Interaction of Na(I), Ni(II) and Cu(II) with 2-cyano-2-(hydroxyimino)acetic acid: spectroscopic and theoretical studies.

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Streszczenie

Sodium(I) salt as well as nickel(II) and copper(II) complexes of 2-cyano-2-(hydroxyimino)acetic acid (**1a**) have been prepared and characterized by infrared, Raman and EPR spectra. Molecular structures of the compounds in the solid state are proposed. The bidentate **1a** ligand chelates the copper and nickel ions through the oxime nitrogen and the carboxyl oxygen atoms to form a *trans* bis-complexes. However, two sodium ions are bonded to the deprotonated oximic as well as carboxylic groups. Equilibrium geometries, atomic charges, harmonic vibrational frequencies with potential energy distribution (PED), infrared and Raman intensities are calculated for all compounds studied here by using the hybrid functional of DFT (B3LYP) with 6-311++G(d,p) and LanL2DZ basis sets, for sodium and transition metal ions complexes, respectively. The computed properties are compared to the experimental values.

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