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Theoretical Studies on Electrophilic Aromatic Substitution Reaction for 8-Hydroxyquinoline

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ABSTRACT

Theoretical investigations of organic molecules for the objective of their structural stability are the most important techniques in this regards. Recently calculations and simulation reactions utilizing theoretical studies become attractive conventional method for the researchers. Density function theory (DFT) method was used to study the reaction of 8-hydroxyquinoline with 4-ethoxycarbonyl-benzene diazonium chloride as electrophilic aromatic substitution reaction. To study any reaction there are two explanations: first explanation depends on the reactant molecules and second explanation depends on the stability of the product molecules. Determine the stability of the molecule by comparing the energies (total energy, energy level of (HOMO), and energy gap), we have three stable molecules, are: HQ-7-YBAEE (II) for the total energy, HQ-6-YBAEE (II) for the energy level of (HOMO) and HQ-2-YBAEE (II) for the energy gap. The molecule HQ-4-YBAEE (II) is always at least stability in all data.

Key words: Electrophilic, 8-Hydroxyquinoline, DFT, HOMO, Energy gap, Total energy.

INTRODUCTION

Theoretical studies had been quite used to investigate the reaction mechanism, explain the reaction products and clarify chemical reactions mystery. Theoretical studies are valuable approaches to explore the mechanism of reactions in the molecules and their electronic structures levels in addition to electronic parameters that acquired by means of theoretical calculations employ the computational methods of quantum chemistry [1,2]. The improvement in theoretical