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The thermodynamic parameters derived material [1,5-b] tetrazolo [1,2,4] Terry inflorescences (TTA) with boron nitride nano- cages in different conditions of temperature , density functional theory method.

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Abstract

In this study the reaction of the derivative , material [1,5-b] tetrazolo [1,2,4] Terry inflorescences (TTA) with boron nitride nano- cages in different conditions of temperature , density functional theory methods were studied . For this purpose, the material on both sides were geometrically optimized reaction , then the calculation of the thermodynamic parameters were performed on all of them . The values of ΔH, ΔG, ΔS the reaction at different temperatures for different products together, these parameters in the raw material is obtained . And finally, the best temperature for the synthesis of derivatives of explosives, according to the results of thermodynamic parameters were evaluated .

Keywords: Enthalpy of formation , TTA, boron nitride cage

1. Introduction

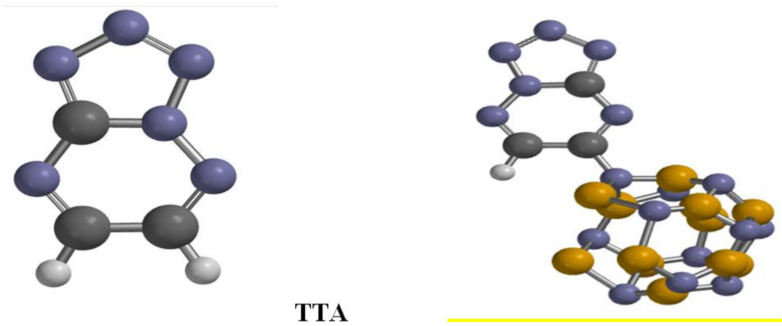
tetrazole cyclic and aromatic compounds , has four atoms of nitrogen and carbon . Which are used in military industries . These compounds are released by burning large amounts of gas N2 so little pollution to the environment and green are the explosives . Today, many scientists in the world investigating the energetic materials with high density tetrazole times , Environmental hazards these reactions are commonly used to lower fossil energy materials And has a high carbon content because during the process of burning fossil fuel carbon emissions of carbon dioxide , carbon monoxide and unburned carbon particles such as Produce a lot of soot pollution in the environment and create a lot of problems . The nitrogen-rich compounds are used in various industries . The nitrogen-rich compounds are used in various industries .

Table 1. Some chemical properties calculated in the B3lyp / 6-31g to material **[1,5-b]** tetrazolo **[1,2,4]** Terry inflorescences(**TTA)** and its derivatives with boron nitride cage

	Temperature=298.15K , pressure=1 atm	
	TTA	TTA-B12N12
ENERGY(au)	-435.171624	-1145.11262
E HOMO(eV)	-8.97	-4.42
E LUMO (eV)	3.39	1.02
Dipole Moment (debye)	5.97	3.01
Weight(amu)	122.091	404.892
Volume(A^3)	100.17	327.08
Area (A^2)	120.73	289.18
ZPE (KJ/mol)	204.48	540.31
H° (au)	-435.637672	-1318.70204
CV (J/mol)	80.58	312.28
S° (J/mol)	316.68	523.12
G° (au)	-435.673634	-1318.76145

2. calculations and results

Computational study material derived synthesis**[1,5-b]** tetrazolo **[1,2,4]** Terry inflorescences(TTA) with boron nitride nono-cages in different conditions of temperature, studied by density functional theory, the operation was performed using the software Gaussian 98 and Gaussian view And Spartan. 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:



TTA **TTA-B12N12**

Figure 1. optimized molecules material **[1,5-b]** tetrazolo **[1,2,4]** Terry inflorescences (TTA) and its derivative with boron nitride nono-cages

3.Calculation results

Computational Investigation of the reaction products of [1,5-b] tetrazolo [1,2,4] Terry inflorescences (TTA) with boron nitride nono-cages in different conditions of temperature, studied by density functional theory, the operation was performed using the software Gaussian 98 and Gaussian view And Spartan . 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:

$$TTA + B_{12}N_{12} \rightarrow TTA\ B_{12}N_{12}\ +1/2H_2 \quad (1)$$

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

calculated enthalpy values for raw materials and products in process synthesis. For calculating and obtain the change in enthalpy in the reaction A+B→C+D from the Equation 2 is used .

$$\Delta Hf = \Sigma H_{Products} - \Sigma H_{Reactants} \quad (2)$$

Given the following reactions

$$TTA + B_{12}N_{12} \rightarrow TTA\ B_{12}N_{12}\ +1/2H_2$$

Enthalpy of formation values obtained through calculation software Spartan , is as follows :

$$\Delta H_f = [H_{TTA\ B12N12} + 1/2H_{H2}] - [H_{TTA} + H_{B12N12}] \quad (3)$$

Table 2 . Enthalpy of formation calculated at the level B3lyp / 6-31g for derivative material [1,5-b] tetrazolo [1,2,4] Terry inflorescences (TTA) with boron nitride nono-cages

	Enthalpy(kJ/mol)
Temperature	TTA B12N12
300	38.3934
310	38.9438
320	39.43345
330	39.8884
340	40.28725
350	40.65725
360	40.9992
370	41.3137
380	41.5909
390	41.82095
400	42.02545

Enthalpy of formation calculated at the level B3lyp / 6-31g for derivatives material [1,5-b] tetrazolo [1,2,4] Terry inflorescences (TTA) with boron nitride nono-cages , Always Positive in all temperature range 300 to 400 degrees Kelvin .

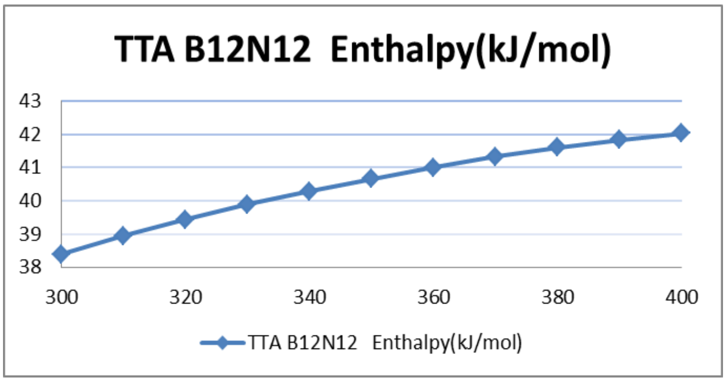


Figure 2. diagram the enthalpy changes for the synthesis of derivatives material [1,5-b] tetrazolo [1,2,4] Terry inflorescences (TTA) with boron nitride nono-cages at different temperatures.

The positive ΔHf the show, Derived synthesis process material **[1,5-b]** tetrazolo **[1,2,4]** Terry inflorescences (TTA) with boron nitride nano- cage insertion at temperatures ranging from 300 to 400 Kelvin ، And by increasing the amount of heat released endothermic reaction temperature becomes lower. figure 2).

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

The results of the calculations show that the entropy values for raw materials and goods in process synthesis were calculated . To calculate and obtain the entropy changes in reaction A+B→C+D the following equation is used .

$$\Delta S_f = \Sigma S_{Products} - \Sigma S_{Reactants} \qquad (4)$$

Given the two reactions

$$TTA + B_{12}N_{12} \rightarrow TTA\ B_{12}N_{12} + 1/2H_2$$

The entropy values obtained through calculation software Gaussian , generally the following:

$$\Delta S_f = [S_{TTA\ B12N12} + 1/2S_{H2}] - [S_{TTA} + S_{B12N12}] \qquad (5)$$

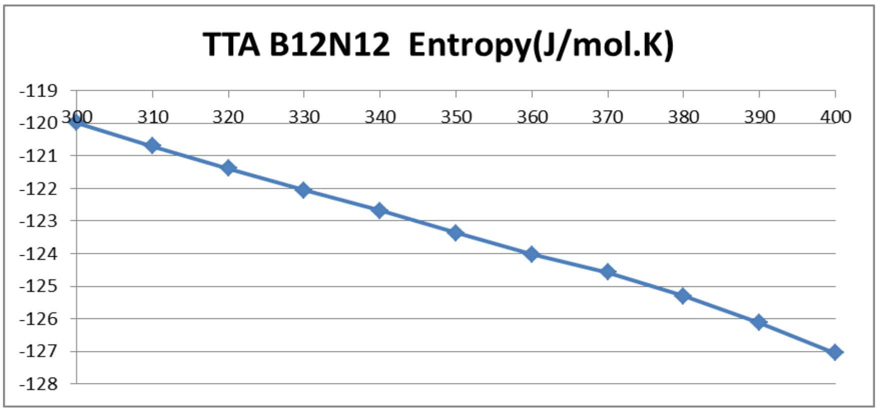


Figure 3. Diagram of the entropy changes for the synthesis of derivatives material [1,5-b] tetrazolo [1,2,4] Terry inflorescences (TTA) with boron nitride nono -cages at different temperatures.

ΔSf positive value indicates that the process of synthesis derived material [1,5-b] tetrazolo [1,2,4] Terry inflorescences (TTA) with boron nitride nono -cages at different temperatures have a negative entropy . Figure 3 .

6.Calculate and verify specific heat capacity (CV)

The results of the calculations show , specific heat capacity CV values for raw materials and goods in process synthesis were calculated showed the following procedure .

$$B_{12}N_{12}\ TTA > TTA \qquad (6)$$

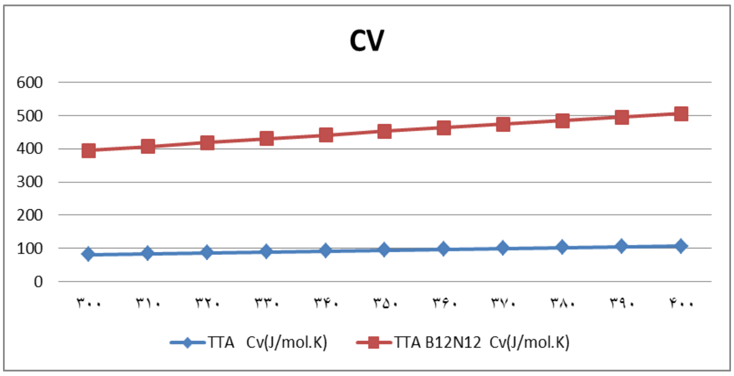


Figure 4. Diagram changes in specific heat capacity CV raw material [1,5-b] tetrazolo [1,2,4] Terry inflorescences (TTA), and its derivatives with boron nitride nono -cages at different temperatures.

Table 3. Specific heat capacity calculated at the level B3lyp / 6-31g for raw material [1,5-b] tetrazolo [1,2,4] Terry inflorescences (TTA), and its derivatives with boron nitride nono -cages at different temperatures.

	Cv(J/mol.K)	
Temperature	TTA	TTA B12N12
300	81.081	313.9806
310	83.7797	323.0873
320	86.4696	332.0586
330	89.1469	340.892
340	91.8081	349.5856
350	94.4501	358.1378
360	97.0699	366.5477
370	99.6648	374.8142
380	102.2322	382.937
390	104.77	390.9157
400	107.276	398.7502

Values of specific heat capacity change , CV raw material [1,5-b] tetrazolo [1,2,4] Terry inflorescences (TTA), and its derivatives with boron nitride nono -cages at different temperatures indicates that the product has specific heat capacity CV values higher, in the same conditions by taking more heat than the raw material increases its temperature . Figure (4) .

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

The results of the calculations show 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→C+D from the following formula is used:

$$\Delta G_f = \Sigma G_{Products} - \Sigma G_{Reactants} \quad (7)$$

Given the reaction

$$TTA + B_{12}N_{12} \rightarrow TTA\ B_{12}N_{12} + 1/2H_2$$

The values of Gibbs free energy obtained through calculation software Gaussian, is as follows:

$$\Delta G_f = [G_{TTA\ B12N12} + 1/2G_{H2}] - [G_{TTA} + G_{B12N12}] \quad (8)$$

Table 4 . Gibbs free energy of formation calculated at the level B3lyp / 6-31g for raw material [1,5-b] tetrazolo [1,2,4] Terry inflorescences (TTA), and its derivatives with boron nitride nono -cages at different temperatures.

	G(kJ/mol)
Temperature	TTA B12N12
300	30.2786
310	31.9207
320	33.52075
330	35.1083
340	36.64855
350	38.20955
360	39.75735
370	41.26555
380	42.8228
390	44.3881
400	46.0004

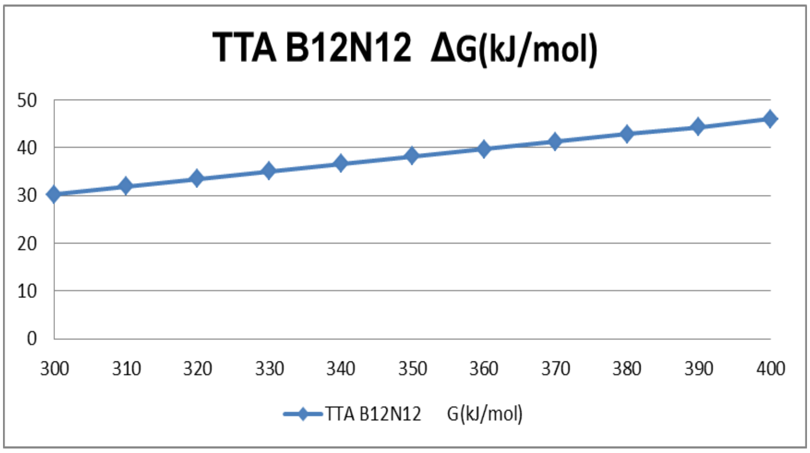


Figure 5. Diagram of the ΔG_f changes for the synthesis of derivatives material [1,5-b] tetrazolo [1,2,4] Terry inflorescences (TTA) with boron nitride nono -cages at different temperatures.

ΔGf negative values indicate that the process of synthesis derived material **[1,5-b]** tetrazolo **[1,2,4]** Terry inflorescences (TTA) With boron nitride nano- cages at different temperatures , it can not be done spontaneously and with increasing temperature , Gibbs free energy so more positive reaction than is done at higher temperatures (Figure 5) .

8. Discussion and conclusion

The results of the calculations show that in the process of synthesis of derivatives of **[1,5-b]** tetrazolo **[1,2,4]** Terry inflorescences (TTA) with boron nitride nono -cages at different temperatures , the amount of ΔHf negative at all temperatures, the amount of ΔHf positive at all temperatures, indicating that this process is endothermic And with increasing temperature the amount of heat released is less , the materials are thermodynamically more positive heat of formation , Unstable and thus are more active nitrogen-containing energetic materials , Metastable molecules with high activity is obvious that the heat of formation is positive for these substances in the environment and sustainable divided into smaller molecules And high energy are produced . Sometimes tensile energy release pressure release energy circles The process of formation of explosive energy and negative entropy and entropy rate decreased with increasing temperature . Changes in specific heat capacity CV shows specific heat capacity of raw material **[1,5-b]** tetrazolo **[1,2,4]** Terry inflorescences (TTA) to its derivatives with boron nitride cage There are at different temperatures lower doses This means less heat than the products on the same terms by taking its temperature increases. CV lower specific heat of the material TTA represents more energetic than it is derived The values also indicate changes in Gibbs free energy ΔGf That the process is calculated at various temperatures 300 to 400 degrees Kelvin , are not spontaneous Gibbs free energy of more positive with increasing temperature so the reaction at higher temperatures , less done.

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