# **CHEMISTRY** A European Journal



# **Accepted Article**

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Authors: Jean'ne Shreeve, Yongxing Tang, Chunlin He, Gregory H. Imler, and Damon Parrish

This manuscript has been accepted after peer review and appears as an Accepted Article online prior to editing, proofing, and formal publication of the final Version of Record (VoR). This work is currently citable by using the Digital Object Identifier (DOI) given below. The VoR will be published online in Early View as soon as possible and may be different to this Accepted Article as a result of editing. Readers should obtain the VoR from the journal website shown below when it is published to ensure accuracy of information. The authors are responsible for the content of this Accepted Article.

To be cited as: Chem. Eur. J. 10.1002/chem.201703930

Link to VoR: http://dx.doi.org/10.1002/chem.201703930

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## Energetic 1,2,5-oxadiazolo-pyridazine and its N-oxide

Yongxing Tang,<sup>[a]</sup> Chunlin He, <sup>[a]</sup> Gregory H. Imler,<sup>[b]</sup> Damon A. Parrish,<sup>[b]</sup> and Jean'ne M. Shreeve\*<sup>[a]</sup>

Dedication ((optional))

**Abstract:** Achieving an energetic compound which exhibits high performance and insensitivity is important in the field of energetic materials and remains a major challenge. Here we find that oxidation of 4,7-diaminopyridazino[4,5-*c*]furoxan (**5**) with a mixture of 50% hydrogen peroxide and trifluoroacetic anhydride gives rise to 6-amino-7-nitro-[1,2,5]oxadiazolo[3,4-*c*]pyridazine (**7**) and its N-oxide derivative (**8**). The oxidation of **5** with hypofluorous acid (HOF) was also studied. Compound **8** displays an energetic performance compared to TATB and insensitive properties (*IS*: 36 J and *FS*: >360 N). Such excellent properties make **8** attractive for high performance applications where insensitivity is important.

With the advent of numerous strategies for design and synthesis of high energy density materials, the challenging optimum balance between detonation performance and sensitivity has come into focus.[1] Most well-established strategies involving enforced layer-by-layer stacking,<sup>[2]</sup> intramolecular hydrogen bonds,[3] 3D metal organic frameworks (MOFs),[4] and cocrystallization<sup>[5]</sup> show reasonable prospects. From the view point of synthetic methodology, the introduction of a nitro group while maintaining the stability of the molecule is an efficient method. The synthesis of novel energetic compounds containing vicinal C-NH<sub>2</sub>/C-NO<sub>2</sub> functionalities gives an unprecedented entry to extend the variety of insensitive energetic compounds by condensation of nitroacetonitrile with the diazonium moiety.<sup>[6]</sup> Meanwhile, the incorporation of the N-oxide component has been shown to be an efficient method to improve the detonation performance.[7]

Based on previous oxidation studies using HOF<sup>[8]</sup> or a mixture of 50% hydrogen peroxide and trifluoroacetic anhydride,<sup>[7a, 7g]</sup> we selected 4,7-diaminopyridazino[4,5-c]furoxan (**5**) as the substrate, which could be converted to the nitro substituted compound **A** (Scheme 1). Compound **A** had been discussed theoretically, and showed promising properties in the application of solid composite propellants.<sup>[9]</sup> During our attempts to synthesize **A** through the oxidation reaction of **5** (Scheme 1) with different oxidizing reagents, we quite surprisingly found the formation of 6-amino-7-nitro-[1,2,5]oxadiazolo[3,4-c]pyridazine (**7**) and its N-oxide (**8**). Both of them comprise a five-membered ring fused to a six membered ring having vicinal C–NH<sub>2</sub>/C–NO<sub>2</sub> groups, which showed high stability and insensitive properties. Now we describe these new findings involving oxidation of 4,7-

[a] Dr. Y. Tang, Dr. C. He, Prof. Dr. J. M. Shreeve Department of Chemistry, University of Idaho, Moscow, Idaho, 83844-2343, United States Fax: (+1) 208-885-9146
E-mail: jshreeve@uidaho.edu
[b] Dr. G. H. Imler, Dr. D. A. Parrish Naval Research Laboratory, 4555 Overlook Avenue, Washington,

D.C. 20375, United States

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diaminopyridazino[4,5-c]furoxan (5) with HOF or a mixture of 50% hydrogen peroxide and trifluoroacetic anhydride which does not undergo the expected oxidation reaction.





Initially, 4,7-diaminopyridazino[4,5-c]furoxan (5) was synthesized based on the literature.<sup>[10]</sup> Nitration of cyanoacetic acid (1) with a mixture of 100% nitric acid and trifluoroacetic acid gave 3,4-cyanofuroxan (2) which when reacted with hydrazine monohydrate resulted in the intermediate 3-cyanofuroxan-4carbamidrazone (3). Compound 3, when treated with acetic acid, gave rise to 4,7-diaminopyridazino[4,5-c]furoxan diacetate (4). Finally, 4,7-diaminopyridazino[4,5-c]furoxan (5) was synthesized by neutralization of 4 with solid sodium carbonate.

Two different common oxidants were used in attempts to introduce the nitro group into 5 which would enhance the density thus improving the detonation performance. When hypofluorous acid (HOF) was the oxidizer, 4-cyano-3-(N'nitrocarbamimidoyl)furoxan (6) was isolated. However, with a mixture of 50% hydrogen peroxide and trifluoroacetic anhydride, two novel fused heterocyclic rings, 6-amino-7-nitro-[1,2,5]oxadiazolo[3,4-c]pyridazine (7) and its N-oxide derivative (8) were formed and isolated. These products may result from complex oxidation reactions with the concomitant rearrangement of the furoxan ring.<sup>[11]</sup>In addition, 4,7-diaminopyridazino[4.5c]furoxan trifluoroacetate (9) was also formed at a high yield. The structures of 6-9 were confirmed by single crystal X-ray diffraction analysis.

Suitable crystals of **6**–**8** for X-ray diffraction analysis were obtained by slow evaporation from a solution of **6** in acetonitrile and a solution of **7** or **8** in ethyl acetate/hexane, respectively. Compound **6** crystallizes in the orthorhombic space group Pna2<sub>1</sub> with a crystal density of 1.813 g cm<sup>-3</sup> at 150 K. The crystal asymmetric unit consists of two independent molecules (*Z* = 8) is shown in Figure 1. The parameters of the two molecules in the

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crystal agree well with each other. The largest difference is 0.08 Å in the N-oxide moiety (N13-O14: 1.261 (5) Å and N27-O28: 1.179 (5) Å). The details are given in the Supporting Information. In addition, one cyano group is located in the same plane with furoxan with a torsion angle N10-C9-C8-N11 of 179.8°, while the other cyano group is twisted out of the furoxan ring with a torsion angle N24-C-23-C22-N25 of 12.3°.



Figure 1. Molecular structure of 6 (drawn with 50% probability)

Compound 7 crystallizes in the monoclinic space group Cc and has a calculated density of  $1.822 \text{ g cm}^{-3}$  at 150 K (Figure 2). The bond lengths and the bond angles on the furazan ring and pyrazine ring are between typical C–N/N–N single and C=N/N=N double bonds due to the aromaticity. Among them, the bond lengths of N8-C9 and N7-N8 are 1.376(3) and 1.270(2) Å, respectively. In the structure, there are three types of hydrogen bonds including an intramolecular hydrogen bonds (N6-H6A...O11 and N6-H6B...N12).



Figure 2. Molecular structure of 7 (drawn with 50% probability)

Compound **8** crystallizes in the orthorhombic space group Fdd2 and has a calculated density of 1.909 g cm<sup>-3</sup> at 150 K. As can be seen in Figure 3, the crystal asymmetric unit also consists of two independent molecules (Z = 32). In the two molecules, the amino groups, the nitro groups and the fused heterocyclic ring attached thereto lie in one plane. The bond lengths of the N-oxide moiety are 1.253(6) (N22-O23) and 1.255(6) (N8-O9) Å, respectively. In comparison with **7**, the presence of the N $\rightarrow$ O moiety in **8** increases the neighboring bond lengths. (N8-C10/N22-C24, viz., 1.414(7)/1.392(8) Å in **8** 

vs. 1.376(3) Å in 7; N7-N8/N21-N22: 1.290(7)/1.309(7) Å in 8 vs. 1.270(2) Å in 7). The molecules of 8 in the crystal form an extensive network of hydrogen bonds, especially, the adjacent nitro group and the amino group form intramolecular H-bonds via N(6)-H(6B)...O(2) and N(20)-H(20B)...O(16), which is one of the main reasons for stabilizing the molecules and increasing the density.





Since **7** and **8** may find application in the field of energetic materials, their properties including thermal stability, detonation performance and sensitivities were studied. The results are given in Table 1. The onset decomposition temperature of **7** and **8** are 186 and 175 °C, respectively. The measured density by a gas pycnometer for **7** is 1.79 g cm<sup>-3</sup>. As expected, the introduction of the N $\rightarrow$ O moiety increases the density; **8** is at 1.84 g cm<sup>-3</sup>. The gaseous state heats of formation of both compounds were calculated using G2 method. The solid state heats of formation were predicted based on the literature.<sup>[12]</sup> The values for **7** and **8** are 417.8 and 368.7 kJ mol<sup>-1</sup>, respectively.

 Table 1. Physicochemical and energetic properties of compounds 7– 8

 compared with TATB

	ρ <sup>[a]</sup> (gcm ³)	<i>Dv</i> <sup>[b]</sup> (m/s)	P <sup>[c]</sup> (GPa)	<i>∆H</i> f <sup>[d]</sup> (kJ/mol)/(kJ/g)	T <sub>dec</sub> <sup>[e]</sup> (°C)	/S <sup>[f]</sup> (J)	FS <sup>[g]</sup> (N)
7	1.79	8396	29.4	417.8/2.29	186	>50	>360
8	1.84	8695	32.9	368.7/1.86	175	36	>360
ТАТВ	1.93	8504	31.7	-154.2/-0.60	350	50	353

[a] Density measured by a gas pycnometer at 25 °C; [b] Calculated detonation velocity; [c] Calculated detonation pressure; [d] Calculated molar enthalpy of formation in solid state; [e] Temperature of decomposition (onset); [f] Impact sensitivity; [g] Friction sensitivity.

The detonation velocity and pressure were calculated by using EXPLO5 V6.01 code.<sup>[13]</sup> Compound **7** is calculated to have a detonation velocity of 8396 m s<sup>-1</sup> and a detonation pressure of 29.4 GPa. In comparison, **8** has a better detonation performance with a detonation velocity of 8695 m s<sup>-1</sup> and a detonation pressure of 32.9 Gpa, which are superior to those of the traditional insensitive explosive, TATB.

For initial safety considerations, the impact sensitivity and friction sensitivity were tested.<sup>[14]</sup> As shown in Table 1, both of  $\bf{7}$ 

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and  ${\bf 8}$  are insensitive. The impact sensitivity of  ${\bf 7}$  is more than 50 J, while the impact sensitivity of  ${\bf 8}$  is 36 J. Both have friction sensitivity of > 360 N.

In summary, the oxidation of ring system (**5**) was studied. By using hypofluorous acid (HOF), a ring-opening product (**6**) was formed, while using a mixture of 50% hydrogen peroxide and trifluoroacetic anhydride led to the formation of two novel fused compounds **7** and **8**. Both of them show good detonation properties; especially the detonation performance of **8** is better than that of TATB while meanwhile it exhibits low sensitivities (*IS*: 36 J; *FS*: >360 N). This attractive oxidation reaction may provide a promising route for constructing new fused rings with excellent properties. The detailed mechanism and further studies along these findings are currently under study in our laboratories.

#### **Experimental Section**

*Caution!* Compounds 7 and 8 are potential energetic materials. Although we have had no difficulty in handling these compounds during the synthetic procedure, personal protective equipment such as leather gloves, blast shields and safety glasses should be used at all times.

#### Synthesis of 4-cyano-3-(N'-nitrocarbamimidoyl)furoxan (6)

A 20% fluorine mixture (in gaseous nitrogen) was bubbled through a mixture of acetonitrile (40 mL) and water (4 mL) at -15 °C in a dry-ice bath for 0.5 h. The solution was added to a suspension of **5** (0.25 g, 1.5 mmol) in acetonitrile (2 mL). The reaction mixture was stirred at 0 °C for 0.5 hour and the solvent was removed by air. The residue was added to water (30 mL), the precipitate was filtered to give a crude product, **6**. The pure product could be obtained by slow evaporation of the solution of **6** in acetonitrile. Colorless solid (0.15 g, 52% yield). *T*<sub>m</sub>: 158 °C. *T*<sub>d</sub> (onset): 162 °C. <sup>1</sup>H NMR:  $\delta$  9.79 (s, 1H), 9.78 (s, 1H) ppm. <sup>13</sup>C NMR:  $\delta$  149.7, 134.0, 110.1, 107.5 ppm. IR (KBr):  $\dot{v}$  3382, 3283, 3175, 2245, 1667, 1615, 1570, 1470, 1381, 1264, 1242, 1107, 1087, 1027, 922, 851, 808, 780. 737, 677, 655 cm<sup>-1</sup>. Elemental analysis for C4H<sub>2N6</sub>O<sub>4</sub> (198.10): Calcd C 24.25, H 1.02, N 42.42 %. Found: C 24.54, H 1.08, N 42.41 %.

#### Synthesis of 6-amino-7-nitro-[1,2,5]oxadiazolo[3,4-c]pyridazine (7), 6-amino-7-nitro-[1,2,5]oxadiazolo[3,4-c]pyridazine 4-oxide (8), and 4,7-diaminopyridazino[4,5-c]furoxan trifluoroacetate (9)

Trifluoroacetic anhydride (4 mL, 28 mmol) was added dropwise to a slurry of 50% hydrogen peroxide (1.3 mL, 25 mmol) in methylene chloride (20 mL) with stirring at <10 °C. Compound **5** (1.0 g, 5.9 mmol) was added at 0 °C and stirred for 30 min and continued for 10 hours at room temperature. The solvent was removed and the concentrated solution was added to water (60 mL). The solution was extracted with ethyl acetate (20 mL × 3). The combined organic phase was dried over anhydrous magnesium sulfate and the solvent was concentrated. The residue was separated by column chromatography (EtOAc/*n*-hexane = 1 : 4) to give **7** and **8**. The water phase was evaporated slowly to give **9** as yellow crystals.

7: Brown solid (0.11 g, 10% yield). *T*<sub>d (onset)</sub>: 186 °C. <sup>1</sup>H NMR (*d*<sub>6</sub>-DMSO): δ 8.81 (s, 1H), 8.40 (s, 1H) ppm. <sup>13</sup>C NMR (*d*<sub>6</sub>-DMSO): δ 161.5, 152.6, 136.0, 106.7 ppm. IR (KBr):  $\tilde{v}$  3416, 1637, 1561, 1465, 1403, 1354, 1303, 1255, 1140, 986, 950, 918, 790, 764, 717, 675, 647 cm<sup>-1</sup>. Elemental analysis for C<sub>4</sub>H<sub>2</sub>N<sub>6</sub>O<sub>3</sub> (182.10): Calcd C 26.38, H 1.11, N 45.09 %. Found: C 25.96, H 1.22, N 46.15 %.

**8**: Red solid (0.25 g, 21% yield).  $T_{d \text{ (onset)}}$ : 175 °C. <sup>1</sup>H NMR( $d_6$ -DMSO):  $\delta$  10.29 (s, 1H), 9.80 (s, 1H) ppm. <sup>13</sup>C NMR ( $d_6$ -DMSO):  $\delta$  167.5, 156.0, 144.0, 108.9 ppm. IR (KBr):  $\tilde{\nu}$  3413, 3303, 1629, 1543, 1499, 1457, 1425, 1384, 1353, 1285, 1239, 1147, 992, 908, 808, 771,672, 569 cm<sup>-1</sup>. Elemental analysis for C<sub>4</sub>H<sub>2</sub>N<sub>6</sub>O<sub>4</sub> (198.10): Calcd C 24.25, H 1.02, N 42.42 %. Found: C 24.82, H 1.17, N 42.34 %.

 ${\bf 9}\text{-}H_2\text{O}:$  Yellow crystals (1.07 g, 60% yield).  $\textit{T}_m:$  94 °C.  $\textit{T}_d$  (onset): 170 °C.  $^1\text{H}$  NMR ( $\textit{d}_6\text{-}\text{DMSO}$ ):  $\delta$  10.08 (br), 8.13-8.89 (m) ppm.  $^{13}\text{C}$  NMR ( $\textit{d}_6\text{-}\text{DMSO}$ ):  $\delta$  157.1, 154.9, 152.5, 148.8, 110.2, 108.7 ppm. IR (KBr):  $\tilde{\nu}$  3433, 3410, 3297, 1697, 1669, 1612, 1473, 1435, 1354, 1193, 1157, 1069, 1044, 840, 797, 760, 726, 706, 689, 637, 588, 555 cm^{-1}. Elemental analysis for C<sub>6</sub>H<sub>7</sub>F<sub>3</sub>N<sub>6</sub>O<sub>5</sub> (300.15): Calcd C 24.01, H 2.35, N 28.00 %. Found: C 24.01, H 2.45, N 28.19 %.

#### Acknowledgements ((optional))

This work was supported by the Office of Naval Research (N00014-16-1-2089) and the Defense Threat Reduction Agency (HDTRA 1-15-1-0028). We are also grateful to the M. J. Murdock Charitable Trust, Reference No.: 2014120: MNL:11/20/2014 for funds supporting the purchase of a 500 MHz NMR spectrometer. We thank Prof. Richard V. Williams and Dr. Gang Zhao for the discussion of mechanism.

**Keywords:** energetic materials • furoxan • furazan • pyridazine • N-oxide

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The oxidation reactions of 4,7diaminopyridazino[4,5-c]furoxan (5) gave unexpected products. The oxidant products, 6-amino-7-nitro-[1,2,5]oxadiazolo[3,4-c]pyridazine (7) and its N-oxide derivative (8) exhibit good detonation performance and insensitive properties, which may find potential application in insensitive energetic materials.



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