



The thermodynamic parameters derived material [1,5-b] tetrazolo [1,2,4] Terry inflorescences (TTA) with boron nitride nano- cages in different conditions of temperature , density functional theory method.

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Abstract

In this study the reaction of the derivative , material [1,5-b] tetrazolo [1,2,4] Terry inflorescences (TTA) with boron nitride nano- cages in different conditions of temperature , density functional theory methods were studied . For this purpose, the material on both sides were geometrically optimized reaction , then the calculation of the thermodynamic parameters were performed on all of them . The values of ΔH , ΔG , ΔS the reaction at different temperatures for different products together, these parameters in the raw material is obtained . And finally, the best temperature for the synthesis of derivatives of explosives, according to the results of thermodynamic parameters were evaluated .

Keywords: Enthalpy of formation , TTA, boron nitride cage

1. Introduction

tetrazole cyclic and aromatic compounds , has four atoms of nitrogen and carbon . Which are used in military industries . These compounds are released by burning large amounts of gas N₂ so little pollution to the environment and green are the explosives . Today, many scientists in the world investigating the energetic materials with high density tetrazole times , Environmental hazards these reactions are commonly used to lower fossil energy materials And has a high carbon content because during the process of burning fossil fuel carbon emissions of carbon dioxide , carbon monoxide and unburned carbon particles such as Produce a lot of soot pollution in the environment and create a lot of problems . The nitrogen-rich compounds are used in various industries . The nitrogen-rich compounds are used in various industries .