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Conformational stability, spectroscopic (FT-IR, FT-Raman) analysis, fukui function, Hirshfeld surface and docking analysis of Naphthalene-2-lyoxy acetic acid by density functional theory

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Abstract

The experimental and theoretical study on the structure and vibrations of Naphthalene-2-lyoxy acetic acid (NLA) are presented. The FT-IR and FT-Raman spectra of the title compound have been recorded in the region 4000-0 cm^{-1} and 3500-100 cm^{-1}. The molecular structure, vibrational wave numbers infrared intensities and Raman intensities were calculated using DFT (B3LYP) method with LANL2DZ and LANL2MB basis sets. The conformational behavior of the molecule was also investigated. The vibrational wave numbers were calculated using DFT quantum chemical calculations. The data obtained from the wave number calculations are used to assign vibrational bands obtained through an experiment. The stability of the molecule arising from charge delocalization and hyper-conjugative interaction has been analyzed by NBO analysis. The HOMO and LUMO analysis were used to verify the charge transfer at intervals the molecule and quantum chemical parameters connected to the title compound. From the MEP analysis, it is clear that the ring and are possible sited for electrophilic attack and the positive regions are localized at all the hydrogen atoms as possible sites for nucleophilic attack. Fukui function and Mulliken analysis on atomic charges of the title compound have been discussed. The Hirshfeld surface analysis and fingerprint plots are reported the title molecule and reveal that the structures are stabilized intermolecular interactions. It is clear from the docking studies that NLA has inhibition capability toward the plant growth protein target 4Y31, 4PSB and 4QOK.

Keywords: Vibrational spectra; HOMO-LUMO; MEP; NBO; Hirshfeld; Docking.

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