Third-order Nonlinear Optical Properties of Copper(II)bis{2-[(4-iodophenyl)iminomethyl]-6-methoxy-phenolate}

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Copper(II)bis{2-[(4-iodophenyl)iminomethyl]-6-methoxy-phenolate} has been synthesized, characterized by UV-visible spectroscopy, and its crystal structure determined by X-ray diffraction. The Cu atom is situated on a twofold axis and the geometry around the metal centre can be described as distorted square planar with a *trans* configuration. The absorption maxima are shorter than 450 nm, giving rise to good optical transparency in the visible and near IR. To reveal the microscopic third-order NLO properties, the static second hyperpolarizabilities have been evaluated by using the *ab initio* time-dependent Hartree-Fock (TDHF) method. According to the results, the title complex exhibits non-zero γ values, implying microscopic third-order NLO behavior.

Key words: Copper(II) Complex, Time-Dependent Hartree-Fock, Static Third-Order Hyperpolarizability, UV-visible Spectroscopy, *ab initio* Calculation