Journal of Applied, Physical and Bio-Chemistry Research (JAPBR)
Vol. 1, Issue 2, Dec 2015, 17-22

THEORETICAL STUDY FOR SOME CYCLIZATION OF IMINE COMPOUNDS 5-MEMBERED RINGS BY USING AB INTIO CALCULATIONS(RHF -MODEL)

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ABSTRACT

This study involved the adoption of the program (Gaussian 09) at (B3LYP/6-311G)to use the method of calculation the total (Ab initio of method) according to the Hartree – Fock method (RHF) , for the purpose of the expense of dimensional geometric (lengths and angles bond) when the geometry of a balanced, functions thermodynamic and some physical properties for derivatives of Imine Compounds 5-Membered Rings 3-(thiophene-2-yl)-2-p-tolylimidin-4-one .

Calculation results have shown that the compound **B**($C_{18}H_{16}N_2O_3S$) has highest value of thermodynamic functions (E^0 , H^0 , G^0 , A^0 , C_V , C_P,S^0) .

For [**A**($C_{14}H_{14}N_2OS$) , **B**($C_{18}H_{16}N_2O_3S$) , **C**($C_{17}H_{14}N_2O_3S$) , **D**($C_{16}H_{16}N_2O_2S$)] molecules the calculated some of physical properties (dipole moment μ in Debye), orbital energies (E_{HOMO} , E_{LUMO} in e V), IP (in e V) , (measurement stability ΔE) , hardness η and Electron Affinity E_A).Also For these molecules the calculated (ΔHf^0 (in kJ/mole)by using (semi-empirical method PM3 model in MOPAC program). Calculation results have shown that the compound **B**($C_{18}H_{16}N_2O_3S$) the lower value of the heat of formation (the more Stability) , and the compound **C**($C_{17}H_{14}N_2O_3S$) has less value of (E_{LUMO} , IP , η) as well as has less value ΔE (more activity than other compounds). ,This difference in results come according to the difference of substituted groups.

KEYWORDS: RHF study, Imine Compounds, Thermodynamics Functions and Hardness