COMBINED EXPERIMENTAL AND THEORETICAL STUDIES ON THE VIBRATIONAL AND ELECTRONIC SPECTRA OF 5-QUINOLINECARBOXALDEHYDE

MUSTAFA KUMRU, MUSTAFA KOCADEMIR, TAYYIBE BARDAKCI, *Department of Physics, Fatih University, Istanbul, Turkey*.

Experimental and theoretical investigations have been performed on the structure, vibrational and electronic spectra of 5-quinolinecarboxaldehyde (5QC). The 4000-50 cm^{-1}region FT-IR and FT-Raman and the 190-1100 nm region UV–Vis spectra of 5QC were recorded at the room temperature. Structural and spectroscopic properties of the cis and trans conformers of 5QC were calculated by Hartree-Fock (HF) and B3LYP density functional methods using the 6-311++G(d,p) basis set. Although calculated B3LYP frequencies are found to be closer to the experimental frequencies than the HF calculation results, scaled frequencies of both HF and B3LYP levels are in good agreement with the experimental spectra. The time-dependent density functional theory (TDDFT) is also used to find excitation energies, absorption wavelength, oscillator strengths and HOMO and LUMO energies of the title molecule.

Keywords: FT-IR, FT-Raman, and UV-vis spectra; HF; DFT, HOMO-LUMO.

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