Second-Order Nonlinear Optical Properties of Tetradentate Schiff base Complexes

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Quadratic non-linear optical properties of new unsymmetrical Ni(II), Cu(II), Zn(II) and VO(II) complexes with $[N_2O_2]$ chelate tetradentate ligands are presented. The complexes were synthesized by template condensation of 1-phenylbutane-1,3-dione mono-*S*-methylisothiosemicarbazone with o-hydroxybenzaldehyde or its 5-phenylazo-derivative. The crystal structure of some complexes was determined by using synchrotron radiation (XRD1 beamline at ELETTRA, Trieste).

Large values of hyperpolarizability, as obtained for these complexes by the solution-phase dc electric-field-induced second harmonic (EFISH) generation method, together with their high stability constants, make them promising candidates for successful applications in the field of optoelectronic technologies.

The values of theoretical hyperpolarizability, calculated through both Finite Field and Time Dependent DFT methods, are also presented.

Keywords: transition-metal complexes, nonlinear optical properties, theoretical calculations