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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  $\pi$ -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  $\gamma$  amplitudes of compounds **1-Ph**, **2-PyQ** and **3-TTF** are  $429.6 \times 10^{-36}$ ,  $1871.7 \times 10^{-36}$  and  $967.5 \times 10^{-36}$  esu, respectively, at M06/6-311G\* level of theory. Interestingly, in present investigation the  $\gamma$  amplitude of the best-studied NLO compound **2-PyQ** is 257 times larger than that of para nitroaniline ( $7.279 \times 10^{-36}$  esu) at the same M06/6-311G\* level

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