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Quantum chemical, spectroscopic and third order nonlinear optical investigations on 3-(3-bromophenyl)-1-imidazol-1-yl-propenone

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Imidazole is a five-membered heterocyclic moiety that possesses three carbon, two nitrogen, four hydrogen atoms, and two double bonds. It contains two nitrogen atoms, in which one nitrogen bears a hydrogen atom, and the other is called pyrrole type nitrogen. Due to the presence of a positive charge on either of two nitrogen atom, it shows two equivalent tautomeric forms. Among the different heterocyclic compounds, imidazole is better known due to its broad range of chemical and biological properties. Imidazole has become an important synthon in the development of new drugs. In this study, 3-(3-bromophenyl)-1-imidazol-1-yl-propenone have been prepared and characterized in a systematic manner. For synthesised molecule, atomic charges, frontier orbital energies and the thermodynamic properties have been calculated with theoretical Density Functional method. The synthesised molecule has been subjected to NMR, FTIR and UV analysis. The molecule shows interesting nonlinear optical (NLO) properties by the Z-scan technique. This study evokes the interest of researchers regarding the development of imidazole based tempting NLO compounds that could be beneficial in modern hi-tech applications.

Keywords: Imidazole, DFT, FTIR, nonlinear optics