**CRYSTAL STRUCTURE, DFT AND THIRD ORDER NON-LINEAR OPTICAL STUDIES OF AN ORGANIC 2-AMINOPYRIDINIUM CYANOACETATE SINGLE CRYSTAL**

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**Abstract**

In the ground state of 2-aminopyridinium cyanoacetate, the molecular geometry and vibration have been resolved by using B3LYP method with 6-31+g(d) basis set. The natural bond orbital (NBO) analysis has been carried out to address the intra and intermolecular hydrogen bonding in the molecule. The HOMO-LUMO energy has been elucidated to show the charge transfer interaction which arises within the molecule. The wide-range optical transparency of the compound in the entire visible region ensures the optical quality with a lower cut-off wavelength was analysed experimentally using UV-visible spectrometer. The molecular electrostatic potential mapping has been generated to analyze the mutual interaction. The non-linear optical (NLO) property of the title compound was investigated using Z-scan analysis.

Key Words: NBO, HOMO-LUMO, DFT, MESP, Z-scan