01

Structural, Spectroscopic, Electronic Analysis with Nonlinear Optical Activity of L-Methionine L-Methioninium Hydrogen Maleate: a DFT tudy*

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The molecular structure parameters, vibrational wavenumbers, ^{1}H NMR and ^{13}C NMR chemical shifts of L-methionine L-methioninium hydrogen maleate (LMLMHM) were carried out by using density functional theory (DFT) B3LYP and PBEPBE method using 6-311++G(d,p) basis set. The complete structural analysis such as geometric parameters, vibrational data, NMR chemical shifts of LMLMHM were in good agreement with reported experimental findings. The stability of the molecule arising from charge transfer and hyper-conjugative interaction were researched using natural bonding orbital (NBO), and frontier molecular orbital (FMO) analysis. The electrophilic and nucleophilic sides of the title compound were investigated by using molecular electrostatic potential and Mulliken charge populations. The nonlinear optical features were investigated from the dipole, polarizability and hyperpolarizability values at the same theory levels. The computational finding suggests that mentioned compound has a potential to be used as a nonlinear optical materials.

Keywords: L-methionine L-methioninium hydrogen maleate, density functional theory.

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