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DFT study of the structure, spectra and some molecular properties of 5-substituted uracil derivatives: A brief review*

Sunila Abraham[1], M Alcolea Palafox[2], Kaushal Rani[3], Ravinder Kumar[4], R A Yadav[5], S P Singh[6], Preeti Mishra[3]and V K Rastogi[3]

[1]*Post Gradúate and Research Department of Physics, Christian College, Chengannur- 689 122, India*

[2]*Departamento de Química-Fisica. Facultad de Ciencias Químicas. Universidad Complutense, Madrid- 28040. Spain*

[3]*Indian Spectroscopy Society, KC- 68/1, Old Kavinagar, Ghaziabad-201 002, India*

[4] *Department of Physics, Shyam Lal College (Dehli University) Shahadara- 110 032, India*

[5]*Department of Physics, Banaras Hindu University, Varanasi-221 005, India*

[6] *Department of Physics, Dr B R Ambedkar College, Mainpuri-205 001, India*

In this work, optimized molecular structure and the vibrational spectra of uracil and its main 5-monosubstituted derivatives, 5-XU (X = F, Cl, Br, I, CH_3, NH_2 and NO_2 attached to C5), were compared. MEP, ESP and HOMO and LUMO energies for these 5-substituted uracil derivatives were computed for the first time. The FTIR spectra were studied with the support of DFT (B3P86, B3LYP, B3PW91, MPW1PW91) calculations using several basis sets. The effects of substitution of X on the carbon atom in position-5 of the uracil ring on the structural parameters, atomic charges and vibrational wavenumbers of uracil were analyzed and substituent-property relationships were established. In addition, several correlations between the structure and spectral parameters were also shown and sites of the nucleophilic and electrophilic attacks were located and compared. Several general conclusions were underlined on these derivatives

Keywords: Uracil, 5-substituted uracils, Geometry, Vibrational spectra, Nucleophilic and Electrophilic attack.

1 Introduction

Nucleic acid bases are constituents of DNA and RNA and play an important role in genetic code transformation. Uracil (U) and its derivatives are constituents of the genetic material which play a fundamental role in basic biological processes. From the structural [1-6] and spectroscopic [6-11] points of view, uracil is very important. The bioactivity of 5-substituted uracils also induces exceptional interest in their biochemistry and pharmacology. In the present investigation, structure, spectra and some molecular properties of uracil and its monosubstituted derivatives, 5-XU (X = F, Cl, Br, I, CH_3, NH_2 and NO_2 attached to C5) are studied.

Among the 5-XUs, halogen-substituted uracils play special attention. Transformation of uracil into a 5-halouracil molecule leads to significant changes in its chemical and spectroscopic properties and *in vivo* activity. The halogenated pyrimidines were synthesized in the 1950s as potential antitumor agents because uracils change the interaction of nucleic acids with proteins by inducing various biological phenomena [12].

* Part of Ph D work of Ms Kaushal Rani

Corresponding author :

e mail: alcolea@ucm.es. (M A Palafox); v_krastogi@rediffmail.com (V K Rastogi)