

Article

Computational Studies of Energetic Property Peculiarities in Trinitrophenyl-Substituted Nitramines

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Abstract: This research was performed using Becke's three-parameter hybrid functional approach with non-local correlation provided by Lee, Yang, and Parr and the cc-pVTZ basis set. The geometry, total energy, and heat of formation of the most stable conformers of the nitramines under study were obtained to obtain the density, resistance to shock stimuli, detonation pressure, and velocity of the materials under study. The results obtained allow us to predict new multipurpose energetic materials with a good balance between energy and stability. Our findings show that *N*-(2-nitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2,4,6-trinitrophenyl)-*N*-[(3,4,5-trinitro-1*H*-pyrazol-1-yl)methyl]nitramine, *N*-(2,2-dinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2,2,2-trinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, and *N*-(trinitromethyl)-*N*-(2,4,6-trinitrophenyl)nitramine possess better explosive properties and a greater stability compared to tetryl, although they remain sensitive to shock stimuli. Referring to the results obtained, we recommend new tetryl analogs containing dinitroethyl, trinitroethyl, and trinitromethyl substituents for practical usage.

Keywords: aromatic nitramines; trinitrophenyl; energetic properties; stability; resistance to shock stimuli



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1. Introduction

The global market for high-energy materials has been constantly growing [1–8]. During the 2017–2022 period, it grew from nearly USD 23.8 billion to USD 31.2 billion [9]. This growth is primarily related to the usage of these materials in the mining, quarrying, and construction industries [10–12]. From a practical point of view, the energetic compound should be powerful, stable, insensitive to mechanical stimuli, and provide a large quantities of energy release during intentional detonation [2–4]. Hence, new functionalized compounds with unique improved properties are required for the development of advanced energetic materials [13–16]. In this context, the study of high energy materials is performed in several fields [17–20]. First, this study is carried out aiming to create new or modify existing materials, understand their potential risks, and develop strategies to minimize or mitigate those risks [21–37]. Second, the potential health effects of exposure to high-energy materials, including the short-term and long-term effects on human health, and identifying strategies to reduce these risks are the focus of the research [38]. Third, the potential environmental impacts of these materials, including their persistence in the environment, bioaccumulation in ecosystems, and effects on wildlife and ecosystems are also investigated [39]. As a result of previous studies, strategies for emergency response and cleanup in the event of an accident or spill involving hazardous materials are developed. All of the above studies require data on the structure, chemical stability, possible degradation pathways, etc.

2,4,6-Trinitrophenylmethyl nitramine or tetryl (C₇H₅N₅O₈) is a high-energy material that has been used to make detonators and explosive booster charges and brisant explosive

compositions (melt-cast mixture tetratol (80% tetryl and 20% TNT) and PTX-1 (mixture of 30% RDX, 50% Tetryl and 20% TNT)), mostly during World War I and World War II [40]. Tetryl is more easily detonated than ammonium picrate or TNT, being about as sensitive as picric acid [41]. It has been approved as the standard bursting charge for small-caliber projectiles since it gives a much better fragmentation than TNT [40]. However, tetryl appears to break down rapidly in some soils and could reach surface and underground waters where it may dissolve or/and associate with small particles of suspended solids, sediments, or organic debris [42]. Bulk TNT production generates a serious industrial problem with environmental pollution (so-called “pink water”) [43–45]; thus, the design of a new high-energy material also demands the development of new, clean chemical processes [46,47]. Importantly, modern technologies including the application of the clean nitration agent, N_2O_5 , allow more “green” and efficient synthesis processes for new nitramine production. Furthermore, easily recyclable alternatives such as ionic liquids and supercritical fluids (including CO_2) have attracted attention as potential and more environmentally friendly substitutes for the liquid phases in nitramine production processes [48–50]. As the demand for high-energy materials continues to grow, there is a rising interest in exploring the potential of tetryl to create nitramines, which possess more favorable energetic properties and an improved chemical and thermal stability [51–56], i.e., it is possible to modify tetryl in such way that its energetic properties remain the same or even better, while its chemical stability or resistance to degradation increases.

Currently, we obtain that the thermal stability and resistance to shock stimuli of tetryl is directly CH_2 chain length dependent, while its explosive properties become worse due to this chain increase. The results of our studies also exhibited that in tetryl with different $-CH_2$ chain lengths ($n = 1-5$) ((2,4,6-trinitrophenyl-(O_2N) $N(CH_2)_n$ H), the chain length should not be longer than three or the detonation pressure of these compounds would not be below that of TNT [57]. The stability of the compounds increases more significantly than the worsening of the explosive properties. So, the question arises whether other substituents could improve not only the energetic properties of tetryl but also its stability and resistance to shock stimuli.

It is known that azide functional group incorporation into high-energy materials increases energy levels, enhances the nitrogen content, and lowers environmental hazards by releasing nontoxic N_2 gas during detonation [22]. Similar effects are achieved by incorporation of other nitrogen-rich substituents into energetic molecules, such as azole rings (pyrazole, triazole, tetrazole, or tetrazine) [24,25,54]. Incorporation of the listed explosophores substantially improves the density and oxygen balance, and thus results in excellent energetic/detonation characteristics. Notably, the excessive accumulation of explosophoric groups can lead to an increased sensitivity to mechanical stimulation and a thermal factor, decreasing the stability and safety of the designed target materials and complicating their potential practical use, instead of their high-performance characteristics, so various functional groups must be used to balance the properties of high-energy materials [26–35].

In this respect, we continue our study of a series of secondary aromatic nitramines, possessing as the main substituents the traditional 2,4,6-trinitrophenyl moiety, by varying the substitutes attached to the nitramine group nitrogen, aiming to improve the chemical stability and resistance to shock stimuli. The new target molecules can be divided into two main groups: (a) where the substituent is a simple or branched alkyl group and (b) where the substituent contains in its structure additional important explosophoric fragments such as nitro, fluoro, or azido groups to increase the energy and brisance. The first group is targeted to the design of new perspective melt cast energetic materials for the substitution of currently used TNT or DNAN, while group (b) is targeted for the design of high-energy materials with increased power as replacements of the currently used nitramine RDX. As the result of the current work, several perspective structures with a good balance between high energy and low sensitivity were selected.

Thus, this study is performed because there is a lack of information on the dependence of the stability and energetic properties of aromatic nitramines on the substituents. The results of our study will indicate the modification of the tetryl by substituents in such a way that their stability and resistance to shock stimuli of the aromatic nitramines remain high along with their energetic properties. The insight gained from this research could pave the way for the development of new and improved high-energy materials in the future. We also predict that the results of these studies shed some light on the degradation pathways of the materials under study.

2. Materials and Methods

As mentioned above, the study was performed aiming to exhibit the influence of various substituents' stability and energetic properties of tetryl. The used methodology in this research does not differ from that presented in our recently published paper [57]. So, to obtain reliable results, several different conformers of each molecule under study were designed. The conformers are different due to the position of the substituents with respect to the core molecules. It is necessary to point out that in some cases, only one of the above positions is possible because of steric effects. Berny optimization without any symmetry constraints (all bonds length, angles, and dihedral angles are changed) was applied to find an equilibrium point. A vibrational frequency analysis was performed to be sure that the energy minima are reached and the structure of the most stable conformer is definitely found. Becke's three-parameter hybrid functional approach with non-local correlation provided by Lee, Yang, and Parr (B3LYP) and the cc-pVTZ basis set implemented in a GAUSSIAN package was applied in our studies [58–60]. This approach appropriately describes the geometric and electronic structure of various molecules and their derivatives [61–71]. First, we compare the total energy of the conformers investigated. The conformers with the lowest total energy were selected for further study. Second, to compare the thermal stability of the nitramines with different chemical compositions, the binding energy per atom was calculated and compared. This energy indicates the amount of energy required to separate an atom from a system of particles and is calculated by the following:

$$\frac{E - \sum_i E_i}{N}$$

where E is the total energy of the molecule under study, E_i is the total energy of the atoms consisting of this molecule, and N is the number of atoms. A larger value of N shows a higher thermal stability. Third, to evaluate the stability related to the chemical properties and aging of the compounds investigated we calculated the HOMO–LUMO gap, chemical hardness, and softness, as well as the electronegativity. It is known that compounds with a larger HOMO–LUMO gap and chemical hardness are more resistant to undergoing chemical reactions or to being transformed by an external perturbation, such as an applied electric field. On the other hand, a low chemical softness value denotes a high tendency of the molecule to degrade, while a higher electronegativity reflects a higher tendency of the compound to form a bond [72,73]. The activation energy of the compounds was also evaluated, as the difference in the total energies of transitional and ground states. This energy, i.e., the minimum amount of energy that must be provided for the compounds to chemically react, could also be assessed as an indicator of chemical stability.

The energetic properties of the compounds under study were obtained by using a reliable and low computationally demanding approach. The reliability of the approach used was checked earlier by a comparison of the theoretical and experimental results of the detonation velocity of tetryl. In short, the detonation velocity calculated by us applying the above approach coincides well with the 7.59–7.7 km/s presented by other researchers. Additionally, it is an experimentally confirmed conclusion followed by the above approach results that TNTs energetic properties are better than those of *N*-(2,4,6-trinitrophenyl)-1*H*-1,2,4-triazol-3-amine, and its properties are better than tetryl [74–78].

The oxygen balance [79] and impact sensitivity were calculated to evaluate the resistance to impact. For the fluorine-containing high-energy materials, the equation to evaluate the oxygen balance was corrected into oxygen–fluorine balance because of the introduction of another oxidant fluorine element [80]. The impact sensitivity was obtained with the following:

$$\log h_1 = (11.76a + 61.72b + 26.89c + 11.48d)/M$$

$$\log h_2 = (47.33a + 23.50b + 2.357c - 1.105d)/M$$

where a , b , c , and d indicate the number of C, H, N, and O atoms, respectively, and M is the molar mass of the compounds [81–83]. Larger values of these parameters indicate a large resistance to impact.

The density of the materials under investigation was obtained by the approach suggested by M.S. Keshavarz [84,85]. We demonstrated that in some cases the density obtained by this approach gives more reliable results than that calculated by the division of molecular weight by molar volume (calculated by the division of molar in additive increments).

To predict the energetic properties of the compound investigated, we calculated the detonation velocity and pressure. It is necessary to mention that there are a lot of methods to assess detonation velocities, but there is no one named as the most precise approach. We would like to point out that when using the same approach, one can ensure that the statistical errors in the detonation velocities for each molecule will be similar. This allows us to compare the detonation velocities of the compounds studied here, regardless of the model used to compute them, and subsequently rank these molecules. Thus, the detonation velocity was calculated by the following:

$$D_1^2 = -393.6877 - 0.2454 \left(\frac{E * N}{M} \right) - 114.0793 \frac{E}{M} \quad (1)$$

where N is the number of $-NO_2$ groups in the molecule, E is the total energy in a.u., and M is the molar mass in g/mol. These equations are given by Türker [86].

The very well-known Kamlet–Jacobs equation of the detonation velocity was also used to calculate this parameter [87].

$$D_3 = 1.01\varphi^{1/2}(1 + 1.30\rho) \quad (2)$$

where $\varphi = nM^{1/2}Q^{1/2}$

where n is the number of moles of gaseous products of detonation per gram of explosive, M is the average molecular weight of the gas found from the chemical reaction equations with an assumed equilibrium composition, Q is the heat of detonation in calories per gram of explosive, and ρ is the loading density. The values obtained by this approach are marked as D_3 .

We emphasize the data obtained by different approaches allow us to reveal general features and avoid unexpected errors.

The detonation pressure was evaluated by the following:

$$P(\text{kbar}) = 15.58 (D \rho / (1.01(1 + 1.30 \rho)))^2$$

where D is the detonation velocity and ρ is the density of the compounds.

3. Results

The views of the compounds and their chemical composition are presented in Appendix A and as supporting information in Table S1. The parameters reveal the chemical and thermal stability which are presented in Table 1.

Table 1. The parameters describe the chemical and thermal stability of the compounds under study. The parameters are presented in the order of increasing chemical hardness. The results are discussed in the next section of this paper.

Compound	Binding Energy per Atom, eV	HOMO–LUMO Gap, eV	Hardness, eV	Softness, eV	Electronegativity, eV	Hardness Index Y
<i>N</i> -[(1,2,4,5-tetrazin-3-yl)methyl]- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	5.65	2.90	1.45	0.35	5.65	0.76
<i>N</i> -(trifluoromethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	5.07	3.35	1.67	0.30	7.26	0.82
<i>N</i> -(2-azidoethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	5.58	3.43	1.72	0.29	5.90	0.83
<i>N</i> -(2-methoxyethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	5.08	3.65	1.82	0.27	5.90	0.85
<i>N</i> -(3-methoxypropyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	5.04	3.70	1.85	0.27	5.86	0.85
<i>N</i> -prop-2-en-1-yl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	5.29	4.20	2.10	0.24	6.12	0.89
<i>N</i> -prop-2-yn-1-yl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	5.82	4.23	2.11	0.24	6.18	0.89
<i>N</i> -butan-2-yl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	5.08	4.26	2.13	0.24	6.12	0.89
<i>N</i> -(2-methylpropyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	5.08	4.28	2.14	0.23	6.18	0.89
<i>N</i> -tert-butyl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	5.44	4.32	2.16	0.23	6.12	0.89
<i>N</i> -(2-nitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	5.19	4.33	2.17	0.23	6.47	0.89
Tetryl	4.84	4.31	2.17	0.23	6.19	0.89
<i>N</i> -(2-nitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine ¹	5.42	4.43	2.21	0.23	6.52	0.9
<i>N</i> -(2,4,6-trinitrophenyl)- <i>N</i> -[(3,4,5-trinitro-1 <i>H</i> -pyrazol-1-yl)methyl]nitramine	5.44	4.50	2.25	0.22	6.70	0.9
<i>N</i> -[(1 <i>H</i> -tetrazol-5-yl)methyl]- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	5.58	4.58	2.29	0.22	6.54	0.9
<i>N</i> -[(1 <i>H</i> -tetrazol-5-yl)methyl]- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	5.19	4.62	2.31	0.22	6.83	0.91
<i>N</i> -(2,2-dinitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	5.18	4.62	2.31	0.22	6.46	0.91
<i>N</i> -(2-fluoro-2,2-dinitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	5.19	4.63	2.32	0.22	6.80	0.91
<i>N</i> -(trinitromethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	4.94	4.72	2.36	0.21	6.88	0.91

¹ denotes second conformer of *N*-(2-nitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine.

We also obtained the activation energy of the compounds under study as an additional parameter to reveal their stability and foresee the minimum amount of energy required to activate molecules of high-energy materials to a condition in which they can undergo a chemical transformation from a solid to a gaseous state. We predict that structural changes in the ground and transition states could indicate the weakest bond to be decomposed first. The obtained values of the activation energies are presented in Table 2.

Table 2. The activation energy of the compounds under study.

Compound	Activation Energy, eV
<i>N</i> -(2-methoxyethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	0.06
<i>N</i> -(3-methoxypropyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	0.09
<i>N</i> -butan-2-yl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	0.08
<i>N</i> -(2-methylpropyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	0.11
<i>N</i> -prop-2-yn-1-yl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	0.03
<i>N</i> -tert-butyl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	0.10
<i>N</i> -(2-azidoethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	0.0003
<i>N</i> -(2-nitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	0.02
<i>N</i> -(2-fluoro-2,2-dinitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	0.09
<i>N</i> -(2,2-dinitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	0.05
<i>N</i> -(2,2,2-trinitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	0.12
<i>N</i> -(trinitromethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	0.05
<i>N</i> -[(1 <i>H</i> -tetrazol-5-yl)methyl]- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	0.17
<i>N</i> -(trifluoromethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	0.91
<i>N</i> -[(1,2,4,5-tetrazin-3-yl)methyl]- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	0.14

The results that exhibit resistance to impact are presented in increasing order in Table 3.

Table 3. The parameters describe the resistance to the impact of the compounds and the oxygen balance (OxB). The results are discussed in the next section of this paper. These parameters for tetryl are equal to 1.096 (log h_1), 1.573 (log h_2), and -47.36 (oxygen balance).

Compound	log h_1	log h_2	OxB, %
<i>N</i> -(trinitromethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	1.212	0.904	-3.79
<i>N</i> -(2-nitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	1.460	1.091	-14.67
<i>N</i> -(2-fluoro-2,2-dinitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine			-21.51
<i>N</i> -(trifluoromethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine			-25.80
<i>N</i> -(2,4,6-trinitrophenyl)- <i>N</i> -[(3,4,5-trinitro-1 <i>H</i> -pyrazol-1-yl)methyl]nitramine	1.422	1.179	-26.22
<i>N</i> -(2,2-dinitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	1.658	1.277	-26.59
<i>N</i> -(2,2,2-trinitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	1.908	1.510	-41.60
<i>N</i> -[(1 <i>H</i> -tetrazol-5-yl)methyl]- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	1.848	1.432	-47.30
<i>N</i> -[(1,2,4,5-tetrazin-3-yl)methyl]- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	1.845	1.484	-49.24
<i>N</i> -(2-azidoethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine.	2.020	1.548	-51.43
<i>N</i> -prop-2-yn-1-yl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	1.770	1.756	-64.27
<i>N</i> -prop-2-en-1-yl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	2.153	1.895	-68.97
<i>N</i> -(2-methoxyethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	2.363	2.001	-72.26
<i>N</i> -(3-methoxypropyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	2.706	2.125	-76.47
<i>N</i> -(2-methylpropyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	2.803	2.232	-85.05
<i>N</i> -tert-butyl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	2.803	2.232	-85.05

The detonation pressure and velocity were obtained to exhibit the energetic properties of the compound under study. These parameters are given in Tables 4 and 5.

Table 4. The detonation velocity of the compounds given in increasing order in accordance with the results obtained by the Kamlet–Jacobs equation (D_2).

Compounds	Detonation Velocity, km/s	
	D_1	D_2
<i>N</i> -(trifluoromethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	*	6.935
<i>N</i> -(2-fluoro-2,2-dinitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	*	7.338
<i>N</i> -(2-methylpropyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	6.908	7.098
<i>N</i> -butan-2-yl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	6.908	7.098

Table 4. Cont.

Compounds	Detonation Velocity, km/s	
	D ₁	D ₂
<i>N</i> -tert-butyl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	6.908	7.098
<i>N</i> -prop-2-yn-1-yl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	7.610	7.212
<i>N</i> -prop-2-en-1-yl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	7.447	7.277
<i>N</i> -[(1,2,4,5-tetrazin-3-yl)methyl]- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	7.592	7.364
<i>N</i> -(3-methoxypropyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	7.235	7.368
<i>N</i> -[(1 <i>H</i> -tetrazol-5-yl)methyl]- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	7.782	7.595
<i>N</i> -(2-methoxyethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	7.588	7.606
<i>N</i> -(2-azidoethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	7.720	7.617
Tetryl	8.070	7.880
<i>N</i> -(2-nitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	8.305	8.088
<i>N</i> -(2,4,6-trinitrophenyl)- <i>N</i> -[(3,4,5-trinitro-1 <i>H</i> -pyrazol-1-yl)methyl]nitramine	8.767	8.265
<i>N</i> -(2,2-dinitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	8.778	8.473
<i>N</i> -(2,2,2-trinitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	9.144	8.780
<i>N</i> -(trinitromethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	9.421	9.012

** indicates that the approach used is not applicable to compounds containing fluorine atoms. *N*-(trifluoromethyl)-*N*-(2,4,6-trinitrophenyl)nitramine and *N*-(2-fluoro-2,2-dinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine are not discussed due to the different approach used to evaluate their density.

Table 5. The detonation pressure given in increasing order in accordance with the results obtained by using D₂.

Compounds	Detonation Pressure, kbar	
	p(D ₁)	p(D ₂)
<i>N</i> -(trifluoromethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	*	216.882
<i>N</i> -(2-fluoro-2,2-dinitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	*	220.918
<i>N</i> -tert-butyl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	199.991	211.144
<i>N</i> -(2-methylpropyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	200.000	211.145
<i>N</i> -butan-2-yl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	199.998	211.145
<i>N</i> -prop-2-yn-1-yl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	248.109	222.866
<i>N</i> -prop-2-en-1-yl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	236.714	226.074
<i>N</i> -(3-methoxypropyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	221.521	229.753
<i>N</i> -(2-methoxyethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	247.144	235.389
<i>N</i> -[(1,2,4,5-tetrazin-3-yl)methyl]- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	254.580	239.506
<i>N</i> -(2-azidoethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	262.825	255.849
<i>N</i> -[(1 <i>H</i> -tetrazol-5-yl)methyl]- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	268.861	256.065
Tetryl	318.370	273.110
<i>N</i> -(2-nitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	304.896	289.190
<i>N</i> -(2,4,6-trinitrophenyl)- <i>N</i> -[(3,4,5-trinitro-1 <i>H</i> -pyrazol-1-yl)methyl]nitramine	346.394	307.834
<i>N</i> -(2,2-dinitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	346.370	322.740
<i>N</i> -(2,2,2-trinitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	380.715	351.033
<i>N</i> -(trinitromethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine	408.716	374.006

** indicates that the approach used is not applicable to compounds containing fluorine atoms. *N*-(trifluoromethyl)-*N*-(2,4,6-trinitrophenyl)nitramine and *N*-(2-fluoro-2,2-dinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine are not discussed due to the different approach used to evaluate their density.

4. Discussion

As mentioned above, this study is a continuation of our work associated with the energetic properties of mostly C_aH_bN_cO_d group derivatives. Several compounds with substituents consisting of F were investigated too, to foresee fluorine atoms' influence on the stability of the nitramines, although they do not belong to C_aH_bN_cO_d group compounds and therefore there are some limits to the approaches applied.

The results obtained indicated that the stability of the nitramines decreased sufficiently when they are bonded to a -CH₂C₂HN₄ substituent. Only with this substituent is the hardness index below 0.8, which indicates the lower stability of this nitramine in comparison

with others (Table 1). The main reason for this decrease is the very low chemical stability that indicates a HOMO–LUMO gap equal to 2.892 eV and a chemical hardness of 1.447 eV, which is significantly different from other nitramines under study.

The data on binding energy per atom presented in Table 1 clearly show that the thermal stability of trinitrophenyl derivatives increases due to substituents (Table 2). However, we do not find any clear relationship between the binding energy per atom and the atom number in the compound or their rates with respect to each other to find some common features for the most effective design of high-energy materials. An analysis of the HOMO–LUMO gap indicates that the chemical stability is higher than that of tetryl only for a few compounds, such as *N*-(2,2,2-trinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2,4,6-trinitrophenyl)-*N*-[(3,4,5-trinitro-1*H*-pyrazol-1-yl)methyl]nitramine, *N*-[(1*H*-tetrazol-5-yl)methyl]-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2,2,2-trinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2,2-dinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2-fluoro-2,2-dinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, and *N*-(trinitromethyl)-*N*-(2,4,6-trinitrophenyl)nitramine. The data on the chemical hardness of these compounds reveal their higher resistance to deformation or changes, although the information on their chemical softness and electronegativity indicates increased a tendency to form chemical bonds in comparison to tetryl. It is necessary to mention that the hardness indexes of the compounds mentioned as stabler than tetryl are in the range of 0.90–0.91 (Table 1). This also indicates that *N*-(2-nitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2,4,6-trinitrophenyl)-*N*-[(3,4,5-trinitro-1*H*-pyrazol-1-yl)methyl]nitramine, *N*-[(1*H*-tetrazol-5-yl)methyl]-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2,2,2-trinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2,2-dinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2-fluoro-2,2-dinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, and *N*-(trinitromethyl)-*N*-(2,4,6-trinitrophenyl)nitramine are generally high-stability compounds. This index for tetryl is equal to 0.89, lower than that mentioned above. Hence, we may conclude that the substituents $-\text{CH}_2\text{CH}_2\text{NO}_2$, $-\text{CH}_2-3,4,5-(\text{NO}_2)_3\text{C}_3\text{N}_2$, $-\text{CH}_2-\text{CHN}_4$, $-\text{CH}_2-\text{C}(\text{NO}_2)_3$, $-\text{CH}_2-\text{CH}(\text{NO}_2)_2$, $-\text{CH}_2-\text{CF}(\text{NO}_2)_2$, and $\text{C}(\text{NO}_2)_3$ increase the thermal and chemical stability of tetryl along with increasing its electronegativity. As mentioned above, the tendency of the tetryl to form a chemical bond with the above-mentioned substituents increases along with their thermal stability. Referring to these findings, we predict a faster aging and higher requirements for the safe storage of tetryl containing the substituents $-\text{CH}_2\text{CH}_2\text{NO}_2$, $-\text{CH}_2-3,4,5-(\text{NO}_2)_3\text{C}_3\text{N}_2$, $-\text{CH}_2-\text{CHN}_4$, $-\text{CH}_2-\text{C}(\text{NO}_2)_3$, $-\text{CH}_2-\text{CH}(\text{NO}_2)_2$, $-\text{CH}_2-\text{CF}(\text{NO}_2)_2$, and $\text{C}(\text{NO}_2)_3$.

The activation energy was calculated too. We do not associate the differences between activation energies as a factor that has a negative impact on the performance–sensitivity trade-off because in practice this criterion cannot easily be taken into account for the design of optimized explosives [88].

We assume that the ignition of the compounds with a low activation energy does not require a large amount of energy; thus, the reaction zone in detonation waves supplies the sustaining energy, the detonation front initiates the chemical reaction by compression and the diffusion of both heat and species and thus inherently the reaction is self-sustained, leading to extremely rapid combustion reactions. Shortly, the transitional length from deflagration to detonation could be shorter for low-activation energy compounds in comparison with that of high-activation energy ones. Referring to the results obtained, the activation energy of *N*-(2-azidoethyl)-*N*-(2,4,6-trinitrophenyl)nitramine is the lowest. This compound could be addressed to the azide groups due to the azidoethyl group presence. The intrinsic instability of organic azides is very well known, and it makes their properties difficult to measure, and experimental work has to be carried out with care [89]. The activation energy of *N*-(trifluoromethyl)-*N*-(2,4,6-trinitrophenyl)nitramine is the highest among the investigated compounds. This compound consists of trifluoromethyl groups (CF_3) which introduce properties into organic compounds that include a high thermal stability, a high chemical resistance, a low surface energy, and a high electronegativity [90]. These results indirectly confirm our presumption that low-activation-energy compounds could be more sensitive and unstable.

The activation energy of other compounds varies from 0.02 to 0.16 eV. There is no doubt that the substituents influence the activation energy, but ways to reach the transition state are also important. An analysis of the transition state of the compounds under study indicates that the ground state of low-activation-energy (0.02–0.10 eV) compounds differs from transition state only due to the rotation of NO₂ groups. In the case of the higher activation energy compounds, the substituent positions due to bending or/and rotation are changed along with NO₂ group rotations. For example, in the case of *N*-tert-butyl-*N*-(2,4,6-trinitrophenyl)nitramine, the substituent and NO₂ groups positions are different in the ground and transition state due to bending and rotation. The geometrical structures in the transition state of *N*-(2-methoxyethyl)-*N*-(2,4,6-trinitrophenyl)nitramine and *N*-(3-methoxypropyl)-*N*-(2,4,6-trinitrophenyl)nitramine are different from that of the ground state only due to the position of -C₃H₇O and -C₄H₉N substituents. These structural transformations could be the reason that the reaction zone in detonation waves cannot supply the sustaining energy and the detonation front does not initiate a chemical reaction. This is because the use of the vast majority of the detonation wave energy is used for the above transformations.

It is well known that the oxygen balance of TNT, a standard reference for many purposes, is equal to -74% [91], and that of tetryl is -47.36%. The data presented in Table 3 indicate that compounds with substituents rich in oxygen in comparison to carbon are more brisant and stronger than tetryl and even TNT, but they also are more sensitive to shock stimuli. Referring to the results of our investigation, we may state that *N*-[(1,2,4,5-tetrazin-3-yl)methyl]-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2-azidoethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-prop-2-yn-1-yl-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-prop-2-en-1-yl-*N*-(2,4,6-trinitrophenyl)nitramine, and *N*-(2-methoxyethyl)-*N*-(2,4,6-trinitrophenyl)nitramine are stronger and more brisant than tetryl, while *N*-(3-methoxypropyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-butan-2-yl-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2-methylpropyl)-*N*-(2,4,6-trinitrophenyl)nitramine, and *N*-tert-butyl-*N*-(2,4,6-trinitrophenyl)nitramine possess better brisance and strength properties than TNT. Let us remind you that shock stimuli may have various forms, such as impact, friction, heat, or electrical energy, depending on the specific type of high-energy materials and their sensitivity to different initiation methods. Hence, the oxygen balance indicates that the above compounds could be more sensitive than tetryl, and, in some cases, TNT, to specific stimuli. For example, it is more probable that *N*-(2-azidoethyl)-*N*-(2,4,6-trinitrophenyl)nitramine could be sensitive to heat and friction because its binding energy per atom, chemical hardness, and softness are the lowest in comparison to those of the other compounds. Moreover, its activation energy is the lowest.

The calculated parameters representing the resistance to shock stimuli also show the higher sensitivity to shock impact of *N*-[(1,2,4,5-tetrazin-3-yl)methyl]-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2-azidoethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-prop-2-yn-1-yl-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-prop-2-en-1-yl-*N*-(2,4,6-trinitrophenyl)nitramine, and *N*-(2-methoxyethyl)-*N*-(2,4,6-trinitrophenyl)nitramine than tetryl. It is necessary to mention that patterns of the resistance to shock stimuli obtained by different approaches are slightly different (Table 3 and Figures 1 and 2). This could be because the approach applied was created considering specific compounds that do not fit completely our investigated ones. These differences are not significant, which indicates that a value of the correlation coefficient that is higher than 0.94 reflects only a 6% difference in the ranking of the compounds under study with respect to their resistance to shock stimuli. We considered the above inaccuracies to conclude that the resistance to shock stimuli of *N*-prop-2-yn-1-yl-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-prop-2-en-1-yl-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2-methoxyethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(3-methoxypropyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-butan-2-yl-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2-methylpropyl)-*N*-(2,4,6-trinitrophenyl)nitramine, and *N*-tert-butyl-*N*-(2,4,6-trinitrophenyl)nitramine is lower than that of tetryl. Thus, the impact of stimulating the above-mentioned compounds is higher, along with a higher thermal stability, than that of tetryl.

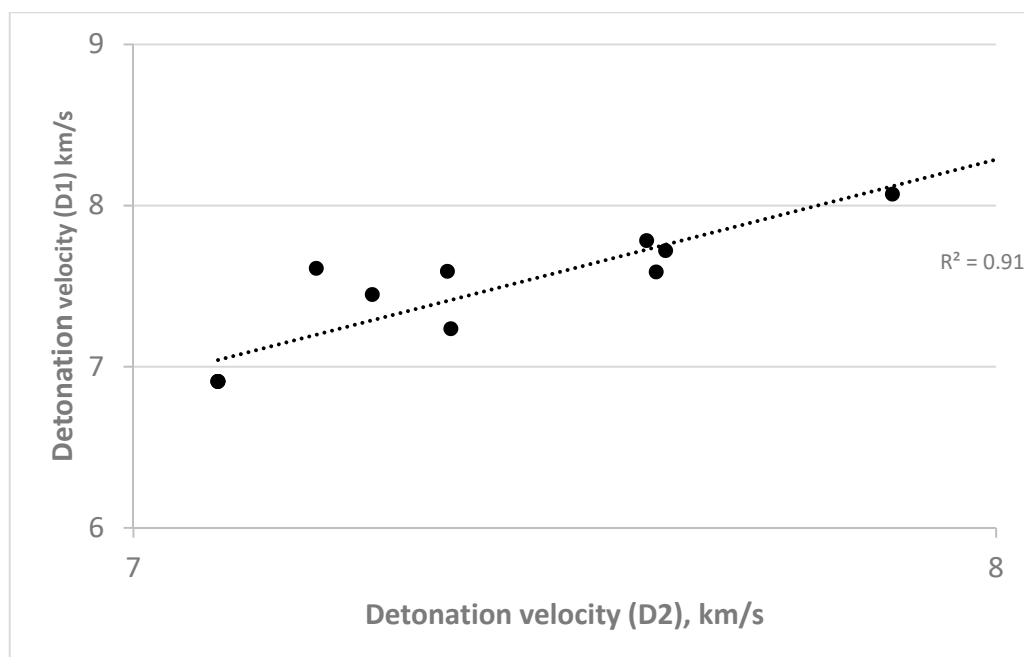


Figure 1. The relationship between the detonation velocity calculated by Equation (1) (D1) and Equation (2) (D2). The correlation coefficient R^2 is equal to 0.91, indicating a strong relationship. Non-coincidences can be addressed by the deviations in the density and other parameter calculations.

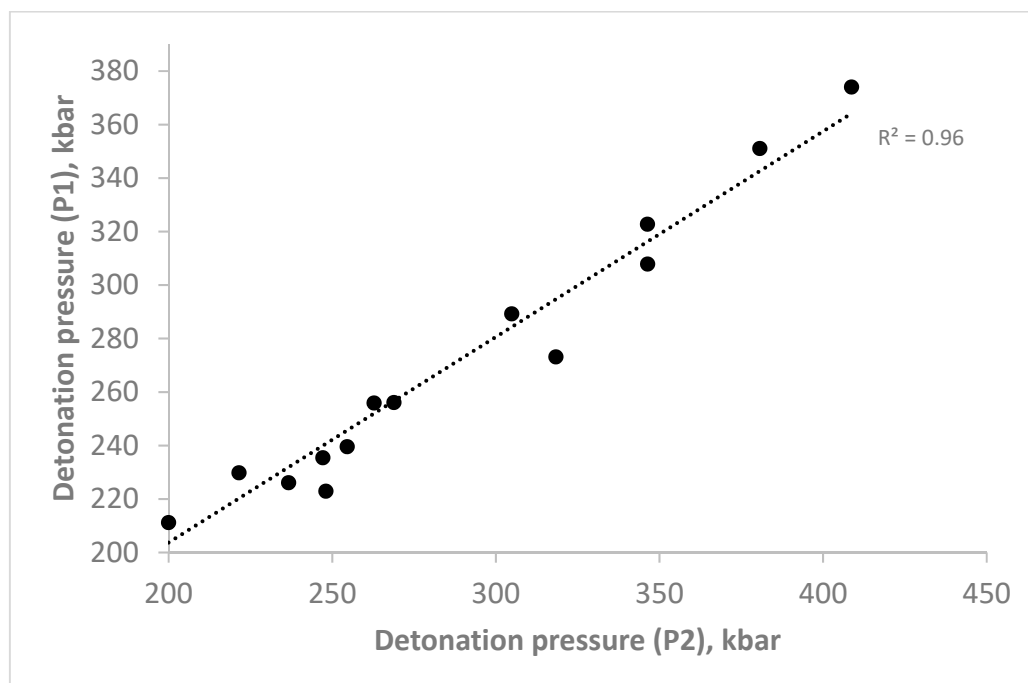


Figure 2. The relationship between the detonation pressures when they are calculated by Equation (1) (P1) and Equation (2) (P2). The correlation coefficient R^2 is equal to 0.96, indicating a strong relationship. Non-coincidences can be addressed by the deviations in calculations of the detonation velocity.

To present as many precise values as possible of parameters describing the explosive properties of the compounds, we calculated their density by using M.S. Keshavarz's [81,82] approach. The densities obtained lie in the range of 1.64–1.91 g/cm³. The values coincide well with crystal densities of 1.7–1.9 g/cm³ that are generally used at high fractions of theoretical maximum density [89]. However, the above approach is not acceptable for

compounds containing F. The density of these compounds was obtained by using the results of molar volume obtained by a B3LYP/cc-pVTZ approach. We pointed out that the detonation velocity is evaluated by using two approaches, and one of them is the density independent (see Equation (1)). Hence, a comparison of the obtained values of the detonation velocity allows one to observe significant inaccuracies if they are present. Indeed, the sequences of increasing detonation velocity of the compounds under study are slightly different (Table 4 and Figure 1). This could be because the approach applied was created considering specific compounds that do not completely match with our investigated ones and/or the limits of the approach used for density calculations. These differences are not significant, which indicates the value of the correlation coefficient. This coefficient is higher than 0.91 and reflects only a 9% difference in the ranking of the compounds under study with respect to their detonation velocity. However, these differences do not influence the main conclusion that *N*-(2-nitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2,4,6-trinitrophenyl)-*N*-[(3,4,5-trinitro-1*H*-pyrazol-1-yl)methyl]nitramine, *N*-(2,2-dinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2,2,2-trinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, and *N*-(trinitromethyl)-*N*-(2,4,6-trinitrophenyl)nitramine possess better explosive properties than tetryl. Moreover, *N*-(2-fluoro-2,2-dinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine is also has a higher energy than tetryl, which is exhibited in the values of D_2 (Table 4). Considering the experimentally obtained detonation velocity of 6.9 km/s of TNT [92], we can foresee that the above compounds also possess better energetic properties than TNT. It is necessary to mention that the detonation velocities calculated vary from 6 to 9 km/s, while those for high explosives vary from 1.01 km/s to 9.89 km/s. The values of the detonation velocity indicate that the compounds under investigation are highly energetic despite the fact that the explosive effectiveness of tetryl in some cases decreases due to the substituents.

We also find that the detonation velocity is related to the ratio of oxygen atoms to carbon atoms, i.e., the detonation velocity is the highest when the oxygen number is exceeded by the number of carbon atoms (Figure 3). However, the sensitivity of the oxygen-rich compounds is also increased, as indicated by the oxygen balance (Table 3).

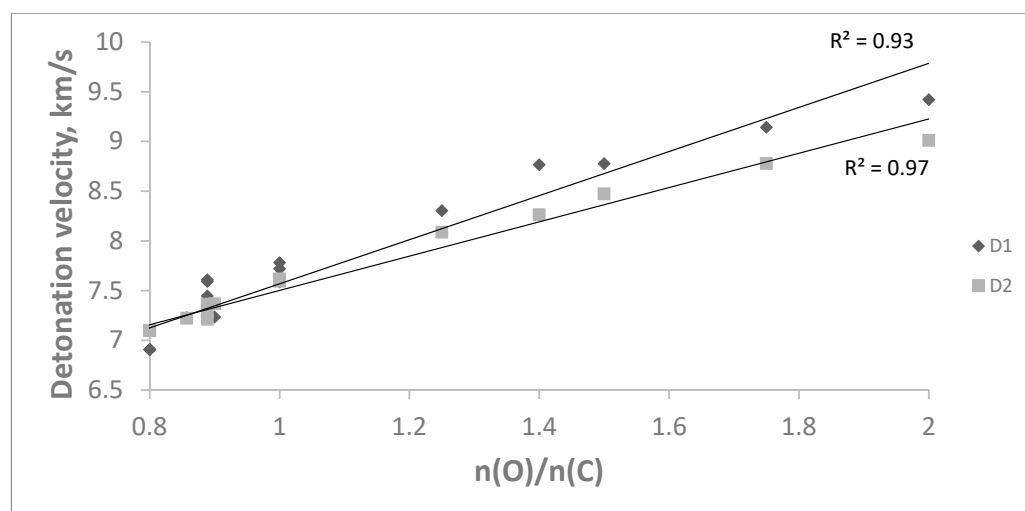


Figure 3. The relationship between the detonation velocity when calculated by Equation (1) (D1) and Equation (2) (D2) and the oxygen rate with respect to the carbon number in the compounds. The correlation coefficient R^2 is equal to 0.93 and 0.97, indicating a strong relationship between the detonation velocity and the number of oxygen atoms with respect to carbon atoms.

Similar conclusions follow from an investigation of the detonation pressure (Table 4). Only a few investigated compounds' explosive properties are better than those of tetryl. They are *N*-(2-nitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2,4,6-trinitrophenyl)-*N*-[(3,4,5-trinitro-1*H*-pyrazol-1-yl)methyl]nitramine, *N*-(2,2,2-trinitroethyl)-*N*-(2,4,6-trinitro-

phenyl)nitramine, *N*-(trinitromethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, and *N*-(2-fluoro-2,2-dinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine. On the other hand, only *N*-tert-butyl-*N*-(2,4,6-trinitrophenyl)nitramine's, *N*-(2-methylpropyl)-*N*-(2,4,6-trinitrophenyl)nitramine's, and *N*-butan-2-yl-*N*-(2,4,6-trinitrophenyl)nitramine's properties are worse in comparison with TNT, whose detonation pressure is equal to 210 kbar at 1.63 g/cm³ density in a solid and is used as a standard. The detonation pressure's dependence on the ratio of oxygen atoms to carbon atoms was also obtained (Figure 4).

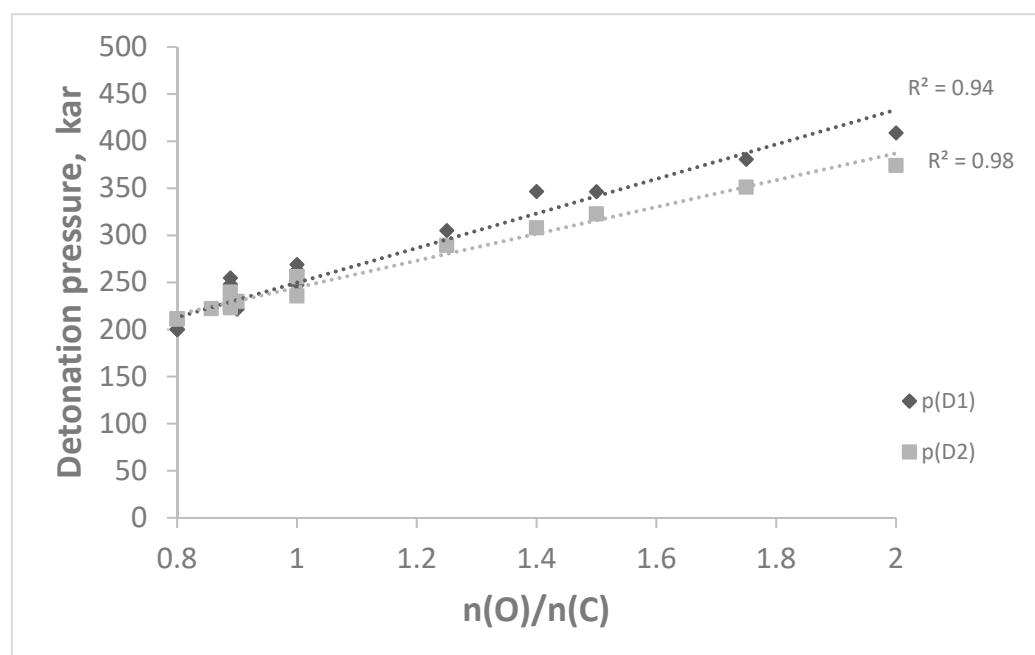


Figure 4. The relationship between the detonation pressure $p(D1)$ and $p(D2)$ when the detonation velocity is calculated by Equation (1) (D1) and Equation (2) (D2), respectively, and the oxygen rate with respect to the carbon number in the compounds. The correlation coefficient R^2 is equal to 0.75 and 0.80, indicating a strong relationship between the detonation velocity and the number of oxygen atoms with respect to carbon atoms.

We pointed out that a summary of the results of our study reveals that *N*-(2-nitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2,4,6-trinitrophenyl)-*N*-[(3,4,5-trinitro-1*H*-pyrazol-1-yl)methyl]nitramine, *N*-(2,2-dinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2,2,2-trinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, and *N*-(trinitromethyl)-*N*-(2,4,6-trinitrophenyl)nitramine possess better explosive properties and are more stable than tetryl. Additionally, we speculate that the compound $C_aH_bN_cO_d$ will be stable, along with having improved explosive properties, if the ratio of oxygen atoms to carbon atoms is between 1.2 and 2.

5. Conclusions

This work was conducted to investigate how varying the substituents attached to the nitramine group nitrogen enhance the stability, resistance to shock stimuli, and explosive properties of a series of secondary aromatic nitramines. These nitramines have the traditional 2,4,6-trinitrophenyl moiety as the main substituent. Based on the obtained results, the following groups can be identified as substituents that increase the thermal and chemical stability of tetryl, while also increasing its electronegativity: $-CH_2CH_2NO_2$, $-CH_2-3,4,5-(NO_2)_3C_3N_2$, $-CH_2-CHN_4$, $-CH_2-C(NO_2)_3$, $-CH_2-CH(NO_2)_2$, $-CH_2-CF(NO_2)_2$, and $C(NO_2)_3$. The higher electronegativity when compared to tetryl indicates a faster aging and greater requirements for the safe storage of tetryl containing these substituents.

The transformations that occur during the activation of these compounds might explain why the reaction zone in detonation waves cannot supply sufficient sustaining

energy and why the detonation front fails to initiate a chemical reaction. This conclusion is derived from an analysis of the activation energy and the shapes of the molecules in the ground and transition states, and it must be confirmed experimentally.

Our findings show that *N*-(2-nitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2,4,6-trinitrophenyl)-*N*-[(3,4,5-trinitro-1*H*-pyrazol-1-yl)methyl]nitramine, *N*-(2,2-dinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, *N*-(2,2,2-trinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine, and *N*-(trinitromethyl)-*N*-(2,4,6-trinitrophenyl)nitramine possess better explosive properties and a greater stability compared to tetryl, although they remain sensitive to shock stimuli.

We propose that the explosive properties of other compounds can be improved by increasing the number of oxygen atoms in such a way that the ratio of oxygen atoms to carbon atoms ranges from 1.2 to 2.

The calculated detonation properties show that introducing an aliphatic chain of additional NO₂ groups to tetryl and increasing their number can be a very convenient way to improve the explosive performance of our designed tetryl analogs. An analysis of the results reveals that the introduction of a N₃ group to the alkyl sidechain can dramatically increase the sensitivity and shock stability of the new energetic materials.

Generally, most of our designed high-energy materials have better explosive properties than TNT and even the parent tetryl. Moreover, *N*-(2,2,2-trinitroethyl)-*N*-(2,4,6-trinitrophenyl)nitramine and *N*-(trinitromethyl)-*N*-(2,4,6-trinitrophenyl)nitramine are close in detonation performance to standard alicyclic nitramines RDX and HMX.

Taking the sensitivity, stability, and detonation performance into account, new tetryl analogs containing dinitroethyl, trinitroethyl, and trinitromethyl substituents could be recommended as candidates for practical realization by chemical synthesis.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/en16135180/s1>.

Author Contributions: Conceptualization, J.S. and J.T.; methodology, J.T.; validation, J.S. and J.T.; formal analysis, J.S. and J.T.; investigation, J.S.; resources, J.T.; data curation, J.S. and J.T.; writing—original draft preparation, J.S. and J.T.; writing—review and editing, J.S. and J.T. All authors have read and agreed to the published version of the manuscript.

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Data Availability Statement: The data supporting the reported results can be obtained upon request to the authors.

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Conflicts of Interest: The authors declare no conflict of interest.

Appendix A

Table A1. A view of the molecules under study and their name, structure, chemical composition, and molecular weight (g/mol).

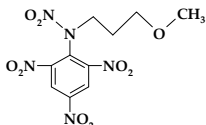
No.	Name	Structural Formula	Molecular Formula	Molecular Weight	Molecular Composition
1.	<i>N</i> -(3-methoxypropyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine		C ₁₀ H ₁₁ N ₅ O ₉	345.222	C 34.79% H 3.21% N 20.29% O 41.71%

Table A1. Cont.

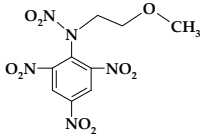
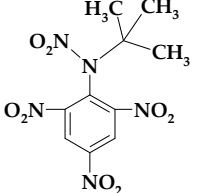
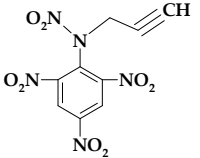
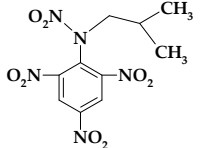
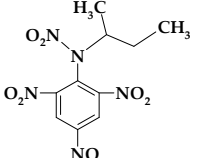
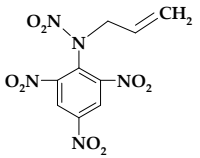
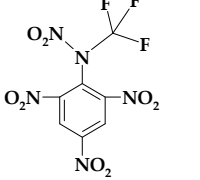
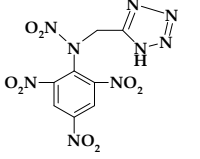
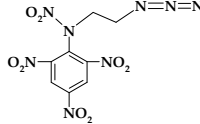
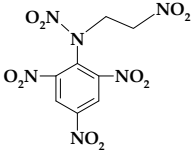
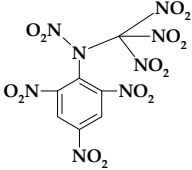
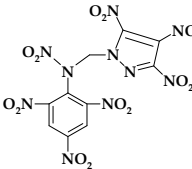
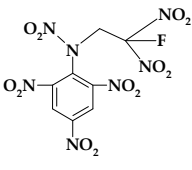
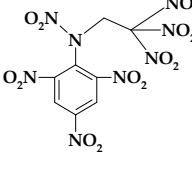
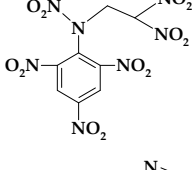
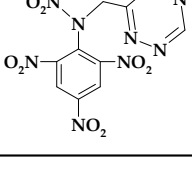
No.	Name	Structural Formula	Molecular Formula	Molecular Weight	Molecular Composition
2.	<i>N</i> -(2-methoxyethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine		C ₉ H ₉ N ₅ O ₉	331.196	C 32.64% H 2.74% N 21.15% O 43.48%
3.	<i>N</i> -tert-butyl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine		C ₁₀ H ₁₁ N ₅ O ₈	329.223	C 36.48% H 3.37% N 21.27% O 38.88%
4.	<i>N</i> -prop-2-yn-1-yl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine		C ₉ H ₅ N ₅ O ₈	311.165	C 34.74% H 1.62% N 22.51% O 41.13%
5.	<i>N</i> -(2-methylpropyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine		C ₁₀ H ₁₁ N ₅ O ₈	329.223	C 36.48% H 3.37% N 21.27% O 38.88%
6.	<i>N</i> -butan-2-yl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine		C ₁₀ H ₁₁ N ₅ O ₈	329.223	C 36.48% H 3.37% N 21.27% O 38.88%
7.	<i>N</i> -prop-2-en-1-yl- <i>N</i> -(2,4,6-trinitrophenyl)nitramine		C ₉ H ₇ N ₅ O ₈	313.181	C 34.52% H 2.25% N 22.36% O 40.87%
8.	<i>N</i> -(trifluoromethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine		C ₇ H ₂ F ₃ N ₅ O ₈	341.115	C 24.65% H 0.59% F 16.71% N 20.53% O 37.52%
9.	<i>N</i> -[(1 <i>H</i> -tetrazol-5-yl)methyl]- <i>N</i> -(2,4,6-trinitrophenyl)nitramine		C ₈ H ₅ N ₉ O ₈	355.181	C 27.05% H 1.42% N 35.49% O 36.04%
10.	<i>N</i> -(2-azidoethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine		C ₈ H ₆ N ₈ O ₈	342.182	C 28.08% H 1.77% N 32.75% O 37.41%

Table A1. Cont.

No.	Name	Structural Formula	Molecular Formula	Molecular Weight	Molecular Composition
11.	<i>N</i> -(2-nitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine		C ₈ H ₆ N ₆ O ₁₀	346.167	C 27.76% H 1.75% N 24.28% O 46.22%
12.	<i>N</i> -(trinitromethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine		C ₇ H ₂ N ₈ O ₁₄	422.136	C 19.92% H 0.48% N 26.54% O 53.06%
13.	<i>N</i> -(2,4,6-trinitrophenyl)- <i>N</i> -[(3,4,5-trinitro-1 <i>H</i> -pyrazol-1-yl)methyl]nitramine		C ₁₀ H ₄ N ₁₀ O ₁₄	488.197	C 24.60% H 0.83% N 28.69% O 45.88%
14.	<i>N</i> -(2-fluoro-2,2-dinitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine		C ₈ H ₄ FN ₇ O ₁₂	409.155	C 23.48% H 0.99% F 4.64% N 23.96% O 46.92%
15.	<i>N</i> -(2,2,2-trinitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine		C ₈ H ₄ N ₈ O ₁₄	436.163	C 22.03% H 0.92% N 25.69% O 51.36%
16.	<i>N</i> -(2,2-dinitroethyl)- <i>N</i> -(2,4,6-trinitrophenyl)nitramine		C ₈ H ₅ N ₇ O ₁₂	391.165	C 24.56% H 1.29% N 25.07% O 49.08%
17.	<i>N</i> -[(1,2,4,5-tetrazin-3-yl)methyl]- <i>N</i> -(2,4,6-trinitrophenyl)nitramine		C ₉ H ₅ N ₉ O ₈	367.192	C 29.44% H 1.37% N 34.33% O 34.86%

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