



The Energetic, Check of Derived Boron Nitride Nano-cage with (HMX) in Different Conditions of Temperature by Density Functional Theory Method

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Abstract

In this study the synthesis of the derivative of boron nitride nano-cages with energetic material (HMX) 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 was 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: Explosives , HMX, Boron nitride cage, Thermodynamic parameters and Density functional theory

1. Introduction

HMX (Octogen) is an acronym for High Melting explosive. It is also known as octogen and cyclotetramethylene-tetranitramine, as well as by other names. It is a colorless solid that dissolves slightly in water. Only a small amount of HMX (Octogen) will evaporate into the air; however, it can occur in air attached to suspended particles or dust. The taste and smell of HMX (Octogen) are not known [1-5]. HMX (Octogen) does not occur naturally in the environment. It is made from other chemicals known as hexamine, ammonium nitrate, nitric acid, and acetic acid. HMX (Octogen) explodes violently at high temperatures. Because of this property, HMX (Octogen) is used in various kinds of explosives, rocket fuels, and burster chargers [6-11]. A small amount of HMX (Octogen) is also formed in making cyclotrimethylene-trinitramine (RDX), another explosive similar in structure to HMX (Octogen) [12-15].

Table 1. Some chemical properties calculated in the B3lyp / 6-31g to material cyclotetramethylene-tetranitramine inflorescences (HMX) and its derivatives with boron nitride cage

	Temperature=298.15K , pressure=1 atm		
	HMX	B-B ₁₂ N ₁₂ HMX	N-B ₁₂ N ₁₂ HMX
	C ₄ H ₈ N ₈ O ₈	C ₄ H ₈ B ₁₂ N ₁₄ O ₈	C ₄ H ₈ B ₁₂ N ₁₄ O ₈
ENERGY(au)	-1174.25745	-2057.39529	-2057.65141
E HOMO(eV)	-8.61	-7.11	-11.51
E LUMO (eV)	4.87	-0.52	-1.60
Dipole Moment (debye)	3.46	12.47	4.13
Weight(amu)	296.156	578.957	578.957
Volume(A ³)	212.85	439.23	439.53
Area (A ²)	247.60	417.03	399.71
ZPE (KJ/mol)	569.59	901.38	897.72
H° (au)	-1174.02492	-2057.02529	-2057.2823
CV (J/mol)	258.53	496.55	502.04
S° (J/mol)	503.47	692.90	703.99
G° (au)	-1174.08209	-2057.10398	-2057.36225

2. calculations and results

Computational study material derived synthesis cyclotetramethylene-tetranitramine inflorescences (HMX) with boron nitride nano-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 [16-20]. All calculations are done in the level B3lyp / 6-31g at 300 to 400 degrees Kelvin, and the atmospheric pressure, the Studied reaction is:

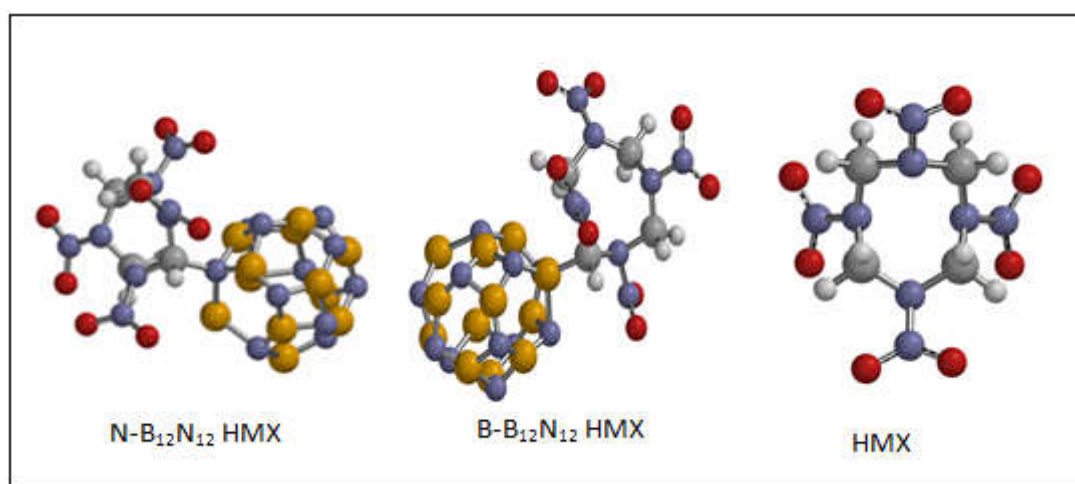


Figure 1. optimized molecules material cyclotetramethylene-tetranitramine inflorescences (HMX) and its derivative with boron nitride nano-cages

3. Calculation results

Computational Investigation of the reaction products of cyclotetramethylene-tetranitramine inflorescences (HMX) 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:

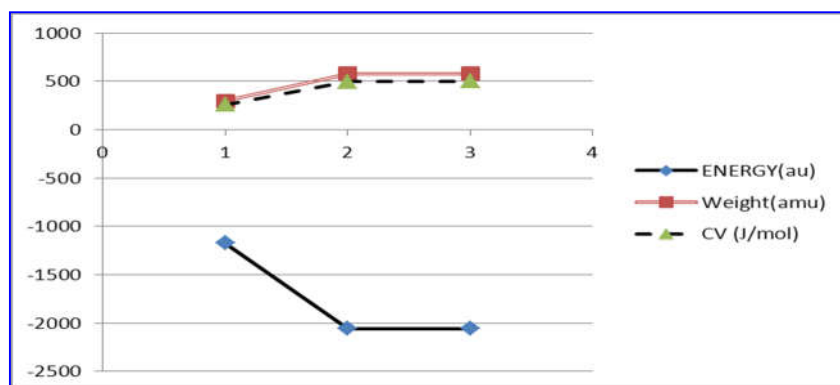
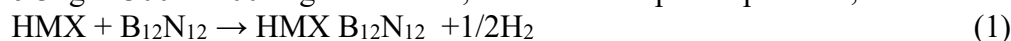


Figure 2. diagram the comparing the molecular mass, internal energy and specific heat capacity of explosives cyclotetramethylene-tetranitramine inflorescences (HMX) with boron nitride nono-cages In the case of boron nitride connection.

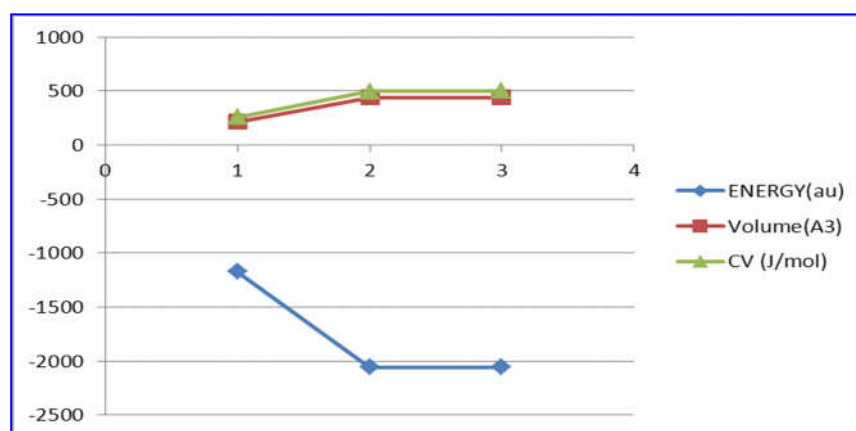


Figure 3. diagram the comparing the molecular Volume, internal energy and specific heat capacity of explosives cyclotetramethylene-tetranitramine inflorescences (HMX) with boron nitride nono-cages In the case of boron nitride connection.

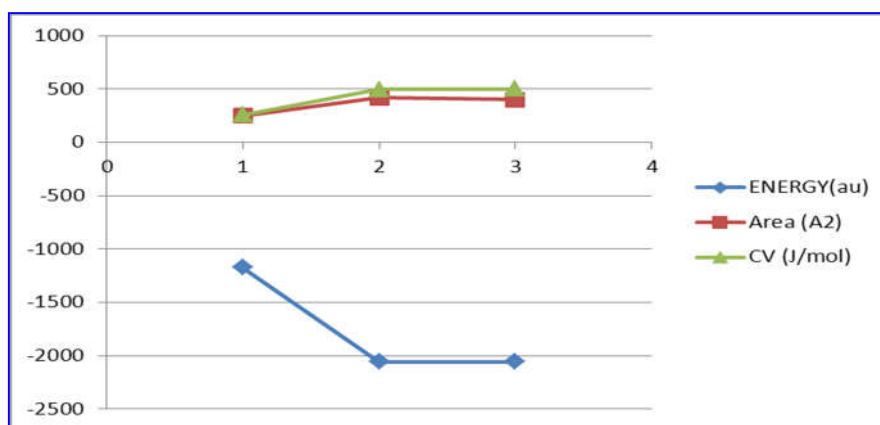


Figure 4. diagram the comparing the molecular area, internal energy and specific heat capacity of explosives cyclotetramethylene-tetranitramine inflorescences (HMX) with boron nitride nano-cages In the case of boron nitride connection.

As well as the results of calculations showed that by increasing the molecular weight of the material HMX derivatives in connection with its cage, boron nitride, boron and nitrogen specific heat capacity increases, And by increasing the molecular weight and the molar enthalpy and molar Gibbs free energy reduced form (5-6). Also check out the molar entropy showed that by increasing the molecular weight increases. Figure (7)

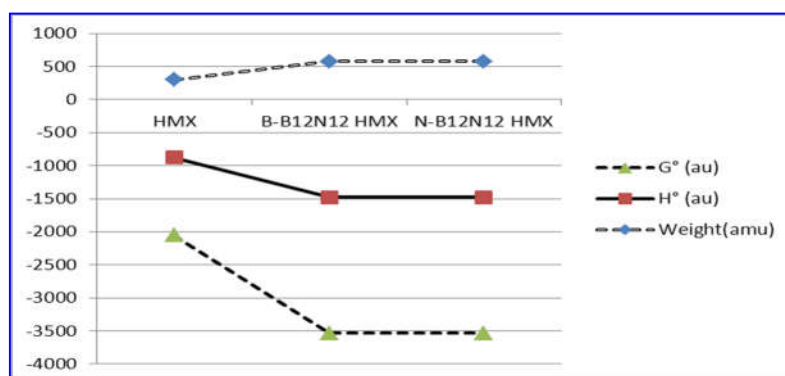


Figure 5. diagram the comparing the molar enthalpy and molar Gibbs free energy and molecular mass, of explosives cyclotetramethylene-tetranitramine inflorescences (HMX) with boron nitride nano-cages In the case of boron nitride connection.

4. 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 .



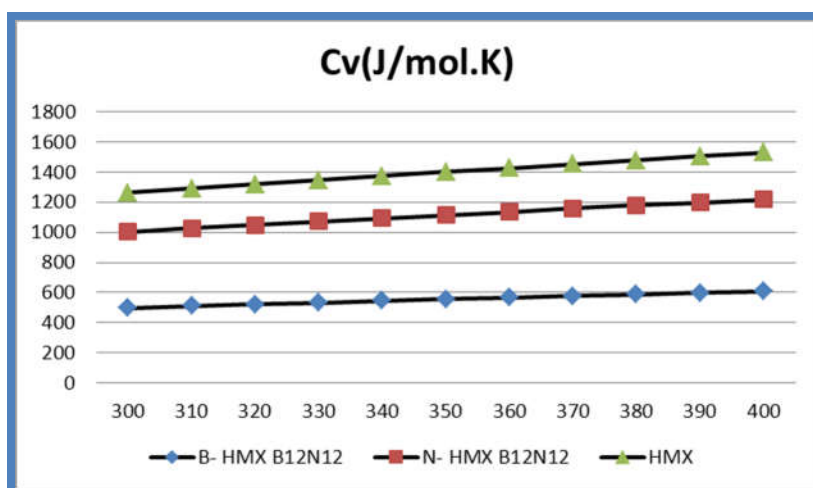


Figure 6. Diagram changes in specific heat capacity CV raw material of explosives cyclotetramethylene-tetranitramine inflorescences (HMX) , and its derivatives with boron nitride nano -cages at different temperatures.

Table 2. The changes in specific heat capacity CV raw material of explosives cyclotetramethylene-tetranitramine inflorescences (HMX) , and its derivatives with boron nitride nano -cages at different temperatures.

Temperature	Cv(J/mol.K)		
	B- HMX B12N12	N- HMX B12N12	HMX
300	498.7311	504.1339	259.4897
310	510.4359	515.3908	264.6706
320	521.9738	526.5073	269.8246
330	533.3466	537.485	274.9533
340	544.5559	548.3249	280.0574
350	555.6031	559.0276	285.1369
360	566.4893	569.5934	290.1911
370	577.2155	580.022	295.2188
380	587.7823	590.313	300.2182
390	598.1902	600.4658	305.1874
400	608.4395	610.4794	310.1241

The values of specific heat capacity change , CV raw material cyclotetramethylene-tetranitramine inflorescences (HMX) , and its derivatives with boron nitride nano -cages at different temperatures indicates that Nanostructures by adding to the explosive HMX specific heat capacity CV at different temperatures in all cases to increased raw material form .Figure (6) .

5. Discussion and conclusion.

The results of the calculations show that after addition different nanostructure with same carbon number to explosive material (HMX), specific heat capacity of its derivatives increases. The other hand various derivatives with respect to the amount of specific heat capacity at different temperatures show the following trends:

$$CV_{N-HMX B12N12} > CV_{B-HMX B12N12} > CV_{HMX} \quad (3)$$

Since the number of atoms in the nanostructure used in this study are considered identical, so the resulting molecular mass derivatives is equal, But according to the size and shape of each of the nano structures of molecules derived nanostructures are different, on the other hand nano-structural changes in the volume of derivatives molecules show the following trends:

$$V_{N-HMX B12N12} > V_{B-HMX B12N12} > V_{HMX} \quad (4)$$

And also compares the level of molecules, nano-structured derivatives show the following trends:

$$A_{B-HMX B12N12} > A_{N-HMX B12N12} > A_{HMX} \quad (5)$$

Compare the process of increasing the amount of specific heat capacity, volume and surface of molecules of different nanostructures with the same atom derivatives and show In the same condition in terms of molecular weight molecules increase the volume greater than the increase in the level of the increase in specific heat capacity molecule is effective. We know that Specific heat capacity (CV) The amount of heat that a mole of the material to a temperature increase of one degree, Obviously the more energetic of the value of specific heat capacity is lower CV. So is concluded derived from the boron compound bound energetic than those derived from the nitrogen attached so the increase is as follows:

$$E_{HMX N} > E_{B-HMX B12N12} > E_{N-HMX B12N12} \quad (6)$$

Compare the values of thermodynamic parameters examined in this study confirms these results.

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