COMBINED EXPERIMENTAL AND THEORETICAL STUDIES ON THE VIBRATIONAL SPECTRA OF SOME QUINOLINECARBOXALDEHYDE MOLECULES-I

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Combined experimental and theoretical studies have been performed on the structure and vibrational spectra (FT-IR, FT-Raman, Dispersive Raman spectra including far region) of some quinolinecarboxaldehyde molecules. Hartree-Fock (HF) and density functional B3LYP calculations have 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 quinolinecarboxaldehyde. The B3LYP frequencies are closer to the experimental frequencies than the HF frequencies, but scaled frequencies of both HF and B3LYP agree almost perfectly with the experimental frequencies. The *cis* conformer has been found more stable than the *trans* conformer. The scaled vibrational frequencies of *cis* conformer also agree slightly better than those of the *trans* conformer with the experimental frequencies.

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