TOPOLOGICAL ANALYSIS AND FREQUENCY DEPENDENT HYPERPOLARIZABILITY CALCULATIONS OF FDDNP: A DFT STUDY

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Abstract. The topological and first-hyperpolarizability properties of 2-(1-{6-[(2-fluoroethyl)(methyl)amino]-2-naphthyl}ethylidene)malononitrile (FDDNP) were studied using DFTB3LYP method. The static and dynamic electronic (hyper)polarizabilities of conformers were calculated and a simple two-state model was employed to explain the first hyperpolarizability differences in two conformers. The second harmonic generation property was evaluated at the typical wavelengths of Cr:forsterite, Nd:YAG(neodymium-doped yttrium aluminium garnet) and Ti:sapphire lasers to predict the compound conformers potency for second harmonic generation imaging in biological studies.