**SPECTROSCOPIC INVESTIGATION AND NON LINEAR OPTICAL STUDY ON 2,6-DICHLORO-N-(4-METHYLPHENYL)BENZAMIDE**

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ABSTRACT:

 This study uses a spectroscopic theoretical quantum chemistry technique to analyze the structure of 2,6-DICHLORO-N-(4-METHYLPHENYL)BENZAMIDE . On the basis of optimal geometry, spectroscopic behaviour, chemical reactivity and intramolecular hydrogen bonding, the basic structural features of 2,6-dichoro-N-(4-methylphenyl)Benzamide have been investigated. To determine the most reactive site and the charge transfer that occurs within the molecules, HOMO-LUMO analysis was carried out. The delocalization of charge within the molecule caused by intramolecular interactions is explained by the natural bond orbital (NBO) study. The molecular electrostatic potential (MEP) surface map, which additionally identifies the nucleophilic and electrophilic region or sites was used to anticipate the overall image of the accumulation of charges on individual molecule atoms. The quantitative analysis of electrophilicity and nucleophilicity indicies were done by Hirshfeld surface analysis. To show the non-linear optical active nature of the material hyperpolarizability calculations were carried out. The lower energy gap indicates eventual charge transfer interaction taking place within the molecule and high value of polarizability shows more NLO active nature of title compound.

Key words: optimized geometry, HOMO-LUMO, NLO