Study of Structure, IR spectra Molecular Polarizatity and Electronic Energy of a drug molecule

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***Abstract*: There are large number of biological activities, like antiviral, anticancer, antimicrobial and antibiotic activities. A number of bisfuramidine compounds have been found to be endowed with antitumour, anti-*Pneumocystis carinii pneumonia* (PCP) activity which binds within the malleable minor groove of the duplex DNA in A/T rich regions. There are no imaginary freq it means molecule is fully optimised all the study have been done using dft .The geometry of the molecule and optimisation is done by B3LYP.HOMO AND LUMO is found by DFT The harmonic vibrational frequencies of the molecule w. The vibrational spectra of the molecule is calculated through B3LYP/6-31G* method in 400-3200 cm^{-1} region.**

***Keywords*: Geometry Optimization; HOMO-LUMO; Analysis of IR.**

1. Introduction

In all the biological object DNA plays basic for improvement and is active for all biological system].DNA is a genitic material so it is called as transporter .so as a genetic material, genitic properties are transferred through DNA. Genetic character and involves in gene expression, replication, and by the small molecul *etc.* Caring process is done by interacting with DNA. Binding of drug with DNA maybe covelent, and non-covalent in this study, I have taken drug molecule 1d86 of minor groove Highest occupied orbital and Lowest unoccupied molecular orbital is used for Reactions and molecular spectra. Density functional theory is used in vibrational spectra and molecular structure.

Methodology

2 Electronic structure calculation

Gaussian03 program is used for the calculations of all the electronic structure properties of the molecule. Optimization of the molecule is done with the help of B3LYP from density from optimized coordinates electronic energy ground state energy are calculated and Homo and vibrational energy are also calculated. The density functional theory is in mathematical form

$$E_{xc} = (1-a_0)E_x^{ISDA} + a_0 E_x^{HF} + a_x \Delta E_x^{B88} + a_c E_c^{LYP} + (1-a_c)E_c^{VWN} \quad \ldots\ldots\ldots (1)$$

Here first term is exchange Second one is Hartree-Fock and third term is Becke's exchange energy.fourth and six terms are Lee,Yang,Par corrections terms.

2D structure is given below

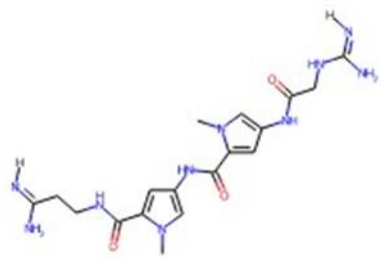


Fig- I

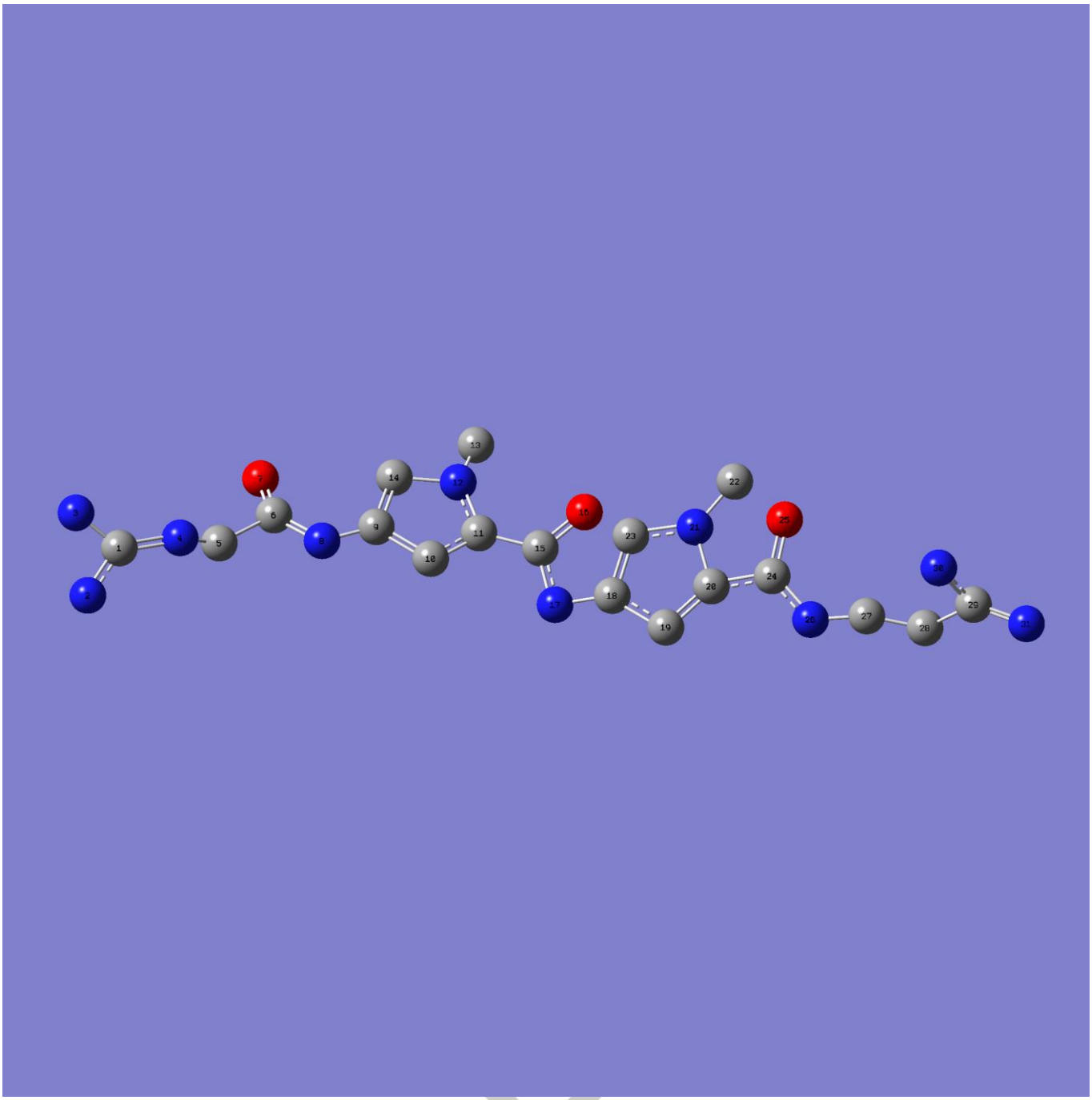
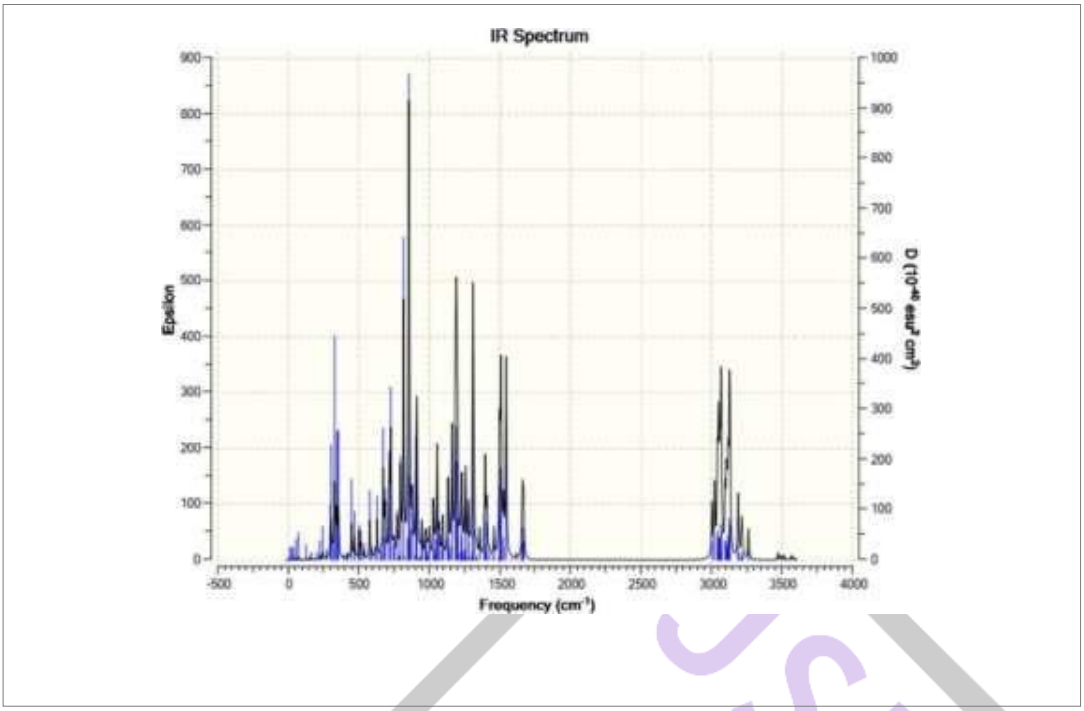


Fig- 2

3D structure of 1D86 molecule with DNA or Drug with DNA as shown in l

3

IR SPECTRA



Result and Discussion-

IR of a molecule is due to transition between vibrational energy levels due to alsorption of radiation. Frequency versus intensity spectra has been found in this work shown in the fig. The theoretically calculated - and practically calculated spectra are nearly same.all the values are given in the fig.Range of IR frequency in the fig is sp from 400 to 3500cm -1

Conclusion

All geometrical parameters calculated through B3LYP/6-31G* method and are approximately same with experimental values. The MEP map gives evident that electrophilic ability strengthens and nucleophilic ability become poor as one move radially outwards from the center of the molecule. Small values of HOMO and LUMO energy gaps means that the charge transfer interactions taking place within the molecule. Computed IR values are in good agreement with those of experimental values.

Objective

Study and analysis of drug molecules and after that DRUG-DNA interaction.

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