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Vibrational analysis of Zotepine 2-[-3-chlorodibenzo(b)(1)benzothepin-5-yl)oxy]-N,N-dimethyl ethanamine

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Abstract

Zotepine is a atypical antipsychotic drug indicated for acute and chronic schizophrenia. It has been used in Germany sincr 1990 and Japan since 1982 The optimized geometry and their properties such as equilibrium energy, frontier orbital energy, dipole moment and vibrational frequencies have been used to understand the activity of Zolepine. The calculated highest occupied molecule orbital or HOMO and the lowest un-occupied molecular orbital or LUMO energies shows that charge transfer within the molecule. The vibrational spectra of IR and Raman have been interpreted with the help of B3LYP level of theory with the 6-31G basis set from the Density function theory.

Keyword Vibrational spectra, DFT, HOMO, LUMO,antipsychotic

Introduction

Method, material and theory

Density functional theory (DFT) has become very popular in recent years. This is justified based on the pragmatic observation that it is less computationally intensive than other methods with similar accuracy. The premise behind DFT is that the energy of a molecule can be determined from the electron density instead of a wave function.

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DFT is a computational quantum mechanical modeling method used in physics, chemistry and material sciences. In the present contribution, the properties that can be calculated with DFT, such as geometries, energies, spectroscopic properties. Density functional theory (DFT) calculations have been performed to predict the IR and Raman spectra for the molecule. Fourier transform infrared (FTIR) and Raman spectra of the compound have been obtained experimentally. All FTIR and Raman bands of the compound obtained experimentally were assigned based on the modeling results obtained at the B3LYP/6-31G level.

In general, ab initio calculations give very good qualitative results and can yield increasingly accurate quantitative results as the molecules in question become smaller. The advantage of ab initio methods is that they eventually converge to the exact solution once all the approximations are made sufficiently small in magnitude.

DFT was applied using the B3LYP which is the keyword for the hybrid functional, which is a linear combination of the gradient functional proposed by Becke and Lee, Yang and Parr, together with the Hartree Fock local exchange function. Calculations were performed using the Gaussian 09. Gaussan is a general purpose computational chemistry software package. A basis set in theoretical and computational chemistry is a set of functions (called basis functions) that is used to represent the electronic wave function in the density-functional theory The DFT methods with 6-31G basis set calculations were made first to optimize the structures. The vibrational frequencies and non-linear optical properties were calculated by means of DFT methods at the corresponding optimized geometries. All the calculations converged to an optimized geometry which corresponds to a true energy minimum as revealed by the lack of imaginary values in the calculate vibration frequencies. Vibration frequencies are calculated using B3LYP/6-31G.

Optimized geometrical structure of zotepine is shown in figure1.

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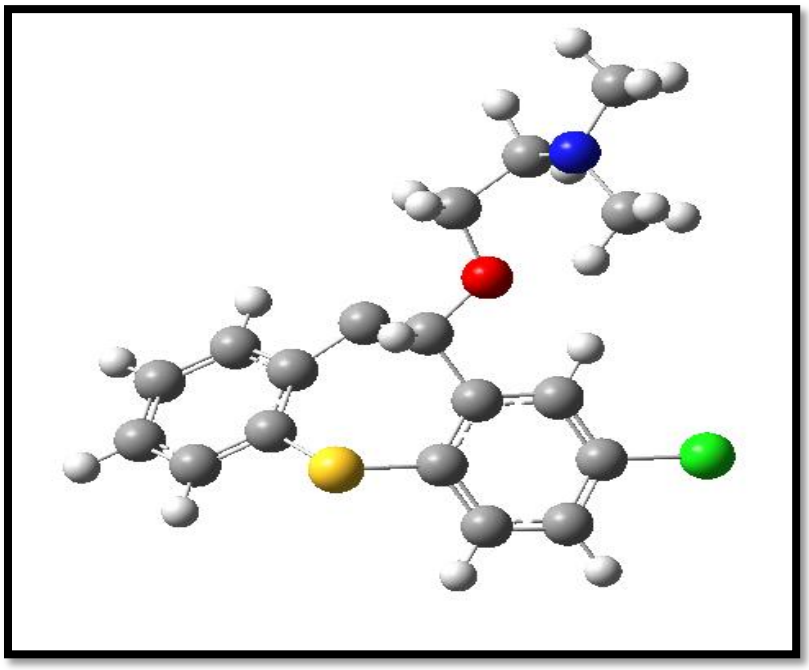

Fig 1

IR and RAMAN Spectroscopy

Infrared spectroscopy (IR spectroscopy or vibrational spectroscopy) involves the interaction of infrared radiation with matter. It covers a range of techniques, mostly based on absorption spectroscopy. An IR spectrum can be visualized in a graph of infrared light absorbance (or transmittance) on the vertical axis vs. frequency or wavelength on the horizontal axis. Optimized geometric structure of IR Spectra of Zotepine is shown in figure-2.

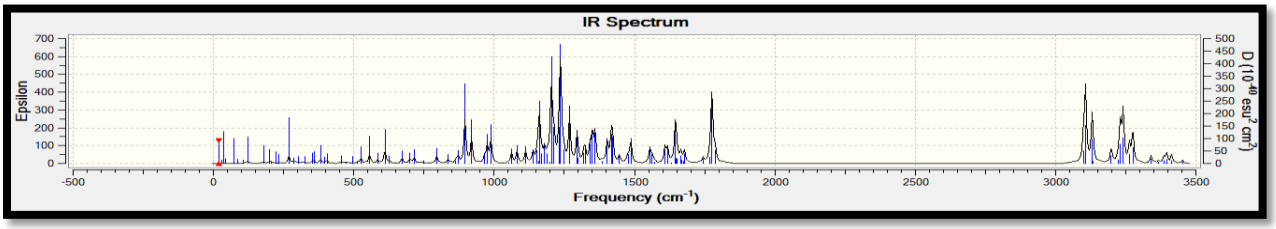

Fig 2

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A RAMAN spectrum is a plot of the intensity of RAMAN scattered radiation as a function of its frequency difference from the incident radiation (usually in units of wavenumbers, cm^{-1}). This difference is called the **RAMAN shift**, because it is a difference value, the Raman shift is independent of the frequency of the incident radiation. Optimized geometric structure of Raman Spectra of Zotepine is shown in figure3.

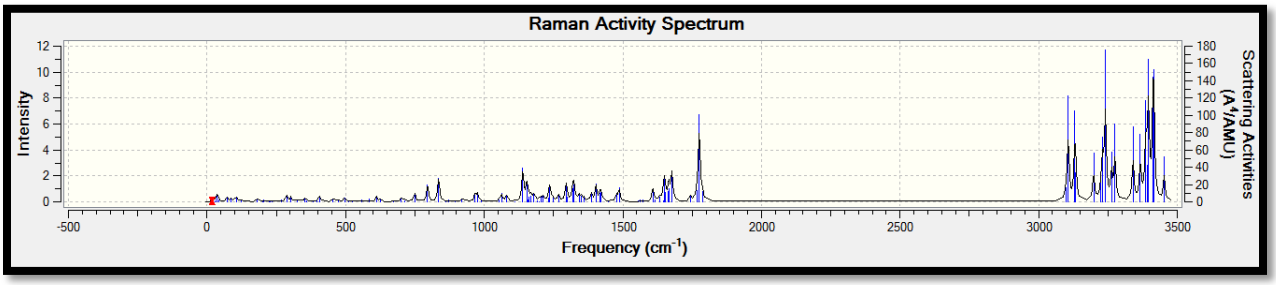

Fig 3

DEPOLARIZATION SPECTRA-

The depolarization ratio is the intensity ratio between the perpendicular component and the parallel component of the Raman scattered light. Two polarizations occur i.e. p- polarization and u- polarization. The optimized spectra of p-depolarization and u-depolarization are shown in the fig-4 and fig-5.

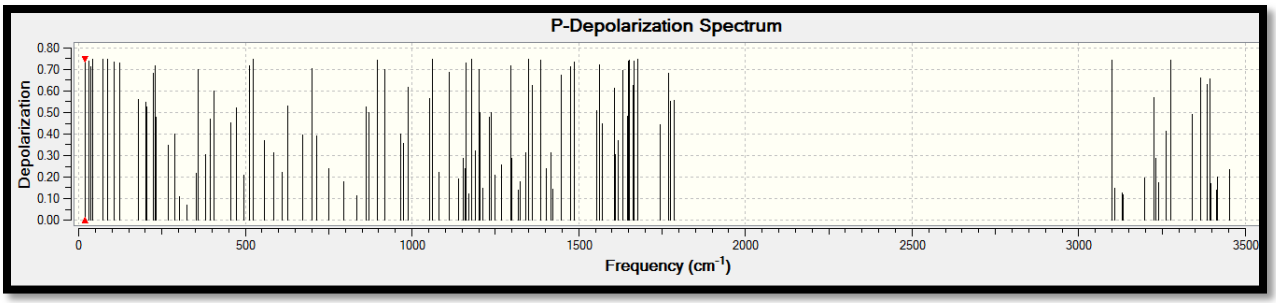

Fig 4

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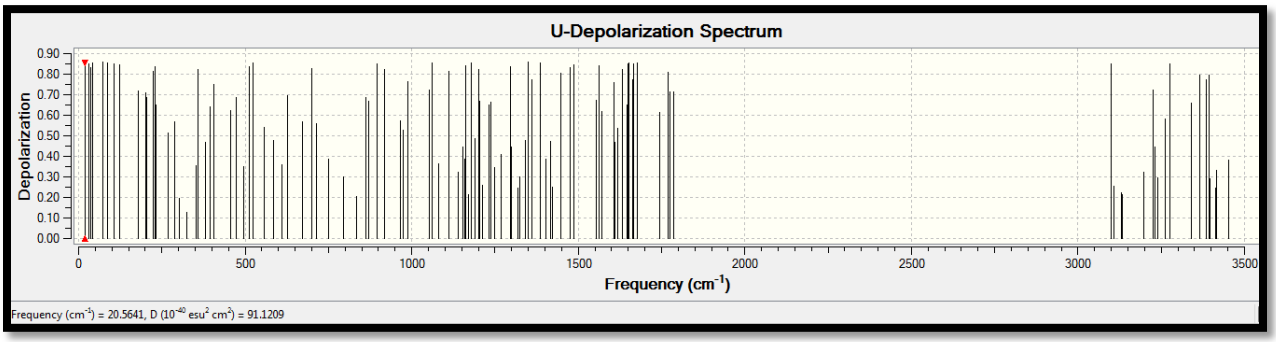

Fig 5

Theoretically computed ground state optimized parameters

Parameters	Zotepine(B3LYP/6-31G)
Energy (in a.u.)	-1646.73318231
Dipole moment (in Debye)	2.9866

1 Debye = $3.34*10^{-30}$ cm.

1 ***a.u.*** of ***energy*** = 1hartree = 4.360×10^{-18} J. = 27.211***eV*** = 2625kJ/mol = 627.5kcal/mol.

Molecular Orbital Energies

The most important orbitals in a molecule are the frontier molecular orbitals, called highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO).These orbitals determine the way the molecule interacts with other species. The frontier orbital gap helps characterize the chemical reactivity and kinetic stability of the molecule. A molecule with a small frontier orbital gap is more polarizable and is generally associated with a high chemical reactivity, low kinetic stability and is also termed as soft molecule.

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The density plot of the HOMO and LUMO of zolepine is calculated at B3LYP/6-31G level of theory and are shown in Figure 6and 7.

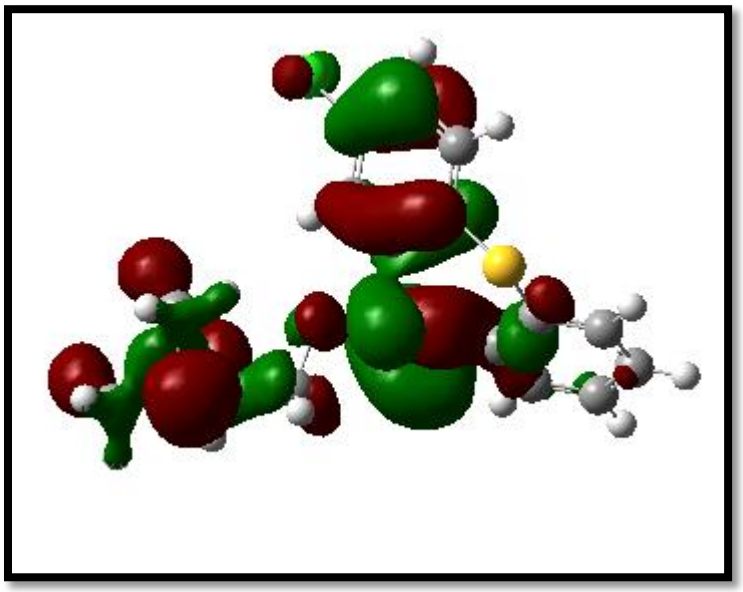

Fig 6

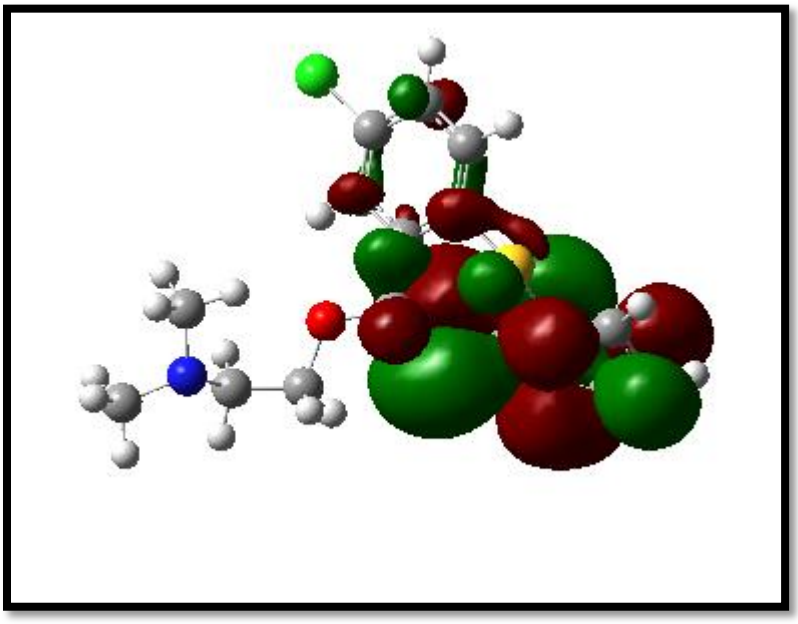

Fig7

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Bond length and Bond angle

In molecular geometry, bond length or bond distance is the average distance between nuclei of two bonded atoms in a molecule. It is a transferable property of a bond between atoms of fixed types, relatively independent of the rest of the molecule. Molecular geometries can be specified in terms of bond lengths and bond angles. The bond length is defined to be the average distance between the nuclei of two atoms bonded together in any given molecule. A bond angle is the angle formed between three atoms across at least two bonds. Such as bond lengths and bond angle are the optimized structural parameters, so these parameters were determined at B3LYP level theory with 6-31G basis set and they are presented in a table. Bond length table and graph of Zotepine is given below.

Atom	Bond Length
S(21)-C(03)	1.84016
S(21)-C(09)	1.8335
C(13)-Cl(22)	1.82865
O(23)-C(07)	1.46391
O(23)-C(24)	1.4698
N(30)-C(31)	1.46888
N(30)-C(27)	1.47347
N(30)-C(35)	1.46813

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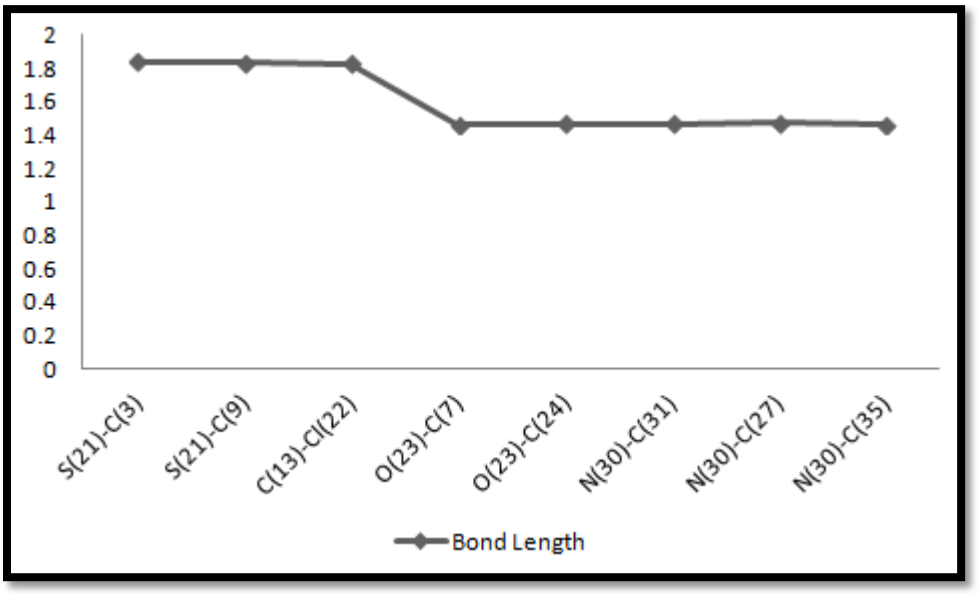

Atom	Bond Angle
C(3)-S(21)-C(9)	100.726
C(14)-C(13)-Cl(22)	118.994
C(12)-C(13)-Cl(22)	119.054
C(7)-O(23)-C(24)	117.66
O(23)-C(24)-H(26)	109.611
C(35)-N(30)-C(31)	112.74
C(27)-N(30)-C(31)	113.797
N(30)-C(35)-H(37)	110.328

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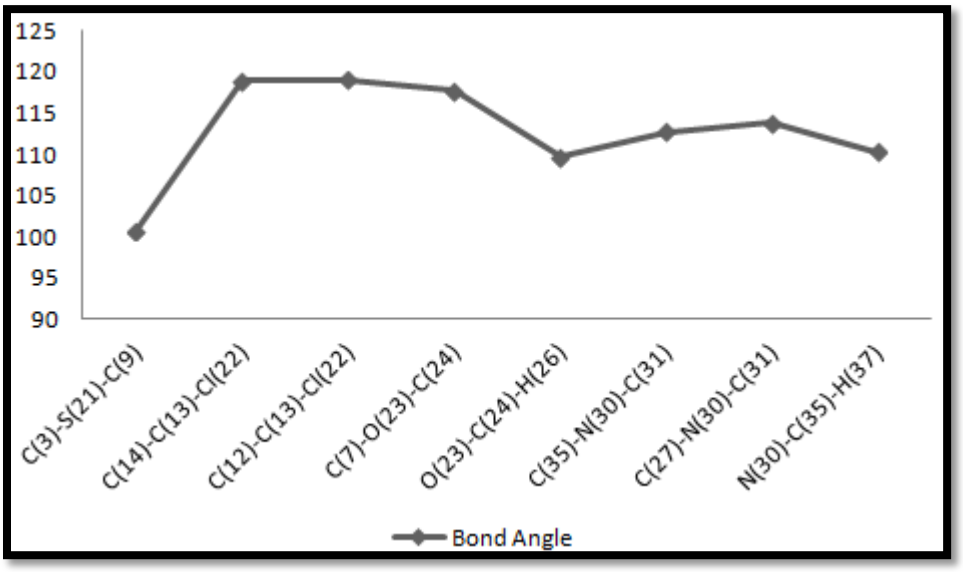

Conclusion: Simulation work of Zotepine is in the process. Simulation report of Zolepine we will reported very soon.

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