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THEORETICAL, COMPUTATIONAL AND ELECTRONIC PROPERTIES OF A BIOLOGICALLY ACTIVE COMPOUND MESOMILE

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Abstract-The DFT method employed to predict its electronic properties such as electronic transitions by HOMO-LUMO energies,various global reactivity and selectivity descriptors (chemical potential,electronegativity,chemical hardness, softness and electophilicity index)also calculated. Quantum chemical calculations of energies, geometrical structure and vibrational wave number of Mesomile were carried by B3LYP/6-311G(d,p) basis set.

I. Introduction

Vibrational spectroscopy is used in organic chemistry, for the identification of functional groups of organic compounds, for studies on molecular conformation, reaction kinetics, etc. A method can be proposed on the basis of frequency agreement between the computed harmonics and the observed fundamentals. Mesomile is used as an insecticide. They offer certain environmental and toxicological properties which are especially important in public health use [1,2]. Mesomile is very high mobile in soil. On increasing the concentration of mesomile decreases and Fe^{2+} and H_2O_2 can both accelerate degradation [3]. Density Functional Theory (DFT) is popular for the calculation of molecular structures vibrational frequencies and energies of molecules. Hence, the present investigations aim to study the HOMO-LUMO enrgy gap, the global reactivity descriptors like chemical potential, electronegativity, chemical hardness, softness and electophilicity index can be calculated for Mesomile using DFT/B3LYP utilizing 6-311G(d,p).

II. Computational details

The DFT computations for the Mesomile was carried out in the Gaussian 09 program package using "ultrafine" integration grids. The calculations were performed at the B3LYP level with the standard 6-311 G(d,p) basis set in order to derive the optimized geometry, vibrational wave numbers and natural bond orbital analysis of Mesomile.

III. Result and Discussion

A. Optimized geometry

The calculated data of Mesomile is in close agreement with the experimental values [table1].

Table 1: Selected optimized parameters of for Mesomile

Bond length(A^0)			Bond Angle(^{0})			Dihedral angle(^{0})		
Mesomile	Experimental value	Calculateded value	Mesomile	Experimental value	Calculated value	Mesomile	Experimental value	Calculated value
C_2-S_5	1.803	1.829	C_2-S_5	111.6	112.1	N_{11}-O_{12}-C_{13}	110.5	112.9
S_5-C_6	1.733	1.785	S_5-C_6-C_7	121.3	121.9	O_{12}-C_{13}-O_{14}	110.5	112.9
C_{13}-N_{15}	1.373	1.359	C_2-S_5-C_6	103.5	102.9	O_{12}-C_{13}-O_{14}	124.8	125.5

The bond length S5-C6 is increased by $0.052A^0$ because of the substitution of methyl group. The C_6-N_{11}(1.279 Aº) is relatively short compared to other C-N bonds.This shows the double bond character . The various bond angles and dihedral angles are found to be satisfactory agreement with the reported standard values.

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B. Frontier Molecular Orbitals

The highest Molecular orbital (HOMO) represents the outermost orbitals filled by electrons and behaves as an electron donor, while in the lower unoccupied molecular orbital (LUMO) considers as the first empty innermost orbital unfilled by electron behaves as an electron acceptor. The energy gap between HOMO and LUMO indicates the molecular chemical stability and is a critical parameter to determine molecular electrical transport properties. In this study,HOMO-LUMO energies and their 3D plots of the title compound are shown in fig.2

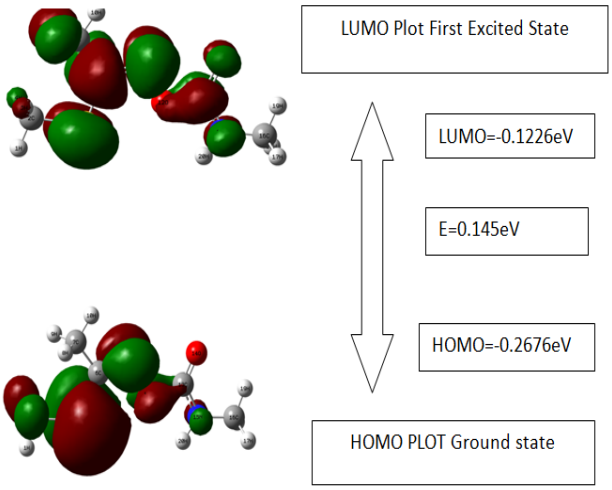

Fig.2.Highest occupied and Lowest unoccupied molecular orbital orbital Mesomile obtained by B3LYP/6-311G(d,p).

The narrow energy gap between HOMO and LUMO facilitates intramolecular charge transfer which makes the material to be bioactive[4]

C. Global Reactivity Descriptors

The global reactivity descriptors like chemical potential, electronegativity, chemical hardness, softness and electophilicity index and local reactivity descriptor like Fukui functions can be calculated on mesomile using DFT. In simple molecule theory approaches, the HOMO energy is related to the ionization potential (I) by Koopman's theorem and LUMO energy has used to estimate the electron affinity (A)[5].

Electron affinity (A)=-E_{LUMO}

The average value of HOMO and LUMO energies is related to electronegativity(χ) defined by Mulliken[6].

Electronegativity (χ)= (I+A)/2

Electronegativity is decribed as negative of the electornic chemical potential.

Where μ is chemical potential takes the average value of ionisation potential (I) and electron affinity (A)[7].

Chemical Potential=-(I+A)/2

The electronic Chemical Potential is the parameter which describes the escaping tendency of electrons from an equilibrium system.Thus the frontier molecular orbital analysis also provided the details on chemical stability, chemical hardness and electronegativity of the molecule in B3LYP methods with 6-311G (d,p)basis set are presented in table 1. In addition,the HOMO and LUMO energy is related to the hardness(g) and softness(r)[8].

Global hardness (η)= (I-A)/2

Global softness(S)=1/2 η

Electrophilicity Index (ω)=μ^2/2η

Electrophilicity index is one of the important quantum chemical descriptors in describing toxicity or biological activities of the molecules in the context of development of Quantitative Structure Activity Relashionship(QSAR)analysis.

Table.1:Global reactivity descriptors data for mesomile at B3LYP/6-311G(d,p)level

E_{HOMO}	-0.2676 eV
E_{LUMO}	-0.1226 eV
Chemical hardness(η)	-0.0725 eV
Softness(s)	-0.0363 eV
Chemical Potential(μ)	0.1951 eV
Electronegativity(χ)	-0.1951 eV
Electrophilicity(ω)	-0.2625 eV

The electrophilicity of mesomile describes the biological activity. Considering the chemical hardness, if one molecule has large HOMO-LUMO gap, it is a hard molecule; small HOMO-LUMO gap, it is a soft molecule. We can also relate the stability of molecule of hardness, which means that the molecule with least HOMO- LUMO gap means, it is more reactive. This shows that the title compound shows more bioactive. The local reactivity descriptor like Fukui function indicates the preferred regions where a chemical molecule will amend its density when the numbers on electrons are modified or indicates the tendency of the electronic density to deform at a given position upon accepting or donating electrons.

IV. CONCLUSION

The equilibrium geometries of Mesomile were determined and analyzed at the DFT level. The DFT calculated values of the Vibrational wave number agrees well with experimental data. The HOMO–LUMO energy gap clearly reveals the structure activity relation of the molecule. The results shows the bioactive nature of the molecule . The electronic properties such as electronic transitions by HOMO and LUMO energies,various global reactivity such as chemical hardness,chemical potential,softness,elecrophilicity index of the title molecule precisely.

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