Electronic Supplementary Material (ESI) for Soft Matter.

Supporting Information

A novel bis-component AIE smart gel high selectively and sensitively detect CN^-, Fe^{3+} and $H_2PO_4^-$

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Materials and methods

All cations were used as the perchlorate salts, while all anions were used as the Tetrabutyl ammonium salts, which were purchased from Alfa Aesar and used as received. Fresh double distilled water was used throughout the experiment. Nuclear Magnetic Resonance (NMR) spectra were recorded on Varian Mercury 400 instruments. Mass spectra were recorded on a Bruker Esquire 6000 MS instrument. The infrared spectra were performed on a Digilab FTS-3000 Fourier transform-infrared spectrophotometer. The morphologies of the gel were characterized using field emission scanning electron microscopy (FE-SEM, UL TRA plus). The X-ray diffraction analysis (XRD) was performed in a transmission mode with a Rigaku RINT2000 diffractometer equipped with graphite monochromated CuKa radiation (λ = 1.54073 Å). Fluorescence spectra were recorded on a Shimadzu RF-5301PC spectrofluorophotometer.

General Procedure

Preperation of the bis-component AIE-gel TG

The mixture of **TNA** (12.86 mg, 1.6 $\mathscr{S}$ 10^{-5} M) and G (7.14 mg, 1.6 $\mathscr{S}$ 10^{-5} M) were added into a binary solution of DMSO and H_2O (V/V, 7.4 : 2.6, 0.275 mL), the mixture was heated dissolve, then cooled it to room temperature, obtaining stable bis-components gel **TG**.

^{1}H NMR experiments

(1) ^{1}H NMR titration experiments of guest G to host TNA. The **TNA** (5 mg, 1.3 × 10^{-2} M) was dissolved in the DMSO-d_6 (0.5 mL), then, a series of different equivalent of guest **G** (0.1 M) were added into the solution of **TNA** and recorded their ^{1}H NMR respectively.

(2) The concentrations-dependent ^{1}H NMR of TG (TNA/G, 1 : 1, n/n): A series of DMSO-d_6 (0.5 mL) solutions of **TG** with different concentrations (7.57 mM; 12.6 mM; 17.7 mM; 27.8 mM) were prepared. Then record their ^{1}H NMR respectively.

(3) ^{1}H NMR titration experiments of TG to CN$^-$. The **TG** (1.3 × 10^{-2} M) was dissolved in the DMSO-d_6 (0.5 mL), then a series of **CN$^-$** (0.1 M, DMSO-d_6) were added into the solution of **TG** and recorded their ^{1}H NMR respectively.

Preperation of TG-Fe

The Fe^{3+} of 0.2 equiv. was added into the **TG** (0.275 mL), the mixture was heated dissolve, then cooled it to room temperature, obtaining stable **TG-Fe**.

Inductively coupled plasma (ICP) experiment

The xerogel of **TG** (2.0 mg) was suspended in a dilute aqueous solution of Fe^{3+} (1×10^{-5} M, 10.0 mL). After the mixture was stirred at room temperature for 1 h, we separated the precipitate by centrifugation (20 min) and obtained the supernatant and using the supernatant for ICP analysis.

Calculation formula of LOD

Formula 1: Linear Equation: y = Ax + B

Formula 2: $$\delta = \sqrt{\frac{\sum (x_i - \bar{x})^2}{n-1}} \ (n = 20)$$

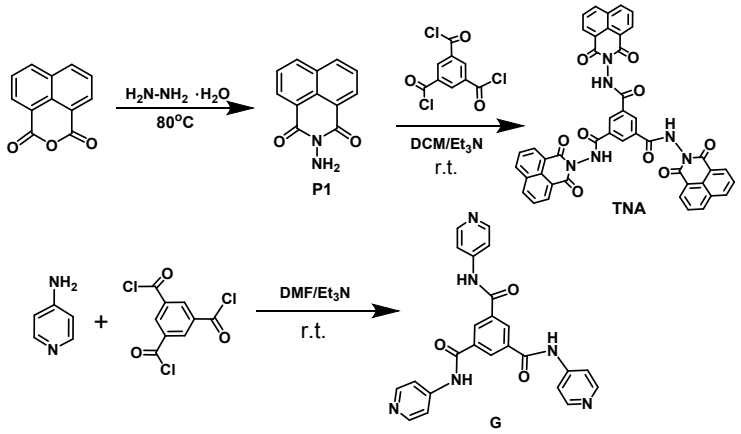
Formula 3: $$LOD = K \frac{\delta}{s} \ (K = 3)$$

Formula 4: S = A × 10^6

Calculate method of adsorption percentage

Adsorption percentage (%) = $\left(1 - \frac{C_1 \times V_1}{C_0 \times V_0}\right)$ × 100%

(State: C_1 is the residual concentration of Fe^{3+}, C_0 is the initial concentration of Fe^{3+}, $V_1 = V_0$).



Scheme S1 Synthesis of **TNA** and **G**.

TNA and **G** were synthesized according to our previous reported method, [S1, S2] respectively.

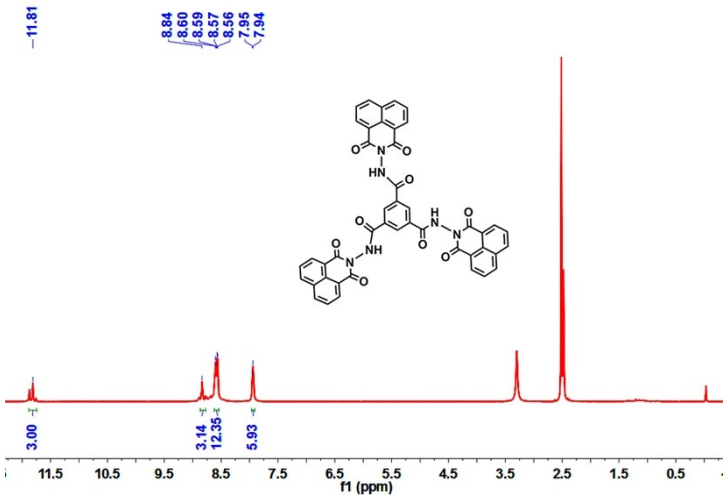


Fig. S1 ^{1}H NMR Spectrum of **TNA** in DMSO-d_6 (600 MHz, 298K).

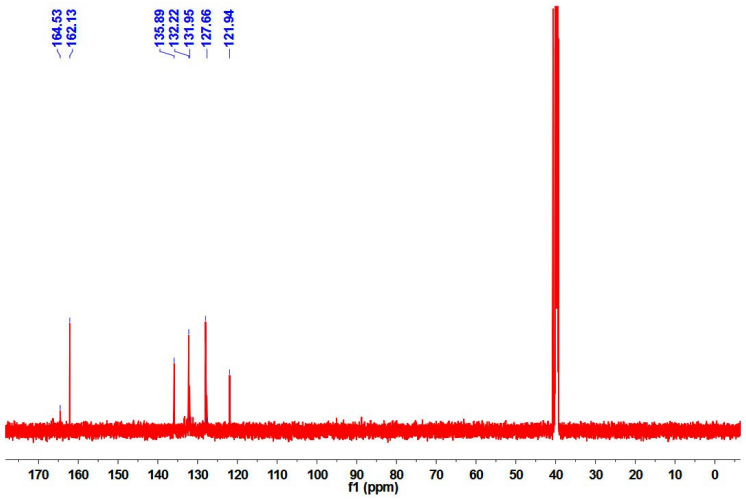


Fig. S2 ^{13}C NMR Spectrum of **TNA** in DMSO-d_6 (150 MHz, 298K).

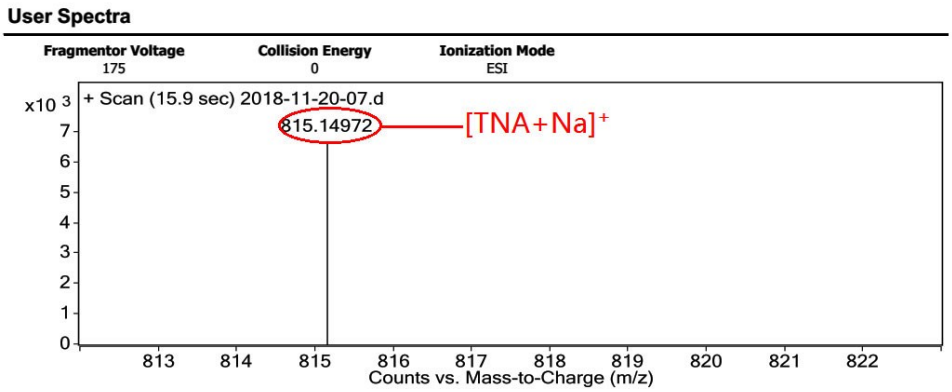


Fig. S3 Mass spectrum of **TNA**.

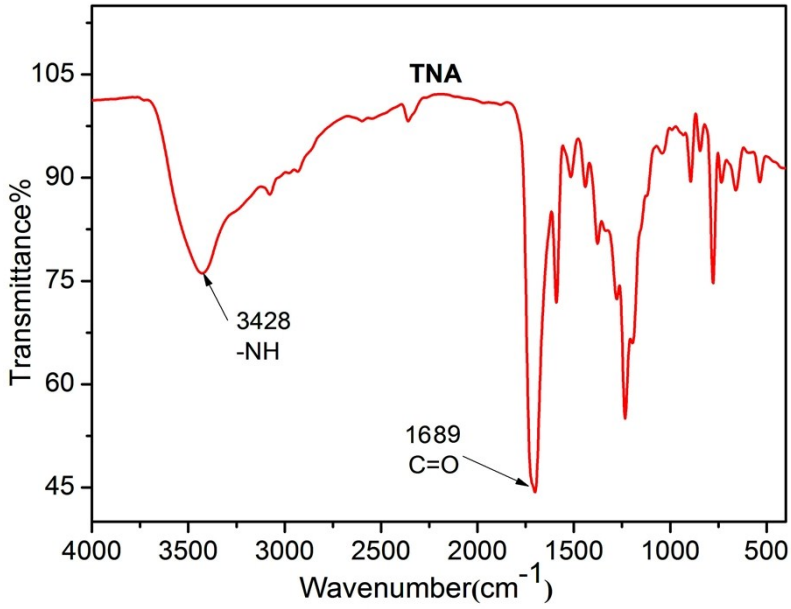


Fig. S4 FT-IR spectrum of **TNA** in KBr disk.

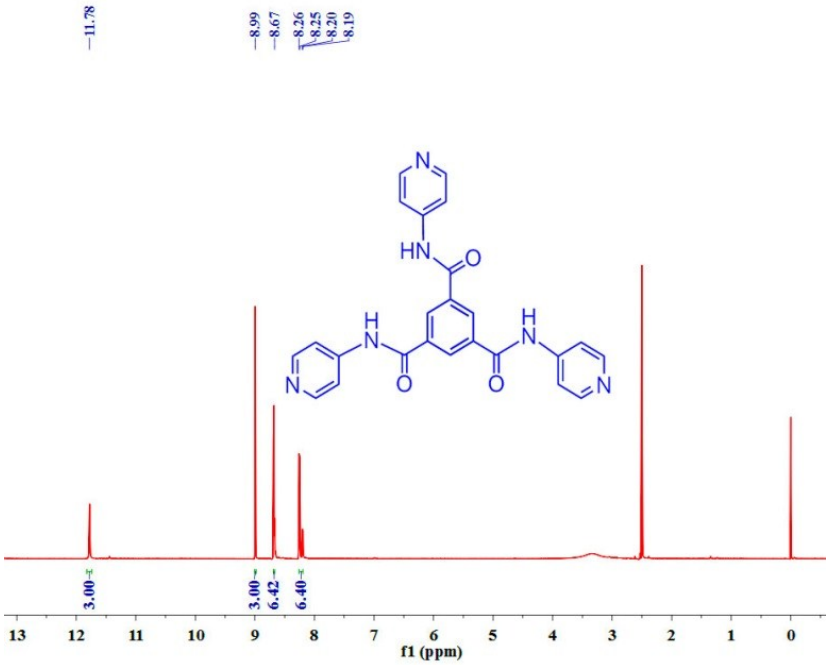


Fig. S5 ^{1}H NMR spectrum of **G** in DMSO-d_6 (400 MHz, 298K).

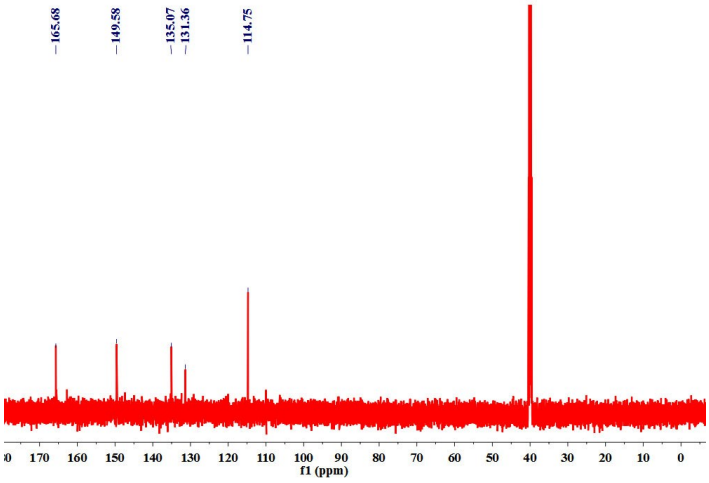


Fig. S6 ^{13}C NMR spectrum of **G** in DMSO-d_6 (150 MHz, 298K).

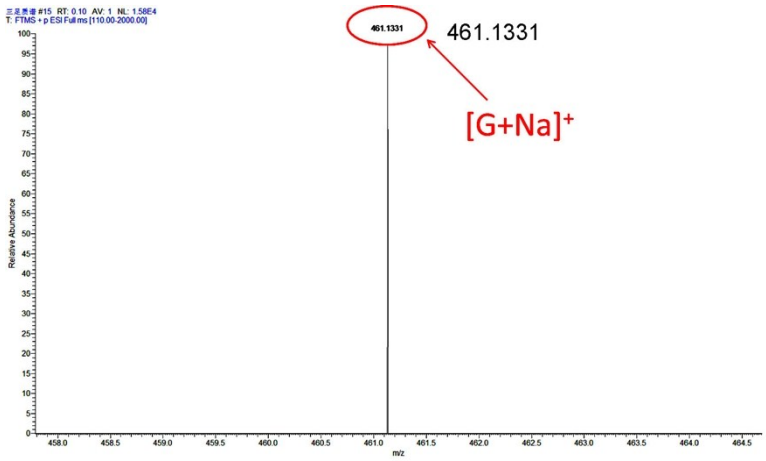


Fig. S7 Mass spectrum of **G**.

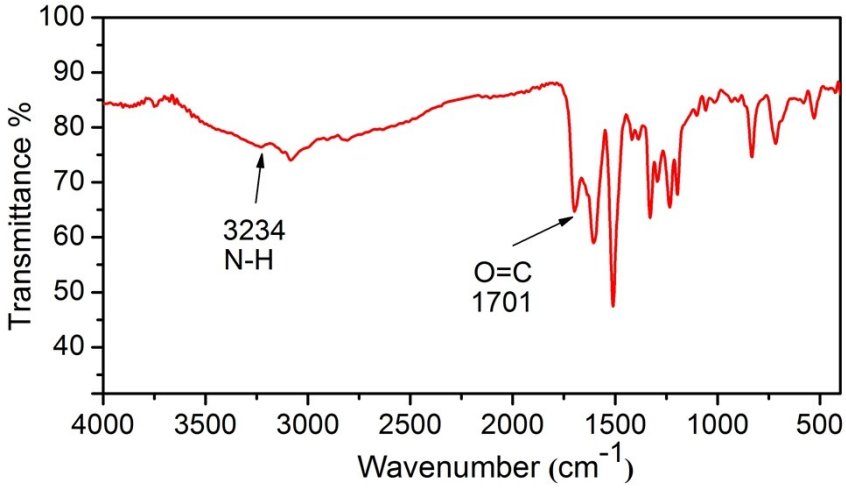


Fig. S8 FT-IR spectrum of **G** in KBr disk.

Table S1 Gelation properties of **TG** in organic solvents.

Entry	Solvents	State[a]	CGC[b](%)	T_{gel}[c] (°C, wt/v %)
1	methanol	P	\	\
2	ethanol	P	\	\
4	n-butyl alcohol	P	\	\
5	n-propanol	P	\	\
6	n-hexanol	P	\	\
7	formic acid	P	\	\
8	acetic acid	P	\	\
9	propanoic acid	P	\	\
10	hexylic acid	P	\	\
11	butyric acid	P	\	\
12	$CHCl_3$	P	\	\
13	DMF	S	\	\
14	DMF/H_2O	P	\	\

15	DMSO	S	\	\
16	**DMSO/H_2O (7.4 : 2.6)**	**G**	**7**	**90-92 °C (7%)**
17	acetonitrile	P	\	\
18	cyclohexanol	p	\	\
19	cyclohexane	P	\	\
20	n-hexane	P	\	\

[a]G, P, and S denote gelation, precipitation and solution, respectively.
[b]The critical gelation concentration (wt %, 10 mg/ml = 1.0 %).
[c]The gelation temperature (°C).

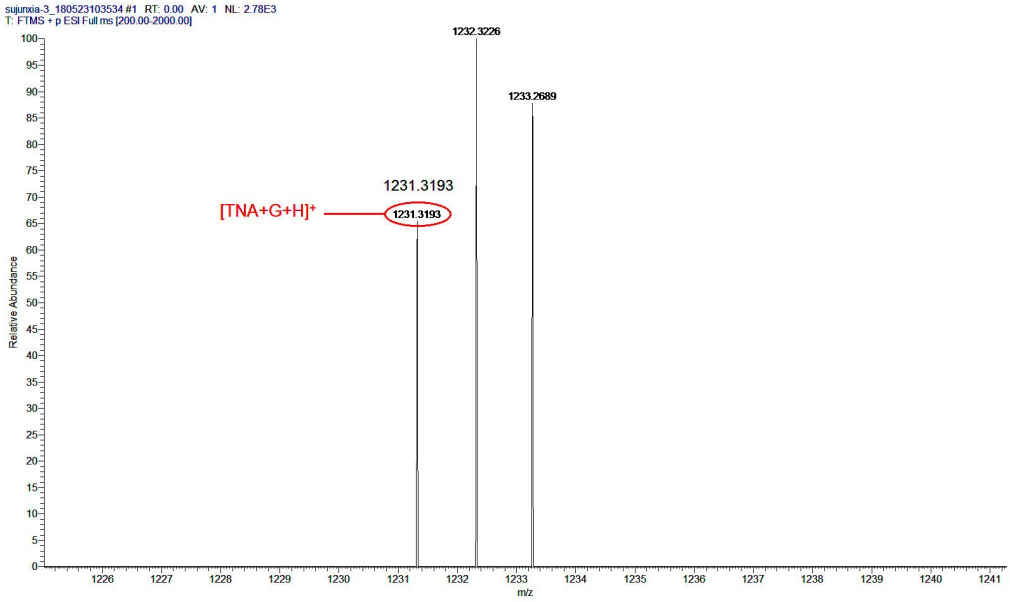


Fig. S9 Mass spectrum of **TG**.

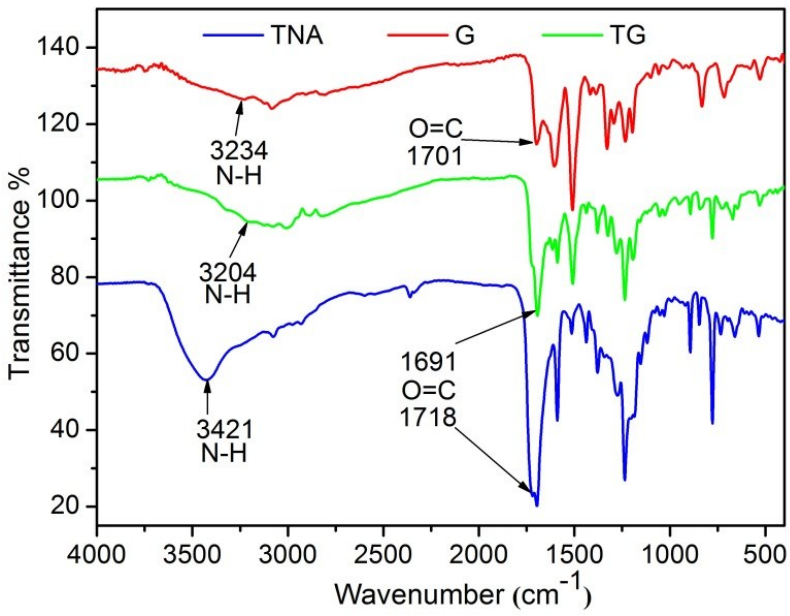


Fig. S10 FT-IR spectra of **TNA**, **G** and **TG**.

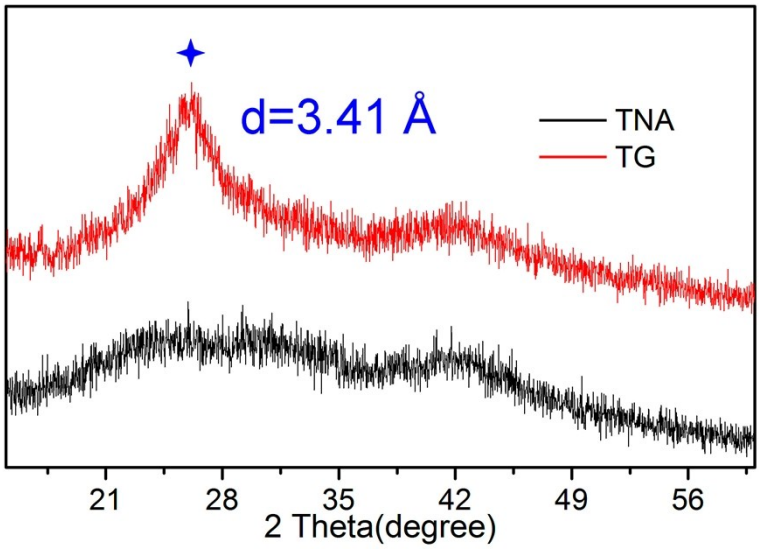


Fig. S11 XRD pattern of the **TNA** and **TG**.

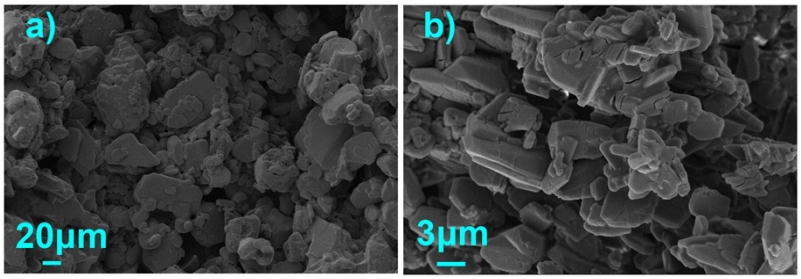


Fig. S12 FE-SEM images of a) **TNA** and b) **G**.

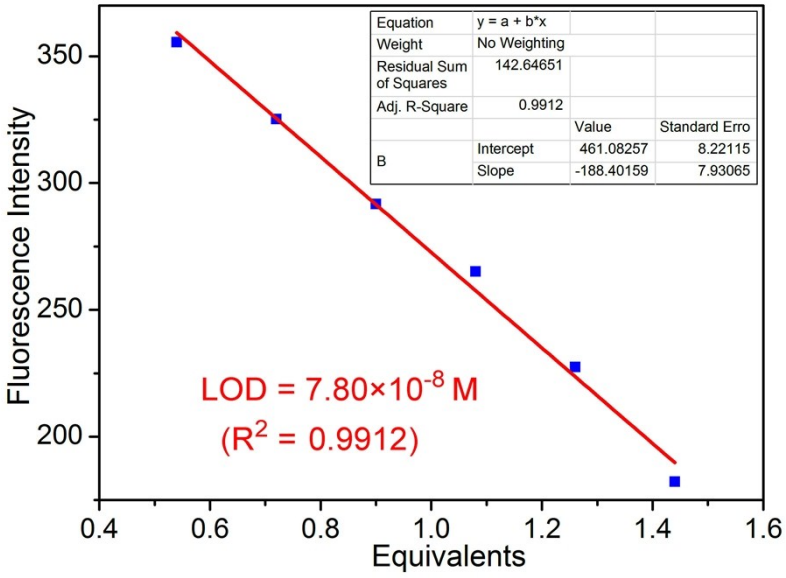


Fig. S13 Fluorescent spectrum linear range for CN^- by addition of various

concentrations of CN^- to **TG**.

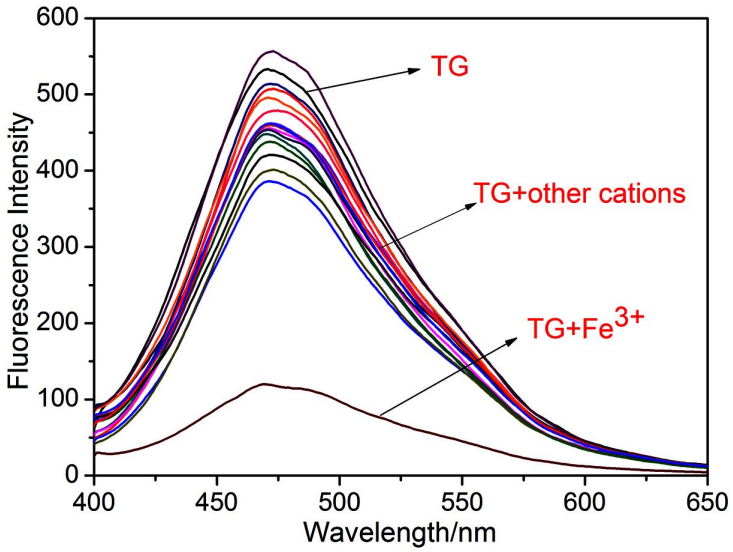


Fig. S14 Fluorescent spectra changes (λ_{ex} = 380 nm) of **TG** with addition of different cations aqueous solution.

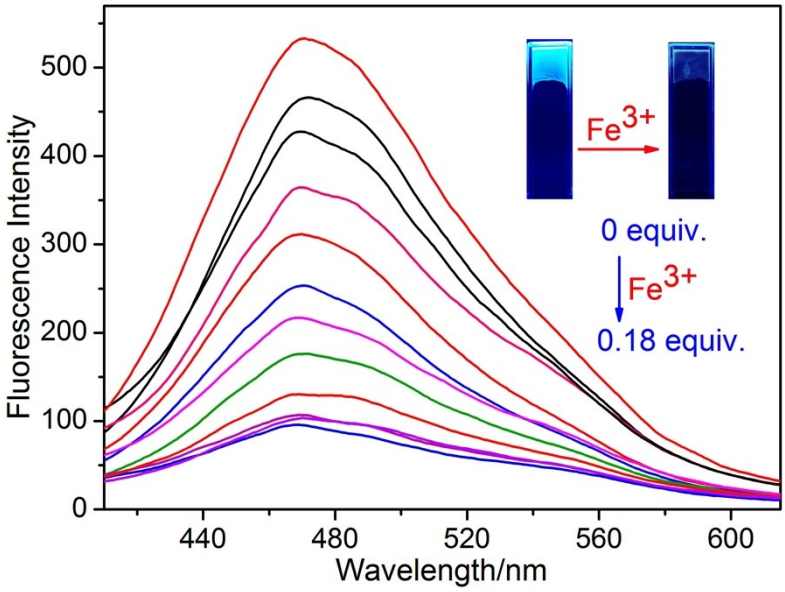


Fig. S15 Emission spectra of **TG** with increasing amounts of Fe^{3+}.

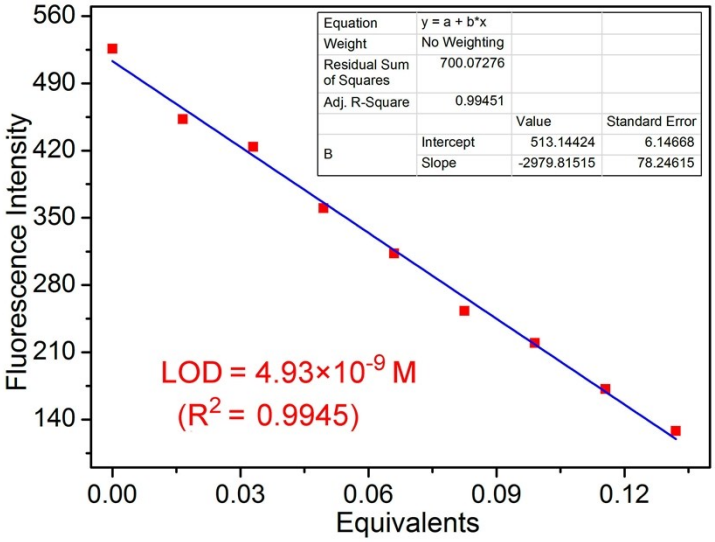


Fig. S16 Fluorescent spectrum linear range for Fe^{3+} by addition of various concentrations of Fe^{3+} to **TG**.

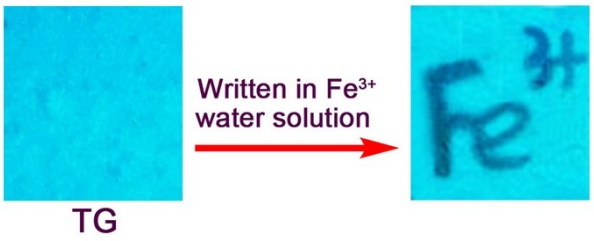


Fig. S17 Photograph of **TG**-based film fluorescently detect Fe^{3+} in water solution.

Table S2 The ICP data of **TG** with Fe^{3+}.

Ion	Initial concentration (M)	Residual concentration (M)	Absorbing rate (%)
Fe^{3+}	1×10^{-5}	4.1×10^{-7}	95.89 %

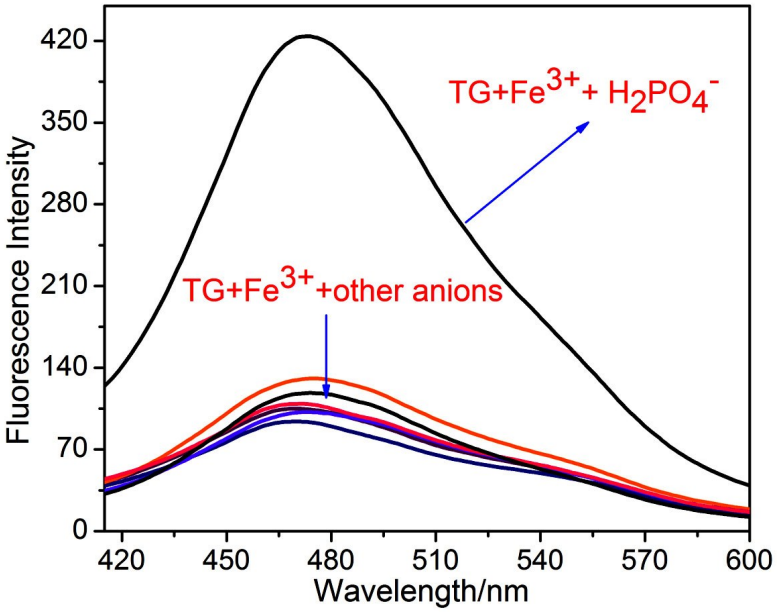


Fig. S18 Fluorescent spectra changes (λ_{ex} = 380 nm) of **TG-Fe** with addition of different anions aqueous solution.

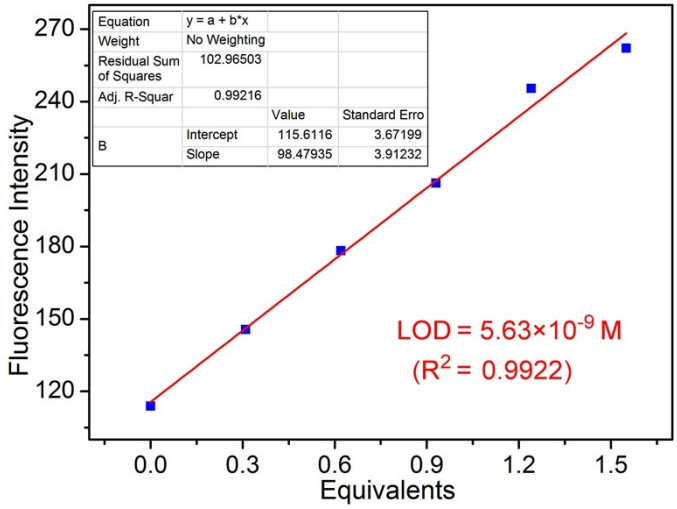


Fig. S19 Fluorescent spectrum linear range for $H_2PO_4^-$ by addition of various concentrations of $H_2PO_4^-$ to **TG-Fe**.

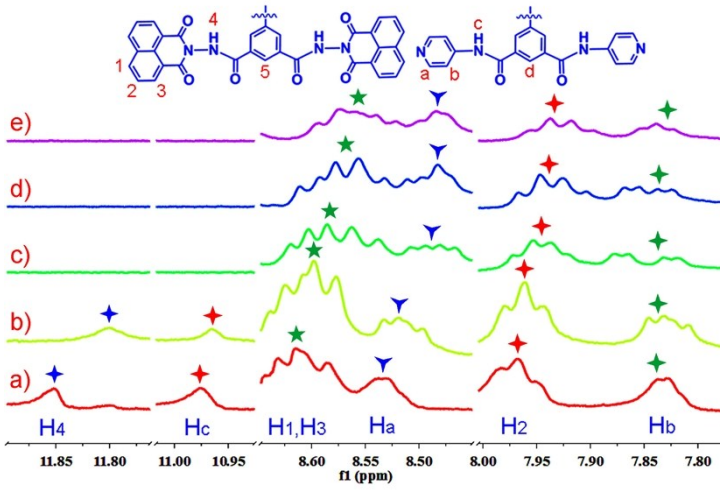


Fig. S20 Partial ^{1}H NMR spectra of 5.0 mg **TG** in DMSO-d_6 with different equivalent CN^- (a) 0 equiv.; (b) 0.2 equiv.; (c) 0.4 equiv.; (d) 1.0 equiv.; (e) 2.0 equiv.

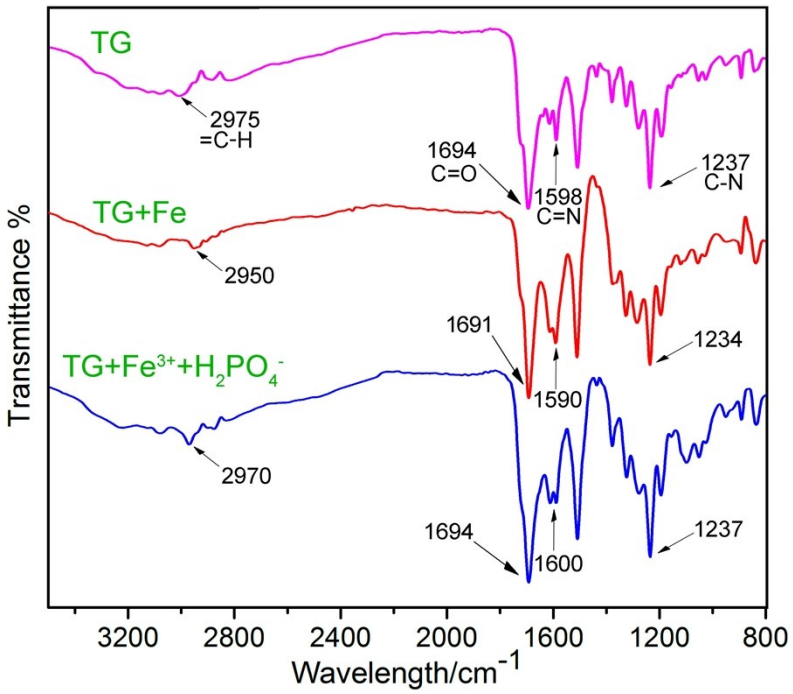


Fig. S22 FT-IR spectra of **TG**, **TG** + Fe^{3+} and **TG-Fe** + $H_2PO_4^-$.

Notes and references

S1 Y. Q. Fan, J. Liu, Y. Y. Chen, X. W. Guan, J. Wang, H. Yao, Y. M. Zhang, T. B. Wei, Q. Lin, *J. Mater. Chem. C.*, 2018, **6**, 13331-13335.

S2 Q. Lin, G. F. Gong, Y. Q. Fan, Y. Y. Chen, J. Wang, X. W. Guan, J. Liu, Y. M. Zhang, H. Yao, T. B. Wei, *Chem. Commun.*, 2019, **55**, 3247-3250.