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The Theoretical studies of molecular orbitals, spectroscopic and thermodynamic properties of Antifungal drug

Joy Sarkar
Department of Chemistry, University of Lucknow, Lucknow 226007, Uttar Pradesh, India

Introduction:

The local indexes (softness, hardness, chemical potential, condense Fukui functions and electronegativity, etc.), global and absorption spectrum analysis (UV/Visible), and thermodynamic parameters (Heat capacity, Entropy, etc) of an antifungal drug were theoretically computed. In this work also, electronic structure, frontier molecular orbital energies were calculated. The images of molecular orbitals were developed with the help of the Gauss View 5.0.9 program package. The reactive site prediction and hydrogen bond interaction analysis were determined by using the Fukui function analysis. In this study, DFT/B3LYP/6-31+G and DFT/CAM-B3LYP/6-31+G (d, p) methods were used. Main Keywords: Absorption spectrum analysis, Frontier molecular orbital energies, Fukui function, Molecular geometry, Thermodynamic parameters.

Objectives:

An aurone is a heterocyclic chemical compound that is a kind of flavonoid. [1] There are two isomers of the molecule, with (E) - and (Z)-configurations. The molecule contains a benzofuran element associated with a benzylidene linked in position 2. In aurone, a chalcone-like group is attached to a 5-membered ring instead of the 6-membered ring more typical of flavonoids. Structural isomers are exhibited in Figure 1.

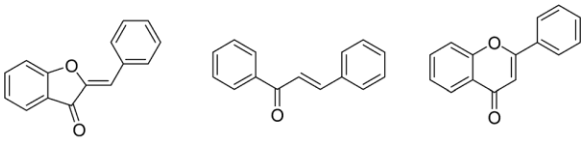

Figure 1. General Structure of aurone, chalcone and flavone molecular scaffolds

They are found in vegetables and especially in fruits and flowers where they responsible for their coloration. The biosynthesization of aurone takes place from chalcones by the use of enzyme aureusidin synthase. With their pigmentation role, aurones show a large multiplicity of biological activities, like antifungal, antibacterial, insect antecedent, antioxidant, and anticancer activities. Moreover, they have also been described as inhibitors of tyrosinase acetylcholinesterase, hepatitis C virus RNA-dependent RNA polymerase, histone deacetylase, monoamine oxidase, and ABCG2, and as inducers of NAD(P) H:quinone oxidoreductase 1. Aurones shows unique properties like photochemical and photophysical, these properties make them useful in a various applications such as fluorescent labels and probes in biology and medicine. In recent years, DFT method has been largely used in electronic transition energy predictions. It appears as one of the best successful methods in terms of the balance between the accuracy and the computational cost.

Results:

Quantum chemical calculations such as optimization of drug and molecular orbital energy calculation of molecules have been accomplished by using Becke's three-parameter exchange function (B3) with Lee-Yang-Parr correlation function with 6-31 G (d) by DFT theory. The Gaussian 09 software of the program has been used for various calculations. First, the drug is optimized then by the optimized structure of drug, geometrical parameters are used for the calculation of energy (HOMO and LUMO), energy gap, molecular electrostatic potential (MESP) to characterize the stability of the molecule and reactive sites of the molecule. HOMO and LUMO are types of molecular orbital. HOMO molecular orbital is standing for highest occupied molecular orbital, LUMO molecular orbital is standing for lowest unoccupied molecular orbital. The gap between HOMO and LUMO is known as the HOMO-LUMO gap.

The interaction among HOMO and LUMO of reacting groups is responsible for the electron transition as defined by FMO. HOMO energy is interrelated to the ionization potential and LUMO energy is associated to the electron affinity. More value of HOMO energy is proportional to give electrons to the suitable acceptor molecule of low empty molecular orbital energy. The less value of LUMO energy show more chance to accept electrons. So, the energy gap among HOMO and LUMO is a significantly stability index. The less value of energy gap shows higher electronic transition and vice versa.

The HOMO - LUMO energy is calculated at DFT B3LYP/3-21G level and the plot of frontier orbital energy gap for drug is shown in Figure 3. The energy of HOMO and LUMO are: - 6.0108 eV and -2.3197ev eV respectively and the energy gap (ΔE) is 3.6911 eV. The Energy gap gives information about the chemical activity of the drug

Conclusions:

In this study theoretical analysis of geometries and electronic properties of Aurone is performed using DFT/B3LYP method at a 6-31G (d) basis set. The effect of the substituted group on the structure and electronic properties are studied.

The stabilization energy and the calculated HOMO and LUMO energies indicated charge transfer in the molecule, which in turn indicated its bioactive properties.

Thus the theoretical study indicates that these molecules are polar and active molecule and they may interact with its environment strongly. The indications of the theoretical study reveal useful information about the reactivity of such molecules and give good information about the active sites in the molecules and clarify the sites of molecules that undergo nucleophilic substitution or electrophilic substitution reactions.