

Frontier molecular orbitals (FMO) and molecular electrostatic potential (MEP) surface of 2-(4-chlorophenyl)-1-((furan-2-yl) methyl)-4,5-dimethyl-1H-imidazole using DFT method

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ABSTRACT

The FMO and MEP surface of 2-(4-chlorophenyl)-1-((furan-2-yl)methyl)-4,5-dimethyl-1H-imidazole (FDI) was calculated at B3LYP/6-31G(d,p) basis set. The calculated HOMO-LUMO energy gap shows the stability of the molecule. Molecular electrostatic potential (MEP) was studied for predicting the reactive sites.

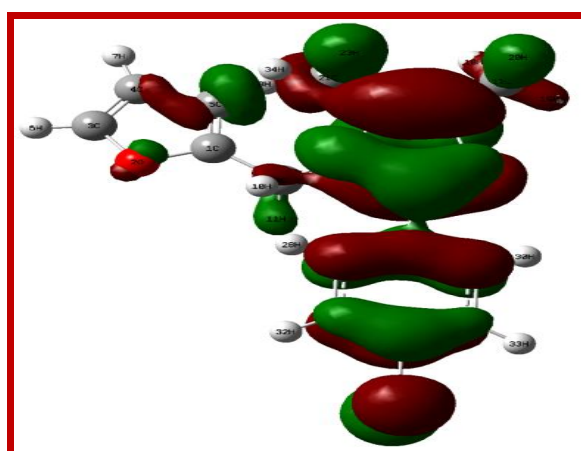
SCHEME



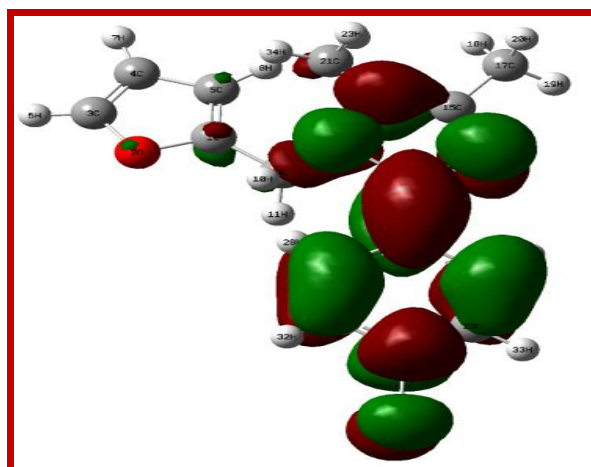
RESULTS AND DISCUSSION

HOMO - LUMO Analysis

HOMO = -5.2822 eV



Energy gap = 4.0106 eV



LUMO = -1.2715 eV

Fig 1. The HOMO-LUMO Energy diagram of FDI

The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) plots of the FDI compound is shown in Fig. 1. The frontier molecular orbital gap helps to characterize the chemical reactivity and kinetic stability of the molecule[1-8]. The energy gap between HOMO and LUMO indicates the molecular chemical stability. The red color indicates the negative charge and green color indicates positive charge for the title molecule. The HOMO is orbital that indicates as an electron donor and the LUMO is the orbital that indicates as an electron acceptor[9-12]. The HOMO indicates the charge density localized all over the imidazole and the full phenyl ring except hydrogen and furfuryl ring. The LUMO part is present on imidazole and chloro substituted phenyl ring except furfuryl ring[13-19]. Their corresponding energy value is -5.2822 eV and -1.2715 eV respectively. The calculated HOMO and LUMO energies clearly show that charge transfer occurs within the molecule. The calculated HOMO-LUMO energy gap value is found to be 4.0106 eV[20-29].

Molecular electrostatic potential

Molecular electrostatic potential (MEP) gives information about the net electrostatic effect produced at that point by total charge distribution (electron + proton) of around the molecule [30-39]. Moreover, MEP surface helps to identify the reactivity of wide variety of chemical systems in both electrophilic and nucleophilic reactions, hydrogen bonding interactions and the study of biological recognition processes [2,3]. It also helps visual understanding of relative polarity of the molecule. An electron density isosurface mapped with electrostatic potential surface predicts the size[40-45], shape, charge density and reactive sites of the molecules. The different values of the electrostatic potential at the surface are represented by different colors; red indicates regions of most electro negative electrostatic potential, blue indicates regions of most positive electrostatic potential and green indicates

regions of zero potential. The electrostatic potential increases in the order red < orange < yellow < green < blue [1].

To predict reactive sites for electrophilic and nucleophilic attack for the investigated molecule, MEP surface is plotted over optimized FDI at B3LYP/6-31G(d,p) basis set. From Fig. 2 shows that the electrostatic potential contour map of FDI. As easily can be seen in FDI molecule has several possible sites for electrophilic (the electrophilic sites are most electro negative and are represented as red color) and nucleophilic attack (the nucleophilic sites are most positive and are represented as blue color). We concluded that the oxygen groups behaves electrophiles region and it denoted as red colour. Like wise, the nucleophiles region was graphically in blue color. The regions over the rings are neutral as represented in green colour. These regions give information about intermolecular interactions [4].

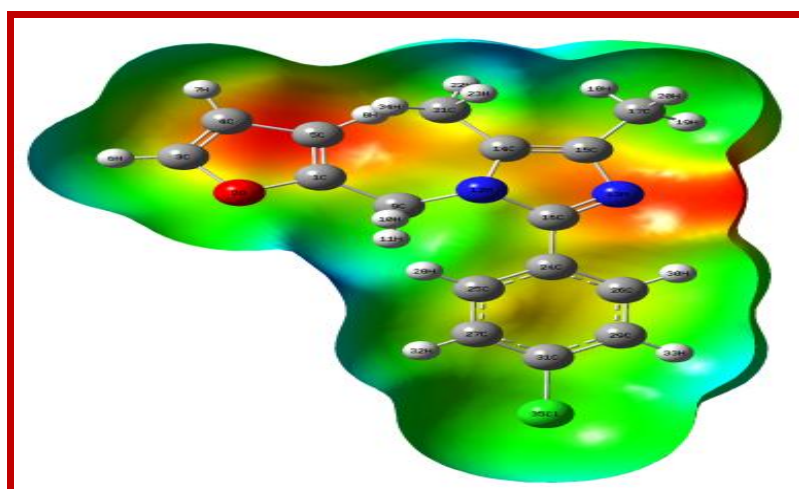


Fig 2. MEP diagram of FDI

CONCLUSION

The complete vibrational assignments of 2-(4-chlorophenyl)-1-((furan-2-yl)methyl)-4,5-dimethyl-1H-imidazole was performed for first time to using quantum chemical calculation. Geometrical parameters were calculated at DFT/B3LYP/6-31G(d,p) level of

theory and also compared with the related XRD data. The HOMO-LUMO energy gap is calculated at 4.0106 eV. This small energy gap indicates that FDI molecule has a good chemical stability of the present system. MEP surface performed from the reactive sites of the FDI molecule.

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