Energetic Materials

International Edition: DOI: 10.1002/anie.201701659
German Edition: DOI: 10.1002/ange.201701659

A Facile and Versatile Synthesis of Energetic Furazan-Functionalized 5-Nitroimino-1,2,4-Triazoles

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Abstract: *An analogue-oriented synthetic route for the formulation of furazan-functionalized 5-nitroimino-1,2,4-triazoles has been explored. The process was found to be straightforward, high yielding, and highly efficient, and scalable. Nine compounds were synthesized and the physicochemical and energetic properties, including density, thermal stability, and sensitivity, were investigated, as well as the energetic performance (e.g., detonation velocities and detonation pressures) as evaluated by using EXPLO5 code. Among the new materials, compounds **4–6** and **11** possess high densities, acceptable sensitivities, and good detonation performances, and thereby demonstrate the potential applications as new secondary explosives.*

In the last decade, considerable attention has been directed toward the synthesis of energetic heterocyclic compounds with excellent performance characteristics, such as a positive heat of formation, high density, high detonation velocity and pressure, high thermal stability, and low sensitivity towards external forces.[1] The need for highly energetic materials continues to expand, and of particular interest are nitrogen-containing heterocycles (triazole, furazan, etc.) in combination with energetic substituents such as nitro (-NO_2), nitrate (-ONO_2), and nitramine (-$NHNO_2$) functionalities because of their satisfactory comprehensive performances.[2] The compounds functionalized with nitramino groups have been theoretically and experimentally investigated as energetic materials.[3] 3,3′-Dinitramino-4,4′-bifurazan (**1**: $\nu_D = 9086\,\mathrm{m\,s^{-1}}$; $P = 40.3$ GPa) and 3,3′-dinitramino-5,5′-bis(1*H*-1, 2, 4-triazole) (**2**: $\nu_D = 8355\,\mathrm{m\,s^{-1}}$; $P = 30.0$ GPa) are two representative nitramino-based energetic compounds which show excellent detonation properties.[3a,b] Unfortunately, these compounds are highly sensitive towards external mechanical stimuli (impact sensitivity for **1** and **2** is 1.5 and 3 J, respectively), and it greatly limits their practical applications.[4]

Quantum chemical calculations give rise to the most appropriate method to understand the relationship between impact sensitivity and the charge distribution in energetic materials.[5] Politzer and co-workers have applied general interaction properties functions (GIPF), based on quantum chemical calculations, to the correlation and prediction of a number of properties of energetic molecules.[5] According to Pauling’s electroneutrality postulation, the electrostatic potential of a molecule under steady-state conditions tends to be as uniform as possible.[6] Therefore, the GIPF electrostatic balance parameters (ν), which can be obtained from ab initio methods, should be close to 0.2500. Deviations from this value suggests either instability or sensitivity.[6] In our prestudy, the GIPF balance parameters of several classic energetic materials along with some nitramino-functionalized azoles have been calculated by application of this method. The GIPF balance parameter (ν) for the very insensitive explosive 2,4,6-triamino-1,3,5- trinitrobenzene (TATB) has the maximum value of 0.2500, whereas the corresponding values for **1** and **2** are much lower than 0.2500, and is thus in agreement with their high sensitivity. Unexpectedly, compounds which are structurally similar to **1** and **2**, compounds such as nitramino-functionalized azoles, 3-amino-4-(5-nitramino-1, 2, 4-triazol-3-yl)furazan (**3**), 3-nitro-4-(5-nitramino-1, 2, 4-triazol-3-yl)furazan (**4**), and 3-nitramino-4-(5-nitramino-1, 2, 4-triazol-3-yl)furazan (**5**), have balance parameters of 0.2325, 0.2143, and 0.1951, respectively (close to 0.2500). Based on quantum chemical calculations, furazan-functionalized 5-nitroimino-1, 2, 4-triazoles should possess a fine balance between high detonation performance and low sensitivity.

Commonly, the most practical method to prepare nitramino-containing 1, 2, 4-triazoles has been the nitration of 5-amino-1,2,4-triazoles by either 100% HNO_3 or other strongly acidic systems.[3b,7] The precursors of 5-amino-1,2,4-triazoles are usually synthesized by condensation of carbonyl compounds with either aminoguanidine hydrochloride or hydroxyacetimidamides with cyanogen bromide.[8] The drawbacks of these procedures include narrow applicability to substrates, harsh reaction conditions, and the inefficiency in synthesis scale-up. Herein, we report the straightforward and scalable synthesis, and characterization of a series of energetic compounds consisting of the 5-nitramino-1,2,4-triazole moiety and furazan/furoxan rings substituted with methyl, amino, azo, nitro, and nitramino functional groups. The

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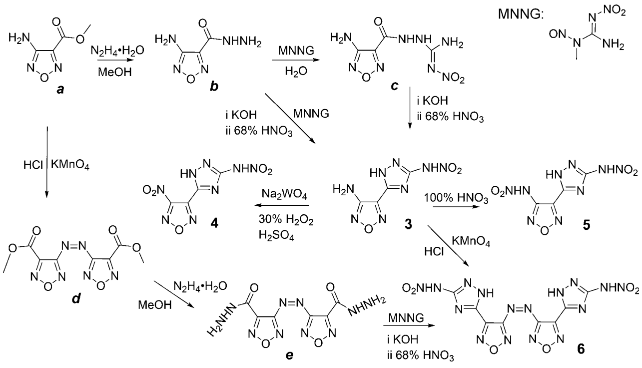
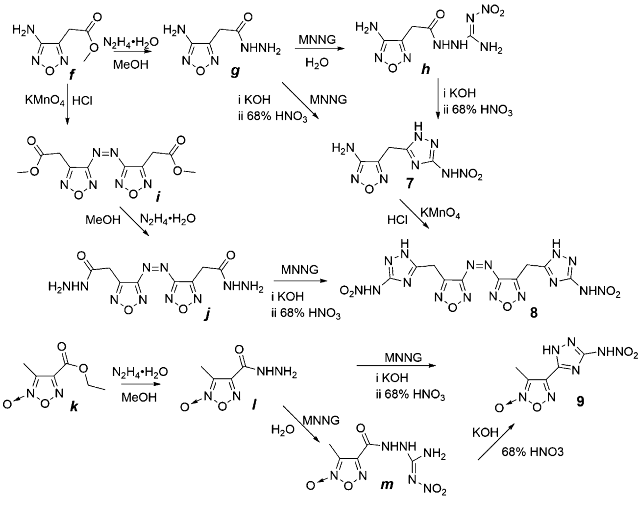
Supporting information and the ORCID identification number(s) for the author(s) of this article can be found under: https://doi.org/10.1002/anie.201701659.

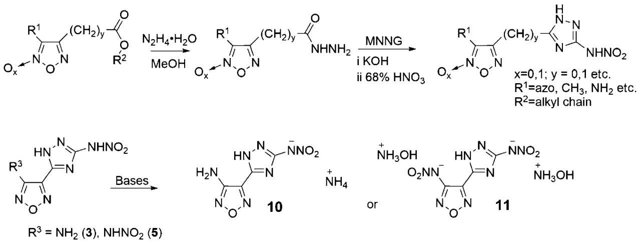
methodology is based on condensation of the readily and commercially available 1-methyl-1-nitroso-2-nitroguanidine (MNNG) with furazan-functionalized carboxylic acid hydrazides.[9] In the initial case (Scheme 1), compound ***b*** reacts with MNNG in aqueous solution to give the nitroguanidyl-functionalized intermediate ***c***, from which **3** was synthesized through intramolecular cyclization by refluxing in aqueous alkaline solution. The compounds **4** and **5** were prepared by treating **3** with 30% hydrogen peroxide and 100% nitric acid, respectively. Notably, the one-pot synthesis of **3** from ***b*** was demonstrated, and further increases the efficiency of this procedure. The azo-derivative **6** can be obtained from **3** through an oxidative coupling reaction with acidic potassium permanganate. Additionally, the reaction of ***e***, obtained from ***d***, and MNNG also provides a feasible route to **6**. The broader applicability of this synthetic strategy was exemplified for three additional substrates (Scheme 2), that is, methyl-2-(4-amino- furazan-3-yl)acetate (***f***) bis(methylacetate)-azofurazan (***i***), and 4-(ethoxycarbonyl)-3-methyl-furoxan (***k***). By using the one-pot procedure with MNNG, 3-amino-4-(5-nitramino-1, 2, 4-triazol-3-yl)methylfurazan (**7**), bis(5-nitramino-1,2,4-triazol-3-methyl)-azofurazan (**8**), and 3-methyl-4-(5-nitramino-1, 2, 4-triazol-3-yl)furoxan (**9**) were obtained. The variations of the substrates are shown in Scheme 3. The reactions of MNNG with furazan/furoxan-based carboxylic acid hydrazides provide convenient approaches to synthesize furazan-functionalized 5-nitroimino-1,2,4-triazoles, which are compounds of potential interest for energetic material applications. Energetic salts most often possess higher thermal stability, and lower vapor pressure and acid-induced corrosivity than their neutral precursors. Hence, a monoammonium salt (**10**) of **3** and dihydroxylammonium salt (**11**) of **5** were also prepared by typical acid-base reactions (Scheme 3). The structures of **3–11** are well-supported by ^{1}H NMR, ^{13}C NMR, and IR spectroscopy, and elemental analysis. The compounds **3–5** were further investigated by single-crystal X-ray crystallography.



Scheme 1. Synthesis route to 3-amino-4-(5-nitramino-1,2,4-triazol-3-yl)furazan (**3**) and its azo derivative (**6**), 3-nitro-4-(5-nitramino-1, 2, 4-triazol-3-yl)furazan (**4**), and 3-nitramino-4-(5-nitramino-1, 2, 4-triazol-3-yl)furazan (**5**).



Scheme 2. Synthesis route of 3-amino-4-(5-nitramino-1,2,4-triazol-3-yl)methylfurazan (**7**), bis(5-nitramino-1,2,4-triazol-3-methyl)-azofurazan (**8**), and 3-methyl-4-(5-nitramino-1,2,4-triazol-3-yl)furoxan (**9**).



Scheme 3. Variations of the substrates of this synthesis strategy and the preparation of the energetic salts **10** and **11**.

Suitable crystals of **3**·H_2O, **4**·acetone, and **5**·H_2O for single-crystal X-ray diffraction were obtained through slow evaporation from solvents. In Figure 1, the crystal structures of these compounds are displayed. The crystals of **3**·H_2O and **5**·H_2O crystallize in the monoclinic space group $P2_1/c$, which contains one lattice water molecule, whereas **4**·acetone crystallizes in the triclinic space group $P\bar{1}$. Based on the crystal structures, the C–C bridged rings, and the amino and nitranimo moieties of **3**·H_2O and **5**·H_2O are nearly planar.

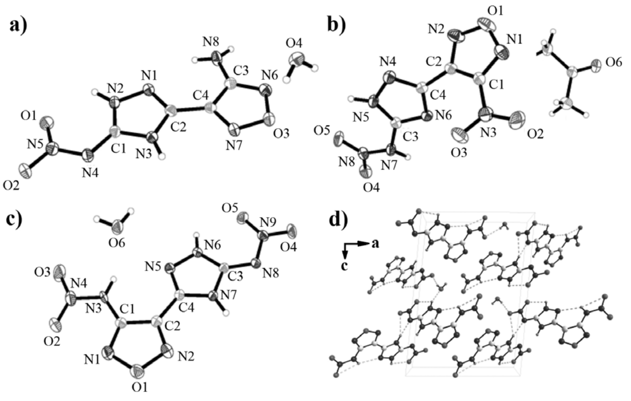


Figure 1. The molecular structures of a) **3**·H_2O, b) **4**·acetone, and c) **5**·H_2O.[13] Thermal ellipsoids shown at 50% probability. d) Depicted are the inter- and intramolecular hydrogen bonds for **5**·H_2O.

Among these crystals, **5**·H_2O has the highest crystal density of 1.896 $g\,cm^{-3}$, in spite of the presence of a water molecule in the structure. With a lone electron pair associated with the nitrogen atom (N3) attached to the furazan ring of **5**·H_2O, they form p-π conjugation between the nitrogen atoms and the aromatic ring, so that the lengths of the C1−N3 (1.375 Å) bonds approach the length of the C=N (1.350 Å) double bond. The hydrogen-bonding interactions in **3**·H_2O, **4**·acetone, and **5**·H_2O are extensive. Additional details involving the crystal structures, including CCDC numbers,[13] and the polymorph **3**·DMF are provided in the Supporting Information.

The thermal stabilities of the newly prepared furazan-functionalized 5-nitroimino-1,2,4-triazoles were determined using differential scanning calorimetry (DSC) measurements. As shown in Table 1, all the compounds decompose without melting, with **3** and **7** being exceptions as they melt at 158.8 and 170.2 °C, respectively, and then decompose. Amino-functionalized compounds decompose at higher temperatures (**3**: $T_d = 195.5$ °C; **7**: $T_d = 196.8$ °C) than the other neutral energetic compounds. In addition, **5** ($T_d = 128.7$ °C) has the lowest decomposition temperature. This undesirable thermal behavior most likely arises from the presence of a second nitramino moiety in the furazan ring. As expected, the ionic derivatives **10** ($T_d = 242.8$ °C) and **11** ($T_d = 196.9$ °C) have the best thermal stabilities among the new materials.

Density is a critical physical parameter for energetic materials. The experimental densities of **3–11** are in the range of 1.680 to 1.920 $g\,cm^{-3}$. It should be noted that the densities of **4–6** and **11** fall within the range designated for new high-energy-density materials (1.8–2.0 $g\,cm^{-3}$), and are comparable with the common high explosives RDX and HMX. Oxygen balance is the index of the deficiency, that is, the excess of oxygen in a compound required to convert carbon into either carbon dioxide or carbon monoxide, and all hydrogen into water. Based on CO_2, **3–11** exhibited negative OB values ranging between −26.43 % (**4**) and −70.74 % (**7**). In the case of OB_{co}, **4** (0) and **11** (−7.43 %) possess similar values to that of RDX (0) and HMX (0). Among these compounds, **5** (80.12 %) and **11** (82.83 %) exhibit higher combined nitrogen and oxygen content values, which are comparable to those of RDX (81.04 %) and HMX (81.04 %).

Heat of formation (HOF) plays an important role in evaluating the performance of energetic materials. The heats of formation of **3–11** were calculated based on appropriate isodesmic reactions by using Gaussian 09 program package (more details about the calculations of heats of formation can be found in the Supporting Information).[10] As summarized in Table 1, all new energetic compounds exhibit positive heats of formation ranging from 327.3 $kJ\,mol^{-1}$/1.01 $kJ\,g^{-1}$ (**11**) to 1274.4 $kJ\,mol^{-1}$/3.03 $kJ\,g^{-1}$ (**6**), and are much higher than those of TNT, RDX, and HMX. The reason for these higher values is attributed to the large number of C−N, N−N, and N−O bonds within the structures of **3–11**.

In the case of energetic materials, the value of energetic performance depends to a great extent on the detonation velocity (ν_D) and detonation pressure (P). Based on experimental densities and calculated heats of formation, detonation properties were determined using EXPLO5 (v6.01).[11] The calculated detonation velocities and pressures fall in the range from 8079 to 9258 $m\,s^{-1}$, and from 24.9 to 39.0 Gpa, respectively. The compounds **4** (9025 $m\,s^{-1}$), **5** (9258 $m\,s^{-1}$), and **11** (9135 $m\,s^{-1}$) exhibit excellent detonation velocities, and they are comparable to that of HMX (9144 $m\,s^{-1}$). These values are due to high density and high combined nitrogen and oxygen content for these compounds. The high detonation pressure of **5** (39.0 GPa) is slightly lower than that of HMX (39.2 GPa). To perform a more thorough evaluation of the energetic compounds, impact and friction sensitivity measurements were made using a standard BAM Fallhammer and a BAM friction tester.[12] The compounds **3–11** were found to be less impact sensitive (18 J to ≥ 40 J) than TNT. In addition, the friction sensitivity is higher than 250 N for all compounds. As shown in Figure 2, the GIPF balance parameters of **1–9** showed a relatively consistent trend with their experimental sensitivity values. Two energetic compounds (**7** and **9**) with measured IF values above 40 J show higher GIPF

Table 1: Properties of **3–11** compared to 2,4,6-trinitrotoluene (TNT), 1,3,5-trinitroperhydro-1,3,5-triazine (RDX), octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX), and TATB.

Compd	T_m[a] [°C]	T_d[b] [°C]	ρ[c] [$g\,cm^{-3}$]	N+O[d] [%]	OB_{CO_2}[e] [%]	OB_{CO}[f] [%]	$\Delta_f H_m$[g] [$kJ\,mol^{-1}$]/[$kJ\,g^{-1}$]	ν_D[h] [$m\,s^{-1}$]	P[i] [GPa]	IS[j] [J]	FS[k] [N]
3	158.8	195.5	1.740	75.43	−52.80	−20.87	467.52/2.20	8332	27.7	35	360
4	–	163.2	1.851	79.30	−26.43	0	524.66/2.17	9025	36.0	20	280
5	–	128.7	1.920	80.12	−28.00	−3.11	548.82/2.13	9258	39.0	18	250
6	–	174.3	1.873	76.17	−45.69	−15.24	1274.4/3.03	8973	34.9	28	280
7	170.2	196.8	1.695	70.77	−70.74	−35.40	449.0/1.99	8079	24.9	>40	>360
8	–	196.3	1.704	71.40	−64.25	−28.57	1206.2/2.69	8125	26.0	31	300
9	–	180.5	1.741	71.34	−59.88	−24.67	443.8/1.95	8236	28.2	>40	>360
10	–	242.8	1.680	75.95	−59.37	−31.14	328.2/1.43	8130	24.6	>40	>360
11	–	196.9	1.850	82.83	−27.24	−7.43	327.3/1.01	9135	36.6	36	360
TNT	80.5	295	1.65	60.79	−73.97	−24.67	−67.0/−0.30	6881	19.5	15	353
RDX	–	204	1.800	81.04	−21.61	0	70.3/0.32	8795	34.9	7.4	120
HMX	–	280	1.905	81.04	−21.69	0	70.4/0.25	9144	39.2	7.4	120
TATB	–	360	1.930	69.75	−55.8	−18.6	−137.5/−0.54	8114	31.2	50	>360

[a] Melting point. [b] Thermal decomposition temperature (onset) under nitrogen (determined by the DSC exothermal peak, 5 °C min^{-1}). [c] Density measured by gas pycnometer at 25° C. [d] Combined nitrogen and oxygen content. [e] Oxygen balance [%] based on CO_2 for $C_aH_bN_cO_d$: OB [%] = $1600\times(d-2a-b/2)/M_W$, M_W = molecular weight. [f] Oxygen balance [%] based on CO for $C_aH_bN_cO_d$: OB [%] = $1600\times(d-a-b/2)/M_W$. [g] Calculated molar enthalpy of formation in solid state. [h] Detonation velocity. [i] Detonation pressure. [j] Impact sensitivity. [k] Friction sensitivity.

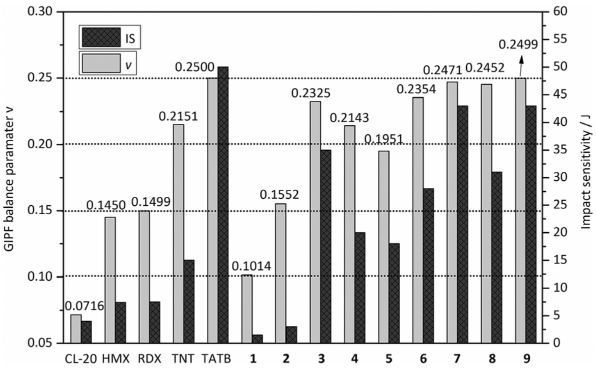


Figure 2. The general interaction properties function balance parameters and impact sensitivities of representative nitramino-functionalized energetic compounds compared with classic explosives and targeted furazan-functionalized 5-nitroimino-1,2,4-triazoles. CL-20 (hexanitrohexaazaisowurtzitane).

balance parameters of 0.2471 and 0.2499, which are close to 0.25 and indicate that this approach may be a powerful means for the insensitive energetic materials design. The most promising compounds for practical use as new secondary explosives are compounds **4**–**6** and **11**. These compounds possess high densities, acceptable sensitivities, and good detonation performances.

In conclusion, inspired by the recently reported highly energetic compounds functionalized with nitramino groups, a series of furazan-functionalized 5-nitroimino-1,2,4-triazoles were designed and synthesized. One-pot reactions based on condensation of readily and commercially available 1-methy-1-nitroso-2-nitroguanidine with furazan-functionalized carboxylic acid hydrazides were developed. The advantages of the new strategy were illustrated to be the availability of the substrates, the high efficiency of the reaction step, and the possibility of scalable synthesis using a green chemical process. The new compounds exhibit reasonable physical properties. The compounds **3**–**11** possess high measured densities, high heats of formation, and excellent detonation velocities and detonation pressures. Also, **4**, **5**, and **11** exhibit superior detonation performance relative to RDX and are comparable to HMX. Importantly, all the novel furazan-functionalized 5-nitroimino-1,2,4-triazoles exhibit low impact sensitivities (18 to more than 40 J) and friction sensitivities (250 to more than 360 N). These features make them potentially interesting candidates for further investigation as secondary energetic materials. New advances in the synthesis of energetic 5-nitroimino-1,2,4-triazoles are expected to emerge in the foreseeable future by utilization of the new strategy.

Acknowledgments

This work was supported by the Office of Naval Research (N00014-16-1-2089), the Defense Threat Reduction Agency (HDTRA1-15-1-0028), the National Natural Science Foundation of China (No. 21376121, 21676147), and the Priority Academic Program Development of Jiangsu Higher Education Institutions (PAPD).

Conflict of interest

The authors declare no conflict of interest.

Keywords: density functional calculations · energetic materials · heterocycles · structure elucidation · X-ray diffraction

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[13] CCDC 1479423 (**3**·H_2O), 1479439 (**4**), and 1491824 (**5**·H_2O) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

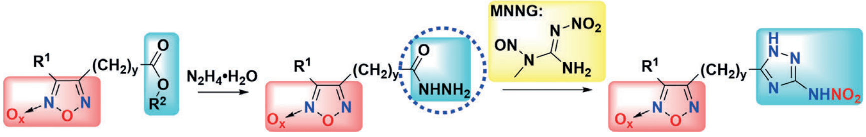
Manuscript received: February 14, 2017
Revised: March 15, 2017
Final Article published: ■■ ■■, ■■■■

Communications

Energetic Materials

Z. Xu, G. Cheng, H. Yang,* X. Ju, P. Yin, J. Zhang,* J. M. Shreeve* ___ ■■■■–■■■■

A Facile and Versatile Synthesis of Energetic Furazan-Functionalized 5-Nitroimino-1,2,4-Triazoles



High energy: An analogue-oriented synthetic route for the formulation the title compounds was developed. The process was found to be straightforward, high yielding, and highly efficient, and scalable for the synthesis of high-performance energetic materials.