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Investigating the Energy Efficiency of TEX High Energy Derivatives with Different Carbon Fuller Nano Structures under Different Temperature Conditions by DFT Method

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Abstract

In this study, high energy energy derivatives of TEX with different carbon-containing fullerenes at different temperature conditions were studied using density functional theory. For this purpose, the materials were first geometric optimized, then the thermodynamic parameters were calculated for all of them. Then, the process of changing the energy-dependent parameters such as specific heat capacity, enthalpy, entropy and Gibbs free energy relative to molecular mass, molecular volume and measured level in this study at a given temperature, were evaluated against each other.

Keywords: High energy energy derivatives, TEX, Functional density theory.

1. Introduction

TEX is an energetic explosive that has the same high speed and high explosive pressure, mechanical sensitivity and thermal stability. In recent years, new energetic materials have been taken into consideration, due to their special properties, they are widely used in military applications. TEX is made up of white to slightly yellow crystals that are impregnated with brown or different colors. As an explosive, TEX draws attention to its relatively high density. Its high density is due to its ISO structure and a compact crystal network of nitro groups that fill the gap between the cages. These high-performance materials are very useful in the production of pyrotechnic products with diameters, and they are less sensitive to heat and shock. On the other hand, the environmental hazards of these compounds are lower and better performance of the proportion of high-energy fossil fuels that burn in the process of burning out a large amount of carbon dioxide (CO2), carbon monoxide (CO) and unpolluted carbon particles, such as soot. Nitrogen-rich