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Assembly of Nitrofurazan and Nitrofuroxan Frameworks for High-Performance Energetic Materials

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Abstract: The design of novel energetic materials with improved performance, optimized parameters and environmental compatibility remains a challenging task. In this study, new high energy materials based on the isomeric dinitrobi-1,2,5-oxadiazole structures comprising of nitrofurazan and nitrofuroxan subunits were synthesized. Due to planarity and strong non-covalent interactions, materials reveal the high density values as determined by single-crystal X-ray diffraction. Thermal, impact, and friction sensitivity of both isomers are close to that for nitroesters. High density, high heat of formation, and good oxygen balance regard the synthesized compounds as promising explosives and highly-energetic oxidizers.

Common energetic materials from 2,4,6-trinitrotoluene (TNT) to 1,3,5,7-tetranitro-1,3,5,7-tetrazocane (HMX) synthesized about a century ago bring its energy mainly from the carbon backbone oxidation. Contrary, recently developed explosives comprise the various heterocycles with high-nitrogen content aiming to increase the power mainly due to N₂ formation.^[1] These synthetic efforts are driven by a search for a combination of the high performance, safe handling with a lower environmental impact in a single compound.^[2] More specifically, the promising explosive should combine the high values of density, heat of formation, detonation parameters, oxygen balance, thermal stability and, along with that, possess the low sensitivity toward impact and friction.^[3] Unfortunately, in practice the convergence of these properties remains a challenging task.^[4] A variety of moieties were

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proposed during the development of the energetic materials, among them the 1,2,5-oxadiazole (furazan) and its N-oxide (furoxan) frameworks stand out due to high positive heats of formation and active oxygen atoms.^[1,3a] In last few years these motifs were successfully incorporated in a number of modern primary and secondary high-energy materials, mainly by the efforts of the Shreeve's team,^[5] Klapötke's team^[6] and some other research groups.^[7] Recently synthesized energetic materials incorporating a few nitro-1,2,5-oxadiazole moieties are shown in Figure 1. Dinitroazofuroxan (DNAFO) representing two nitrofuroxan fragments linked by an azo bridge has an excellent energetic performance and zero oxygen balance, however its synthesis includes multistep reaction sequence with low overall yield.^[8] Bis(nitrofurazanyl)furoxan (BNFF)^[9] comprising two nitrofurazan units, coupled by the C-C bond with a furoxan ring lower parameters has including moderate density. Dinitrobifurazan (DNBF) has seemingly confused high thermal stability (250 °C) along with a moderate density and high sensitivity.^[10] Only few crystals of dinitrobifuroxan (DNBFO) were isolated and characterized by X-ray diffraction.[6a] Despite of its high calculated detonation performance, the synthesis of DNBFO is hardly scalable and no parameters such as mechanical sensitivity was reported so far. Overall, the analysis of literature reveals that tradeoff between the synthesis simplicity, high performance and low sensitivity is still not reached for 1,2,5oxadiazole-based explosives, which are of urgent interest as a platform in the design of novel energetic materials. As a logical step in the development of the nitro-1,2,5-oxadiazole structures the alliance of nitrofurazan and nitrofuroxan frameworks linked via C-C bond (structures **1a,b**) is proposed. Hence, here we present is of novel high-performance compounds 1(3)-(3-nitrofurazan-4-yl)furoxans, their hanical sensitivity, and theoretical on performance.

Figure 1. Several prospective 1,2,5-oxadiazole based high-energy materials.

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Having an experience in the synthesis and reactivity of furoxans,^[11] we decided to develop a synthetic strategy (Scheme 1) to the target 3-nitro-4-(4-nitrofurazan-3-yl)furoxan 1a. It is based on the readily available furazan precursor - amidoxime 2, which can be easily obtained by the cascade reactions of malononitrile.^[12] Amidoxime 2 was then transformed to the chloroximinofurazan 3 according to a known procedure.^[13] Amino group in compound 3 was oxidized to the nitro group with a mixture of conc. H₂O₂-H₂SO₄ under mild conditions. The resulted chloride 4 was involved in one-pot cascade process including acylation of dinitromethane sodium salt followed by nitrosation of the formed intermediate 5 and the subsequent regioselective intramolecular cyclization of the nitrosation product with the formation of the target compound 1a. To prepare the isomeric 4nitro-(4-nitrofurazan-3-yl)furoxan 1b a possibility of the 3nitroisomer 1a to undergo thermal isomerization was studied. The thermal isomerization of 4-aryl-3-nitrofuroxans into 3-aryl-4nitrofuroxans is carried out by refluxing of 3-nitroisomer in toluene for 3 hours.^[14] However, these conditions proved to be unsuitable for the preparation of 4-nitroisomer 1b since 3-nitroisomer 1a decomposed significantly. Refluxing of compound 1a in CCl₄ for 90 hours was found to be an appropriate approach enabling to obtain the 4-nitroisomer 1b in high yield (Scheme 1). Importantly, the developed protocols enable to synthesize the target energetic materials in gram scale avoiding isolation of very sensitive intermediates.

Synthesized compounds **1a,b** were characterized by spectral (IR, ¹H, ¹³C, ¹⁴N NMR spectroscopy and mass spectrometry) and analytical methods. The position of nitro group namely at C(3) or C(4) carbon atoms of the furoxan ring was defined by ¹⁴N NMR spectra, which may serve as a reliable tool to differ nitrofuroxan isomers.^[14] The chemical shift of the nitro group at the C(3) carbon of the furoxan ring in compound **1a** (-38.9 ppm) is located more upfield than the corresponding chemical shift of the nitro group at the furazan one (-37.4 ppm) (Fig. 2, top). In the ¹⁴N NMR spectrum of compound **1b** this correlation is inverted and the signal of the nitro group at the C(4) carbon of the furoxan ring moved downfield significantly (-36.4 ppm), while the chemical shift of the nitro group at the furazan ring is rather the same (-37.8 ppm) (Fig. 2, bottom). Thus, the ¹⁴N NMR spectroscopy resolves the isomerization process of the 3-nitrofuroxan framework.

Finally, the structures of the dinitrobi-1,2,5-oxadiazoles **1a** and **1b** were confirmed by a single-crystal X-ray diffraction study (Figs. 3,4). Analysis of X-ray diffraction data revealed that the



Figure 2. ¹⁴N NMR spectra of dinitrobi-1,2,5-oxadiazoles 1a and 1b in acetoned₆.

density of **1a** and **1b** crystals is high, but slightly different, i.e., 1.981 and 2.026 g cm⁻³ for **1a** and **1b** at 100 K. According to the structural analysis and DFT calculations (see refs.^[15] for more detailed description of the approach and Supporting information for the discussion) this difference can be rationalized by the formation of a quite strong intramolecular contact between the O(1) atom of the nitroxyl fragment and the nitro group oxygen atom in **1a** (i.e., the O(1)...O(3) distance is 2.707 Å, the interaction energy is 15.5 kJ mol⁻¹). Namely, the oxygen atoms can be involved in short intermolecular contacts only if this interaction is not formed (as in 4-nitroisomer **1b**).

The morphology of synthesized energetic dinitrobi-1,2,5oxadiazoles **1a,b** were additionally characterized by scanning electron microscopy (SEM). Powder of compound **1a** is comprised with plate-like particles around 10 μ m. Contrary, sample **1b** has a coarser elongated particles (ca. 50 μ m) (SEM images are presented in Supporting information).



Scheme 1. Synthesis of the dinitrobi-1,2,5-oxadiazoles 1a and 1b.

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Figure 3. The general view of the **1a** molecule. Atoms are represented by probability ellipsoids of atomic vibrations (p=0.5). The short intramolecular contact corresponding to non-covalent interactions is shown by dashed lines.



Figure 4. The general view of the 1b molecule. Atoms are represented by probability ellipsoids of atomic vibrations (ρ =50%).

Thermal behavior of the isomers 1a and 1b was studied with differential scanning calorimetry (DSC) and pressure DSC.^[16] Bi-1,2,5-oxadiazole 1a has a lower melting point comparing to 1b isomer, viz., 96 and 102 °C, however its decomposition onset is higher - 146°C and 140°C, respectively (Table 1). Based on the mechanical sensitivity values, both compounds are more sensitive than nitramines (RDX and HMX) approaching the nitroesters (PETN: 3.3 J, 70 N for impact and friction sensitivity, respectively). Kamlet-Jacobs method^[17] used to calculate the detonation velocity and the Chapman-Jouguet pressure revealed the title compounds are superior compared to commonly used RDX and HMX. Since the dinitrobi-1,2,5-oxadiazoles 1a,b have higher oxygen content and oxygen balance than DNBF, RDX and HMX, they can be used as energetic oxidizers. Combustion performance for model compositions with active and hydrocarbon binders was obtained using thermodynamic calculations (Section S6, Supporting information). The optimized metal-free compositions based on 1a,b reveal the 258-259 s of specific impulse at chamber pressure 4 MPa. Comparison with the results for nitramines proves the high potential of the nitrofuroxannitrofurazan based materials, i.e., 1a, 1b and DNBF, DNBFO.

In summary, we present the synthesis of 3-nitro-4-(3nitrofurazan-4-yl)furoxan through a one-pot acylation/nitrosation/cyclization cascade of the 3-(chloroximino)-4-nitrofurazan. 3-Nitrofuroxan motif in the synthesized structure was isomerized almost quantitatively to the corresponding

Table 1. Functional properties of dinitrobi-1,2,5-oxadiazoles 1a,b compared to DNBF, DNBFO, RDX, and HMX.

	1a	1b	DNBF	DNBFO	RDX	HMX
Formula	$C_4N_6O_7$	C4N6O7	C4N6O6	$C_4N_6O_8$	$C_3H_6N_6O_6$	$C_4H_8N_8O_8$
FW [g mol ⁻¹] ^[a]	244	244	228	260	222	296
ρ [g cm ⁻³] ^[b]	1.920	1.934	1.85 ^[n]	1.970 ^[p]	1.806	1.910
T _m [°C] ^[c]	96	102	85 ^[n]	-	204	280
T _{dec} [°C] ^[d]	146	140	250 ^[n]	140 (est.) ^[p]	204	280
IS [J] ^[e]	2.6	2.8	-	-	8	7
FS [N] ^[f]	67	82	-	-	140	150
N [%] ^[g]	34.43	34.43	36.84	32.31	37.84	37.84
$\Omega_{ ext{CO}}$ [%] ^[h]	19.67	19.67	14.04	24.62	0	0
Ω _{CO2} [%] ^[i]	-6.56	-6.56	-14.04	0	-21.61	-21.61
$\Delta H^{0}{}_{f}$ [kJ mol ⁻¹] ^[j]	417.5	417.5	413.5 ^[o]	448.9 ^[p]	70.3	74.8
<i>D</i> [km s ⁻¹] ^[k]	9.18	9.23	9.22 ^[0]	9.53 ^[p]	8.80	9.14
<i>Р</i> _с , [GPa] ^[]	38.8	39.4	35.6 ^[o]	41.2 ^[p]	34.9	39.2
/ _{SP} [S] ^[m]	259	259	257	263	251	250

[a] Molar weight. [b] Density at 298 K. [c] Melting temperature (DSC). [d] Decomposition temperature (pressure DSC, 5 K min⁻¹). [e] Impact sensitivity (according to STANAG 4489^[18]). [f] Friction sensitivity (according to STANAG 4487^[19]). [g] Nitrogen content. [h] Oxygen balance toward carbon monoxide ($\Omega_{CO2} = nO - xC - yH/2(1600/FW)$). [j] Oxygen balance toward carbon dioxide ($\Omega_{CO2} = nO - 2XC - yH/2(1600/FW)$). [j] Calculated heat of formation via the additive method.^[20] [k] Calculated detonation velocity. [l] Calculated detonation Chapman-Jouguet pressure. [m] Calculated specific impulse for a model composition (4/0.1 MPa). [n] Ref.^[50]. [o] Ref.^[50].

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4-nitrofuroxan subunit. Detailed analysis of the functional properties of isomeric dinitrobi-1,2,5-oxadiazoles reveals that this type of coupled hydrogen-free high energetic molecules represents the attractive features as a high energy content and high density, providing the performance exceeding the nitramines. Presented synthetic data and detailed characterization appeared to be an important step toward the development of a nitrofuroxan-and nitrofurazan-based energetic materials. Described energetic alliance of nitrofurazan and nitrofuroxan scaffolds resulted in an excellent combination of easy access, high performance and acceptable sensitivity. Therefore, these compounds may serve as well alternative to the known commonly used explosives and, thus, may be considered to find real-life applications as a new generation secondary energetic materials.

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Conflict of interest

The authors declare no conflict of interest.

Keywords: energetic materials • explosives • nitrogen heterocycles • oxadiazoles • structure elucidation

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Novel highly energetic heterocyclic assemblies, incorporating 1,2,5oxadiazole motif, were prepared through a step-economical and gramscalable procedure. A unique set of energetic properties, including high density, high positive heat of formation (+417.5 kJ mol⁻¹), positive oxygen balance (+19.7%) and moderate sensitivity provides a high performance (e.g. detonation velocity 9.23 km s⁻¹) and an opportunity to replace commonly used explosives.



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