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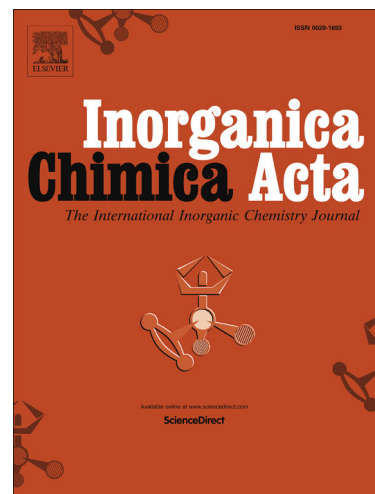
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# Synthesis, structural variation, photophysical, electrochemical and DFT studies of CuX (X= I, Br and Cl) mixed ligand complexes of an azino-pyridyl ligand and triphenylphosphine

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## Abstract

Three new copper(I) coordination oligomers  $[\text{Cu}_2(\text{L})_2(\mu\text{-I})_2(\text{PPh}_3)_2]_2$  (**1**),  $[\text{Cu}_2(\mu\text{-L})(\mu\text{-Br})_2(\text{PPh}_3)_2 \cdot \text{CH}_2\text{Cl}_2]_\infty$  (**2. CH<sub>2</sub>Cl<sub>2</sub>**) and  $[\text{Cu}_2(\mu\text{-L})(\mu\text{-Cl})_2(\text{PPh}_3)_2]_\infty$  (**3**) have been synthesized by reactions of equimolar CuX (X = I, Br and Cl), PPh<sub>3</sub> and the polydentate azino-pyridyl ligand **L**. These complexes have been characterized by elemental analyses, IR, UV–Vis and NMR spectroscopy. The crystal structures of the complexes **1** and **2. CH<sub>2</sub>Cl<sub>2</sub>** have been determined by single-crystal X-ray analysis and it has been found that complex **1** is a dimer with  $\text{-}\{\text{Cu}^{\text{I}}(\mu\text{-I})\text{-Cu}^{\text{I}}\text{-}$  rhomboid core whereas complex **2. CH<sub>2</sub>Cl<sub>2</sub>** is a 1-D co-ordination polymer containing bridged  $\text{Br}^{-1}$  ion as well as the ligand **L**. Matching of X-ray powder pattern of **3** with the simulated powder data obtained from the single crystal of **2. CH<sub>2</sub>Cl<sub>2</sub>**, and DFT studies reveal that the complex **3** is also a 1-D co-ordination polymer like complex **2. CH<sub>2</sub>Cl<sub>2</sub>**. At room temperature in dichloromethane the ligand **L** is non-emissive whereas the complexes **1**, **2** and **3** are photoluminescent. The  $E_{1/2}$  values of the  $\text{Cu}^{\text{I}}\text{-Cu}^{\text{II}}$  couple of **1**, **2** and **3** are 1.06 V, 0.85 V and 0.81 V (vs. Ag/AgCl in 1 M KCl, scan rate 100 mV s<sup>-1</sup>) respectively. DFT and Hirshfeld surfaces computational studies have also been performed for **1**, **2** and **3**.

Keywords: Dimer, copper(I), 1-D coordination polymer; crystal structure, azino-pyridyl ligand, electrochemistry and Hirshfeld surfaces studies.

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