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Determination of Amino-1,2,3,4-tetrazole (PAT) from the reaction of Article 5 - Amino-1,2,3,4-tetrazole with Chloride Pyr-Chloride

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Abstract

In this research, the synthesis of Article 5 -Pacrylamino-1,2,3,4-tetrazole (PAT) from the reaction of the 5-amino-1,2,3,4-tetrazole with chloride picral in various temperature conditions was studied by the method of density functional theory it placed. 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 H, ΔG, ΔSΔ of this reaction are 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

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Keywords: 5 - Amino-1,2,3,4-tetrazole (PAT), Synthesis, 5-Amino-1,2,3,4-tetrazole, Chloride Pyridine.

1. Introduction

Many researchers around the world are researching and testing on high-energy, high-tech materials based on tetrazole. These high-energy materials are widely used in the production of pyrotechnic materials with diameters, gas generators and propellants, and are less sensitive to heat and shock than others. And are widely used in the military field. The tetrazoles are ring and aromatic compounds, which include four nitrogen atoms and one carbon. These compounds are widely used in various industries, including military industries. These compounds release large amounts of N2 gas after combustion, and therefore have little pollution to the environment and are considered to be a green explosive. By introducing tetrazoles into the structure of polymeric chains, the energy properties of polymers can be increased. So far, various methods have been reported for the synthesis of polytetrazoles, most of them tetrazoles are hanging and attached to the main chain. In the case of the use of functionalized tetrazole rings as monomers, the rings can be inserted into the main polymer structure of the chain. The environmental hazards of these compounds are lower compared to high-energy fossil materials that are commonly used and have high carbon content, which during the burning process generate large amounts of carbon dioxide carbon dioxide and carbon-free carbon particles such as soot, which in the environment pollution And they cause a lot of problems. Nitrogen-rich compounds in propulsion systems, fire extinguishing systems and air bag systems, as well as missile and military fuel systems. In this research, the synthesis of Article 5-Pyrrolamino-1,2,3,4-tetrazole (PAT) from the reaction of the 5-amino-1,2,3,4-tetrazole with chloride picrilic acid under different temperature conditions was studied using the functional density theory method [1-5].

Table 1). Some chemical properties calculated at B3lyp / 6-31g levels for 5-picyril amino-1,2,3,4-tetrazole (PAT) and 1 and 5 diaminoto-tetrazole (CH4N6).

mperature=298.15K, pressure=1 atm		
	REACTANT	PRODUCT
	$C_6H_2ClN_3O_6$	$C_7H_4N_8O_6$
ENERGY	-1293.06017 au	-1145.11262 au
ENERGY(aq)	-1293.06073 au	-1145.12608 au
SOLVATION ENERGY	-1.48 kJ/mol	-35.33 kJ/mol
E HOMO	-11.88eV	-10.72 eV
E LUMO	-0.61 eV	-0.62 ev
Dipole Moment	0.29 debye	5.39 debye
weight	247.550 amu	296.159 amu
volume	175.80 A^3	215.73 A^3
Area	202.66 A^2	244.04 A^2
POLARIZABILITY	52.98	56.49
ZPE	268.96 KJ/mol	421.15 KJ/mol
H°	-1292.94620 au	-1144.93837 au
CV	185.70 J/mol	237.93J/mol
S°	431.43 J/mol	473.26 J/mol
G°	-1292.99519 au	-114499212 au

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 Amino-1,2,3,4-tetrazole (PAT) , 5 - Amino-1,2,3,4-tetrazole and Chloride Pyr-Chloride 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 [6-10].

3. Calculations and results

Computational Computation of Synthesis of Compound 5-Amino-1,2,3,4-tetrazole (PAT) from the reaction of Article 5 - Amino-1,2,3,4-tetrazole with Chloride Pyr-Chloride under different temperature conditions was studied by the method of density functional theory The operation was carried out using the Gaucin 98 and Gosvio software. The compounds were initially optimized by density functional theory method in the base series (6-31g). Then, IR studies were carried out to calculate the thermodynamic parameters related to the process. All calculations at B3lyp / 6-31g levels of 300 to 400 degrees Kelvin and one pressure The atmosphere has been investigated. The reaction **is:**

$$C_6H_2ClN_3O_6 + CN_5H_3 \rightarrow C_7H_4N_8O_6 + HCl$$

Calculating and analyzing 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. Relation (1)

$$\Delta H = H_{\text{پایانی}} - H_{\text{آغازی}}$$

Now with regard to the reaction

$$C_6H_2ClN_3O_6 + CN_5H_3 \rightarrow C_7H_4N_8O_6 + HCl$$

The form of enthalpy obtained by calculating Gaussian software is as follows

Relation (2)

$$\Delta H_f = [H_{C7H4N8O6} + H_{HCl}] - [H_{C6H2ClN3O6} + H_{CN5H3}]$$

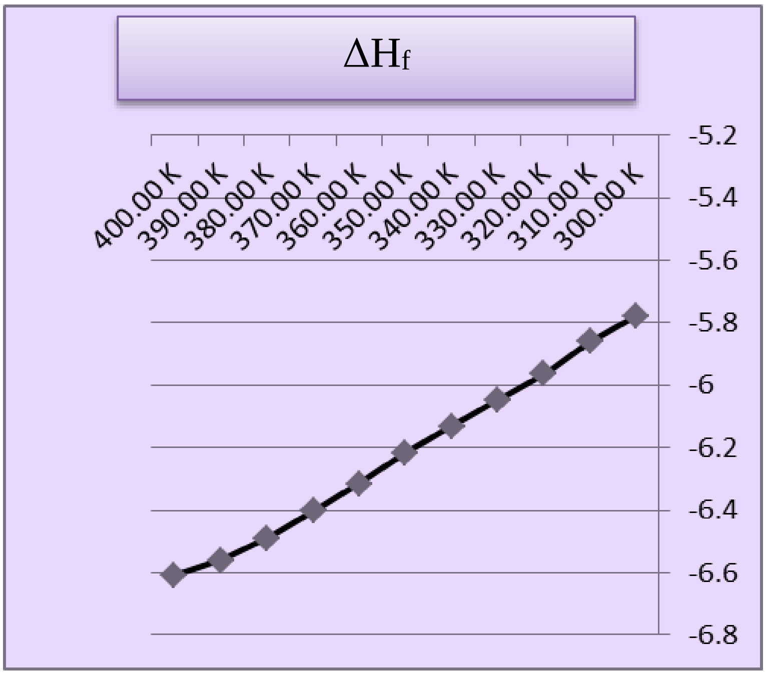

Figure (1) Annealing Modification Chart for Synthesis of Article 5-Amino-1,2,3,4-tetrazol (PAT) from the reaction of Substance 5 - Amino-1,2,3,4-tetrazole with Chloride Pyrriline at Different Temperatures

The amount of ΔHf shows that the process of synthesis of 5-picrolamino-1,2,3,4-tetrazole (PAT) from the reaction of substance 5 - amino-1,2,3,4-tetrazole with chloride picril at different temperatures of thermoplastic and with increasing The reaction temperature is greater than the released heat (Fig. 1.)

Calculate and check the values of entropy changes (ΔS)

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

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

Now with regard to the reaction

$$C_6H_2ClN_3O_6 + CN_5H_3 \rightarrow C_7H_4N_8O_6 + HCl$$

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

$$\Delta S_f = [S_{C7H4N8O6} + S_{HCl}] - [S_{C6H2ClN3O6} + S_{CN5H3}]$$

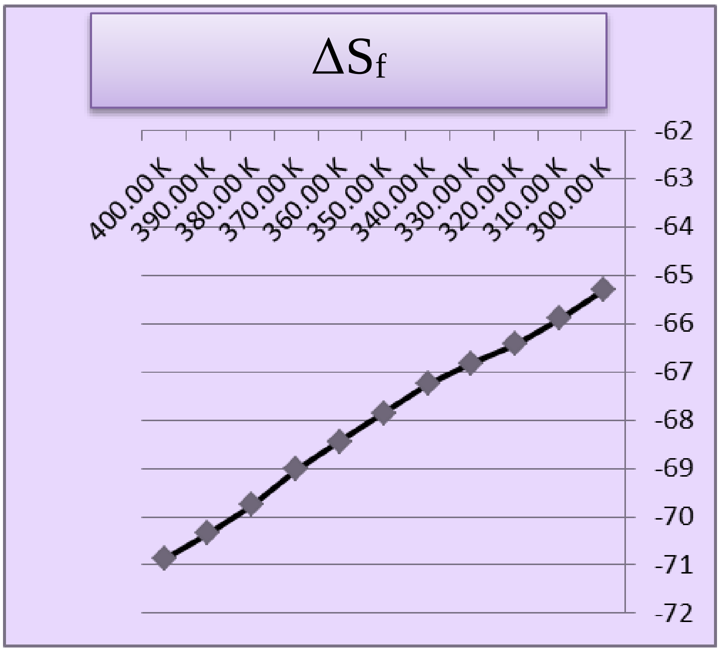

Fig. 2 shows the formation of entropy changes for synthesis of 2 and 6 (diamino) 3 and 5 di nitropyridine (C5H5N5O4) at various temperatures

The amount of ΔSf shows that the process of synthesis of matter-5-picyrylamino-1,2,3,4-tetrazole (PAT) from the reaction of substance 5 - amino-1,2,3,4-tetrazole with chloride picril has negative entropy at various temperatures. Which increases the temperature of the entropy. figure 2**.**

Calculating and checking the specific heat capacity of the CV:

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

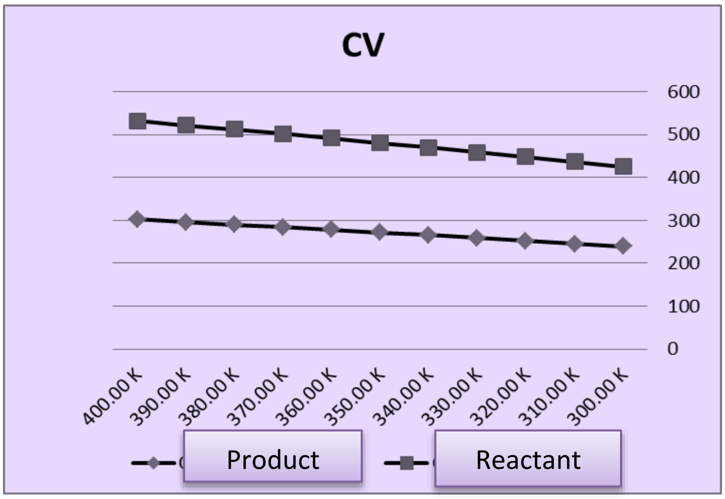

Fig 3. Specific CV Heat Capacity Chart Diagram in Article 2, Article 5 - Amino-1,2,3,4-tetrazol (PAT) and Primary Material 5-Amino-1,2,3,4-tetrazole at various temperatures

Specific changes in CV heat capacity in Article 5, Amino-1,2,3,4-tetrazol (PAT) and primary substance 5-amino-1,2,3,4-tetrazole, at different temperatures, indicate that the product has a capacity value The special heat of a CV is less, that is, under the same conditions, it will increase with less heat than the initial material of the heating (Fig. 3**)** [11-14].

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Calculating and checking the values of Gibbs free energy changes (Δ G)

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

$$C_6H_2ClN_3O_6 + CN_5H_3 \rightarrow C_7H_4N_8O_6 + HCl$$

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

$$\Delta G_f = [G_{C7H4N8O6} + G_{HCl}] - [G_{C6H2ClN3O6} + G_{CN5H3}]$$

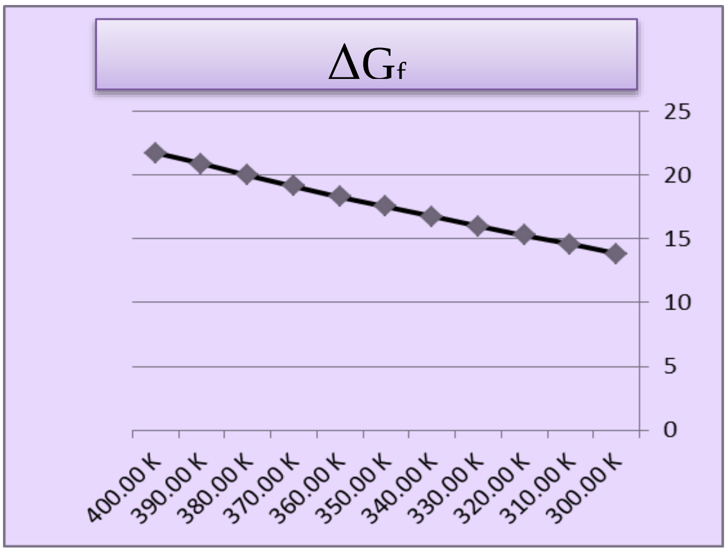

Fig. 3 shows a diagram of the formation of ΔGf for the synthesis of material. 5-Amino-1,2,3,4-tetrazole (PAT) from reaction of the substance 5 - amino-1,2,3,4-tetrazole with chloride picril at various temperatures

The values of ΔGf indicate that the synthesis process of Article 5 -Pacrilamino-1,2,3,4-tetrazole (PAT) from the reaction of Substance 5 - Amino-1,2,3,4-tetrazole with chloride picrilic acid at various temperatures was independently As the temperature increases, Gibbs free energy changes are more positive, so the reaction is better at lower temperatures. Fig. 3.

Discussion and Conclusion

The results of the calculations show that in the process of the synthesis of Article 5, the amino-1,2,3,4-tetrazole (PAT) of the reaction of the 5-amino-1,2,3,4-tetrazole with chloride picril at various temperatures, The enthalpy is a negative reaction that indicates that the process is thermosensitive, and with increasing reaction temperature the amount of released heat increases and the amount of antiseptic ΔSf is negative, which indicates that this process has decreased significantly and with increasing entropy temperature, the values Specific CV Heat Capacity Changes in Article 5-Amino-1,2,3,4-Tetrazole (PAT) and Primary Material 5-Amino-1,2,3,4-tetrazole at various temperatures indicate that the product has The values of the specific heat capacity of a particular CV are lower, that is, under the same conditions, it will increase with less heat than that of the primary material, which indicates the high energy content of the original product relative to the primary material, and finally, the quantities of ΔGf show that the synthesis process The desired effect is self-sustaining and with increasing process temperature, Gibbs free energy changes become more positive, so the reaction is better at lower temperatures.

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