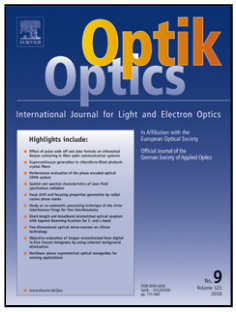

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A Comparative Analysis of the Optical and Nonlinear Optical Properties of Cross-shaped Chromophores: Quantum Chemical Approach

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Abstract

Using the first principles calculations, optical and nonlinear optical (NLO) properties are calculated for three crossed shaped chromophores having alike benzoic acid π-conjugated side chains but different central cores i.e. phenyl in **1-Ph**, pyrazino[2,3-*g*]quinoxaline in **2-PyQ** and tetrathiafulvalene in **3-TTF**. Molecular geometries are effectively reproduced and compared to their experimental crystallographic structures. The third-order NLO polarizability is calculated with three different DFT functionals including M06, PBE0 and B3LYP and using 6-311G* basis set. Our calculated third-order NLO polarizability amplitudes and their comparison to those of standard and contemporary NLO chromophores indicate that all the three compounds have remarkably larger NLO response. The γ amplitudes of compounds **1-Ph**, **2-PyQ** and **3-TTF** are 429.6×10^{-36}, 1871.7×10^{-36} and 967.5×10^{-36} esu, respectively, at M06/6-311G* level of theory. Interestingly, in present investigation the γ amplitude of the best-studied NLO compound **2-PyQ** is 257 times larger than that of para nitroaniline (7.279×10^{-36} esu) at the same M06/6-311G* level