Electronic Supplementary Material (ESI) for Dalton Trans.

Electronic Supplementary Information

A Perfectly Aligned 6₃ Helical Tubular Cuprous Bromide Single Crystal for Selective Photo-catalysis, Luminescence and Sensor for Nitro-explosive

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	Compound	1	
Cu(1)-Br(1)	2.500(2)	Cu(2)-Br(1)	2.463 (3)
Cu(1)-Br(2)	2.372(2)	Cu(2)-Br(3)	2.5063(18)
Cu(1)-Br(3)	2. 929(1)	Cu(2)-Br(4)	2.539(3)
Cu(1)-Br(5d)	2.376(2)	Cu(2)-Br(3a)	2.5063(18)
Cu(3)-Br(2)	2.396(2)	Cu(3)-Br(4)	2.5491(19)
Cu(3)-Br(5)	2.427(2)	Cu(3)-Br(3)	2.759(3)
Cu(2)-Cu(1)	2.955(3)	Cu(3)-Cu(1)	3.1151(1)
Cu(2)-Cu(3)	2.976(2)		
Br(5d)-Cu(1)-Br(2)	128.12(10)	Br(1)-Cu(2)-Br(3a)	115.44(6)
Br(5d)-Cu(1)-Br(1)	110.12(9)	Br(1)-Cu(2)-Br(3)	115.44(6)
Br(2)-Cu(1)-Br(1)	112.90(9)	Br(3a)-Cu(2)-Br(3)	104.65(10)
Br(5d)-Cu(1)-Br(3)	100.053(1)	Br(1)-Cu(2)-Br(4)	107.07(10)
Br(2)-Cu(1)-Br(3)	98.745(2)	Br(3a)-Cu(2)-Br(4)	106.83(7)
Br(1)-Cu(1)-Br(3)	101.122(2)	Br(3)-Cu(2)-Br(4)	106.83(7)
Br(2)-Cu(3)-Br(5)	116.6(3)	Br(2)-Cu(3)-Br(3)	106.1(3)
Br(2)-Cu(3)-Br(4)	115.9(4)	Br(5)-Cu(3)-Br(3)	107.8(3)
Br(5)-Cu(3)-Br(4)	106.7(3)	Br(4)-Cu(3)-Br(3)	102.5(2)
Cu(1)-Cu(2)-Cu(1a)	106.27(11)	Cu(3)-Cu(2)-Cu(3a)	108.296(2)
Cu(1)-Cu(2)-Cu(3)	63.360(1)	Cu(2)-Cu(3)-Cu(1)	57.985(1)
Cu(2)-Cu(1)-Cu(3)	58.655(1)		

 Table S1. Bond lengths [Å] and angles [deg] of 1.



Figure S1. The PXRD patterns of simulated, before and after photocatalytic experimental for **1**.



Figure S3. (a) View of coordination environment of the copper ions, (b) the tortoiseshell-like Cu_5Br_{10} unit in 1.



Figure S4. (a) Electron-density distribution of HOMO and (b) LUMO for anion $[Cu_5Br_6]^-$ cluster.



Figure S5. (a) Emission spectra and (b) emission intensities ($\lambda_{em} = 530$ nm) of **1** in different solvents when excited at 358 nm, 1-6 corresponding to different solvents from anisole, phemethylol, toluene, benzene, chlorobenzene to NB.



Figure S6. UV-vis diffuse reflectance spectrum of 1.



Figure S7. Band-edge positions of **1** relative to the energy levels of various redox couples in water.



Figure S8. Color change photograph of MO dye solution during photodecomposition by 1, the ratio of remaining MO dye with time in presence of 1, TiO_2 and ZnO nanorods monitored by UV-vis spectra.



Figure S9. Color change photograph of KR dye solution during photodecomposition by 1, the ratio of remaining KR dye with time in presence of 1, TiO_2 and ZnO monitored by UV-vis spectra.



Figure S10. Color change photograph of MB dye solution during photodecomposition by 1, the ratio of remaining MB dye with time in presence of 1, TiO_2 and ZnO monitored by UV-vis spectra.



Figure S11. Color change photograph image of RhB dye solution during photodecomposition by 1, the ratio of remaining RhB dye with time in presence of 1, TiO_2 and ZnO monitored by UV-vis spectra.



Figure S12. The remaining concentration of MO after photocatalytic reaction compound **1** as photocatalyst over 6 cycles.



Figure S13. (a) Single crystalline photo of 1, (b) photos after photocatalytic reaction by TiO_2 and 1 as photocatalysts.