

## Supporting Information

*for*

### A terbium(III)-organic framework for highly selective sensing of cytidine triphosphate

Xi Juan Zhao, Rong Xing He and Yuan Fang Li\*

Education Ministry Key Laboratory on Luminescence and Real-Time Analysis, School of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715, China. E-mail: [liyf@swu.edu.cn](mailto:liyf@swu.edu.cn), Tel: (+86) 23 68254659, Fax: (+86) 23 68367257.

#### 1. Materials and methods

**1.1 Materials.** Tb(NO<sub>3</sub>)<sub>3</sub>·5H<sub>2</sub>O, Eu(NO<sub>3</sub>)<sub>3</sub>·5H<sub>2</sub>O, 2, 3-pyrazinedicarboxylic acid and cytidine were purchased from Aldrich. Adenosine 5'-triphosphate disodium salt (ATP), cytidine 5'-triphosphate disodium salt hydrate (CTP), uridine 5'-triphosphate trisodium salt hydrate (UTP), guanosine 5'-triphosphate disodium salt hydrate (GTP), Cytidine 5'-monophosphate disodium salt (CMP), and cytosine were all purchased from Sigma. The other inorganic salts were obtained from commercial sources in China. [Tb<sub>2</sub>(2,3-pzdc)<sub>2</sub>(ox)(H<sub>2</sub>O)<sub>2</sub>]<sub>n</sub> and [Eu<sub>2</sub>(2,3-pzdc)<sub>2</sub>(ox)(H<sub>2</sub>O)<sub>2</sub>]<sub>n</sub> were synthesized according to the reported procedures.<sup>1</sup>

**1.2 Methods.** Powder X-ray diffraction patterns were collected on an XD-3 X-ray diffractometer (Beijing, China) using Cu K $\alpha$  radiation ( $\lambda = 1.5406 \text{ \AA}$ ). The IR spectra were obtained as KBr pellets on Shimadzu 8300 FTIR spectrophotometer. The scanning electron microscope (SEM) images were observed with a Hitachi S-4800 scanning electron microscope (Tokyo, Japan) operating at 30.0 kV. UV-vis spectra were measured on a U-3010 spectrophotometer, and the fluorescence spectra were measured on an F-4600 spectrophotometer. <sup>31</sup>P NMR spectra were measured with AVANCE AV-300 (BRUKER, Swiss). N<sub>2</sub> adsorption-desorption isotherms of the samples were obtained on a surface area analyzer (Quantachrome Autosorb-1, USA) at 77 K. The samples were outgassed at room temperature under a pressure of 10<sup>-3</sup> Torr for at least 5 h. Raman spectra were taken with HORIBA LabRAM HR (785 nm).

## 2. Supporting figures

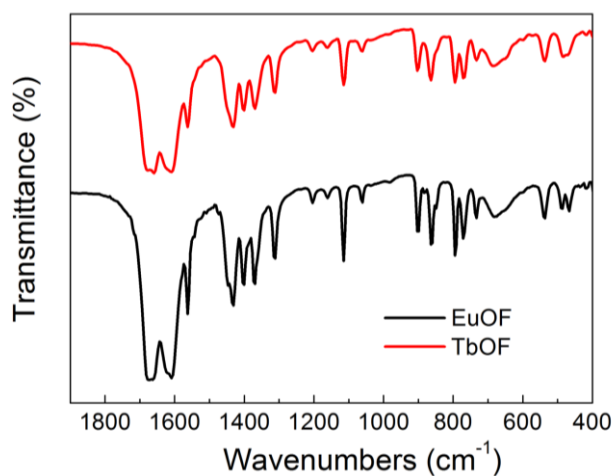


Figure S1. The IR spectra of  $[\text{Ln}_2(2,3\text{-pzdc})_2(\text{ox})(\text{H}_2\text{O})_2]_n$  ( $\text{Ln} = \text{Tb}, \text{Eu}$ ).

$[\text{Tb}_2(2,3\text{-pzdc})_2(\text{ox})(\text{H}_2\text{O})_2]_n$  (KBr,  $\text{cm}^{-1}$ ): 1679, 1658, 1620, and 1608 ( $\nu_{\text{as}}\text{CO}_2^-$ ), 1562 (s), 1448 (s), 1431 (s), 1401 (s), 1369, and 1311 (s-m,  $\nu_{\text{s}}\text{CO}_2^-$ ).

$[\text{Eu}_2(2,3\text{-pzdc})_2(\text{ox})(\text{H}_2\text{O})_2]_n$  (KBr,  $\text{cm}^{-1}$ ): 1680, 1660, 1620, and 1606 ( $\nu_{\text{as}}\text{CO}_2^-$ ), 1562 (s), 1446 (s), 1438 (s), 1401 (s), 1369, and 1311 (s-m,  $\nu_{\text{s}}\text{CO}_2^-$ ).

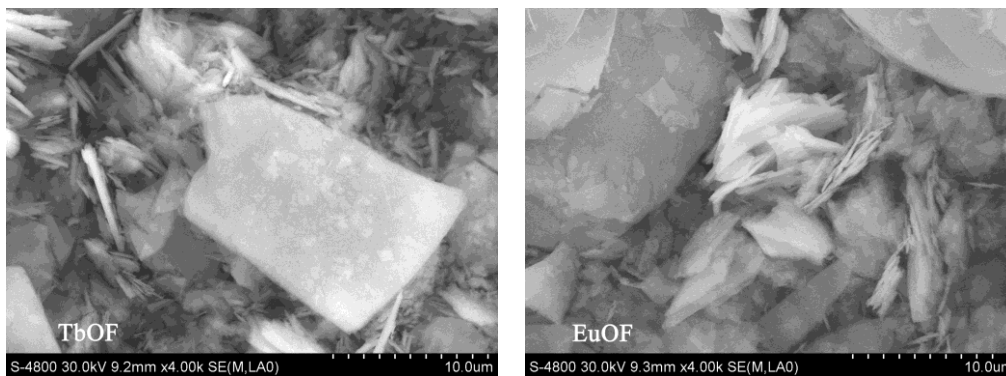


Figure S2. SEM images of  $[\text{Ln}_2(2,3\text{-pzdc})_2(\text{ox})(\text{H}_2\text{O})_2]_n$  ( $\text{Ln} = \text{Tb}, \text{Eu}$ ).

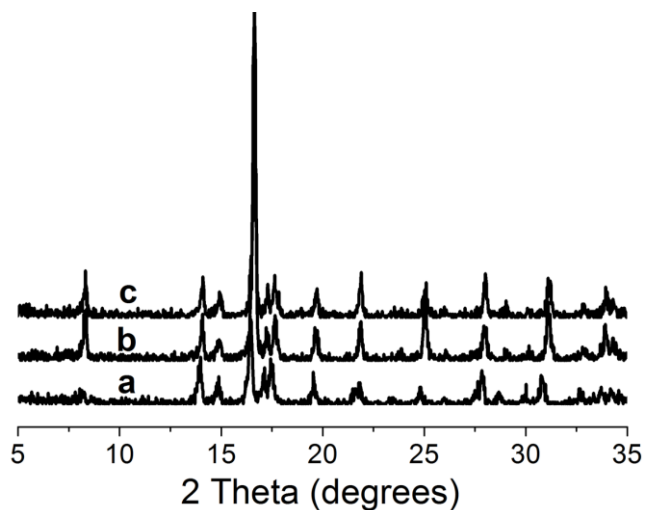


Figure S3. The powder X-ray diffraction (PXRD) of the synthesized EuOF (a), TbOF (b) and TbOF after reacting with CTP (c).

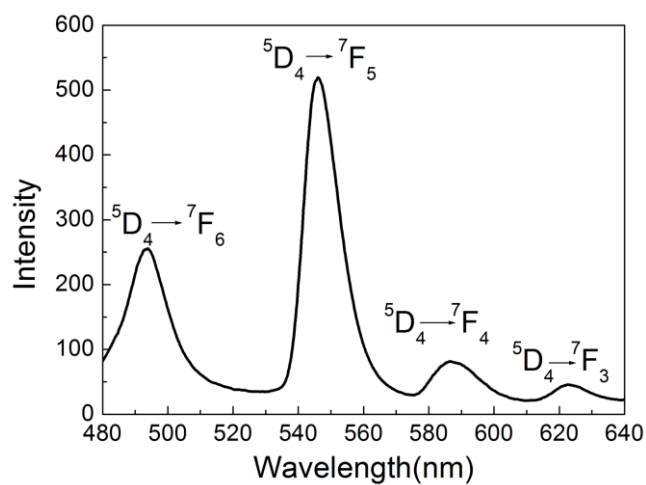


Figure S4. Luminescence spectrum of TbOF dispersed in DMF with excitation at 330 nm. The ratio of DMF and H<sub>2</sub>O is 1:1 (V/V).

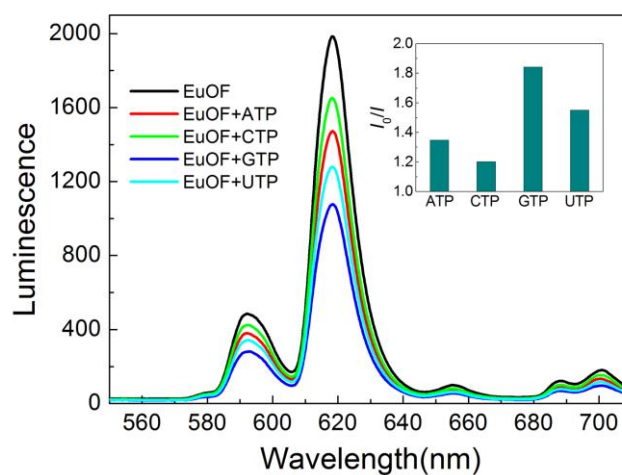


Figure S5. Luminescent changes of the EuOF dispersed in DMF upon the addition of ATP, CTP, GTP, and UTP at the same concentration of  $7.5 \times 10^{-4}$  mol/L with excitation at 365 nm. Inset is the comparison of  $I_0/I$  at 618.4 nm. The ratio of DMF and H<sub>2</sub>O is 1:1 (V/V).

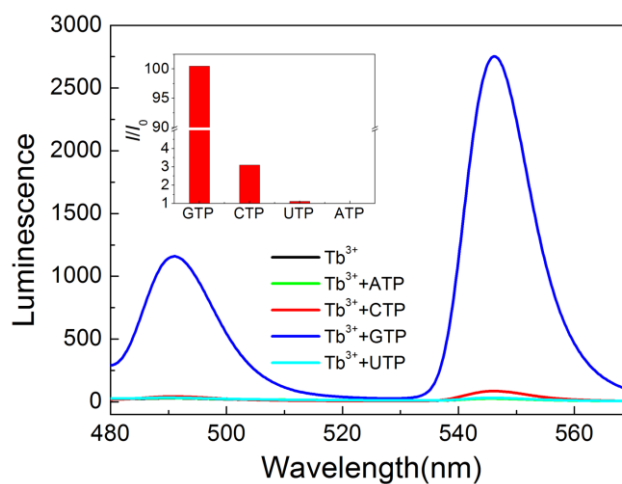


Figure S6. Luminescent responses of Tb(III) dissolved in DMF to CTP, GTP, UTP and ATP with excitation at 300 nm. Inset is the comparison of  $F/F_0$  at 546.0 nm. The ratio of DMF and H<sub>2</sub>O is 1:1 (V/V).  $c_{\text{anions}}, 7.5 \times 10^{-4}$  mol/L.

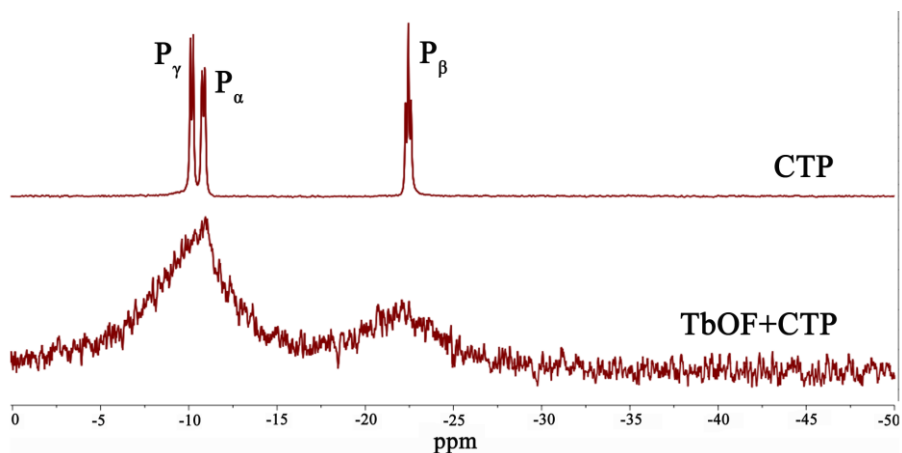


Figure S7.  $^{31}\text{P}$  NMR spectra of CTP in the absence and presence of TbOF carried out in  $\text{D}_2\text{O}$ .

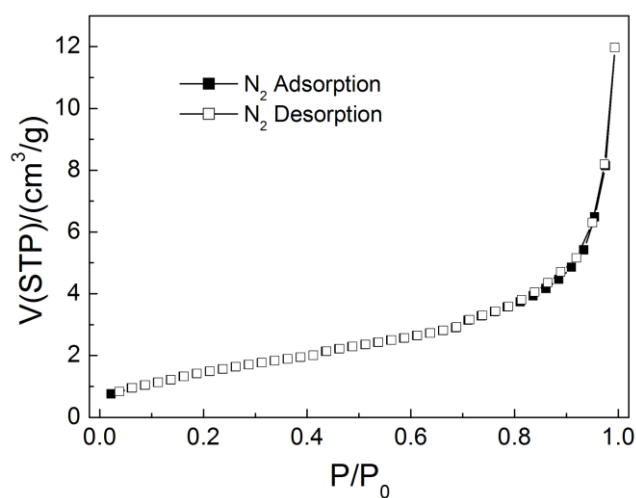


Figure S8.  $\text{N}_2$  adsorption-desorption isotherms of TbOF at 77 K. Adsorption, ■; Desorption, □.

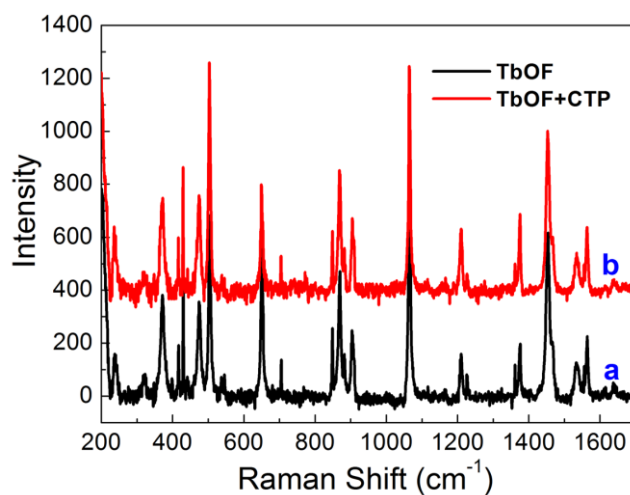


Figure S9. Raman spectra of TbOF before (a) and after (b) reacting with CTP.

Reference:

1. P. C. R. Soares-Santos, L. Cunha-Silva, F. A. A. Paz, R. A. S. Ferreira, J. Rocha, L. D. Carlos and H. I. S. Nogueira, *Inorg. Chem.*, 2010, **49**, 3428-3440.