ChemTech

International Journal of ChemTech Research
CODEN(USA): IJCRGG, ISSN: 0974-4290, ISSN(Online):2455-9555
Vol.10 No.9, pp299-305,2017

Electronic Structure, Thermodynamics functions and Physical properties forthiadiazolderivativesringby usingAbIntiocalculations(RHF-Model).

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Abstract: This study involved the adoption of the program (Gaussian 03) 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, some physical properties, charges for derivatives ring 4-(1,3,4-thiadiazol-2-yl)benzene-1,3-diols.

Calculation results have shown that the compound($R\text{-}NO_2$) has less value of thermodynamic functions (E^0 , H^0 , G^0 , A^0) but the compound ($R\text{-}OCH_3$)) has highest value of heat capacity and Entropy (C_V , C_P,S^0) .The results showed that both nitrogen atoms (N_9 , N_8) had the highest negative charge when the compound($R\text{-}NO_2$) which makes it a strong legend when Linked to metal and the formation of the complex.

For ($R\text{-}CH_3$, $R\text{-}NO_2$, $R\text{-}OCH_3$, R-OH) 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 Δ) , hardness η and Electron Affinity E_A).Also For these molecules the calculated (ΔH_f^0 (in kJ/mole)by using (semi-empirical method AM1 model in MOPAC program). Calculation results have shown that the compound (R-OH) the lower value of the heat of formation (the more Stability)as well as has high value of the (ΔE , η , E_A),While the compound $R\text{-}NO_2$ has less ΔE that means this compound more active than other compounds ,This difference in results come according to the difference of substituted groups.

Key words:RHF study,4-(1,3,4-thiadiazol -2-yl)benzene -1,3-diols ,thermodynamics functions.

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