

Electronic Supplementary Information

**Tri-pillar[5]arene-based multi-stimuli responsive
supramolecular polymer for fluorescent detection and
separation of Hg²⁺**

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Table of Contents

Materials and methods

Synthesis of gelator **JP5**.

Fig. S1 ^1H NMR Spectrum of **JP5**.

Fig. S2 ^{13}C NMR Spectrum of **JP5**.

Fig. S3 Mass Spectrum of **JP5**.

Table S1 Gelation property of supramolecular polymer **JP5**.

Fig. S4 Fluorescence spectra of supramolecular polymer **JP5G** in gelled state and solution in cyclohexanol (5% w/v).

Fig. S5 FT-IR spectra of powder **JP5**, xerogel of supramolecular polymer **JP5G** and xerogel **JP5G+Hg²⁺**.

Fig. S6 Powder XRD patterns of powder **JP5**, xerogel **JP5G**, and xerogel **JP5G+Hg²⁺**.

Fig. S7 Photographs of supramolecular polymer **JP5G** in cyclohexanol (5% w/v) and supramolecular polymers of **JP5G** in the presence of various cations (Hg^{2+} , Zn^{2+} , Pb^{2+} , Cd^{2+} , Ca^{2+} , Mg^{2+} , Al^{3+} , Tb^{3+} , La^{3+} , Ba^{2+} , Eu^{3+} $n_{\text{JP5G}}: n_{\text{cations}}=1:1$) under UV light.

Fig. S8 The association constant (K_a) express for the complexation between **JP5** and Hg^{2+} .

Table S2 The ICP data of xerogel **JP5G** with Hg^{2+} .

Materials and instruments

All reagents we used were analytical and commercial grade without doing anything. All metal ions were prepared from the perchlorate salts. They were all purchased from Sigma-Aldrich Chemical and were stored in a vacuum desiccator. Melting points were measured by an X-4 digital melting point apparatus. Fluorescence spectra were recorded on a Shimadzu RF-5310. ^1H NMR spectra were recorded on a Mercury-600BB spectrometer at 600 MHz and ^{13}C NMR spectra were recorded on a Mercury-600BB spectrometer at 151 MHz with CDCl_3 as solvent. Mass spectra were performed on a Bruker Esquire 3000 plus mass spectrometer (Bruker-Franzen Analytik GmbH Bremen, Germany) equipped with ESI interface and ion trap analyzer. The X-ray diffraction analysis (XRD) were performed in a transmission mode with a Rigaku RINT2000 diffractometer equipped with graphite monochromated CuK α radiation ($\lambda = 1.54073 \text{ \AA}$). The infrared spectra were performed on a Digilab FTS-3000 Fourier transform-infrared spectrophotometer.

The preparation of responsive film based on JP5G

The Hg^{2+} responsive film based on **JP5G** was prepared by pouring the heated cyclohexanol solution of **JP5** (5% 10 mg/mL = 1%) onto a clean glass surface and drying in the air. Then, writing on the film with a writing brush dipped in Hg^{2+} aqueous (0.1 M).

Synthesis and characterizations of compound **JP5**

Synthesis of gelator **JP5**

1. Compound **PQ**

Compound **PQ** was synthesized according to our previous work^[1]

2. Compound **JP5**

Compound **PQ** (0.48 g, 0.6 mmol) and dichloromethane (10 mL) were added into a 100 ml round-bottomed flask, 5 ml dichloromethane solution of trimesoyl chloride (0.053 g, 0.2 mmol) was added dropwise at the atmosphere of ice bath. Then the mixture was reacted at room temperature for 12 hours. Finally, filtered and washed filter cake with dichloromethane, we could get a kind of white solid (0.36 g, 70 %). m. p. 53-54°C. ¹H NMR (600 MHz, *d*₆-DMSO), δ 10.81 (s, 3 H, -NH), δ 10.30 (s, 3 H, -NH), δ 8.58 (s, 3 H, ArH), δ 6.94-6.73 (m, 30 H, ArH), δ 4.56 (s, 6 H, -OCH₂), δ 3.80-3.66 (m, 111 H, 81 -OCH₃, 30 -ArCH₂). ESI-MS m/z: [**JP5**+H]⁺ calcd for 2583.0673; Found 2583.0696.

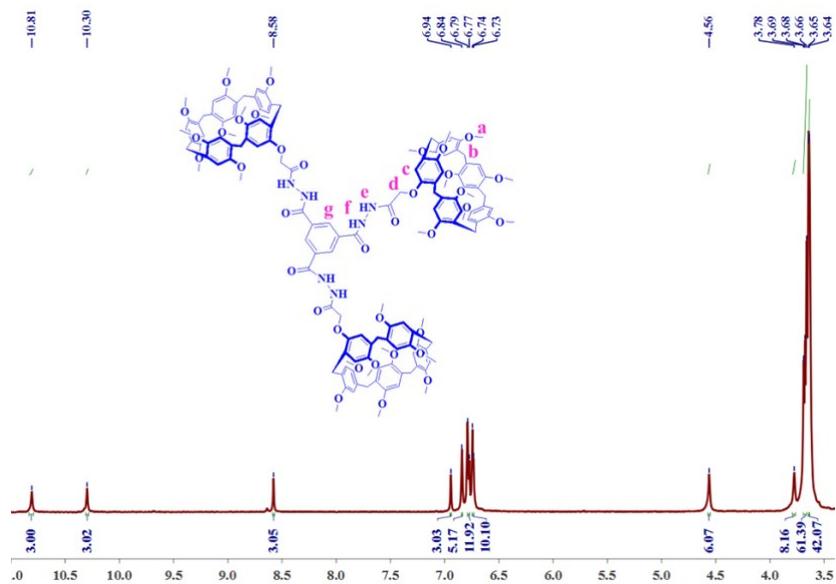


Fig. S1 ¹H NMR Spectrum of JP5.

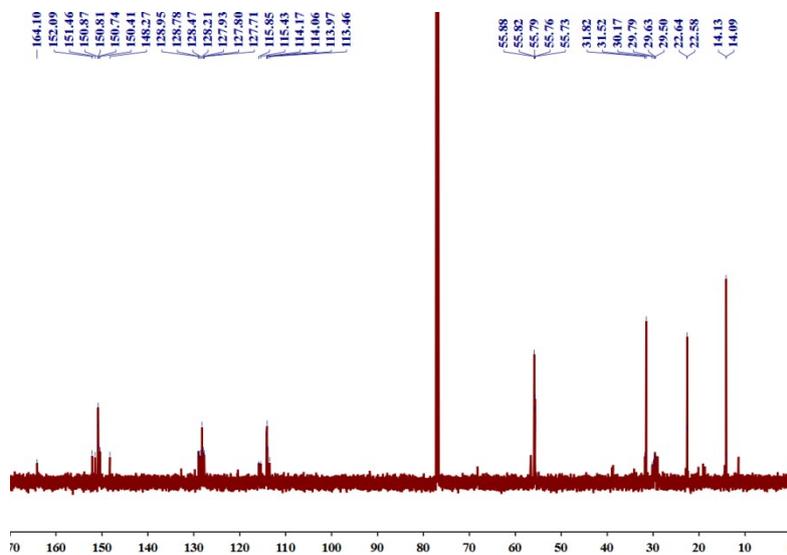


Fig. S2 ¹³C NMR Spectrum of JP5.

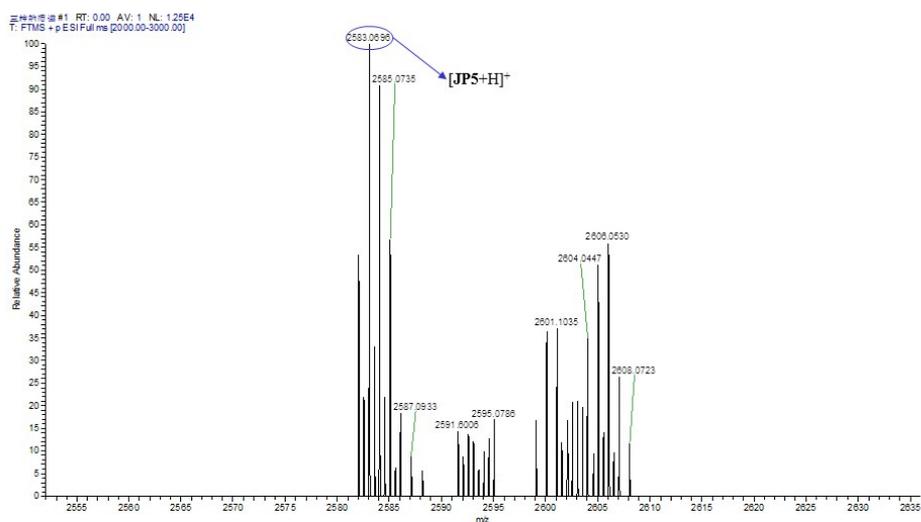


Fig. S3 Mass Spectrum of **JP5**.

Table S1 Gelation properties of supramolecular polymer **JP5**

Entry	Solvent	State ^a	CGC ^b (%)	Tgel ^c (°C, wt%)
1	Water	P	\	\
2	Cyclohexanol	G	5%	58~60°C
3	Isoamyl alcohol	P	\	\
4	Ethylene glycol	P	\	\
5	Isopropanol	P	\	\
6	N-propanol	P	\	\
7	Butanol	P	\	\
8	Tert-butanol	P	\	\
9	N-hexanol	P	\	\
10	Ethanol	P	\	\
11	Acetonitrile	P	\	\
12	Dichloromethane	P	\	\
13	Chloroform	P	\	\
14	DMF	S	\	\
15	THF	S	\	\
16	DMSO	S	\	\

^aG P and S denote gelation, precipitation and solution, respectively, c = 0.8%.

^bThe critical gelation concentration (wt%, 10mg/ml = 1.0%).

^cThe gelation temperature(°C).

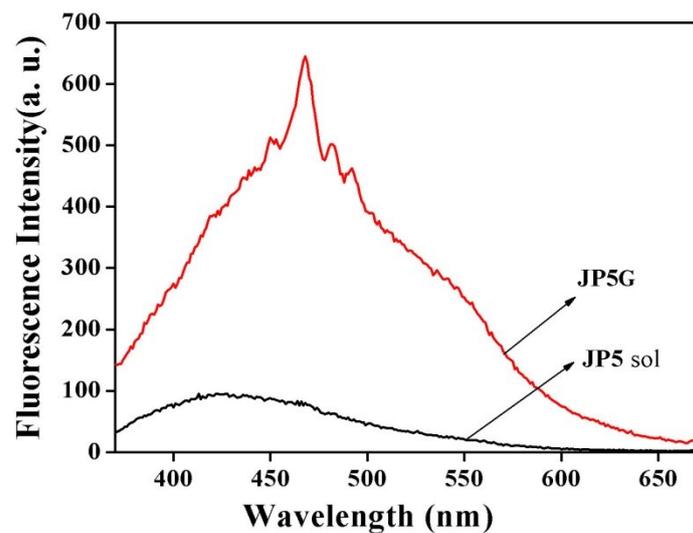


Fig. S4 Fluorescence spectra of supramolecular polymer **JP5G** in gelated state and solution in cyclohexanol (5% w/v).

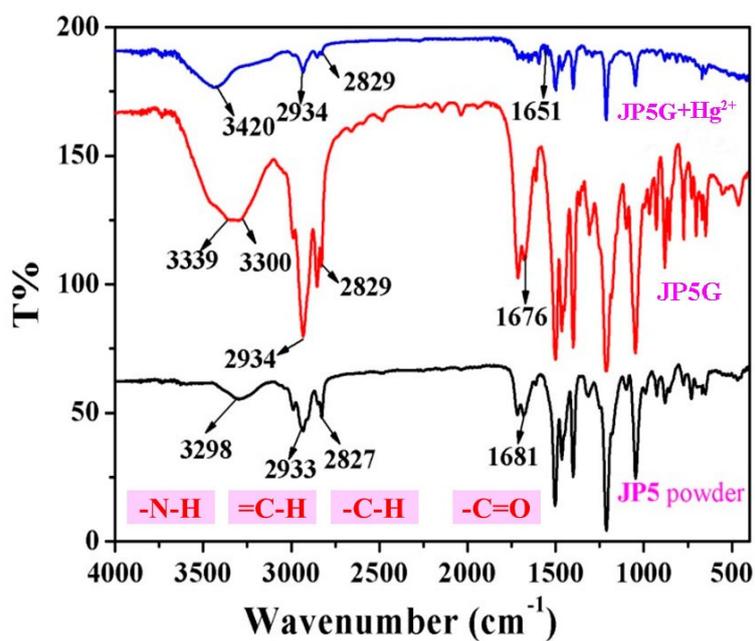


Fig. S5 FT-IR spectra of powder **JP5**, xerogel of supramolecular polymer **JP5G** and xerogel **JP5G+Hg²⁺**.

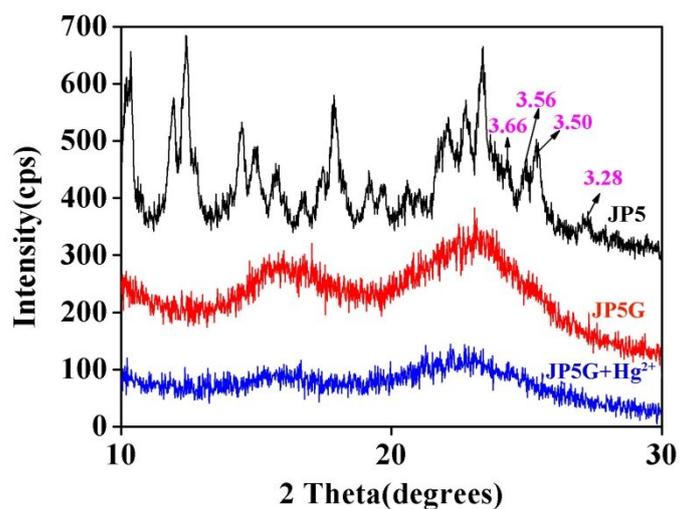


Fig. S6 Powder XRD patterns of powder **JP5**, xerogel **JP5G**, and xerogel

JP5G+Hg²⁺.

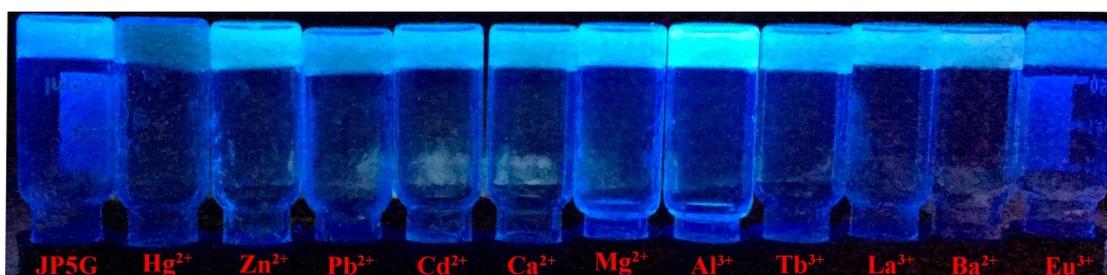


Fig. S7 Photographs of supramolecular polymer **JP5G** in cyclohexanol (5% w/v) and supramolecular polymers of **JP5G** in the presence of various cations (Hg²⁺, Zn²⁺, Pb²⁺, Cd²⁺, Ca²⁺, Mg²⁺, Al³⁺, Tb³⁺, La³⁺, Ba²⁺, Eu³⁺ n_{JP5G}: n_{cations}=1:1) under UV light.

$$\log \frac{I - I_{\min}}{I_{\max} - I} = \frac{1}{3} \log Ka + \log[B1]$$

Fig. S8 The association constant (Ka) express for the complexation between **JP5** and Hg²⁺.

Where I is the observed the fluorescence intensity of **JP5** at the fixed concentrations of Hg²⁺. I_{\max} and I_{\min} are the corresponding maximum and minimum, respectively, $1/3$

is complex ratio between **JP5** and Hg^{2+} , [B1] is the corresponding concentration of Hg^{2+} .

Ion	Initial concentration (mg/ml)	Residual concentration (mg/ml)	Absorbing rate (%)
Hg^{2+}	0.8	0.15	81.3

Table S2 The ICP data of xerogel **JP5G** with Hg^{2+} .

[1] Q. Lin, X. M. Jiang, L. Liu, J. F. Chen, Y. M. Zhang, H. Yao, T. B. Wei, *Soft Matter*, 2017, **13**, 7222-7226.