

The Effects of BTTN, TMETN and DEGDN Molecules on the Explosion Properties of PETN Molecule

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Abstract: Molecular modelling is an appreciated tool that brings valuable data on physical and chemical characteristics of materials that eliminates the necessity of conducting any experiment. This method allows the calculation of the performance of energetic molecules to be synthesized. In the work, the detonation parameters of the energetic organic compounds Pentaerythritol tetranitrate (PETN), Butanetriol trinitrate (BTTN), Trimetylolethane trinitrate (TMETN) and Diethyleneglycol dinitrate (DEGDN) has theoretically been calculated and some values compared with the literature values. Moreover, three hypothetical molecules combining PETN with other explosive molecules have been designed. The density functional theory (DFT) with B3LYP 6-31G (d,p) basis set was employed for the calculation of the detonation properties. It has been concluded that all molecules have the effect of increasing the explosion parameters of PETN.

PETN Molekülünün Patlama Özelliklerine BTTN, TMETN and DEGDN Moleküllerinin Etkileri

Anahtar Kelimeler

Yoğunluk fonksiyonu teorisi,
Patlama hızı,
Patlama basıncı,
Patlama ısısı,
Oksijen içeriği

Öz: Moleküler modelleme deney yapmaksızın moleküllerin fiziksel ve kimyasal özellikleri hakkında değerli veriler sunan bir araçtır. Bu yöntem sentezlenecek enerjik moleküllerin performanslarının hesaplanmasına olanak sağlamaktadır. Çalışmada enerjik organik bileşik olan Pentaeritritol tetranitrat (PETN), Bütantriol trinitrat (BTNN), Trimetiloletan trinitrat (TMETN) ve Dietilen glikol dinatrat (DEGDN) moleküllerinin patlama parametreleri kuramsal olarak hesaplanmış ve bazı değerler literatür değerleriyle karşılaştırılmıştır. Ayrıca PETN ve diğer moleküller arasında farklı üç boyutlu moleküller modellenmiştir. Patlama özelliklerinin hesaplanması için B3LYP 6-31G (d,p) temel seti ile yoğunluk fonksiyonel teorisi (YFT) kullanılmıştır. Tüm moleküllerin PETN' nin patlama parametrelerini artırıcı etkide bulunduğu sonucuna ulaşılmıştır.

1. Introduction

Explosives are unstable energetic molecules that can be initiated by heat, spark, flame, shock, impact, friction or by any energy pulse. Upon initiation, explosion occurs resulting in an immediate expansion of gaseous products emitting heat and great change in pressure. This phenomenon is called an explosion. The reaction enthalpy can be defined with the difference products and reactants. The reaction heat is defined as the "heat of explosion" when an energetic molecule is activated to gaseous products at constant pressure. The explosives consist of high percent of carbon (C), hydrogen (H), oxygen (O) and nitrogen (N). When an

explosive molecule is burnt in abundant oxygen, CO₂ and H₂O which are the highest oxidation states of C and H, respectively, are produced. The nitrogen content of the explosive is converted to molecular nitrogen (N₂) because the internal energy of N₂ is lower than the nitrogen oxides compounds such as NO, NO₂, N₂O₃ etc. Since the nitro (-NO₂) and nitrate ester (-ONO₂) functional groups in an explosive are the primary sources of oxygen, they contribute to the detonation or combustion processes [1].

The specific and sensitive manufacturing of energetic materials (explosives, propellants, and pyrotechnics,

for example) is an essential research area for their usage in the military, defense, and industrial domains.

The two concepts of energy and stability are incompatible. Various chemical additives can be added to the explosive material to enhance or reduce them, or new explosives can be created by modifying the substituents in the present structure [1, 2].

Because the synthesis of energetic materials is hazardous and characterization is challenging, theoretical techniques are frequently employed to determine the pyrotechnical features of explosive materials. This technique not only gives advice for experimental synthesis and reduces experimental blindness, but it also pre-evaluates performance and shows the link between structures and qualities [1-3].

Pentaerythritol tetranitrate (PETN, $C_5H_8O_{12}N_4$) is a thermally stable explosive molecule, which can be synthesized by mixing pentaerythritol with concentrated nitric acid by efficient stirring and cooling. It is a powerful explosive which shows considerable bristle on detonation. It is the most stable and least reactive of the common nitrate ester explosives. Since PETN is highly sensitive to friction and impact, it is generally desensitized by using wax. This mixture is employed in boosters, detonation cord and as a base charge in detonators. Synthetic polymers can be mixed with PETN to produce plastic bonded explosives (PBXs) such as Semtex-1A. A cast mixture of PETN and Trinitrotoluene (TNT) in equal proportions is known as pentolite and has been extensively used as a military energetic material. The physical, chemical and explosive properties of PETN commend its use as a high explosive [2, 3].

1, 2, 4 - Butanetriol trinitrate (BTTN, $C_4H_7N_3O_9$) is a significant liquid nitrate ester molecule. The BTTN molecule as an additive to propellant formulations enhance mechanical properties of propellant at low temperatures. Therefore, BTTN could be introduced as an alternative to nitroglycerin (NG) [4, 5].

Diethylene glycol dinitrate (DEGDN, $C_4H_8N_2O_7$) is a nitrated alcohol ester that has colorless, odorless, viscous, oily properties. It is synthesized by the reaction of concentrated HNO_3 upon diethylene glycol. Although it is chemically similar to many strong explosives, plain diethylene glycol dinitrate is extremely difficult to ignite and will not detonate. When mixed with nitrocellulose and extruded under pressure, DEGDN can be used as a smokeless powder for artillery and a solid propellant for rockets [6].

Trimethylolethane trinitrate (TMETN, $C_5H_9N_3O_9$), also called metriol trinitrate (METN, MTN, METRTN) or nitro-pentaglycerin, is a nitrate ester explosive molecule served as an alternative to nitroglycerin. It is an odorless oily liquid and used as a plasticizer in most solid propellants and smokeless powders. It can be

initiated especially by electrostatic discharge, impact or friction and can be used as a viscous plasticizer together with nitrocellulose [7]. TMETN, DEGDN and BTTN have recently been considered as substitutes for nitroglycerin in rocket propellants [2]. The chemical structures of PETN, BTTN, DEGDN and TMETN are shown in Figure 1.

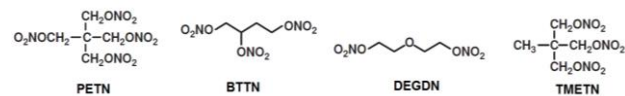


Figure 1. The chemical structures of PETN, BTTN, DEGDN and TMETN

In this current study, the detonation parameters of the explosive molecules, Pentaerythritol tetranitrate (PETN), Butanetriol trinitrate (BTTN), Diethylene glycol dinitrate (DEGDN) and Trimethylolethane trinitrate (TMETN) has computationally been calculated and compared with the literature values. Three unique hypothetical molecules have been designed. First molecule has been designed as the combination of two well-known energetic materials: PETN and BTTN; the second one is the combination of PETN and TMETN; third one is the combination of PETN and DEGDN. The main goal of the study is to observe the effects of BTTN, TMETN and DEGDN molecules on explosive properties of PETN. The idea of pairing these widespread molecules to design explosive molecules with better explosive characteristics has inspired us to study them. The density functional theory at B3LYP 6-31G (d, p) basis set was employed for the determination of the detonation properties of these hypothetical molecules.

2. Material and Method

The first structure optimization calculations of molecules considered in the present study were achieved by the following sequence: MM2 method, PM3 method, STO and HF 6-31G (d, p) and finally DFT-B3LYP 6-31G (d, p) level were used [8-12]. These basis sets were chosen because they give consistent results for forecasting ground and transition state geometries, as well as thermochemistry, in non-cyclic straight chain structures [13-17]. No imaginary frequencies have been observed in single point energy calculations. The zero point vibrational energies (ZPE) were added to the calculated energy values to find the total electronic energies. The heat of formation values of all the chemical structures were determined by the PM3 method in Spartan'08 [18]. All these computations were performed at standard temperature and pressure (STP) [19]. The molar density of the molecule is defined as the ratio of molar mass to molar volume. The molar volumes of the molecules were calculated as the average of 100 single point calculations on optimized molecule geometry. Almost all organic compounds can be studied with the present approach [20].

3. Results

3.1. Geometries

All the structures currently under consideration are assumed as candidates of effective explosives (See Figure 2). The B3LYP 6–31G (d, p) basis set was used to optimize the geometries shown in Figure 2. The nature of the stationary point has been characterized using harmonic vibrational analyses. The results revealed that the optimized molecules all have minimum energy without an imaginary frequency on the potential energy surface. Figure 2 shows the geometry optimized chemical structures.

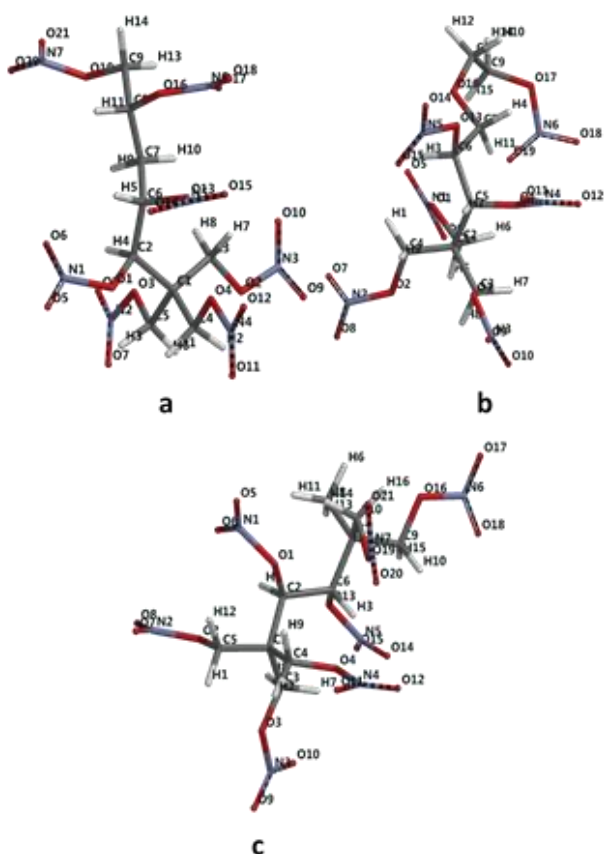


Figure 2. The optimized geometry of a. PETN-BTTN- b. PETN-DEGDN c. PETN-TMETN

3.2. Explosive properties

Detonation parameters are required for acquiring a fundamental understanding of a material's energetic performance. The detonation pressure (P) and detonation velocity (D) are the two significant parameters, which are utilized to calculate the performance of explosive materials. These parameters were calculated using the empirical Kamlet-Jacobs [21-25] equations as follows:

$$D = 1.01 (N M_{ave}^{1/2} Q^{1/2})^{1/2} (1 + 1.30 \rho) \quad (1)$$

$$P = 1.558 \rho^2 N M_{ave}^{1/2} Q^{1/2} \quad (2)$$

where each term in equations 1 and 2 has the following definition: D is detonation velocity (km/s); P

is detonation pressure (GPa); ρ is density of a compound (g/cm^3); N is moles of gaseous detonation products per gram of explosive; M_{ave} is average molecular mass of gaseous products; Q is chemical energy of detonation (kJ/g). The parameters N, M_{ave} and Q are determined based on the chemical structure of each explosive (see Table 1) [26]. In Table 1, M denotes the compound's molecular mass (in g/mol), and ΔH_{of} denotes the compound's gas phase standard heat of formation (in kJ/mol). The heats of formation in the gas state of all the molecules considered in the current work were calculated by Parametric Method-3 (PM3) on structurally optimized geometries [27-29].

Table 1. Calculating the N, M_{ave} and Q parameters of $\text{C}_a\text{H}_b\text{O}_c\text{N}_d$ type explosives using stoichiometric relationships

Paramt.	Stoichiometric relations		
	$c \geq 2a + b/2$	$2a + b/2 > c \geq b/2$	$b/2 > c$
N	$(b + 2c + 2d)/4M$	$(b + 2c + 2d)/4M$	$(b + d)/2M$
M_{ave}	$4M/(b + 2c + 2d)$	$(56d + 88c - 8b)/(b + 2c + 2d)$	$(2b + 28d + 32c)/(b + d)$
$Q \times 10^{-3}$	$(28.9b + 94.05a + 0.239\Delta H_{of}^g)/M$	$[28.9b + 94.05c - 5(c/2 - b/4) + 0.239\Delta H_{of}^g]/M$	$(57.8c + 0.239\Delta H_{of}^g)/M$

The molar volume of molecules was determined using the Gaussian 03 software's Monte Carlo approach [20]. The Ω symbol shows percent of oxygen balance of the energetic materials in this work. The predicted density data and detonation characteristics of PETN, BTTN, TMETN, DEGDN and the uniquely designed molecules pair molecules are listed in Table 2. All molecules are stoichiometrically consistent with $2a + b/2 > c \geq b/2$ relation. Consequently, relations in the second column of Table 1 have been employed in the calculations. Wu et al. [30] developed two series of novel energetic molecules by substituting carbon atoms in the rings of RDX and HMX compounds with varying quantities of boron atoms, and their performance was studied theoretically using the density functional theory approach (DFT-B3LYP 6-31G (d, p) level). The findings revealed that features including electrical structure, formation heat, density, and sensitivity may all be altered. The burst velocity (8.85 km/s) and burst pressure (36.9 GPa) were both found to be higher than the main structure.

The density data in parenthesis have been obtained from ref [31]. The correctness of the method is supported by the closeness of the estimated density data produced with the methodology utilized in this work (DFT - B3LYP 6–31G (d, p)) to the experimentally acquired data.

As seen from Table 2, the presence of PETN causes a remarkable increase in the density of PETN-BTTN, PETN-TMETN, PETN-DEGDN pair molecules. Consequently, the presence of PETN also resulted in a

Table 2. The density and the detonation parameters of explosives calculated at the B3LYP/6-31G (d,p) basis set

	ρ g/cm ³	N mol/g	M _{ave} g/mol	ΔH_f° kJ/mol	Q kJ/g	D km/s	P GPa	Ω %
PETN	1.76 (1.77*)	0.0316	30.4	-357.2 (-386.6**)	1651 (1629**)	8.83 (8.30**)	34.16 (33.50**)	-10.13
BTTN	1.70 (1.74*)	0.0321	29.16	-304.5	1610	8.57	31.51	-16.59
TMETN	1.63 (1.64*)	0.0323	26.90	-298.7	1569	8.13	27.64	-34.49
DEGDN	1.53 (1.58*)	0.0331	25.54	-369.1	1449	7.63	23.32	-40.79
PETN-BTTN (C ₉ H ₁₃ O ₂₁ N ₇)	2.11	0.0311	30.96	-532.7	1675	10.05	49.05	-10.09
PETN-TMETN (C ₁₀ H ₁₅ O ₂₁ N ₇)	1.97	0.0312	29.86	-500.2	1667	9.47	41.86	-18.27
PETN-DEGDN (C ₉ H ₁₄ O ₁₉ N ₆)	1.98	0.0314	29.63	-625.5	1606	9.45	41.89	-18.81

significant rise of D and P of pair molecules. It is clear from the calculations that the introduction of PETN molecules to BTTN, TMETN or DEGDN molecules yield more powerful explosives with higher detonation characteristics.

3.3. Heat of detonation

The heat of detonation (ΔH_d°) is the huge energy released as heat upon detonation reaction. It is the energy difference between the products and the explosive itself, as stated by Hess Law [32, 33] and shown in equation 3. Kistiakowsky and Wilson rules were applied to molecules to clarify the identification and amount of gaseous decomposition products [34, 35]. In the formula ΔH_f° is the standard formation enthalpy.

In the calculations the following standard formation enthalpy values are used: $\Delta H_f^\circ \text{H}_2\text{O}(\text{g}) = -242$ kJ/mol; $\Delta H_f^\circ \text{CO}(\text{g}) = -111$ kJ/mol; $\Delta H_f^\circ \text{CO}_2(\text{g}) = -394$ kJ/mol. The standard formation enthalpies of explosives have been calculated by PM3 method and listed in Table 2.

$$\Delta H_d^\circ = \sum \Delta H_f^\circ(\text{det. products}) - \sum \Delta H_f^\circ(\text{exp.}) \quad (3)$$

The moles of detonation products have been calculated by Kistiakowsky and Wilson rules and presented in Table 3. The presence of PETN in the new designed molecules increased the heat of detonation tremendously as seen from Table 3. Similar to the studies in the literature [30, 36-38], it is seen that the explosion heat values increase by changing the substitution groups of energetic materials or adding new groups. This means that the new energetic materials obtained will generate more heat compared to the original explosives. This means that the detonation will produce more heat when compared to those of original explosives PETN, BTTN, TMETN and DEGDN.

3.4. Explosive power and power index

The two main reaction products of an explosive reaction are heat and hot gas. The volume of explosive

product gases can be used to estimate the amount of work done by energetic materials. Standard parameters must be established to determine the volume of produced gas since the gas volume fluctuates with temperature.

The standard conditions (Pressure=1atm and Temperature 298.15 K) also enable the explosive scientists to perform evaluations among the different energetic materials. To calculate how much gas was released per gram of explosive, the molar mass was divided by the total volume of gas generated during the explosion [39-42]. Total moles of produced gas have been calculated and listed in Table3. Multiplication with 22.4 dm³/mol gives the total volume of product gases.

The explosive power value can be calculated using the heat of explosion "Q" and the volume of created gas "V," as shown in equation 4. The power index can be calculated as shown in equation 5.

$$\text{Explosive Power} = QV \quad (4)$$

$$\text{Power Index \%} = QV / Q_{PA}V_{PA} \quad (5)$$

The explosive power results were then compared to a conventional explosive's explosive power. Table 3 displays the power index values of PETN, BTTN, TMETN, DEGDN and the pair molecules. The compounds under consideration have power index values ranging from 107 to 111 percent and they are listed in the order below: TMETN>BTTN> PETN-TMETN> PETN-DEGDN>DEGDN> PETN> PETN-BTTN. The results have shown that there is no significant difference in power index values in the pair molecules because of the chemical similarities (all are aliphatic nitrates) between the parent molecules and pair molecules.

4. Discussion and Conclusion

In this study, PETN, BTTN, TMETN, DEGDN, and three different pair explosive compounds have been studied computationally. The corrected absolute and relative

Table 3. The power index values of molecules and the decomposition products of molecules projected by the Kistiakowsky and Wilson Rules

Molecule	Chemical Formula	Products and moles						ΔH°_d kJ/mol	Q kJ/g	V dm ³ /g	QV	Power Index %
		H ₂ O	N ₂	CO	CO ₂	C	O ₂					
PETN	C ₅ H ₈ N ₄ O ₁₂	4.0	2.0	2.0	3.0	-	-	-2015	1651	0.78	1286.8	107
BTTN	C ₄ H ₇ O ₉ N ₃	3.5	1.5	3.0	1.0	-	0.25	-1270	1610	0.86	1383.6	115
TMETN	C ₅ H ₉ O ₉ N ₃	4.5	1.5	4.5	-	0.5	-	-1290	1569	0.92	1446.4	125
DEGDN	C ₄ H ₈ O ₇ N ₂	4.0	1.0	3.0	-	1.0	-	-932	1449	0.91	1324.0	110
PETN-BTTN	C ₉ H ₁₃ O ₂₁ N ₇	6.5	3.5	3.5	5.5	-	-	-3595	1675	0.77	1283.9	106
PETN-TMETN	C ₁₀ H ₁₅ O ₂₁ N ₇	7.5	3.5	6.5	3.5	-	-	-3415	1667	0.83	1377.5	114
PETN-DEGDN	C ₉ H ₁₄ O ₁₉ N ₆	7.0	3.0	6.0	3.0	-	-	-2916	1606	0.83	1339.6	111

total energies of the geometry optimized structures were determined at the B3LYP 6-31G (d,p) basis set. The obtained results show that by combining BTTN, TMETN, DEGDN, and PETN, it is feasible to significantly increase density, detonation velocity, and pressure. All the investigated pair compounds showed better explosive properties than parent molecules. The recently designed pair molecules are all alternatives to their parent molecules. They're all potential high-explosives candidates. May the current study will inspire organic chemists to synthesize these pair molecules and test the explosive characteristics experimentally.

Declaration of Ethical Code

In this study, we undertake that all the rules required to be followed within the scope of the "Higher Education Institutions Scientific Research and Publication Ethics Directive" are complied with, and that none of the actions stated under the heading "Actions Against Scientific Research and Publication Ethics" are not carried out.

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