Electronic Supplementary Material for CrystEngComm

An Infinite Photoluminescent Coordination Nanotube $[CuSCN(L)]\bullet(DMF)_{0.5}$

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Supporting Information

Contents:

Materials and Methods

1,3-Imidazolidine-2-thione was prepared according to the literature method (Allen C.F.H.; Eden C.O.; Van Allen, J. *Organic Syntheses*, Col. Vol. III, Wiley, New York, **1959**, p. 394). All other reagents and solvents were commercially purchased without further purification. Infrared spectra were obtained in KBr disks on a Bruker Vector 22 spectrophotometer with KBr pellets in the 4000 - 400 cm^{-1} region. Thermal analysis (TG) was carried out in a nitrogen stream using Seiko Extar 6000 TG/DTA equipment with a heating rate of 10 °C/min. XRD patterns were measured with Cu Kα radiation using a Rigaku D/max-RA diffractometer. Photoluminescence analyses were performed on a Hitachi 850 fluorescence spectrophotometer.

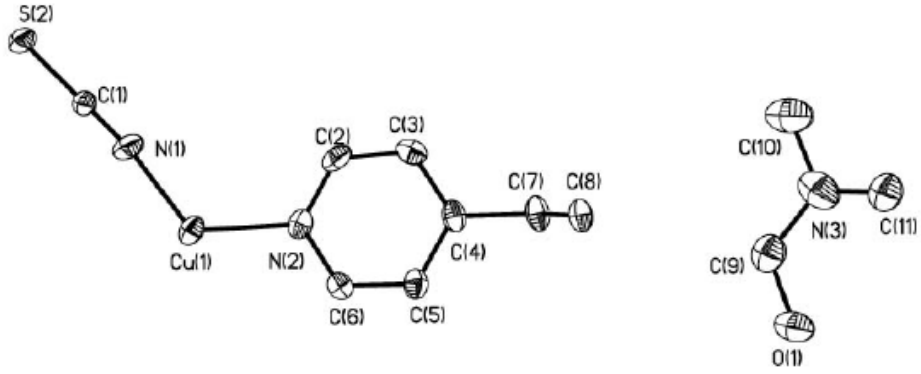

Figure S1. An ORTEP drawing of the asymmetric unit of complex **1** at the 50% probability (H atoms are omitted for clarity).

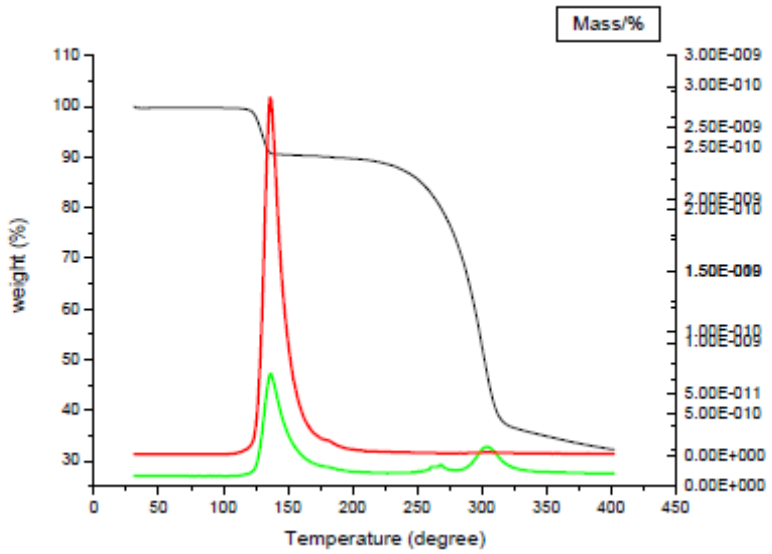

Figure S2. TG-MS profiles of complex **1** obtained with imidazolidine-2-thione, thiourea or hexahydropyrimidine-2-thione showing the release of the DMF guest molecules (m/z: 73, red line; m/z:44, green line) around 120ºC.

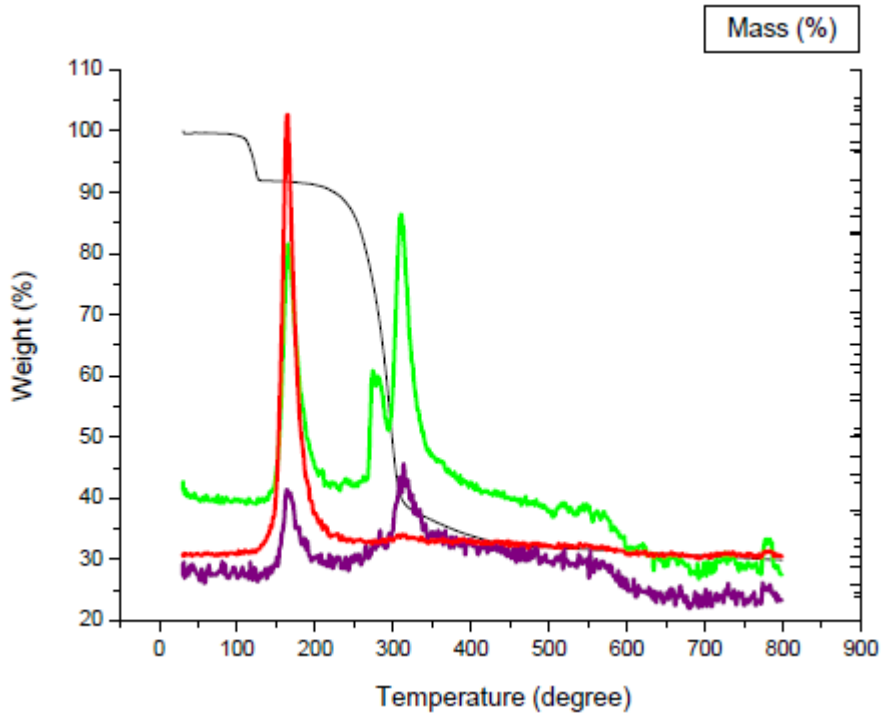

Figure S3. TG-MS profiles of complex **1** exchanged with CH_3CH_2OH, showing the release of the DMF guest molecules (m/z: 73, red line; m/z: 44, green line) and CH_3CH_2OH (m/z: 45, purple line) around 120ºC.

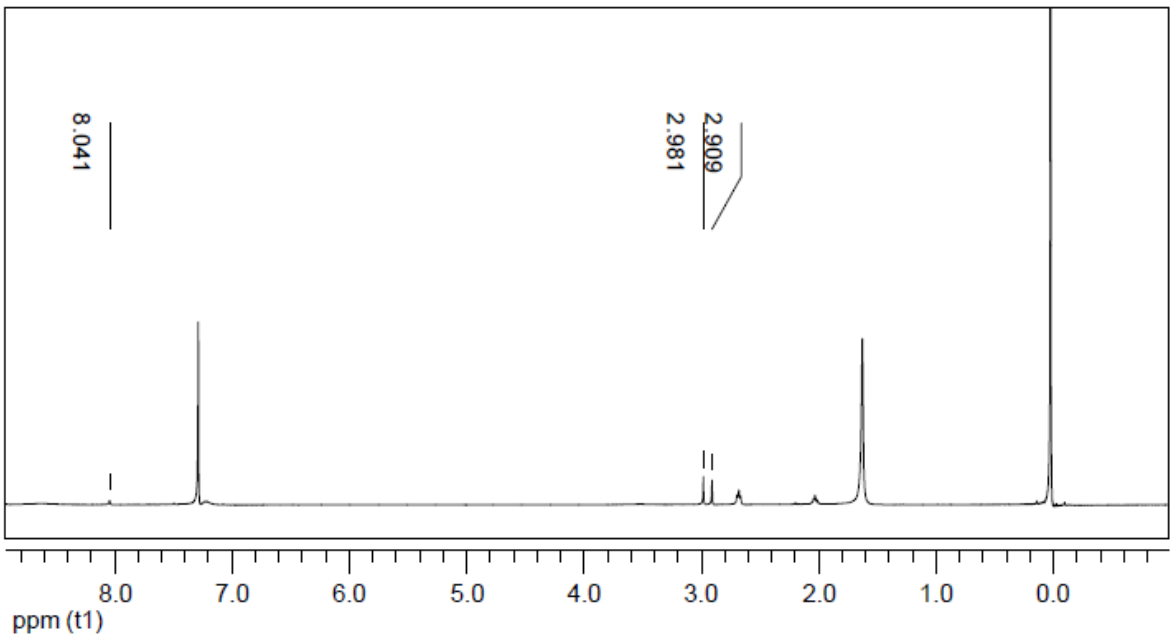

Figure S4. ^1H NMR spectrum of complex **1** obtained with thiourea/ imidazolidine-2-thione after immersed in $CDCl_3$ for three days at room temperature, showing the release of DMF molecules.

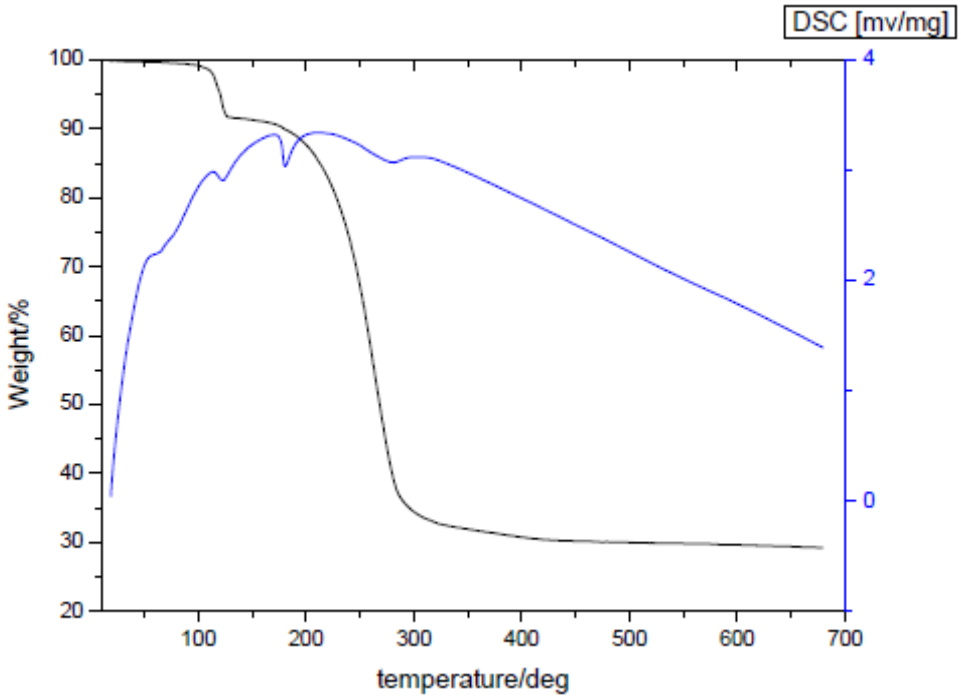

Figure S5. TGA-DTA curves of complex **1** under nitrogen.

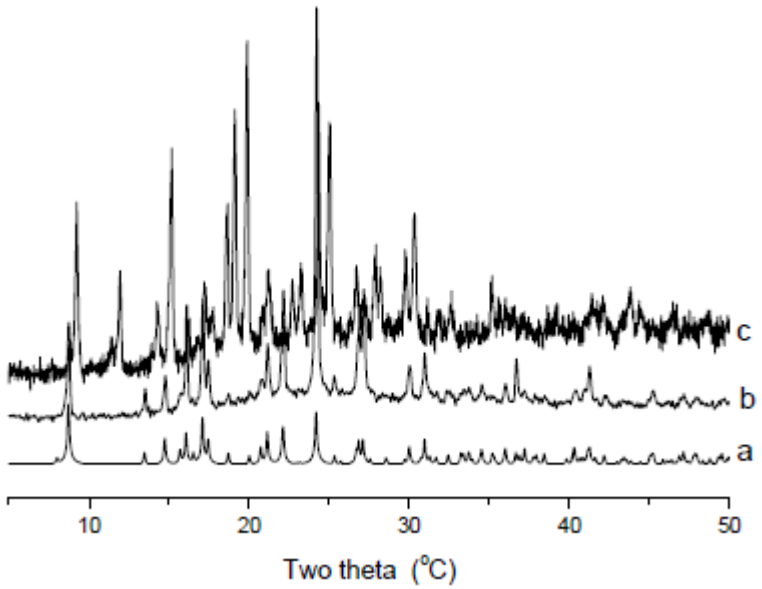

Figure S6. PXRD patterns for **1**: (a) the simulated, (b) the as-synthesized, (c) after removal of guest solvent molecules.

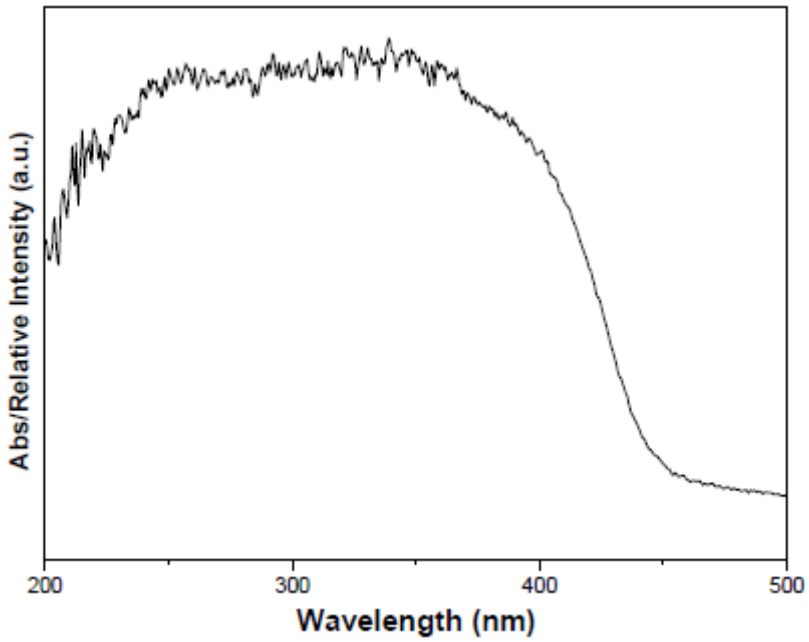

Figure S7. Solid state UV absorption spectrum of complex **1** at room temperature.