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QUANTUM COMPUTATIONAL AND SPECTROSCOPIC ANALYSIS OF SULFAMETHAZINE

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Abstract:

The complete molecular structure properties of Sulfamethazine was performed with the help of DFT method using 6-31+ G (d, p) basis set. The presence of functional groups were obtained by the FT-IR spectral studies. The electronic property was calculated from the time-dependent density functional theory (TD-DFT) calculation. The chemical shift was obtained by the ^{1}H and ^{13}C spectral analysis. The molecular interaction of frontier orbitals emphasizes the modification of chemical properties of the compound through the reaction path.

Key Words: DFT, FT-IR, UV-Vis, HOMO-LUMO & NMR

1. Introduction:

Density Functional Theory (DFT) is a computational method that derives properties of the molecule based on a determination of the electron density of the molecule. Unlike the wave function, which is not a physical reality but a mathematical construct, electrondensity is a physical characteristic of all molecules.The most significant advantage to DFT methods is a significant increase in computational accuracy without the additional increase in computing time. DFT methods such as B3LYP/6-31G+(d,p) are oftentimes considered to be a standard model chemistry for many applications [1]. Heterocycles are an important class of compounds, making up more than half of all known organic compounds. Heterocycles are present in a wide variety of drugs, most vitamins, many natural products, biomolecules, and biologically active compounds, including antitumor, antibiotic, anti-inflammatory, antidepressant, antimalarial, anti-HIV, antimicrobial, antibacterial, antifungal, antiviral, antidiabetic, herbicidal, fungicidal, and insecticidal agents. Also, they have been frequently found as a key structural unit in synthetic pharmaceuticals and agrochemicals [2]. Pyrimidines (PMN) are found in medically important compounds, such as antiviral, antitumor and cardiovascular agents [3].PMN is also used along with other drugs for the treatment of opportunistic infections in patients with AIDS. Owing to the pharmaceutical applications of pyrimidine derivative, the main objective to study the molecular structure, spectral behaviour was studied for the Sulfamethazine compound.

2. Computational Details:

In the present work, the hybrid method B3LYP are carried out using the basis sets 6-31+G(d,p).[4] All these calculations are performed using GAUSSIAN 09W [5] program package. The ^{1}H and ^{13}C NMR isotropic shielding are calculated with the GIAO method [6] using the optimized parameters and the functional groups obtained from B3LYP/6-311++G(2d,2p) method.The electronic properties; HOMO-LUMO energies, absorption wavelengths and oscillator strengths are calculated using B3LYP method of the time-dependent DFT (TD-DFT)[7,8].

3. Result and Discussion:

3.1 Molecular Geometry: The optimized geometrical parameters were calculated for the title compound.Generally, the molecular structure of Sulfamethazine belongs to C1 point groupsymmetry. The global minimum energy of the structure is -1233.37025903 a.u. All the C-C bonds were appeared between the ranges 1.38-1.39Å whereas the C12-C13 atom shows the increased bond length which is due to the attachment of electronegative atom. In the similar manner, the attachment of methyl group increases the bond length to 1.504 Å for the C15-C18 and C16-C19. The SO_2group in the molecule increases the bond length for the C11-N4 atoms while the other C-N bonds are lies in the ranges about 1.351Å. Presence of amine group also increases the bond to 1.38Å for the C12- 7N. The optimized structure of the sulfamethazine is shown in the Figure 1.

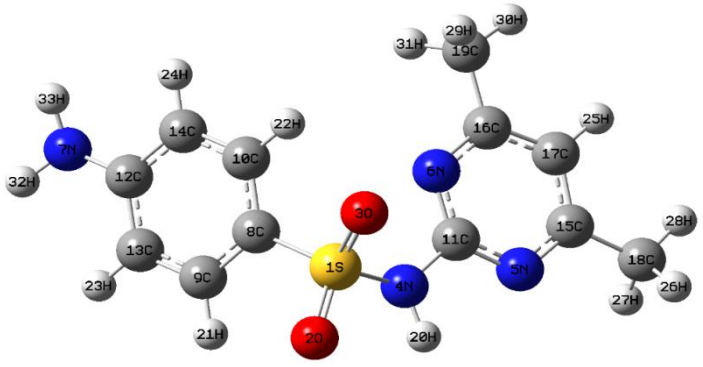

Figure 1: Optimized molecular structure of Sulfamethazine.

3.2 FT-IR Spectral Analysis: In order to obtain the spectroscopic signature of the Sulfamethazine, the computational calculations are performed for frequency analysis. The molecule, has C1 point group symmetry, consists of 33 atoms, so it has 93 normal vibrational modes. The N-H stretching vibrations were appeared at 3541, 3439, 3434 cm^{-1}. The peak at 3096, 3079, 3071, 3043

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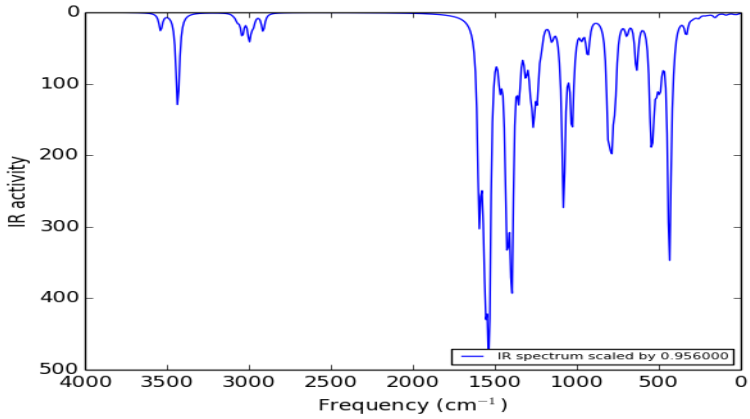
and 3042cm^{-1} are ascribed to the ring C-H vibrations. The substituent of methyl group in the compound exhibits their bands at 3000, 2999, 2977, 2975, 2916, 2915cm^{-1}. The stretching vibrations of amine group was appeared at 1596, 1573 cm^{-1}.The bands at 1397cm^{-1} was due to the C-N stretching vibrations. The S=O stretching mode was appeared at 1241 cm^{-1}. The band at 1081cm^{-1}was due to presence of C-S stretching vibrations. The complete vibrations of FT-IR spectrum is shown in the Figure 2.



3.3 UV-Visible and HOMO-LUMO Analysis: The electronic absorption spectra of Sulfamethazinewere computed with the help of the time-dependent density functional theory (TD-DFT) calculation. The observed and simulated UV–Vis spectra of the title compound is shown in Fig. 3. The absorption bands (λ_{max}) were found to be 276, 271, 263 nm which was due to the $\pi \rightarrow \pi^*$ transitionin the title compound The band gap energy was calculated for the maximum absorption and it is found to 4.7262eV. The HOMO-LUMO energy gap ia an important stability index and reflects the chemical reactivity of a molecule [9].The energy gap between the HOMO-LUMO has been used to prove the bioactivity from the intra molecular charge transfer [10,11]. The HOMO-LUMO band gap energy was calculated and it is 4.98eV.The HOMO-LUMOplot is shown in the Fig 4. The higher band bap energy suggested that the title compound have a bioactive property. The band gap energy of UV-Vis and HOMO –LUMO analysis confirms the excited electrons are appeared in the same region.

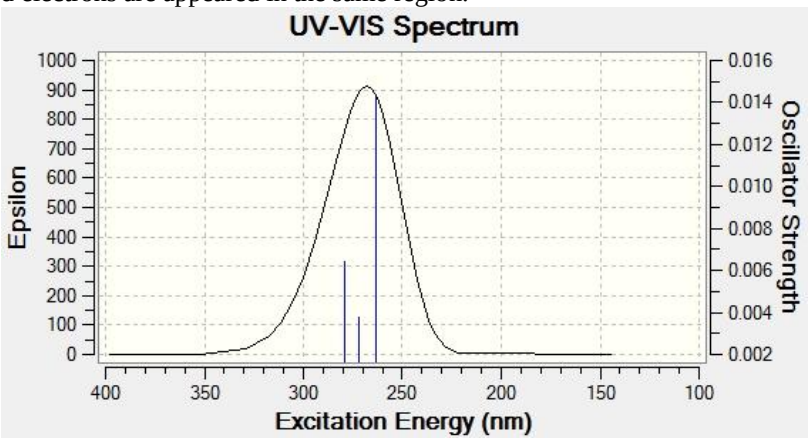


Figure 3: UV-Vis spectrum of Sulfamathazine

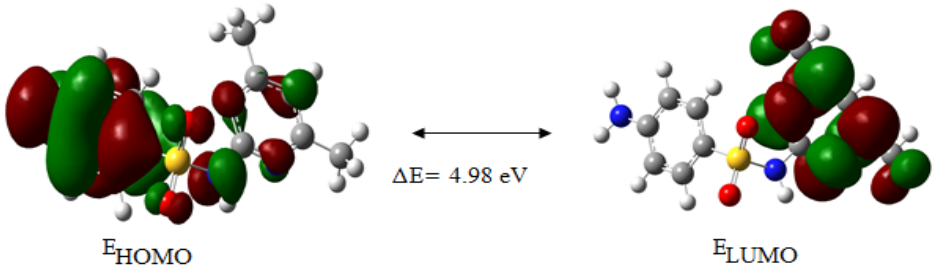


Figure 4: HOMO-LUMO plot of Sulfamathazine

3.4 ^{1}H and ^{13}C NMR Spectral Analysis: The NMR serves as a great resource in determining the structure of an organic compound by revealing the hydrogen and carbonskeleton. In order to explain a complete assignment and analysis of ^{1}H and ^{13}C NMR spectra, theoretical calculations on chemical shift of the title compound are done by gauge independent atomic orbital (GIAO) method at B3LYP/6-311++G(2d,2p) level.The range of 13C-NMR chemical shift for analogous organic molecules is usually >100 ppm [12-14]. Due to the attachment of methyl group in the C15 and C16 atom increases the higher chemical shift to 157 and 156 ppm respectively. All the carbon atoms were appeared with in the range whereas the methyl group carbon and

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protons atoms are appeared in lower chemical shift which are gathered in the Table 1 and the corresponding spectra are shown in the Figure 5.

Atoms	Theoretical TMS B3LYP/6-311+G(2d,p) GIAO	Atoms	Theoretical TMS B3LYP/6-311+G(2d,p) GIAO
15-C	157	22-H	8.7
16-C	156	21-H	8.1
11-C	147	20-H	7.2
12-C	136	23-H	6.9
8-C	123	24-H	6.9
10-C	120	25-H	6.7
9-C	117	32-H	3.8
17-C	99	33-H	3.8
13-C	98	29-H	2.8
14-C	97	26-H	2.7
18-C	15	31-H	2.6
19-C	15	27-H	2.6
		30-H	2.1
		28-H	2.1

Table 1: Theoretical isotropic chemical shifts calculated using B3LYP/6-311+G(2d,p) (with respect to TMS, all values in ppm) for Sulfamethazine

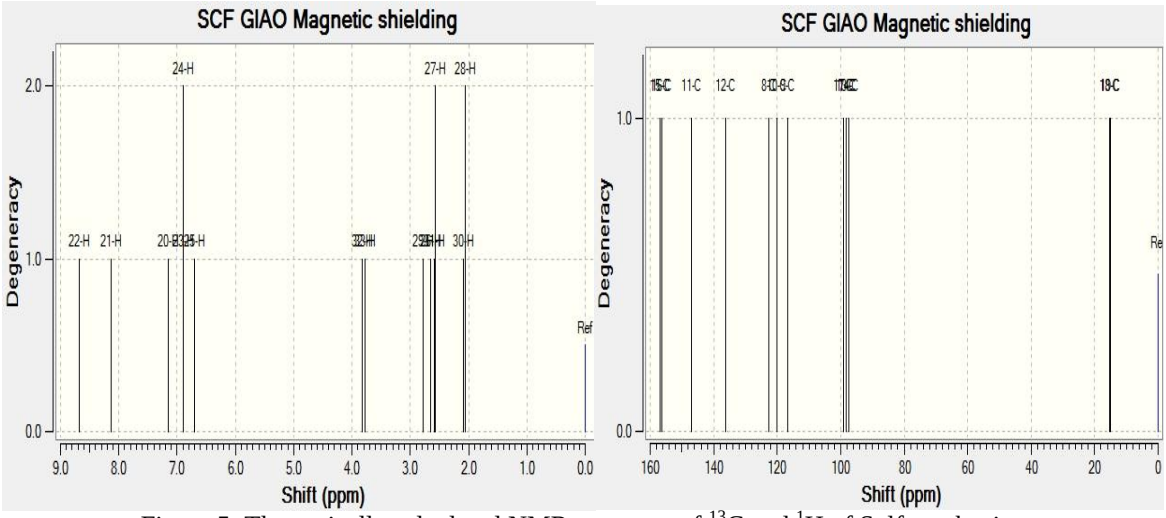

Figure 5: Theoretically calculated NMR spectrum of ^{13}C and ^{1}H of Sulfamethazine

4. Conclusion:

In the present investigation, the molecular structural information were performed from the optimized structureusing DFT calculations at B3LYP/6-31+G (d,p) level. FT-IR, ^{13}C NMR and ^{1}H NMR spectra of the Sulfamethazine are calculated and the vibrational frequencies are assigned depending upon their expectedregion.The higher band energy from the HOMO-LUMO and UV-Vis spectral analysis (4.9800 eV and 4.7262eV respectively) suggested that the title compound have a biological behaviour.

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