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Halogenated Methoxy- and Methyl-benzoic Acids: Joint Experimental and DFT Study For Molecular Structure, Vibrational Analysis, and Other Molecular Properties

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Abstract : Extensive research into the optimized structure and molecular properties of 3-Flouro-2-methylbenzoicacid(FMB), 3-Chloro-2-methoxybenzoicacid (CMB), and 3-Bromo-2-methylbenzoicacid (BMB) was carried out using FT-IR, FT-Raman and UV-Visible spectra, as well as theoretically using the DFT approach with B3LYPfunctional in conjunction with 6-311++G(d,p) basis set. The optimized structure was determined by evaluating torsional scans about free rotation bonds. Structure parameters, harmonic vibrational frequencies, potential energy distribution(PED), and infrared and Raman intensities were computed. The computational results from the DFT approach, such asFT-IR, FT-Raman, and UV-Visible spectra, were compared with the experimental results and found good agreement. Observed and calculated frequencies agreed with an rms error of 8.42, 6.60, and 6.95 cm-1 for FMB, CMB, and BMB, respectively. Unambiguous vibrational assignments were made for all fundamentals using PED and eigenvectors. The electronic HOMO-LUMO, H-bonding, and strong conjugative interactions across different molecular entities are discussed using experimental and simulated Ultraviolet-Visible spectra. The title molecules' molecular properties such as dipole moment, mean polarizability, and first-order hyperpolarizability, were calculated to study their non-linear optical (NLO) behavior. The chemical reactivity descriptors and mapped electrostatic surface potential (MESP) were also evaluated. Natural bond orbital (NBO) analysis was used to examine the stability of molecules resulting from hyperconjugative interactions and charge delocalization.

Keywords : ftir/raman spectra, DFT, NLO, homo-lumo, NBO, halogenated benzoic acids
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