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Molecular Electrostatic Potential in Z-3N(2-Ethoxyphenyl), 2-N'(2-Ethoxyphenyl) Imino Thiazolidin-4-one Molecule by Ab Initio and DFT Methods

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Abstract : In the present work we are interested in the determination of the Molecular electrostatic potential (MEP) in Z-3N(2-Ethoxyphenyl), 2-N'(2-Ethoxyphenyl) imino thiazolidin-4-one molecule by ab initio and Density Functional Theory (DFT) in the ground state. The MEP is related to the electronic density and is a very useful descriptor in understanding sites for electrophilic attack and nucleophilic reactions as well as hydrogen bonding interactions. First, geometry optimization was carried out using Hartree–Fock (HF) and DFT methods with 6-311G(d,p) basis set. In order to get more information on the molecule, its stability has been analyzed by natural bond orbital (NBO) analysis. Mulliken population analyses have been calculated. Finally, the molecular electrostatic potential (MEP) and HOMO-LUMO energy levels have been performed. The calculated HOMO and LUMO energies show also the charge transfer within the molecule. The energy gap obtained is about 4 eV which explain the stability of the studied compound. The obtained molecular electrostatic potential from the two methods confirms the nature of the electron charge transfer at the molecular shell and locate the electropositive part and the electronegative part in molecular scale of the title compound.

Keywords : DFT, ab initio, HOMO-LUMO, organic compounds
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