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Molecular Structure, Vibrational Spectroscopic Analysis of Levofloxacin by Density Functional method

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Abstract

The Fourier transform infrared (FT-IR) spectra of Levofloxacin has been recorded and analysed. The equilibrium geometry, bonding features and harmonic frequencies of the title molecule is investigated with the help of ab initio and density functional theory (DFT) method using B3LYP levels employing 6-31 G(d,p) basis sets. The difference between the observed and scaled wavenumber values is very small. The first order hyperpolarizability (â) and other related properties (á and µ) of Levofloxacin have been examined using density functional theory (DFT). The calculated values show that the molecule might have non-linear optical (NLO) behaviour with non-zero values. The molecular HOMO-LUMO composition, their respective energy gaps, MESP Contours and Surfaces has also been drawn to explain the activity of Levofloxacin. Thermodynamic properties (heat capacity, entropy and enthalpy) of the title compound were calculated. In general, there is a good agreement between experimental and calculated normal modes of vibration have been observed.

Keywords: *Density functional theory; HOMO-LUMO ; Hyperpolarizability; Levofloxacin. Non linear optical properties; Polarizability.*

1. INTRODUCTION

Levofloxacin is a broad spectrum antibiotic ofthe fluoroquinolone drug class. Its spectrum of activity includes most strains of bacterial pathogens responsible for respiratory, urinary tract, gastrointestinal, and abdominal infections (Nelson *et al*. 2007; Kawahara 1998). Levofloxacin is valued for this broad spectrum of activity, excellent tissue penetration, and for their availability in both oral and intravenous formulations. The aim of the work is to investigate the molecular structure, vibrational study of the molecule under study due to its biological and pharmaceutical importance.

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2. EXPERIMENTAL

2.1 Structure and Spectra

The sample was obtained from M/s. Sigma Aldrich Co., with a stated purity of 99% and was used as such without further purification. The Fourier transform infrared spectra are recorded using Perkin Elmer spectrometer in KBr dispersion in the range of 4000 to 400 cm^{-1}. The molecular structure of Levofloxacin has been given in Fig.1.

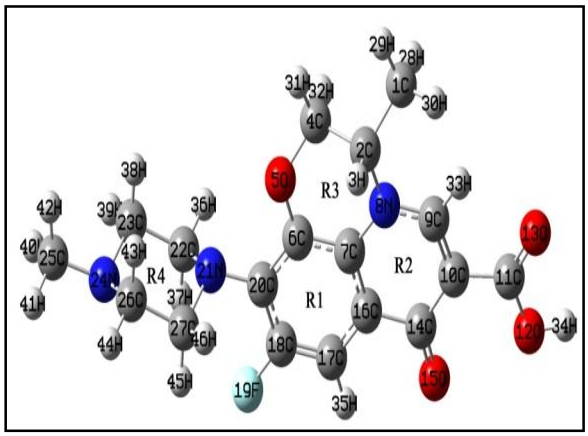

Fig. 1: Molecular structure and numbering scheme of Levofloxacin

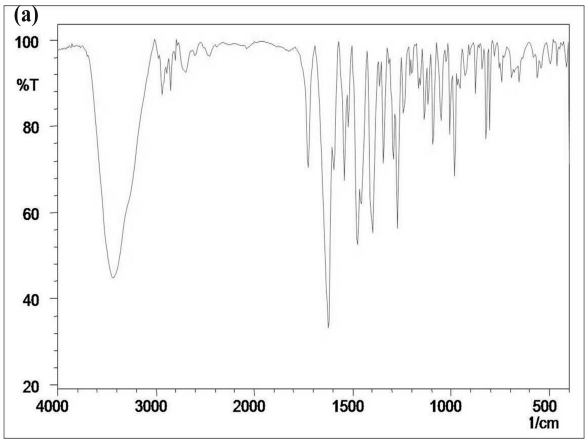

Fig. 2: Experimental FT-IR of Levofloxacin

The experimental and calculated FT-IR spectra are given in Fig.2.

2.2 Computational Details

In the present work, the density functional method (DFT) has been employed using Becke's three parameter hybrid exchange functional (Becke, 1993) with the Lee-Yang –Parr correlation functional (Lee *et al.* 1998) to optimize the structure of the molecule and also to calculate the electronic structure of the title molecule. The entire calculations were performed at ab-initio Hartree fock(HF) and DFT method using B3LYP levels at 6-31 G(d,p) basis sets on a Pentium V/ 1.6GHz personal computer using Gaussian 03W program package (Frisch *et al.* 2003) and applying geometry optimization. Initial geometry generated was minimized at the Hartree Fock level using 6-31 G(d,p) basis set and again reoptimized at DFT/B3LYP levels at 6-31G (d,p) basis set. The vibrational modes are assigned using Gauss-View molecular visualization program package.

2.3 Polarizability and First Order Hyperpolarizability

In the present study of the title molecule, the calculated the dipole moment (μ), polarizability (α) and the first order hyperpolarizability (β) are correlated and discussed. The total intrinsic hyperpolarizability β_{Total} and a component of the first hyperpolarizability are found along the direction of the dipole moment. It is noticed that the biggest values of hyperpolarizability in âxxx direction with a value of 1216.1790 esu and subsequently delocalization of electron cloud is more in that direction. The maximum â value may be due to ð electron cloud movement from donor to acceptor (Kleinman, 1962).

2.4 Vibrational Assignments

In Levofloxacin, the structure of Levofloxacin into three rings R1, R2,R3 and R4 as shown in Fig. 1. After applying a uniform scaling factor, the theoretical calculation reproduces the experimental data well. Vibrational assignments are based on the observations of the animated modes in Gauss View and assignments reported in the literature.

In the present study, the O-H stretching band is observed at 3420 cm^{-1} from DFT/B3LYP method and a very sharp band at 3421 cm^{-1} in FT-IR spectrum is assigned to O-H stretching mode. The O-H in-plane bending and out of plane bending vibrations are assigned to 1393 cm^{-1} and 1380 cm^{-1} respectively from

DFT/B3LYP calculations and in IR spectrum a band observed at 1396 is assigned to O-H bending mode. The O-H in-plane and out-of-plane bending vibrations are increased in value because of the hydrogen bonding through the carbonyl groups (Alkorta *et al.* 1996).

In the present work, the band observed at 1208 cm^{-1} in FT-IR has been assigned to C-N stretching vibrations and theoretically computed value at 1208 cm^{-1} is in good agreement (Karpagam *et al.* 2009).

The C-H stretching mode is observed in the region 2934-2917 cm^{-1} from DFT/B3LYP method and a medium band in FT-IR spectrum observed at 2935 cm^{-1} is assigned to CH stretching mode and is in good agreement. The asymmetric stretching of CH_2 is observed as weak band in IR Spectrum as 2848 cm^{-1} and in DFT method it is observed at 2835 cm^{-1}. The intensity enhancement and blue shifting of the methyl stretching wave numbers are due to the influence of electronic effect resulting from the hyperconjugation and induction of methyl group in the aromatic ring (Padmaja *et al.* 2009).

3. FRONTIER MOLECULE ORBITALS

The frontier orbital gap helps to characterize the chemical reactivity of the molecule. HOMO and LUMOs determine the way in which it interacts with other species. The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) are the main orbitals that take part in chemical stability (Gunasekaran *et al.* 2008). The homo represents the ability to donate an electron and lumo as an electron acceptor represents the ability to accept an electron. HOMO is located on Ring R4 and LUMOs are located on the rings R1,R2,R3 as shown in Fig.3 and in the case of given molecule, the electronegative region (red) is towards the outer part and near the oxygen which is adjacent to ring R1 and R2 and moderate positive region (green) is located nearly over whole molecule.

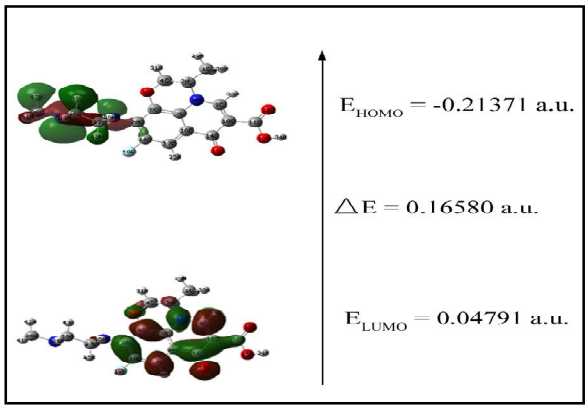

Fig. 3: HOMO and LUMO analysis of Levofloxacin

4. CONCLUSION

In the present work, we have calculated the geometric parameters, vibrational frequencies, frontier molecular orbitals, molecular electrostatic potential contours and surfaces and the nonlinear properties of Levofloxacin using DFT/B3LYP method. Vibrational spectral analysis of Levofloxacin was performed and DFT/B3LYP /6-31 G(d,p) showed better agreement with the experimental spectrum. Nonlinear Optical (NLO) behaviour of the examined molecule was investigated by the determination of the dipole moment μ, the polarizability α, and the hyperpolarizability β, using the DFT/B3LYP /6-31 G(d,p) method. According to HOMOs figures, the bands are predicted as an $\pi \rightarrow \pi^*$ transition. The molecular electrostatic potential contours and surfaces have also been drawn to explain the activity of Levofloxacin molecule. There is a good agreement between experimental and calculated normal modes of vibration have been observed.

REFERENCES

Alkorta, I., Perez, J. J., Molecular polarization potential maps of the nucleic acid bases, *Int. J. Quantum Chem.*, 57, 123-135 (1996).

Becke, A. D., Density-functional thermochemistry. III. The role of exact exchange, *J. Chem. Phys*., 98, 5648-5652 (1993).

Kawahara, S., Chemotherapeutic agents under study, *Nippon Rinsho*., 56, 3096-3099 (1998).

Kleinman, D. A., Nonlinear Dielectric Polarization in Optical Media, *Phys. Rev*., 126, 1977 (1962).

Lee, C., Yang, W., Parr, R.G., Development of the Colle-Salvetti conelation energy formula into a functional of the electron density, *Phys.Rev. B*., 37, 785-789 (1988).

Nelson, J. M., Chiller, T. M., Powers, J. H., Angulo, F. J., Fluoroquinolone-resistant Campylobacter species and the withdrawal of fluoroquinolones from use in poultry: a public health success story, *Clin Infect Dis*., 44, 977-80 (2007).

Padmaja, Amalanathan, M., Ravikumar, C., Hubert Joe, I., Density functional theory calculations and vibrational spectral analysis of 3, 5-(dinitrobenzoic acid), *Spectrochim Acta. Part A*., 74, 349-356 (2009).