Cuprophilicity Induced Cocrystallization of $[Cu_2(4,4'-bpy)(CN)_2]_n$ Sheets and $[Cu(SCN)]_n$ Chains into a Three-Dimensional Pseudo-polyrotaxane

Xian-Ming Zhang, * Zhen-Ming Hao, Hai-Shun Wu

School of Chemistry & Material Science, Shanxi Normal University, Linfen 041004, P. R. China. Fax: Int. code +86 357 2051402; E-mail: zhangxm@dns.sxtu.edu.cn

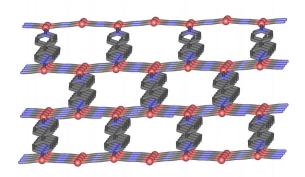


Fig. S1 View of stacking of $[Cu_2(4,4'-bpy)(CN)_2]_n$ along the *c*-axis direction showing the channels.

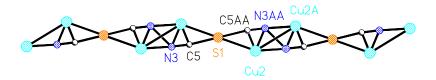


Fig. S2 View of the disordered [Cu(SCN)]_n chain.

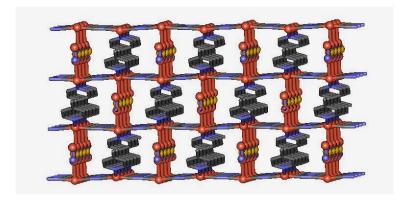


Fig. S3 View of the 3-D pseudo-polyrotaxane along the c-axis direction showing dually disordered [Cu(SCN)]_n chains penetrating 2-D [Cu₂(4,4'-bpy)(CN)₂]_n layers and unsupported Cu^I-Cu^I interactions.

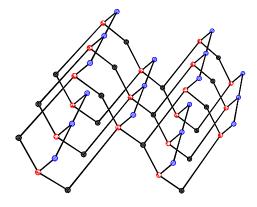


Fig. S4 Schematic view of the 3-D trinodal (3,4)-connected net. The three different nodes are shown in red, black and blue color, respectively.

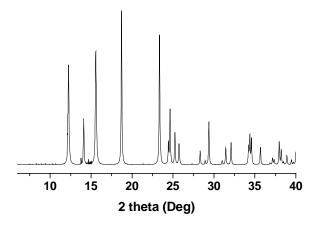


Fig. S5 X-ray powdered diffraction pattern of 1.

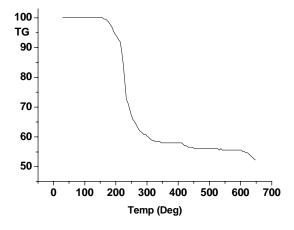


Fig. S6 TGA curve of 1 in air at the heating rate of 10 °C per minute.

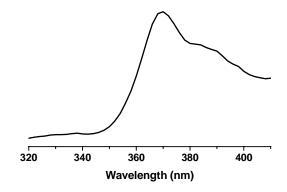


Fig. S7 Photoluminescent emission spectrum of 1 $\lambda_\text{ex} = 220$ nm at room temperature.

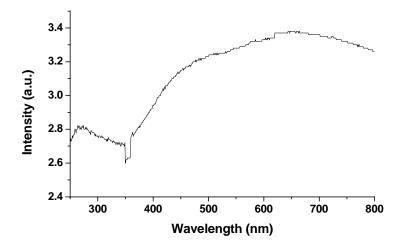


Fig. S8 The Solid UV-vis spectrum of 1 in KBr pallet.