**STRUCTURAL, SPECTROSCOPICAL INVESTIGATION AND NON LINEAR OPTICAL STUDY OF (2E)-1-(3-CHLOROPHENYL)-3-(4- CHLOROPHENYL)PROP-2-EN-1-ONE**

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Abstract:

This study aims about the structural and spectral analysis of (2E)-1-(3-Chlorophenyl)-3-(4-chlorophenyl)prop-2-en-1-one which was performed using DFT with B3LYP/6-311G(d,p)level of theory. The electronic properties such as molecular electrostatic potential (MEP) and HOMO-LUMO analysis were executed to identify the charge transfer taking place within the molecule. The natural bond orbital (NBO) analysis was carried out to explain the delocalization of charges that is taking place within the molecule due to intramolecular interactions. Hirshfeld analysis was carried out to investigate the intermolecular interaction in crystal structure and percentage of close contact within the molecule. To show the non-linear optical active nature of the material hyperpolarizability calculations were carried out. High value of first-order hyperpolarizability shows more NLO active nature of the title compound.

Keywords: DFT, NBO, MEP, HOMO-LUMO, NLO.