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Original Research Article

A DFT Investigation on The Reaction of tetrazolo [1,5-b][1,2,4]triazine with 1,5-diaminotetrazole and glyoxal in Different Temperatures

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ABSTRACT

In this article, synthesis of the explosive synthesis of tetrazolo [1,5-b][1,2,4]triazine from the reaction of 1,5-diaminotetrazole with glyoxal in different conditions of temperature, with density functional theory method were studied. For this purpose, at first the material contained in the both sides of reaction were geometrically optimized, then the calculation of the thermodynamic parameters performed on all of them. The amount of ΔH, ΔS and ΔG of this reaction at different temperatures in form of sum of parameters discrepancy in the products than reactants is obtained. And finally, the best temperature for the synthesis of explosive according to the obtained thermodynamic parameters were evaluated.

Keywords: tetrazolo [1,5-b][1,2,4]triazine , Density Functional Theory; 1; 5-diaminotetrazole; glyoxal; Thermodynamic parameters

Introduction

In recent years, new energetic materials considered and due to the special properties, have many applications in the military field. Currently many researchers around the world with high density based on energetic materials such as Tetrazole doing research, this energetic materials in the production of pyrotechnics with less smoke, gas generators and engines are widely used and also less sensitive to heat and shock of their show. Another benefit of this combination compared to conventional energetic substances, they are green [1-20]. Because these reactions were less environmental hazard and let it show better performance. Energetic materials commonly used fossil that often have high carbon content. During the process of burning large amounts of carbon dioxide (CO_2), carbon monoxide (CO) and unburned carbon particles such as soot produce and environmental pollutants and pollution and create a lot of problems. Nitrogen-rich compounds widely used in propulsion systems, fire extinguishing systems and airbag systems as well as fuel for missiles and military systems. In this study, the synthesis of tetrazolo [1,5-b][1,2,4]triazine from the reaction of 1,5-diaminotetrazole with glyoxal is studied under different conditions of temperature, density functional theory method. Some chemical properties calculated in the level of B3lyp / 6-31g for tetrazolo [1,5-b][1,2,4]triazine($C_3H_2N_6$) and 1,5-diaminotetrazole (CH_4N_6) is shown Table 1 [21-39].

Table1. Some chemical properties calculated in B3lyp / 6-31g to Material tetrazolo [1,5-b] [1,2,4]triazine($C_3H_2N_6$) and 1,5-diaminotetrazole (CH_4N_6)

	Temperature=298.15K , pressure=1 atm	
	The main raw material	The main product
	CH_4N_6	$C_3H_2N_6$
Energy()	-364.696118 au	-438.785083 au
Solvation Energy()	-76.24 kJ/mol	-83.65 kJ/mol
E HOMO()	-9.80eV	-11.10 eV
E LUMO()	4.39 eV	-0.59 ev
Dipole Moment	6.59 debye	7.14 debye
weight	100.085 amu	122.091 amu
volume	80.65 A^3	98.45 A^3
Area	110.03 A^2	118.82 A^2
Polarizability	44.59	46.61
ZPE	225.23 KJ/mol	194.68 KJ/mol
H°	-364.603783 au	-438.704933 au
CV	87.88 J/mol	80.88 J/mol
S°	315.69 J/mol	313.90 J/mol
G°	-364.639632 au	-438.740579 au

Calculations and Results

Reviews the calculation of the synthesis of tetrazolo [1,5-b][1,2,4]triazine from the reaction of 1,5-diaminotetrazole with glyoxal under different conditions of temperature, studied by density functional theory, the operation was performed using the software Gaussian 98 and Gaussian view. First, compounds were optimized in a series of basic using density functional theory (6-31g) and then IR studies are done in order to calculate thermodynamic parameters of the process. All calculations are done in the level B3lyp / 6-31g at 300 to 400 degrees Kelvin, and the atmospheric pressure, the Studied reaction is:

$$CH_4N_6+C_2H_2O_2 \rightarrow C_3H_2N_6+2\ H_2O$$

Calculate and verify the values of changes in enthalpy (ΔH):

By using Gaussian 98 program were calculated enthalpy values for raw materials and products in process synthesis. For calculating and obtain the change in enthalpy in the reaction $A + B \rightarrow AB$ from the following formula is used:

Equation 1: $\Delta H = H_{product} - H_{reactant}$

With regards to reaction $CH_4N_6+C_2H_2O_2 \rightarrow C_3H_2N_6+2H_2O$, Enthalpy values obtained through calculation software Gaussian, is as follows:

Equation 2: $\Delta H_f = [H_{C3H2N6}+2H_{H2O}] - [H_{CH4N6} + H_{C2H2O2}]$

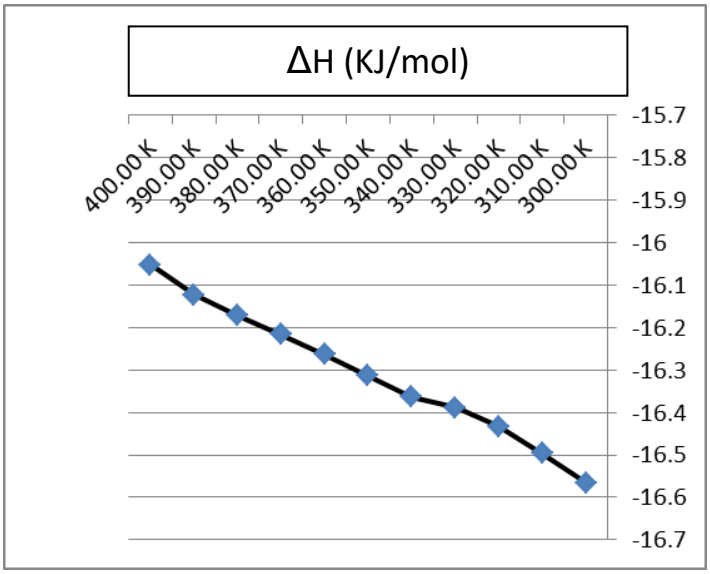

Figure1. Diagram of the enthalpy changes for the synthesis material material tetrazolo [1,5-b] [1,2,4]triazine from the reaction of 1,5-diaminotetrazole at different temperatures.

Values of ΔH_f are indicating that in synthesis of tetrazolo [1,5-b][1,2,4]triazine from the reaction of 1,5-diaminotetrazole with glyoxal under different conditions of temperature, Terms of exothermic and the reaction temperature by increasing the amount of heat released is less (Figure 1).

Calculate and assess the values of change in entropy (ΔS)

By using Gaussian 98 program were calculated entropy values for reactants and products in process synthesis. For calculating and obtain the change in entropy in the reaction A + B → AB from the following formula is used:

Equation 3: $\Delta S_{AB} = [S_{AB}] - [S_A + S_B]$

With regards to reaction $CH_4N_6+C_2H_2O_2 \rightarrow C_3H_2N_6+2H_2O$, Entropy values obtained through calculation software Gaussian, is as follows:

Equation 4: $\Delta S_f = [S_{C3H2N6}+2S_{H2O}] - [S_{CH4N6} + S_{C2H2O2}]$

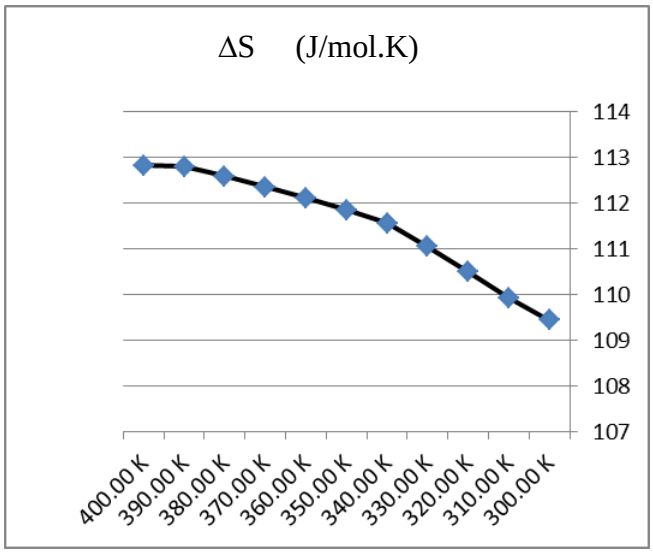

Figure 2. Diagram of the entropy changes for the synthesis material material **tetrazolo [1,5- b] [1,2,4]triazine from the reaction of 1,5-diaminotetrazole** at different temperatures.

Values of ΔS_f are indicating that in synthesis of **tetrazolo [1,5-b][1,2,4]triazine from the reaction of 1,5-diaminotetrazole with glyoxal** at different temperatures. Positive entropy is increased with increasing temperature irregularities in Figure 2 .

Calculate and verify specific heat capacity (CV)

By using Gaussian 98 program were calculated the specific heat capacity CV values for reactants and products in process synthesis.

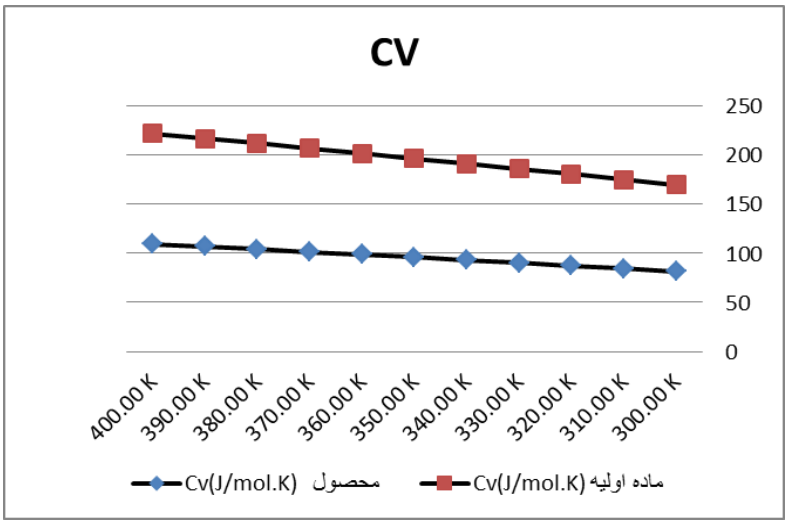

Figure 3. Diagram of the Specific heat capacity change (C_V) for the synthesis reaction of material tetrazolo [1,5-b][1,2,4]triazine from the reaction of 1,5-diaminotetrazole at different temperatures.

Values of the specific heat capacity CV in product material **tetrazolo [1,5-b][1,2,4]triazine** And raw material **1,5-diaminotetrazole** at different temperatures indicates that the product have specific heat capacity CV values, less than the reactant in the same conditions (Figure 3).

Calculate and verify the values of Gibbs free energy (ΔG)

By using Gaussian 98 program were calculated the values of Gibbs free energy (ΔG) for reactants and products in process synthesis. For calculating and obtain the change in values of Gibbs free energy (ΔG) in the reaction A + B → AB from the following formula is used:

Equation 4: $\Delta G_{AB} = [G_{AB}] - [G_A + G_B]$

With regards to reaction $CH_4N_6+C_2H_2O_2 \rightarrow C_3H_2N_6+2\ H_2O$, The values of Gibbs free energy obtained through calculation software Gaussian, is as follows:

Equation 5: $\Delta G_f = [G_{C3H2N6}+2G_{H2O}] - [G_{CH4N6} + G_{C2H2O2}]$

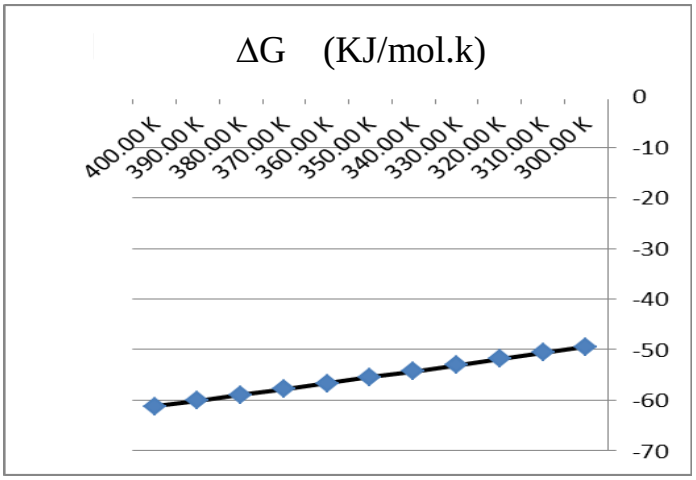

Figure 4. Diagram of Gibbs free energy changes (ΔGf) for the synthesis reaction of material tetrazolo [1,5-b][1,2,4]triazine from the reaction of 1,5-diaminotetrazole at different temperatures.

Values of ΔG_f indicates that the synthesis of of tetrazolo [1,5-b][1,2,4]triazine from the reaction of 1,5-diaminotetrazole with glyoxal under different conditions of temperature are positive, so the reaction be spontaneous and with increasing temperature, the Gibbs free energy changes are more negative, so the reaction is best done at higher temperatures (Figure 3).

Discussion and conclusion

Results of the calculation for synthesis of tetrazolo [1,5-b][1,2,4]triazine from the reaction of 1,5-diaminotetrazole with glyoxal under different conditions of temperature, is shown that ΔH_f Negative at all temperatures, which suggests that this process is exothermic and the heat released by increasing the reaction temperature becomes lower The positive entropy and entropy rate increased with increasing temperature In other words, the The irregularities has increased . Changes in specific heat capacity CV The product tetrazolo [1,5-b][1,2,4]triazine from the reaction of 1,5-diaminotetrazole with glyoxa At different temperatures indicates that the product has specific heat capacity CV values less This means that the same conditions, taking less heat than raw material increases its temperature That's more energetic This suggests that the material is the product of the raw material ΔGf values also show that , This process is done spontaneously

at different temperatures And the temperature rise becomes more negative Gibbs free energy changes So the reaction at higher temperatures , done better shape (3) .

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