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N-Trinitroethyl-substituted azoxyfurazan: high detonation performance energetic materials†

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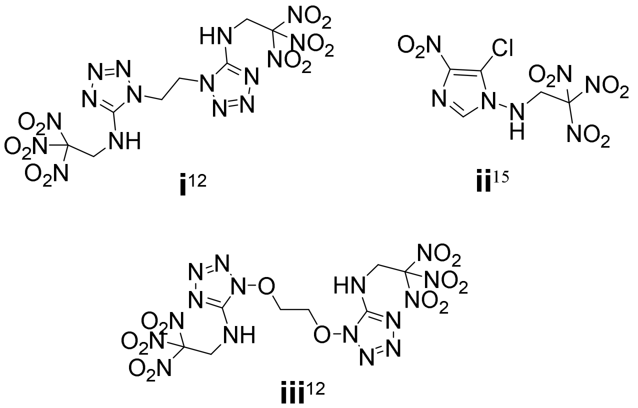
The azoxyfurazan derivatives based on the trinitroethyl functionality were synthesized. These energetic *N*-trinitroethyl-substituted azoxyfurazan were fully characterized by using ^{1}H and ^{13}C NMR spectroscopy, IR, elemental analysis, differential scanning calorimetry (DSC), thermogravimetric analysis (TG) as well as single crystal X-ray diffraction, and, in case with *N*-trinitroethylamino azoxyfurazan **4**, with ^{15}N NMR spectroscopy. Furthermore, compound **4** and nitramine **5** have been tested with their responses to impact, friction, and electrostatic discharge. The donation pressures and velocities of the azoxyfurazan derivatives were calculated, ranging from 35.8 GPa to 41.2 GPa and 8861 m s^{-1} to 9458 m s^{-1}, respectively. Additionally, compound **5** having an oxygen balance of near zero (+2.5%), exhibits favorable measured density (1.92 g cm^{-3}) and excellent detonation property ($\Delta_f H_m$, 962.1 kJ mol^{-1}; *P*, 41.2 GPa; *D*, 9458 m s^{-1}). Thus, these compounds could be potential high detonation performance of energetic materials.

Introduction

High-energy density materials (HEDMs) are the focus of advanced energetic materials research aimed at future needs in the defense and space sectors.[1] Fundamental properties such as high nitrogen content, high density, high heat of formation, high detonation velocity and pressure, good oxygen balance, high thermal stability and low sensitivity, must be considered during the development of these energetic ingredients.[2] However, the development of such materials is complex, owing to the fact that the contradictory nature of high detonation performance and low sensitivity usually poses interesting but challenging problems for the synthesis of new HEDMs.[3] Therefore, it is necessary to find suitable strategies to guide the synthesis of energetic materials.

Polynitrofunctionalized compounds are one of the most significant structural motifs in HEDMs.[4-10] Owing to the presence of polynitro fragments in the molecules, most of them have positive oxygen balance values and high densities.[11] Energetic materials containing trinitroethyl moieties have high density and good detonation performance.[12-20] Moreover, they can be readily synthesized by the addition of trinitroethanol[21] (or trinitromethane and formaldehyde[22,23]) to an amine. Recently, some tetrazole and imidazole derivatives containing trinitroethyl fragments have been reported. However, further nitration of these compounds is difficult to be achieved because the effect of the electron-withdrawing of tetrazole and imidazole rings (Fig.1).[12,15]

The furazan ring is an effective fragment for improving the performance of explosives, a fact that is probably attributable to its high density, high positive heat of formation, and good oxygen balance.[24] The design of new energetic compounds based on a combination of amino furazan with an explosophore group of trinitroethyl has attracted considerable interest.[16-20] Recently, two *N*-nitration product of furazan-derived compounds (Fig. 2, **iv** and **v**) with the trinitroethyl functionality have been reported, which were obtained by the one-pot reaction using ionic liquids as solvents.[18] Actually, nitrating trinitroethyl amine compounds to obtain nitroamine compounds has not been widely concerned.[19] In addition, the additional oxygen atom coordinated to the azo group was considered which not only enhances density and performance, but also tends to stabilize the entire molecule.[25,26] As shown in figure 2(**vi**, **vii**), two examples of azoxyfurazan derivatives bearing the trinitroethyl group were reported recently, but their detonation properties are not quite satisfying.[16,17]



i[12] ii[15] iii[12]

Fig. 1 Tetrazole derivatives containing a trinitroethyl group.

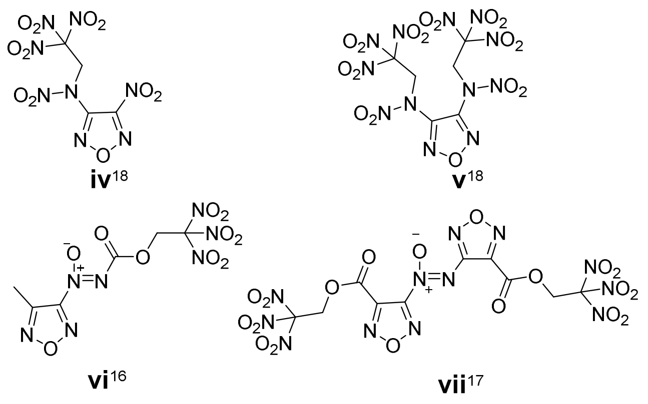


Fig. 2 Furazan-derivatives containing one or two trinitroethyl groups.

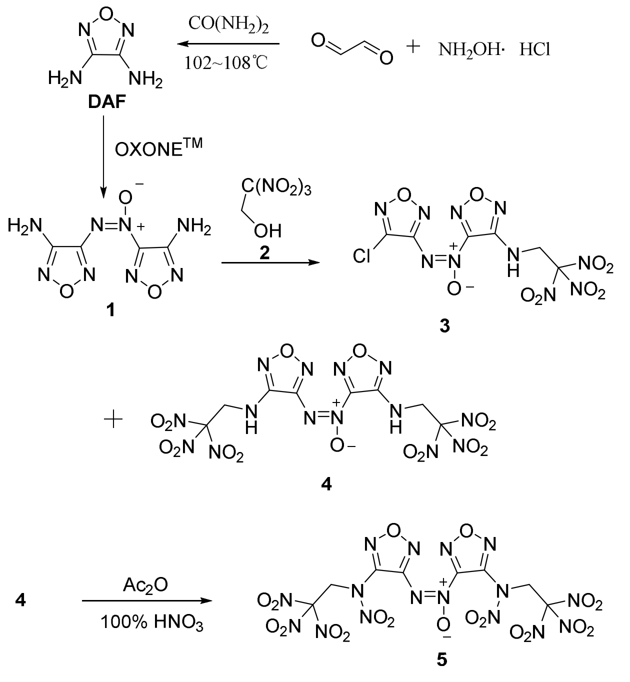
In a continuing effort to search for more powerful, better thermal stability, eco-friendly energetic materials, we are interested in designing and synthesizing some trinitroethyl derived compounds based on azoxyfurazan containing a high percentage of both oxygen and nitrogen content and owning good oxygen balance. Herein we describe the synthesis of two trinitroethyl derivatives of azoxyfurazan and one *N*-nitration product which contain one or two trinitroethyl fragments and display potentially significant physical and energetic properties. These compounds exhibit high densities, high heats of formation, and thereby excellent detonation properties.

Results and Discussion

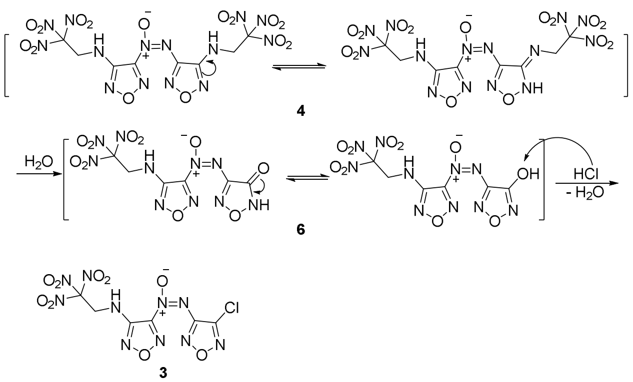
Synthesis

The raw material 3,3’-diamino-4,4’-azoxyfurazan **1** was readily synthesized according to the literature, which can be obtained by treatment of OXONE^{TM} (a strong oxidant) with 3,4-diamino furazan (DAF).[27,28] To afford trinitroethyl derivatives of azoxyfurazan, we opted to use the Mannich reaction of electron deficient trinitroethanol which was synthesized according to the method reported previously[29] and the weak base **1** under acidic condition (Scheme 1). When reaction temperature is below 70 °C, the reaction of trinitroethanol with 3,3’-diamino-4,4’-azoxyfurazan **1** affords a low yield of *N*,*N*’-bis(2,2,2-trinitroethyl)-3,3’-diamino-4,4’-azoxyfurazan **4** (≤30%) in 1M hydrochloric acid. Enhancing of temperature from 70 °C to 100 °C is favorable to improve yield of **4** to 89.55 % with the reaction time of 5 days. Interestingly, further extension of reaction time resulted in yield decline of **4** accompanied by the generation of byproduct **3.** The identification of byproduct **3** is proved be monochloro-adduct of trinitroethyl derivatives of azoxyfurazan **4** by X-ray diffraction analysis. The plausible mechanism for the formation of **3** from product **4** could be involved two elementary steps (Scheme 2). The first step involves the formation of ketone intermediates **6** by hydrolyzation of imine **4,** which was formed by the proton transformation from secondary amine of compound **4**. At the second step, the hydroxyl group of intermediates **6** was attacked by hydrochloric acid to form byproduct **3**.

After condensation on the azoxyfurazan **1** with trinitroethanol **2**, the resulting secondary amine **4** was subjected to nitration to give *N*,*N*'-bis(2,2,2-trinitroethyl)-3,3'-dinitramino-4,4'-azoxyfurazan **5** by 100% nitric acid and acetic anhydride. When the acetic anhydride was dropped into the 100 % nitric acid solution, the reaction temperature should be strictly controlled at 0~5 °C avoiding the nitrification progress reaction growing extremely violent.



Scheme 1 Synthesis of trinitroethyl substituted amino azofurazan (**3**-**4**) and nitroamino furazan (**5**).



Scheme 2 A plausible mechanism for synthesis of **3**.

NMR spectoroscopy

The structures of the three new compounds (**3-5**) were supported by ^{1}H, and ^{13}C NMR spectroscopic data. In the ^{1}H NMR spectra of compounds **3** and **4**, the proton signals of -NH- groups attached to the furazan ring appeared at 5.63 and 5.41 ppm, respectively. These proton signals of -NH- groups and -CH$_2$- groups show as triplets and doublets, respectively, owing to the coupling of -NH- group and -CH$_2$- group. Furthermore, in the ^{1}H NMR spectra of compound **5**, the proton signals were easily assigned because only two singlets occurred at δ= 6.16 ppm and δ= 6.23 ppm; they were shifted downfield compared to the parent molecule **4** (δ≈ 5.41 ppm). In the ^{13}C NMR spectra of the three new compounds, the signals of carbon atoms bonded to three nitro groups were found at 124-127 ppm, while

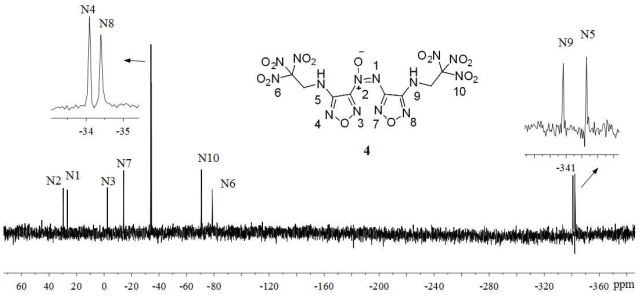


Fig. 3 ^{15}N NMR spectra of compound **4**.

those in the furazan ring appeared between 146 and 162 ppm. The carbon atoms in the furazan rings are influenced by the conjugated system so that their electron cloud density decreases a lot, which result in the signals of them shifted downfield more than 20 ppm compared to those of quaternary carbon atoms(-C(NO_2)$_3$).

The ^{15}N NMR spectra of compound **4** was measured in $(CD_3)_2CO$ solution and chemical shifts are given with respect to CH_3NO_2 as an external standard. As shown in fig. 3, the spectra of compound **4** displays ten signals. The assignments in the ^{15}N NMR spectrum are based on the signals of the other nitrogen atoms in the furazan ring and trinitroethyl group in the literature.[16-20] The asymmetric bridging azoxy moiety causes different ^{15}N signals between two furazan rings and two kinds of nitro groups attached to trinitromethyl as well as the two amino groups. The nitrogen signals (N5 and N9) of the -NH- group appears at the highest field (δ= -342.3 ppm, -340.9 ppm). The signals for N2, which has oxygen as a neighbor in the azoxy linkage, appear as expected at lower field compared to N1.

X-ray crystallography

Single crystals of the compounds **3**-**5** suitable for single-crystal X-ray diffraction, were obtained by slow evaporation of CH_2Cl_2 solutions. Their crystallographic data are summarized in Table 1, and structures are displayed in Fig. 4, 5 and 6, respectively. Further information about crystal-structure determinations is given in the supporting information†. As expected and found in the three structures discussed in this work, the furazan ring is nearly planar, building an aromatic system, which can be seen since the mean deviation of them are in the range of 0.0004 Å-0.0098 Å.

As can be seen in Table 1, **3** crystallizes in the orthorhombic *Pbca* space group with a calculated density of 1.887 g cm^{-3}. The crystal cell of **3** contains separate molecules of **3** without water or solvent molecule (Fig. 4 a). The distance between N1 and N2 (1.283 Å) falls in the range between N=N double bonds (1.290 Å) and N≡N triple bonds (1.095 Å), which is the result of the decrease electron cloud density on N=N1A bond owing to a π-π conjugation system between N1=N2 bond and furazan ring. The lengths of the C-N bonds in the trinitromethyl (1.510-1.526 Å) are longer than the other C-N bond distances in the furazan ring and the substituted amino (1.293-1.437 Å). The length of C(5)-Cl(1) bond is 1.687(2) Å and is shorter than a normal C-Cl bond (1.77 Å), which is arising from the conjugation system between a lone electron pair of the chlorine atoms Cl(1) and furazan ring. And, the dihedral angle between the two furazan rings is 4.32^{o}, which indicate that they are planar (Fig. 4 a). The packing structure of **3** is influenced by strong hydrogen bonds. These extensive hydrogen bonds (N5-H5…O3 2.875(3) Å, N5-H5…N2 2.858(3), C(3)-H(3A)…N(4) 2.835(3), C(3)-H(3A)…O(1) 3.431(3)) are presented in Figure 4(b) along the c axis (Fig. 4 b), which extend the structure into a 3D supramolecular structure, and make an important contribution to enhance the thermal stability of the complex.

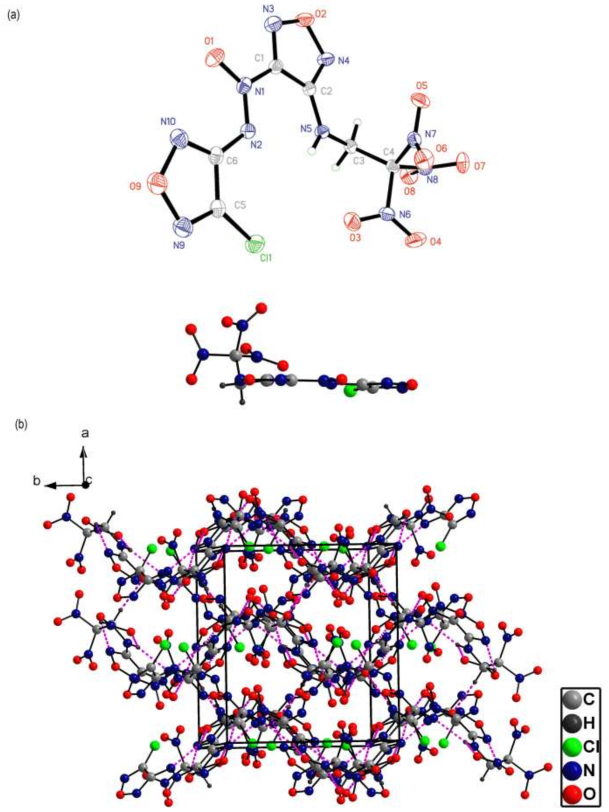


Fig. 4 (a) Molecular structure of **3**. Hydrogen atoms are shown, but are unlabeled for clarity. (b) Ball and stick packing diagram of **3** viewed down the *c* axis. Dashed lines indicate strong hydrogen bonding.

Compound **4** crystallizes in the monoclinic space group *C2/c* with one molecule in the unit cell, and has a calculated density of 1.855 g cm^{-3} (173(2) K). In the unit cell, there are two oxygen atoms bearing the azo group. The length of -N=N(O)- bond is 1.277(3) Å which is slightly shorter than that of **3**. The lengths of the C-N bonds in the trinitromethyl are in the range of 1.517 Å -1.527 Å and are significantly elongated relative to a normal C-N single bond (1.47 Å).[30] With a lone electron pair of the nitrogen atoms (N4) attached to the furazan ring, they can form a p-π conjugation between the nitrogen atoms and the aromatic ring, so that the lengths of C2-N4 (1.360 Å) bonds are approaching the length of C=N (1.350 Å) double bond. The bi(1,2,5-oxadiazole) ring system shows a planar arrangement, which is reflected in the dihedral angles of almost 0^{o} and ±180^{o} (C1-N2-O2-N3 0.1(2)^{o}, O2-N3-C2-N4 -176.69(19)^{o}, O2-N2-C1-N1 177.70(19)^{o}). However, the trinitro group is twisted out of the furazan ring plane with torsion angles of N5-C4-C3-N4, -49.06^{o}; N6-C4-C3-N4, 71.98^{o}; N7-C4-C3-N4, 168.35^{o}. Interestingly, the amino connected to the furazan ring are lie in the furazan planner (Fig. 5a). As shown in fig. 5(b), crystal packing of **4** shows that the 3D network is *S*-shaped. It can be

Table 1. Crystallographic data for the compounds **3-5**.

	3	**4**	**5**
CCDC number	994773	994770	994775
Empirical formula	$C_6H_3ClN_{10}O_9$	$C_8H_7N_{14}O_{15}$	$C_8H_4N_{16}O_{19}$
Formula weight	394.63	539.28	628.27
T[K]	170(2)	173(2)	173(2)
Crystal size [mm^3]	0.34 × 0.32 × 0.13	0.20 × 0.18 × 0.12	0.38 × 0.21 × 0.16
Crystal system	Orthorhombic	Monoclinic	Monoclinic
Space group	Pbca	C2/c	$P2_1/n$
a [Å]	11.3577(6)	21.343(4)	7.6635(6)
b [Å]	9.9015(6)	7.8125(16)	9.5134(7)
c [Å]	24.7060(14)	11.766(2)	15.1332(12)
α [°]	90	90	90
β [°]	90	100.11(3)	99.571(3)
γ [°]	90	90	90
V [Å^3]	2778.4(3)	1931.4(7)	1087.94(15)
Z	8	4	2
λ(Å)	0.71073	0.71073	0.71073
ρ_{calcd} [mg m^{-3}]	1.887	1.855	1.918
μ [mm^{-1}]	0.356	0.178	0.189
F (000)	1584	1092	632
θ range [°]	3.19 - 26.38	1.94 - 27.87	3.22 - 25.90
Index ranges	$-12 \le h \le 14$	$-28 \le h \le 28$	$-9 \le h \le 8$
	$-12 \le k \le 12$	$-10 \le k \le 10$	$-11 \le k \le 11$
	$-29 \le l \le 30$	$-14 \le l \le 15$	$-18 \le l \le 18$
Reflections collected	15508	11713	6057
Independent reflections/R_{int}	2806 / 0.0556	2303 / 0.0447	2074 / 0.0412
Completeness to θ [%]	98.5	99.9	98.0
Goodness-of-fit on F^2	1.037	1.142	1.019
R_1(F) ($I > 2\sigma(I)$) [a]	0.0439	0.0505	0.0350
wR_2 [all date] [b]	0.1120	0.1076	0.0727
Largest diff. peak / hole [e Å^3]	0.370 / -0.343	0.205 / -0.256	0.162 / -0.236

[a] $R_1=\Sigma|F_o| - |Fc|/\Sigma|F_o|$. [b] $wR_2=\{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$

clearly seen that intramolecular hydrogen bonds between the -NH- group (N4) and the oxygen atoms (O1) of azoxy group combined with intramolecular hydrogen (N4-H4…O1 2.784(4), N4-H4…O5 2.795(2), C3-H3A…N3 2.867(3)) form a complex three-dimensional network.

Compound **5** crystallizes in the monoclinic crystal system in the space group $P2_1/n$. The calculated density is 1.918 g cm^{-3} (173 K) which shows higher than that of **4** owing to the addition of two nitro groups. The crystal structure of **5** is similar to that of **3** and **4** in which the length of the C-N bonds joining the trinitroethyl groups are also longer than that of furazan ring and the substituted amino (such as C4-N7 1.530 Å, C4-N8 1.529 Å, and C4-N9 1.526 Å). However, the distances (1.452 Å) between N5 (N6) and C2 (C6) are longer than the similar bond length in compound **4** (C2-N4 1.360 Å), which is because the p-π conjugation between the nitrogen atoms and the aromatic ring is destroyed resulting from strong electron-withdrawing effect on the nitrogen atoms (N5, N12) by the nitro group in the nitroamino moiety. Besides, the two furazan rings are parallel rather than planar owing to the twist of N1 atom (Fig. 6a). The -N-NO_2 group is out of the furazan ring plane with dihedral angles of 65.175° and 41.764°. The presence of weak attractive electrostatic interactions (short contacts) between the nitro groups within the trinitromethyl moieties (such as N15…O15= 2.47 Å, N14…O19= 2.53 Å, N12…O1= 2.81 Å, N9…O8= 2.55 Å, N8…O6= 2.66 Å, N7…O10= 2.65 Å, N7…O7= 2.87 Å) are shorter than the sum of van der Waals radii (N, O= 3.07 Å),[31] which make an important contribution to improve the crystal density. The packing of the atoms of compound **5** is dominated by a three-dimensional network, which are connected by strong intermolecular hydrogen bonds (C3-H3B…N4 2.800(16) Å, C3-H3A…O3 2.71(2) Å) and intramolecular hydrogen bonds (C3-H3B…O15 2.56(15) Å, C3-H3A…N3 2.705(17) Å). A view of the hydrogen bonds along the a axis is shown in Fig. 6(b).

Physical and energetic properties

To assess the thermal stability of the new materials, thermogravimetric analysis (TG) and differential scanning calorimetry (DSC) measurements were carried out for these new compounds at a heating rate of 5 °C min^{-1} using dry nitrogen as an atmosphere in ranging from 30 °C to 400 °C (Fig. S1-S3†). Compound **3** melted at 185.5 °C, the endothermic stage occurs at a temperature range of 180.2-188.7 °C and decomposed at 209.2 °C, which shows that the compound melts without decomposition. Compounds **4** and **5** decomposed without melting at 190.2 °C and 144.6 °C,

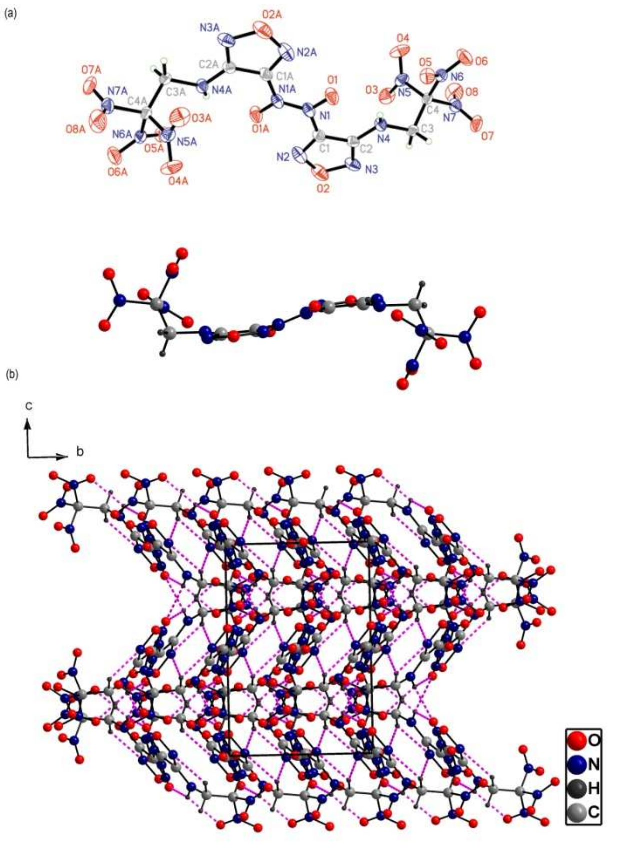


Fig. 5 (a) Molecular structure of **4**. Hydrogen atoms are shown, but are unlabeled for clarity. (b) Ball and stick packing diagram of **4** viewed down the *a* axis. Dashed lines indicate strong hydrogen bonding.

respectively. Compound **3** is slightly more thermally stable than that of **4** due to one side trinitroethyl group attached to compound **3** was substituted by a chlorine atom in which the lone electron pair on the chlorine atom could conjugate with the furazan. There are two steps in the decomposition of compound **5**. One decomposition progress occurs at 144.6 ^{o}C and the other appeared at 193.1 ^{o}C. Therefore, these studies show that **3** and **4** presented here have higher thermal stabilities than that of **5**, which is attributed to the "explosophore" of nitramino groups in compound **5**. The weight losses of compound **3** and **4** are 73.9 % and 99.8 %, respectively, which both correspond to the thermal decompositions of the molecules. Compound **5** has two steps of weight loss which has a total weight loss of 99.9%.

Oxygen balance (OB) is used to indicate how clean a compound combust completely to N_2, H_2O and CO_2 etc. Compound **3** possesses a negative OB value of -18.2%, which is less negative than that of RDX (-21.6%) (Table 2). With the increase in the number of nitro group, it is found that compound **4** (-11.9 %) has a less negative OB than **3**. Moreover, after nitration of **4**, compound **5** has an oxygen balance of near zero (+2.5 %), which can almost make full use of chemical energy. Both nitrogen and oxygen content is another very important property of energetic materials. All the three compounds in this study have a relatively high both nitrogen and oxygen content which range from 71.99% to 84.06%.

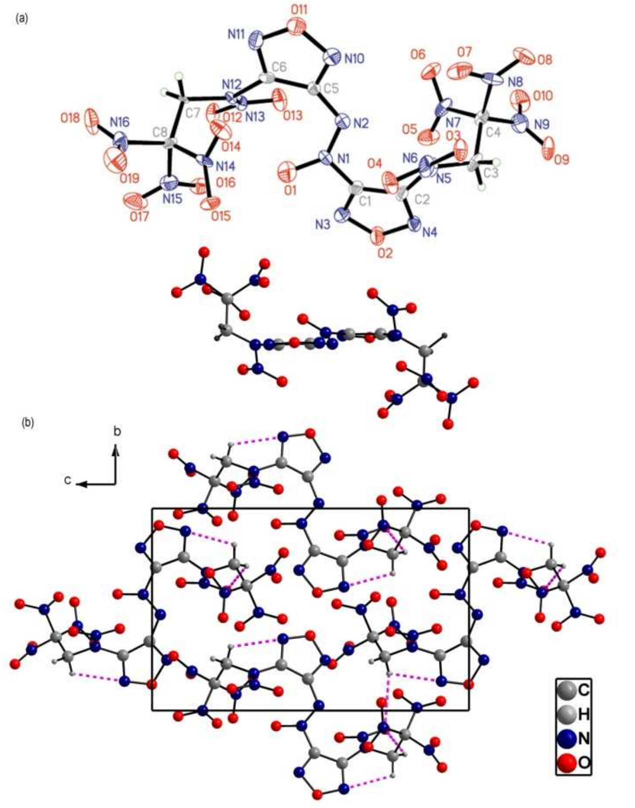


Fig. 6 (a) Molecular structure of **5**. Hydrogen atoms are shown, but are unlabeled for clarity. (b) Ball and stick packing diagram of **5** viewed down the *a* axis. Dashed lines indicate strong hydrogen bonding.

Heat of formation is an important parameter in evaluating the performance of energetic compounds, which were calculated by using the Gaussian 09 suite of program.[33] The geometry optimizations of the molecules and frequency analyses were accomplished by using the B3LYP[34] with the 6-311+G** basis set.[35] Atomization energies were calculated by the CBS-4M.[36] All the optimized structures were characterized to be true local energy minima on the potential energy surface without imaginary frequencies. The calculated heats of formation are summarized in Table 2. It can be seen that all of the trinitroethyl derivatives exhibit positive heats of formation, with **5** having the highest value of 962.1 kJ mol^{-1}, which is more ninefold than that of HMX. Followed by the compound **3** and **4**, the heats of formation are also remarkably high, which is almost sevenfold of HMX (104.8 kJ mol^{-1}). The heat of formation of compound **5** was higher than that of **3** and **4**, which was a result of the higher both nitrogen and oxygen content of compound **5**.

With the data for molecular weight, density from X-ray diffraction and gas pycnometer (25 ^{o}C), and heat of formation in hand, the detonation velocity (*D*) and pressure (*P*) of the resulting compounds were calculated with Kamlet-Jacobs (K-J) equations. (See ESI†) Their detonation performance data are summarized in Table 2. The detonation pressures of compounds **3-5** lie in the range between *P*=35.8 to *P*=41.2 GPa (compared with RDX 35.2 GPa, and HMX 40.3 GPa). Detonation velocities lie in the range between 8861 m s^{-1} and 9458 m s^{-1} (compared with RDX 8977 m s^{-1} and HMX 9320 m s^{-1}). Among them, owing to high density and high heat of formation,

Table 2. Physical properties of trinitroethyl derivatives of furazan and azofurazan

Comp.	T_{dec}[a] [°C]	ρ[b] [g cm^{-3}]	N+O[d] [%]	ΔH_f[e] [kJ mol^{-1}]	D[f] [m s^{-1}]	P[g] [GPa]	IS[h] [J]	FS[i] [N]	ESD[j] [J]	OB[k] [%]
3	209.2	1.887[c]	71.99	719.6	8861	35.8	-	-	-	-18.2
4	190.2	1.84	81.02	759.8	9041	36.7	7.9	130	0.29	-11.9
5	144.6	1.92	84.06	962.1	9458	41.2	3.2	80	0.12	+2.5
RDX	230	1.82	81.06	92.6	8977	35.2	7.5 [l]	120[l]	0.1-0.2 [l]	-21.6
HMX	287	1.91	81.06	104.8	9320	39.6	7.0 [l]	112 [l]	0.2 [l]	-21.6

[a] Thermal decomposition temperature under nitrogen gas, peak of maximum (DSC, 5 °C min^{-1}); [b] Density measured by gas pycnometer (25 °C); [c] Density from X-ray diffraction; [d] Both nitrogen and oxygen content; [e] Heat of formation calculated with Gaussian 09; [f] Calculated detonation velocities; [g] Calculated detonation pressure; [h] Impact sensitivities; [i] Friction sensitivity; [j] Electrostatic sensitivity; [k] Oxygen balance (OB, %) for $C_aH_bN_cO_d$: OB=1600×(d-$2a$-$b/2$)/M_w, M_w= molecular weight (based on carbon dioxide); [l] Ref. 32.

compound **5** exhibits excellent detonation performances (P=41.2 GPa, D=9458 m s^{-1}), which are better than that of HMX.

The measurements of impact sensitivities and friction discharge of the furazan derivatives **4** and **5** were realized by using the standard BAM method.[37] Additionally, they were tested for sensitivity toward electrical discharge by using an ESD JGY-50 III electric spark tester. The sensitivity of compound **4** (7.9 J) is comparable to that of RDX (7.5 J). The nitration product **5** is more sensitive (4.0 J) than HMX (7.0 J). As can be seen from Table 2, similar trends are observed in the electrostatic discharge and friction discharge sensitivity results. The electrostatic sensitivities for compounds **4** and **5** are 0.29 and 0.12 J, respectively, showing that compound **4** is less sensitive to electrical discharge than HMX (0.2 J) and compound **5** is more sensitive than RDX (0.1-0.2 J). In addition, compound **4** is less sensitive to friction (130 N) while the friction sensitivity of HMX is 112 N. Undoubtedly, compound **5** is sensitive to friction (80 N).

Conclusions

In summary, *N*,*N*'-bis(2,2,2-trinitroethyl)-3,3'-diamino-4,4'-azoxyfurazan **4** and *N*,*N*'-bis(2,2,2-trinitroethyl)-3,3'-dinitramino-4,4'-azoxyfurazan **5** were synthesized and fully characterized by ^{1}H, ^{13}C NMR spectroscopy, IR, and single crystal X-ray diffraction. These trinitroethyl derivatives have good both nitrogen and oxygen content, good oxygen balance, which exhibit high densities, moderate thermal stability and high detonation velocities (8861 m s^{-1} to 9458 m s^{-1}) and detonation pressures (35.8 GPa to 41.2 GPa), may serve as a promising alternative to some known explosive such as RDX. Especially, compound 5 having an oxygen balance of near zero (+2.5 %), exhibits superior detonation properties ($\Delta_f H_m$, 962.1 kJ mol^{-1}; D, 9458 m s^{-1}; P, 41.2 GPa) to HMX. These properties suggest that trinitroethyl derivatives might be of interest for future applications as environmentally friendly and nitrogen-rich energetic materials.

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Notes and references

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† Footnotes should appear here. These might include comments relevant to but not central to the matter under discussion, limited experimental and spectral data, and crystallographic data.

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N-Trinitroethyl-substituted azoxyfurazan: high detonation performance energetic materials

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Detonation property: High nitrogen energetic compounds with good oxygen balance are reported. These compounds display excellent detonation properties and extra high heat of formation. Especially, an *N*-nitrated trinitroethylamino azoxyfurazan derivative reported here possesses oxygen balance of near zero (+2.5 %) and exhibits outstanding properties ($\Delta_f H_m$, 962.1 kJ mol^{-1}; D, 9458 m s^{-1}; P, 41.2 GPa).