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Posted Date: 11 October 2025

doi: 10.20944/preprints202510.0879.v1

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Article

Theoretical Design of Acridone-Core Energetic Materials: Assessment of Detonation Properties and Potential as Insensitive, Thermally Stable High-Energy Materials

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Abstract

In this study, we investigated the impact of incorporating energetic substituents such as $–NO_2$, $–NH_2$, –Cl, –F, N-methyl-N-nitro ($CH_3–N–NO_2$), and picryl on the detonation performance and stability of acridone-based compounds. The DFT B3LYP/cc-pVTZ method was employed to evaluate key molecular properties, including the HOMO–LUMO gap, cohesive energy, chemical hardness, and electronegativity. Based on these parameters, changes in chemical and thermal stability were assessed. The results highlight the significant influence of both the type and position of substituents on the energetic performance and stability of the compounds studied. Notably, the acridone derivative bearing a picryl group and four $–NH_2$ substituents exhibited energetic properties superior to those of TNT. However, the analysis of stability and sensitivity—based on oxygen balance—suggests that such substitutions generally reduce stability. This reduction, however, is dependent on both the nature and number of substituents introduced.

Keywords: high energy materials (Ex); acridones; energetic groups; detonation properties; density; stability

1. Introduction

Acridone, a heterocyclic aromatic scaffold featuring a carbonyl group and a secondary amine, possesses a unique, planar heterocyclic ring system containing nitrogen, which can exist in both protonated and unprotonated forms [1,2]. Owing to these structural characteristics, the acridone core has attracted considerable interest from medicinal chemists worldwide. In the past years, increased knowledge and understanding of the mode of action of acridone derivatives have driven sustained and dynamic research into their potential, mostly as anti-cancer agents. However, the use of acridone in co-crystallization technology for the development of high-energy materials has attracted significant attention as a promising strategy to balance explosive performance with safety considerations, including sensitivity to heat, impact, shock, and friction. Recently, Sen et al. demonstrated that co-crystallization of trinitrotoluene (picryl) and picric acid (PIC) with acridine (ACR) enhanced the properties of these high-energy materials, suggesting its potential as an insensitive explosive [3]. They also state that these newly formed compounds exhibit excellent thermal stability, demonstrating that salt formation and crystallization are two strategies to modulate thermal stability, and the conformers play a vital role in the performance of the target products.

The advanced compound 3-nitro-1,2,4-triazol-5-one (NTO), when co-crystallized with acridine (ACR), demonstrated good thermal stability and excellent impact insensitivity. Moreover, the

 doi:10.20944/preprints202510.0879.v1

obtained detonation velocity and pressure values confirm its potential as a high-performance explosive [4]. Despite the potential of co-crystals to combine high heats of formation, desirable detonation performance, good thermal stability, and low sensitivity to impact and shock, few studies have been conducted in this direction. Therefore, we designed and conducted theoretical studies to evaluate the influence of substitutions on the stability and detonation performance of acridone-based polynitro derivatives, to predict their potential as safe and powerful high-energy materials. In our investigation, the energetic and stability properties of Tetranitroacridone or 2,4,5,7-Tetranitro-10H-acridin-9-one according to IUPAC nomenclature (Acri1) were evaluated upon substitution with selected functional groups such as NO_2, -NH_2, -Cl, -F, N-methyl-N-nitro (CH_3-N-NO_2), and Picryl. The selection of functional groups was considered on their expected impact on detonation performance. For example, in many reported cases, the incorporation of -NH_2 leads to an improvement in the thermal stability of the high-energy materials, while -NO_2 enhances energetic properties [5–15]. The effects of fluorine and chlorine substitutions were also established, as these halogens are known to improve detonation performance through bond reinforcement, altered decomposition pathways, greater energy output, and enhanced structural stability, often accompanied by reduced sensitivity to unintended initiation [16,17]. Methylation of the compound reduces sensitivity to mechanical stimuli and thermal decomposition, making energetic materials safer and more manageable [18,19]. On the other hand, nitrogen-rich compounds typically exhibit high sensitivity to external stimuli, but they also demonstrate excellent detonation performance [20]. Additionally, 1,3,5-trinitrobenzene derivatives, such as picric acid, are used in the formulation of energetic materials. Owing to their high thermal stability and elevated melting points, compounds containing trinitrobenzene groups are particularly suitable for applications in explosives and related energetic systems, but they have not been investigated as thoroughly [21].

We hope that our study will help reveal the most promising strategy for synthesizing co-crystals to create advanced, safe, and cost-effective materials that meet hazardous material requirements.

2. Materials and Methods

Investigations were performed using the B3LYP functional with the cc-pVTZ basis set, as implemented in GAUSSIAN [22–24]. This approach yielded results consistent with experimental data [25–33]. The most stable conformations were obtained by Berny geometry optimization, followed by vibrational frequency analysis to confirm true minima. The total energy of the conformers was compared to identify the most stable ones. The selected conformers were then further analyzed.

Stability and sensitivity were assessed through key descriptors: cohesive energy per atom, HOMO–LUMO gap, chemical hardness, electronegativity, hardness index, and oxygen balance [34]. Cohesive energy (BDE) indicated thermal stability, while the HOMO–LUMO gap and hardness reflected electronic stability. Electronegativity was used to gauge bond-forming propensity and predict the aging compounds.

Densities of the compounds were predicted using three approaches:

- Politzer's equations [35]. , which incorporate the 0.001 e/bohr^3 isosurface and surface potential balance;
- Calculated from molecular weight and B3LYP/cc-pVTZ molar volume;
- ACD/ChemSketch [36], where density is estimated using a machine-learning algorithm trained on compounds with known densities, expressed as a function of molecular volume, electronic properties, and intermolecular interaction patterns. The obtained densities were compared.

The energetic performance of the materials was assessed through detonation pressure and velocity, calculated using several approaches developed for Cl/F-containing compounds [37–39]. Predictions obtained with the method of [39] were notably higher than those from the equations in [37,38]. The latter yielded values for CaHbOcNd in close agreement with the established Kamlet–Jacobs approach. Therefore, in this study, we present detonation parameters evaluated using the equations described in [37,38]. Sensitivity to shock was estimated from the oxygen balance, calculated according to formulae presented in [40,41]. It is used for compounds that contain F or Cl.

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Aiming to combine two valuable practical properties of modern high-energy materials, an application of ortho-amino-nitro groups present in the acridone moiety (responsible for the decreased sensitivity to mechanical stimuli) was additionally modified at N-9 with specific Picryl or 3,5-diamino-picryl fragments, known as markedly increasing thermal stability [42]. Similar methods in molecular design were previously successfully applied for the design of famous thermally resistant energetic molecules such as 3,5-Dinitro-N,N′-bis(2,4,6-trinitrophenyl)-2,6-pyridinediamine (PYX) (therm. decomp. 360 °C)[] or PL-1 (2,4,6-Tris(3′,5′-Diamino-2′,4′,6′-trinitrophenylamino)-1,3,5-triazine, therm. decomp. 337 °C) [43–45].

3. Results and Discussion

3.1. Stability

3.1.1. Thermal Stability

Figure 1 depicts the molecular skeleton together with the electrostatic potential, which was used to investigate the influence of substitutions on stability and detonation properties.

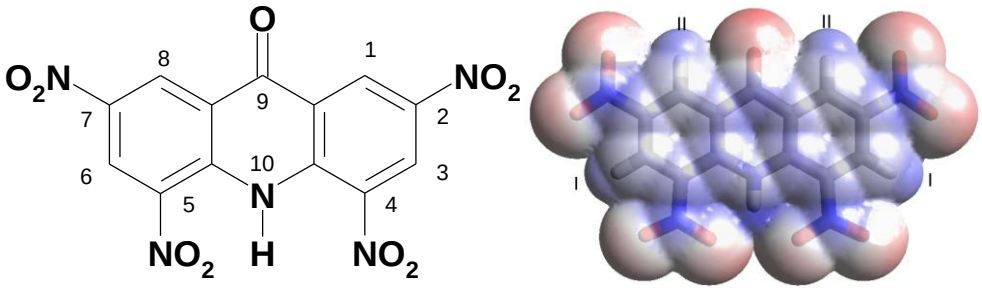

Figure 1. The molecular skeleton (on the left) together with the electrostatic potential (on the right). The deep red regions indicate areas of the highest electron density, whereas the deep blue regions correspond to the lowest electron density. I ir II indicates the position of the substitutions.

This compound contains -NO_2 groups, making it a potential high-energy material. Moreover, there are several areas, marked as I and II in Figure 1, for the substitutions. Based on the electron distribution in the compounds, we predict that the more favorable position for substitution is site I, which is slightly more positive than site II and is surrounded by less negative regions (Figure 1). So, the substitutions firstly filled site I, and later site II. From a chemical perspective, the preferential occupation of site I may also be related to reduced steric hindrance and increased stabilization through electronic effects. Additionally, Picryl or other energetic fragments can be introduced in place of the hydrogen atom of the N–H group [3,4]. This introduction allows us to examine how stability and detonation properties change when not only the molecular skeleton but also the introduced molecule is substituted. It is also important to note that, in some cases, the introduction of substitutions leads to significant changes in the structure of the skeleton molecule. The core (benzene rings) bends and becomes non-planar. To illustrate these structural changes, we provide the coordinates of each studied compound in the supplementary materials, enabling more detailed analysis, while in Appendix 1, there are abbreviations, chemical compositions, and skeletons of each compound. The importance of molecular structure for stability is well known and is also confirmed by our results. For example, the difference between conformers Acri2 and Acri2_II lies in the position of the hydrogen atoms in the OH substituent. While the thermal stability of these compounds is the same, their chemical stability differs (Table 1). Notably, the hardness index of the investigated compounds is higher than or close to 0.8 (Table 1), which indicates their overall high stability, although variations reveal which substitutions may reduce or increase this stability.

Our results of cohesive energy (BDE) show that only F substitutions leave the thermal stability of Acri1 unchanged. In most cases, the thermal stability of the compounds is slightly lower, although

 doi:10.20944/preprints202510.0879.v1

it decreases significantly in the case of Acri15 **(**Table 1**).** Moreover, compounds with fewer substitutions are more thermally stable, whereas more complex substituents tend to reduce this stability to a greater extent than simpler ones (Table 1, Figure 2). For instance, a compound with four NCH_3NO_2 substituents shows the lowest thermal stability of all compounds investigated. These results are in good agreement with previous research [46,47].

Table 1. The parameters described the chemical and thermal stability. Here, BDE is cohesive energy, Hard-chemical hardness, Elec – electronegativity, Gap – the gap between the highest occupied and the lowest unoccupied orbitals, Ind – hardness index.

Abderviation	Substitutions	Gap, eV	Hard, eV	Elec, eV	Ind	BDE
Acri1	None	3.79	1.90	5.96	0.86	5.94
Acri2	2 OH	3.46	1.73	6.04	0.83	5.83
Acri2_II		3.64	1.82	5.92	0.85	5.83
Acri7	4 HO	3.88	1.94	5.88	0.87	5.75
Acri3	2 Cl	3.82	1.91	5.96	0.86	5.82
Acri8	4 Cl	3.20	1.60	5.58	0.80	5.68
Acri4	2 F	3.90	1.95	6.07	0.87	5.93
Acri9	4 F	4.06	2.03	6.16	0.88	5.92
Acri5	2 NH_2	3.47	1.74	5.58	0.83	5.84
Acri10	4 NH_2	3.65	1.83	5.13	0.85	5.76
Acri6	2 NCH_3NO_2	3.68	1.84	6.08	0.85	5.55
Acri11	4 NCH_3NO_2	3.41	1.71	6.26	0.83	5.35
Acri12	Picryl	3.21	1.60	6.34	0.81	5.86
Acri13	Picryl and 2 NH_2	3.22	1.61	5.85	0.81	5.81
Acri14	Picryl and 4 NH_2	3.11	1.55	5.54	0.79	5.78
Acri15	2 NH_2 in Picryl and 4 NH_2	2.99	1.50	5.24	0.78	4.76

Notably, the thermal stability of the Picryl-containing compound (Acri12) decreases significantly when the Picryl group is substituted by $–NH_2$ (Acri15) but remains approximately the same when the core of the compound is substituted by $–NH_2$ (Acri13 and Acri !4). The results coincide well with the conclusions drawn from the experimental research presented in [48–51].

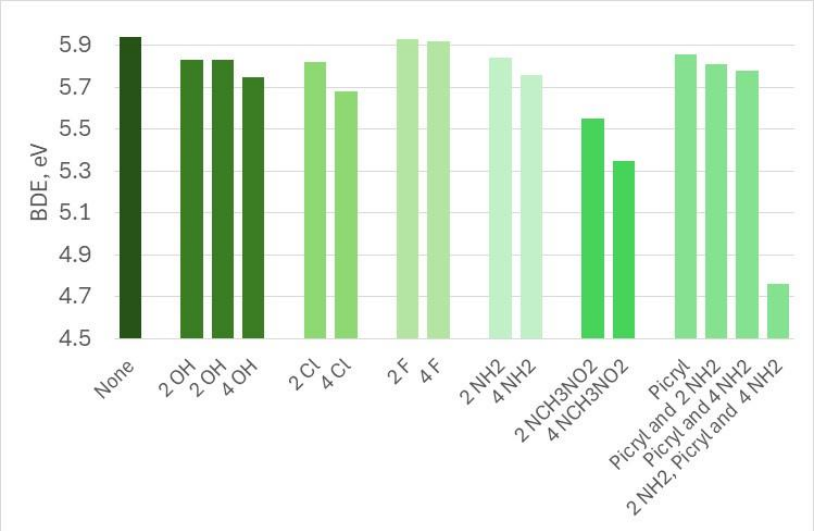

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Figure 2. Effect of substitutions and their number on thermal stability, as reflected by the cohesive energy.

In summary, we conclude that Acri1 is thermally stable, and substitutions such as –Cl, –F, –NH_2, –NO_2, or -Picryl do not significantly affect this property. However, thermal stability may decrease when the substituent contains –NO_2 groups (e.g., N–NO_2–CH_3 or Picryl with additional amino groups), most likely because strong electron-withdrawing effects weaken the substituent's structure and increase its susceptibility to thermal degradation. The analysis further revealed that the thermal stability of Acri1 is not affected by the position of the substituents.

3.1.1. Chemical Stability

HOMO–LUMO gap and chemical hardness analyses reveal the same trend in the influence of substitutions on the chemical stability of the studied compounds (Table 1, Figure 3). While the HOMO–LUMO gap reflects stability and chemical hardness indicates reactivity, both parameters describe the reactivity potential of the compounds. Hence, we focus our discussion on the changes in the HOMO–LUMO gap due to substitutions.

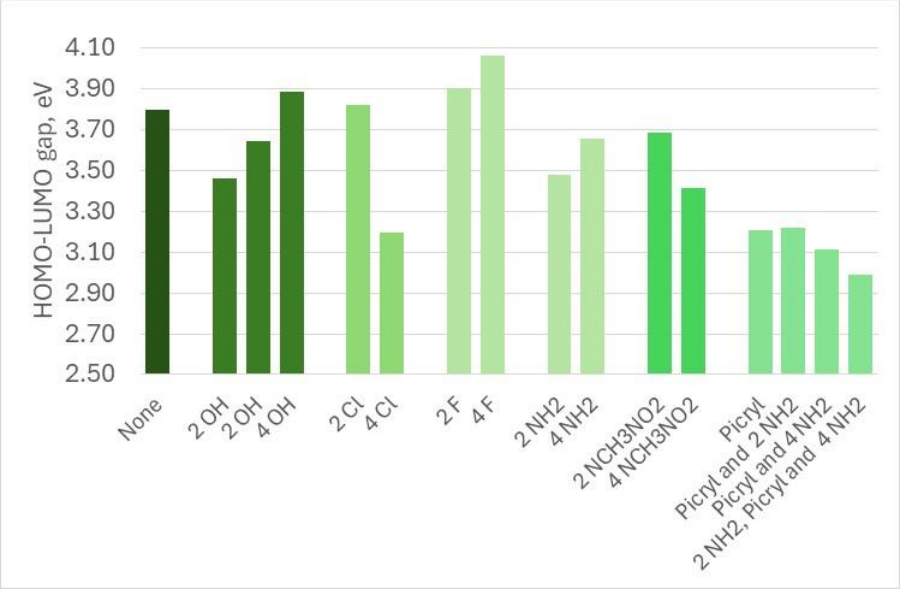

Figure 3. Effect of substitutions and their number on chemical stability, as reflected by the HOMO–LUMO gap.

Generally, Acri1 becomes less chemically stable upon substitution, except when four –OH or –F groups are present (Figure 3). An increasing number of hydrogen-bond-forming substitutions enhances chemical stability, provided that other effects, such as steric hindrance, do not prevail. This trend is clearly reflected in the HOMO–LUMO gap and chemical hardness of the compounds containing Picryl: substitution of the core molecule with two –NH_2 groups slightly increases stability, whereas further increasing the number of such substitutions leads to decreased chemical stability. The importance of both the presence and the placement of hydrogen bonds is also illustrated by the results obtained for Acri2, Acri2_II, and Acri7. Acri2 and Acri2_II differ only in the position of the OH hydrogen: in Acri2 the hydrogen bonds form a V-shaped arrangement, while in Acri2_II they adopt a cyclic motif. The Acri7, where four hydrogen bonds form cycle arrangements, is chemically more stable than Acri2_II and Acri1. Since larger substituents cause greater steric hindrance, which can reduce chemical stability, an increasing number of Cl substituents leads to lower stability. Additionally, relatively weaker bonding compared to fluorine may also be the reason for the higher chemical stability of compounds with F substitutions, which tends to increase chemical stability through strong, stable bonds and favorable electronic effects [52]. A compound combining high chemical stability with highly electronegative substituents typically exhibits strong covalent bonding,

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low susceptibility to spontaneous degradation, and resistance to aging, while maintaining the potential for selective reactivity under extreme conditions.

The electronegativity of compounds such as Acri2, Acri4, Acri6, Acri11, Acri9, and Acri12 is higher than that of Acri1 (Figure 4), reflecting a stronger tendency to attract electrons.

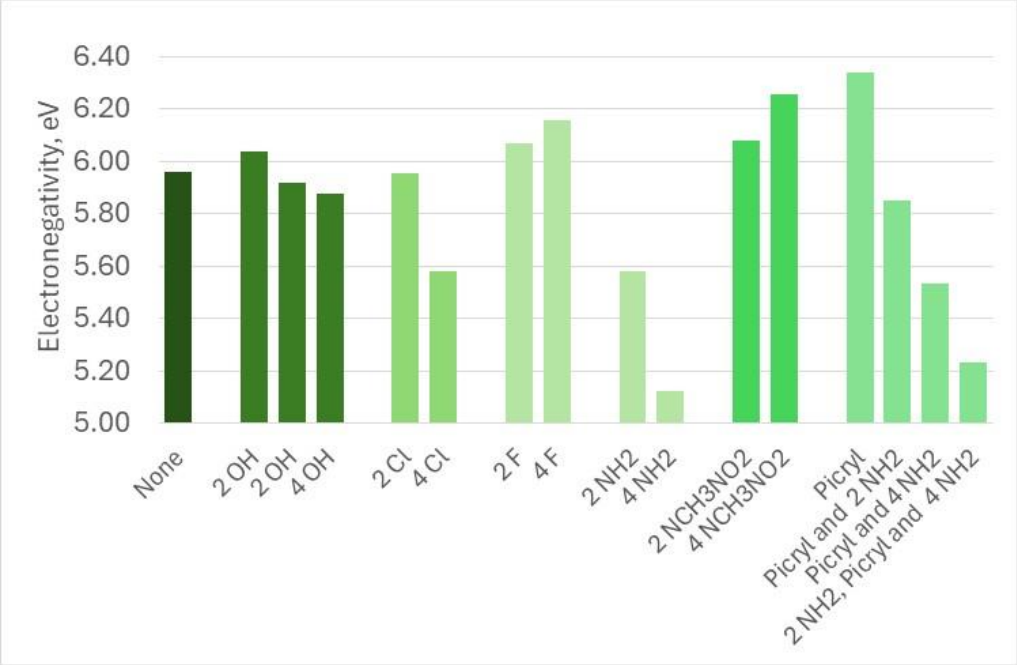

Figure 4. Effect of substitutions and their number on electronegativity.

Considering the low chemical and thermal stability, as well as the high electronegativity, of Acri2, Acri6, Acri11, and Acri12, we propose that these compounds are likely to degrade more rapidly than Acri1. In contrast, the selective reactivity and degradation of Acri4 and Acri9 are expected to depend on the environmental and chemical context. The analysis of the charge distribution illustrates these observations: in the compounds Acri2, Acri6, Acri11, and Acri12 the electron-deficient areas are located on the outer part of the compounds, whereas in Acri4 and Acri9, these regions are concentrated in the inner molecular structure (see Supplementary Materials).

The degradation of the remaining compounds could also be faster than that of Acri1 due to their higher instability despite their electronegativity. Thus, only –F substitutions enhance Acri1 stability and reduce its degradation rate. Notably, the position of the substituents plays a significant role in chemical stability. The compound bearing a picryl group and the one substituted with -NO_2 group are markedly more reactive compared to the others.

3.2. Sensitivity

We obtained oxygen balance (OB) to predict the sensitivity of the compounds under study (Figure 5). It is well established that compounds with highly negative oxygen balances tend to exhibit reduced sensitivity, likely due to the presence of unbalanced reactive fragments during decomposition [53–56]. This statement is supported by our results, which show that an increase in reactive fragments leads to increased sensitivity. For instance, compounds bearing four chlorine or fluorine substituents exhibit higher sensitivity compared to those with only two such groups.

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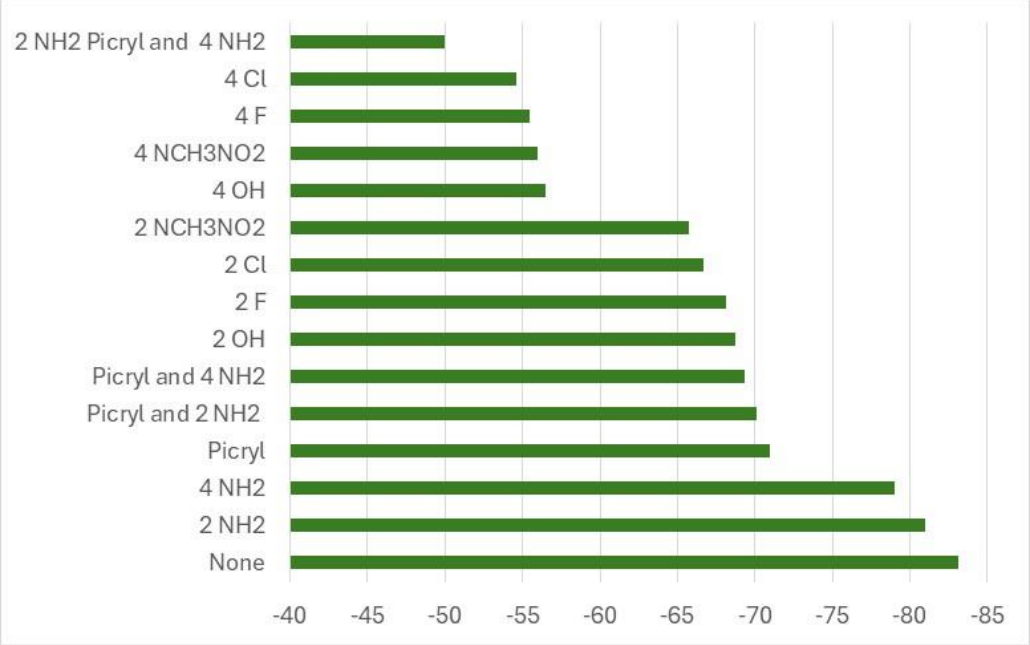

Figure 5. Effect of substitutions and their number on the impact of the stimuli.

It is important to note that OB of TNT is –73.97%, while that of RDX is -21.61%. The comparison of these values with those of the studied compounds shows that all compounds investigated are substantially less sensitive than RDX, but only Acri1, Acri5, and Acri10 exhibit lower sensitivity than TNT. This implies that the compounds are more resistant to external stimuli such as impact or friction than RDX although only a few outperform TNT in terms of insensitivity. Given that moderately sensitive materials generally have an OB between –30% and –20%, it can be stated that all of the compounds studied fall within the insensitive category.

3.3. Detonation Properties

3.3.1. Density

Material density plays a key role in determining the detonation products, which directly influence detonation pressure and velocity [57]. As described in the *Materials and Methods* section, density was calculated using three different approaches. Among them, Politzer's method, combined with rigorously validated B3LYP quantum chemical calculations, captures intermolecular interactions that are critical for accurate density modeling [58]. The results are summarized in Table 2. As expected, different approaches yield different values. In the majority of cases, these differences do not exceed 5–6%, which is considered an acceptable deviation. However, in some instances, the densities calculated using the ACD/ChemSketch approach exceed those from other methods by more than 9%. Considering that experimentally measured densities can vary by more than 10% under different conditions, we speculate that the computational approaches applied here provide reasonably trustworthy results. For confirmation, the density of TNT is generally stable but can vary from approximately 1.57 to 1.67 g/cm³ depending on temperature, pressure, and physical state. Similarly, the experimentally determined density of CF3N3 has been reported in the range of 1.716–1.816 g/cm³, while the value estimated using ACD/ChemSketch is 1.77 g/cm³ [59,60]. It is also important to note that the calculated densities fall within the range of 1.62 to 1.94 g/cm³, which is consistent with the reported values for substituted acridone derivatives [61].

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Table 2. The density obtained. Here, ϱ_{gaus}, is calculated from molecular weight and B3LYP/cc-pVTZ molar volume, ϱ_{Kev} is evaluated by Politzer's equations [35], and ϱ_{acd} is obtained by the approach implemented in ACD/ChemSketch [36].

Abderviation	Substitutions	ϱ_{gaus}, g/cm^3	ϱ_{Kev}, g/cm^3	ϱ_{acd},g/cm^3
Acri1	None	1.70	1.60	1.82
Acri2	2 OH	1.98	1.89	2.01
Acri2_II		1.95	1.86	2.01
Acri7	4 HO	1.91	1.81	2.20
Acri3	2 Cl	1.81	1.72	1.93
Acri8	4 Cl	2.10	2.02	2.02
Acri4	2 F	1.84	1.75	1.92
Acri9	4 F	1.83	1.73	2.01
Acri5	2 NH_2	1.88	1.79	1.92
Acri10	4 NH_2	1.66	1.56	2.02
Acri6	2 NCH_3NO_2	1.85	1.75	1.91
Acri11	4 NCH_3NO_2	1.71	1.61	1.96
Acri12	Picryl	1.75	1.65	1.95
Acri13	Picryl and 2 NH_2	1.94	1.85	2.02
Acri14	Picryl and 4 NH_2	2.14	2.06	2.09
Acri15	2 NH_2 in Picryl and 4 NH_2	1.96	1.87	2.15

Analysis of the calculated densities indicates that the density of Acri1 increases upon substitution, most likely due to a greater rise in overall molecular weight compared to volume. Indeed, most compounds exhibit larger calculated volumes compared to Acri1, and only the volumes of both conformers of Acri2 and Acri5 are found to be lower. In these cases, the increase in density appears to result from tighter molecular packing, promoted by molecular shape and intermolecular interactions such as hydrogen bonding or dipole–dipole forces, which reduce molecular volume and thereby enhance density [62]. Notably, contradictory results were obtained in the case of Acri10. The density calculated using molecular weight and B3LYP/cc-pVTZ-derived molar volume, as well as the value estimated via Politzer's equation, is lower than that of Acri1. However, the density obtained using the ACD/ChemSketch approach is higher. These findings indicate that the ACD/ChemSketch method may more accurately account for empirical influences—such as molecular packing, steric effects of substituents, and crystal lattice interactions—that affect density in the solid state. On the other hand, the observed discrepancy may also reflect the variability in the density of the same compound when crystallized under different conditions.

No clear trend was observed between density and the type or number of substitutions. However, the results confirm that density increases when the rise in molecular weight outweighs the increase in molecular volume, particularly when the substituents are flexible enough to adapt their shape and promote intermolecular interactions.

3.3.2. Detonation Velocity and Pressure

High-energy materials generally exhibit detonation velocities in the range of 1.01 to 9.89 km/s. TNT, a widely used reference explosive, has a typical detonation velocity of ~6.9 km/s. In contrast, RDX and HMX achieve higher detonation velocities of 8.7 km/s and 9.1 km/s, with associated detonation pressures of approximately 33.8 GPa and 39.3 GPa, respectively, compared to ~ 21.0 GPa for TNT [63,64]. The detonation pressure and velocity of compounds consisting of one or two benzene

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rings annelated with N-heterocycle fall within the range of 20–25 GPa and 6.6–8.0 km/s, respectively [63,65].

The compounds under investigation generally exhibit lower detonation pressure compared to TNT (Table 3). An exception is Acri14, whose detonation pressure is higher than that of TNT and comparable to that of the aforementioned nitrogen-rich compounds, but significantly lower than that of RDX and HMX. Thus, based on the analysis of the detonation pressure, a parameter reflecting shockwave intensity, the compounds under study are unlikely to be effective explosives. While the detonation velocities of the compounds fall within the range typical of high-energy materials, only Acri14 and Acri15 exhibit values significantly exceeding that of TNT (Table 4). These compounds along with -NH_2 substitutions contain picryl groups, and such substituent is often associated with detonation velocities and pressures comparable to, or intermediate between, those of TNT and RDX. Furthermore, the significant exothermic decomposition observed in compounds with picryl substituents suggests a high energy output. So, the high detonation pressure and velocity of Acri14 and Acri15 could be related to the decomposition of picryl. It implies that when these compounds are initiated, chemical reactions will begin when the bonds between the core molecules and picryl and its substitutions begin to break. These first reactions generate highly reactive intermediate species that promote further decomposition of the core molecule and the sequence of exothermic reactions that give rise to thermal runaway. The comparison of the detonation pressure and velocity of the rest compound supports this finding. First, the detonation pressures and velocities of Acri12 and Acri13 are lower than those of Acri14, despite all three containing picryl groups. The primary difference between these compounds lies in the number of –NH_2 substituents. The absence or insufficient number of these substituents may result in an unbalanced formation of highly reactive intermediate species, which is inadequate to promote the effective decomposition of the molecular core. Second, the analysis of detonation pressures and velocities indicates lower values for compounds with the strongest bonds between the core molecule and its substituents. For example, Acri3 and Acri4—both containing strong C–Cl or C–F bonds—exhibit some of the lowest detonation pressures and velocities among the compounds studied.

Table 3. Detonation pressures calculated using different density estimation methods. Here, $\mathbf{P_{gaus}}$, is the pressure calculated using density derived from molecular weight and B3LYP/cc-pVTZ-optimized molar volume; $\mathbf{P_{Kev}}$ is the pressure obtained using density estimated via Politzer's equation [35], and $\mathbf{P_{acd}}$ is the pressure based on density calculated with the ACD/ChemSketch approach [36].

Abderviation	Substitutions	P_{gaus}, GPa	P_{Kev}, GPa	P_{acd}, GPa
Acri1	None	9.76	8.49	11.43
Acri2	2 OH	14.45	13.06	14.91
Acri2_II		13.98	12.58	14.91
Acri7	4 HO	14.03	12.56	19.05
Acri3	2 Cl	11.53	10.33	13.28
Acri8	4 Cl	15.93	14.67	14.70
Acri4	2 F	12.22	10.86	13.35
Acri9	4 F	12.56	11.09	15.31
Acri5	2 NH_2	14.29	12.81	15.07
Acri10	4 NH_2	12.40	10.79	19.03
Acri6	2 NCH_3NO_2	16.15	14.44	17.26
Acri11	4 NCH_3NO_2	16.64	14.62	22.19
Acri12	Picryl	12.92	11.33	16.33
Acri13	Picryl and 2 NH_2	11.53	10.33	13.28

 doi:10.20944/preprints202510.0879.v1

Acri14	Picryl and 4 NH_2	24.36	22.49	23.02
Acri15	2 NH_2 in Picryl and 4 NH_2	18.91	17.12	23.06

Table 4. Detonation velocity calculated using different density estimation methods. Here, D_{gaus}, is is the detonation velocity calculated using density derived from molecular weight and B3LYP/cc-pVTZ-optimized molar volume; D_{Kev} is the velocity obtained using density estimated via Politzer's equation [35], and D_{acd} is the velocity based on density calculated with the ACD/ChemSketch approach [36].

Abderviation	Substitutions	D_{gaus}, km/s	D_{Kev}, km/s	D_{acd}, km/s
Acri1	None	5.70	5.48	5.98
Acri2	2 OH	6.43	6.23	6.49
Acri2_II		6.36	6.16	6.49
Acri7	4 HO	6.37	6.15	7.04
Acri3	2 Cl	5.99	5.80	6.26
Acri8	4 Cl	6.63	6.46	6.46
Acri4	2 F	6.10	5.89	6.27
Acri9	4 F	6.15	5.92	6.55
Acri5	2 NH_2	6.41	6.19	6.52
Acri10	4 NH_2	6.13	5.88	7.04
Acri6	2 NCH_3NO_2	6.66	6.43	6.81
Acri11	4 NCH_3NO_2	6.73	6.45	7.42
Acri12	Picryl	6.21	5.96	6.69
Acri13	Picryl and 2 NH_2	5.99	5.80	6.26
Acri14	Picryl and 4 NH_2	7.66	7.45	7.51
Acri15	2 NH_2 in Picryl and 4 NH_2	7.02	6.79	7.52

Based on the results obtained, it can be concluded that the detonation performance of acridone-based compounds is potentially improved by incorporating picryl-like groups along with appropriate substitutions on the core structure.

4. Conclusions

The studies were carried out to evaluate the influence of substitutions on the stability and detonation performance of acridone-based polynitro derivatives and to assess their potential as safe, high-energy materials. The results show that Acri1 is thermally stable, and substitutions with –Cl, –F, $–NH_2$, $–NO_2$, or –Picryl do not significantly affect this property, although its compounds with the substituent contain $–NO_2$ groups are less thermally stable. We also found that the position of electron-deficient areas influences chemical stability. Based on this, Acri2, Acri6, Acri11, and Acri12 are predicted to degrade more rapidly than Acri1, while only –F substitution improves Acri1 stability and reduces its degradation rate. Notably, compounds bearing a picryl group or substituted with $–NH_2$ are markedly more reactive than the others.

Based on the BO analysis, all of the studied compounds can be classified as insensitive. The detonation performance of acridone-based compounds is potentially enhanced by incorporating picryl-like groups together with appropriate substitutions on the core structure. However, while substitutions on the core molecule do not significantly affect the stability of acridone-based compounds, modifications to the picryl-like substituents lead to a marked decrease in stability.

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The planar structure of Acri1 and its proposed ability to form hydrogen bonds suggest that it could be used for co-crystal production. Moreover, the properties of acridone-based co-crystals may be further improved through substitutions on this compound or on the substituted fragment.

Supplementary Materials: The following supporting information can be downloaded at the website of this paper posted on Preprints.org.

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

Funding: This research received no external funding.

Data Availability Statement: The data presented in this study are available on request from the corresponding author due to access restrictions.

Acknowledgments: The numerical calculations with the GAUSSIAN09 package were performed using the resources of the Information Technology Research Center of Vilnius University and the supercomputer "VU HPC" of Vilnius University in the Faculty of Physics location.

Conflicts of Interest: The funders had no role in the design of the study, in the collection, analyses, or interpretation of data; in the writing of the manuscript; or in the decision to publish the results.

Abbreviations

The following abbreviations are used in this manuscript:

BDE	Cohesive energy per atom
HOMO-LUMO gap	Difference between the highest occupied and the lowest unoccupied orbitals
OB	Oxygen Balance (calculated to CO_2)
PYX	3,5-Dinitro-N,N′-bis(2,4,6-trinitrophenyl)-2,6-pyridinediamine

Acri1	$C_{13}H_5N_5O_9$	2,4,5,7-Tetranitroacridin-9(10 *H*)-one
Acri2	$C_{13}H_5N_5O_{11}$	3,6-Dihydroxy-2,4,5,7-tetranitroacridin-9(10 *H*)-one
Acri3	$C_{13}H_3Cl_2N_5O_7$	3,6-Dichloro-2,4,5,7-tetranitroacridin-9(10 *H*)-one
Acri4	$C_{13}H_3F_2N_5O_7$	3,6-Difluoro-2,4,5,7-tetranitroacridin-9(10 *H*)-one
Acri5	$C_{13}H_7N_7O_9$	3,6-Diamino-2,4,5,7-tetranitroacridin-9(10 *H*)-one
Acri6	$C_{15}H_9N_9O_{13}$	3,6-Bis[methyl(nitro)amino]-2,4,5,7-tetranitroacridin-9(10 H)-one
Acri7	$C_{13}H_5N_5O_{13}$	1,3,6,8-Tetrahydroxy-2,4,5,7-tetranitroacridin-9(10 *H*)-one
Acri8	$C_{13}HCl_4N_5O_9$	1,3,6,8-Tetrachloro-2,4,5,7-tetranitroacridin-9(10 *H*)-one
Acri9	$C_{13}HF_4N_5O_9$	1,3,6,8-Tetrafluoro-2,4,5,7-tetranitroacridin-9(10 *H*)-one
Acri10	$C_{13}H_9N_9O_9$	1,3,6,8-Tetraamino-2,4,5,7-tetranitroacridin-9(10 *H*)-one

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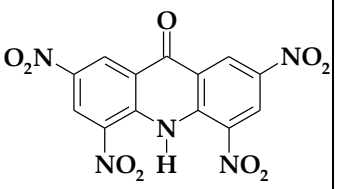
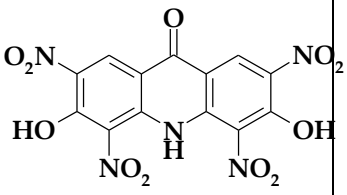
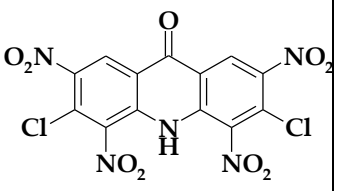
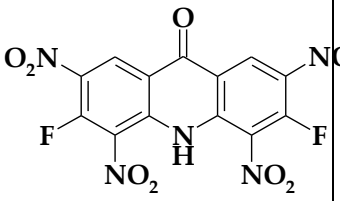
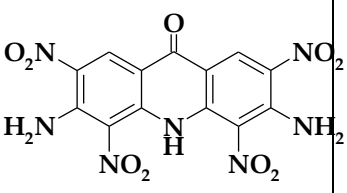
Acri11	$C_{17}H_{13}N_{13}O_{17}$	1,3,6,8-Tetrakis[methyl(nitro)amino]-2,4,5,7-tetranitroacridin-9(10 *H*)-one
Acri12	$C_{19}H_6N_8O_{15}$	10-Picryl-2,4,5,7-tetranitroacridin-9(10 *H*)-one
Acri13	$C_{19}H_8N_{10}O_{15}$	10-Picryl-3,6-Diamino-2,4,5,7-tetranitroacridin -9(10 *H*)-one
Acri14	$C_{19}H_{10}N_{12}O_{15}$	10-Picryl-1,3,6,8-tetraamino-2,4,5,7-tetranitroacridin -9(10 *H*)-one
Acri15	$C_{19}H_{12}N_{14}O_{15}$	10-(3′,5′-Diamino-picryl)-1,3,6,8-tetraamino-2,4,5,7-tetranitroacridin -9(10 *H*)-one

Appendix A

Structural formulas of designed acridone-based energetic materials, their molecular weights, and calculated elemental composition data are presented in **Table 1**:

Assign.	*Structure	Mol. formula	MW	Calculated elemental composition data				
				C, %	H, %	F or Cl, %	N, %	O, %
Acri1		$C_{13}H_5N_5O_9$	375.21	41.62	1.34	0	18.67	38.36
Acri2		$C_{13}H_5N_5O_{11}$	407.21	38.34	1.24	0	17.20	43.22
Acri3		$C_{13}H_3Cl_2N_5O_9$	444.10	35.16	0.68	15.97 (Cl)	15.77	32.42
Acri4		$C_{13}H_3F_2N_5O_9$	411.19	37.97	0.74	9.24 (F)	17.03	35.02
Acri5		$C_{13}H_7N_7O_9$	405.24	38.53	1.74	0	24.19	35.53

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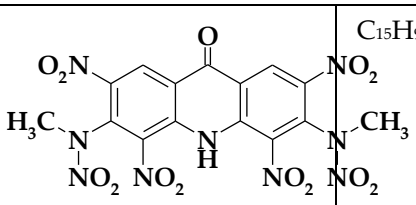
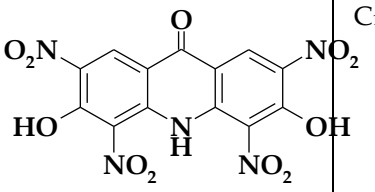
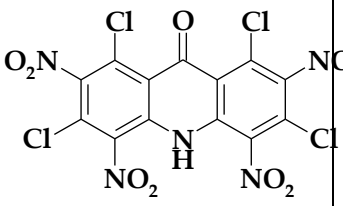
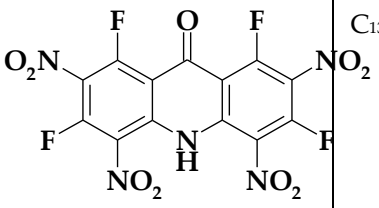
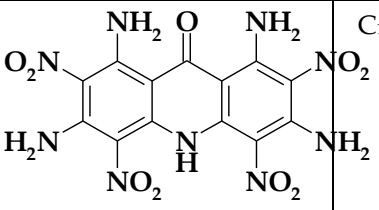
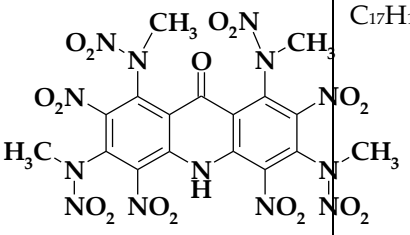
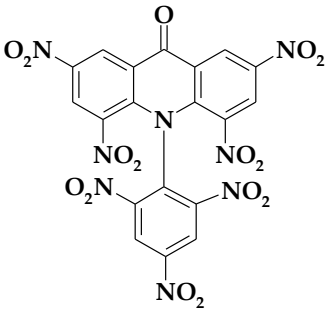
Acri6		$C_{15}H_9N_9O_{13}$	523.29	34.43	1.73	0	24.09	39.75
Acri7		$C_{13}H_5N_5O_{11}$	407.21	38.34	1.24	0	17.20	43.22
Acri8		$C_{13}HCl_4N_5O_9$	512.99	30.44	0.20	27.64 (Cl)	13.65	28.07
Acri9		$C_{13}HF_4N_5O_9$	447.17	34.92	0.23	16.99 (F)	15.66	32.20
Acri10		$C_{13}H_9N_9O_9$	435.27	35.87	2.08	0	28.96	33.08
Acri11		$C_{17}H_{13}N_{13}O_{17}$	671.37	30.41	1.95	0	27.12	40.51
Acri12		$C_{19}H_6N_8O_{15}$	586.30	38.92	1.03	0	19.11	40.93

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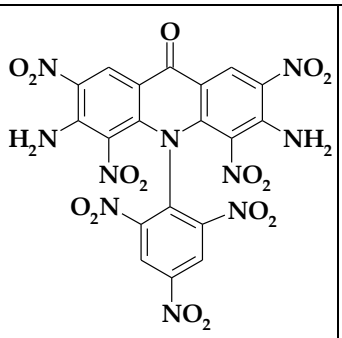
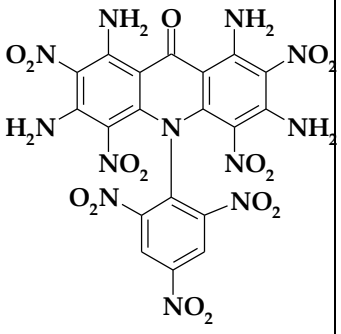
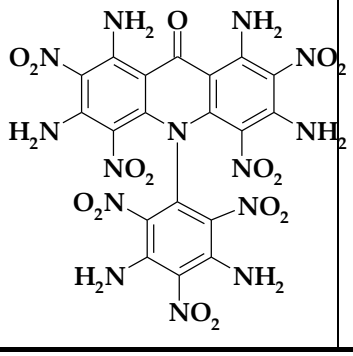
Acri13		$C_{19}H_8N_{10}O_{15}$	616.33	37.03	1.31	0	22.73	38.94
Acri14		$C_{19}H_{10}N_{12}O_{15}$	646.36	35.31	1.56	0	26.00	37.13
Acri15		$C_{19}H_{12}N_{14}O_{15}$	676.39	33.74	1.79	0	28.99	35.48

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