## عنوان مقاله:

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


## محل انتشار:

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## خلاصه مقاله:

In thisresearch, the formed reaction derivative of matter [b-5,1] Tetrazolo [4,2,1] Teriazine (TTA) with boron nitride 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 ΔS, ΔH and ΔG 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



## کلمات کلیدی:

Formation enthalpy changes, [b-5, 1] Tetrazolo [4, 2, 1] Teriazine (TTA), Boron nitride cage, density functional theory