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Molecular structure, NBO, first order hyperpolarizability and HOMO-LUMO analysis of 7-Azathieno[2,3-c]cinnoline

V.P.Gopika[1], G.Havisha[1], S.Muthu[2]*, M. Raja[3], R. Raj Muhamed[3]

[1]Department of Chemical Engineering, Sri Venkateswara College of Engg, Sriperumbudur,Tamilnadu, India
[2]Department of Physics, Govt Thirumagal Mills College, Gudiyattam,Vellore, India
[3]Department of Physics, Jamal Mohamed College (Autonomous), Trichy-20, India

Abstract: In this work, we reported a theoretical investigations on molecular structure of 7-Azathieno[2,3-c]cinnoline(7AC). The molecular geometry and NBO have been calculated by using density functional theory B3LYP method with 6-311++G(d,p) basis set. Stability of the molecule arising from hyper-conjugative interactions and charge delocalization has been analyzed using natural bond orbital analysis (NBO). The calculated HOMO and LUMO energies show that charge transfer within the molecule. Molecular electrostatic potential(MEP) and the first order hyperpolarizability were also performed. The electron density-based local reactivity descriptor such as Fukui functions are calculated to explain the chemical selectivity or reactivity site in title compound. The molecule orbital contributions were investigated by using the total density of states (TDOS) and sum of α and β electron density of states ($\alpha\beta$DOS). The thermodynamical properties (heat capacity, entropy and enthalpy) of the 7AC at the different temperatures were calculated in gas phase.
Keywords: *DFT; NBO; Fukui function; Thermodynamic Properties.*

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