

MS15-P30 Thiolate halide copper(I) 2D coordination polymers with thermochromic luminescent properties

Josefina Perles¹, Javier Troyano², Carlos Zaldo³, Félix Zamora², Salomé Delgado²

1. Laboratorio de Difracción de Rayos X de Monocristal, Servicio Interdepartamental de Investigación, Universidad Autónoma de Madrid, 28049 Madrid, Spain

2. Departamento de Química Inorgánica, Facultad de Ciencias, Universidad Autónoma de Madrid, 28049 Madrid, Spain

3. Departamento de Materiales Fotónicos, Instituto de Ciencia de Materiales de Madrid (CSIC), 28049 Madrid, Spain

email: josefina.perles@uam.es

The design of coordination compounds and, particularly, coordination polymers^{1,2} as advanced materials is one of the most exciting and promising topics in materials science. The physical properties of this type of compounds are strongly dependent on the nature of the constituents, both the metal center and the ligands used to construct the polymer in the solid state. However, the structure itself in the solid state also plays a crucial role. In the case of coordination polymers, the obtention of a flexible framework can lead to small changes in the crystal packing under different experimental conditions, which may in turn affect the properties.

Three new 2D polymeric copper(I) thiolates with formula $[\text{Cu}_3\text{X}(\text{HT})_2]_n$ (X= Cl, Br, I; HT= 4-mercaptophenol) have been synthesised by solvothermal procedures. The crystal structures of these coordination polymers have been solved by single crystal X-ray diffraction. They display a similar layered structure with the hydroxyl groups from the HT ligands joining the polymeric sheets by hydrogen bonds.

These compounds present a strong orange emission at room temperature. A reversible thermochromic effect is observed on cooling, stronger in the iodine derivative. The emission changes from orange, at room temperature, to green at lower values. Photoluminescence in these coordination polymers has been studied at different temperatures, and the disappearance of the lower energy band is observed with decreasing temperature, together with an increase in the intensity of the more energetic band. Changes in the luminescent properties are associated with the structural modifications observed in the crystal structures solved both at room temperature and at 110 K.

1-Kitagawa, S.; Noro, S.: *Comprehensive Coordination Chemistry*, 2004; Vol. 7.

2-Batten, S. R.; Neville, S. M.; Turner, D. R.: *Coordination polymers: Design, analysis and application*; Royal Society of Chemistry, 2008.

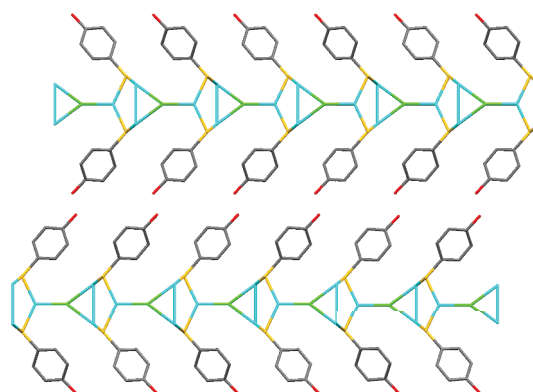


Figure 1. Layered structure of $[\text{Cu}_3\text{Cl}(\text{HT})_2]_n$ at room temperature viewed along the c axis. Hydrogen atoms have been omitted for clarity.

Keywords: coordination compounds, photoluminescence, framework flexibility