Second-order Nonlinearities of Anionic 3-dicyanomethylen-5,5-dimethyle-1-[2-(4-hydroxyphenyl)ethenyl)]-cyclohexene

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Résumé en anglais	Due to the connecting one π-conjugated group with the two backside donor and acceptor groups, anionic 3-dicyanomethylen-5,5-dimethyle-1-[2-(4-hydroxyphenyl)ethenyl)]-cyclohexene (1) might possess nonlinear optical (NLO) properties. To estimate the potential for second-order NLO behaviour; the electric dipole moments and dispersion-free dipole polarizabilities and first hyperpolarizabilities have been determined by density functional theory (DFT) at B3LYP/6-31++G(d, p) level. Quantum mechanical calculations using time-dependent Hartree-Fock (TDHF) procedure have been utilized to evaluate frequency-dependent second-order nonlinearities of 1. The one-photon absorption (OPA) characterization of 1 has been theoretically obtained by means of configuration interaction (CI) with 6-31G basis set. Our theoretical results on the maximum OPA wavelength, second-order susceptibilities and corresponding microscopic NLO responses are accorded with the previous experimental observations of the investigated compound. The highest occupied molecular orbitals, the lowest unoccupied molecular orbitals and the HOMO-LUMO band gaps for 1 have been also examined by DFT/B3LYP method.
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