

A novel 3D Cu(I) coordination polymer based on Cu_6Br_2 and $\text{Cu}_2(\text{CN})_2$ SBUs: in situ ligand formations and naked-eye colorimetric sensor of NB and 2-NT

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Figure caption

Table S1 Bond lengths (Å) and Angles (deg) for compound **1**

Fig. S1 Experimental and simulated X-ray diffraction patterns of compounds **1**

Fig.S2 The DG-DTG curve of compound **1**

Fig. S3 Fluorescence titration of compound **1** dispersed in ethanol by gradual addition of 0.1 M solution of DNCB in ethanol

Fig. S4 Fluorescence titration of compound **1** dispersed in ethanol by gradual addition of 0.1 M solution of TNP in ethanol

Fig. S5 The film of compound **1** on the glass substrate (a) under daylight, (b) under UV illumination, (c) after the addition of 50 μL 0.1molL^{-1} 2-NT under UV illumination

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1			
Br(1)-Cu(2)	2.6777(14)	N(4)#3-Cu(1)-N(4)#4	107.8(2)
Br(1)-Cu(3)	2.7056(15)	C(1)-Cu(1)-C(1)#2	111.1(2)
Br(1)-Cu(4)	2.7515(11)	N(4)#3-Cu(1)-C(1)#2	94.76(16)
Br(1)-Cu(4)#1	2.7515(11)	N(4)#4-Cu(1)-C(1)#2	94.76(16)
C(1)-Cu(1)	1.940(8)	N(1)-Cu(2)-N(5)#5	118.39(14)
C(1)-Cu(1)#2	2.430(8)	N(1)-Cu(2)-N(5)#6	118.39(14)
Cu(1)-N(4)#3	2.012(4)	N(5)#5-Cu(2)-N(5)#6	108.7(2)
Cu(1)-N(4)#4	2.012(4)	N(1)-Cu(2)-Br(1)	109.3(2)
Cu(1)-C(1)#2	2.430(8)	N(5)#5-Cu(2)-Br(1)	99.24(12)
Cu(1)-Cu(1)#2	2.5048(19)	N(5)#6-Cu(2)-Br(1)	99.24(12)
Cu(2)-N(1)	1.936(6)	N(2)#1-Cu(3)-N(2)#7	159.0(3)
Cu(2)-N(5)#5	2.035(4)	N(2)#1-Cu(3)-Br(1)	100.51(13)
Cu(2)-N(5)#6	2.035(4)	N(2)#7-Cu(3)-Br(1)	100.51(13)
Cu(3)-N(2)#1	1.894(4)	N(3)#7-Cu(4)-N(3)	143.2(2)
Cu(3)-N(2)#7	1.894(4)	N(3)#7-Cu(4)-Br(1)#1	112.19(13)
Cu(4)-N(3)#7	1.955(4)	N(3)-Cu(4)-Br(1)#1	96.06(13)
Cu(4)-N(3)	1.955(4)	N(3)#7-Cu(4)-Br(1)	96.06(13)
Cu(4)-Br(1)#1	2.7515(11)	N(3)-Cu(4)-Br(1)	112.19(13)
N(2)-Cu(3)#1	1.894(4)	Br(1)#1-Cu(4)-Br(1)	80.15(4)
N(4)-Cu(1)#8	2.012(4)	N(1)-C(1)-Cu(1)	179.8(7)
N(5)-Cu(2)#9	2.035(4)	N(1)-C(1)-Cu(1)#2	111.3(6)
Cu(2)-Br(1)-Cu(3)	86.04(4)	C(1)-Cu(1)-N(4)#3	120.96(14)
Cu(2)-Br(1)-Cu(4)#1	125.44(2)	C(1)-Cu(1)-N(4)#4	120.96(14)
Cu(4)#1-Br(1)-Cu(4)	99.85(4)		

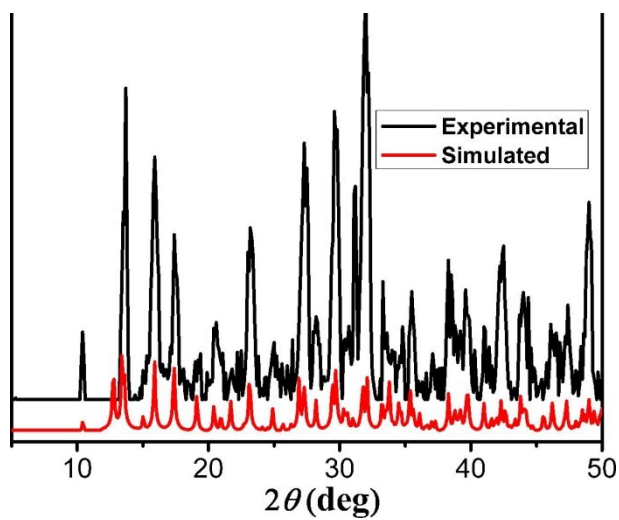


Fig. S1 Experimental and simulated X-ray diffraction patterns of compounds 1

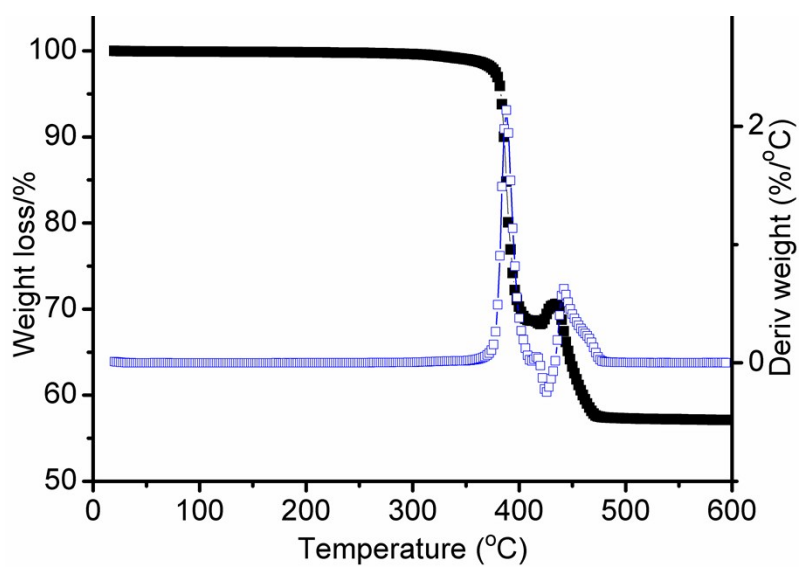


Fig.S2 The DG-DTG curve of compound 1

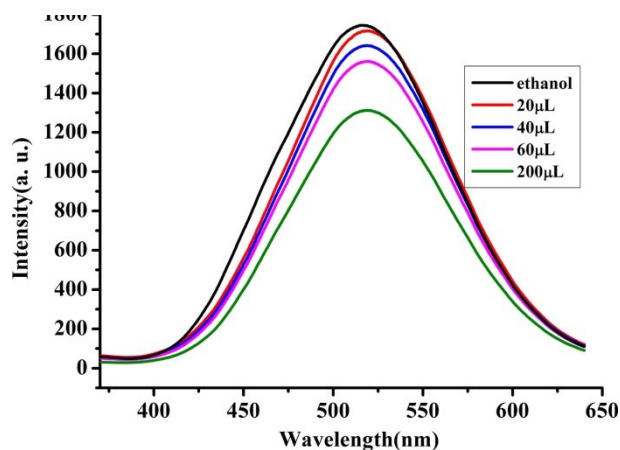


Fig. S3 Fluorescence titration of compound **1** dispersed in ethanol by gradual addition of 0.1 M solution of DNCB in ethanol

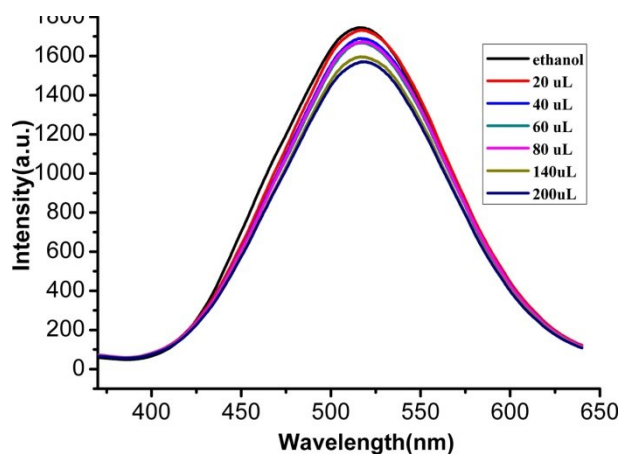


Fig. S4 Fluorescence titration of compound **1** dispersed in ethanol by gradual addition of 0.1 M solution of TNP in ethanol

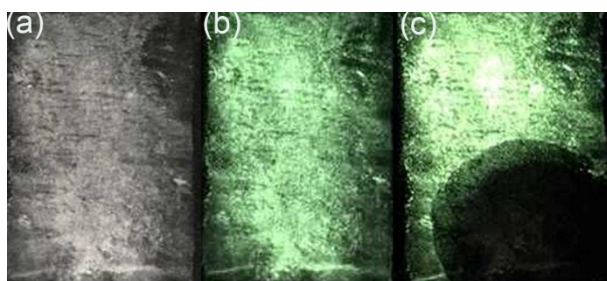


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