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Computational Investigation of the Efference of Different Fullerenes on Aktogen High Energy

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Abstract

In this research, HMX energy derivatives with different carbon-containing fullerenes in different temperature conditions were studied using density functional theory. For this purpose, the materials were first geometric optimized, then the thermodynamic parameters were calculated for all of them. Then, the process of changing the energy-dependent parameters such as specific heat capacity, enthalpy, entropy and Gibbs free energy relative to molecular mass, molecular volume and measured level in this study at a given temperature, were evaluated against each other.

Keywords: Aktogen, High energy energy derivatives, HMX

1. Introduction

The HMX explosive, also known as octogeny, has been considered in recent years because of its special properties and applications in the military field. Many researchers around the world are currently studying high-energy high-energy materials, these high-energy materials used in the manufacture of cogeneration products, and gas generators used in propulsion engines, tend to be less sensitive to heat and shock. The other advantages of these compounds are the greenness of the high-energy fossil materials and their environment. Because high-energy fossil materials have high carbon content, which during the burning

process generate large quantities of carbon dioxide (CO2), carbon monoxide (CO) and carbon-free carbon particles such as carbon black, which are pollutants of the environment and pollution and many problems To create. Nitrogenous high-energy compounds are used extensively in propulsion systems, fire extinguishing systems, airbags for cars and fuel, missiles, and military systems. In this research, HMX energy derivatives with different carbon-containing fullerenes in different temperature conditions have been studied using the method of density functional theory [1-10].

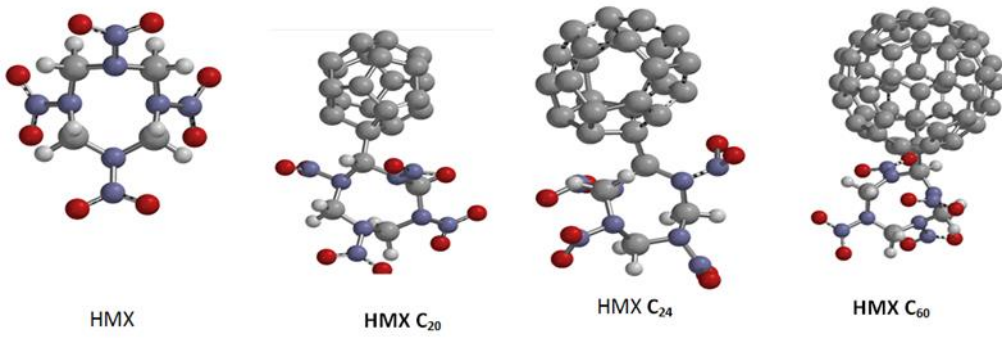

Fig 1. View of Aktogen (HMX) and HMX C_{20} ،HMX C_{24} ،HMX C_{60}

Table 1. Some chemical properties calculated at B3lyp / 6-31g levels for HMX, HMX C20, HMX C24, HMX C60

	Temperature=298.15K , pressure=1 atm			
	HMX	HMX C_{20}	HMX C_{24}	HMX C_{60}
	$C_4H_8N_8O_8$	$C_{24}H_7N_8O_8$	$C_{28}H_7N_8O_8$	$C_{64}H_7N_8O_8$
ENERGY(au)	-1174.25745	-1920.74541	-2070.00333	-3417.62616
E HOMO(eV)	-8.61	-10.50	-9.42	-9.10
E LUMO (eV)	4.87	-4.10	-3.73	-2.96
Dipole Moment (debye)	3.46	17.46	17.26	8.96
Weight(amu)	296.156	535.368	583.412	1015.808
Volume(A^3)	212.85	417.97	458.98	798.44
Area (A^2)	247.60	393.63	412.22	622.59
ZPE (KJ/mol)	569.59	885.65	919.34	1655.37
H° (au)	-1174.02492	-1920.38679	-2069.62976	-3416.96377
CV (J/mol)	258.53	403.26	454.61	676.74
S° (J/mol)	503.47	606.58	637.54	758.52
G° (au)	-1174.08209	-1920.45567	-2069.70216	-3417.04991

2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [11-13]. 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 Aktogen on Fullerene were designed primarily using of Gauss View 5.0.8 and nanotube modeler 1.3.0.3 soft wares. The interaction effects of Aktogen on Fullerene were investigated

through attachment to three different base positions. All these calculations are done under the assumption of standard state of gas phase, pressure of 1 atmosphere, and temperature of 25 degrees centigrade. The calculations are performed, using a Pentium 4 PC with a Windows 7 OS and a Core i5 processor.

3. Calculations and results

The computational study of high-energy HMX derivatives with different carbon-containing fullerenes was studied using functional density theory. This operation was performed using Gaussian 98 and Gossive 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 done. The results of the calculations showed that with increasing molecular mass, molecular volume and molecular surface of HMX material to explosive derivatives with different nanostructures, carbon has the same specific heat capacity, and, of course, internal energy also decreases. Fig. 2- 4.

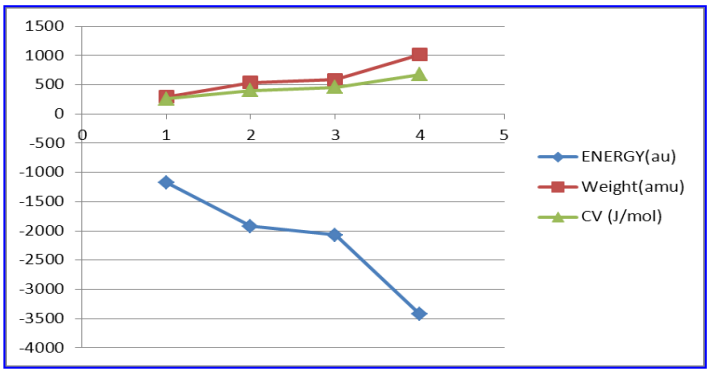

Fig 2. The comparison of the molecular mass, internal energy and specific heat capacity of the HMX explosive and its derivatives with different carbon-containing fullerenes

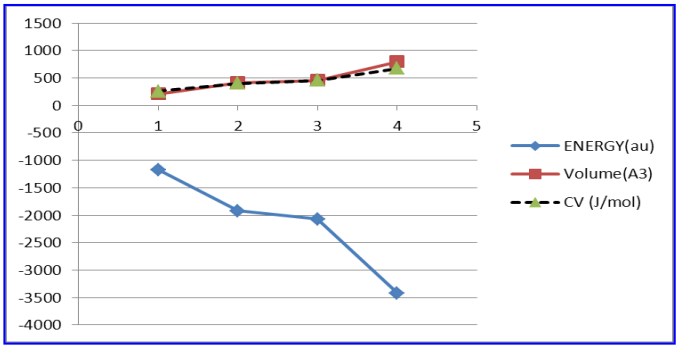

Fig 3 Comparison of the molecular volume, internal energy and specific heat capacity of the HMX explosive and its derivatives with different carbon-containing fullerenes

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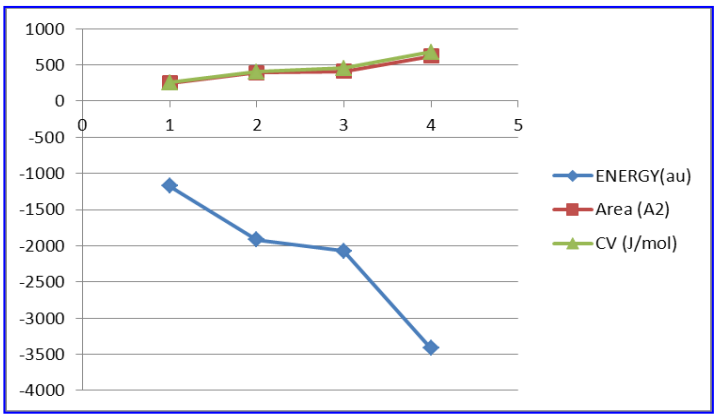


Fig4 The comparison of the molecular level, internal energy and specific heat capacity of the HMX explosive and its derivatives with different carbon-containing fullerenes

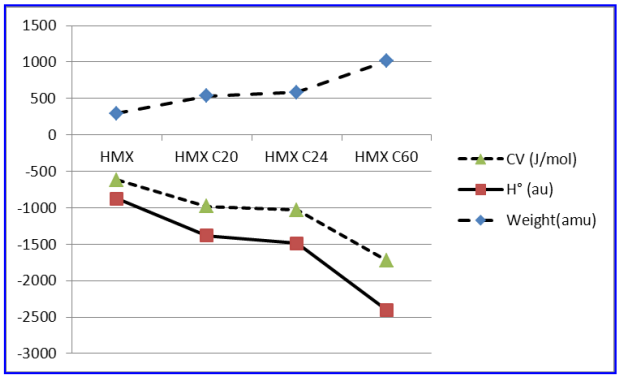
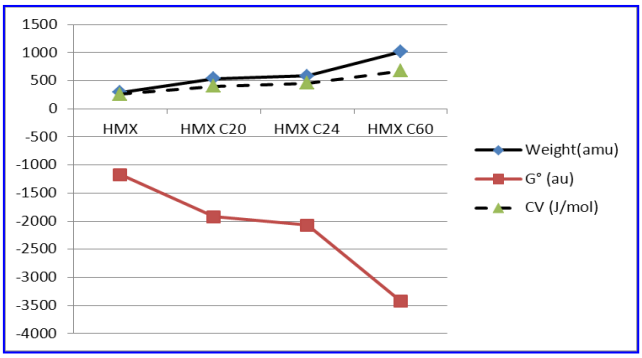


Figure 5 Comparison of molecular enthalpy, molecular mass and specific heat capacity of HMX explosives and its derivatives with different carbon-based fuller nano structures



.Fig 6 Gibbs free energy graph, molecular mass and specific heat capacity of HMX explosives and their derivatives

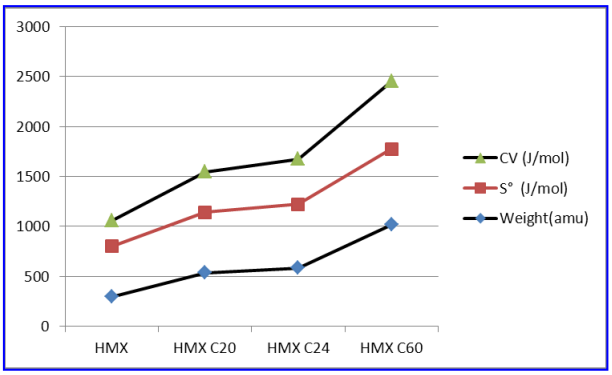


Fig. 7 Chart of the molecular entropy, molecular mass and specific heat capacity of the HMX explosive and its derivatives with fullerenes

Also, the results of the calculations showed that increasing the molecular mass from HMX to the derivatives of explosives with different carbon-containing fullerenes increases the specific heat capacity, but with increasing molecular mass, the molten enthalpy and the free energy of molybdenum energy decreases Figure 5-6. The molecular entropy study also showed that with increasing molecular mass, molecular volume and molecular surface, HMX material increases to explosive derivatives with different carbon-based fuller nano structures. Fig. 7.

4. Calculate and check the specific heat capacity of the CV at various temperatures:

Using the Gaussian 98 program, the values of CV specific heat capacity for HMX explosives and their derivatives with different carbon nanoparticles used in this study were calculated at a temperature range of 300 to 400 Kelsius, each 10 ° C once.

Table 2: Specific Heat Capacity Changes for HMX Explosives and its Derivatives with Different Carbon Fuller Nano Structures at Different Temperatures

	Cv(J/mol.K)			
Temperature	HMX	HMX C20	HMX C24	HMX C60
300	259.4897	405.4588	457.1748	681.4718
310	264.6706	417.3303	470.9563	706.9409
320	269.8246	429.1425	484.6266	732.2047
330	274.9533	440.884	498.172	757.2405
340	280.0574	452.5442	511.58	782.0281
350	285.1369	464.1127	524.8392	806.549
360	290.1911	475.5801	537.9393	830.7865
370	295.2188	486.9374	550.8711	854.7257
380	300.2182	498.1761	563.6262	878.353
390	305.1874	509.2885	576.1974	901.6564
400	310.1241	520.2673	588.578	924.625

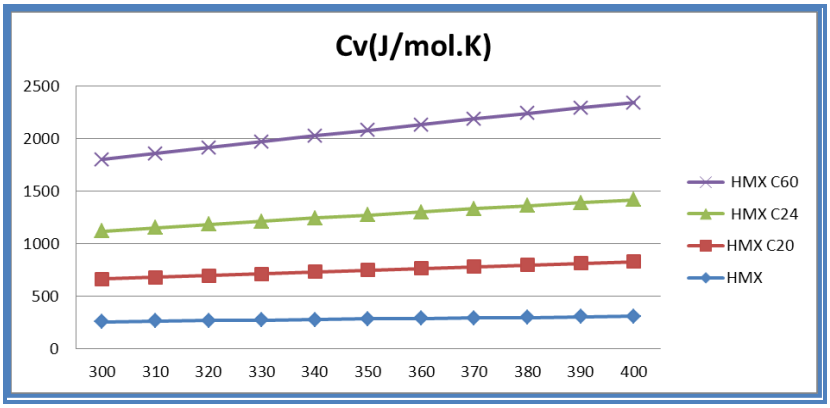


Fig 8: Chromium CV variation diagram for HMX explosives and its derivatives Fuller nano-structures with different carbon at various temperatures

Changes in the specific CV heat capacity values in an HMX explosive and its derivatives with different carbon nanoparticles used at various temperatures show that, by adding nanomaterials to the HMX explosive at different temperatures, the specific heat capacity of CV in all cases is The raw material has been increased, and on the other hand, in all cases examined by increasing the temperature, the specific heat capacity of the CV increases (Fig. 8)

5.Discussion and Conclusion

The results of the calculations show that the HMX explosive after adding various carbon-based fullerene nanostructures to its specific heat capacity increases. On the other hand, various derivatives are increased due to the increase in their specific heat capacity at different temperatures of the following process Show:

Cv HMX C60> Cv HMX C24> Cv HMX C20> Cv HMX

Since the number of carbon nanoparticles used in this study is considered differently, therefore, the molecular mass of the derivatives is different, and according to the shape of each of the nanostructures,

the volume and level of the molecules of the derivatives of the nanostructures are also different On the other hand, the variations in the volume of molecules of derivatives of different nanostructures with the same carbon number show the following trend:

$V_{HMX\ nano\ cone\ sheet} > V_{HMX\ Nano\ Cone} > V_{HMX\ Ger} > V_{HMX\ C20}$

Also, the comparison of the level of the molecules of various nanostructure derivatives with the number of carbon is similar to the following:

$A_{HMX\ Nano\ Cone\ Sheet} > A_{HMX\ Nano\ Cone} > A_{HMX\ Ger} > A_{HMX\ C20}$

Comparing the incremental trend of the specific heat capacity, the volume and the surface of the molecules of the various nano-structures derivatives with the different carbon numbers and their coordination, shows that under different conditions, increasing the molecular mass, volume and surface of the molecule increases the amount of specific heat capacity of the molecule. We know that the specific heat capacity of a CV is the amount of heat that is given to a mole of matter to rise to a temperature of one degree, it is evident that the more energy the material is, the less the specific heat of its CV. Therefore, it is concluded that the molecules of derivatives of different nanostructured nanostructures with different carbon numbers of HMX explosives have molecular mass, volume and surface area. The product is less energy efficient.

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