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## **Electronic Supplementary Information**

### Novel 3D cesium(I) based EMOF of nitrogen-rich triazole derivatives as

### a "green" orange-light pyrotechnics

Tingwei Wang,<sup>a,b</sup> Jinyang Zhou,<sup>b</sup> Qi Zhang,<sup>\*b</sup> Lin Zhang,<sup>a</sup> Shunguan Zhu,<sup>\*a</sup> and Yan Li<sup>\*a</sup>

<sup>a</sup> School of Chemical Engineering, Nanjing University of Science and Technology, Xiaolingwei 200, Nanjing 210094, P. R. China

<sup>b</sup> Institute of Chemical Materials, China Academy of Engineering Physics, Sichuan, Mianyang 621900, P. R. China

Corresponding authors' emails: : jackzhang531@caep.cn (Q.Z.); zhusg@mail.njust.edu.cn (S. Z.); yanli@njust.edu.cn (Y. L.)

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## **Experimental Section**

#### **Materials and Equipments**

During the course of the experiment, the reagents used (analytical grade) were purchased from the reagents factory and used without further purification. Single crystal X-ray diffraction data was collected by using Rigaku supernova single X-ray diffractometer area detector ( $Mo_{Ka'}$ , 0.71073 Å). The thermal behavior of the compound was analyzed by a differential scanning calorimeter (TGA / DSC2, METTLER TOLEDO STAR system) under the conditions of a heating rate of 5 K·min-1 and a gas atmosphere of N2. Infrared (IR) spectra were measured on a Nicolet islo spectrometer (Equipped with KBr discs) with a measurement range of 4000 - 400 cm <sup>-1</sup>. The mechanical sensitivities (including impact sensitivity and friction sensitivity) of the material were determined by the standard step method of the drop weight device with a BAM DFH-10 device with a weight drop of 5 kg. The constant pressure reaction heat is measured by an oxygen bomber (IKA@ C5000). The wavelength and purity of the pyrophoric light was tested using the SGX-III Transient Fast Spectrophotometric System.

#### Synthesis of N-(5'-amino-1H,1'H-[3,3'-bi(1,2,4-triazol)]-5-yl)nitramide (HABTNA)

Add 3-amino-1H-1,2,4-triazole-5-carbohydrazide (ATCA) 2.1 g (14.8 mmol) to a 100 mL threenecked flask and suspend in 20 mL of deionized water. 4.35 g (water content 50%, 30 mmol) MNNG was suspended in 20 mL of methanol and slowly added dropwise to the reaction solution. The reaction solution is heated to 80 °C and refluxed for 2 h. After the reaction is completed, the temperature is cooled to below 50 °C, and an aqueous KOH solution (KOH/H<sub>2</sub>O = 2.8 g/15 mL) is slowly added, and the temperature is raised to 80 °C for 3 h. After the reaction was completed, it was cooled to room temperature, and the pH was adjusted to 4 with HNO<sub>3</sub>. A yellow precipitate was obtained by suction filtration, washed twice with anhydrous ethanol and dried to give a yellow solid (yield: 93%). IR (KBr,  $\nu$ /cm<sup>-1</sup>): 3206 (m), 2957 (m), 2767 (w), 1698 (s), 1510 (m), 1314 (m), 1252 (w), 1229 (w), 1076 (s), 1038 (m), 850 (w), 974 (s), 767 (s),710 (s); MS (ESI), *m/z*: 209.9 [C<sub>4</sub>H<sub>4</sub>N<sub>9</sub>O<sub>2</sub><sup>-</sup>]; <sup>13</sup>C NMR (125 MHz, D<sub>2</sub>O/NaOH-*d*<sub>2</sub>, 25 °C)  $\delta$  :161.9, 163.08, 154.5, 155.32.

#### Synthesis of the EMOF 1

0.211 g (1 mmol) of the substance 2 was suspended in distilled water at 80 ° C, and the CsOH solution (0.1 M) was slowly added dropwise until the reaction solution became clear. Waiting for the reaction solution to cool naturally, and the water is slowly volatilized, the orange-red crystal of the substance 3 can be obtained (yield: 64%). IR (KBr,  $\nu$ /cm<sup>-1</sup>): 3469(m), 3407(m), 3312(m), 3155(m), 1647(m), 1621(m), 1582(m), 1518(s), 1452(s), 1385(s), 1322(s), 1247(s), 1147(m), 1068(s), 972(s), 855(m), 762(s), 710(m); elemental analysis (%) calcd for C<sub>4</sub>H<sub>6</sub>N<sub>9</sub>O<sub>3</sub>Cs (M= 361.09 g mol<sup>-1</sup>): C 13.29, H 1.66, N 34.89; found C 13.41, H 1.71, N 34.91.

#### **Thermal analysis**

The melting temperature or decomposition temperature of the complex (about 0.8 mg sample) were determined by thermogravimetric and scanning calorimetry (TG-DSC) at a heating rate of 10  $^{\circ}$ C·min <sup>-1</sup> under a N<sub>2</sub> atmosphere.

#### **Oxygen bomb calorimetry**

The standard molar combustion enthalpy  $(\Delta_C H^{\theta}_m)$  can be obtained from the constant pressure reaction heat  $(\Delta_C U)$  according to the **equation 1**. According to the principle of Hess' law, the standard molar generation enthalpy  $(\Delta_f H^{\theta}_m)$ can be obtained based on the **equation 2 and 3**. **Equation 2** represents the complete combustion reaction equation for MOFs. [CO<sub>2</sub>(g):-393.51 kJ·mol<sup>-1</sup>; Cs<sub>2</sub>O(s):-345.77 kJ·mol<sup>-1</sup>; H<sub>2</sub>O(l):-285.85 kJ·mol<sup>-1</sup>]

$$\Delta_C H^{\theta}{}_m = \Delta_C U + \Delta n R T \tag{1}$$

 $\Delta_n = n_g$ (products)- $n_g$ (reactants), ( $n_g$  is the sum of the total moles of gas in the product or reactant,  $R = 8.314 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$ , T = 298.15 K)

$$C_{4}H_{6}N_{9}O_{3}Cs(s) + 17 / 4O_{2}(g) = 4CO_{2}(g) + 1 / 2Cs_{2}O(s) + 3H_{2}O(l) + 3N_{2}(g)$$
(2)

$$\Delta_{\rm f} H^{\theta}_{\rm m}(\text{compound}) = \sum \Delta_{f} H^{\theta}_{\rm m}(\text{products}) - \Delta_{c} H^{\theta}_{\rm m}(\text{compound})$$
(3)

The various detonation characteristics of the ECPs were predicted using the modified Kamlet-Jacbos (K-J) ( eq 4-6) equations which is a commonly used equation for predicting the detonation velocity and pressure of high energy composites. According to the parameters required in Equation 1-3, the obtained data is accurately brought into the formula, and the detonation parameters of the ECPs can be obtained.

$$D = 1.01 (NM^{1/2}Q^{1/2})^{1/2} (1+1.30\rho)$$
(4)

$$P = 1.55 \rho^2 N M^{1/2} Q^{1/2} \tag{5}$$

$$Q = \frac{-[\Delta H_f (\text{detonation production}) - \Delta H_f (\text{explosive})]}{\text{formula weight of explosive}}$$
(6)

D: detonation velocity , km·s<sup>-1</sup>); P: detonation pressure, GPa;  $\rho$ : density, g·cm<sup>-3</sup>;  $\Delta H_{f}$ : heat of formation, kJ·mol<sup>-1</sup>); Q: heat of detonation, J·g<sup>-1</sup>); N: moles of detonation gases per gram of explosive, mol·g<sup>-1</sup>); M: average molecular weight of gases, g·mol<sup>-1</sup>)

#### Producing and photographing of pyrotechnic agents

Weigh compound 1, Al powder and ADN accurately according to the ratio, which are 500 mg, 100 mg and 380 mg, respectively. Place them in a mortar and mix carefully. The 20 mg of epoxy binder was dissolved in 10 ml of acetone and slowly dripped into the mixed powder. Mix all kinds of materials evenly and place them in a fume hood to dry naturally. The control group also weighs the individual component materials in proportion, and the preparation method is exactly the same as that described above.

Approximately 100 mg of the pyrotechnic agents was placed in an aluminum crucible having a diameter of 1 cm. Hang the crucible at an appropriate height and use an alcohol lamp to heat it and ignite the pyrotechnic agent. Use the camera to record the color of the flaming .

#### Flame test

Weigh about 400 mg of pyrotechnic agent and place it in an open evaporating dish. The wavelength of light was measured while igniting the drug using a nitrocellulose sheet. The control group is first measured and the obtained data is used as a blank control. Then measure the data of

the experimental group. Using the data obtained by the control group, subtract the blank group data to get the most realistic wavelength of light.

## Supplementary Figures S1-S5



Figure S1 <sup>13</sup>C NMR spectra of ATCA.



Figure S2 <sup>13</sup>C NMR spectra of HABTNA.



Figure S3 Status of EMOF 1 before (a) and after (b) hygroscopic test.



Figure S4 The images of the burning of the white flame.



Figure S5 Comparison of single crystal and powder X-ray diffraction of EMOF 1.

# Supplementary Table S1

Table S1	Crystallogra	ohic data	for	EMOF	1
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Formula	$C_4H_6CsN_9O_3$		
<i>M</i> <sub>w</sub> [g mol <sup>-1</sup> ]	361.09		
Crystal size [mm <sup>3</sup> ]	0.220 x 0.200 x 0.180		
Crystal system	Monoclinic		
Space group	P2 <sub>1</sub> /c		
unit call dimensions	a=7.09549(18)Å,b=10.8347(3)Å,c[Å]=12.9313(3)Å		
	α[Å]=90, <i>β</i> [Å]=89.883(2),γ[Å]=90		
<i>V</i> [[Å <sup>3</sup> ]	994.12(4)		
Ζ	4		
$\rho_{calc}[g \text{ cm}^{-3}]$	2.413		
μ[mm <sup>-1</sup> ]	3.743		
F(000)	688.0		
Data/restraints/parameters	2497 / 0 / 163		
GOF on F <sup>2</sup>	1.026		
CCDC			