**SPECTROSCOPIC INVESTIGATION AND NON LINEAR OPTICAL STUDY ON N-4-METHOXY-2-NITROPHENYL ACETAMIDE
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**Abstract**
 This study uses a spectroscopic theoretical quantum chemistry to analyze the structural characteristics of N-4-Methoxy-2-nitrophenyl acetamide(NMNA). On the basis of optimized geometry, spectroscopic behaviour, intermolecular interactions and intramolecular hydrogen bonding, the basic structural features of NMNA have been investigated. The HOMO-LUMO analysis was carried to resolve the most reactive site and charge transfer that occurs with in the molecule. The inter and intramolecular interactions accountable for the stabilization of the material was done via NBO analysis. Molecular electrostatic potentials (MEP) was performed to analyse the reactive area of the title molecule. Intermolecular contacts and molecular surface contours were analysed by using Hirshfeld and 2D fingerprint plot analysis. To confirm the nonlinear optical active nature of the compound hyperpolarizability calculations were carried out. The large value of first order hyperpolarizability proves the NLO activity of the title compound.
**Keywords:** DFT, NLO, HOMO-LUMO, NBO.