Theoretical Study of Reactions with Electrophiles Substitutions: by B3lyp-Dft Density Function Calculation

Dr. Rashed Taleb Rasheed  
Applied Sciences Department, University of Technology / Baghdad  
Email: r_awsy@yahoo.com  
Hadeel Salah Mansoor  
Applied Sciences Department, University of Technology / Baghdad  
Aseel Salah Mansoor  
Pharmaceutical Department, Al-Rasheed University/Baghdad  
Dr. Emad A. Yousif  
Department of Chemistry, College of Sciences, AL-Nahrain University/Baghdad

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ABSTRACT

Density functional theory (DFT), using the B3LYP functional was utilized to study the molecular properties (benzene molecule was a reference) of 1,3,5-Trihydroxybenzene (THB) compound in order to determine the relationship between molecular structure and electrophiles substitutions (nitration) efficiencies to get 2-nitro 1,3,5-Trihydroxybenzene (NTHB), 2,4-Dinitro 1,3,5-Trihydroxybenzene (DNTHB) and 2,4,6-Trinitro 1,3,5-Trihydroxybenzene (TNTHB) respectively. The best geometry for all molecules was investigated at (6-31G) basis sets. The total energies, ionization potentials, electron affinities, energy gaps, hardness and softness were calculated for the studied molecules. The electronic properties for all molecules were investigated by Gaussian (03) program.

Keywords: DFT, Electrophones Substitution, Nitration, Molecular Properties.