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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

Highly-fossil enriched fossil fuels or commonly used fossil fuels often contain high carbon content, which during the burning process generate large quantities of carbon dioxide (CO2), carbon monoxide (CO) and carbon-free carbon particles such as carbon black, which pollutant They are environmentally friendly and cause many pollution and problems. The more thermodynamic materials have a more positive heat formation, the more unstable and thus more active, nitrogen-containing high-energy materials are high-activity semi-stable molecules whose heat formation is positive, and, in the case of these materials, they decompose into smaller and more stable molecules. High energy is produced from them. Occasionally, the release of tensile energy from pressure rings is a source of energy release and explosion. Nitrogen-rich compounds are a bunch of high-energy compounds that are widespread due to their high nitrogen content. The main product of the combustion process is nitrogen gas (N2), the most abundant gas in the atmosphere, so there will be no environmental pollution problems associated with the use of these compounds. On the other hand, nitrogen-rich compounds in propulsion systems, fire extinguishing systems and airbag systems, as well as missile and military fuel systems, have been widely used [1-7]. In this study, the 3,6-D-amino-tetrazine (primary material) reaction with nitric acid and sodium azide was studied under different temperature conditions by functional density theory for the synthesis of heterocyclic explosives (ATTz) (main product). Is Figure (1)[8].

2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [9]. Geometries for all compounds are computed by means of the density functional theory (DFT) with Becke's three-parameter functional (B3) plus Lee, Yang, and Parr (LYP) correlation functional. For all atoms, the standard 6-31G basis set is utilized. The structures of **3,6-D-aminotrazine with nitric acid and sodium azid** were designed primarily using of Gauss View 5.0.8 and nanotube modeler 1.3.0.3 soft wares. The interaction effects of Fluoxetine on Fullerene were investigated [10-13].

3. Results

Investigation of the synthesis of heterocyclic explosives (ATTz) from 3,6-D-amino-tetrazine reaction with nitric acid and sodium azide under different temperature conditions was carried out using the functional density theory method using Gaussian 98 and Gossive software. The compositions were first optimized by density functional theory in the base series (6-31g). Then, IR studies were performed to calculate the thermodynamic parameters [14-16]. All calculations were carried out at a B3lyp / 6-31g surface temperature of 300 to 400 degrees Kelvin and atmospheric pressure. The reaction Examined is:

$$C2H4N6 + NaNO2 + NaN3 \rightarrow C2H2N8 + H2 + 1/ 2N2$$

4. Calculate and check the values of enthalpy changes (ΔH)

Using the Gaussian 98 program, the enthalpy values for raw materials and products were calculated in the synthesis process. The following equation is used to calculate and obtain enthalpy changes in the reactions A + B → AB. $\Delta H_{AB} = [H_{AB}] - [H_A + H_B]$

Now with regard to the reaction

$$C_2H_4N_6+NaNO_2+NaN_3\rightarrow C_2H_2N_8+H_2+1/2N_2$$

The amounts of enthalpy formed by calculating Gaussian software are as follows:

$$\Delta H_f = [H_{C2H2N8}+H_{H2}+1/2H_{N2}]-[H_{C2H4N6}+H_{NaNO3}+H_{NaN3}]$$

Fig2. The formation of enthalpy changes for the synthesis of heterocyclic bombs (ATTz) from the reaction of 3,6-dinamo-tetrazine with nitric acid and sodium azide at various temperatures

The value of ΔH_f indicates that the heterocyclic explosive (ATTz) process of the 3,6-D-amino-tetrazine reaction with Nitric acid and sodium azide are heated at different temperatures and, with increasing reaction temperatures, the amount of enthalpy changes is more negative (Fig. 2).

5. Calculate and check the values of entropy changes (ΔS):

Using the Gaussian program 98, entropy values for raw materials and products were investigated in the synthesis process. The following equation is used to calculate and obtain entropy variations in the reactions of A + B → AB.

Relationship (3): $\Delta S\ AB = [S_{AB}] - [S_A + S_B]$

Given the reaction:

C2H4N6 + NaNO2 + NaN3 → C2H2N8 + H2 + 1 / 2N2

The entropy values obtained by calculating Gaussian software are as follows:

Relationship (4):

$$\Delta S_f = [S_{C2H2N8}+S_{H2}+1/2S_{N2}] -[S_{C2H4N6}+ S_{NaNO3} +S_{NaN3}]$$

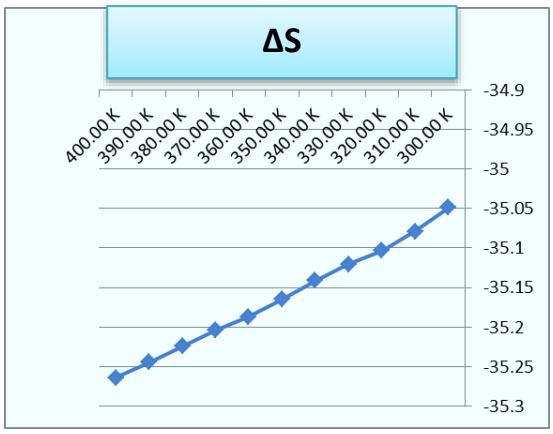

Fig. 3: Entropy Changes Chart The formation of heterocyclic (ATTz) explosive from 3,6-D-amino-tetrazine reaction with nitric acid and sodium azide at various temperatures

The amount of ΔSf indicates that the heterocyclic explosive formation (ATTz) of the reaction of 3,6-diaminototazine with nitric acid and sodium azide has a negative entropy at different temperatures, which, with increasing temperature, decreases the disorder. Fig. 3.

Calculating and checking the specific heat capacity of the CV:

Using the Gaussian program 98, the specific CV heat capacity values for raw materials and products in the synthesis **process were investigated and calculated.**

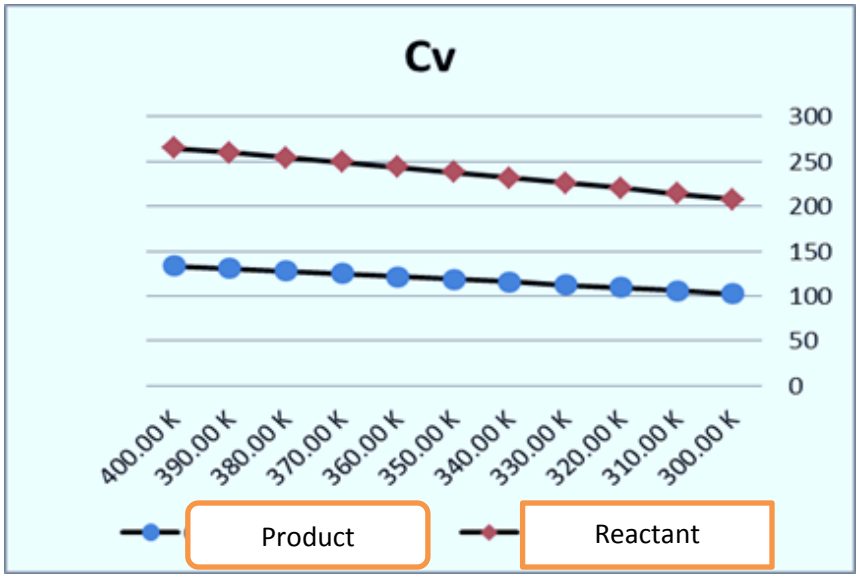

Fig. 4 shows the variation of the specific CV heat capacity in the heterocyclic product (ATTz) relative to the 3,6-D-amino-tetrazine starting material at various temperatures

The changes in the specific heat capacity of the CV in the ATC (ATC) relative to the 3,6-D-amino-tetrazine substance at different temperatures indicate that the product has a lower CV-specific capacity, that is, under the same conditions, by taking less heat than the substance The initial heating rate increases. Therefore, the material of the original product is much more energetic than the original material. Figure (4)

6 .Calculate and verify the values of Gibbs free energy changes ΔG

Using the Gaussian program 98, Gibbs free energy (G) (Δ) was calculated for raw materials and products in the synthesis process. To calculate and obtain Gibbs free energy variations G (Δ), in the reactions A + B → AB, the following equation is used.

$$\Delta G_{AB} = [G_{AB}] - [G_A + G_B]$$

Now with regard to the reaction

$$C2H4N6 + NaNO2 + NaN3 \rightarrow C2H2N8 + H2 + 1 / 2N2$$

The Gibbs free energy generated by calculating Gaussian software is as follows:

Relationship (5): $\Delta G_f = [G_{C2H2N8} + G_{H2} + 1/2G_{N2}] - [G_{C2H4N6} + G_{NaNO3} + G_{NaN3}]$

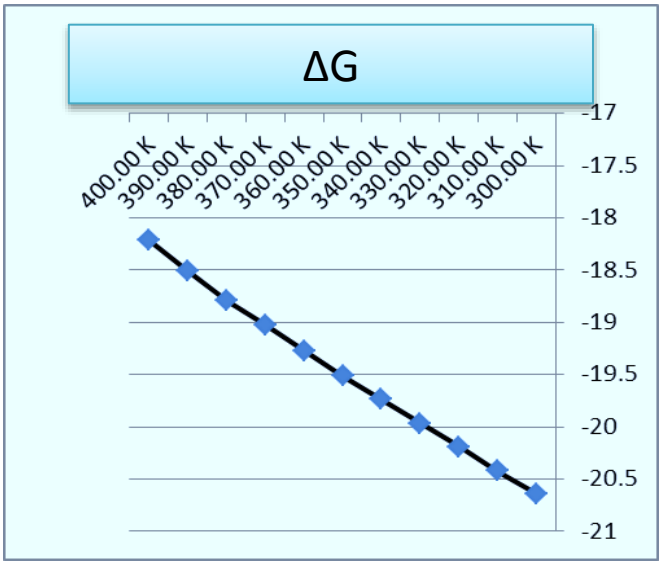

Fig. 5 shows a diagram of formation of ΔGf for heterozygous explosives (ATTz) from the reaction of 3,6-D-amino tetrazine with nitric acid and sodium azid at various temperatures

ΔGf values indicate that the ATC synthesis process of 3,6-D-amino-tetrazine reaction with nitric acid and sodium azide at different temperatures is self-sustaining and, with increasing temperature, Gibbs-free energy changes So the reaction is better done at higher temperatures. Fig. 5.

7. Discussion and Conclusion

The results of the calculations show that in the process of synthesis of heterocyclic explosives (ATTz) from the reaction of 3,6-dinamo-tetrazine with nitric acid and sodium azid at various temperatures, the heterocyclic explosive (ATTz) process of the 3,6-dino-amine reaction Tetrazine with nitric acid and sodium azide at different temperatures and with increasing temperature reaction conditions, the amount of enthalpy changes is negatively affected. At different temperatures, negative entropy is observed. As the temperature rises, the degree of irregularity decreases. CV capacity variations of the product have capacitance values The special heat of a CV is less, that is, under the same conditions, by getting fewer heat than the primary substance of the test increase. Therefore, the material of the original product is much more energetic than the original material. The values of ΔGf also indicate that this process can be carried out at different temperatures by itself and by increasing the temperature, the Gibbs free energy changes become more positive, so the reaction at lower temperatures is better.

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