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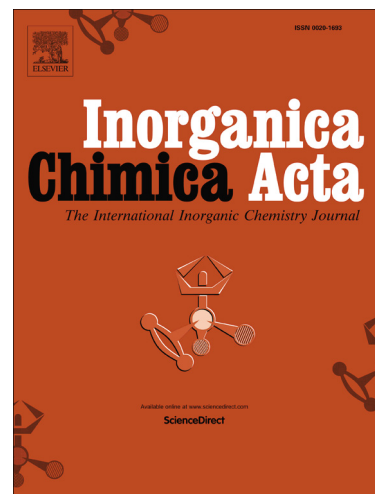
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# Non-Innocent Ground State Electronic Structure of a Polynuclear Copper Complex with Picolinate Bridges

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## Abstract

A mononuclear copper complex  $[\text{Cu}^{\text{II}}(\text{asN4Py})(\text{MeCN})](\text{O}_3\text{SCF}_3)_2$  (**1**) and its mixed mono- and trinuclear  $[\text{Cu}(\text{pic})_2(\text{ClO}_4)_2][\text{Cu}_3(\text{asN4Py})_2(\text{pic})_2(\text{ClO}_4)_2](\text{ClO}_4)$  derivatives (**2**) were synthesized containing *N,N*-bis(2-pyridylmethyl)-1,2-di(2-pyridyl)-ethylamine (asN4Py) chiral ligands and 2-picolinate (pic) bridges. The structures were elucidated using single crystal X-ray diffraction and spectroscopic methods. Due to the non-trivial assignments of the formal Cu oxidation states, the d-electron count and the location of electron holes were assigned by broken-symmetry electronic structure calculations using a spectroscopically validated, hybrid density functional theory with saturated basis set. The ground state description of the mononuclear complexes is trivial; thus, they were used to validate the computational level of theory and the modelling approach. The experimental structure of the trinuclear complex can only be described by considering two asymmetric resonance structures in the crystal structure containing  $\text{Cu}^{\text{II}}\text{-Cu}^{\text{II}}\text{-Cu}^{\text{I}}/\text{Cu}^{\text{I}}\text{-Cu}^{\text{II}}\text{-Cu}^{\text{II}}$  metal centres.

**Keywords:** Copper(II); Pentadentate; Chiral; X-ray crystal structure; Computation.

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