

Experimental and Theoretical Investigation of 5-para-nitro-benzylidene-thiazolidine-2-thione-4-one Molecule

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Development of novel therapeutics for the treatment of microbial infections has become a clinical imperative [1,2] and new heterocycle compounds which contain in their structure a series of structural units similar to those of Linezolid are proposed and used to discover new antimicrobial leads. In this connection, thiazolidines derivatives were obtained by replacing the oxygen atom of the oxazolidinone ring with a bulkier sulfur atom.

In this work, experimental methods (FT-IR, Raman and NMR spectroscopies, and X-ray diffraction technique) coupled with quantum chemical calculations based on density functional theory (DFT) are used for structural and electronic characterization of 5-para-nitro-benzylidene-thiazolidine-2-thione-4-one (5p-NBTT), a new synthesized compound with antimicrobial activity.

The molecular vibrations of 5p-NBTT were investigated by FT-IR and FT-Raman spectroscopies. In parallel, quantum chemical calculations based on Density Functional Theory (DFT) are used to determine the geometrical, energetic and vibrational characteristics of the molecule. Different conformers and tautomers of 5p-NBTT have been analyzed by theoretical methods and their relative stability is discussed. The molecular electrostatic potential of this molecule has been calculated and used for predicting site candidates of electrophilic attack.

The ¹H and ¹³C NMR spectra of 5p-NBTT were obtained in DMSO solution and they were also calculated using the GIAO (Gauge-Including Atomic Orbitals) method. Proton NMR spectrum of this molecule in solution shows an unexpected proton chemical shift at 13.0 ppm. This signal is attributed to the proton bound to the nitrogen atom and this very important deshielding can be explained by assuming a relatively strong hydrogen bond of 5p-NBTT with the solvent molecules, realized through NH group [3].

X-ray diffraction technique indicates that 5p-NBTT crystallizes with one tetrahydrofuran (THF) solvent molecule, forming a 1:1 5p-NBTT•THF complex in the monoclinic space group C2/c, with Z = 8 and cell parameters: $a = 29.496 \text{ \AA}$, $b = 7.276 \text{ \AA}$, $c = 14.873 \text{ \AA}$, $\alpha = 90.00^\circ$, $\beta = 95.161^\circ$ and $\gamma = 90.00^\circ$.

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