



Investigating the Energy Efficiency of TEX High Energy Derivatives with Different Carbon Fuller Nano Structures under Different Temperature Conditions by DFT Method

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Abstract

In this study, high energy energy derivatives of TEX with different carbon-containing fullerenes at 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: High energy energy derivatives, TEX, Functional density theory.

1. Introduction

TEX is an energetic explosive that has the same high speed and high explosive pressure, mechanical sensitivity and thermal stability. In recent years, new energetic materials have been taken into consideration, due to their special properties, they are widely used in military applications. TEX is made up of white to slightly yellow crystals that are impregnated with brown or different colors. As an explosive, TEX draws attention to its relatively high density. Its high density is due to its ISO structure and a compact crystal network of nitro groups that fill the gap between the cages. These high-performance materials are very useful in the production of pyrotechnic products with diameters, and they are less sensitive to heat and shock. On the other hand, the environmental hazards of these compounds are lower and better performance of the proportion of high-energy fossil fuels that burn in the process of burning out a large amount of carbon dioxide (CO₂), carbon monoxide (CO) and unpolluted carbon particles, such as soot. Nitrogen-rich

compounds have been used extensively for fire extinguishing, air bags, rocket fuel, and military systems (1-6). In this research, high energy energy derivatives of TEX with different carbon-containing fullerenes at different temperature conditions have been studied using density functional theory [1-10].

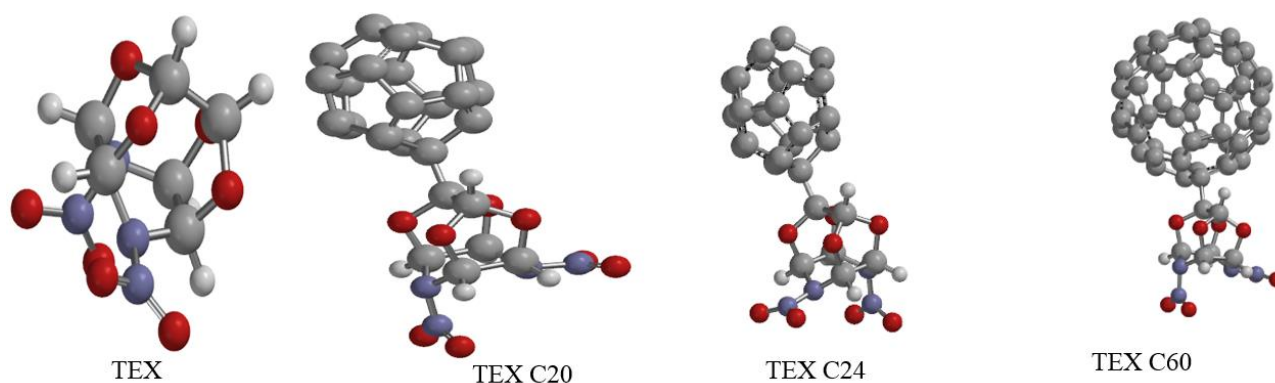


Fig 1. View of TEX derivatives with different carbon monoxide TEX C20, TEX C24, TEX C₆₀

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

	Temperature=298.15K , pressure=1 atm			
	TEX	TEX C ₂₀	TEX C ₂₄	TEX C ₆₀
	C ₆ H ₆ N ₄ O ₈	C ₂₆ H ₅ N ₄ O ₈	C ₃₀ H ₅ N ₄ O ₈	C ₆₆ H ₅ N ₄ O ₈
ENERGY(au)	-1033.38647	-1779.90773	-192933714	-3276.79133
E HOMO(eV)	-8.45	-10.49	-9.45	-8.99
E LUMO (eV)	-5.19	-3.78	-4.02	-2.70
Dipole Moment (Debye)	3.18	16.17	10.03	5.69
Weight(amu)	262.134	501.346	549.390	981.786
Volume(A ³)	182.55	389.03	429.24	767.70
Area (A ²)	199.15	352.25	375.71	579.74
Polarizability	53.01	71.35	74.91	39.89
ZPE (KJ/mol)	493.97	808.27	846.19	1579.08
H° (au)	-1033.188	-1779.58265	-1928.99477	3276.16230
CV (J/mol)	185.30	334.69	393.19	604.82
S° (J/mol)	418.84	532.77	581.78	684.02
G° (au)	-1033.24	-1779.65	-1929.06084	-3276.23998

2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [11-12]. 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 TEX 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 TEX 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. 2. Calculations and results

The computational study of high-energy TEX derivatives with different carbon-containing fullerenes was studied using functional density theory. The operation was performed using Gaussian 98 and Gauss view 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 by increasing the molecular mass, molecular volume and molecular surface of the TEX material, the explosive derivatives with different nanostructures increase the carbon content of the specific heat capacity, and, of course, the internal energy decreases. Fig. 2- 4.

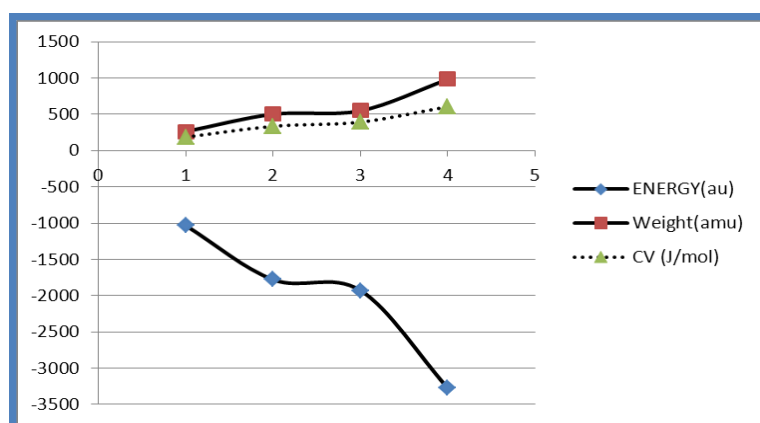


Fig 2. The comparison of the molecular mass, internal energy and specific heat capacity of the TEX explosive and its derivatives with different carbon-containing fullerenes

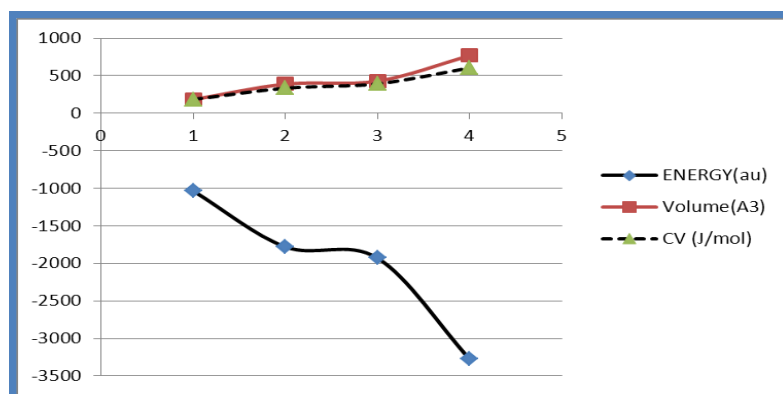


Fig 3. Comparison of the molecular volume, internal energy and specific heat capacity of the TEX explosive and its derivatives with different carbon-containing fullerenes

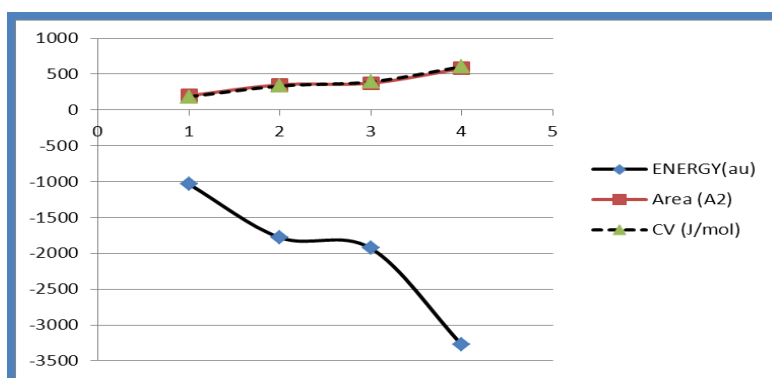


Fig 4. The comparison of the molecular level, internal energy and specific heat capacity of the TEX explosive and its derivatives with different carbon-containing fullerenes

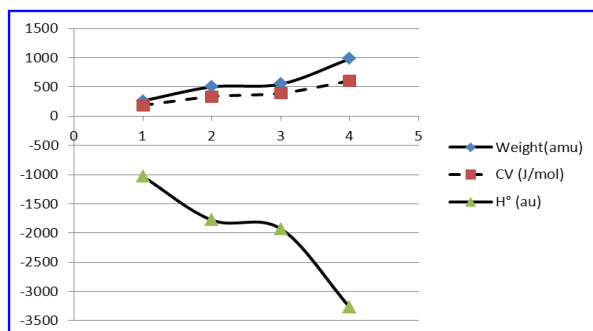


Fig 5. The comparison of molecular enthalpy, molecular mass and specific heat capacity of the TEX explosive and its derivatives with different carbon-based fullerene nanostructures

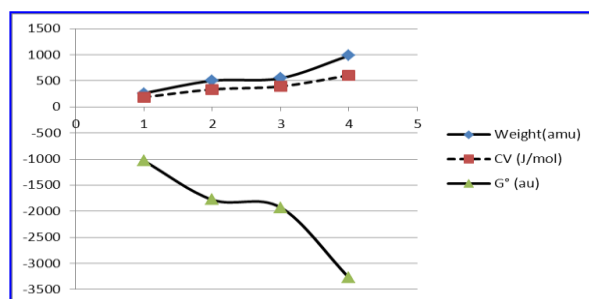


Fig. 6 Graph of the energy of molybdenum free molecule, molecular mass and specific heat capacity of the TEX explosive and its derivatives with different carbon-containing fullerenes

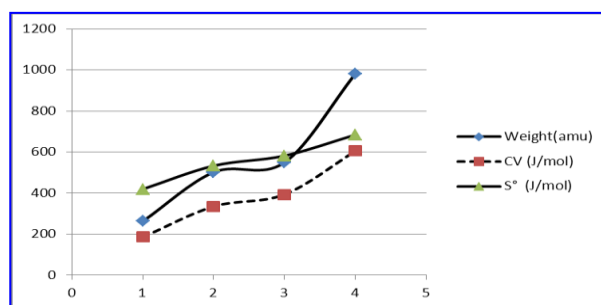


Figure 7 The comparison of molecular entropy, molecular mass and specific heat capacity of the TEX explosive and its derivatives with different carbon-containing fullerenes

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

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

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

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

Temperature	Cv(J/mol.K)			
	TEX	TEX C20	TEX C24	TEX C60
300	186.3191	336.9306	395.6305	609.6045
310	191.8472	349.0286	408.9493	635.366
320	197.3745	361.0873	422.1988	660.9462
330	202.8957	373.09	435.3609	686.3167
340	208.4049	385.0209	448.4188	711.4513
350	213.8962	396.865	461.357	736.3266
360	219.3638	408.6086	474.1614	760.9212
370	224.8019	420.239	486.8194	785.2158
380	230.2049	431.7446	499.3194	809.1935
390	235.5672	443.1148	511.6512	832.8388
400	240.8838	454.34	523.8057	856.1382

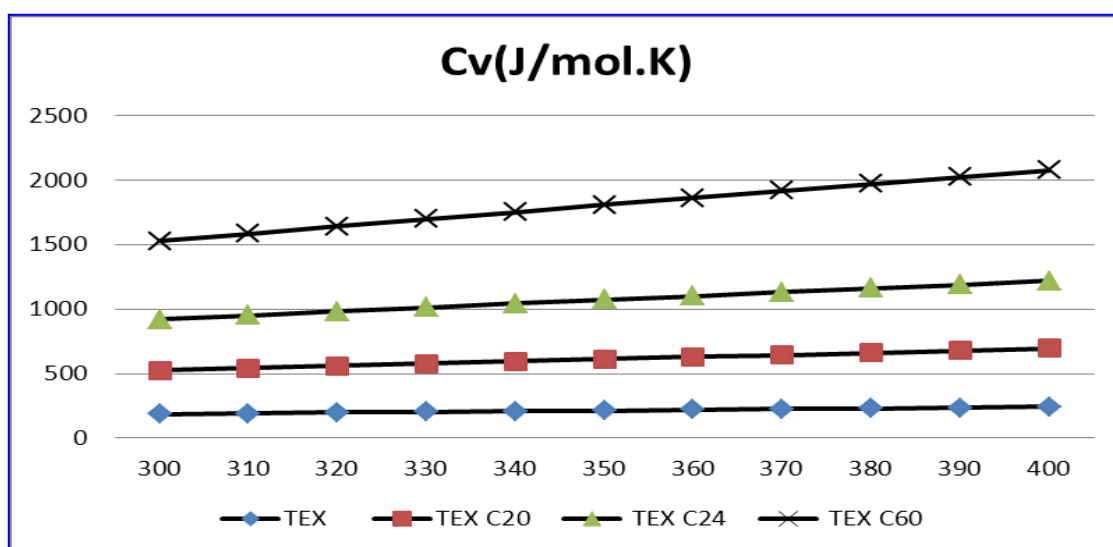


Fig8. Changes in CV Special Heat Capacity for Explosive TEX and its Derivatives Fullerene Nanostructures with Different Carbon at Different Temperatures

Changes in the specific CV heat capacity values of the TEX explosive and its derivatives with different carbon nanotubes, used at various temperatures, show that, with the addition of nanostructures to the TEX 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)

4. Conclusion

The results of the calculations show that the TEX explosive after adding different carbon-based fullerene nanostructures to that specific heat capacity of the derived derivatives increases. On the other hand, different derivatives, due to the increase in their specific heat capacity at different temperatures, are as follows. Show:

$$C_{V \text{ TEX C60}} > C_{V \text{ TEX C24}} > C_{V \text{ TEX C20}} > C_{V \text{ TEX}}$$

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:

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

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

$$A_{\text{TEX nano cone sheet}} > A_{\text{TEX Nano Cone}} > A_{\text{TEX Ger}} > A_{\text{TEX C20}}$$

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 nanosized nanostructures with different carbon numbers of TEX explosives have molecular mass, volume and surface area. The product is less energy efficient. Table 1. Comparison of the values of other thermodynamic parameters studied in this study confirms the results.

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