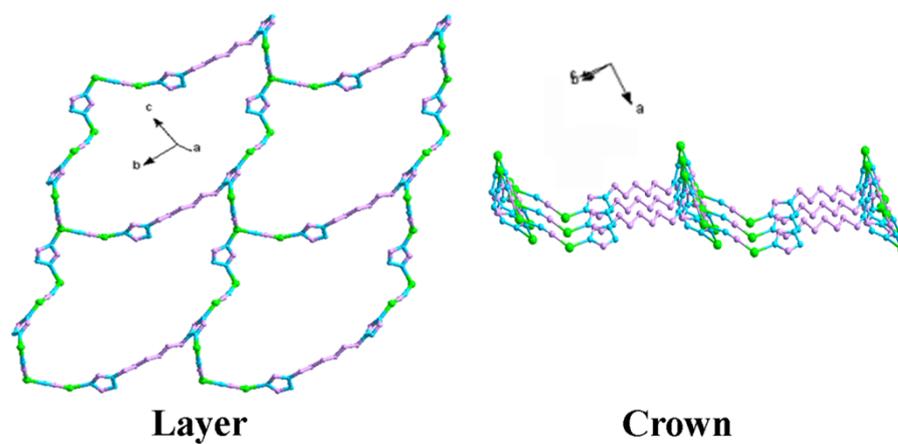


Fig. S6 Eleven-membered metal ring units in the polymer 2.

2. Physical characterization

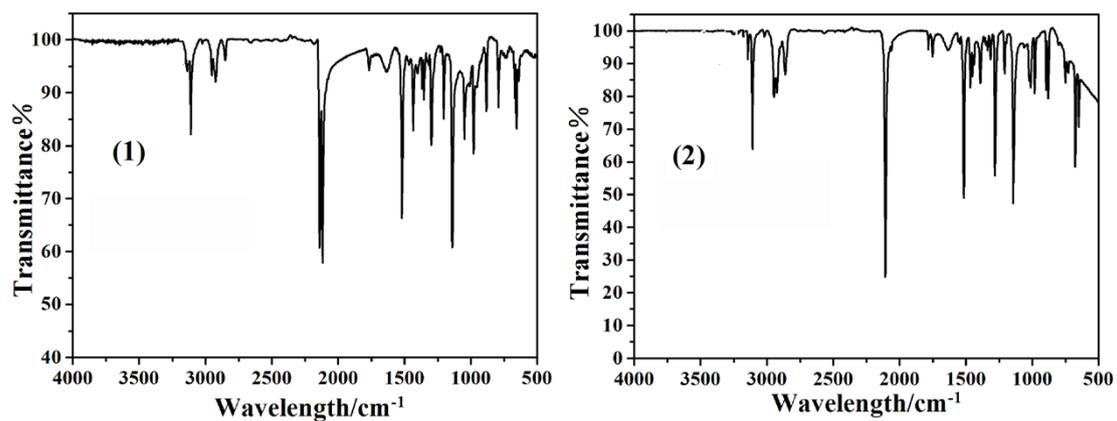


Fig. S7 The IR spectra of polymers 1 and 2.

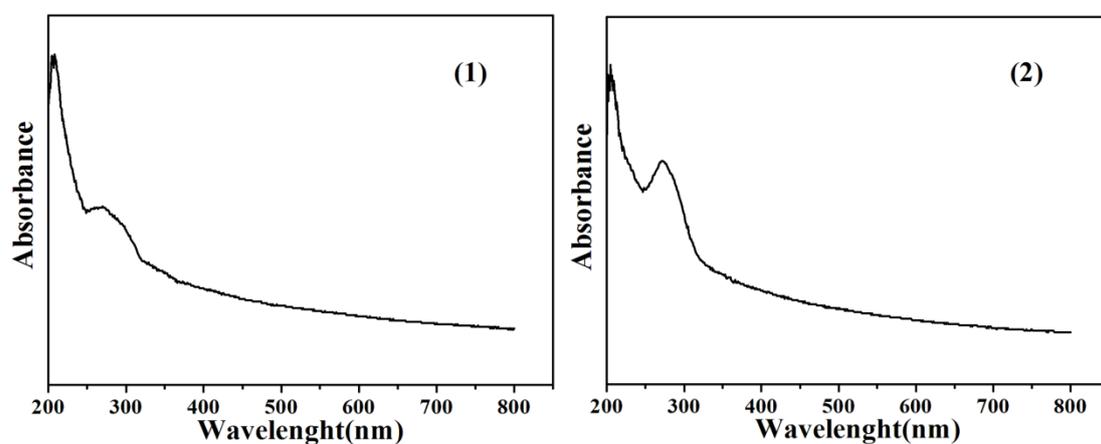


Fig. S8 Solid state UV-vis spectra of polymers 1 and 2.

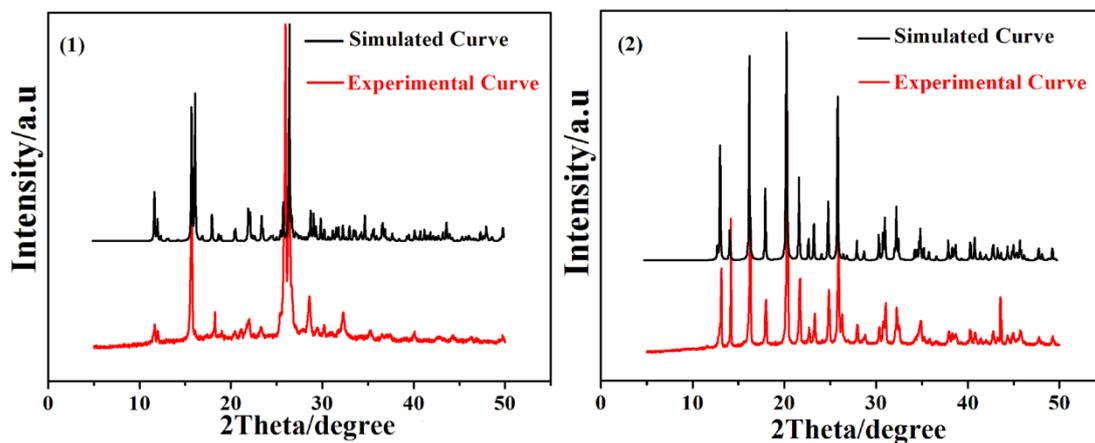


Fig. S9 The PXRD contrast curves of (1) polymer 1 and (2) polymer 2.

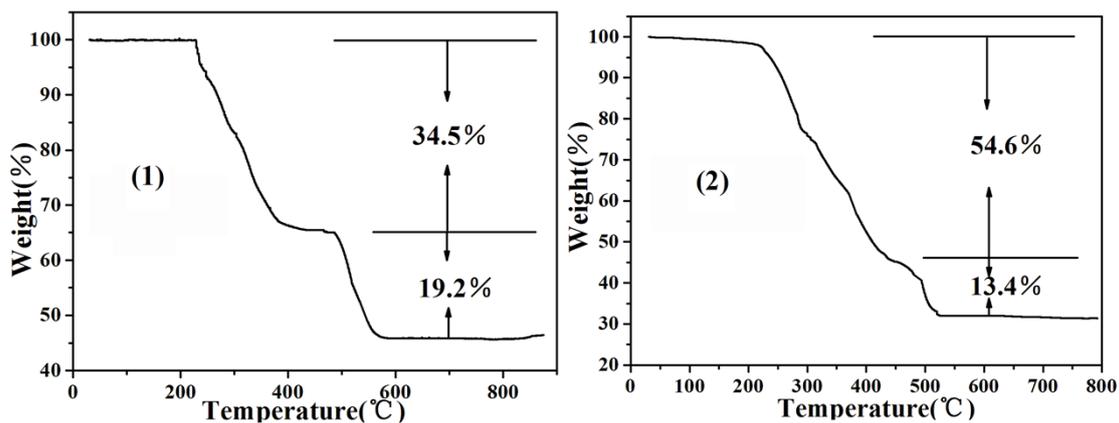


Fig. S10 TG curve of polymers 1 and 2.

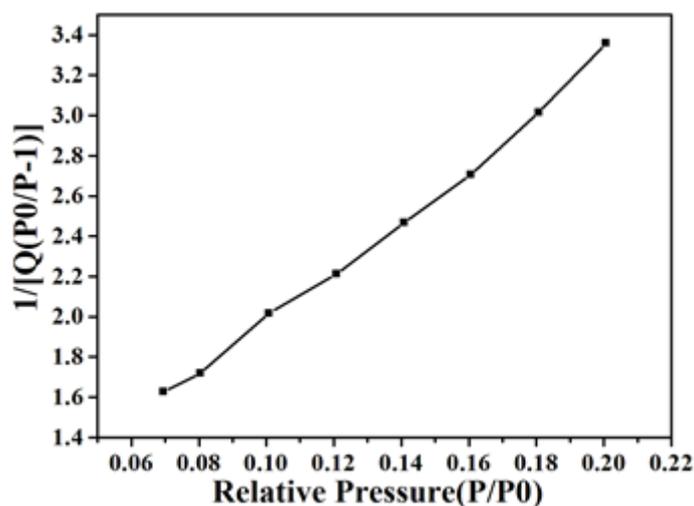


Fig. S11 The linear relationship diagram of the BET in polymer 2.

3. Structural data

Table S1 Selected bond lengths (Å) and bond angles (°) of polymers 1 and 2

Polymer 1			
Cu(3)-N(10)	1.864(5)	Cu(2)-C(12)#1	1.848(6)
Cu(3)-N(8)	1.889(6)	Cu(2)-C(5)	1.921(5)
Cu(3)-N(9)	2.071(5)	Cu(2)-N(1)	2.020(4)
Cu(1)-C(6)	1.862(6)	Cu(4)-N(5)	1.876(5)
Cu(1)-C(10)	1.915(6)	Cu(4)-N(4)	1.904(6)
Cu(1)-N(7)	1.999(4)	Cu(4)-N(3)	2.092(4)
N(10)-Cu(3)-N(8)	148.4(2)	C(12)#1-Cu(2)-C(5)	128.5(2)
N(10)-Cu(3)-N(9)	112.2(2)	C(12)#1-Cu(2)-N(1)	129.8(2)

N(8)-Cu(3)-N(9)	99.18(19)	C(5)-Cu(2)-N(1)	101.6(2)
C(6)-Cu(1)-C(10)	126.8(2)	N(5)-Cu(4)-N(4)	150.6(2)
C(6)-Cu(1)-N(7)	129.0(2)	N(5)-Cu(4)-N(3)	110.2(2)
C(10)-Cu(1)-N(7)	104.2(2)	N(4)-Cu(4)-N(3)	98.55(19)

Symmetry transformations used to generate equivalent atoms: #1 $x+1, y+1, z$ #2 $x, y+1, z$ #3 $x, y-1, z$
#4 $-x+2, y-1/2, -z+3/2$ #5 $-x+2, y+1/2, -z+3/2$ #6 $x-1, y-1, z$

Polymer 2

Cu(1)-C(6)	1.877(4)	Cu(1)-N(2)#2	2.348(3)
Cu(1)-N(4)#1	1.988(3)	N(4)-Cu(1)#3	1.988(3)
Cu(1)-N(3)	2.075(3)	N(2)-Cu(1)#4	2.348(3)
C(6)-Cu(1)-N(4)#1	124.36(15)	N(4)-C(6)-Cu(1)	174.9(4)
C(6)-Cu(1)-N(3)	126.39(14)	C(6)-N(4)-Cu(1)#3	167.6(3)
N(4)#1-Cu(1)-N(3)	99.54(13)	C(4)-N(3)-Cu(1)	135.7(3)
C(6)-Cu(1)-N(2)#2	112.01(15)	C(5)-N(3)-Cu(1)	121.5(2)
N(4)#1-Cu(1)-N(2)#2	96.81(13)	C(5)-N(2)-Cu(1)#4	121.8(2)
N(3)-Cu(1)-N(2)#2	88.74(12)	N(1)-N(2)-Cu(1)#4	134.5(2)

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

Table S2 Bond-valence sum calculations values in polymers 1 and 2.

Polymer 1	
Cu1	1.362
Cu2	1.359
Cu3	1.143
Cu4	1.097
Polymer 2	
Cu1	1.249