Molecular Structure, Vibrational Spectra and Chemical Shift Properties of $C_{12}H_9ClO_4$ and $C_{12}H_9BrO_4$ Crystals by Density Functional Theory and *ab initio* Hartree-Fock Calculations

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The molecular geometry, vibrational spectra, and gauge including atomic orbital (GIAO), individual gauges for atoms in molecules (IGAIM), and continuous set of gauge transformations (CSGT) ^{1}H and ^{13}C chemical shift values of ethyl 6-chloro-2-oxo-2*H*-chromene-3-carboxylate ($C_{12}H_9ClO_4$–(I)) and ethyl 6-bromo-2-oxo-2*H*-chromene-3-carboxylate ($C_{12}H_9BrO_4$–(II)) in the ground state have been calculated by using the Hartree-Fock (HF) and density functional method (B3LYP) with 6-31G+(d,p) basis set. The results of the optimized molecular structure are presented and compared with the experimental X-ray diffraction. The computed vibrational frequencies were used to determine the types of molecular motions associated with the spectra of the experimental bands observed. Also, calculated ^{1}H and ^{13}C chemical shift values were compared with the experimental ones.

Key words: Ethyl 6-chloro-2-oxo-2*H*-chromene-3-carboxylate; Ethyl 6-bromo-2-oxo-2*H*-chromene-3-carboxylate; DFT; HF; ^{1}H (^{13}C) NMR; Structure Elucidation; Vibrational Assignment.