



Original Research Article

A DFT Investigation on The Reaction of tetrazolo [1,5-b][1,2,4]triazine with 1,5-diaminotetrazole and glyoxal in Different Temperatures

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ABSTRACT

In this article, synthesis of the explosive synthesis of tetrazolo [1,5-b][1,2,4]triazine from the reaction of 1,5-diaminotetrazole with glyoxal in different conditions of temperature, with density functional theory method were studied. For this purpose, at first the material contained in the both sides of reaction were geometrically optimized, then the calculation of the thermodynamic parameters performed on all of them. The amount of ΔH , ΔS and ΔG of this reaction at different temperatures in form of sum of parameters discrepancy in the products than reactants is obtained. And finally, the best temperature for the synthesis of explosive according to the obtained thermodynamic parameters were evaluated.

Keywords: tetrazolo [1,5-b][1,2,4]triazine , Density Functional Theory; 1; 5-diaminotetrazole; glyoxal; Thermodynamic parameters

Introduction

In recent years, new energetic materials considered and due to the special properties, have many applications in the military field. Currently many researchers around the world with high density based on energetic materials such as Tetrazole doing research, this energetic materials in the production of pyrotechnics with less smoke, gas generators and engines are widely used and also less sensitive to heat and shock of their show. Another benefit of this combination compared to conventional energetic substances, they are green [1-20]. Because these reactions were less environmental hazard and let it show better performance. Energetic materials commonly used fossil that often have high carbon content. During the process of burning large amounts of carbon dioxide (CO₂), carbon monoxide (CO) and unburned carbon particles such as soot produce and environmental pollutants and pollution and create a lot of problems. Nitrogen-rich compounds widely used in propulsion systems, fire extinguishing systems and airbag systems as well as fuel for missiles and military systems. In this study, the synthesis of tetrazolo [1,5-b][1,2,4]triazine from the reaction of 1,5-diaminotetrazole with glyoxal is studied under different conditions of temperature, density functional theory method. Some chemical properties calculated in the level of B3lyp / 6-31g for tetrazolo [1,5-b][1,2,4]triazine(C₃H₂N₆) and 1,5-diaminotetrazole (CH₄N₆) is shown Table 1 [21-39].