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Research Article

Detonation Parameters of the Pentaerythritol Tetranitrate and Some Structures Descriptors in Different Solvents - Computational Study

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ABSTRACT

Pentaerythritol tetranitrate (PETN, $C_5H_8N_4O_{12}$) is a relatively stable explosive nitrate ester molecule. It has been widely used in various military and public industrial productions. In this study, the solubility tendency of PETN in different organic solvents was investigated theoretically. Several physicochemical parameters of PETN such as density, detonation pressure, temperature, rate and products of detonation reaction were investigated using the B3LYP functional and basic set of polarization functions (d, p) containing 6-31G**. The obtained results have been compared with the literature values. Furthermore, the stability and reactivity of PETN in acetone, diethyl ether, ethanol, tetrahydrofuran, toluene and methylene chloride were examined. Results revealed toluene is a good solvent to increase the explosive properties of PETN.

Keywords: *Density Functional Theory, Organic Solvents, PETN*

Pentaeritritol Tetranitratın Patlama Parametreleri ve Farklı Çözücülerdeki Bazı Yapı Tanımlayıcıları - Hesaplamalı Çalışma

ÖZ

Pentaeritritol tetranitrat (PETN, $C_5H_8N_4O_{12}$) nispeten kararlı bir patlayıcı nitrat esteridir. Çeşitli askeri ve kamuya ait endüstriyel üretimlerde yaygın olarak kullanılmaktadır. Bu çalışmada, PETN'nin farklı organik çözücülerdeki çözünürlük eğilimi teorik olarak araştırılmıştır. PETN'nin yoğunluk, patlama basıncı, sıcaklık, hız ve patlama reaksiyonunun ürünleri gibi çeşitli fizikokimyasal parametreleri, 6-31G ** içeren B3LYP fonksiyonel ve temel polarizasyon fonksiyonları seti (d, p) kullanılarak araştırılmıştır. Elde edilen sonuçlar literatür değerleri ile karşılaştırılmıştır. Ayrıca, PETN'nin aseton, dietil eter, etanol, tetrahidrofuran, toluen ve metilen klorit içindeki stabilitesi ve reaktivitesi benzer şekilde incelenmiştir. Sonuçlar PETN'in patlayıcı özelliklerini arttırmak için, toluenin iyi bir çözücü olduğunu ortaya çıkardı.

Anahtar Kelimeler: *Yoğunluk Fonksiyonu Teorisi, Organik Çözücüler, PETN*

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I. INTRODUCTION

The theoretical calculations have been extensively performed instead of the experimental studies. Especially, density functional theory (DFT) has been employed. It re-formulates the Schrödinger equation [1] which is described as a mathematical approximation that makes up the base of quantum mechanical matter definition from the perspective of wave-like properties of particles in a field. Thus it has been possible to clarify probable solutions in terms of chemical reactions [2]. It was established by Hohenberg and Kohn [3] almost sixty years ago. They declared that whole ground state properties can be presented as function of charge density. It must be minimized in energy. Then, Kohn and Sham put forth an alternative solution for available operations by modifying basic equations to collect dense electron relations in an 'exchange-correlation' functional [4]. Theoretical calculations support and/or predict the expensive experimental works. Density Functional Theory (DFT) is a successful tool defining specific features [5-14]. DFT provides many benefits such as time and money, aiming to define or even estimate the properties of molecular and condensed matter systems. Various computer programs have been developed that can be used in the field of molecular modeling (HyperChem, TeraChem, Scigress, Samson, Mopac, Gaussian, Spartan, etc.). Several properties such as structures, energies, chemical effects, state changes, IR-UV-NMR spectra, enzyme-surface interactions of molecules can be obtained quickly and reliably in many areas [5-14]. So, most physical parameters of various molecules can easily be determined in this way. have a great impact in this field because easily every these molecules due to their explosive properties. Since researchers cannot operate experimental procedures on organic explosive molecules easily, they usually employ DFT to characterize these molecules.

It is good start with a brief explanation of what is meant by explosives. Explosive is an energetic material that may explode when interacted with an energy pulsation of any sort. This causes the explosion on its own, not with any aid from external reactants. An explosion causes an immediate release of heat and gas. There are three main characteristics of an explosive that are generally investigated: First of all, it is a detonated chemical material or combination that is energetically unstable. It is inflamed by shock, heat friction and a number of other factors, in addition some of these factors together may also cause an explosion. Secondly, it decomposes immediately in a detonation when it is flamed. Lastly, following detonation, a significant amount of pressurized hot gases are produced, they become larger at size quickly and forcefully enough to withstand restricting effects. Although there are a lot of products that have explosive characteristics, this paper focuses on pentaerythritol tetranitrate (PETN).

PETN is one of the simplest molecules containing both fuel and oxidant of the same molecule, and the chemical structure is presented in Fig. 1. Some properties of the PETN molecule are indicated in Table 1 [15]. It is thermally very stable. It was first synthesized by Tollens and Wiegand at 141°C [16].

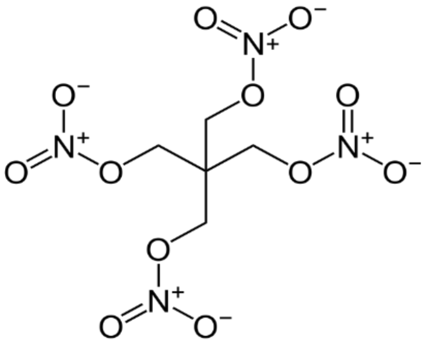


__Figure 1.__ Molecular structure of pentaerythritol tetranitrate (PETN).

Commercially avaliable nanocrystalline PETN is synthesized through the reaction of acetaldehyde and formaldehyde using a sol-gel process. Four equivalent formaldehyde and one equivalent acetaldehyde react in an aqueous solution containing calcium hydroxide or barium hydroxide at 65-70 °C to form PETN. Three molecules of the formaldehyde react with three hydrogens of acetaldehyde, while the fourth acts as a reducing agent, converting the aldehyde group to alcohol and is oxidized itself to formic acid. Then it is mixed at 70 °C for two hours (the mixture turns a slightly yellow color), sulfuric acid is added to precipitate calcium, finally, it is filtered. Then vacuum evaporation is used for crystallization. Pentaerythritol crystallizes from water in white tetragonal crystals (Figure 2). PETN can also be produced commercially by many patented methods [17-24]. 100 grams of pentaerythritol is added to 400 mL nitric acid by keeping the temperature 25 - 30 °C. It is completed gradually by adding 400 mL of concentrated sulfuric acid while product separation and mixing continues. Crude PETN (85-90 % of theoretically) is filtered directly from the mixture and washed with 50 % sulfuric acid first and then with water [25].

Table 1. *Some properties of the PETN molecule [15].*

Property	**Value**	**Unit**
Color	Colorless crystal solid	
Chemical formula	$C_5H_8N_4O_{12}$	
Molecular mass	316.1	*(g/mol)*
Energy of formation	-1509	*(kJ/kg)*
Enthalpy of formation	-1683	*kJ/kg*
Oxygen balance	-10.1 %	
Nitrogen content	17.72 %	
The volume of explosive gases	780	*(L/kg)*
Specific energy	1205	*(kJ/kg)*
Crystal density at 20 °C	1.76	*(g/cm^3)*
Melting temperature	286.3	*(°C)*
Fusion heat	36.4	*(kcal/kg)*
Specific combustion temperature	0.26	*kcal/kg*
Detonation velocity (ρ=1.7 g/cm^3)	8400	*(m/s)*
Detonation temperature	396	*(°F)*
Impact sensitivity	3	*(Nm)*
Friction sensitivity	60	*(N)*

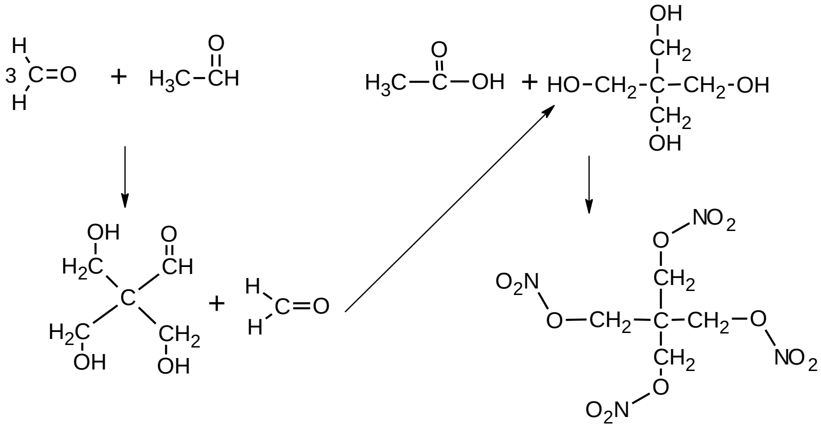


Figure 2. *Production mechanism of PETN.*

It can be mixed with nitrocellulose or synthetic rubber to be plastic moulded. It can be burnt above 100 °C emitting flaming red smoke and it can be burnt faster above approximately 210 °C [26]. Besides PETN can be added to gelatinous industrial explosives and this mixture can be used for seismic exploration [27].

II. MATERIAL AND METHODS

The initial geometry optimization of PETN structure was obtained with the help of molecular mechanics (MM). The semi-empirical PM3 self-consistent fields molecular orbital (SCF-MO) method [28, 29] at the restricted level [30]. Subsequently, optimization was obtained at Hartree-Fock (HF) level with the usage of several basis sets in a hierarchical manner (STO-3G, 3-21G, 6-31G* and 6-31G**) [31]. Then, geometry optimization was obtained by using the DFT method and 6-31G*,6-31G** basis sets respectively. Because, these basis sets reveal reliable results for determining the ground state and transition state geometries and thermochemistry [9, 10, 32-35]. The molecular geometry was optimized and the structure obtained was given in Figure 3. In DFT calculations, B3LYP comprises hybrid HF and local spin density (LSD) exchange functions with Becke's gradient correlation to LSD exchange [36, 37]. The correlation term of B3LYP comprises Vosko, Wilk, Nusair (VWN3) local correlation functional [38] and Lee, Yang, Parr (LYP) correlation functional [39]. DFT / B3LYP level 6-31G ** base set and Gaussian 03 computer program [40] Monte Carlo method was applied to determine thermodynamic properties and the average molecular volume of PETN molecule optimized in a vacuum. The ballistic characteristics for example, density, detonation velocity (D), detonation pressure (P), reaction temperature, reaction and products of PETN molecule were calculated using the B3LYP functional and basic set of polarization functions (d, p) containing 6-31G** and compared with the literature data (Table 5). Furthermore, we investigate the stability, the reactivity of PETN in different organic solvents (acetone, diethyl ether, ethanol, tetrahydrofuran (THF), toluene and methylene chloride) by using the mentioned functional and basis set. Finally, frontier orbital energy levels, dipole moment, electronegativity and chemical hardness values of PETN molecule were calculated at DFT / B3LYP level 6-31G ** for each organic solvents (Table 6).

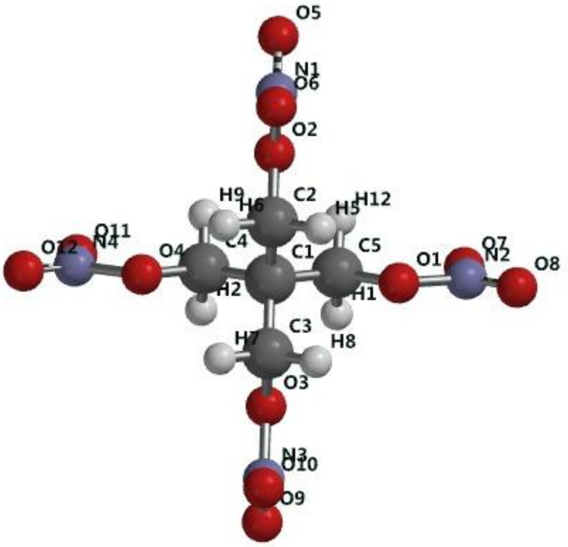


Figure 3. *Optimized pentaerythritol tetranitrate molecule (PETN).*

III. RESULTS AND DISCUSSION

A. DENSITY

In theoretical studies, Monte Carlo is the most commonly used method for calculating the density, which is one of the properties affecting the explosive properties of energetic compounds [41-44]. First, the possible geometric shape of the explosive molecule is defined and the estimated volume has been calculated 100 times to determine the average volume. In order to calculate the average density, the ratio between molar mass and the average volume was used. In this study, Monte Carlo method in Gaussian 03 computer program was used to calculate the average volume of PETN molecule. Probable gas products that may occur a consequence of the explosion reaction can be estimated by the help of the Kistiakowsky-Wilson rules shown in Table 2 [15].

Table 2. *Kistiakowsky–Wilson Rules [15].*

Order	Condition	Reaction
1	Oxygen atoms oxidize ‘H’ atoms to ‘H_2O’ molecules	$2H + O \rightarrow H_2O$ (g)
2	Remaining ‘O’ atoms oxidize all ‘C’ atoms to CO molecules	$C + O \rightarrow CO$ (g)
3	Remaining ‘O’ atoms oxidize all ‘CO’ molecules to ‘CO_2’molecules	$CO + O \rightarrow CO_2$ (g)
4	Excess of O, H, N atoms are converted to O_2, H_2 and N_2 Any excess C stays as C (solid)	$2H \rightarrow H_2$ (g) $2N \rightarrow N_2$ (g) $2O \rightarrow O_2$ (g)

When the PETN molecule is applied to the Kistiakowsky-Wilson Rules, the possible reaction products are estimated below given in equation 1;

$$C_5H_8N_4O_{12}\,(s) \rightarrow 2CO\,(g) + 4H_2O\,(g) + 3CO_2\,(g) + 2N_2\,(g) \tag{1}$$

As seen in equation 1, carbon atoms are converted to carbon monoxide, if any oxygen remains then hydrogen is than oxidized to water, if any oxygen still remains then carbon monoxide is oxidized to carbon dioxide, all the nitrogen is converted to nitrogen gas [15].

H_2O, CO_2, N_2 molecules are very stable products in explosion reactions. The more gas that is released as a product in explosion reactions, the greater the temperature of the explosion.

When the explosion reaction occurs, the energy released is named the detonation heat. It is equal to internal energy change if it occurs at a constant volume, or the enthalpy change if it occurs at a constant pressure [45]. In the detonation reaction, firstly, the bonds between the atoms constituting the explosive charge break off and a rapid bond formation occur to form new products. The explosion occurs in the form of chain reactions and the enthalpy change during multi-stage chain reactions is equal to the mathematical sum of the enthalpy changes in the steps. This is known as the Hess Law, and the heat of the explosion can be determined using equation 2 below [46-49].

$$\Delta H_d^o = \Sigma\Delta H_f^o(\text{products}) - \Sigma\Delta H_f^o(\text{energetic material}) \tag{2}$$

Another characteristic that can be calculated theoretically the standard enthalpy of formation (ΔH_f^o). The PM3 quasi-experimental molecular orbital method is used to approximate the standard enthalpy value of formation [50]. The method gives quite satisfactory results in the calculation of standard formation enthalpy [51, 52].

B. THE DETONATION VELOCITY AND THE DETONATION PRESSURE

When assessing the energy efficiency of explosive chemicals, there are two fundamental characteristics to take into consideration. Most significant concepts in this matter are detonation velocity (D) and detonation pressure (P). For the aim of finding out the effectiveness of energetic matters these ballistic parameters (D, P) are used. In an explosion, supersonic waves emerge and heat is released into the environment, which causes a rapid rise in pressure [53]. As a matter of fact, an explosive's detonation is a consequence of a set of complex relations that happen amidst the chemistry and hydrodynamics. Along with the detonation wave, there is an immediate increase in pressure and temperature.

In a matter of microseconds, detonation energy is released as kinetic energy and heat. When an explosive is detonated, a supersonic wave is generated around the initiation point then it is spread throughout the energetic materials, causing it to decompose exothermically. The detonation energy moves to the atmosphere, pushing an impulsive and extreme pressure similar to that of a powerful mechanical blast. In certain cases, when the explosive is combined with solid materials such as iron balls, nails, rocks etc the efficency is enhanced with regards to this change. The gaseous materials begin to expand because of the degree to which the medium is hot in terms of temperature and it functions around the enclosing atmosphere once the shock wave has spread away from the explosive. The detonation pressure is formed by the amount of the gas expansion. Theoretically D and P values of an explosive might be determined with the help of Kamlet-Jacobs equations given below; [54-57]

$$D = 1.01\ (N\ M^{1/2}\ Q^{1/2}\ )^{1/2}\ (1+1.30\ \rho) \qquad (3)$$

$$P = 1.558\ \rho^2\ NM^{1/2}\ Q^{1/2} \qquad (4)$$

where D is detonation velocity (km/s), P is detonation pressure (GPa), ρ is the density of the compound (g/cm^3), N is a mole of gaseous detonation products per gram of explosive (mol/g), M_{ave} is the average molar mass of gas products (g/mol), Q is the chemical energy of detonation (kJ/g).

Calculation methods of N, M and Q parameters are given in Table 3. We know that we face some problems because experimental techniques are inadequate for the calculation of Q and ρ parameters of some molecules. As per the principle of thermodynamic laws, the Q was determined using the deduction of reactant formation energies from product formation energies. The ρ was determined by dividing the molecular mass by the average molecular volume. The volume was described as inside a contour of 0.001 electrons Bohr^3 density that was evaluated using a Monte Carlo integration. This approach has been applied to a wide range of CHNO molecules. [41-44, 58-60].

Table 3. *Stoichiometric relations for calculation of N, M and Q parameters of $C_aH_bO_cN_d$ type explosives [56].*

	Stoichiometric relations		
Parameter	$c \geq 2a + b/2$	$2a + b/2 > c \geq b/2$	$b/2 > c$
N	$(b + 2c + 2d)/4M$	$(b + 2c + 2d)/4M$	$(b + d)/2M$
M	$4M/(b + 2c + 2d)$	$(56d+88c–8b)/(b+2c+2d)$	$(2b + 28d + 32c)/(b + d)$
$Q\times10^{-3}$	$(28.9b+94.05a+0.239\Delta H_f^o)/M$	$[28.9b+94.05(c/2-b/4)+0.239\Delta H_f^o]/M$	$(57.8c+0.239\Delta H_f^o)/M$

ΔH_f^o is the standard enthalpy of formation of the compound in kJ/mol

C. OXYGEN BALANCE/CONTENT

The mass percentage of the amount of oxygen they have in order to form stable products such as CO, H_2O and N_2 from explosive substances is defined as oxygen balance. In other words, the mass of the oxygen in the explosive is the surface of the explosive. The sensitivity of an energetic materials depends on their oxygen content [15, 46]. Although the calculation formulas of oxygen content are different in some studies [15, 46, 53], the results obtained are not different from each other. The oxygen content calculation formula for the percent area is given in equation 5 and the oxygen contents of some known explosives are given in Table 4.

$$\%\ \Omega = \frac{\mu_0}{\mu_{exp}}\left(c - 2a - \frac{b}{2}\right)x100 \qquad (5)$$

where μ_0 is the molar mass of oxygen, μ_{exp} is the molar mass of explosive, a, b, c, d are the number of carbon, hydrogen, oxygen and nitrogen atoms in the molecule [$C_aH_bO_cN_d$] respectively.

Table 4. *Oxygen values of some explosives [50].*

Explosive	**Chemical formula**	**Oxygen balance**
Ammonium nitrate	NH_4NO_3	19.90
Nitroglycerine	$C_3H_5N_3O_9$	3.50
EGDN	$C_2H_4N_2O_6$	0.00
PETN	$C_5H_8N_4O_{12}$	-10.13
RDX	$C_3H_6N_6O_6$	-21.60
HMX	$C_4H_8N_8O_8$	-21.62
Nitroguanidine	$CH_4N_4O_2$	-30.70
Picric acid	$C_6H_3N_3O_7$	-45.40
Tetryl	$C_7H_5N_5O_8$	-47.39
TATB	$C_6H_6N_6O_6$	-55.80
HNS	$C_{14}H_6N_6O_{12}$	-67.60
TNT	$C_7H_5N_3O_6$	-74.00

As can see in Table 5 and Table 6, some detonation parameters of PETN molecule are calculated using the B3LYP functional and basic set of polarization functions (d, p) containing 6-31G** and compared with the literature data.

Table 5. *Some theoretical results were obtained for the PETN molecule in the gas phase.*

μ_w *(g/mol)*	**ρ** *(g/cm$^{3)}$*	**N** *(mol/g)*	**M** *(g/mol)*	ΔH_f^o *(kJ/mol)*	**Q** *(kJ/g)*	**D** *(km/s)*	**P** *(GPa)*	ΔH_d^o *(kJ/mol)*	**Ω** *(%)*
316.14	1.758	0.0316	30.4	-357.15	1651.30	8.830	34.16	-2011.55	-10.13

In Table 5, μ_w is molecular mass, ρ is the density of the compound, N is moles of gaseous detonation products per gram of explosive, M is the average molar mass of gas products, ΔH_f^o is standard heat of formation, Q is chemical energy of detonation, D is detonation velocity, P is detonation pressure, ΔH_d^o is detonation heat, Ω is oxygen balance (content), respectively. The calculation of ΔH_d^o is achieved according to equation 2. In this equation, $\Sigma\Delta H_f^o(\text{products})$ is equal to (4xΔH_{H2O}^o + 2xΔH_{CO}^o + 3xΔH_{CO2}^o + 2xΔH_{N2}^o = 4x(-241.8 kj/mol) + 3x(-393.5 kj/mol) + 2x(-110.5 kj/mol) + 0 = -2368.7 kj/mol; $\Sigma\Delta H_f^o(\text{energetic material})$ is equal to -357.15 kj/mol which is calculated according to PM3 quasi-experimental molecular orbital method.

Table 6. *Some literature values for the PETN molecule in the gas phase [54, 61-68].*

	Ref. [54]	Ref. [61]	Ref. [62]	Ref. [63]	Ref. [64]	Ref. [65]	Ref. [66]	Ref. [67]	Ref. [68]
ρ *(g/cm^3)*	1.765	1.780	1.770	1.770	1.763	1.845	1.760	1.778	1.760
D *(km/s)*	8.160	8.260	8.080	8.300	8.274	8.843	8.481	8.564	8.270
P *(GPa)*	30.41	30.00	28.70	33.50	31.50	33.80	30.44	31.39	33.70

Furthermore, we investigate the stability, the reactivity of PETN in different organic solvents (acetone, diethyl ether, ethanol, tetrahydrofuran (THF), toluene and methylene chloride) by using the mentioned functional and basis set. Therefore, HOMO and LUMO energy levels, dipole moment, electronegativity and chemical hardness values of PETN molecule were calculated at DFT / B3LYP level 6-31G ** for each organic solvents.

The highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO) and the energy difference between them have been used in the understanding of organic reactions and chemical stability [69]. The tendency to donate an electron is reflected by the HOMO, while the tendency to receive an electron is reflected by the LUMO. In addition to HOMO & LUMO, there are some other chemical reactivity descriptors, such as electronegativity (χ) and chemical hardness (η) as defined by Koopman's theorem [3, 36, 70-74]. Electronegativity (χ), which is a measure of the power of an atom or a group of atoms to attract electrons, can be calculated from $\chi = -1/2(E_{HOMO} + E_{LUMO})$ [75, 76]. Chemical hardness (η), known as the resistance of an atom to charge transfer, can be calculated as $\eta = -1/2\ (E_{HOMO} - E_{LUMO})$ [76-78]. HOMO, LUMO, Δ (LUMO–HOMO), dipole moment, electronegativity (χ), chemical hardness (η) and maximum charge transfer parameter [$\Delta N_{max} = -(E_{HOMO} + E_{LUMO})/2(E_{LUMO} - E_{HOMO})$] values of PETN molecule in different solvents are given in Table 7.

Table 7. *Dipole moment, HOMO, LUMO, Δ (LUMO-HOMO), electronegativity (χ) and chemical hardness (η) values of PETN, calculated at the B3LYP 6-31G** (d,p) theoretical level.*

Solvent	**Dipole Moment** *(Debye)*	**HOMO** *(eV)*	**LUMO** *(eV)*	**LUMO–HOMO** *(eV)*	***χ*** *(eV)*	***η*** *(eV)*	**ΔN_{max}**
Acetone	4.11	-8.79742	-2.17120	6.62622	5.48431	3.31311	0.82767
Diethyl ether	4.12	-8.78404	-2.15696	6.62708	5.4705	3.31354	0.82548
Ethanol	4.21	-8.87699	-2.22447	6.65252	5.55073	3.32626	0.83438
THF	4.24	-8.82215	-2.21129	6.61086	5.51672	3.30543	0.83449
Toluene	3.76	-8.90862	-2.33856	6.57006	5.63259	3.28503	0.85594
Methylene Chloride	3.92	-8.85411	-2.25783	6.59628	5.55597	3.29814	0.84229

It is easier for high HOMO energy molecules to donate their electrons than low HOMO energy molecules, making them more reactive in oxidation reactions. On the other hand, molecules having low LUMO energy are more convenient to accept electrons than molecules with high LUMO energy [79]. The sensitivity of explosives has a relation with the LUMO–HOMO energy gap. If it has narrowed the gap of the explosive is more sensitive [80-82]. A simple description of the electronegativity is the force of an atom to attract bonding electrons. In the case of 2 atoms that have a covalent bond, the electronegative one will attract strongly the shared electrons. The chemical hardness value of a compound is known to be related to its kinetic stability [83, 84] and it is recognized that the harder compounds have higher kinetic stability [44, 85, 86].

As seen in data from Table 7; electronegativity is aligned from large to small;

PETN in Toluene > PETN in Methylene Chloride > PETN in Ethanol > PETN in THF> PETN in Acetone > PETN in Diethyl ether.

Chemical Hardness (η) is large to small;

PETN in Ethanol > PETN in Diethyl ether > PETN in Acetone > PETN in THF> PETN in Methylene Chloride > PETN in Toluene.

According to the literature [87,88] the more electronegative compound is, the less susceptible it is to oxidation and that the hard molecules have a greater frontier orbital gap (ΔE) than the soft molecules.

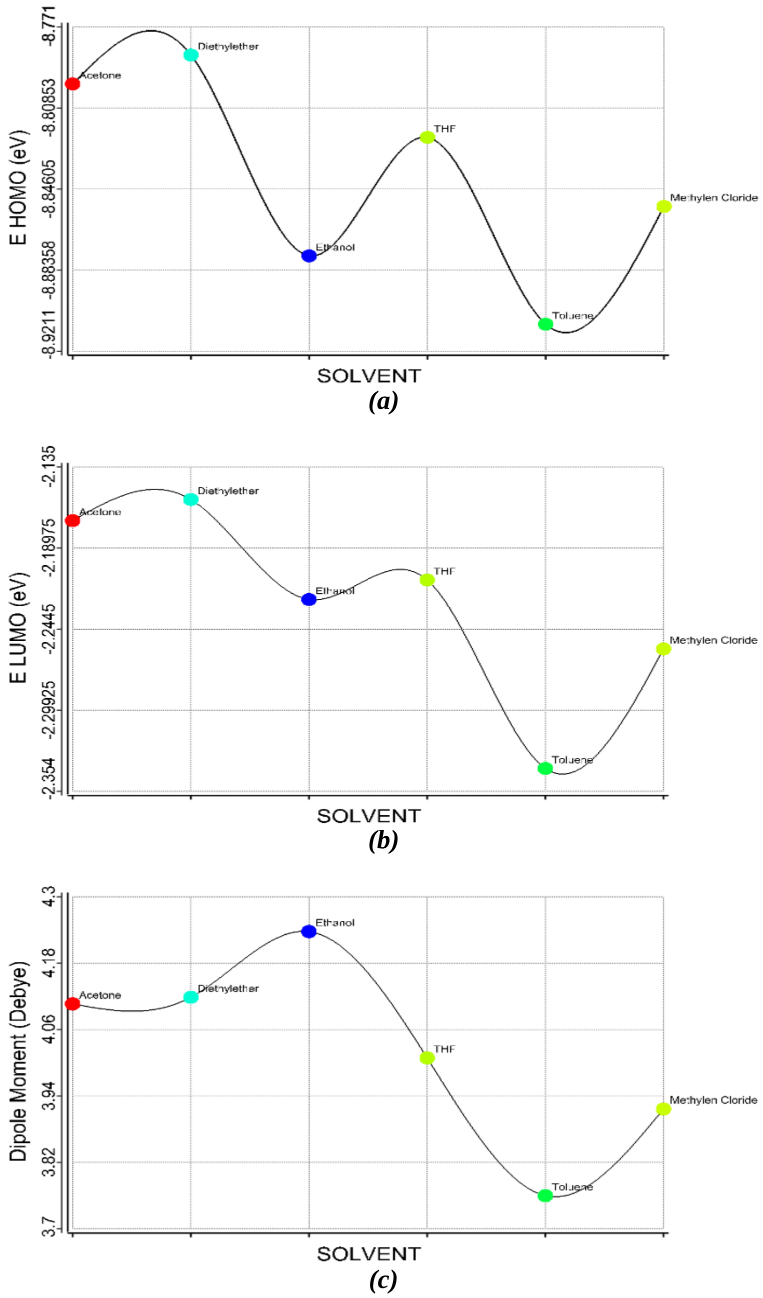
As seen in data from Table 7; Stability; (LUMO–HOMO difference) is from large to small;

PETN in ethanol> PETN in Diethyl ether > PETN in Acetone > PETN in THF> PETN in Methylene Cloride > PETN in Toluene.

Polarity: (Dipole moment)

PETN in THF > PETN in ethanol > PETN in Diethyl ether > PETN in Acetone > PETN in Methylene Cloride > PETN in Toluene.

The lowest chemical hardness value (≅3.28 eV), the highest electronegativity value (≅5.63 eV) and the lowest LUMO–HOMO value (≅6.57 eV) for PETN dissolved in toluene were calculated (Table 7 and Figure 4). With these results, we can say that PETN molecule has a more unstable structure than other organic solvents studied in Toluene. So, it can interact with other molecules more easily. PETN in ethanol has a large frontier orbital gap so it has low chemical reactivity and high kinetic stability. Our theoretical results show that the PETN has more stability in ethanol than the other solvents. The ΔE of PETN in toluene narrow and not stable. So, it is more sensitive to explode. The solvents-PETN investigations are also classified according to ΔN_{max} values, decreasing as PETN in Toluene > PETN in Methylene Chloride > PETN in Ethanol > PETN in THF> PETN in Acetone > PETN in Diethyl ether. These theoretical trends would be in good agreement with the enhanced explosive reactivity of PETN [89-90].



(a)

(b)

(c)

Figure 4. *E_{HOMO} (eV)* ***(a)****, E_{LUMO} (eV)* ***(b)*** *and Dipole moment* ***(c)*** *values of PETN for each solvent.*

IV. CONCLUSION

An energetic material in the organic solvent is more prone to detonate than its pure form. The rate and pressure of the detonation can be related to the molecular structure both of the chemicals containing solvent. The interaction between solute and solvent molecules would be minimum in order to experience a detonation having maximum brisance. Toluene without any functional group was found theoretically the most convenient solvent to prepare an unstable explosive mixture PETN solution. Since the theoretically calculated energy gap of PETN in toluene is narrow, it is more sensitive to explode. The detonation rate and pressure can also change depending on the density, the number of gaseous products, the average molar mass of those, oxygen content, and enthalpy change by detonation reaction.

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