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NONLINEAR OPTICAL PROPERTIES OF CHROMOPHORES WITH INDOLIZINE

DONORS: THEORETICAL STUDY

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Abstract

New class of nonlinear optical chromophores with donors containing indolizine moiety is proposed. Dipole moment and first hyperpolarizability values of the chromophores, which are analogs of FTC, CLD and OLD chromophores, containing 1-methyl-2-phenylindolizin-3-yl (MPI-3) or 3-methyl-2-phenylindolizin-1-yl (MPI-1) donors (instead of diethylaminophenyl), 3-cyano-2-dicyanomethylene-5,5-dimethyl-1,5-dihydrofuran-4-yl (TCF) acceptor, and 2,5-divinylthiophene, octatetraene and 2,2'-divinylbithiophene π -electron bridge, are calculated by DFT technique. Chromophores with named donors and acceptors and 3,7-divinylquinoxalin-2-one π -electron bridge are also studied. In most cases higher values of first hyperpolarizability were obtained for chromophores with (MPI-3) donor, this being in accordance with the electron

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