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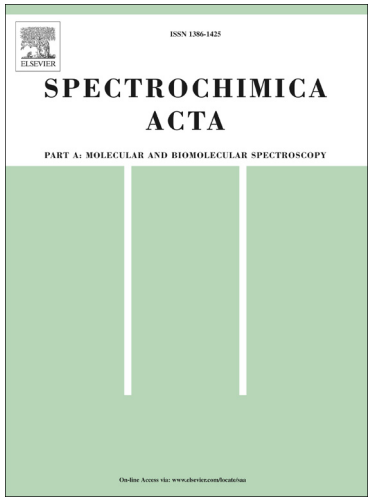

FT-IR and Raman Spectra, *ab initio* and density functional computations of the vibrational spectra, molecular geometries and atomic charges of uracil and 5-halogenated uracils (5-X-uracils; X= F, Cl, Br, I)

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FT-IR and Raman Spectra, *ab initio* and density functional computations of the vibrational spectra, molecular geometries and atomic charges of uracil and 5-halogenated uracils (5-X-uracils; X= F, Cl, Br, I)

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Abstract

Raman (200–4000 cm^{-1}) and FT-IR (400–4000 cm^{-1}) spectra of uracil and 5-halogenated uracils (5-X-uracils; X= F, Cl, Br, I) have been recorded and analyzed in the range 200–4000 cm^{-1}. The optimized molecular geometries, atomic polar tensor (APT) charges and vibrational characteristics have been studied theoretically using restricted Hartree–Fock (RHF) and density functional theory (DFT) methods. *Ab initio* and DFT calculations [using Becke's exchange in conjunction with Lee-Yang-Parr's correlation functional and Becke's three-parameter hybrid method (B3LYP)] were carried out to study the optimized molecular fundamental vibrational frequencies for uracil and 5-halogenated uracils by employing Gaussian-03 program. Gauss View software was used to make the vibrational analysis. Raman and IR spectra have been computed theoretically for the uracil and 5-halogenated molecules. The fundamental vibrational frequencies along with their corresponding intensities in IR and Raman activities and depolarization ratios of the Raman lines have also been calculated using the RHF and DFT methods employing different basis sets. Quantum chemical calculations