

Theoretical Study of IR and Raman Spectra of 5-Hydroxy Uracil

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Ab initio calculations were used to investigate the interactions of nucleosides with 5-hydroxy uracil. 5-hydroxy uracil could form a stable base pair. Quantum chemical methods have been employed to carry out vibrational frequencies for 5-hydroxy uracil. The assignment of each calculated fundamental has been assigned using band intensities and depolarization ratios for the Raman lines. We have calculated optimized geometrical parameters, atomic charges, fundamental frequencies and their corresponding IR and Raman intensities and Raman depolarization ratios. The influences of the presence of the OH group in 5-hydroxy uracil molecule on the geometries and normal modes of the parent molecule (Uracil) have been differentiated.

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