DETERMINATION OF STRUCTURAL AND VIBRATIONAL PROPERTIES OF 5-QUINOLINECARBOXALDEHYDE USING EXPERIMENTAL FT-IR, FT-RAMAN TECHNIQUES AND THEORETICAL HF AND DFT METHODS

MUSTAFA KUMRU, MUSTAFA KOCADEMIR, TAYYIBE BARDAKCI, *Department of Physics, Faculty of Arts and Sciences, Fatih University, 34500 Buyukcekmece, Istanbul, Turkey*.

Quinoline derivatives have been used in several pharmaceuticals. They have vital roles in regulating the functions of DNA and cancerous cells. Its necessary to determine the structures and spectroscopic properties of quinoline derivates. In this study, the FT-IR (including mid and far regions) and FT-Raman spectra of 5-quinolinecarboxaldehyde have been investigated. Hartree-Fock (HF) and density functional B3LYP calculations have also been employed with the 6-311++G(d,p) basis set for investigating the structural and spectroscopic properties of the cis and trans conformers of 5-quinolinecarboxaldehyde. Experimental and theoretical results have been compared and the results are in good agreement with each other.

Keywords: 5-quinolinecarboxaldehyde; Vibrational Spectroscopy; FT-IR spectra; FT-Raman spectra; Vibrational Modes; HF; DFT

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