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Investigation of Barrier Potential, Structure (Monomer & Dimer), Chemical Reactivity, NLO, MEP, and NPA Analysis of Pyrrole-2- Carboxaldehyde Using Quantum Chemical Calculations

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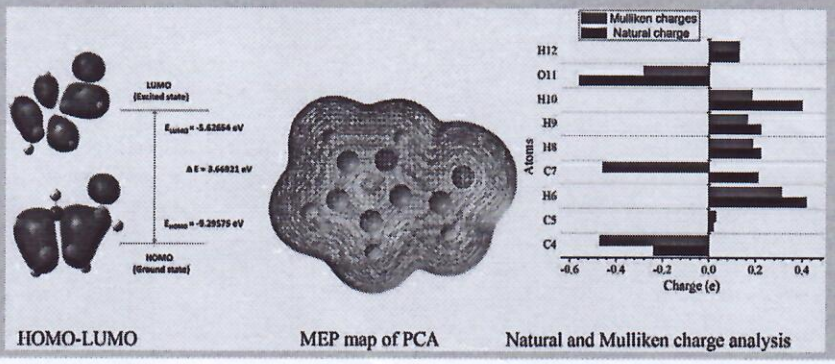
ABSTRACT

In this work, the structural conformation of pyrrole-2-carboxaldehyde was evaluated using potential energy surface (PES) scan employing DFT computations using B3LYP method with 6-311++G(d,p) level of basis set. The molecule assumed *cis* form in conformational ground state being more stable than the *trans* by 15.21 kJ mol^{-1} due to the orientation of the N–C–C = O dihedral angle. Existence of hydrogen bonds due to intra- and inter-molecular interactions was envisaged. The geometrical parameters of optimized monomeric and dimeric forms have been computed. The computational structural parameters of monomer are in good agreement with its experimental counterparts. The HOMO-LUMO energies were employed for determination of chemical reactivity descriptors. The electronic properties such as frontier molecular orbitals and Global reactivity descriptors were predicted using TD-DFT method. The local reactivity descriptors such as Fukui functions were investigated to determine the electrophilic and nucleophilic attacks within the molecule. The calculated first order hyperpolarizability value exhibited its suitability for non-linear optical applications. Furthermore, the electrophilic and nucleophilic regions of the molecule were studied by molecular electrostatic potential and Fukui functions. ^{1}H and ^{13}C NMR chemical shifts were evaluated using GIAO method employing the same level of theory. NPA analysis and thermodynamic parameters were also calculated.



HOMO-LUMO MEP map of PCA Natural and Mulliken charge analysis

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KEYWORDS
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