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Research Article

Theoretical Investigation of Compounds Based on 1, 2, 4-Triazolo [4, 3-b] [1,2,4,5] Tetrazine as High Energy and Low Sensitivity Energetic Materials

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Abstract

Designing compounds with high energetic performance and low sensitivity at the molecular level is the central challenge in molecular design for energetic materials. Molecular frameworks integrating 1,2,4-triazolo [4,3-b] [1,2,4,5] tetrazine (known as high-energy-density and low-sensitivity module) and monocyclic tetrazoles are constructed to design energetic compounds. A series of energetic compounds are constructed. Density functional theory (DFT) has been used to investigate geometries, frontier molecular orbital energy, heats of formation (HOFs), densities of the title compounds at B3PW91/6-31G (d, f) level. Heats of formation were calculated via isodesmic reactions. Crystal densities were predicted using Politzer's method. Detonation velocity (D) and detonation pressure (P) of the title compounds have been determined based on HOFs and densities through the Kamlet-Jacobs (K-J) equation. The effects of substituents on above properties are presented. Substitution with $-NO_2$, $-ONO_2$, $-NH_2$, $-NHNO_2$, and $-N(NO_2)_2$ groups can increase the heats of formation, densities, detonation velocity and detonation pressure of the compounds. Specifically, the compound substituted with the $-N(NO_2)_2$ group exhibits higher detonation performance than the high-energy explosive RDX, suggesting its potential as a promising high energy material. The results are of significant value, providing theoretical guidance for the molecular design of novel high-energy-density compounds and the optimization of established ones.

Keywords

1,2,4-triazolo [4,3-b][1,2,4,5] Tetrazine, Density Functional Theory, Heats of Formation, Detonation Velocity, Detonation Pressure

1. Introduction

The development of high-energy, insensitive and green energetic compounds has always been a frontier issue in energetic materials research. How to balance the contradiction between high energy and low sensitivity at the micro level of molecular structure remains the core challenge in energetic material molecular design. [1-4] Nitrogen-rich fused-ring energetic compounds exhibit superior structural and performance characteristics compared to monocyclic and linked-ring nitrogen-rich heterocycles [5, 6]. Structurally, fused-ring systems are characterized by more energetic bonds (e.g., N=N, N–N, C–N, and N–O) and greater ring strain, which collectively enhance their thermochemical and deto-

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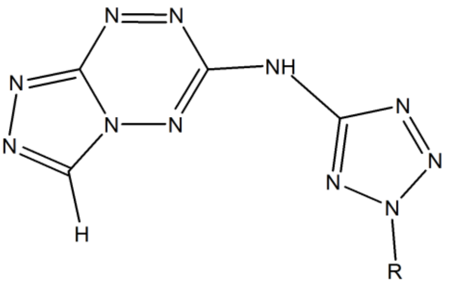
nation properties. These features result in significantly higher heats of formation (HOFs), greater crystal densities, and improved detonation velocities/pressures relative to monocyclic or linked-ring analogs. Furthermore, the coplanar structure of fused-ring systems facilitates extensive delocalized π-electron delocalization across the conjugated framework and promotes intermolecular π-π stacking interactions. These structural attributes not only reduce mechanical sensitivity (e.g., impact sensitivity, friction sensitivity) but also confer enhanced thermal stability (high decomposition temperatures). Collectively, these advantages establish nitrogen-rich fused-ring compounds as competitive candidates for next-generation insensitive high-energy materials (IHEMs).

Experimental results demonstrate that the fused 1,2,4-triazolo[4,3-b][1,2,4,5]tetrazine ring system exhibits superior insensitivity, with an impact sensitivity (*IS*) value exceeding 40 J and a friction sensitivity (*FS*) value surpassing 360 N [1]. These values indicate markedly lower sensitivity compared to conventional explosives such as 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX) (*IS* = 7.5 J, *FS* = 120 N) and 2,4,6-trinitrotoluene (TNT) (*IS* = 15 J, *FS* = 353 N). Thereby the fused 1,2,4-triazolo [4,3-b] [1,2,4,5]tetrazine ring system combines high energy with insensitivity.



Scheme 1. *N-(2H-Tetrazol-5-yl)-[1,2,4]triazolo[4,3-b][1,2,4,5] Tetrazin-6-amine and their derivatives considered in this study.*

T0: R=H T1: R=NO_2 T2: R=ONO_2 T3: R=CH_3
T4: R= OCH_3 T5: R=CN T6: R=N_3 T7: R=NH_2
T8: R= $NHNO_2$ T9: R= $N(NO_2)_2$

In this project, we employ the 1,2,4-triazolo[4,3-b][1,2,4,5] tetrazine fused ring system coupled with nitrogen-rich monocyclic tetrazole units as fundamental building blocks to design derivatives that balance high energy and insensitivity. Density functional theory (DFT) are used to investigate the energy characteristics and stability of these compounds, aiming to screen high-energy and insensitive energetic materials. This research will provide theoretical guidance for the design and performance optimization of energetic materials.

2. Theory and Computational Details

The designed 10 molecules are shown in Scheme 1. Calculations were carried out with the Gaussian 09 program package [7] at B3PW91/6-31G (d, f) level. The geometries of molecules, including the title compounds and the reference species mentioned below to calculate HOFs for the title compounds are optimized without any constraints. Vibrational analysis has been performed for each stationary point to verify a minimum energy structure and to provide zero-point energies (*ZPEs*) and thermal correction (H_T).

2.1. Heats of Formation

The standard heats of formation (HOFs) of a compound at 298.15 K is defined as the enthalpy change when one mole of the substance is formed from its constituent elements in their standard states under standard thermodynamic conditions (1 bar pressure). To compute HOFs at 298.15 K, isodesmic reaction methods have been used. Isodesmic reactions maintain the types and numbers of chemical bonds unchanged during the reaction process. Typically, they allow systematic errors arising from factors such as spin contamination and basis set superposition error (BSSE) in the system's bonding environment to cancel each other out, thus enabling the accurate determination of the standard heat of formation. [8].

2.2. Density

Politzer's crystal electron structure theory, which analyzes the molecular surface electrostatic potential distribution and van der Waals interaction parameters, enhances the accuracy of density predictions for energetic crystals (mean absolute error < 0.03 g cm^{-3}) [9]. In this study, we employ this approach shown below to predict the densities ρ (g cm^{-3}) of our study derivatives with consideration of the intermolecular interactions.

$$\rho = \alpha(M / V_m) + \beta(\nu\sigma^2_{tot}) + \gamma \qquad (1)$$

where *M* is the molecular mass (g mol^{-1}) and V_m represents the molecular volume (cm^3 mol^{-1}) of an isolated gas-phase molecule, defined as the spatial volume enclosed within the 0.001 electrons $bohr^{-3}$ electron density isosurface. ν characterizes the equilibrium ratio between positive and negative electrostatic potential surfaces, σ^2_{tot} represents the variability measure of the electrostatic potential. α, β and γ are the coefficients assigned through fitting eq (1) to the experimental densities of a range of 36 energetic compounds. They are 0.9183, 0.0028, and 0.0443, respectively [9]. The Multiwfn suite [10] was used to calculate surface electrostatic potential quantities.

2.3. Detonation Parameters

Detonation velocity (*D*) and detonation pressure (*P*) are two critical parameters for assessing the explosive performance of energetic materials. The Kamlet-Jacobs (K-J) equation is a well-established computational method originally developed by Kamlet M. J. and Jacobs S. J. to predict energetic material performance [11]. In this study, the K-J equations were employed to predict the detonation velocity and detonation pressure of the derivatives. The calculation formulas are as follows:

$$D = 1.01(NM^{1/2}Q^{1/2})^{1/2}(1+1.30\rho) \tag{2}$$

$$P = 1.558\rho^2 NM^{1/2}Q^{1/2} \tag{3}$$

where D is detonation velocity in km s^{-1}, P is detonation pressure in GPa, also known as Chapman-Jouguet (C-J) pressure, N is molar quantity of gaseous detonation products per unit mass in mol g^{-1}, M is the average molar mass of detonation gas products in g mol^{-1}, Q is chemical energy released per unit mass during detonation, ρ is the crystal density in g cm^{-3}.

2.4. Frontier Molecular Orbital Energy

According to the Frontier Molecular Orbital (FMO) theory, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) are key determinants of a system's chemical reactivity. The molecular orbital energy gap ΔE ($\Delta E = E_{LUMO} - E_{HOMO}$) between the HOMO and the LUMO represents the energy required for electron transition. The higher the energy of HOMO and the lower the energy of LUMO of a compound, the smaller the energy gap ΔE, and the higher the chemical reactivity of the compound.

3. Results and Discussion

3.1. Heats of Formation

In designing isodesmic reactions, [1,2,4] triazolo [4,3-b] [1,2,4,5] Tetrazine and 2H-tetrazole backbone were selected as the reference framework to preserve bond types and quantities, thereby reducing computational errors. The experimental and calculated gas phase HOFs of all reference compounds are listed in Table 1. The isodesmic reactions designed are displayed in Table 2.

Table 1. The gas phase heat of formation ($\Delta H^0_{f,gas}$) of the reference compounds.

Compd.	$\Delta H^0_{f,gas}$	**Compd.**	$\Delta H^0_{f,gas}$
[1,2,4] triazolo[4,3-b]-[1,2,4,5] Tetrazine	683.16 [a]	2H-tetrazole	327.35 [a]
CH_4	-74.6 ± 0.3 [b]	NH_2ONO_2	29.90 [a]
C_6H_6	82.9 ± 0.9 [b]	NH_2OCH_3	-31.33 [a]
NH_3	-45.9 [b]	NH_2CN	138.41 [a]
CH_3NHCH_3	-19.0 ± 2.0 [b]	NH_2N_3	421.12 [a]
NH_2NO_2	-2.38 [a]	NH_2NHNO_2	99.11 [a]
NH_2CH_3	-23.5 [a]	$NH_2N(NO_2)_2$	181.80 [a]
NH_2NH_2	95.35 [a]		

[a] The values are calculated at the G2 level from the atomization reaction.
[b] The experimental HOFs were taken from reference [12].
[c] $\Delta H^0_{f,gas}$ are the gas phase heat of formation in kJ mol^{-1}.

For the isodesmic reactions, the heats of reaction $\Delta H_{298.15K}$ at 298.15K can be calculated through the reaction enthalpies:

$$\Delta H_{298.15K} = \sum_{product} \Delta H^0_{f,gas} - \sum_{reactant} \Delta H^0_{f,gas} \tag{4}$$

where $\sum_{product} \Delta H^0_{f,gas}$ and $\sum_{reactant} \Delta H^0_{f,gas}$ are the sums of the heats of formation for products and reactants in gas at 298.15K, respectively. Since the HOFs of reference compounds are available as shown in Table 1, the HOFs of the title compounds can be obtained if the heats of reaction $\Delta H_{298.15K}$ are known. The $\Delta H_{298.15K}$ can be calculated from the following equations:

$$\Delta H_{298.15K} = \Delta E_{298.15K} + \Delta(PV) = \Delta E_e + \Delta ZPE + \Delta H_T + \Delta nRT \tag{5}$$

where ΔE_e and ΔZPE are the electronic energy difference and the zero-point energy difference between products and reactants at 0K, respectively; ΔH_T is the changes in thermal correction to enthalpies between products and reactants; $\Delta(PV)$ equals ΔnRT for reaction in gas phase. For isodesmic reactions, $\Delta n=0$.

Table 2. *Designed isodesmic work reactions for calculating gas heats of formation of the title compounds.*

Compd.	**Isodesmic work Reactions**
T0	T0+2CH_4→[1,2,4]triazolo[4,3-b][1,2,4,5]tetrazine+2H-tetrazole + CH_3NHCH_3
T1	T1+NH_3+2CH_4→[1,2,4]triazolo[4,3-b][1,2,4,5]tetrazine+2H-tetrazole +NH_2NO_2+CH_3NHCH_3
T2	T2+NH_3+2CH_4→[1,2,4]triazolo[4,3-b][1,2,4,5]tetrazine+2H-tetrazole +NH_2ONO_2+CH_3NHCH_3
T3	T3+NH_3+2CH_4→[1,2,4]triazolo[4,3-b][1,2,4,5]tetrazine+2H-tetrazole +NH_2CH_3+CH_3NHCH_3
T4	T4+NH_3+2CH_4→[1,2,4]triazolo[4,3-b][1,2,4,5]tetrazine+2H-tetrazole +NH_2OCH_3+CH_3NHCH_3
T5	T5+NH_3+2CH_4→[1,2,4]triazolo[4,3-b][1,2,4,5]tetrazine+2H-tetrazole +NH_2CN+CH_3NHCH_3
T6	T6+NH_3+2CH_4→[1,2,4]triazolo[4,3-b][1,2,4,5]tetrazine+2H-tetrazole +NH_2N_3+CH_3NHCH_3
T7	T7+NH_3+2CH_4→[1,2,4]triazolo[4,3-b][1,2,4,5]tetrazine+2H-tetrazole +NH_2NH_2+CH_3NHCH_3
T8	T8+NH_3+2CH_4→[1,2,4]triazolo[4,3-b][1,2,4,5]tetrazine+2H-tetrazole +NH_2NHNO_2+CH_3NHCH_3
T9	T9+NH_3+2CH_4→[1,2,4]triazolo[4,3-b][1,2,4,5]tetrazine+2H-tetrazole +$NH_2N(NO_2)_2$+CH_3NHCH_3

The solid phase heat of formation is required for determining the energetic properties of energetic materials. According to Hess's Law, the solid phase heat of formation can be predicted from the gas-phase heat of formation $\Delta H^0_{\mathrm{f,gas}}$ and the heat of sublimation enthalpy ΔH_{sub} as,

$$\Delta H^0_{\mathrm{f,solid}} = \Delta H^0_{\mathrm{f,gas}} - \Delta H_{\mathrm{sub}} \tag{6}$$

$$\Delta H_{\mathrm{sub}} = aA^2 + b(v\sigma^2_{tot})^{0.5} + c \tag{7}$$

where A is the isosurface area corresponding to an electron density of 0.001 electrons/Bohr^3, v and σ^2_{tot} are defined and provided in the density calculation methodology (Section 2.2). a, b, and c are the coefficients optimized via iterative least-squares minimization. They were determined by the Byrd and Rice method [13] and are 2.670×10^{-4} kcal mol^{-1} Å^{-4}, 1.650 kcal mol^{-1}, and 2.966 kcal mol^{-1}, respectively.

Calculated total energies (E_0), Zero point Energies (ZPE), thermal corrections (H_T), heats of sublimation (ΔH_{sub}) and gas/solid phase heats of formation ($\Delta H^0_{\mathrm{f,gas}}$ and $\Delta H^0_{\mathrm{f,solid}}$) of the title compounds are listed in Table 3.

Table 3. *Calculated total energies (E_0), zero point energies (ZPE), thermal corrections (H_T), heats of sublimation (ΔH_{sub}) and heats of formation ($\Delta H^0_{\mathrm{f,gas}}$ and $\Delta H^0_{\mathrm{f,solid}}$) of the title compounds**

Compd.	E_0	ZPE	H_T	$\Delta H^0_{\mathrm{f,gas}}$	ΔH_{sub}	$\Delta H^0_{\mathrm{f,solid}}$
T0	-756.0581	0.1151	29.31	994.45	27.22	880.55
T1	-960.4292	0.1159	36.33	1119.90	28.84	999.24
T2	-1035.5703	0.1198	39.10	1089.05	31.02	959.26
T3	-795.3635	0.1429	33.75	976.92	27.74	860.87
T4	-870.4824	0.1465	36.53	998.76	29.10	877.02
T5	-848.2194	0.1122	34.01	1249.21	28.36	1130.55

Compd.	$\boldsymbol{E_0}$	***ZPE***	$\boldsymbol{H_T}$	$\Delta H^0_{f,gas}$	ΔH_{sub}	$\Delta H^0_{f,solid}$
T6	-919.5298	0.1167	36.67	1473.05	29.52	1349.54
T7	-811.3607	0.1315	33.44	1091.91	29.00	970.57
T8	-1015.7535	0.1337	38.89	1173.36	31.52	1041.49
T9	-1220.1198	0.1339	46.50	1283.89	34.89	1137.92

* E_0 and *ZPE* are in a.u., H_T, ΔH_{sub} and HOF are in kJ mol^{-1}.

The solid phase heats of formation of different substituted compounds are shown in Figure 1. As shown in Figure 1, the solid phase HOF of compounds T1, T2, T5, T6, T7, T8, and T9 are all greater than that of T0. This indicates that substitutions with $-NO_2$, $-ONO_2$, -CN, $-N_3$, $-NH_2$, $-NHNO_2$, and $-N(NO_2)_2$ groups increase the standard heat of formation compared to the parent compound, except for CH_3 and OCH_3 groups. Notably, the $-N_3$ groups significantly enhance the HOF. Furthermore, comparing the HOF values of T0, T1, and T7–T9 reveals that the heat of formation increases with the number of nitro ($-NO_2$) groups. Furthermore, all compounds exhibit heats of formation exceeding that of HMX (105 kJ mol^{-1}), indicating that the fused-ring framework elevates the heat of formation, and consequently enhances the performance of energetic materials.

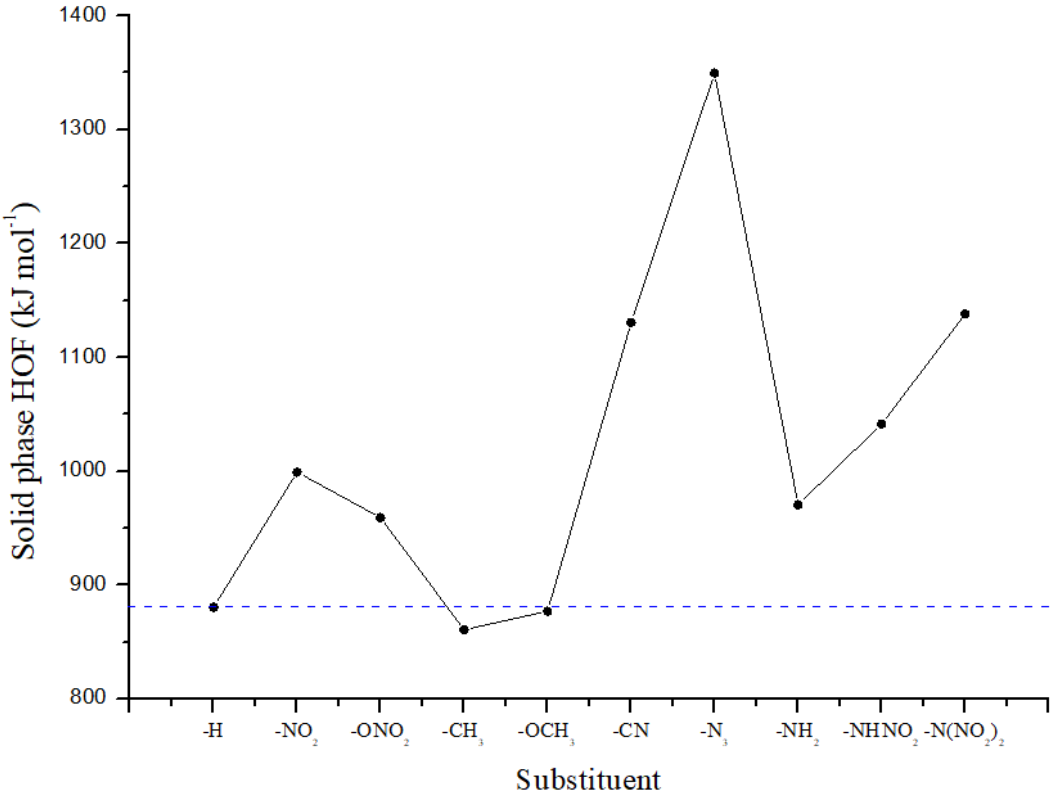


Figure 1. *Comparison of solid phase heats of formation of different substituted compounds.*

3.2. Density

The calculated crystal densities of the title compounds are listed in Table 4. To visually analyze substituent effects on density, Figure 2 was plotted.

It can be seen that substituted compounds exhibit significant density variations. Specifically, the densities of $-NO_2$, $-ONO_2$, $-NHNO_2$, and $-N(NO_2)_2$ substituted compounds are 1.840 g cm^{-3}, 1.867 g cm^{-3}, 1.838 g cm^{-3}, and 1.901 g cm^{-3}, respectively. All values exceed that of unsubstituted compound T0 (1.799 g cm^{-3}) and surpass the density of explosive

RDX (1.82 g cm^{-3}), demonstrating significant density enhancement. This phenomenon is attributed to intra- or intermolecular O ··H hydrogen bonding between hydrogen atom and nitro-group oxygen atom. Critically, the -N$(NO_2)_2$ functionalized compound achieves a density of 1.901 g cm^{-3}, surpassing HMX (1.900 g cm^{-3}). In contrast, -CH_3, -OCH_3, -CN, -N_3, and -NH_2 substituted compounds exhibit reduced densities.

3.3. Detonation Performance and HOMO-LUMO Energy Gap

Detonation velocity and pressure are critical parameters for evaluating the performance of energetic compounds. The values of the title compounds calculated via the K-J equations are tabulated in Table 4. The HOMO-LUMO energy gap is correlated with the sensitivity of energetic materials [14], and the calculated values are also listed in Table 4. Substituents differentially affect detonation performance: -CH_3, -OCH_3 and -CN groups decrease D and P values, whereas -NO_2, -ONO_2, -N_3, -NH_2, -$NHNO_2$, and -N$(NO_2)_2$ groups enhance these detonation parameters. Although the energetic properties of -NO_2、-ONO_2、-N_3、$NHNO_2$ and N$(NO_2)_2$ substituted compounds remain inferior to HMX benchmarks (ρ = 1.90 g cm^{-3}, D = 9.370 km s^{-1}; P = 40.20 GPa), they exhibit considerably higher ρ, D, and P values, which are compared to TNT (ρ = 1.65 g cm^{-3}, D = 7.129 km s^{-1}; P = 21.37 GPa), demonstrating potential as novel energetic materials. Notably, the dinitramino-substituted compound T9 exhibits higher ρ, D, and P values than high-energy explosive RDX (ρ = 1.77 g cm^{-3}, D = 8.882 km s^{-1}; P = 34.64 GPa), along with a larger HOMO-LUMO gap compared to its unsubstituted compound T0. These characteristics fulfill dual requirements for high-performance and low-sensitivity energetic materials, positioning it as a promising superior energetic material.

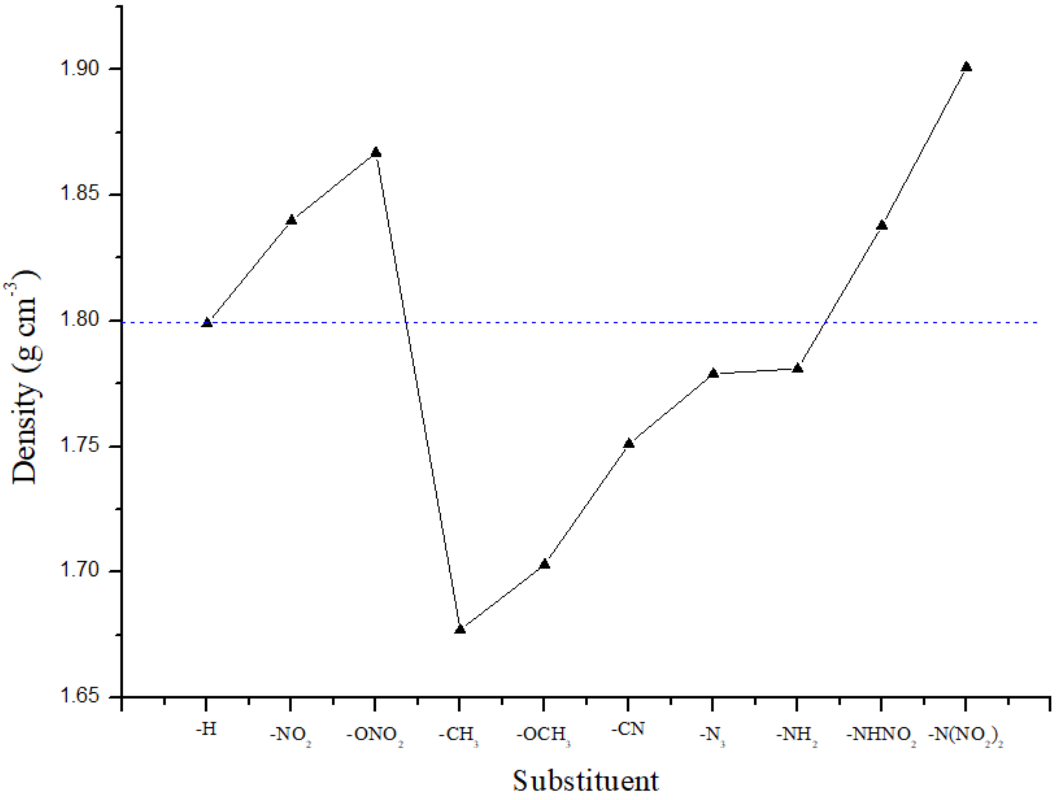


Figure 2. *Comparison of density of different substituted compounds.*

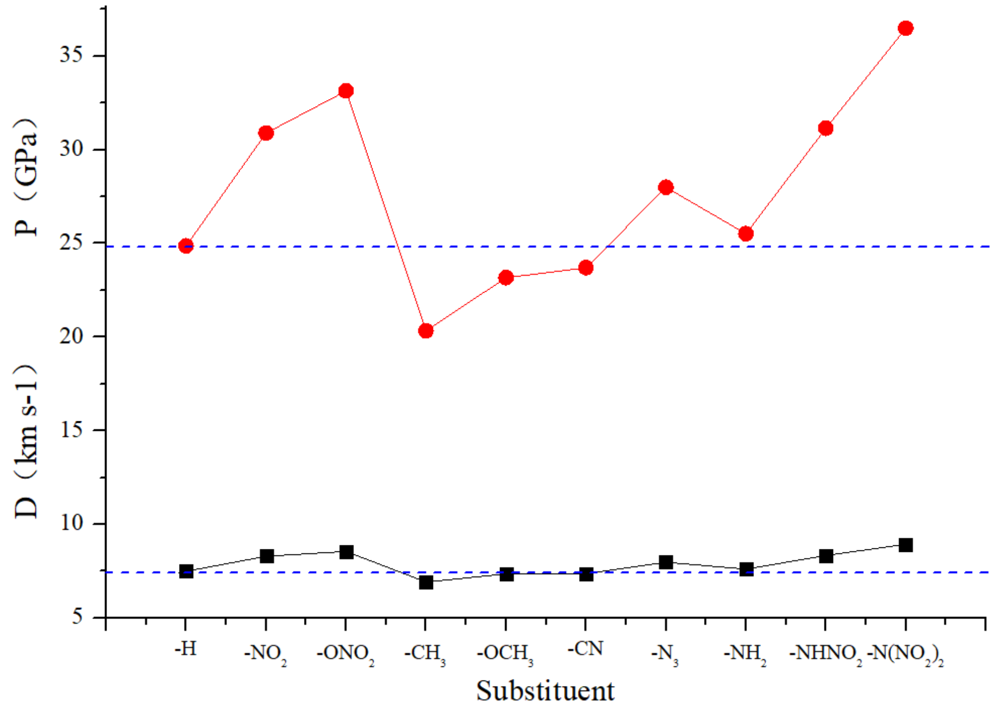


Figure 3. *Detonation velocity and detonation pressure of different substituted compounds.*

Table 4. *Calculated density, detonation performance and molecular orbital energy gap ΔE for designed title compounds*[*]

Compd.	ρ	**D**	**P**	I_s	ΔE
T0	1.799	7.490	24.875	0.868	3.82
T1	1.840	8.291	30.896	0.947	3.95
T2	1.867	8.552	33.147	0.960	3.86
T3	1.677	6.919	20.335	0.852	3.73
T4	1.703	7.351	23.173	0.897	3.76
T5	1.751	7.371	23.702	0.909	3.97
T6	1.779	7.973	27.999	0.957	3.64
T7	1.781	7.610	25.522	0.886	3.65
T8	1.838	8.328	31.149	0.943	3.92
T9	1.901	8.927	36.504	0.984	3.96

[*] ρ is crystal density in g cm^{-3}, D is detonation velocity in km s^{-1}, P is detonation pressure in GPa and ΔE is molecular orbital energy gap in eV.

4. Conclusions

Ten nitrogen-rich fused-ring energetic compounds were constructed based on N-(2H-Tetrazol-5-yl)-[1,2,4]triazolo [4,3-b] [1,2,4,5] tetrazin-6-amine. The DFT-B3PW91 method was used to study the HOMO-LUMO energy gaps, heats of formation, densities and detonation performance.

Heats of formation were calculated via isodesmic reactions, crystal densities were predicted using Politzer's method, and detonation velocities/pressures were calculated using K-J equations. Key findings are summarized as follows:

1. Except for -CH_3 and -OCH_3 groups, substitution with -NO_2, -ONO_2, -CN, -N_3, -NH_2, -$NHNO_2$, and -$N(NO_2)_2$ groups can increase the heats of formation of the compounds.
2. The densities of compounds substituted with -NO_2, -ONO_2, -$NHNO_2$, and -$N(NO_2)_2$ groups are 1.840 g cm^{-3}, 1.867 g cm^{-3}, 1.838 g cm^{-3}, and 1.901 g cm^{-3}, respec-

tively. These values are all higher than that of the unsubstituted compound T_0 (1.799 g cm^{-3}) and exceed the density of the explosive RDX (1.82 g cm^{-3}), indicating a significant improvement in compound density.

3. Detonation performance results show that substitution with $-NO_2$, $-ONO_2$, $-N_3$, $-NH_2$, $-NHNO_2$, and $-N(NO_2)_2$ groups improves the detonation performance. Specifically, the compound substituted with the $-N(NO_2)_2$ group exhibits higher values of density, detonation velocity, and detonation pressure than the high-energy explosive RDX. Additionally, its HOMO-LUMO energy gap is larger than that of the unsubstituted compound, suggesting its potential as a promising high-energy material.

Abbreviations

DFT	Density Functional Theory
HOF	Heat of Formation
D	Detonation Velocity
P	Detonation Pressure
HOMO	Highest Occupied Molecular Orbital
LUMO	Lowest Unoccupied Molecular Orbital

Author Contributions

Xinfang Su is the sole author. The author read and approved the final manuscript.

Data Availability Statement

The data supporting the outcome of this research work has been reported in this manuscript.

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Conflicts of Interest

The authors declare no conflicts of interest.

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