# An interesting 1,2,4-triazole-furazan system: a new family of insensitive energetic materials

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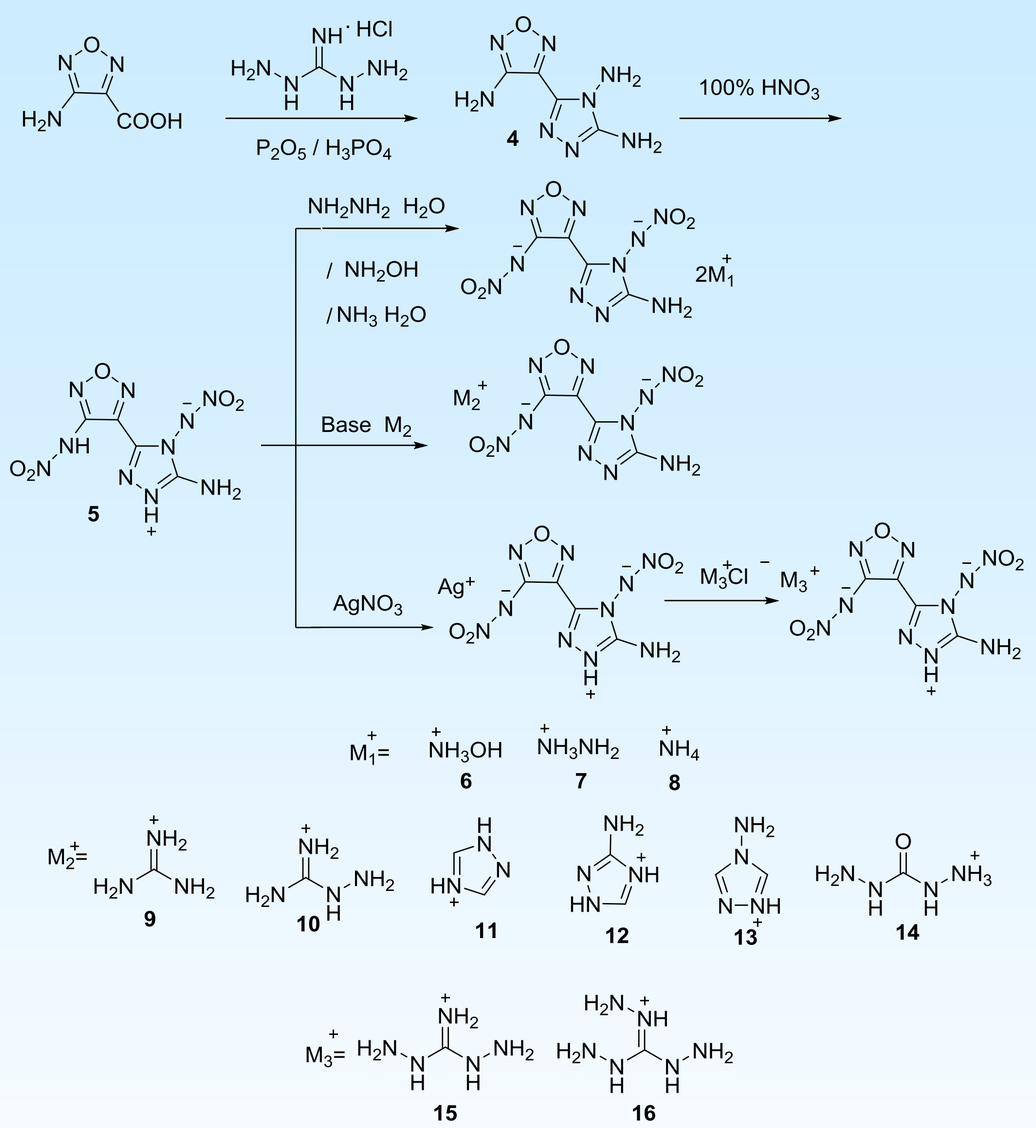
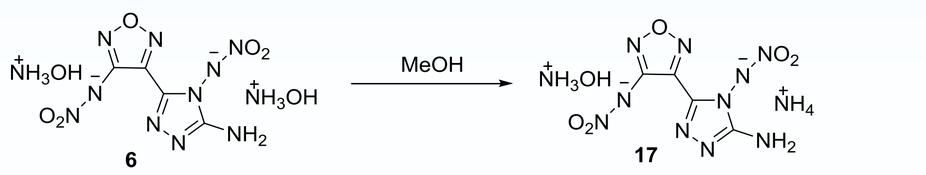
## Introduction

Several efficient ways to achieve the balance between energetic and sensitivity have been well-established: a) formation of energetic salts; b) layer-by-layer stacking; c) blending of energetic rings using alkyl bridges; d) 3D metal organic frameworks; e) cocrystallization; f) intramolecular hydrogen bonds. The nitrogen-rich energetic salts are the hottest topics and these salts with high energy and low sensitivity are important in energetic materials. As we know the introduction of amino groups has a positive effect resulting in an increase in detonation performance and safety. Herein, we report a series of energetic salts based on 3-nitramino-4-(4-nitramino-5-amino-1,2,4-triazol-3-yl)furazan with a system that comprises both nitro and amino groups. Hydroxylammonium salt has good thermal stability, high detonation performance and low sensitivity.

## Synthesis




**Scheme 2** Syntheses of 3-nitramino-4-(4- nitramino-5-amino-1, 2, 4-triazol-3-yl)furazan and nitrogen-rich salts of 3-nitramino-4-(4-nitramino-5-amino-1,2,4-triazol-3-yl)furazan under different conditions




**Scheme 3** Synthesis of Hydroxylammonium Ammonium 3-nitramino-4-(4-nitramino-5-amino-1,2, 4-triazol-3-yl)furazan

**Table 1** Properties of 5-17 and comparison with TATB, RDX and HMX

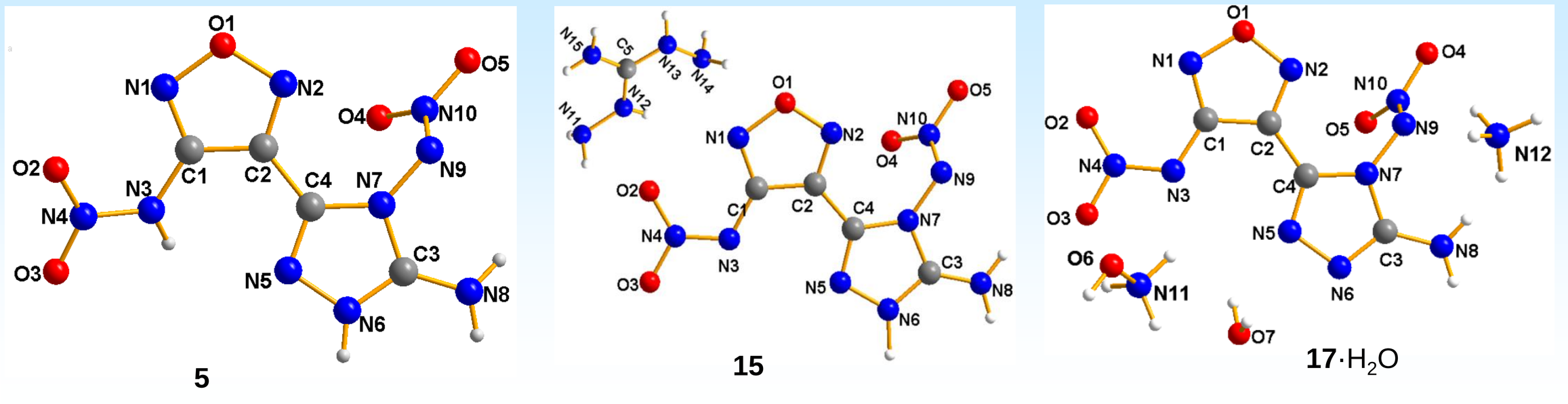
| compound | $T_m$ [a] [℃] | $T_d$ [b] [℃] | $\rho$ [c] [g cm$^{-3}$] | $\Delta H_f$ [d] [kJ mol$^{-1}$]/[kJ g$^{-1}$] | $D$ [e] [m s$^{-1}$] | $P$ [f] [GPa] | IS [g] [J] | FS [h] [N] |
|---|---|---|---|---|---|---|---|---|
| 5 | _ | 114 | 1.812 | 759.8/2.79 | 9091 | 36.5 | 35 | 360 |
| 6 | 69 | 184 | 1.767 | 733.7/2.08 | 9165 | 36.1 | 40 | 360 |
| 7 | _ | 222 | 1.732 | 957.9/2.85 | 9239 | 33.9 | 40 | 360 |
| 8 | _ | 208 | 1.727 | 591.5/1.93 | 8912 | 33.2 | >40 | >360 |
| 9 | _ | 204 | 1.701 | 729.5/2.20 | 8557 | 28.8 | >40 | >360 |
| 10 | 155 | 214 | 1.703 | 917.5/2.65 | 8749 | 30.2 | >40 | >360 |
| 11 | _ | 139 | 1.7 | 1035.5/3.03 | 8525 | 29.3 | >40 | >360 |
| 12 | _ | 208 | 1.698 | 1015/2.85 | 8466 | 28.3 | >40 | >360 |
| 13 | _ | 202 | 1.680 | 1133.5/3.18 | 8536 | 29.0 | >40 | >360 |
| 14 | 166 | 204 | 1.691 | 886.1/2.45 | 8514 | 39.1 | >40 | >360 |
| 15 | _ | 186 | 1.719 | 934.5/2.59 | 8732 | 30.2 | >40 | >360 |
| 16 | _ | 188 | 1.654 | 1041.1/2.77 | 8655 | 28.8 | >40 | >360 |
| 17 | _ | 184 | 1.741 | 632.4/1.96 | 8803 | 31.3 | >40 | >360 |
| TATB | _ | 360 | 1.930 | -137.5/-0.54 | 8114 | 31.2 | 50 | >360 |
| RDX | | 204 | 1.800 | 70.3/0.32 | 8795 | 34.9 | 7.4 | 120 |
| HMX | | 287 | 1.905 | 74.8/0.25 | 9144 | 39.5 | 7.4 | 120 |

[a] Melting point. [b] Decomposition temperature [c] Density measured using a gas pycnometer (25 ° C).[d]Heat of formation. [e] Calculated detonation velocity. [f] Calculated detonation pressure [g] Impact sensitivity. [h] Friction sensitivity.

## Physical and Chemical Properties

The decomposition temperatures of the salts ranged from 139 (**11**) to 222 ° C (**7**). Neutral compound has a low decomposition temperatures of 114° C . Hydrazinium salt 7 is the most thermally stable (222 °C). The calculated detonation velocities lie in the range between 8514 and 9239 m s-1 All compounds (**5-17**) possess good impact and friction sensitivities, which up to 35 J and 360 N, respectively. The most promising compound for industrial scale-up and practical use is the Hydrazinium salt **7**, which has acceptable density (1.732 g cm$^{-3}$), lower sensitivities (40 J, 360 N ), good detonation pressure (33.9 GPa) and ( 9239 m s$^{-1}$). The combination of exceedingly high performance properties, which are comparable to those of HMX.

## Crystal Structure




## Acknowledgement

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