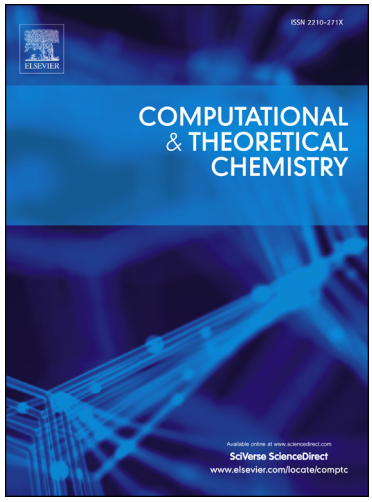

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THEORETICAL PREDICTIONS OF NONLINEAR OPTICAL CHARACTERISTICS OF NOVEL CHROMOPHORES WITH QUINOXALINONE MOIETIES

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Keywords: chromophores with 3,7-divinylquinoxalin-2-one π-bridge, nonlinear optics, quantum chemical calculations, DFT, first hyperpolarizability

Abstract

New class of nonlinear-optical (NLO) chromophores is proposed, containing quinoxalin-2-one moiety in π-electron bridge. The chromophores electric characteristics (dipole moments and molecular polarizabilities) are calculated in the framework of the DFT technique, and *structure-property* relationship is established. The chromophores with donor bound in position 3 to quinoxalin-2-one one through vinyl group demonstrate the greatest NLO characteristics among the molecular systems under study. The calculated values of the first hyperpolarizability for the chromophores with 3,7-divinylquinoxalin-2-one π-electron bridge and TCF and TCP acceptor fragments exceed the corresponding values of the majority of the known world analogues.