

## Study of thermodynamic parameters of (TATB) and its fullerene derivatives with different number of Carbon ( $C_{20}$ , $C_{24}$ , $C_{60}$ ), in different conditions of temperature, using density functional theory

Roya Ahmadi\*

Young Researchers and Elite Clube, Yadegar-e-Imam Khomeini (RAH), Shahre-rey Branch, Islamic Azad University, Tehran, Iran

Received 03 March 2017; revised 28 May 2017; accepted 14 June 2017; available online 02 July 2017

### Abstract

In this research 1, 3, 5-triamino-2, 4, 6-trinitrobenzene (TATB) were attached with different nano structures of fullerene with 20, 24 and 60 carbons producing nano structures with diverse molecular weights. Then by the use of density functional theory methods, thermodynamic parameters of TATB with foregoing nanostructures, in wide of temperature, between 300-400 °K were computed. To this purpose, the materials on both sides of suggested synthesis reactions were geometrically optimized, and then, the calculations of the thermodynamic parameters were performed on all of them. The values of enthalpy, Gibbs free energy and Specific heat capacity for these reactions were obtained. Also important parameters such as energy levels, the amount of HOMO/LUMO values and related parameters including electrophilicity scale, chemical hardness, chemical potential, and the maximum amount of electronic charge transferred were derived. Finally, the effect of type and molecular weight of nano structure fullerene ( $C_{20}$ ,  $C_{24}$ ,  $C_{60}$ ) on explosion properties and other chemical properties of TATB were evaluated.

**Keywords:** Density Functional Theory (DFT); Enthalpy; Fullerene; TATB; Thermodynamic parameters.

### How to cite this article

Ahmadi R. Study of thermodynamic parameters of (TATB) and its fullerene derivatives with different number of Carbon ( $C_{20}$ ,  $C_{24}$ ,  $C_{60}$ ), in different conditions of temperature, using density functional theory. *Int. J. Nano Dimens.* 2017; 8 (3): 250-256.

## INTRODUCTION

1, 3, 5-triamino-2, 4, 6-trinitrobenzene (TATB) is a combustible substance, that was firstly prepared in 1888 by Jackson and Wing, that remain stable at temperatures at least as high as 250 °C, with a high melting point and thermal stability (Fig. 1) [1-2]. TATB is bright yellow color, insoluble in organic solvents. The chemistry of the nitro group has been widely investigated. Aromatic nitro compounds are important in pharmaceutical drugs, agrochemicals, polymers, solvents, perfumes, and etc [3-4].

TATB has been developed for use in lead free primary compositions, many of the high explosives are sensitive to shock and heat, but TNT is insensitive to shock or fire so it is commonly used as a safety weapon. Research is being done to develop non-toxic and environmentally acceptable smoke, because we need to have a clean environment. TATB

\* Corresponding Author Email: [roya.ahmadi.chem@hotmail.com](mailto:roya.ahmadi.chem@hotmail.com)

is a green material and environmentally friendly with less harmful effect, because after combustion of TATB, is produced excessive  $N_2$  gas [5-8].

## EXPERIMENTAL

Computational study of 1, 3, 5-trichloro-2, 4, 6-trinitrobenzene (TATB) with nanostructures of fullerene with 20, 24 and 60 carbons, in different conditions of temperature were done by density functional theory [9]. The operation was performed using the software Gaussian 98 and Gauss view and Spartan. First, compounds were optimized in a series of basic (6-31G) using density functional theory (Fig. 2). Then IR studies were done in order to calculate thermodynamic parameters of the process (Table 1) [10-11]. All of these calculations were done in the level B3LYP/6-31G at 300 to 400 Kelvin, and the atmospheric pressure.

When molecular weight of compounds increased, energy decreased but volume, area and  $C_v$  increased (Fig. 3, Table 1). In this article some properties including energetic levels, HOMO & LUMO levels ( $\epsilon_H, \epsilon_L$ ), electrophilicity ( $\omega$ ), chemical hardness ( $\eta$ ),  $\Delta N_{max}$  and chemical potential properties were investigated. The maximum amount of electronic charge index,  $\Delta N_{max}$ , describes the charge capacity of the molecule that the electrophone system may accept, it is given by (1) equation. A positive value of  $\Delta N_{max}$  index (a.u.) for a compound reveals that acts as an electron acceptor, where as a negative value of  $\Delta N_{max}$  index indicates that acts as an electron donor. The maximum amount of electronic charge and the electrophilicity and indices are related to electronic charge. The electrophilicity Index,  $\omega$ , in

atomic units is a measure of electrophilic power of a molecule it is given by (2) equation. When two molecules react with each other, one molecule behaves as a nucleophile, whereas the other one acts as an electrophone. A higher electrophilicity index shows higher electrophilic power of a molecule. So the quantity of  $\omega$  describes the propensity of the system to acquire additional electronic charge from the environment, which is described by (2) equation. In equations (3) and (4), respectively  $\mu$  and  $\eta$  are the chemical potential and the chemical hardness [12-13].

$$\Delta N_{max} = -\mu / \eta \quad (1)$$

$$\omega = \mu^2 / 2\eta \quad (2)$$

$$\mu \approx (\epsilon_H + \epsilon_L) / 2 \quad (3)$$

$$\eta = (\epsilon_L - \epsilon_H) / 2 \quad (4)$$

The results obtained show that when structure of TATB is Connected to nanostructures of Fullerene with 20, 24 and 60 carbons, the dipole moment of The resulting derivatives are increased (Table 1) [14]. In TATB derivatives HOMO- LUMO Gap (HLG) are less than TATB (Table 1). A small HOMO-LUMO Gap (HLG) means small excitation energies to the excited states. Therefore TATB derivatives are more conductive than TATB (Table 1, Fig 4).

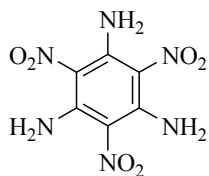


Fig. 1: 1, 3, 5-triamino-2, 4, 6-trinitrobenzene (TATB).

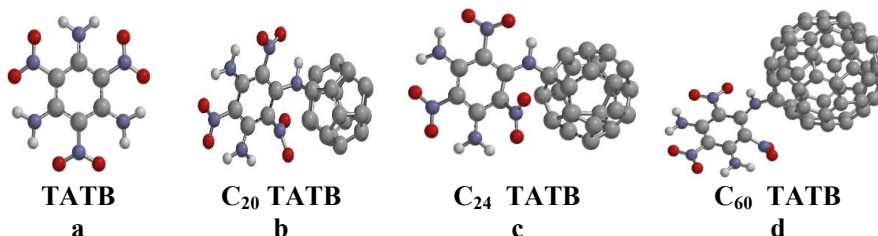


Fig. 2: optimized molecules TATB (a) and its fullerene derivatives with different number of Carbon,  $C_{20}$  TATB (b),  $C_{24}$  TATB(c) and  $C_{60}$  TATB (d).

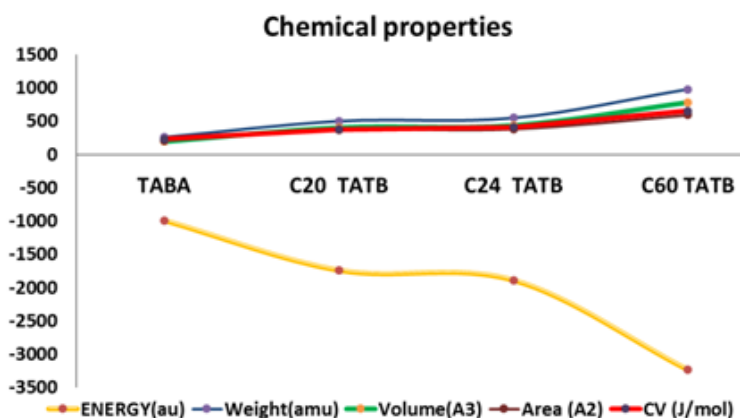


Fig. 3: Compare of some chemical properties, were done for 1, 3, 5-triamino-2, 4, 6-trinitrobenzene (TATB) and its derivatives with  $C_{20}$ ,  $C_{24}$  and  $C_{60}$ , in the computational level B3LYP / 6-31G.

Chemical hardness for TATB derivatives are less than TATB, so these are softer than TATB. Soft molecules with a small gap, can change their electron density more easily than a hard molecule. So they are more reactive than TATB (Table 1). Electrophilicity values (a.u.) in  $C_{60}$  TATB increased. The electrophilicity index is a measure of electrophilic power of a molecule. When two molecules react with each other, one molecule behaves as a nucleophile system, whereas the other one acts as an electrophone system. A higher electrophilicity index shows higher electrophilicity of a molecule; therefore  $C_{60}$  TATB is more strong Lewis acid than TATB (Table 1). Maximum amount of electronic charge index ( $\Delta N_{max}$ ) as mentioned, most electron charge that a system accepts can be calculated by  $\Delta N_{max}$  parameter. The obtained results for this parameter were obtained like the previous parameter, For  $C_{60}$  TATB increased. A positive value

of  $\Delta N_{max}$  indicates that charge flows to system, or our system acts as an electron acceptor, whereas a negative value of  $\Delta N_{max}$  indicates that charge flows from system or our system acts as an electron donor. So TATB derivatives are electron acceptor or a stronger Lewis acid (Table 1) [15-16].

## RESULTS AND DISCUSSIONS

The results of the calculations show that the manner of increasing the density is such as the follows:

$$d_{TATB} > d_{C_{24} TATB} > d_{C_{60} TATB} > d_{C_{20} TATB}$$

As we know the power of explosion in high-energy compound depends on the density directly. Increasing trend of explosive compounds which were investigated is as follows:

$$TATB > C_{24} TATB > C_{60} TATB > C_{20} TATB$$

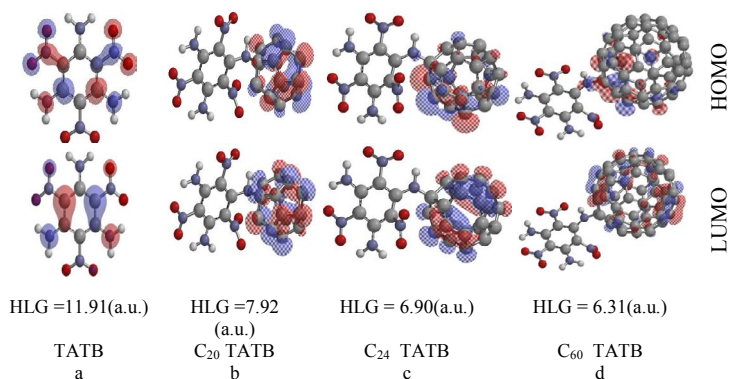


Fig. 4: HOMO and LUMO molecular orbitals and HOMO- LUMO Gap (HLG) of TATB (a),  $C_{20}$  TATB(b),  $C_{24}$  TATB (c), and  $C_{60}$  TATB (d).

Table 1: Some chemical properties were calculated in the B3LYP / 6-31G for of TATB,  $C_{20}$  TATB,  $C_{24}$  TATB and  $C_{60}$  TATB.

|                           | TATB    | $C_{20}$ TATB | $C_{24}$ TATB | $C_{60}$ TATB |
|---------------------------|---------|---------------|---------------|---------------|
| Energy(au)                | -992.92 | -1740.25      | -1889.78      | -3236.26      |
| E HOMO(eV)                | -7.05   | -4.85         | -4.79         | -9.06         |
| E LUMO (eV)               | 4.86    | 3.07          | 2.11          | -2.75         |
| Dipole Moment (Debye)     | 0.00    | 1.35          | 2.58          | 2.48          |
| Weight(amu)               | 258.15  | 498.37        | 546.41        | 977.80        |
| Volume( $\text{\AA}^3$ )  | 190.63  | 401.30        | 434.31        | 779.48        |
| Area ( $\text{\AA}^2$ )   | 209.96  | 371.03        | 378.71        | 589.50        |
| ZPE (KJ/mol)              | 460.56  | 825.00        | 893.99        | 1546.28       |
| $H^\circ$ (au)            | -992.73 | -1739.92      | -1889.42      | -3235.64      |
| $C_v$ (J/mol)             | 227.66  | 373.69        | 406.10        | 650.00        |
| $S^\circ$ (J/mol)         | 444.27  | 566.29        | 589.06        | 724.29        |
| $G^\circ$ (au)            | -992.78 | -1739.99      | -1889.48      | -3235.72      |
| $d=m/v$                   | 1.35    | 1.24          | 1.26          | 1.25          |
| HLG (a.u.)                | 11.91   | 7.92          | 6.90          | 6.31          |
| Chemical Hardness (a.u.)  | 5.96    | 3.96          | 3.45          | 3.16          |
| Chemical Potential (a.u.) | -1.10   | -0.89         | -1.34         | -5.91         |
| Electrophilicity (a.u.)   | 3.57    | 1.57          | 3.10          | 55.01         |
| $\Delta N_{max}$ (a.u.)   | 0.18    | 0.22          | 0.39          | 1.87          |

Calculation and verifying the values of changes in enthalpy ( $\Delta H$ )

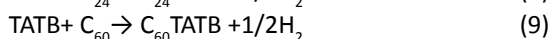
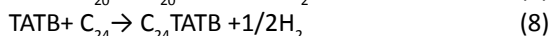
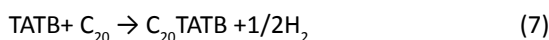
The way to calculate enthalpies of reaction is to calculate heats of formation, and operation of the appropriate sums and difference. Enthalpy values for raw materials and products calculated in process synthesis. For calculating and obtaining of any changes on the enthalpy, Equation 5 is used.

$$\Delta H_f(T, K) = \sum(\epsilon^0_{+H_{corr}})_{Products} - \sum(\epsilon^0_{+H_{corr}})_{Reactants} \quad (5)$$

Sum of electronic and thermal enthalpies =  $\epsilon^0_{+H_{corr}} = H$

$$\Delta H_f(T, K) = \sum(H)_{Products} - \sum(H)_{Reactants} \quad (6)$$

Yielding the following reactions



Enthalpy values obtained through calculation

software Spartan, and then enthalpy of formation values obtained from Equation 10, 11, 12.

$$\Delta H_f = [H_{C_{20}TATB} + 1/2H_{H_2}] - [H_{TATB} + H_{C_{20}}] \quad (10)$$

$$\Delta H_f = [H_{C_{24}TATB} + 1/2H_{H_2}] - [H_{TATB} + H_{C_{24}}] \quad (11)$$

$$\Delta H_f = [H_{C_{60}TATB} + 1/2H_{H_2}] - [H_{TATB} + H_{C_{60}}] \quad (12)$$

Enthalpy of formation calculated at the level B3LYP / 6-31G for derivatives of 1, 3, 5-triamino-2, 4, 6-trinitrobenzene (TATB) with  $C_{60}$  TATB is always positive in all temperature range 300 to 400 Kelvin but for  $C_{20}$  TATB and  $C_{24}$  TATB are always negative in all temperature range 300 to 400 Kelvin (Table 2).

The negative  $\Delta H_f$  shows that, derived synthesis process material 1, 3, 5-triamino-2, 4, 6-trinitrobenzene (TATB) with  $C_{20}$  and  $C_{24}$  are exothermic reaction, but with  $C_{60}$  is endothermic reaction at temperature ranging from 300 to 400 Kelvin (Fig. 5, Table 2).

Table 2: Enthalpy of formation calculated at the level B3LYP / 6-31G for derivatives of 1, 3, 5-triamino-2, 4, 6-trinitrobenzene (TATB) with  $C_{20}$ ,  $C_{24}$  and  $C_{60}$ .

| Enthalpy(kJ/mol) |               |               |               |
|------------------|---------------|---------------|---------------|
| Temperature      | $C_{20}$ TATB | $C_{24}$ TATB | $C_{60}$ TATB |
| 300              | -1951.697378  | -1957.521115  | 639.8432584   |
| 310              | -1951.841878  | -1952.819715  | 639.7231584   |
| 320              | -1951.986978  | -1948.099715  | 639.6040584   |
| 330              | -1952.141878  | -1943.406815  | 639.4615584   |
| 340              | -1952.296678  | -1938.717315  | 639.3030584   |
| 350              | -1952.475278  | -1934.054415  | 639.1786584   |
| 360              | -1952.661678  | -1929.390715  | 639.0665584   |
| 370              | -1952.847778  | -1924.726115  | 638.9313584   |
| 380              | -1953.033678  | -1920.060015  | 638.7928584   |
| 390              | -1953.223678  | -1915.392415  | 638.6512584   |
| 400              | -1953.362778  | -1910.660715  | 638.5686584   |

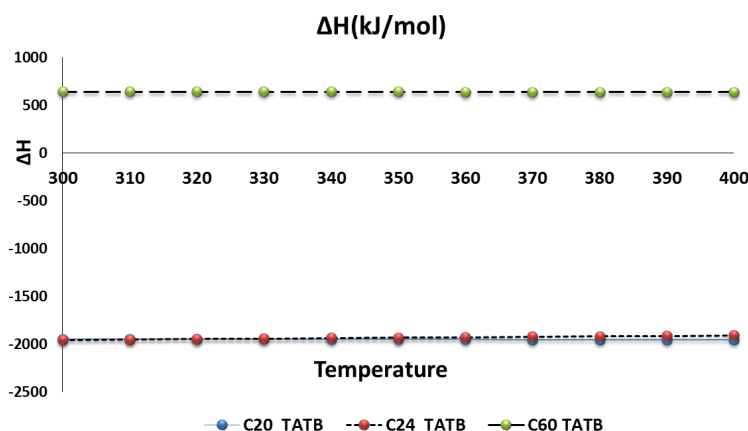


Fig. 5: Diagram of the Enthalpy of formation calculated at the level B3LYP / 6-31G for  $C_{20}$  TATB and  $C_{24}$  TATB  $C_{60}$  TATB at different temperatures.

Table 3: Specific heat capacity ( $C_v$ ) calculated at the level B3LYP / 6-31G for 1, 3, 5-triamino-2, 4, 6-trinitrobenzene (TATB) and its derivative with  $C_{20}$ ,  $C_{24}$  and  $C_{60}$ .

| Cv(J/mol.K) |          |                      |                      |                      |
|-------------|----------|----------------------|----------------------|----------------------|
| Temperature | TATB     | C <sub>60</sub> TATB | C <sub>24</sub> TATB | C <sub>20</sub> TATB |
| 300         | 228.7532 | 654.8054             | 408.6298             | 375.9792             |
| 310         | 234.5778 | 680.6436             | 422.2397             | 388.3011             |
| 320         | 240.3017 | 706.2027             | 435.7092             | 400.4961             |
| 330         | 245.9244 | 731.459              | 449.0265             | 412.5541             |
| 340         | 251.4458 | 756.3921             | 462.1811             | 424.4664             |
| 350         | 256.8658 | 780.9846             | 475.1642             | 436.2251             |
| 360         | 262.185  | 805.2217             | 487.9678             | 447.8234             |
| 370         | 267.4039 | 829.0911             | 500.5851             | 459.2551             |
| 380         | 272.5232 | 852.5823             | 513.0104             | 470.5149             |
| 390         | 277.5438 | 875.6866             | 525.2385             | 481.5984             |
| 400         | 282.4665 | 898.3971             | 537.2654             | 492.5015             |

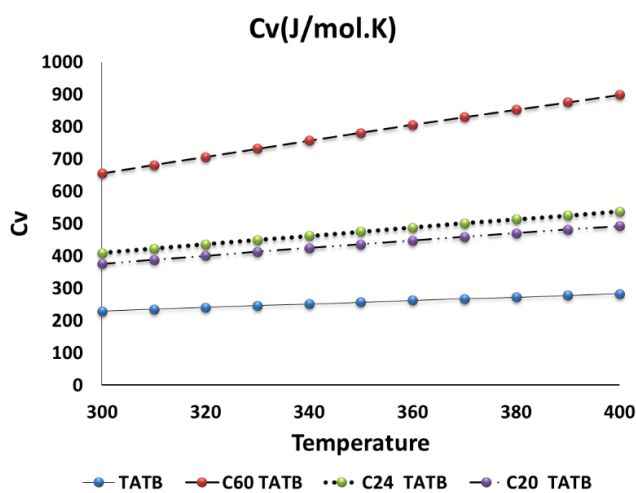


Fig 6. Diagram changes in specific heat capacity  $C_v$  of TATB, and  $C_{20}$  TATB and  $C_{24}$  TATB  $C_{60}$  TATB at different temperatures.

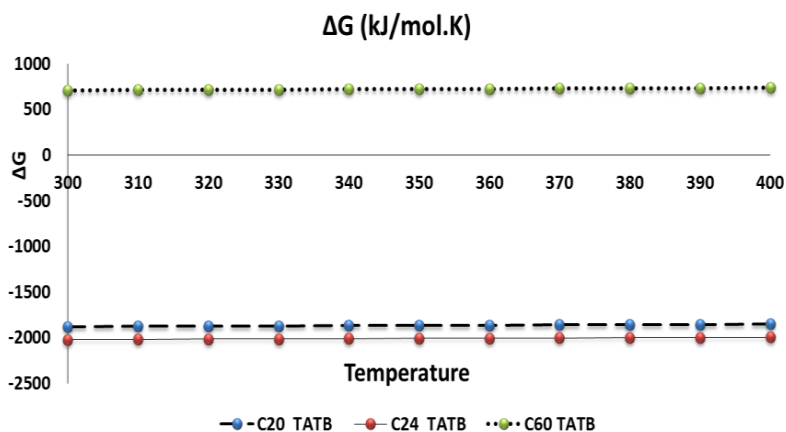


Fig. 7: diagram of the Gibbs Free Energy changes for the synthesis of derivatives material 1, 3, 5-triamino-2, 4, 6-trinitrobenzene (TATB), with  $C_{20}$ ,  $C_{24}$  and  $C_{60}$  at different temperatures (300-400K).

Table 4: Gibbs Free Energy of formation calculated at the level B3LYP / 6-31G for derivative material 1, 3, 5-triamino-2, 4, 6-trinitrobenzene (TATB), with C<sub>20</sub>, C<sub>24</sub> and C<sub>60</sub> at different temperatures.

| Temperature | $\Delta G$ (kJ/mol.K) |                      |                      |
|-------------|-----------------------|----------------------|----------------------|
|             | C <sub>20</sub> TATB  | C <sub>24</sub> TATB | C <sub>60</sub> TATB |
| 300         | -1880.919478          | -2025.131715         | 709.0778584          |
| 310         | -1878.196778          | -2022.286815         | 711.7868584          |
| 320         | -1875.456678          | -2019.386315         | 714.5174584          |
| 330         | -1872.678078          | -2016.500015         | 717.2449584          |
| 340         | -1869.835578          | -2013.553815         | 719.9762584          |
| 350         | -1867.013578          | -2010.609115         | 722.8166584          |
| 360         | -1864.374578          | -2007.766415         | 725.5041584          |
| 370         | -1861.832278          | -2005.020115         | 728.1708584          |
| 380         | -1859.325978          | -2002.338015         | 730.8370584          |
| 390         | -1856.769878          | -1999.601415         | 733.5212584          |
| 400         | -1854.156578          | -1996.770815         | 736.3471584          |

#### Calculation and verifying specific heat capacity(Cv)

The results of the calculations show that specific heat capacity, Cv values calculated for TATB and its derivatives with C<sub>20</sub>, C<sub>24</sub> and C<sub>60</sub> increased following

$$\text{TATB } C_{60} > \text{TATB } C_{24} > \text{TATB } C_{20} > \text{TATB} \quad (13)$$

Values of specific heat capacity changes, Cv of rawmaterial 1, 3, 5-triamino-2, 4, 6-trinitrobenzene (TATB), and its derivatives with C<sub>20</sub>, C<sub>24</sub> and C<sub>60</sub> at different temperatures indicate that the products have a high specific heat capacity Cv values than TATB (Fig.6, Table 3).

#### Calculation and verifying the values of Gibbs free energy ( $\Delta G$ )

The results of the calculations display that the values of Gibbs free energy ( $\Delta G$ ) were calculated for each of the reactants and products in process synthesis. For calculating and obtaining any changes in values of Gibbs free energy ( $\Delta G$ ) in the reaction  $A+B \rightarrow C+D$  the following formula is used

$$\Delta G_f = \sum G_{\text{Products}} - \sum G_{\text{Reactants}} \quad (14)$$

Given the reactions (7, 8, 9), the values of Gibbs free energy obtained through a Gaussian calculation software:

$$\Delta G_f = [G_{C_{20} \text{ TATB}} + 1/2 G_{H_2}] - [G_{\text{TATB}} + G_{C_{20}}] \quad (15)$$

$$\Delta G_f = [G_{C_{24} \text{ TATB}} + 1/2 G_{H_2}] - [G_{\text{TATB}} + G_{C_{24}}] \quad (16)$$

$$\Delta G_f = [G_{C_{60} \text{ TATB}} + 1/2 G_{H_2}] - [G_{\text{TATB}} + G_{C_{60}}] \quad (17)$$

$\Delta G_f$  negative values of the process of synthesis derived material 1, 3, 5-triamino-2, 4, 6-trinitrobenzene (TATB) with C<sub>20</sub> and C<sub>24</sub> at different temperatures indicate that, they can

be done spontaneously, but this process with C<sub>60</sub> at different temperatures is non spontaneously because  $\Delta G_f$  values are positive at different temperatures (Fig. 7, Table 4).

#### CONCLUSION

The results of the calculations show that in the process of synthesis of 1, 3, 5-triamino-2, 4, 6-trinitrobenzene (TATB) with C<sub>20</sub> and C<sub>24</sub> at different temperatures,  $\Delta G_f$  and  $\Delta H_f$  amounts are negative at all temperatures which suggests that, they are exothermic and spontaneously. (Tables 2 and 4). In contrast to  $\Delta H_f$  and  $\Delta G_f$  of C<sub>60</sub> TATB which are positive and its procedure is endothermic at all temperatures and no spontaneously. The comparison of results of C<sub>v</sub> shows that the Heat capacity of 1, 3, 5-triamino-2, 4, 6-trinitrobenzene (TATB) is lower than its derivatives with C<sub>20</sub>, C<sub>24</sub> and C<sub>60</sub> at different temperatures. The specific heat capacity is the amount of heat per unit mass required to raise the temperature by one degree Celsius, So it cause to need low energy to increase the material temperature, less specific heat capacity values define much energetic properties of TATB rather than its derivations. Heat capacity is increased with increasing molecular weight.

$$CV_{C_{60} \text{ TATB}} > CV_{C_{24} \text{ TATB}} > CV_{C_{20} \text{ TATB}} > CV_{\text{TATB}}$$

Density value of TATB and its derivatives with C<sub>20</sub>, C<sub>24</sub> and C<sub>60</sub> have this manner:

$$d_{\text{TATB}} > d_{C_{24} \text{ TATB}} > d_{C_{60} \text{ TATB}} > d_{C_{20} \text{ TATB}}$$

So we can say TATB has more explosive properties than nanostructure derivatives as studied in this paper.

### Novelty of this study

The main objective of this work is to discover the effect of the fullerene with different weight on the chemical properties of TATB by DFT method; many investigators can use the results in their similar work.

### ACKNOWLEDGMENT

We are appreciating and thanking *Young Researchers and Elite Clube*, Islamic Azad University of Yeager-e-Imam Khomeini (Rah) Share Rey.

### CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this manuscript.

### REFERENCES

- [1] Nic Daeid N., Yu H. A., Beardah M. S., (2017), Investigating TNT loss between sample collection and analysis. *Science & Justice*. 57: 95-100.
- [2] Uesawa S., Nakagawa M., Umetsu A., (2016), Explosive eruptive activity and temporal magmatic changes at Yotei Volcano during the last 50,000 years, southwest Hokkaido, Japan. *J. Volcanol. Geotherm. Res.* 325: 27-44.
- [3] Daryaei R., Eslami A., (2017), Settlement evaluation of explosive compaction in saturated sands. *Soil Dynam. Earthq. Eng.* 97: 241-250.
- [4] DeGreeff L. E., Malito M., Katilie C. J., Brandon A., Conroy M. W., Peranich K., Ananth R., Rose-Pehrsson S. L., (2017), Passive delivery of mixed explosives vapor from separated components. *Forensic Chem.* 4: 19-31.
- [5] Gallastegui G., Lara R. M., Elías A., Rojo N., Barona A., (2017), Black slag fixed bed for toluene, ethylbenzene and p-xylene (TEX) biodegradation and meiofauna development. *Int. Biodeterioration & Biodegradation*. 119: 349-360.
- [6] Ghosh P., Roy P., Ghosh A., Jana S., Murmu N. C., Mukhopadhyay S. K., Banerjee P., (2017), Explosive and pollutant TNP detection by structurally flexible SOFs: DFT-D<sub>3</sub>, TD-DFT study and in vitro recognition. *J. Luminesc.* 185: 272-278.
- [7] Gross M. L., Meredith K. V., Beckstead M. W., (2015), Fast cook-off modeling of HMX. *Combust. Flame*. 162: 3307-3315.
- [8] Konstantynovski K., Njio G., Holl G., (2017), Detection of explosives—Studies on thermal decomposition patterns of energetic materials by means of chemical and physical sensors. *Sensors and Actuators B: Chemical*. 246: 278-285.
- [9] Dixit V., Yadav R. A., (2015), DFT-B3LYP computations of electro and thermo molecular characteristics and mode of action of fungicides (chlorophenols). *Int. J. Pharmac.* 491: 277-284.
- [10] Talebian E., Talebian M., (2014), A comparative DFT study on the differences between normal modes of polyethylene and polyethylene glycol via B3LYP Hamiltonian and the Hartree–Fock method in multiple bases. *Optik – Int. J. Light and Electron Optics*. 125: 228-231.
- [11] Yoshimoto M., Matsunaga T., Tanaka M., Kurosawa S., (2016), Determination of thermodynamic parameters for enolization reaction of malonic and methylmalonic acids by using quartz crystal microbalance. *Analyt. Chem. Res.* 8: 9-15.
- [12] Baei M. T., Peyghan A. A., Moghimi M., Hashemian S., (2012), First-principles calculations of structural stability, electronic and electrical responses of GeC nanotube under electric field effect for use in nanoelectronic devices. *Superlat. Microstruc.* 52: 1119-1130.
- [13] Dai X., Meng Y., Xin M., Wang F., Fei D., Jin M., Wang Z., Zhang R., (2012), Energetics and electronic properties of a neutral diuranium molecule encapsulated in C90 fullerene. *Procedia Chem.* 7: 528-533.
- [14] Beheshtian J., Peyghan A. A., Bagheri Z., (2012), Functionalization of [60] fullerene with butadienes: A DFT study. *Appl. Surf. Sci.* 258: 8980-8984.
- [15] Bahrami Panah N., Vaziri R., (2015), Structure and electronic properties of single-walled zigzag BN and B<sub>3</sub>C<sub>2</sub>N<sub>3</sub> nanotubes using first-principles methods. *Int. J. Nano Dimens.* 6: 157-165.
- [16] Jahanbin Sardroodi J., Afshari S., Rastkar Ebrahimzadeh A. R., Abbasi M., (2015), Theoretical computation of the quantum transport of zigzag mono-layer Graphenes with various z-direction widths. *Int. J. Nano Dimens.* 6: 105-109.