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 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, HMX, boron nitride cage

1. Introduction

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HMX (Octogen) is an acronym for High Melting explosive. It is also known as octagon 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. 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. A small amount of HMX (Octogen) is also formed in making cyclotrimethylene-trinitramine (RDX), another explosive similar in structure to HMX (Octogen)\[1-5\].

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

<table>
<thead>
<tr>
<th></th>
<th>Temperature=298.15K , pressure=1 atm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>HMX</td>
</tr>
<tr>
<td>ENERGY(au)</td>
<td>-1174.25745</td>
</tr>
<tr>
<td>E HOMO(eV)</td>
<td>-8.61</td>
</tr>
<tr>
<td>E LUMO (eV)</td>
<td>4.87</td>
</tr>
<tr>
<td>Dipole Moment (debye)</td>
<td>3.46</td>
</tr>
<tr>
<td>Weight(amu)</td>
<td>296.156</td>
</tr>
<tr>
<td>Volume(A\textsuperscript{3})</td>
<td>212.85</td>
</tr>
<tr>
<td>Area (A\textsuperscript{2})</td>
<td>247.60</td>
</tr>
<tr>
<td>ZPE (KJ/mol)</td>
<td>569.59</td>
</tr>
<tr>
<td>H° (au)</td>
<td>-1174.02492</td>
</tr>
<tr>
<td>CV (J/mol)</td>
<td>258.53</td>
</tr>
<tr>
<td>S° (J/mol)</td>
<td>503.47</td>
</tr>
<tr>
<td>G° (au)</td>
<td>-1174.08209</td>
</tr>
</tbody>
</table>

2. calculations and results
Computational study material derived synthesis 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:
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):\[6-11]\):

\[
\text{HMX} + \text{B}_{12}\text{N}_{12} \rightarrow \text{HMX B}_{12}\text{N}_{12} + \frac{1}{2}\text{H}_2
\]

(1)
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 nono-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 nono-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.

\[ B_{12}N_{12} \text{ HMX} \rightarrow \text{HMX} \] (2)

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

<table>
<thead>
<tr>
<th>Temperature</th>
<th>B- HMX B12N12</th>
<th>N- HMX B12N12</th>
<th>HMX</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>498.7311</td>
<td>504.1339</td>
<td>259.4897</td>
</tr>
<tr>
<td>310</td>
<td>510.4359</td>
<td>515.3908</td>
<td>264.6706</td>
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<td>521.9738</td>
<td>526.5073</td>
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<td>533.3466</td>
<td>537.485</td>
<td>274.9533</td>
</tr>
<tr>
<td>340</td>
<td>544.5559</td>
<td>548.3249</td>
<td>280.0574</td>
</tr>
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<td>350</td>
<td>555.6031</td>
<td>559.0276</td>
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<td>360</td>
<td>566.4893</td>
<td>569.5934</td>
<td>290.1911</td>
</tr>
<tr>
<td>370</td>
<td>577.2155</td>
<td>580.022</td>
<td>295.2188</td>
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<tr>
<td>380</td>
<td>587.7823</td>
<td>590.313</td>
<td>300.2182</td>
</tr>
<tr>
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<td>598.1902</td>
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<td>305.1874</td>
</tr>
<tr>
<td>400</td>
<td>608.4395</td>
<td>610.4794</td>
<td>310.1241</td>
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</table>

The values of specific heat capacity change, CV raw material cyclotetramethylene-tetranitramine inflorescences (HMX), and its derivatives with boron nitride nono-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)[12-16].

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:

\[
CV_{N-HMXB12N12} > CV_{B-HMXB12N12} > CV_{HMX} \tag{3}
\]

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:

\[
V_{N-HMXB12N12} > V_{B-HMXB12N12} > V_{HMX} \tag{4}
\]

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

\[
A_{B-HMXB12N12} > A_{N-HMXB12N12} > A_{HMX} \tag{5}
\]

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:

\[
E_{HMXN} > E_{B-HMXB12N12} > E_{N-HMXB12N12} \tag{6}
\]

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

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Reference


8. www. Plasticizer information center, info@plasticisers.org.


