

Synthesis, Structure, Spectroscopic Studies and *ab-initio* Calculations on First Hyperpolarizabilities of N,N'-Bis(2-hydroxy-1-naphthylmethylidene)-1-methyl-1,2-diaminoethane-N,N',O,O'-copper(II)

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N,N'-Bis(2-hydroxy-1-naphthylmethylidene)-1-methyl-1,2-diaminoethane-N,N',O,O'-copper(II) has been synthesized, and characterized by FT-IR and UV/vis spectroscopies. Its crystal structure has been determined by X-ray diffraction analysis. The maximum absorption wavelengths recorded by linear optical experiments are estimated in the UV region to be shorter than 450 nm, showing good optical transparency to the visible light. It may thus possess first hyperpolarizabilities with non-zero values for nonlinear optical (NLO) applications. *Ab-initio* quantum chemical calculations of the electric dipole moments (μ) and the first static hyperpolarizabilities (β) were carried out. The computational results suggest that the complex may indeed have microscopic NLO behavior with non-zero values.

Key words: Copper(II) Complex, UV-visible Spectroscopy, Crystal Structure,
First Hyperpolarizability, Electric Dipole Moment