



## Original Article.

# Evaluating the Thermodynamic Parameters the Derivative [b-5,1] tetrazolo [4,2,1] teriazine (TTA) with Boron nitride nano-cage in Different Temperature Conditions by DFT Method

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### ABSTRACT

In this research, the formed reaction derivative of matter [b-5,1] Tetrazolo [4,2,1] Teriazine (TTA) with Burnitride cage Nano-structure was studied in different temperature conditions by DFT method.

For this purpose, first, the materials on both sides of the reaction were the geometric optimization, then, calculation related to the thermodynamic parameters were done on all them. Then, the values of  $\Delta S$ ,  $\Delta H$  and  $\Delta G$  of this reaction at different temperatures are obtained by the difference in the sum of these parameters in the products to the primary materials and in the final, the best temperature for the synthesis of the explosive material derivative was evaluated according to the resulting thermodynamic parameters

**Keywords:** formed  $\Delta H$ , matter [b-5,1] Tetrazolo [4,2,1] Teriazine (TTA), Burnitride cage

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### Introduction

The Tetrazoles are ring and aromatic compounds with 4 nitrogen atom and carbon atom that applicable in military industries. These compounds release to the large amounts of gas  $N_2$  through burning. So, they have little pollution for the environment and they are except from green explosives materials[1-2]. Today, many scientists around the world are researching on the full energy materials with high density based on Tetrazoles, environmental hazards of these compounds are lower relative to the fossil full energy materials that are commonly used and have high carbon content. Because, fossil fuels produce many soot at during the process of burning gases  $CO_2$ ,  $CO$ , and unburned carbon particles like that there are in the environment pollution and many problems. These nitrogen-rich compounds have been used in different industries. In this research, synthesis derivative of matter [b-5,1] Tetrazolo [4,2,1] Teriazine (TTA) with Burnitride cage has been studied temperature conditions by DFT method [3-5].