

## DFT Study: Investigation of TATB Derivatives as a Candidate of Energetic Materials

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### ABSTRACT

The explosive substances are chemically reactive materials that, when heated or shocked (impact, compression, and friction), produce a great deal of gas and intense heat. They are extensively employed in both industrial and military applications. They must first be conceptually explored before beginning the experimental studies for the development of their properties because the infrastructure and other requirements for experimental investigations are not frequently readily available. In this study the structurally modified 2,4,6-triamino-1,3,5-trinitrobenzen (TATB) molecules were investigated as a candidate of energetic materials via DFT (with B3LYP/6-31G (d,p) basis set). In order to achieve this purpose, theoretically formed molecules were optimized, and after that, ballistic parameters, including detonation pressure (P) and detonation velocity (D), were examined by using Kamlet-Jacobs equations. According to the obtained data, it was found that the molecular alterations mentioned can reduce the sensitivity of TATB's.

## DFT Çalışması: Enerjik Malzeme Adayı Olarak TATB Türevlerinin İncelenmesi

### Araştırma Makalesi

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Patlayıcı maddeler, ısıtıldıklarında veya şoka (darbe, sıkıştırma ve sürtünme) maruz kaldıklarında çok miktarda gaz ve yoğun ısı üreten kimyasal olarak reaktif malzemelerdir. Hem endüstriyel hem de askeri uygulamalarda yaygın olarak kullanılmaktadırlar. Özelliklerinin geliştirilmesi için deneysel çalışmalara başlamadan önce teorik olarak araştırılmaları gerekir. Çünkü deneysel çalışmalar için altyapı ve diğer gereksinimler sıklıkla hazır değildir. Bu çalışmada, yapısal olarak modifiye edilmiş 2,4,6-triamino-1,3,5-trinitrobenzen (TATB) molekülleri, DFT (B3LYP/6-31G (d,p) temel seti ile) aracılığıyla enerjik malzeme adayları olarak incelenmiştir. Bu amaç için teorik

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## Introduction

The exponential growth in global population and economic development over time has significantly fueled the surge in worldwide energy demand. This escalating need for energy has propelled the utilization of various energetic materials across a spectrum of critical sectors, including propulsion, defense, and industrial applications. Comprising a diverse array of substances such as propellants, pyrotechnics, and explosives, these materials harbor substantial chemical energy, capable of being harnessed for diverse purposes. Remarkably versatile, energetic materials manifest in both solid and liquid states, offering adaptable solutions to meet specific operational requirements. Within their chemical composition, one typically finds a symbiotic interplay between fuel and oxidizer elements, either coexisting within the same molecular framework or as distinct entities, facilitating efficient energy release and utilization across a myriad of applications and industries (Pu et al., 2020; Türker, 2020; P. Wang et al., 2020b; Wu et al., 2020; Zhu et al., 2020). These materials release a large quantity of energy to the exterior at once together with a stimulating force like collision, friction, electrostatic discharge (ESD) or electrical spark, shock, and thermal / heating thanks to the chemical structure inside them (Xi et al., 2019; Xiao et al., 2019; Yongjin and Shuhong, 2019; Zhai et al., 2019). The shockwave travels through energetic material as it explodes. At the wave front the material is highly compressed, leading to the temperature rise, which triggers exothermic chemical reactions and create a chemical reaction zoom after the wave front (Bu et al., 2020; Shi et al., 2020). Experimental research into the breakdown of energetic materials by repulsive force is challenging. The governing factors, such as thermochemical processes and kinetic models, may be observable, though.

For this reason, it's crucial to get some theoretical information prior to starting experiments. High sensitivity frequently has a correlation with high detonation performance. The most potent explosives are frequently more susceptible than average to inadvertent triggers like shock or collision leading to unintended detonation. This finding, that is partially obvious, is based on experience, but it is also backed up by thorough research. The fundamental issue is that factors supporting either great performance or poor sensitivity typically work against the other. As a result, designing better explosives frequently involves a "search for balance," as it

was recently put forth. The literature provides an overview of the numerous theoretical techniques that have been employed to forecast the mechanical and spark sensitivity of materials, as well as their benefits and drawbacks, as well as the range of applications for each (Wang et al., 2019a; Wang et al., 2019b; Xi, Mazian et al., 2019; Zhang et al., 2019; Wang and Zhu, 2020a; Borisov et al., 2020; Jeong et al., 2020; Li et al., 2020; Pu et al., 2020). As a complement, the theoretical models for explosives' thermal stability are also briefly introduced. A number of empirical principles, including simple oxygen balance, chemical characteristics, and the ratios of carbon (C) and hydrogen (H) to oxygen (O) for various types of explosive compounds have been claimed to constitute the only foundation for the current ability to forecast sensitivity.

There are four main categories to consider while choosing explosives. First; dynamites, such as granular dynamite (straight, high-density extra, and low-density extra), as well as gelatin dynamite (straight, ammonia, and semi gelatin). Unless a case-specific waiver is secured from the regional blasting officer, use is forbidden by policy. Second; cartridges and bulk items for water gels, emulsions, and slurries. Third; dry Blasting Agents, which include Packaged (waterproof) ANFO (Ammonium nitrate+ fuel oil), Aluminized ANFO, Poured or Bulk ANFO, and Densified ANFO. Lastly; binary Explosives - An explosive that is created in the field by combining two separate items.

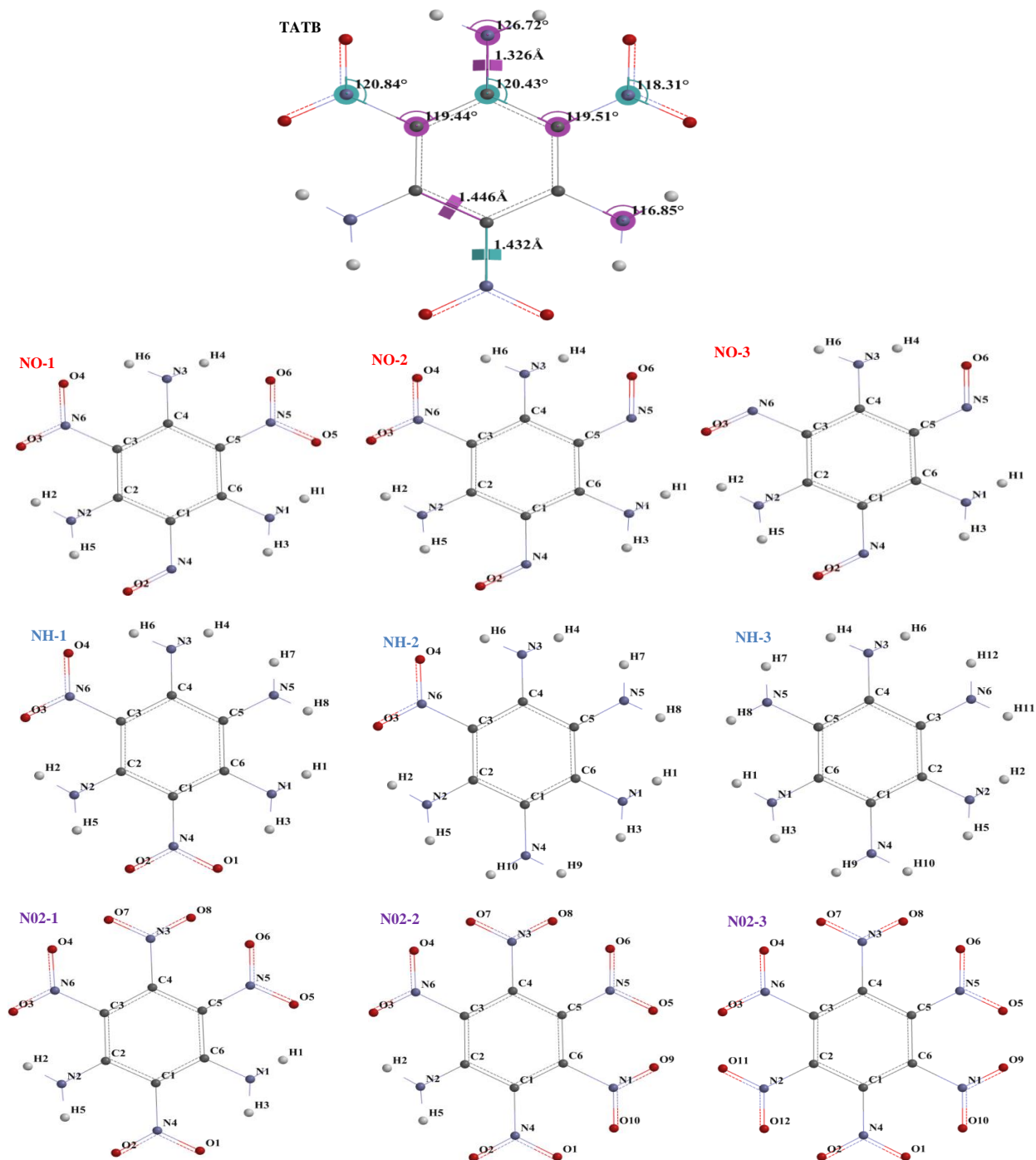
When compared to all explosives, 2,4,6-triamino-1,3,5-trinitrobenzene, also known as TATB, is appealing because to its high temperature safety and resistance to accidental ignition and detonation. In this study, the structurally modified 2,4,6-triamino-1,3,5-trinitrobenzen (TATB) molecules were investigated as a candidate of energetic materials via DFT approach (with B3LYP/6-31G\* (d,p) basis set).

The utilization of theoretical approaches, such as density functional theory (DFT), in the design and modification of energetic materials like 2,4,6-triamino-1,3,5-trinitrobenzen (TATB), offers a practical pathway to enhance safety and efficiency in their synthesis. This study not only underscores the significance of theoretical modeling in advancing energetic materials science but also underscores its pivotal role in promoting safer chemical innovation for diverse practical applications.

The structurally modified 2,4,6-triamino-1,3,5-trinitrobenzen (TATB) molecules would find potential usage in various applications such as explosives, propellants, pyrotechnics, and other energetic materials.

## Materials and Methods

The 3D structure of the TATB and modified molecules were drawn in vacuum using the Spartan 14 program, and using the Hartree-Fock method the STO-3G, 3-21G and 6-31G\* base sets were applied, respectively. Then, geometric optimization of the molecules was performed by applying 6-31G\* basis set, at the level of DFT/B3LYP method. The procedure was frequently obtained in literature (Young, 2001; Türker and Varış, 2013; Wu et al., 2020). The obtained structures were given in Figure 1.



**Figure 1.** The TATB and structurally modified molecules

The density, one of the factors influencing the ballistic properties of energetic molecules, was calculated using the commonly utilized Monte Carlo method (Yang et al., 2013; Wang et al., 2019a; Jeong et al., 2020; Pu et al., 2020). The molar volumes of TATB and the molecules derived from it were calculated 10 times with the help of the Monte Carlo method in the Gaussian 09W package program, and the molar volumes were calculated by taking the arithmetic average. Theoretical density values were determined by dividing the molar mass of the molecules by the average molar volumes found.

N,  $M_{ave}$  and Q values for  $C_aH_bO_cN_d$ -type explosives were calculated with the help of table 1. (N: moles of gas consisting of detonation products per gram of explosive (mol/g),  $M_{ave}$ : average molar mass of the gas products formed (g/mol), Q: chemical energy of explosion (kJ/g)).

**Table 1.** Stoichiometric equations for calculating the N,  $M_{ave}$ , and Q parameters for  $C_aH_bO_cN_d$ -type explosives (Qiu et al., 2006).

Parameter	$c \geq 2a + b/2$	$2a + b/2 > c \geq b/2$	$b/2 \geq c$
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	$(28.9b + 94.05a + 0.239 \Delta H_f^\circ) / M$	$[28.9b+94.05 (c/2 -b/4) + 0.239 \Delta H_f^\circ] / M$	$(57.8c + 0.239 \Delta H_f^\circ) / M$

N: moles of gas consisting of detonation products per gram of explosive (mol/g),  $M_{ave}$ : average molar mass of the gas products formed (g/mol), Q: chemical energy of explosion (kJ/g).

Theoretical detonation velocity (D) and detonation pressure (P) of the TATB and its derived molecules were calculated using the Kamlet-Jacobs equations (Kamlet and Hurwitz, 1968; Fordham, 1980; Qiu et al., 2006; Jeong, 2018) given in Equations 1 and 2.

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

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

D: detonation velocity (km/s), P: detonation pressure (GPa),  $\rho$ : density of the compound (g/cm<sup>3</sup>)

With the help of equation 3 the oxygen content was calculated (Türker and Varış, 2013; Larin et al., 2023).

$$\% \Omega = \frac{\mu_0}{\mu_{pat}} \left( c - 2a - \frac{b}{2} \right) \times 100 \quad (3)$$

Possible gas products that may occur as a result of the explosion reaction, Kistiakowsky-Wilson rules (Akhavan, 1998) (1- Oxygen atoms oxidize 'H' atoms to 'H<sub>2</sub>O' molecules, 2- The remaining 'O' atoms oxidize all 'C' atoms to CO molecules. 3- The remaining 'O' atoms oxidize all the 'CO' molecules into 'CO<sub>2</sub>' molecules, 4- The excess of O, H and N atoms is converted to O<sub>2</sub>, H<sub>2</sub> and N<sub>2</sub>, excess C remains as C(S)) was determined with its help. The determined theoretical values were compared with the literature.

## Results and Discussion

Table 2 listed the bond lengths and bond angles that the 2,4,6-triamino-1,3,5-trinitrobenzene (TATB) molecules B3LYP/6-31G\* (d,p) base set optimization process yielded. As shown in Table 2, the results of the optimization process are consistent with the literature data. Table 3 shows the values for density, explosion velocity, and explosion pressure of the TATB molecule. It can be seen that the values obtained after optimization are in agreement with the literature data and provide information about the accuracy of the optimization process.

**Table 2.** The bond angles and bond lengths obtained in this study for the TATB molecule and obtained from the literature data (°).

Bond Angles	TATB	(Mason et al., 2022)	(David et al., 2011)	(Cady and Larson, 1965)	(Türker, 2019a)
H6-N3-H4	126.72	125.50		124.00	
C6-N1-H1	116.85	117.22		116.00	
C4-C5-N5	119.51		119.40	119.40	
N3-C4-C5	120.43		120.50	120.40	
N6-C3-C4	119.44		119.40	119.40	
O4-N6-C3	120.84		120.60	120.80	
O6-N5-O5	118.31			118.10	
<b>Bond Lengths</b>					
C1-C2	1.45		1.44	1.45	1.44
C1-N4	1.43		1.43	1.43	1.43
C4-N3	1.33	1.32	1.32	1.32	1.32

**Table 3.** The literature data of the values of density, explosion velocity and explosion pressure in the gas phase for the TATB molecule and the values obtained in this study.

	TATB	(Kamlet and Hurwitz, 1968)	(Boddu et al., 2010)	(Brenden et al., 2019)	(Hamilton et al., 2020)
<b>d</b> (g/cm <sup>3</sup> )	1.86	1.80	1.80	-	-
<b>D</b> (km/s)	7.87	7.66	7.66	8.1	7.52
<b>P</b> (GPa)	28.05	27.2	25.9	32.1	27.0

The explosion of energetic materials occurs rapidly. Therefore, the oxygen required for the combustion reaction cannot be supplied from the air, and the reaction continues with the oxygen atoms in the structure of the molecule (Türker, 2019b; Larin et al., 2023; Zaman and Ghosh, 2024). The oxygen balance (%  $\Omega$ - Table 5) calculated with the help of Equation 3 can be expressed as a measure of the oxidizability of the molecule. If the molecule contains more oxygen than is needed, it must have a positive oxygen balance and conversely a negative oxygen balance. All the molecules in this study have a negative oxygen balance, such as TNT (-73.98) and Picric acid (-45.4), which are commonly used in military studies.

**Table 4.** The possible gas molecules that can form after the explosion of the TATB and the molecules derived from it.

	<b>Formula</b>	<b>N<sub>2</sub></b>	<b>H<sub>2</sub>O</b>	<b>CO</b>	<b>CO<sub>2</sub></b>	<b>H<sub>2</sub></b>	<b>C<sub>(k)</sub></b>	<b>N Total gas</b>
TATB	C <sub>6</sub> H <sub>6</sub> N <sub>6</sub> O <sub>6</sub>	3	3	3		-	3	9
NO-1	C <sub>6</sub> H <sub>6</sub> N <sub>6</sub> O <sub>5</sub>	3	3	2		-	4	8
NO-2	C <sub>6</sub> H <sub>6</sub> N <sub>6</sub> O <sub>4</sub>	3	3	1		-	5	7
NO-3	C <sub>6</sub> H <sub>6</sub> N <sub>6</sub> O <sub>3</sub>	3	3	-		-	6	6
NH-1	C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> O <sub>4</sub>	3	4	-		-	6	7
NH-2	C <sub>6</sub> H <sub>10</sub> N <sub>6</sub> O <sub>2</sub>	3	2	-		3	6	8
NH-3	C <sub>6</sub> H <sub>12</sub> N <sub>6</sub>	3	-	-		6	6	9
NO2-1	C <sub>6</sub> H <sub>4</sub> N <sub>6</sub> O <sub>8</sub>	3	2	6		-	-	11
NO2-2	C <sub>6</sub> H <sub>2</sub> N <sub>6</sub> O <sub>10</sub>	3	1	3	3	-	-	10
NO2-3	C <sub>6</sub> N <sub>6</sub> O <sub>12</sub>	3	-	-	6	-	-	9

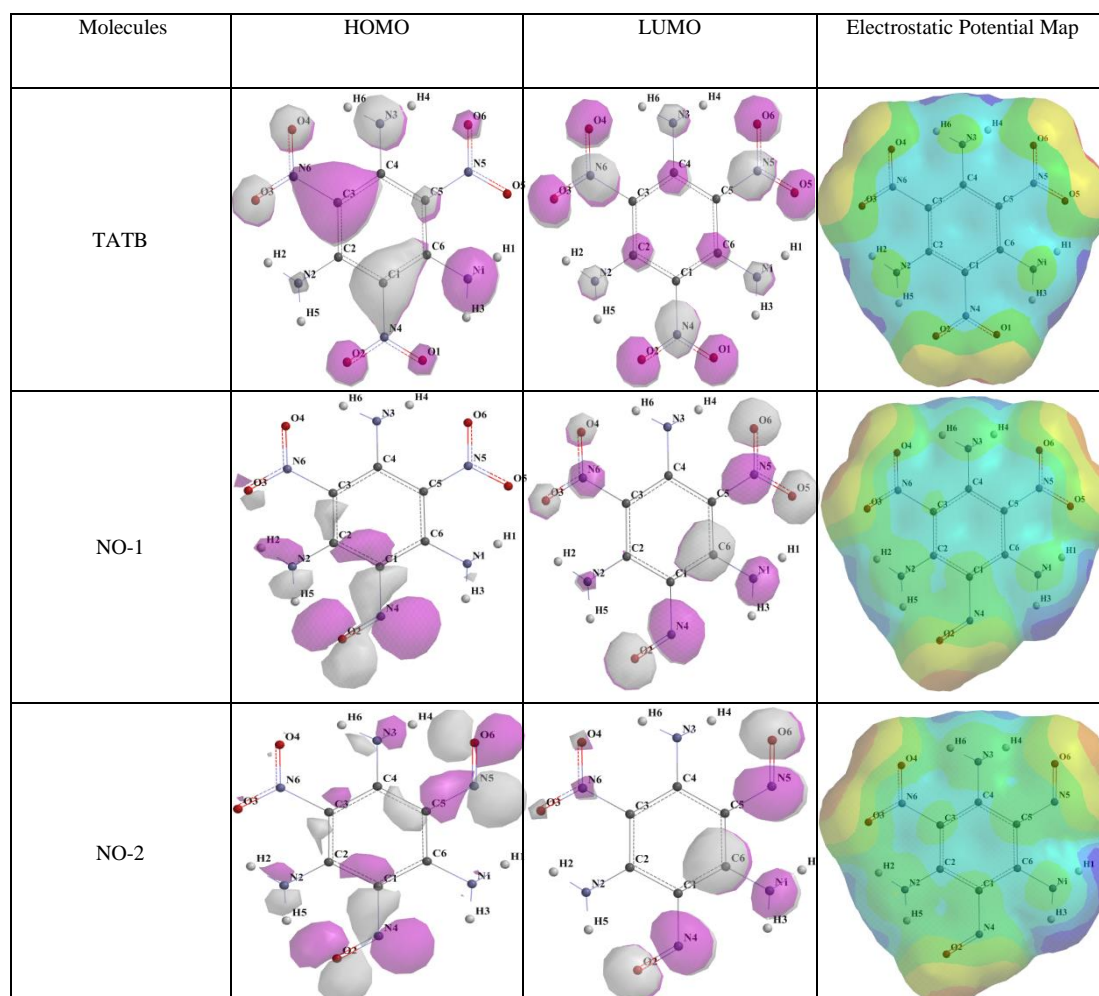
Table 4 presented potential gas molecules that could form in the event that molecules derived from TATB and TATB explode. The table shows that as amino groups (NH<sub>2</sub>) are transformed into nitro groups (NO<sub>2</sub>), more products can be produced while also increasing the sensitivity of the energetic material.

Table 5 was given values produced from theoretical data derived from the 6-31G\* basis set of the DFT/B3LYP approach for the species acquired from TATB and TATB for comparison. The results showed that substituting nitroso (NO) and NH<sub>2</sub> for the nitro groups lowered the TABT molecule's sensitivity. It is observed that when NH<sub>2</sub> are swapped out for nitro ones, sensitivity rises.

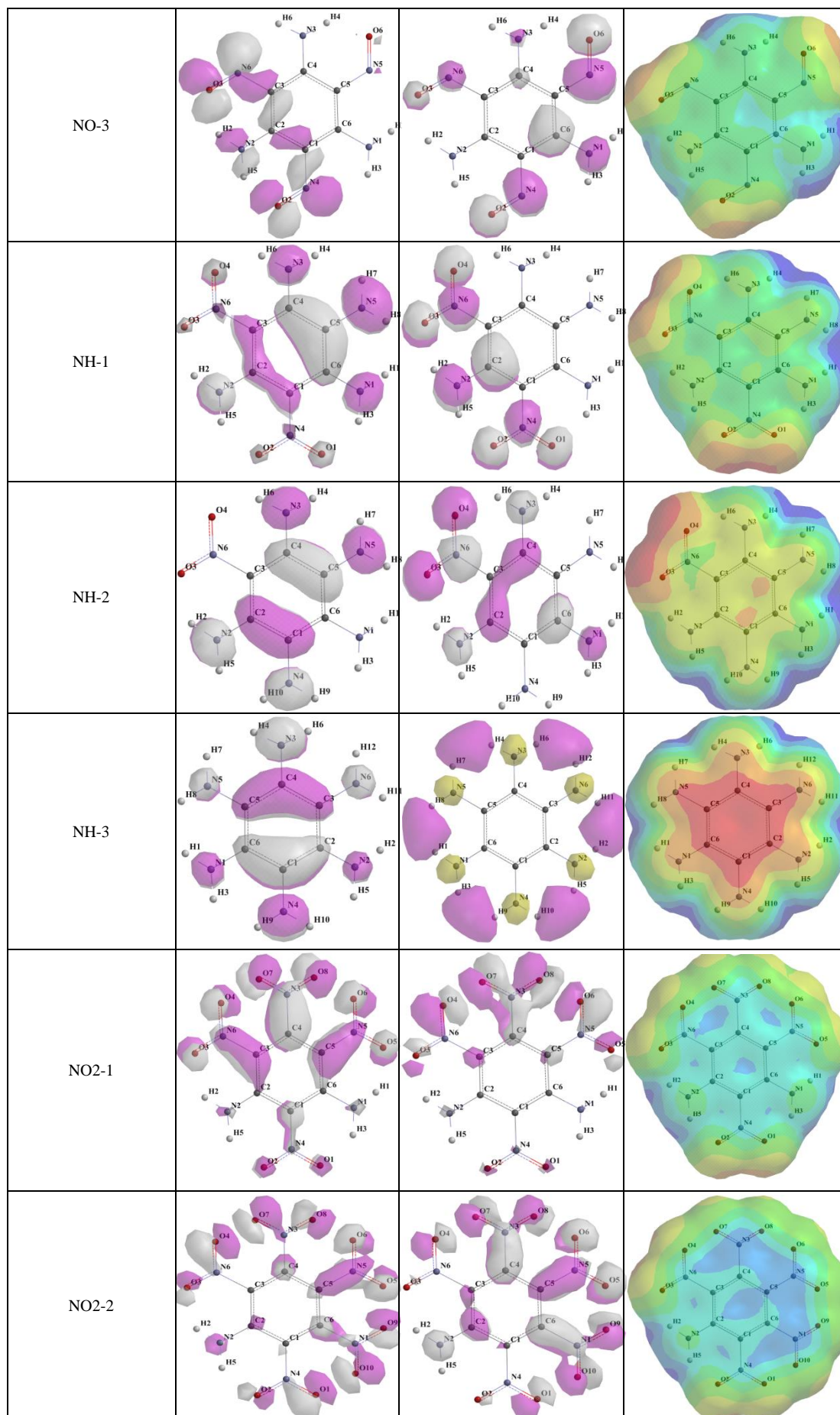
**Table 5.** Theoretical results for TATB and molecules derived from it.

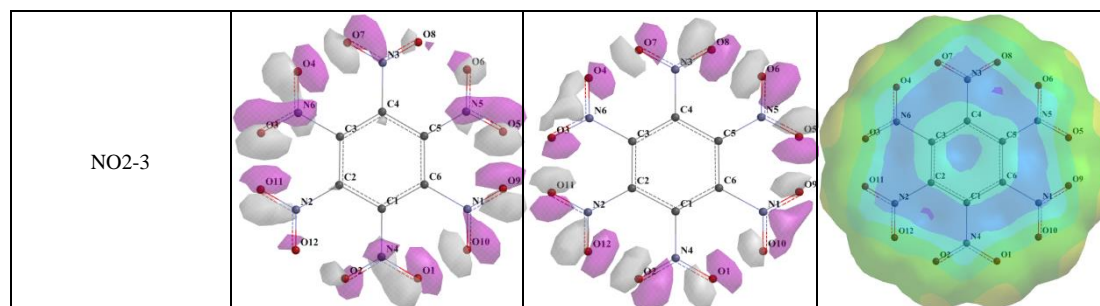
	$\rho$ ( $g/cm^3$ )	% $\Omega$	V ( $cm^3/mol$ )	N ( $mmol/g$ )	M ( $g/mol$ )	Q ( $kJ/g$ )	$\Delta H_f^0$ ( $kJ/mol$ )	D ( $km/s$ )	P ( $GPa$ )
TATB	1.86	-55.78	138.46	29.05	27.20	1168.38	-53.80	7.87	28.05
NO-1	1.83	-66.07	132.23	28.91	26.00	1234.41	131.64	7.77	27.06
NO-2	1.79	-77.82	126.09	28.74	24.62	1238.17	249.32	7.54	25.15
NO-3	1.71	-91.36	122.98	28.55	23.00	1241.69	366.28	7.15	21.95
NH-1	1.75	-84.15	130.23	30.68	22.29	1167.36	147.10	7.36	23.67
NH-2	1.58	-121.09	125.03	32.79	16.62	1066.39	265.37	6.46	17.09
NH-3	1.38	-171.22	121.37	35.67	10.00	904.69	366.19	5.21	10.15
NO2-1	1.94	-33.32	148.35	27.76	31.50	1807.32	514.62	9.16	38.93
NO2-2	2.08	-15.09	152.64	26.72	35.29	2287.24	1031.67	10.37	51.37
NO2-3	2.16	0	160.77	25.85	38.67	2689.43	1556.03	11.12	60.90
*Pikrik asit (1-Hydroxy-2,4,6-trinitrobenzene, PA)								7.85	27.72
*TNT (Trinitrotoluen)								7.37	23.46

\*(Mert, 2021)









**Figure 2.** The  $E_{\text{HOMO}}$ ,  $E_{\text{LUMO}}$  and Electrostatic Potential Map of TATB and Derivatives

The highest energy orbital occupied is known as HOMO, and it is characterized by the molecule's propensity to give electrons. The lowest unoccupied orbital, or LUMO, on the other hand, exhibits the molecule propensity to gain electrons. Figure 2 shows HOMO, LUMO and electrostatic potential maps of the TATB and derived structures. While the HOMO groups were originally centered on carbon (C), oxygen (O) atoms, distributions to nitrogen and oxygen groups were observed with the structural changes made. LUMOS, on the other hand, are initially seen scattered throughout the molecular geometry. In the additions made, dispersions were observed on C, N and O, as can be seen in the last structure, LUMO structures were dispersed on oxygens. The fact that the energy difference between HOMO and LUMO is greater than 1.5 eV indicates that the molecule is stable and durable in terms of thermodynamics. As seen in Table 6, the molecule becomes more sensitive and becomes less stable when nitro groups are substituted for amino groups. Electrostatic potential measurements enable the detection of electron-rich (electrophilic) regions or nucleophilic (nucleophilic) regions, hydrogen bond interactions, and the three-dimensional charge distributions of molecules (Gümüş, 2019; He et al., 2022; Devi et al., 2023). With the modifications made, it can be seen that the electron density zones vary.

**Table 6.** HOMO, LUMO and  $\Delta$  (LUMO-HOMO) values of TATB and its derived molecules calculated at the theoretical level of B3LYP 6-31G\* (d,p).

Compounds	HOMO (eV)	LUMO (eV)	$\Delta E$ (eV)
TATB	-7.24	-2.81	4.43
NO-1	-6.25	-2.83	3.42
NO-2	-6.19	-2.87	3.32
NO-3	-5.66	-2.82	2.84
NH-1	-5.03	-2.02	3.01
NH-2	-3.70	-1.19	2.51
NH-3	-2.85	0.8	3.65
NO2-1	-5.25	-4.08	1.17
NO2-2	-5.23	-4.32	0.91
NO2-3	-5.14	-4.64	0.50

## **Conclusion**

The data on bond lengths and angles acquired by optimizing the TATB molecule at the DFT /B3LYP level at the 6-31G\* base set have been found to be consistent with values from the literature. It was shown that it is possible to decrease an explosive sensitivity without suffering a major performance loss by transforming NO<sub>2</sub> of TATB into NO and NH<sub>2</sub>. Nitroso groups in particular were used to demonstrate this. Conversion of NH<sub>2</sub> to NO<sub>2</sub> can produce explosives with higher power, while increasing sensitivity should be considered. Any of the amino or nitroso added compounds can be employed for low precision applications. In our opinion, employing such theoretical applications will greatly aid in the development of energetic compounds that can be deemed hazardous in a laboratory setting.

## **Conflict of Interest Statement**

There is no conflict of interest.

## **Contribution Rate of Researchers Statement Summary**

All authors contributed equally.

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