

Quantum chemical studies on three novel 1,2,4-triazole *N*-oxides as potential insensitive high explosives

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Abstract Three novel explosives were designed by introducing *N*-oxides into 1,2,4-triazole: 1-amino-3,5-dinitro-1,2,4-triazole-2*N*-oxide (ADT2NO), 1-amino-2,5-dinitro-1,2,4-triazole-3*N*-oxide (ADT3NO), and 1-amino-3,5-dinitro-1,2,4-triazole-4*N*-oxide (ADT4NO). Their detonation performance and sensitivity were estimated by using density functional theory and compared with some famous explosives like 1,3,5,7-tetranitro-1,3,5,7-tetrazocane (HMX) and 1-methyl-2,4,6-trinitrobenzene (TNT). All three designed molecules are more powerful than HMX and less sensitive than TNT, indicating that ADT2NO, ADT3NO, and ADT4NO have high detonation performance as HMX and low sensitivity as TNT, making them being very valuable and may be considered as the potential candidates of insensitive high explosives. Properly introducing *N*-oxides into the energetic triazole derivatives can generate some superior energetic compounds with both high explosive performance and reduced sensitivity.

Keywords Density functional theory · Detonation performance · *N*-oxides · Sensitivity · 1,2,4-triazole

Introduction

Seeking and developing novel high explosives with high detonation performance and low sensitivity always have drawn much attention [1–9]. However, most of the synthesized or designed new explosives have some obvious shortcomings like low density, low energetic properties, bad thermal stability, high sensitivity, or difficulty of synthesis.

Therefore, to meet the continuous requirements for improved energetic materials, further investigations are needed.

Energetic triazole compounds [10–14] are promising candidates of insensitive high explosives because of their positive heats of formation, good thermal stability, and low sensitivity. However, most of them have moderate explosive properties, which would limit their further applications. For instance, their densities and detonation performance are obviously lower than one famous and widely used explosive 1,3,5,7-tetranitro-1,3,5,7-tetrazocane (HMX) [15]. Thus, to improve their practical application value, there is a clear need to use some new strategies to enhance their energy level without damaging the stability and increasing the sensitivity obviously. The introduction of *N*-oxides into the energetic triazole compounds may be an alternative strategy to achieve this goal. This method has been applied to some azacyclo compounds [6, 16–19] such as pyrazine [16] and pyridine [17]. It is found that introducing the *N*-oxides can enhance their detonation velocity and pressure by increasing the density and oxygen balance and can decrease the sensitivity by generating hydrogen bonds. Therefore, properly introducing the *N*-oxides into the energetic triazole compounds may create some energetic materials with both high explosive performance and reduced sensitivity.

In the past several decades, theoretical studies based on quantum chemical treatment have gained acceptance as a useful research tool to screen the candidates of insensitive high explosives, thereby avoiding a lot of expensive and dangerous experimental tests. They can also provide the relationships between molecular structure and property, which in turn can help design better and more efficient laboratory tests. Accordingly, theoretical design of candidate compounds with high energy and insensitivity is the primary step for synthesizing new insensitive high explosives [20].

In this work, three novel explosives with a 1,2,4-triazole and substituent groups (two nitro groups and

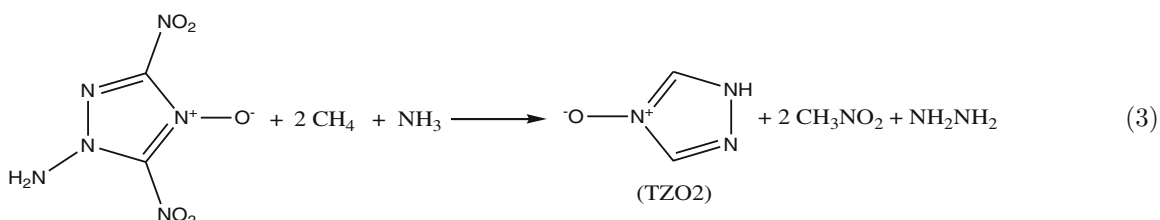
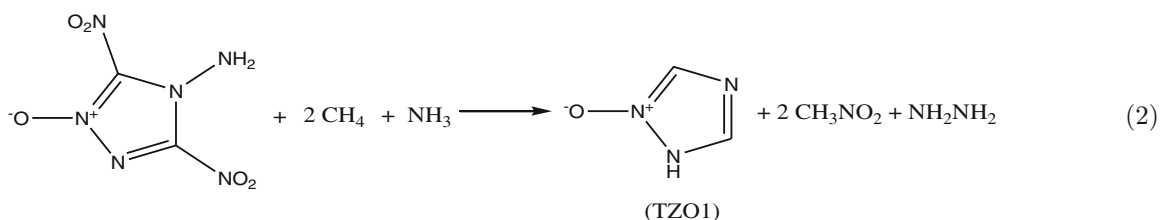
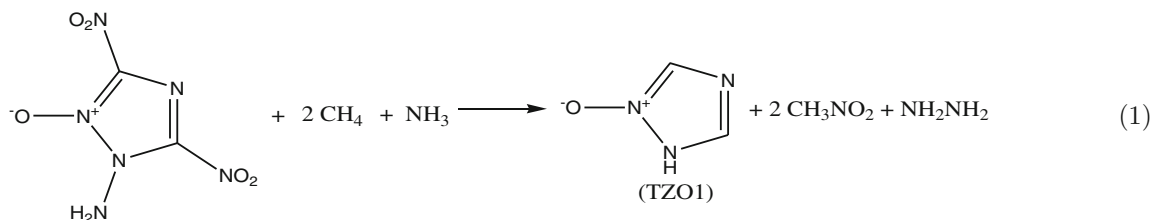
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one amino group) but different positions of *N*-oxides were designed by introducing the *N*-oxides into the 1,2,4-triazole (Fig. 1): 1-amino-3,5-dinitro-1,2,4-triazole-2*N*-oxide (ADT2NO), 1-amino-2,5-dinitro-1,2,4-triazole-3*N*-oxide (ADT3NO), and 1-amino-3,5-dinitro-1,2,4-triazole-4*N*-oxide (ADT4NO). Our purpose is to test whether introducing *N*-oxides into 1,2,4-triazole can produce new insensitive high explosives. Then, the heats of formation, spectral properties, energetic properties, pyrolysis mechanism, and sensitivity of ADT2NO,

ADT3NO, and ADT4NO were studied by using density functional theory (DFT).

Computational methods

The DFT-B3LYP method with 6-311G(d,p) basis set was successfully used to predict the HOFs of many organic systems via isodesmic reactions [6–9, 21]. The isodesmic reactions used to obtain the heats of formation of ADT2NO, ADT3NO, and ADT4NO at 298 K are as follows:



For the isodesmic reaction, heat of reaction ΔH_{298} at 298 K could be calculated from the following equation:

$$\Delta H_{298} = \Delta H_{f,P} - \Delta H_{f,R} \quad (4)$$

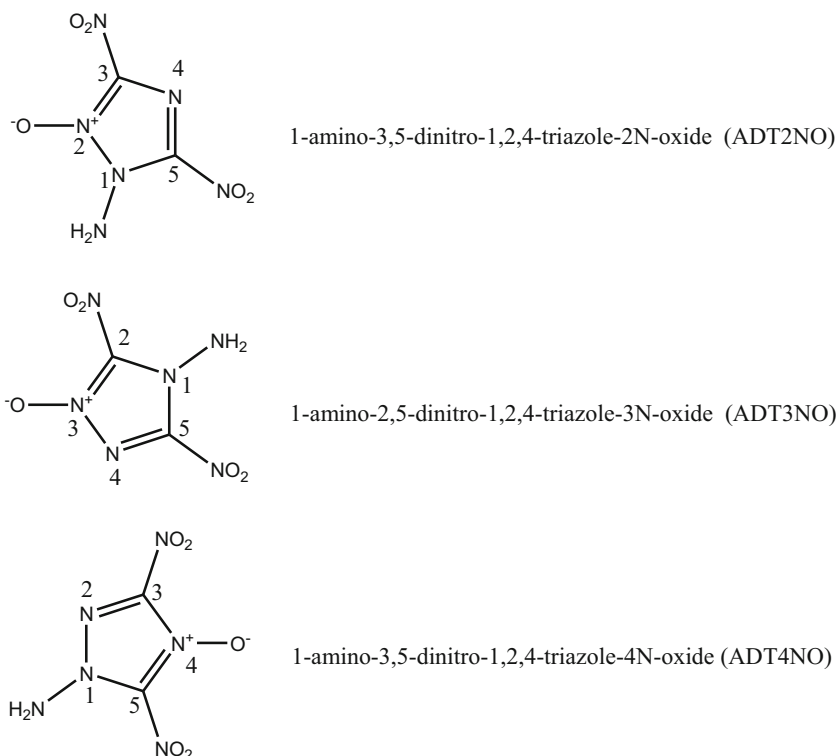
where $\Delta H_{f,R}$ and $\Delta H_{f,P}$ are the HOFs of reactants and products at 298 K, respectively. As the experimental HOFs of TZO1, TZO2, and NH_2NH_2 are unavailable, additional calculations were carried out for the atomization reaction $\text{C}_a\text{H}_b\text{O}_c\text{N}_d \rightarrow a\text{C}(\text{g}) + b\text{H}(\text{g}) + c\text{O}(\text{g}) + d\text{N}(\text{g})$ by using the G2 theory to get an accurate value of ΔH_f . The experimental

heat of formation of reference compounds CH_4 , CH_3NO_2 , and NH_3 are available. Now the most important task is to compute ΔH_{298} . The ΔH_{298} can be calculated using the following expression:

$$\Delta H_{298} = \Delta E_{298} + \Delta(PV) = \Delta E_0 + \Delta E_{\text{ZPE}} + \Delta E_{\text{T}} + \Delta nRT \quad (5)$$

where ΔE_0 is the change in total energy between the products and reactants at 0 K; ΔE_{ZPE} is the difference between the zero-point energies (ZPE) of the products and reactants at

Fig. 1 Molecular frameworks of ADT2NO, ADT3NO, and ADT4NO



0 K; ΔE_T is thermal correction from 0 to 298 K. The $\Delta(PV)$ value in Eq. (5) is PV work term and equals ΔnRT for the reactions of ideal gas. For the isodesmic reaction in this work, $\Delta n = 0$, so $\Delta(PV) = 0$.

According to Hess's law of constant heat summation [22], the solid-phase heat of formation can be obtained from the gas-phase heat of formation ($\Delta H_{f, \text{gas}}$) and heat of sublimation (ΔH_{sub}):

$$\Delta H_{f, \text{solid}} = \Delta H_{f, \text{gas}} - \Delta H_{\text{sub}} \quad (6)$$

Politzer et al. [23, 24] reported that the heat of sublimation correlates with the molecular surface area and the electrostatic interaction index for energetic compounds. The empirical expression of the approach is as follows:

$$\Delta H_{\text{sub}} = aA^2 + b(\nu\sigma_{\text{tot}}^2)^{0.5} + c \quad (7)$$

where A is the surface area of the 0.001 electrons bohr⁻³ isosurface of the electronic density of the molecule, ν describes the degree of balance between positive potential and negative potential on the isosurface, and is a measure of the variability of the electrostatic potential on the molecular surface. The coefficients a , b , and c have been determined by Rice et al.: $a = 2.670 \times 10^{-4} \text{ kcal}\cdot\text{mol}^{-1}\cdot\text{\AA}^{-4}$, $b = 1.650 \text{ kcal}\cdot\text{mol}^{-1}$, and $c = 2.966 \text{ kcal}\cdot\text{mol}^{-1}$ [25]. The

descriptors A , ν , and were calculated by using the computational procedures proposed by Bulat et al. [26]. This approach has been demonstrated to predict reliably the heats of sublimation of many energetic organic compounds [26, 27]. These calculations were carried out at the *ab initio* HF/STO-5G**/HF/STO-3G* level.

The infrared (IR), and ultraviolet-visible (UV-VIS) spectrums were calculated by the B3LYP/6-311G(d,p) method.

The detonation velocity and pressure were estimated by the Kamlet-Jacobs equations [28] as:

$$D = 1.01 \left(N\bar{M}^{1/2} Q^{1/2} \right)^{1/2} \left(1 + 1.30\rho \right) \quad (8)$$

$$P = 1.558\rho^2 N\bar{M}^{1/2} Q^{1/2} \quad (9)$$

where each term in the Eqs. (8) and (9) is defined as follows: D , the detonation velocity (kms⁻¹); P , the detonation pressure (GPa); N , the moles of detonation gases per gram explosive; \bar{M} , the average molecular weight of these gases; Q , the heat of detonation (calg⁻¹); and ρ , the loaded density of explosives (gcm⁻³). For known explosives, their Q and ρ can be measured experimentally; thus their D and P can be calculated according to eq. 8 and eq. 9. However, for some compounds, their Q and ρ cannot be evaluated from experimental measures. Therefore, to estimate their D and P , we first need to

Table 1 Calculated total energies (a. u.) and bond lengths (Å) of ADT2NO, ADT3NO, and ADT4NO

Compound	Total energy	(N-N) _{ring}	(C-N) _{ring}	N-O	N-H	N-NH ₂	C-NO ₂
ADT2NO	-781.8931	1.397	1.305–1.371	1.217–1.238	1.017, 1.024	1.380	1.452, 1.453
ADT3NO	-781.8847	1.364	1.319–1.380	1.214–1.242	1.016, 1.019	1.400	1.419, 1.452
ADT4NO	-781.8761	1.309	1.327–1.393	1.213–1.243	1.017, 1.018	1.391	1.422, 1.446

calculate their Q and ρ . The detonation products are supposed to be only CO₂, H₂O, and N₂, so released energy in the decomposition reaction reaches its maximum.

The theoretical density was obtained using an improved equation proposed by Politzer et al. [29], in which the interaction index $\nu\sigma_{tot}^2$ was introduced:

$$\rho = \alpha \left(\frac{M}{V(0.001)} \right) + \beta \nu (\sigma_{tot}^2) + \gamma \quad (10)$$

where M is the molecular mass (g mol⁻¹) and $V(0.001)$ is the volume of the 0.001 where M is the molecular mass (g mol⁻¹) and $V(0.001)$ is the volume of the 0.001 electronsbohr⁻³ contour of electronic density of the molecule (cm³ molecule⁻¹). The coefficients α , β , and γ are 0.9183, 0.0028, and 0.0443, respectively. These calculations were carried out at the density functional B3PW91/6-31G(d,p) level.

The strength of bonding, which could be evaluated by bond dissociation energy (BDE), is fundamental to understand chemical processes [30]. The energy required for bond homolysis at 298 K and 1 atm corresponds to the enthalpy of reaction A–B(g) → A·(g) + B·(g), which is the bond dissociation enthalpy of the molecule A–B by definition [31]. For many organic molecules, the terms “bond dissociation energy” and “bond dissociation enthalpy” usually appear

interchangeably in the literature [32]. Thus, at 0 K, the homolytic bond dissociation energy can be given in terms of Eq. (11):

$$BDE_0(A-B) = E_0(A\cdot) + E_0(B\cdot) - E_0(A-B) \quad (11)$$

The bond dissociation energy with zero-point energy (ZPE) correction can be calculated by Eq. (12):

$$BDE(A-B)_{ZPE} = BDE_0(A-B) + \Delta E_{ZPE} \quad (12)$$

where ΔE_{ZPE} is the difference between the ZPEs of the products and the reactants.

The free space per molecule in the unit cell, designated ΔV , can be used to estimate the impact sensitivity of an energetic compound [33]. ΔV can be represented as the difference between the effective volume per molecule that would be required to completely fill the unit cell, V_{eff} , and the intrinsic gas phase molecular volume, $V(0.003)$:

$$\Delta V = V_{eff} - V(0.003) \approx V(0.001) - V(0.003) \quad (13)$$

The free space per molecule in the unit cell can also be calculated by a more recent method [34] which was also proposed by Politzer et al.:

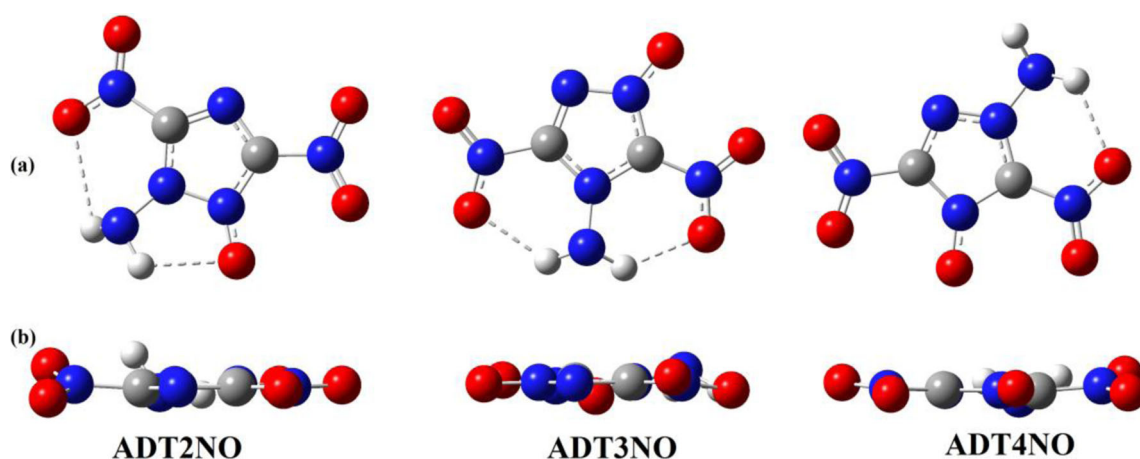
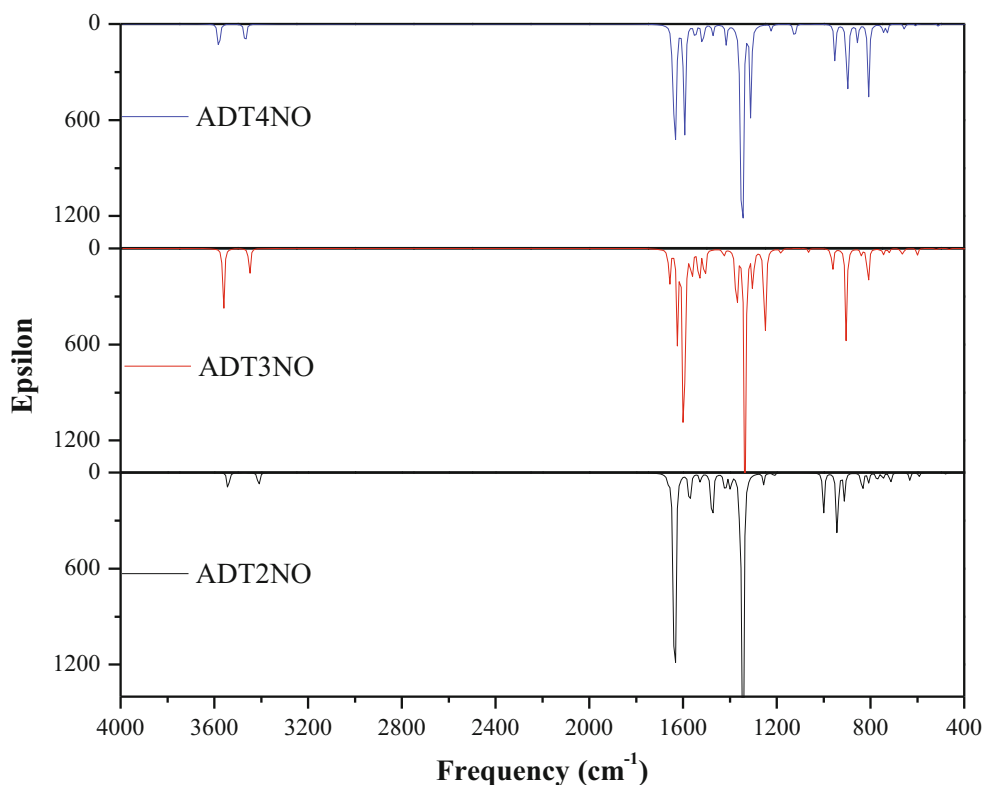


Fig. 2 (a) The optimized structures of ADT2NO, ADT3NO, and ADT4NO. (b) The perspective view of ADT2NO, ADT3NO, and ADT4NO from another viewpoint. White, red, blue, and gray spheres stand for H, O, N, and C atoms, respectively

Fig. 3 The calculated IR spectrums of ADT2NO, ADT3NO, and ADT4NO



$$\Delta V' = V_{eff} - V_{int} = M / \rho - V(0.003) \quad (14)$$

The impact sensitivity (h_{50} , cm) can be estimated by Eq. 15 [35]:

$$h_{50} = \alpha [V_{eff} - V(0.002)]^{1/3} + \beta v \sigma_{tot}^2 + \gamma \quad (15)$$

$V(0.001)$, $V(0.002)$, and $V(0.003)$ is defined as the volume enclosed by the 0.001, 0.002, and 0.003 electrons-bohr⁻³ contour of the molecule's electronic density, respectively. M is the molecular mass and ρ is the crystal density. These calculations were carried out at the density functional B3PW91/6-31G(d,p) level.

The calculations were performed at the B3LYP/6-311G(d,p) level with the Gaussian 03 package [36]. In the geometry optimization, the maximum force was converged less than 0.00045 eV Å⁻¹, the RMS force less than 0.0003 eV

Fig. 4 The calculated UV-VIS (in dimethylsulfoxide solution) spectrums of ADT2NO, ADT3NO, and ADT4NO

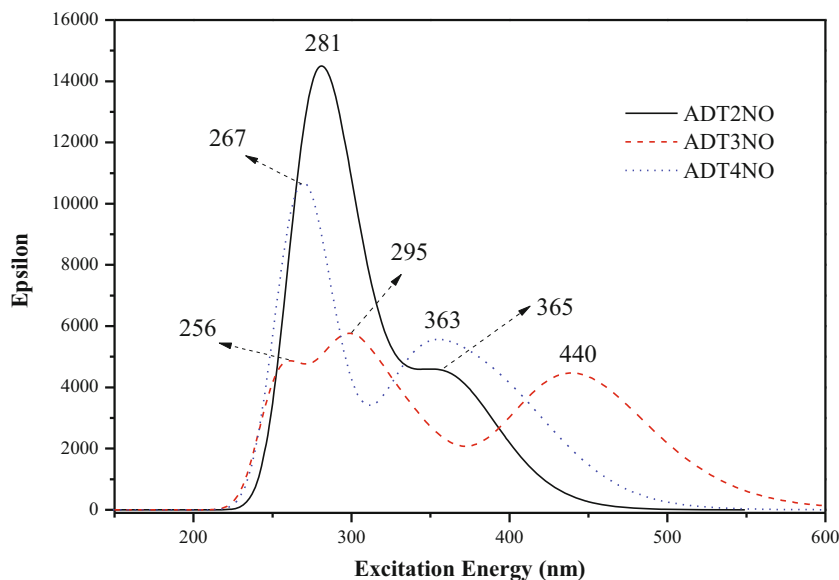


Table 2 Solid-phase HOFs ($\text{kJ}\cdot\text{mol}^{-1}$), densities (ρ , $\text{g}\cdot\text{cm}^{-3}$), Q ($\text{kJ}\cdot\text{g}^{-1}$), D ($\text{km}\cdot\text{s}^{-1}$), and P (GPa) of ADT2NO, ADT3NO, ADT4NO, RDX, and HMX

Compound	HOFs	ρ	Q	D	P
ADT2NO	278.4	1.90	6.9	9.4	40.5
ADT3NO	301.3	1.92	7.0	9.5	41.8
ADT4NO	317.6	1.93	7.1	9.6	42.6
RDX	81.0 (82.6 ^a)	1.81 (1.82 ^b)	6.2 (6.3 ^c)	8.8 (8.7 ^b)	34.6 (34.5 ^b)
HMX	118.5 (105.8 ^a)	1.90 (1.90 ^b)	6.3 (6.2 ^c)	9.2 (9.1 ^b)	39.0 (39.0 ^b)

^a, ^b, ^c Experimental values from ref. [37], [38], and [15], respectively

\AA^{-1} , the maximum displacement less than 0.0018 \AA , and the RMS displacement less than 0.0012 \AA . All of the optimized structures were characterized to be true local energy minima on the potential energy surfaces without imaginary frequencies.

Results and discussion

Molecular geometry

Table 1 lists the calculated total energies and bond lengths of ADT2NO, ADT3NO, and ADT4NO. Their total energy increases in the order of ADT2NO, ADT3NO, and ADT4NO, suggesting that ADT2NO is more stable than ADT3NO and ADT4NO in the gas phase. Among them, ADT2NO has the longest N-N bond in the ring but the shortest C-N bond in the ring, while the case for ADT4NO is just opposite. The N-O and N-H bond lengths are close to each other. ADT3NO has the longest N-NH₂ bond, while ADT2NO has the longest C-NO₂ bonds. Figure 2 displays the optimized structures of ADT2NO, ADT3NO, and ADT4NO. Their structures are

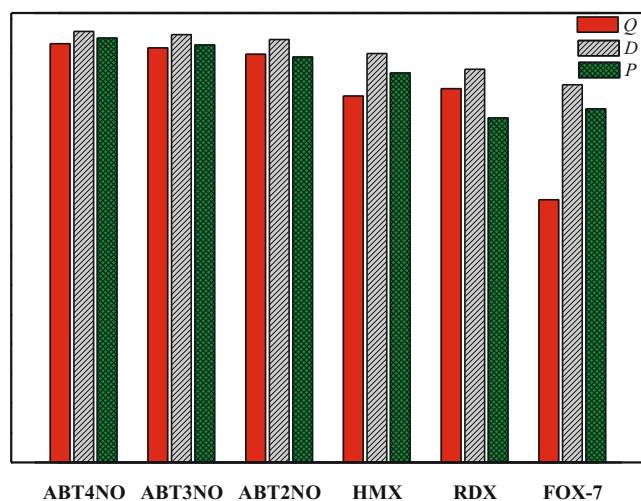


Fig. 5 A comparison of Q , D , and P of ADT2NO, ADT3NO, ADT4NO, RDX, HMX, and FOX-7

planar approximately and there are two intramolecular hydrogen bonds in ADT2NO and ADT3NO and one hydrogen bond in ADT4NO. Therefore, it may be inferred that they have good thermal stability and low sensitivity.

Spectral properties

Figure 3 displays the calculated IR spectrums of ADT2NO, ADT3NO, and ADT4NO. Obviously, the three molecules have similar IR spectra. The strongest peaks at around 1350 cm^{-1} are associated with the C-N stretch, the $N=O$ symmetric stretch motion of C-NO₂ groups, and the stretch of the $N=O$ bond linked with the ring. The strong peaks at around 1620 cm^{-1} correspond to the $N=O$ asymmetric stretch of nitro groups and the stretch of the $N=O$ bond linked with the ring. The several medium strong peaks at around 900 cm^{-1} correspond to the ring expansion and C-N stretching motion. The two weak peaks at around 3400 and 3600 cm^{-1} correspond to the N-H stretch modes.

Figure 4 depicts the calculated UV-VIS (in dimethylsulfoxide solution) spectrums of ADT2NO, ADT3NO, and ADT4NO. In the UV-light region, the wide and strong absorption regions of ADT2NO, ADT3NO, and ADT4NO at around 281 nm, 256 and 295 nm, and 267 nm correspond to the $n \rightarrow \sigma^*$ transition of the amino group, $n \rightarrow \pi^*$ transition of $N=O$ bonds linked with the ring and in the nitro groups, and $\pi \rightarrow \pi^*$ of triazole ring, respectively. In the VIS-light region, the strong peaks at around 363 nm (ADT2NO), 440 nm (ADT3NO), and 365 nm (ADT4NO) are located in the region of purple light, blue light, and purple light, respectively, indicating that ADT2NO, ADT3NO, and ADT4NO probably are yellow-green, yellow, and yellow-green compounds, respectively.

Heats of formation and energetic properties

HOF is an important parameter closely related to the detonation performance of an explosive. Therefore, it is very important to accurately predict it. Table 2 lists the calculated solid-phase HOFs of ADT2NO, ADT3NO, ADT4NO, 1,3,5-trinitro-1,3,5-triazinane (RDX), and HMX along with experimental values [37] of RDX, HMX. The calculated HOFs of

Table 3 Calculated BDE ($\text{kJ}\cdot\text{mol}^{-1}$) of the relatively weak bonds of ADT2NO, ADT3NO, ADT4NO, RDX, and HMX

Compound	N-NH ₂	(N-N) _{ring}	C2-NO ₂	C3-NO ₂	C5-NO ₂	N-NO ₂
ADT2NO	179.2	206.1		251.7	229.3	
ADT3NO	165.9	196.5	167.3		227.6	
ADT4NO	196.9	226.9		168.0	170.0	
RDX						145.5 (145.6 ^a)
HMX						160.4 (160.4 ^a)

^a Calculated values from ref. [27]

RDX and HMX are very close to their experimental values, respectively. ADT2NO, ADT3NO, and ADT4NO have much higher HOFs than RDX and HMX. ADT4NO has the highest HOF among the three designed molecules.

The density (ρ), heat of detonation (Q), and detonation velocity (D) are three important parameters reflecting the performance of the explosives. The calculated densities of ADT2NO, ADT3NO, ADT4NO, RDX, and HMX, and experimental results [38] of RDX, HMX are listed in Table 2. The calculated and experimental values of ρ , Q , D , and P of RDX and HMX are very close to each other. The densities of ADT2NO, ADT3NO, and ADT4NO are obviously higher than that of RDX and are slightly higher than that of HMX, showing that the three designed compounds have high densities. The calculated Q , D , and P of ADT2NO, ADT3NO, and ADT4NO are listed in Table 2. Figure 5 displays a comparison of calculated Q , D , and P of ADT2NO, ADT3NO, and ADT4NO and experimental results of RDX [15, 38], HMX [15, 38], and one famous new insensitive high explosive 1,1-diamino-2,2-dinitroethylene (FOX-7) [15, 39]. Because ADT4NO has higher density and HOF than ADT3NO and

ADT2NO, it possesses higher Q , D , and P than ADT3NO and ADT2NO. Furthermore, ADT2NO, ADT3NO, and ADT4NO all possess higher Q , D , and P than HMX, RDX, and FOX-7, showing that the three designed new explosives all have outstanding detonation performance. In all, the three designed *N*-oxides of 1,2,4-triazole have high HOFs, high density, and high detonation velocity and detonation pressure.

Pyrolysis mechanism, thermal stability, and sensitivity

The stability of the explosives can be evaluated by investigating their pyrolysis mechanism, thermal stability, and sensitivity. The BDE can provide useful information for understanding the stability of energetic materials. Generally, the smaller energy for breaking a bond is, the weaker the bond is, and the easier the bond becomes a trigger bond; that is to say, the corresponding compound is more unstable and its sensitivity is larger. However, it should be noted that the bond energies are not always a good measure of thermal stability since there are various possible mechanisms of decomposition while breaking a trigger linkage is only one of them.

Fig. 6 A comparison of the BDE values of the weakest bonds for ADT2NO, ADT3NO, ADT4NO, RDX, and HMX

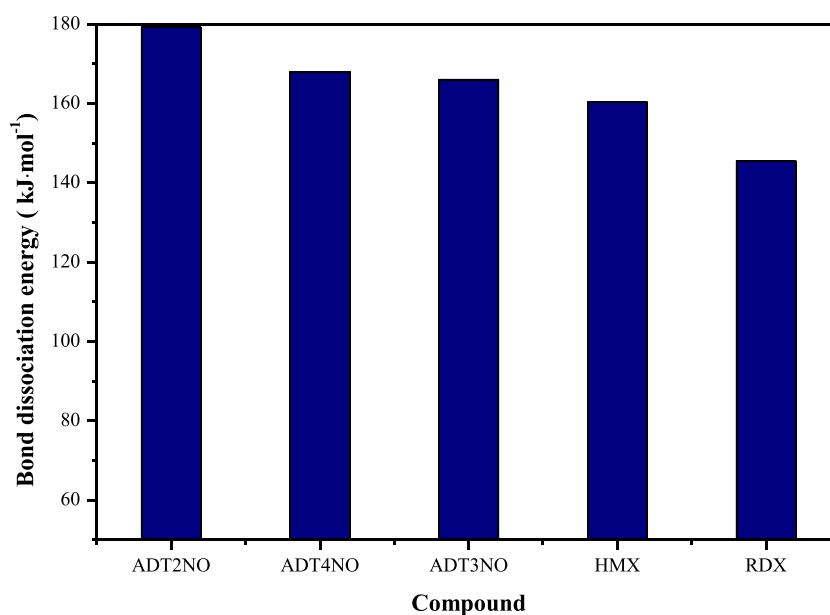


Table 4 ΔV and h_{50} values of ADT2NO, ADT3NO, ADT4NO, and TNT

Compound	ΔV (\AA^3)	$\Delta V'$ (\AA^3)	h_{50} (cm)
ADT2NO	38.4	39.0	130
ADT3NO	37.7	35.8	121
ADT4NO	38.3	36.4	108
TNT	58.1 (58.1 ^a)	58.1 (58.1 ^b)	100 (98 ^c)

^{a, b} Calculated and experimental values from ref. [33], [34], and [40], respectively

Table 3 lists the calculated BDE of several relatively weak bonds of ADT2NO, ADT3NO, ADT4NO, RDX, and HMX. For ADT2NO, the BDE value of the N-NH₂ bond is lower than those of other bonds, indicating that the N-NH₂ bond breaking is an initial decomposition step of ADT2NO. The same is true of ADT3NO. However, the case is different for ADT4NO. The C3-NO₂ bond has lower BDE value than other bonds, suggesting that the cleavage of the C3-NO₂ bond is an initial decomposition step. Figure 6 presents a comparison of the BDE values of the weakest bonds for ADT2NO, ADT3NO, ADT4NO, RDX, and HMX. ADT2NO, ADT3NO, and ADT4NO all have higher BDE values than HMX and RDX, indicating that they have better thermal stability than HMX and RDX. The BDE value of ADT2NO is higher than the other two designed compounds, suggesting that ADT2NO has the best thermal stability among the three new explosives. In all, the three designed molecules have better thermal stability.

The free space per molecule in the unit cell, designated ΔV ($\Delta V'$), can be used to estimate the impact sensitivity of an energetic compound [33, 34]. Generally, the higher the ΔV ($\Delta V'$) value, the more sensitive the compound. Table 4 lists the calculated ΔV ($\Delta V'$) and h_{50} values of ADT2NO, ADT3NO, ADT4NO, and 1-methyl-2,4,6-trinitrobenzene (TNT) [38]. The ΔV and $\Delta V'$ values of ADT2NO, ADT3NO, and ADT4NO are obviously lower than that of TNT. As advised by ref. [34], since the $\Delta V'$ values of ADT2NO, ADT3NO, and ADT4NO are between 30 and

40 \AA^3 , their h_{50} values are between 100 and 150 cm. By using Eq. 15 [35], the estimated h_{50} values of ADT2NO, ADT3NO and ADT4NO are 130, 121, and 108 cm, respectively, which are all higher than that of TNT. This indicates that ADT2NO, ADT3NO, and ADT4NO are more insensitive than TNT. Such low sensitivity is derived from the approximately planar structure and hydrogen bonds. Previous investigations reported [40, 41] that the electrostatic potential (ESP) is related to the impact sensitivity of the explosives and the stability can be expressed as a function of the imbalance between positive and negative regions [42]. In the N-O systems such as the nitro group, the regions of stronger positive potential are concentrated on the nitrogen atom and lead to the atypical imbalance which will lead to high impact sensitivity. However, it is seen from Fig. 7 that the positive potential is dispersed around the amino group, the area between nitro group and amino group and in the triazole ring, which may decrease the impact sensitivity of ADT2NO, ADT3NO, and ADT4NO obviously. In a word, ADT2NO, ADT3NO, and ADT4NO have higher detonation performance than HMX and lower sensitivity than TNT, indicating that their overall performance are outstanding and they may be three very attractive candidates for experiments. Considering the detonation performance and sensitivity, ADT2NO, ADT3NO, and ADT4NO may be considered as the potential candidates of insensitive high explosives. In addition, because their oxygen balance values are equal to zero, they may be used as high energy oxidizers.

Conclusions

In this work, three novel explosives 1-amino-3,5-dinitro-1,2,4-triazole-2*N*-oxide (ADT2NO), 1-amino-2,5-dinitro-1,2,4-triazole-3*N*-oxide (ADT3NO), and 1-amino-3,5-dinitro-1,2,4-triazole-4*N*-oxide (ADT4NO) were designed by

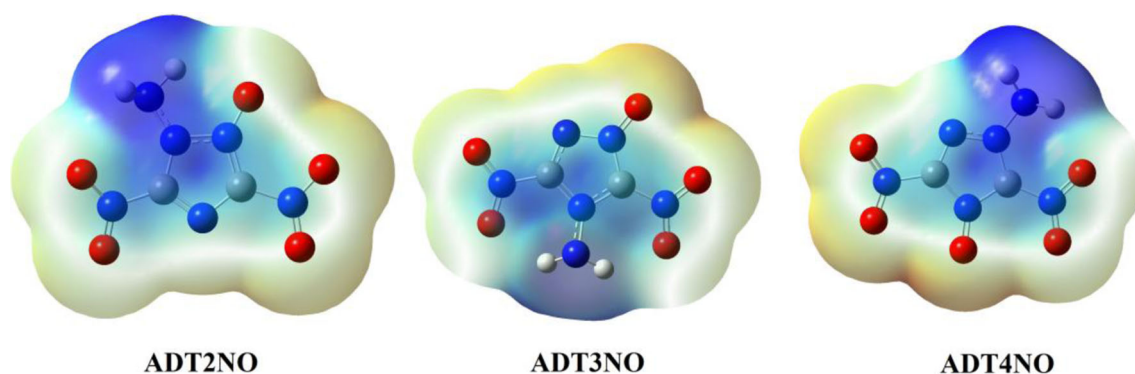


Fig. 7 The electrostatic potential [0.001 electron·bohr⁻³ isosurface, color coding: from yellow (negative) to blue (positive)] of ADT2NO, ADT3NO, and ADT4NO

introducing *N*-oxides into the 1,2,4-triazole. Then, their HOFs, spectral properties, energetic properties, pyrolysis mechanism, and sensitivity were investigated by using DFT. The results indicate that each of them has an approximately planar structure. The N-NH₂ bond breaking is an initial decomposition step of ADT2NO and ADT3NO, while for ADT4NO the C3-NO₂ cleavage is a trigger step. Their HOFs, ρ , Q , D , and P are higher than those of HMX, while their h_{50} values are higher than that of TNT, showing that they are more powerful than HMX and less sensitive than TNT. This makes them very valuable and attractive to experiments and may be considered as the potential candidates of insensitive high explosives. Overall, properly introducing *N*-oxides into the energetic triazole compounds can generate some superior energetic materials with both high explosive performance and reduced sensitivity.

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