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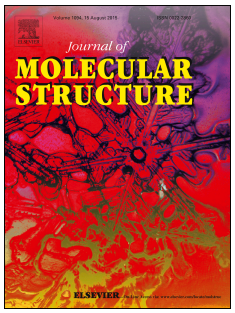

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Synthesis, X-ray crystal structures, electrochemistry and theoretical investigation of a tetradentate nickel and copper Schiff base complexes

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ABSTRACT

New tetradentate mononuclear nickel(II) [NiL] and pentadentate binuclear copper(II) **[$Cu_2L_2H_2O$], H_2O** Schiff base complexes have been synthesized. The crystal structures of [NiL] and **[$Cu_2L_2H_2O$], H_2O** have been determined by X-ray diffraction method showing distorted square-planar geometry for [NiL] and distorted tetragonal pyramid geometry for **[$Cu_2L_2H_2O$], H_2O**. In both complexes, the dehydroacetic acid functional group engages in a deprotonated manner and coordination occurs through the nitrogen atoms of the imine function and the phenolic oxygen. Density Functional Theory calculations are carried out for the determination of the optimized structures. The fundamental vibrational wave numbers are calculated and a good agreement between observed and calculated wave numbers is achieved.