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Investigation of high-energy heterocyclic synthesis as a green fuel from the reaction of 3,6-D-aminotrazine with nitric acid and sodium azid; under different temperature conditions, by DFT method

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Abstract

In this research, the synthesis of heterocyclic explosives (ATTz) from the reaction of 3,6-D-amino-tetrazine with Nitric acid and sodium azide were studied under different temperature conditions using the functional density theory method. For this purpose, the materials were first geometric optimization reaction sides, then the thermodynamic parameters were calculated for all of them. Then, the values of ΔH, ΔG, ΔS of this reaction were obtained at different temperatures as the sum of these parameters in the products to the raw materials. Finally, the best temperature for the synthesis of explosives was evaluated according to the thermodynamic parameters.

Keywords: Explosive, ATTz, Synthesis, 3,6-D-Amino tetrazine.

1. Introduction