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# Ag(I) Energetic Metal-Organic Framework Assembled with the Energetic Combination of Furazan and Tetrazole: Synthesis, Structure and Energetic Performance

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## Abstract

A novel Ag(I) energetic MOF  $[\text{Ag}_{16}(\text{BTFOF})_9]_n \cdot [2(\text{NH}_4)]_n$  (**1**) assembled by Ag(I) ion and furazan derivative, 4,4'-oxybis[3,3'-(1*H*-5-tetrazol)]furazan ( $\text{H}_2\text{BTFOF}$ ), was successfully synthesized and structurally characterized, featuring a three-dimensional porous structure incorporating ammonium cations. The thermal stability and energetic properties were determined, revealing that the 3D energetic MOF occupied outstanding insensitivity ( $\text{IS} > 40 \text{ J}$ ), ultrahigh detonation pressure ( $P$ ) of 65.29 GPa and detonation velocity ( $D$ ) of 11.81 km  $\text{cm}^{-3}$ . In addition, the self-accelerating decomposition temperature ( $T_{\text{SADT}}$ ) and critical temperature of thermal explosion ( $T_b$ ) were also discussed in detail. The finding exemplifies that the assembly strategy plays a decisive role in the density and energetic properties of MOF-based energetic materials.

**Key words:** Energetic materials / Furazan derivative / Detonation performance

## Introduction

Considerable development of energetic materials has been driven by pursuing the simultaneous need of low sensitivity and high heat of detonation, and great advancements have been achieved.<sup>[1-2]</sup> However, it is seeking the new generational energetic materials combined insensitivity and high heat of detonation that has still been challenging. At present, metal-organic frameworks (MOFs) have been paid close attention in the fields of coordination chemistry and material science because of their inherent structural stability, high mechanical strength and intriguing architectures. Based on the structural stability and energetic performance, constructing energetic MOFs with rigid structure and high heat of detonation have attracted much efforts to further investigate their potentially promising applications as new generational explosives.

In the past three years, abundant one-dimensional (1D), two-dimensional (2D) and three-dimensional (3D) energetic MOFs with wonderful energetic properties have been reported.<sup>[1, 3]</sup> As noticed above, nitrogen-rich heterocycle-based energetic compounds have been explored and reported widely, deriving from the significant advantages of nitrogen-rich heterocycle including diverse coordination modes, abundant inherent energetic N-N, N=N, C-N and C=N bonds and superior structural stability.<sup>[3]</sup> In this regard, new generation of energetic compounds with nitrogen-rich heterocycle and nitrogen-rich heterocycle derivatives as energy sources have been attracting continuous interest in the attempt to develop new energetic materials. Nevertheless,

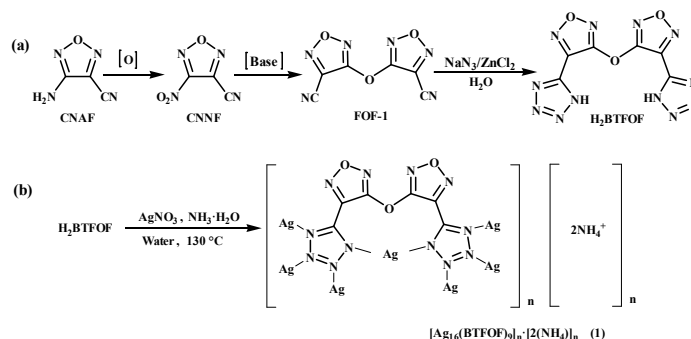
despite the light shed by these studies, taking the inherent structural stability and high mechanical strength of MOFs into consideration,<sup>[4]</sup> further study is expected to synthesize nitrogen-rich heterocycle-based energetic MOFs with excellent energetic properties.

Furazan ligands with high density, high positive heat of formation and good oxygen balance,<sup>[5]</sup> have been employed as the valuable energetic units to design and construct the unique class of energetic MOFs. However, based on the absence of an acidic proton, furazan ring fails to bond with metal ions and thus furazan-based energetic MOFs have received relatively little consideration.<sup>[6]</sup> In this perspective, furazan ring conjugates with nitrogen-rich heterocycles, such as tetrazole or triazole ring, which not only removes acidic proton, but also improves detonation properties.<sup>[7]</sup> As anticipated, energetic MOFs assembled by furazan derivatives and metal ions will possess the exhilarating energetic properties.

In our continuous research aiming at meeting the simultaneous requirements of high thermal stability and high heat of detonation by energetic units coordinating to metal ions,<sup>[8]</sup> it is shown that metal-containing 3D energetic MOFs have been the optimal candidates for new generation of energetic materials because of their tailored architectures and extraordinary energetic properties.<sup>[1(k),1(n), 8(f)]</sup>

Herein, a furazan derivative, 4,4'-oxybis[3,3'-(1H-5-tetrazol)]furazan (H<sub>2</sub>BTFOF) synthesized according to the refs. 7 (Scheme 1(a)), was selected to construct energetic MOFs with the following reasons: 1) The ligand possesses high nitrogen content (*N*% = 57.90), high density ( $\rho = 1.74 \text{ g cm}^{-3}$ ), and high thermal decomposition temperature ( $T_d = 240 \text{ }^\circ\text{C}$ ), which makes a great contribution to the energetic performance; 2) The furazan ring conjugating with tetrazole ring will be help to bond with metal ions to feature high-dimensional frameworks, resulting in high structural stability; 3) The predominant decomposition products are environmentally friendly. From the above, the energetic MOFs with furazan and tetrazole as energy sources, could be the potential high-energy-density materials (HEDM)<sup>[9]</sup>. In addition, taking the high densities and high heats of detonation into consideration, silver(I) ion with coordination diversity and flexibility was employed as the metal ion to prepare energetic MOFs with perfect energetic performance.<sup>[8e]</sup> As expected, an energetic Ag-based coordination polymers,  $[\text{Ag}_{16}(\text{BTFOF})_9]_n \cdot [2(\text{NH}_4)]_n$  (**1**), was successfully synthesized and fully characterized. Structural analysis reveals that compound **1** features a three-dimensional porous structure incorporating ammonium cations. The detailed

synthetic processes of H<sub>2</sub>BTFOF ligand are shown in Supporting Information. The thermal stability, energetic properties, the self-accelerating decomposition temperature ( $T_{\text{SADT}}$ ) and critical temperature of thermal explosion ( $T_b$ ) were also discussed in detail.



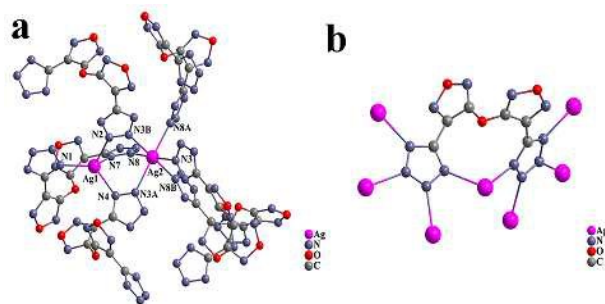
**Scheme 1.** (a) Synthesis of H<sub>2</sub>BTFOF; (b) Synthesis, coordination mode and formula for **1**.

## Results and discussion

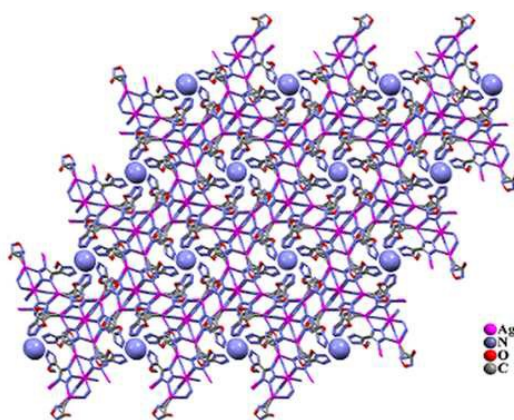
### Structural description

**Crystal Structure of 1.** Compound **1** crystallizes in hexagonal space group,  $P6_3/m$  ( $Z=1$ ) and shows a 3D porous MOF structure with channels incorporating ammonium cations. The calculated density ( $\rho$ ) is 1.997 g cm<sup>-3</sup>. In the asymmetric unit, there are sixteen crystallographically independent Ag(I) ions, nine BTFOF<sup>2-</sup> ligands and two ammonium cations. The Ag(I) ions show two kinds of configuration (Figure 1a). Ag1(I) ion is four-coordinated by four nitrogen atoms [Ag1–N1 = 2.265(7) Å, Ag1–N2 = 2.391(7) Å, Ag1–N4 = 2.331(6) Å and Ag1–N7 = 2.342(8) Å] from four different BTFOF<sup>2-</sup> ligands, forming a tetrahedral geometry. The N–Ag–N bond angles fall into the range of 96.0(3)°–127.1(3)°. While Ag2(I) ion is hexa-coordinated by six nitrogen atoms in an octahedral coordination environment, in which the equatorial plan is defined by four nitrogen atoms (N8, N3, N3B and N8B) from four different BTFOF<sup>2-</sup> ligands [Ag2–N3 = 2.481(6) Å, Ag2–N8 = 2.457(8) Å] and the axial position is occupied by another two nitrogen atoms (N3A and N8A) from another two different BTFOF<sup>2-</sup> ligands. The average of N–Ag–N bond angles is in the range of 87.5(3)°–177.8(3)° (Table S1). And the characteristic binuclear Ag(I) secondary building units (SBUs) were formed obviously as shown in Figure 1b. It is noteworthy that all of nitrogen atoms of two tetrazole rings from BTFOF<sup>2-</sup> ligands participate in coordinating with seven Ag(I) ions, adopting the bidentate chelating and bridging modes. Obviously, the saturated

coordination modes of tetrazole rings certainly have an influence on the thermal stability and sensitivity of framework. In this way, the 3D porous framework structure is constructed by the interlinkages between binuclear SBUs and fantastic BTFOF<sup>2-</sup> ligands, with channels incorporating the ammonium cations (Figure 2). The ammonium cations were further identified and detected through Nessler's Reagent,<sup>[10]</sup> in Supporting Information.



**Figure 1.** (a) Coordination environment of Ag(I) ions; (b) coordination model of ligand (Hydrogen atoms are omitted for clarity).



**Figure 2.** 3D porous framework of **1** with channels incorporating ammonium cations. (Hydrogen atoms are omitted for clarity)

### Thermal decomposition, non-isothermal kinetics analysis and detonation property

**Thermal decomposition of 1.** The TG and DSC curves with the linear heating rate of 10 °C min<sup>-1</sup> under N<sub>2</sub> atmosphere are plotted to explore the thermal decomposition behavior of **1**. As shown in Figure S2, TG curve reveals that the sudden weight loss is observed from 225 °C to 325 °C resulting from the rapid release of energy. Correspondingly, DSC curve shows one main intense

exothermic process at a range between 220 °C to 260 °C with the peak temperature of 258.1 °C (Figure S3), while before that, **1** undergoes the remove of uncoordinated ammonium cations.

### Non-isothermal kinetics analysis

To estimate the thermokinetics stability of **1** in the exothermic decomposition process, DSC experiments were carried out at the heating rates of 2, 5, 8 and 10 °C min<sup>-1</sup> (Figure S3). The basic data for the main exothermic decomposition processes of **1**, including the beginning temperature ( $T_0/^\circ\text{C}$ ), extrapolated onset temperature ( $T_e/^\circ\text{C}$ ), and peak temperature ( $T_p/^\circ\text{C}$ ) at the different heating rates ( $\beta/^\circ\text{C min}^{-1}$ ), are listed in Table 1. Based on the above, Kissinger's method<sup>[11(a)]</sup> and Ozawa-Doyle's method<sup>[11(b),11(c)]</sup> were used to obtain thermokinetics parameters (the apparent activation energy ( $E$ ) and pre-exponential constant ( $A$ )), where the key equations are displayed in Supporting Information. Thus, the Arrhenius equation can be expressed as:  $\ln k = 58.8524 - 275.04 \times 10^3 / (RT)$ , which can be used to estimate the reaction rate of the thermal decomposition process of compound **1**.

**Table 1.** The thermokinetics parameters of the exothermic decomposition process.

| $\beta$<br>(°C min <sup>-1</sup> ) | $T_0$<br>(°C) | $T_e$<br>(°C) | $T_p$<br>(°C) | $T_{00}$<br>(°C) | $T_{e0}$<br>(°C) | $T_{p0}$<br>(°C) | $E_k$<br>(kJ mol <sup>-1</sup> ) | $\log A$<br>(s <sup>-1</sup> ) | $R_k$  | $E_o$<br>(kJ mol <sup>-1</sup> ) | $R_o$  |
|------------------------------------|---------------|---------------|---------------|------------------|------------------|------------------|----------------------------------|--------------------------------|--------|----------------------------------|--------|
| 2                                  | 207.7         | 234.2         | 245.4         |                  |                  |                  |                                  |                                |        |                                  |        |
| 5                                  | 213.1         | 242.5         | 252.7         |                  |                  |                  |                                  |                                |        |                                  |        |
| 8                                  | 217.2         | 247.3         | 256.7         | 204.3            | 228.2            | 239.1            | 277.70                           | 25.59                          | 0.9995 | 272.37                           | 0.9996 |
| 10                                 | 220.8         | 251.0         | 258.1         |                  |                  |                  |                                  |                                |        |                                  |        |

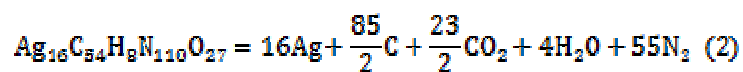
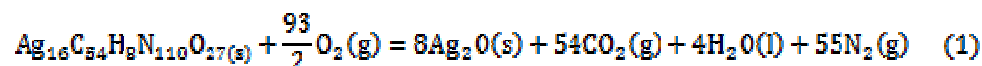
Significantly, the values ( $T_{00}$ ,  $T_{e0}$  and  $T_{p0}$ ) of the initial temperature point corresponding to  $\beta \rightarrow 0$  are obtained and the detailed calculations are listed in Supporting Information.<sup>[12]</sup> Especially, two considerably important parameters, the self-accelerating decomposition temperature ( $T_{\text{SADT}}$ ) and critical temperature of thermal explosion ( $T_b$ ), are necessary for energetic compounds in order to ensure the safety during storage and operations. The  $T_{\text{SADT}}$  and  $T_b$  are respectively 228.2 and 241.2 °C, revealing more perfect thermal stability in the exothermic decomposition stage than common explosives and the known energetic compounds, such as FOX-7 (206.0 and 207.1 °C),<sup>[13]</sup> [Cu(en)<sub>2</sub>H<sub>2</sub>O](FOX-7)<sub>2</sub>·H<sub>2</sub>O (163.3 and 174.8 °C),<sup>[1(g)]</sup> TNPDU (206.29 and 219.54 °C),<sup>[12(b)]</sup> [Cu(NH<sub>3</sub>)<sub>4</sub>](DNANT)<sub>2</sub> (217.9 and 221.0 °C).<sup>[12(a)]</sup> Additionally, the entropies of activation ( $\Delta S^\ddagger$ ),

enthalpies of activation ( $\Delta H^\ddagger$ ), and free energies of activation ( $\Delta G^\ddagger$ ) of **1** can also be calculated respectively as  $240.49 \text{ J mol}^{-1} \text{ K}^{-1}$ ,  $270.78 \text{ kJ mol}^{-1}$ ,  $147.59 \text{ kJ mol}^{-1}$ , which reveal that **1** is thermo-kinetically inert and the exothermic decomposition reaction of **1** would occur if on heating.

### Detonation property

For safety testing, the impact and friction sensitivities of **1** were investigated and the test methods of sensitivities are described in Supporting Information. The collected data were summarized in Table 2. The impact sensitivity of **1** is 40 J, which is lower than that of TNT and those reported energetic coordination polymers. No friction sensitivity is observed up to 360 N for **1**. Compared with the energetic MOFs reported previously, **1** is insensitive to external stimuli. It is most probable that the stable and insensitivity for **1** are attributed to the impacted extended structure produced by metal ions coordination with the ligands.

The constant-volume combustion energy of **1** was determined with a precise rotating-bomb calorimeter (RBC-type II).<sup>[17]</sup> The main experimental procedures had been described previously and shown in Supporting Information in detail.<sup>[8(e)]</sup> The experimental constant volume combustion energies ( $\Delta_c U$ ) of **1** is  $(-7505.04 \pm 1.43) \text{ J g}^{-1}$ , from which the standard molar combustion enthalpy ( $\Delta_c H_m^0$ ) of **1** can be calculated as being  $(-32534.17 \pm 6.23) \text{ kJ mol}^{-1}$ . The combustion reaction equation is listed as equation (1):



Based on the calculated enthalpies of combustion and known enthalpies of formation of the combustion products<sup>[14-15]</sup> determined experimentally,  $\text{Ag}_2\text{O}(\text{s})$ ,  $\Delta_c H_m^0(\text{Ag}_2\text{O}, \text{s}) = (-31) \text{ kJ mol}^{-1}$ ,  $\text{CO}_2(\text{g})$ ,  $\Delta_c H_m^0(\text{CO}_2, \text{g}) = (-393.51 \pm 0.13) \text{ kJ mol}^{-1}$ ,  $\text{H}_2\text{O}(\text{l})$ ,  $\Delta_c H_m^0(\text{H}_2\text{O}, \text{l}) = (-285.830 \pm 0.040) \text{ kJ mol}^{-1}$ , the standard enthalpy of formation of **1**,  $\Delta_f H_m^0$ , was back-calculated from the combustion equation as  $(9893.31 \pm 8.45) \text{ kJ mol}^{-1}$ .

The drastic processes of decomposition and high standard molar enthalpy of formation demonstrate the potential detonation properties of **1**. Based on the largest exothermic principle



proposed by Kamlet-Jacobs,<sup>[14-15]</sup> a new empirical method,<sup>[16]</sup> was selected to investigate the energetic performances of metal-containing explosives without depending on sophisticated computer programs, where the important equations are listed in the Supporting Information. The method used the hypothesis of BKW equation and arbitrary theory of the K-J method, which could be applied to perform the detonation performances of metal compounds containing special elements such as Cd and Ag. Based on the detonation reaction equation (2), the heat of detonation value ( $Q/J\text{ g}^{-1}$ ), detonation pressure ( $P$ ) and detonation velocity ( $D$ ) of **1** was calculated respectively as  $0.8535\text{ kcal g}^{-1}$ ,  $65.29\text{ GPa}$  and  $11.81\text{ km s}^{-1}$ , in which  $D$  and  $P$  show the highest values among the known energetic MOFs and common explosive compounds (Table 2).

**Table 2.** Calculated parameters used in the detonation reactions.

| Compounds                 | $\rho^a/\text{g cm}^{-3}$ | $N^b/\%$ | $T_{\text{dec}}^c/\text{°C}$ | $Q^d/\text{kcal g}^{-1}$ | $D^e/\text{km s}^{-1}$ | $P^f/\text{GPa}$ | $IS^g/\text{J}$ | $FS^h/\text{N}$ |
|---------------------------|---------------------------|----------|------------------------------|--------------------------|------------------------|------------------|-----------------|-----------------|
| <b>1</b>                  | 1.997                     | 35.36    | 225                          | 0.8535                   | 11.81                  | 65.29            | >40             | >360            |
| RDX <sup>[1d]</sup>       | 1.806                     | 37.80    | 210                          | 1.386                    | 8.600                  | 33.92            | 7.5             | 120             |
| TNT <sup>[1d]</sup>       | 1.654                     | 18.50    | 244                          | 0.897                    | 7.178                  | 20.50            | 15              | 353             |
| HMX <sup>[1d]</sup>       | 1.950                     | 37.80    | 280                          | 1.320                    | 8.900                  | 38.39            | 7.4             | —               |
| ATRZ-1 <sup>[1f]</sup>    | 1.680                     | 53.35    | 243                          | 3.618                    | 9.160                  | 35.68            | 22.5            | —               |
| ATRZ-2 <sup>[1f]</sup>    | 2.16                      | 43.76    | 257                          | 1.381                    | 7.773                  | 29.70            | 30              | —               |
| AgNT <sup>[8e]</sup>      | 3.121                     | 25.35    | 305                          | 1.163                    | 7.938                  | 36.47            | >40             | >360            |
| PbTT <sup>[11]</sup>      | 2.519                     | 39.40    | 340                          | 1.359                    | 7.715                  | 31.57            | >40             | >360            |
| CHP <sup>[1d]</sup>       | 1.948                     | 14.71    | 194                          | 1.250                    | 8.225                  | 31.73            | 0.5             | —               |
| NHP <sup>[1d]</sup>       | 1.983                     | 33.49    | 220                          | 1.370                    | 9.184                  | 39.69            | —               | —               |
| CHHP <sup>[1e]</sup>      | 2.000                     | 23.58    | 231                          | 0.750                    | 6.205                  | 17.96            | 0.8             | —               |
| ZnHHP <sup>[1d]</sup>     | 2.117                     | 23.61    | 293                          | 0.700                    | 7.016                  | 23.58            | —               | —               |
| Cu(Htztr) <sup>[2f]</sup> | 2.435                     | 49.08    | 355                          | 3.9582                   | 10.40                  | 56.48            | 32              | >360            |
| CuMAN <sup>[2g]</sup>     | 2.096                     | 47.55    | 242                          | 2.473                    | 8.47                   | 35.32            | —               | —               |

<sup>a</sup> From X-ray diffraction. <sup>b</sup> Nitrogen content. <sup>c</sup> Decomposition temperature. <sup>d</sup> The heat of detonation. <sup>e</sup> Detonation velocity. <sup>f</sup> Detonation pressure. <sup>g</sup> Impact sensitivity. <sup>h</sup> Friction sensitivity. RDX = Hexogen; TNT = Trinitrotoluene; HMX = Octogen; ATRZ-1 = Copper 4,4'-azo-1,2,4-triazole; ATRZ-2 = Silver 4,4'-azo-1,2,4-triazole; AgNTZ = Silver 3-nitro-1H-1,2,4-triazole; PbTT = Lead 3-(tetrazol-5-yl) triazole; CHP = Cobalt hydrazine perchlorate; NHP = Nickel hydrazine perchlorate; CHHP = Cobalt hydrazine hydrazinecarboxylate perchlorate; ZnHHP = Zinc hydrazine hydrazinecarboxylate perchlorate; Cu(Htztr) = Copper 3-(tetrazol-5-yl) triazole; CuMAN = Copper melamine azide.

Obviously, the furazan derivative, 4,4'-oxybis[3,3'-(1H-5-tetrazol)]furazan ( $H_2BTFOF$ ), including tetrazole and furazan groups, not only is propitious to assemble with metal ions for the construction of the energetic MOFs with high density, good thermal stability and low sensitivity, but also is in favour of improving detonation properties, especially detonation pressure ( $P$ ) and detonation velocity ( $D$ ). Compared with common explosives RDX, TNT and HMX, compound **1** occupies the relatively high density. Additionally, based on the inherently structural stability of 3D MOFs, compound **1** shows the good thermal stability at 225 °C and the superior insensitivities, which could be potentially employed in the field of energetic materials. Unfortunately, comparison with the known energetic MOFs, compound **1** exhibits the relatively low heat of detonation probably due to the excessive metal ions in the framework structure. Thus, it would be still great challengeable for construction of energetic MOFs to achieve the largest energetic density with the largest denotation energy.<sup>[8(f)]</sup>

## Conclusions

In conclusion, a novel energetic MOF has been successfully synthesized based on the furazan derivative, 4,4'-oxybis[3,3'-(1H-5-tetrazol)]furazan ( $H_2BTFOF$ ), exhibiting 3D porous framework structure with channels incorporating ammonium cations. The 3D framework structure of **1** displays high nitrogen content (N% = 35.36%), the high density (1.997 g cm<sup>-3</sup>), good thermal stability (225 °C), low sensitivity and superior detonation performance. The thermokinetic investigation for **1** shows the self-accelerating decomposition temperature ( $T_{SADT}$  = 228.2 °C) and critical temperature of thermal explosion ( $T_b$  = 241.2 °C). This study enriches 3D MOFs-based energetic materials using furazan derivative and examples the assembly strategy for constructing new-generation high-performance primary explosives.

## Experimental

Caution: The  $H_2BTFOF$  and the title compound are great hazardous compounds and may explode under certain outside conditions. Although there is no difficulty in our experiment, the compound should be handled in the pyrex glass vessels and proper safety precautions such as safety glasses, face shields, and plastic spatulas, should be taken, particularly when they are prepared on a large scale.

## Materials and instruments

All reagents were purchased commercially and used without further purification. TG and DSC

analysis was conducted on a Netzsch STA 449C instrument with the linear heating rate of 10 °C min<sup>-1</sup> under N<sub>2</sub> atmosphere. Powder X-ray diffraction (PXRD) data were recorded on a Bruker D8 ADVANCE X-ray powder diffractometer (Cu K $\alpha$ , 1.5418 Å). The sensitivity to impact stimuli was determined by the standard staircase method applying fall hammer apparatus with a 2 kg drop weight. The friction sensitivity was determined on a Julius Peter's apparatus. The constant-volume combustion energy of the compound was determined with an RBC-type II rotating-bomb calorimeter.<sup>[17]</sup>

### Synthetic procedures

[Ag<sub>16</sub>(BTFOF)<sub>9</sub>]<sub>n</sub>·[2(NH<sub>4</sub>)]<sub>n</sub> (**1**). In experiment, an attempt to synthesize **1** through one-step hydrothermal reaction succeeded (Scheme 1(b)). A mixture of AgNO<sub>3</sub> (0.0510 g, 0.3 mmol), H<sub>2</sub>BTFOF (0.0145 g, 0.5 mmol) and NH<sub>3</sub>·H<sub>2</sub>O (60  $\mu$ L) in H<sub>2</sub>O (6 mL) was sealed in a 10 mL Teflon-lined stainless autoclave and heated at 130 °C under autogenous pressure for 3 days, then cooled at the rate of 5 °C h<sup>-1</sup> to room temperature, leading to a 3D insensitive energetic MOF (N = 35.36 %, IS > 40 J) with channels incorporating ammonium cations, [Ag<sub>16</sub>(BTFOF)<sub>9</sub>]<sub>n</sub>·[2(NH<sub>4</sub>)]<sub>n</sub> (**1**). Powder X-ray diffraction (PXRD) measurements support its stability in air atmosphere and high phase purity (Figure S1).

### X-ray crystallography

The single crystal X-ray experiment was performed on a Rigaku SCX mini CCD diffractometer equipped with graphite-monochromatized Mo K $\alpha$  radiation ( $\lambda = 0.71073$  Å) using  $\omega$  and  $\phi$  scan mode. The data integration and reduction were processed with SAINT software. Absorption correction based on multiscan was performed using the SADABS program.<sup>[18]</sup> The structures were solved by the direct method using SHELXTL and refined by means of full-matrix least-squares procedures on  $F^2$  with SHELXL-97 program.<sup>[19]</sup> All non hydrogen atoms were refined anisotropically. Other details of crystal data, data collection parameters, and refinement statistics are given in Table 3. The selected bond lengths and angles are listed in Table S1.

**Table 3.** Crystal data and structure refinement details for the compound **1**.

| Compound          | <b>1</b>             |
|-------------------|----------------------|
| Empirical formula | C54 H8 Ag16 N110 O27 |
| Formula weight    | 4355.62              |

|  |                |                 |
|--|----------------|-----------------|
| Temperature                            | 293(2) K       |                 |
| Crystal system                         | Hexagonal      |                 |
| space group                            | $P6_3/m$       |                 |
| $a$ (Å)                                | 15.3657(4)     |                 |
| $b$ (Å)                                | 15.3657(4)     |                 |
| $c$ (Å)                                | 17.7122(5)     |                 |
| $\alpha$ (°)                           | 90             |                 |
| $\beta$ (°)                            | 90             |                 |
| $\gamma$ (°)                           | 120            |                 |
| $V$ (Å <sup>3</sup> )                  | 3621.66(17)    |                 |
| $\rho$ /g cm <sup>-3</sup>             | 1.997          |                 |
| Z                                      | 1              |                 |
| F(000)                                 | 2070           |                 |
| Goodness-of-fit on F <sup>2</sup>      | 1.047          |                 |
| Final $R$ indices [ $I > 2\sigma(I)$ ] | $R_1 = 0.0524$ | $wR_2 = 0.1395$ |
| $R$ indices (all data)                 | $R_1 = 0.0605$ | $wR_2 = 0.1447$ |
| CCDC                                   | 1417165        |                 |

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### Supporting Information

Electronic Supplementary Information (ESI) available: The CIF files give crystallographic data for compound **1**. Details of chemicals and equipments, preparation for **1**, PXRD curve, TG and DSC curves, the detection of the ammonium cations for **1**, nonisothermal kinetic analysis, sensitivity test, oxygen bomb calorimetry, heat of detonation, Table S1 and Figure S1-S3 see in supporting information

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## Graphical Abstract

### Synopsis:

The novel 3D Ag(I) energetic MOF assembled with furazan derivative (4,4'-oxybis[3,3'-(1*H*-5-tetrazol)]furazan) shows low sensitivity, good thermostability and ultrahigh detonation pressure and detonation velocity.

