International Journal of New Chemistry, 2018, 5 (1), 11-18.
Published online March 2018 in http://www.ijnc.ir/.
Original Article

Online ISSN 2383-188X
Open Access

Computational Study of the Mass, Volume and Surface Effects on the Energetic Properties of RDX derivatives with Different Fullerenes (C_{20}, C_{24} and C_{60})

Somayeh Pourkarim* and Hamideh Shahzad

Department of Chemistry, Yadegar-e-Imam Khomeini (RAH) Shahre-rey Branch, Islamic Azad University, Tehran, Iran
*Corresponding Author e-mail Address: s.pourkarim@yahoo.com

Received 6 March 2018; Accepted 10 April 2018; Published 30 April 2018

Abstract

In this study derivatives of energetic matter RDX with Fullerenes has different carbon in different temperature conditions, by Using density functional theory Were studied. For this purpose, at the first, the materials were geometrical optimized, then the calculation related to thermodynamic parameters on all of them were done. Then the process of changes parameters dependents on energy including capacity specific heat, enthalpy, entropy, Gibbs free energy towards Molecular mass, volume molecule, measured level in this study at Certain temperature, relative to each other Was evaluated.

.

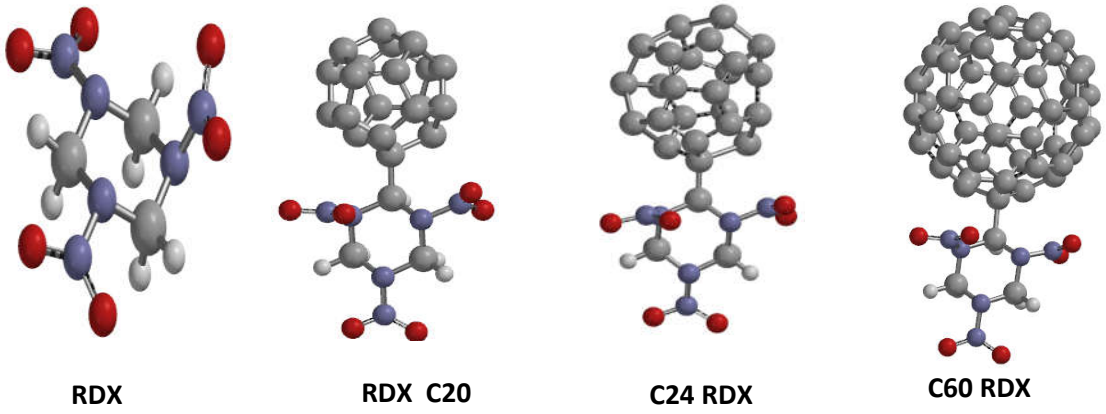
Keywords: Density Functional Theory, Fullerene, C_{20}, C_{24}, C_{60}, RDX and Explosives

1. Introduction

the first time in 1899 years by henning Germany for medical purposes was prepared. its importance as an explosive was marked by Herez in 1920. Herez direct prepare RDX suggested by having nitrous Hexamin. But low efficiency, process was expensive and for mass production wasn't suitable [1-5].

Hill in Pykatny Arsenal in 1925 found the production process RDX that its efficiency was 68%. more improvements in the production of RDX till 1940 wasn't done until Minser a continuous method for

production of RDX Raised and Res and Shisler from Canada offered process that need to Hexamin wasn't as raw matter. at the same time Bachmann process for producing RDX developed of Hexamin which had the highest return [6-12]. Bachmann's products as RDX type B had been known and contains 8 to 12 percent was impurity. Later using The physical properties of this impurity, explosive HMX that as Aktvzhn also was known, found development. In this study derivatives of energetic matter RDX with Fullerenes has different carbon in different temperature conditions, by Using density functional theory Were studied [13-20].



Fig(1): images have been optimized RDX , RDX C204

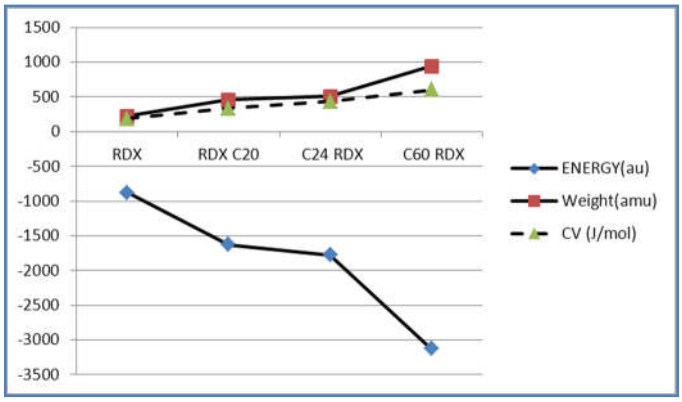
Table (1): Some chemical properties calculated at the level of B3lyp/6-31g for material RDX ،RDX C20 ، RDX C24 ،RDX C60

	Temperature=298.15K , pressure=1 atm			
	RDX	RDX C_{20}	C24 RDX	C60 RDX
ENERGY(au)	-880.703152	-1627.18088	-1776.05429	-3124.06228
E HOMO(eV)	-8.63	-10.66	-9.92	-9.01
E LUMO (eV)	5.13	-3.95	-4.55	-2.85
Dipole Moment (debye)	3.60	13.26	18.29	3.91
Weight(amu)	222.117	461.329	509.373	941.769
Volume(A3)	160.53	367.09	429.55	746.71
Area (A2)	192.71	344.46	385.31	570.66
ZPE (KJ/mol)	427.43	744.09	729.82	1514.25
H° (au)	-880.528656	-1626.87988	-1775.75354	-3123.45752
CV (J/mol)	186.55	331.79	433.8	602.59
S° (J/mol)	433.17	542.89	624.17	694.72
G° (au)	-880.577846	-1626.94153	-1775.82442	-3123.53641

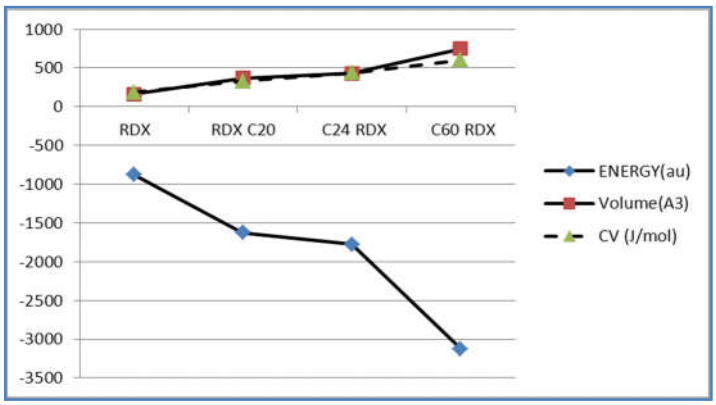
2. Calculations and results:

study computational derivatives of energetic matter RDX with Fullerenes has different carbon, by Using density functional theory Were studied, the operation using Gaussian software and Gauss View was done. The compounds at first by Using density function theory in the series (6 - 31 g) were optimized then IR studies in order to calculate the thermodynamic parameters related to the process has been done. all calculations at the level of B3lyp / 6 - 31 g 300 temperature to 400 K and 1 atm has been done. The results of calculations showed with

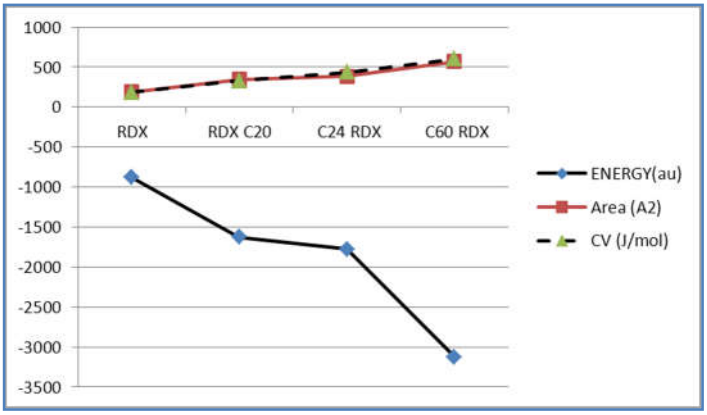
increase of molecular mass, molecular volume and the level of molecules of matter RDX to an explosive derivatives with different nanostructures has similar carbon capacity specific heat will increase and Of course internal energy is also low (2 - 4).



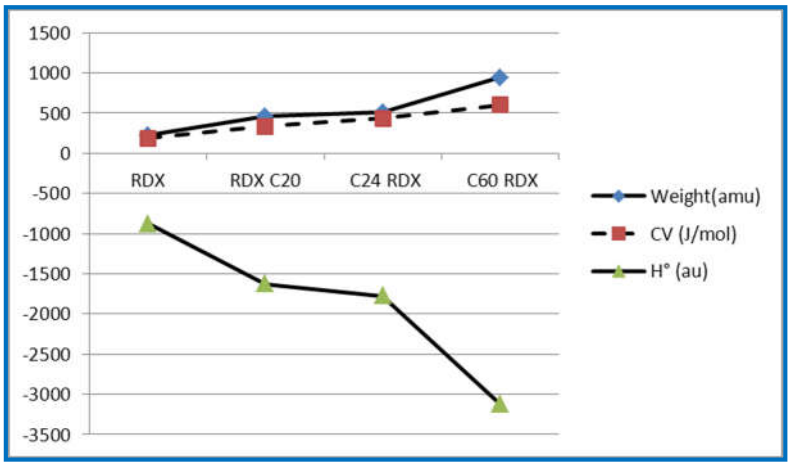
Fig(2): chart of compare molecular mass, internal energy and capacity specific heat of explosives RDX and its derivatives were used with Fullerenes has different carbon



Fig(3): chart compare of molecular volume internal energy and capacity specific heat of explosives RDX and its derivatives were used with Fullerenes has different carbon



Fig(4): chart compare of molecular level internal energy and capacity specific heat of explosives RDX and its derivatives were used Fullerenes has different carbon



Fig(5**):** chart compare of enthalpy, molecular mass and capacity specific heat of explosives RDX and its derivatives were used with nanostructures Fullerene has different carbon

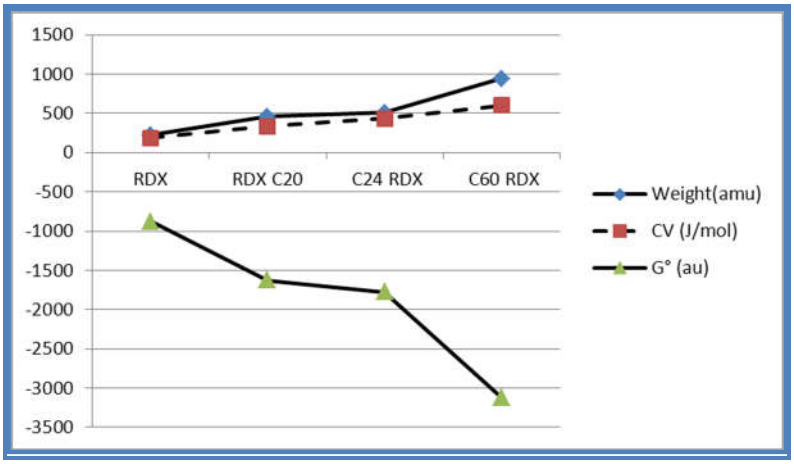
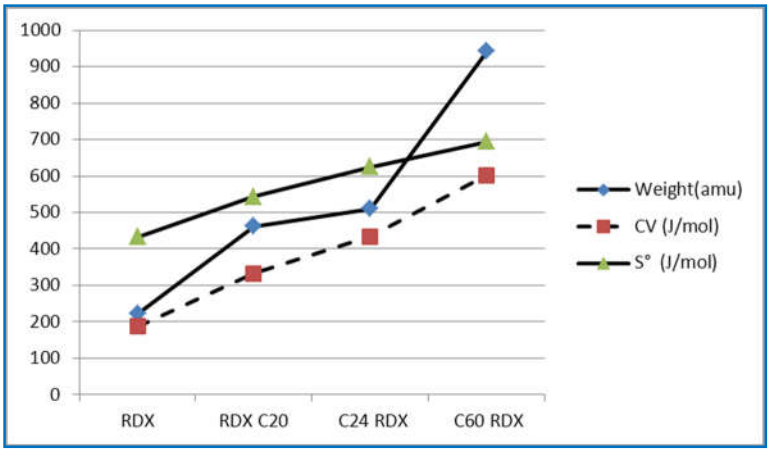


Fig (6) chart compare of free energy Gibbs Muley, molecular mass and capacity specific heat of explosives RDX and its derivatives were used with Fullerenes has different carbon



Fig(7) chart compare of Muley entropy, molecular mass and capacity specific heat of explosives RDX and its derivatives were used with Fullerenes has different carbon

Also study of results of obtained from calculations showed with increase of molecular mass , from the matter of RDX to explosive derivatives with Fullerenes has different carbon, capacity specific heat will increase, But increase molecular,mass, rate enthalpy Muley and free energy Gibbs Muley decreases (5 - 6).

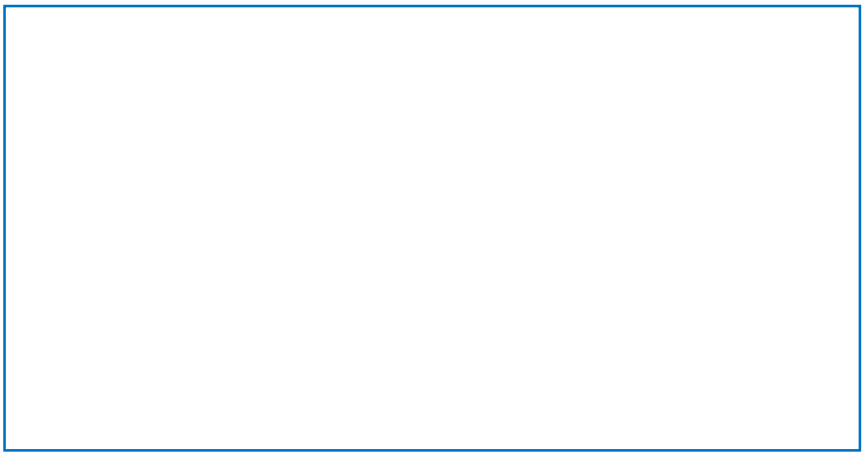
Also study of entropy Muley showed with increase of molecular mass , molecular volume and the level of molecules from the matter RDX to explosive derivatives with different nanostructures has similar carbon will increase (7).

3. calculation and study Special heat capacity CV at different temperatures

By using of Gaussian software 98 capacity specific heat CV for explosive RDX and its derivatives with different nanostructures has similar carbon were used in this study in temperature range 300 to 400 K, every 10 degree once was calculated.

Table(2): changes capacity specific heat of explosives RDX and its derivatives with different nanostructures Fullerene has different carbon in different temperatures

	Cv(J/mol.K)			
Temperature	RDX	RDX C20	C24 RDX	C60 RDX
300	187.2671	333.7288	436.0358	607.077
310	191.1575	344.1805	448.0039	631.2314
320	195.0306	354.5894	459.8101	655.1978
330	198.8871	364.9433	471.4482	678.952
340	202.727	375.2304	482.9129	702.4724
350	206.5499	385.4403	494.1996	725.7396
360	210.355	395.5628	505.3044	748.7361
370	214.1412	405.5888	516.2238	771.4465
380	217.9069	415.5098	526.9551	793.8569
390	221.6505	425.3182	537.4959	815.955
400	225.3701	435.007	547.8444	837.73



Fig(8) diagram changes capacity specific heat C_V for of explosives RDX and its derivatives used with different nanostructures Fullerene has different carbon in different temperatures

values changes capacity specific heat CV in explosives RDX and its derivatives with different nanostructures has similar carbon used in different temperatures shows that, with the addition of nanostructures to the explosive matter RDX in different temperatures capacity specific heat CV in all cases towards the raw matter have increased and on the other hand in all cases were studied with increases temperature capacity special heat will increases. Fig(8).

4. Discussion and deduction

the results of calculations shows that explosives RDX after the addition of nanostructures Fullerenes has different carbon to it capacity specific heat its derivatives increases, on the other hand, different derivatives with to increase the amount of capacity specific heat them at different temperatures below trend shows:

Cv RDX C60>Cv RDX C24> Cv RDX C20> Cv RDX

because the number of carbons in nanostructures were used in this research were considered different, So the resulting derivatives molecular mass is different, and according to the figure of each of nanostructures, the amount of the volume and the level of molecules derivatives nanostructures is different, on the other hand, changes the volume of the molecules of different structures of nano derivatives with the number of similar carbon the process below shows:

V RDX C60>VRDX C24> V RDX C20> V RDX

and also compare the level of molecules nano derivatives of different structures with the number of similar carbon below shows:

A RDX C60>A RDX C24> A RDX C20> A RDX

compare the incremental process amount of capacity specific heat, the volume and the level of molecules nano derivatives of different structures with the number of different carbon and coordination together they show in different conditions with the increase molecular mass the volume and the surface of molecule the amount of capacity specific heat molecule will increase [21-27].

We know the capacity specific heat CV is the amount of heat that give to a mole of matter till its temperature increase one degrees, Obviously whatever matter be energetic its capacity specific heat value CV is less. so the result is taken whatever molecules nano derivatives of different fullerene structures with the number of different carbon with explosive RDX has the molecular mass, volume and the surface are more the resulting product energy is low Table (1)

Compare the values other thermodynamic parameters Case Study in this research the aforementioned results will confirm.

Acknowledgment

We are appreciating and thanking Islamic Azad University of Yeager-e-Imam Khomeini (Rah) Share Rey.

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