



# Multistimuli responsive supramolecular polymer networks via host-guest complexation of pillararene-containing polymers and sulfonium salts

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## ABSTRACT

A stimuli-responsive supramolecular polymer network has been constructed based on the host-guest interactions between the copolymer **poly-P[5]A** with pendent pillararene units and bis(sulfonium) dication guest **G2**. The formation mechanism of the supramolecular polymer network has been explored by the intensive study. With the addition of the competitive molecules and heating, the supramolecular polymer network could be dissociated and lead to clear changes in NMR spectroscopy and viscosity property.

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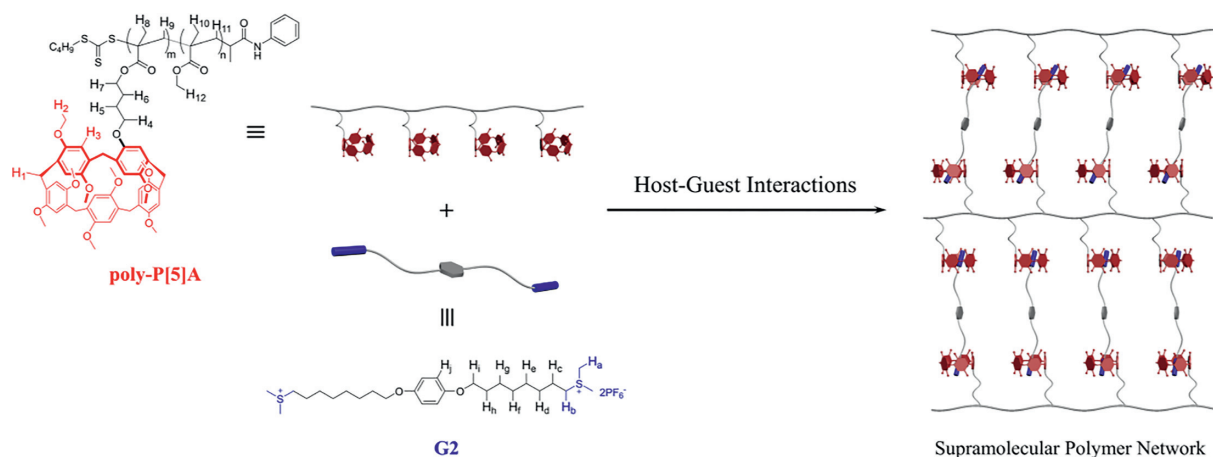
Stimuli-responsive systems have been widely used in the field of functional materials due to their controllable properties upon external stimuli [1,2]. Supramolecular polymer networks, constructed by polymers linked together with non-covalent interactions, have attracted great attention in the field of stimuli-responsive materials due to their reversibility and stimuli-responsiveness properties [3–5]. In recent few years, various non-covalent interactions have been employed to construct supramolecular polymer networks, such as hydrogen bonding [6,7], electrostatic interactions [8], host-guest interactions [9–12],  $\pi$ - $\pi$  stacking [13,14] and metal-ligand coordination [15,16]. Among them, host-guest interactions have been given great attention, which are susceptible to external stimuli, including pH [17], ions [18], light [10], redox [19] and temperature [20]. So these supramolecular polymer materials could be endowed with unique properties and tunability [3]. To date, a variety of supramolecular polymer networks have been successfully fabricated based on the host-guest interactions involved by numerous macrocycles such as crown-ethers [17,18,21], cyclodextrins [22,23], calix[n]arenes [9,24] and cucurbit[n]urils [25,26], which provide a good strategy to prepare stimuli-responsive materials.

Pillar[n]arenes have already attracted great attention in the field of supramolecular chemistry since their first introduction in 2008 by Ogoshi [27,28]. So far, many researches about the host-guest chemistry between pillar[n]arenes and numerous guests have been well studied, such as ammonium salts [29,30], pyridinium salts [31,32], imidazolium salts [33,34]. Based on the host-guest interactions between pillar[5]arenes and these cationic guests, various kinds of supramolecular polymer networks have been reported [35,36]. Sulfonium salts, as valuable reagents, have diverse applications as electrolytes [37], photo-cationic polymerization catalysts [38,39] and versatile reagents in bond-forming or breaking reactions [40]. The host-guest interactions between sulfonium salts and several macrocyclic host molecules have also been investigated [41–43]. However, to the best of our knowledge, the research about the interactions between pillar[5]arenes and sulfonium salts in organic medium has not been reported yet, which leads to a variety of stimuli-responsive materials remaining to be exploited. Therefore, constructing a stimuli-responsive supramolecular polymer network based on the pillar[5]arenes-containing polymers and sulfonium salts is still an attractive task.

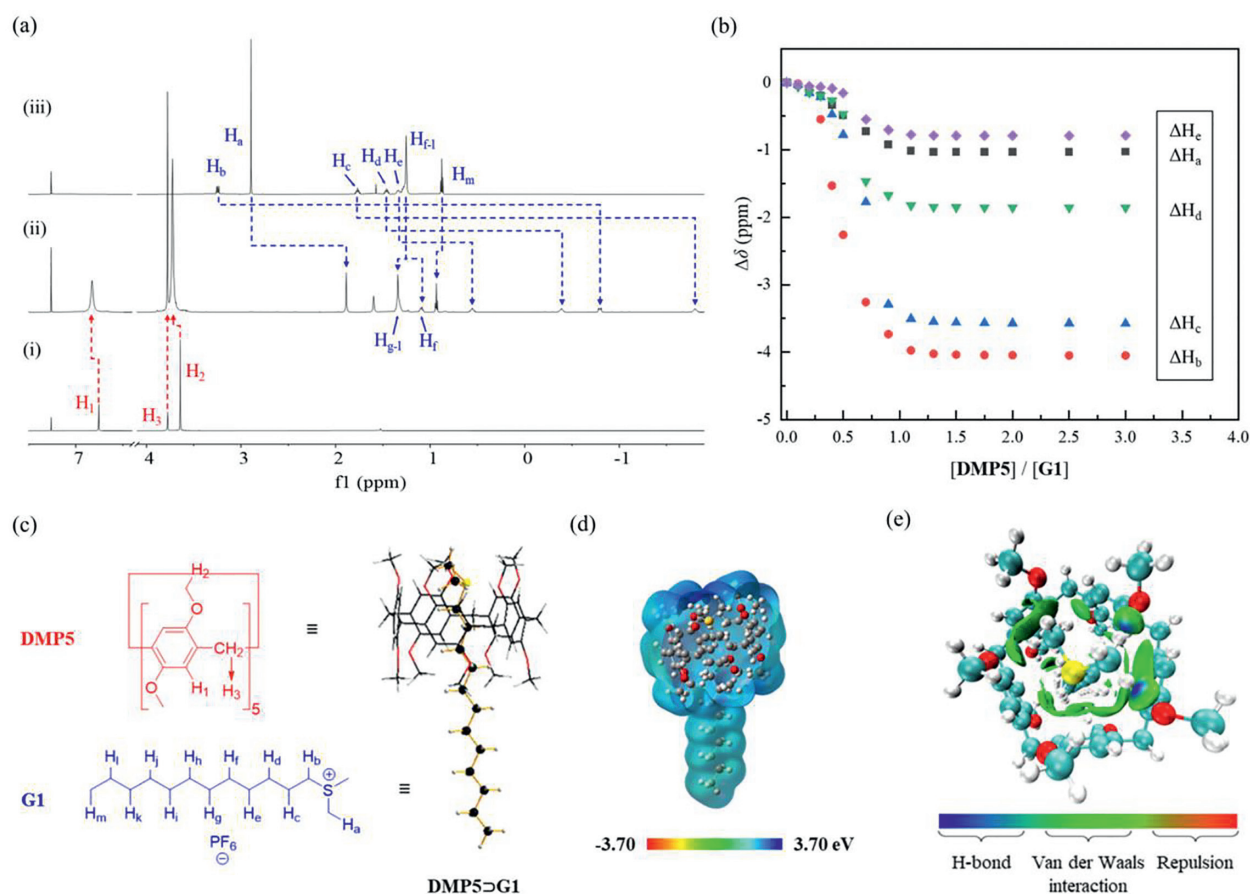
Herein, we reported a new supramolecular polymer network by mixing a copolymer with pendant pillar[5]arenes groups and a bis(sulfonium) dication guest (Scheme 1). The interactions between pillar[5]arenes and sulfonium salts were firstly systematically investigated through the model host and guest. Then we use

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**Scheme 1.** Representation of supramolecular polymer network constructed by copolymer **poly-P[5]A** and bis(sulfonium) guest **G2**.



**Fig. 1.** (a) Partial  $^1\text{H}$  NMR spectra of (i) 10.0 mmol/L **DMP5**, (ii) 10.0 mmol/L **DMP5** + 5.0 mmol/L **G1**, (iii) 10.0 mmol/L **G1** in  $\text{CDCl}_3$  (600 MHz, 298 K); (b) Normalized  $^1\text{H}$  NMR chemical shifts ( $\Delta\delta = \delta_{\text{obsd}} - \delta_{\text{bound}}$ ) of  $\text{H}_3\text{-H}_e$  protons in **G1** at a concentration of 10.0 mmol/L upon addition of **DMP5** (0–3.0 mol equiv.); (c) The side view of the energy-optimized structure of **DMP5**⊃**G1**; (d) The molecular electrostatic potential (ESP) surfaces of **DMP5**⊃**G1**; (E) The top-down view of the noncovalent binding surfaces of **DMP5**⊃**G1** by IGM method. Isosurfaces coloured according to the BGR scheme over the range  $-0.05 < \text{sign}(\lambda_2) \rho < 0.05$  a.u.

reversible addition-fragmentation chain transfer polymerization (RAFT) methods to prepare the target copolymer. Compared to the copolymer, the obtained supramolecular polymer network exhibited great changes in NMR spectroscopy and viscosity property. Moreover, the supramolecular polymer network could be dissociated by different external stimuli including temperature and competing host/guest reagents.

1,4-Dimethoxypillar[5]arenes (**DMP5**) and dodecyl dimethyl sulfonium hexafluorophosphate (**G1**) were chosen as the model

molecules (Fig. 1c). NMR titration experiments were firstly carried out to investigate the interactions between **DMP5** and **G1** (Figs. 1a and b and Fig. S4–S7 in Supporting information). The addition of **DMP5** to **G1** in  $\text{CDCl}_3$  showed significant changes of the magnetic environments of the most protons in **DMP5** and **G1** (Fig. 1a). Only one set of peaks on the NMR time scale indicated the fast-exchange complexation. The plots were constructed to exhibit the normalized chemical shift changes ( $\Delta\delta = \delta_{\text{obsd}} - \delta_{\text{bound}}$ ) for the protons of **DMP5** and **G1** as a function of the increasing

concentration of **DMP5** in the solution of **G1** (Fig. 1b and Fig. S4 in Supporting information). The phenyl protons  $H_1$  and methyl protons  $H_3$  on **DMP5** respectively shifted downfield from 6.76 ppm to 6.88 ppm and 3.65 ppm to 3.78 ppm, while no obvious chemical shift changes of the methylene protons  $H_2$  were observed. The differences of the chemical shift changes for each proton of **G1** revealed their positions in the cavity of **DMP5**. The protons  $H_b$  and  $H_c$  showed greater upfield shift changes ( $\Delta\delta \approx 4.05$  and 3.57 ppm, respectively), which suggested that they inhabited the inner aromatic cavity of **DMP5**. However, the methyl protons  $H_m$  exhibited small downfield shift changes from 0.88 ppm to 0.94 ppm, indicating that they were located in the deshielding regions of **DMP5**. These phenomena suggested the threading of the line guest **G1** into the cavity of **DMP5**. The mole ratio plot based on the chemical shift changes of  $H_m$  on **G1** indicated a 1:1 complexation stoichiometry, while the association constant ( $K_a$ ) was then calculated to be  $4.11 \times 10^3$  L/mol by nonlinear least-squares analysis (Figs. S5–S7 in Supporting information). The electrospray ionization mass spectrum was performed to study the host-guest complex (Fig. S8 in Supporting information). A peak corresponding to  $[\text{DMP5} \supset \text{G1} - \text{PF}_6]^+$  was observed at  $m/z$  981.5545. 2D NOESY spectrum was also performed to confirm the complexation model (Fig. S9 in Supporting information). The cross peaks of  $H_1$  and  $H_{b-d}$  supported the complete inclusion of the sulfonium salts unit into the cavity of **DMP5**. Since **DMP5** provides a rigid and  $\pi$ -rich cavity, the cation- $\pi$  interactions between **DMP5** and **G1** should be the main driving forces [44,45].

To deeply understand the formation mechanism of the complex, the optimized structures of **DMP5**, **G1** and the complex **DMP5**  $\supset$  **G1** were obtained by density functional theory (DFT) studies at the B3LYP/6-31G(d,p) level using the Gaussian 09 package suite [46], Multiwfn software version 3.8 (Fig. 1c and Fig. S10 in Supporting information) [47]. Compared to **DMP5**, the symmetric structure of the **DMP5** of the complex had slightly distorted, indicating the interactions existed between **DMP5** and **G1**. Fig. 1d and Fig. S11 (Supporting information) showed the HOMO, LUMO and electrostatic surface potential (ESP) maps of **DMP5**, **G1** and the complex **DMP5**  $\supset$  **G1**. Both HOMO and LUMO of **DMP5** showed uniform distributions, while in the complex **DMP5**  $\supset$  **G1**, the distributions of the HOMO and LUMO became intricate. The cavity of **DMP5** showed negative charge distributions, while **G1** showed positive charge distributions on the sulfonium moiety. In the complex **DMP5**  $\supset$  **G1**, the positive charge distributions of the **DMP5** fragment were significantly increased because of the charge transfer from **G1** to **DMP5**. So **DMP5** could combine with **G1**, forming cation- $\pi$  interactions [48,49]. Then the noncovalent interaction (NCI) analyses were carried out to reveal the supramolecular interactions between **DMP5** and **G1** by the Independent Gradient Model approach (Fig. 1e and Fig. S12 in Supporting information) [50]. The NCI graph clearly showed multiple C-H...O hydrogen-bonding interactions and van der Waals interactions between **DMP5** and **G1**.

These evidences suggested the good binding ability of **DMP5** with **G1** and drove us to construct the supramolecular polymer network based on the non-covalent interactions between pillar[5]arenes and sulfonium salts.

We used the RAFT polymerization method to generate the copolymer **poly-P[5]A**. Owing to the  $^1\text{H}$  NMR spectrum of **poly-P[5]A**, the ratio of **P[5]A** units to MMA units was around 1:10, which was in good agreement with the feed ratio. The **P[5]A** units concentration was then regarded as the **poly-P[5]A** concentration. The GPC analysis revealed that **poly-P[5]A** had an average molecular weight of 53.0 kDa and PDI of 1.67 (Fig. S2 in Supporting information). Meanwhile, TGA was used to evaluate the thermal stability of **poly-P[5]A**. The mass losses of **poly-P[5]A** in different temperature intervals showed only 1.2% mass loss when up to

200 °C, indicating the good thermal stability of **poly-P[5]A** (Fig. S3 in Supporting information).

Because the bis(sulfonium) guest **G2** was hardly insoluble in chloroform but soluble in acetone, we investigated the host-guest interactions between pillar[5]arene-functionalized monomer **3** and **G2** in  $\text{CDCl}_3/\text{CD}_3\text{COCD}_3$  (2:1, v/v) solvent by  $^1\text{H}$  NMR spectroscopy (Figs. S13–S15 in Supporting information). The protons  $H_{a-f}$  of **G2** showed remarkable upfield shifts due to the shielding effect of **3**, while slight downfield shifts were observed for protons  $H_{9-10}$  of **3**. The 2D NOESY NMR spectroscopy experiment also suggested the NOE correlations between  $H_a$  of **G2** and  $H_{9-10}$  of **3**. The binding behavior of **3** with **G2** provided an opportunity for copolymer **poly-P[5]A** to form a supramolecular polymer network with **G2**.

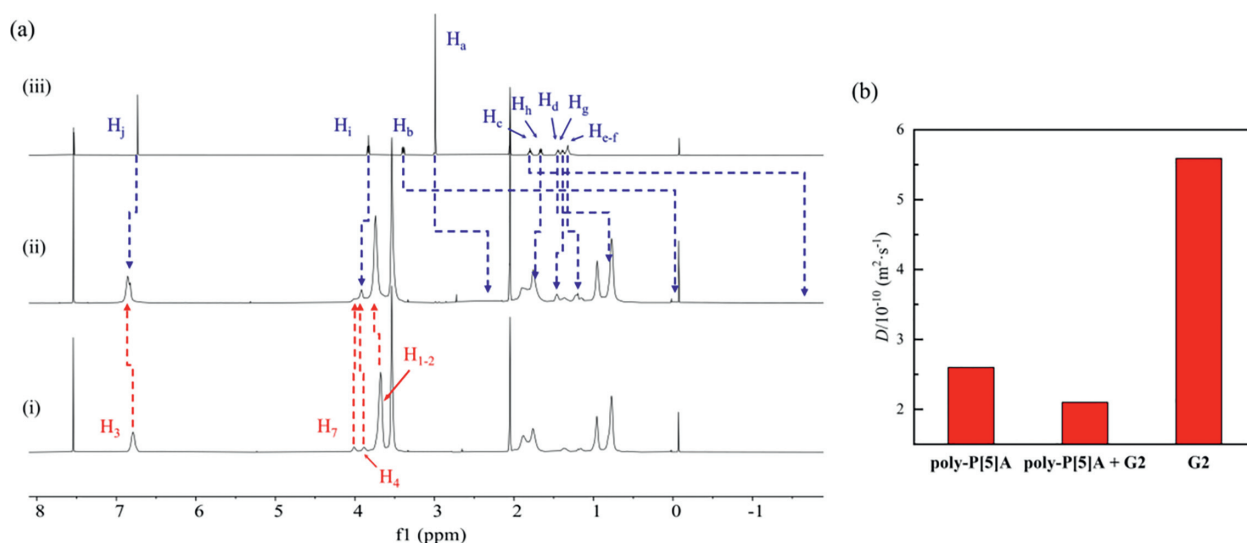
Since the pendant pillar[5]arene groups on **poly-P[5]A** could bind with the sulfonium moiety of **G2** as demonstrated above, a supramolecular network based on pillar[5]arene-sulfonium recognition motifs could be constructed. Firstly, the  $^1\text{H}$  NMR spectroscopy in the mixed solvent ( $\text{CDCl}_3/\text{CD}_3\text{COCD}_3 = 2:1$ , v/v) showed direct evidences of the interactions between **poly-P[5]A** and **G2** (Fig. 2a). The protons  $H_{a-f}$  of **G2** showed remarkable upfield shifts due to the shielding effect of electron-rich cavities of pillararenes, while methoxy protons  $H_2$  of **poly-P[5]A** showed slight downfield shifts. The pendant pillar[5]arene moieties kept good recognition property to sulfonium moieties despite the steric hindrance of the polymer backbone, showing similar behavior to the pillar[5]arene monomer **3**. Since such noncovalent linking behavior would form larger supramolecular aggregates, two-dimensional diffusion-ordered  $^1\text{H}$  NMR spectroscopy (DOSY) experiments were performed to investigate the formation of the supramolecular polymer network. Upon the addition of **G2** into a solution of **poly-P[5]A** in  $\text{CDCl}_3/\text{CD}_3\text{COCD}_3$  (2:1, v/v) solvent, the average diffusion coefficients ( $D$ ) decreased from  $2.60 \times 10^{-10}$  m $^2$ /s to  $2.10 \times 10^{-10}$  m $^2$ /s, suggesting the emergence of the supramolecular polymer network with an increase in the average aggregation size (Fig. 2b and Fig. S16 in Supporting information).

Viscosity measurement is a reliable method to reflect the property of polymers [17]. As the viscosity measurements showed, for the individual **poly-P[5]A**, the correlation between the specific viscosity and the concentration of **poly-P[5]A** was almost linear over the concentration range of 5.3–24.0 mmol/L, suggesting that no significant physical entanglements occurred. However, the specific viscosity of the mixture of **poly-P[5]A** and **G2** increased exponentially with the increase of concentration when risen to around 15.3 mmol/L, indicating the self-assembly process occurred and formed the supramolecular polymer network (Fig. 3) [51].

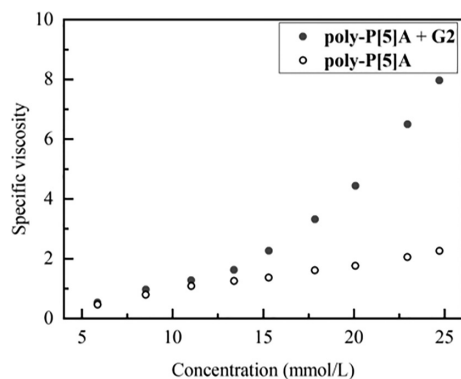
Scanning electron micrography (SEM) was employed to reveal the morphological transformation of the formation of the supramolecular network (Fig. 4). The SEM image of **poly-P[5]A** presented a tightly arranged bubble film. After the addition of **G2**, the SEM image turned to intertangled porous structures, suggesting the formation of a cross-linked network. Transmission electron microscopy (TEM) experiments were also carried out to visualize the structures of the supramolecular polymer network, in which intertangled network structures could be observed (Fig. S17 in Supporting information).

Therefore, the above results further confirmed the formation of the supramolecular polymer network owing to the host-guest interactions between pillar[5]arenes and sulfonium salts.

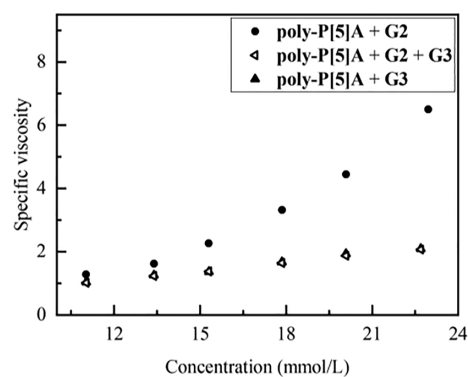
Since the networks were formed through host-guest interactions between the pendant pillararenes and sulfonium groups, they could be dissociated by a variety of external stimuli. First, we investigated the dissociation of the supramolecular polymer network by adding competitive guest molecules. 1,4-Butanedinitrile **G3**, which could strongly bind with pillar[5]arene [52], was chosen as the competitive guest. The transformation of the addition of **G3** into the supramolecular polymer network was firstly studied



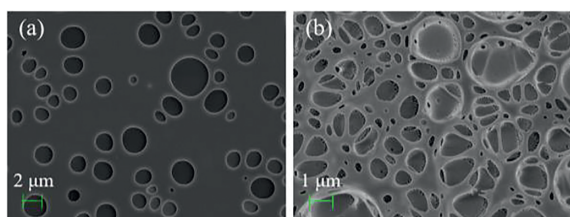
**Fig. 2.** (a)  $^1\text{H}$  NMR spectra of (i) **poly-P[5]A** (10.0 mmol/L), (ii) **poly-P[5]A** (10.0 mmol/L) + **G2** (5.0 mmol/L), (iii) **G2** (10.0 mmol/L) in  $\text{CDCl}_3/\text{CD}_3\text{COCD}_3$  (2:1, v/v, 600 MHz, 298 K); (b) 2D DOSY spectra of **poly-P[5]A** (10.0 mmol/L), **G2** (5.0 mmol/L) and a mixture of **poly-P[5]A** (10.0 mmol/L) + **G2** (5.0 mmol/L) in  $\text{CDCl}_3/\text{CD}_3\text{COCD}_3$  (2:1, v/v, 600 MHz, 298 K).



**Fig. 3.** Specific viscosities of **poly-P[5]A** and a mixture of **poly-P[5]A** + **G2** (1:1 molar ratio) versus the concentration of **poly-P[5]A**.



**Fig. 5.** Specific viscosities of mixtures of **poly-P[5]A** + **G2** (2:1 molar ratio), **poly-P[5]A** + **G2** + **G3** (2:1:2 molar ratio) and **poly-P[5]A** + **G3** (1:1 molar ratio) versus the concentration of **poly-P[5]A**.



**Fig. 4.** SEM images of (a) **poly-P[5]A**; (b) a mixture of **poly-P[5]A** + **G2**.

by  $^1\text{H}$  NMR spectroscopy (Fig. S18 in Supporting information). The protons of **G3** exhibited remarkable upfield shift changes from 2.83 ppm to  $-1.33$  ppm, while the protons of **G2** recovered to the free uncomplexed state, suggesting that **G3** could form a stronger complex with pillar[5]arene and lead to the dissociation of the supramolecular polymer network. The viscosity measurements further confirmed the transformation (Fig. 5). With the presence of **G3**, the specific viscosity of the mixture decreased significantly due to the dissociation of supramolecular aggregates.

Then, the dissociation of the supramolecular polymer network by competitive host molecules was investigated. With the addition of **DMP5** into the solution of **poly-P[5]A** and **G2**, the viscosity of the solution decreased as expected, which was driven by the complexation of free **DMP5** and **G2** (Fig. S19 in Supporting in-

formation). In addition, host-guest complexation is sensitive to temperature. When heated to  $45^\circ\text{C}$ , the protons  $\text{H}_a$  of **G2** exhibited small downfield shift changes, indicating heating behavior led to slight disassembly of the supramolecular polymer network (Fig. S20 in Supporting information).

Since we demonstrated the formation of the supramolecular polymer network, a supramolecular gel could be prepared based on **poly-P[5]A** and **G2**. However, directly mixing **poly-P[5]A** and **G2** (2:1 molar ratio) in  $\text{CHCl}_3/\text{CH}_3\text{COCH}_3$  (2:1, v/v) solvent, we only obtained a slightly yellow solution with high viscosity even the concentration of **poly-P[5]A** was up to 125.0 mmol/L. Since the choice of solvent has a great influence on the preparation of a gel, we screened a variety of solvents. Mixing **poly-P[5]A** with **G2** in pure chloroform, a supramolecular gel was finally obtained.

The gel also could be dissociated by heating and the addition of **G3** or **DMP5**. When **G3** or **DMP5** were directly added to the supramolecular gel and shook for a while, the gel immediately turned to a sol (Fig. 6). And when heated to  $50^\circ\text{C}$  for several minutes, the gel was also dissociated into a transparent solution. Re-formation of the gel could be achieved by cooling and standing for a while.

In conclusion, we have successfully developed a novel supramolecular network *via* host-guest interactions between the

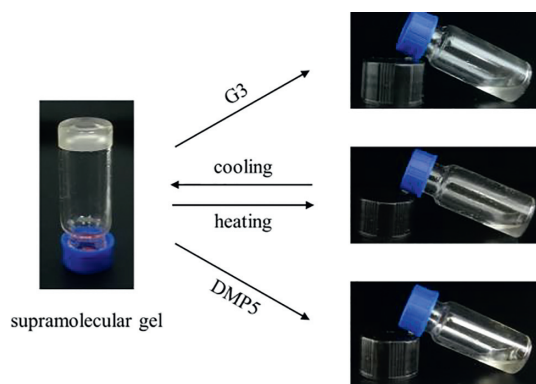


Fig. 6. Reversible gel-sol transition of supramolecular gel.

copolymer **poly-P[5]A** and bis(sulfonium) dication guest **G2**, which is the first time that the sulfonium salts have been introduced to fabricate a supramolecular polymer network. The network exhibited significant changes both in NMR spectroscopy and viscosity property compared to the copolymer **poly-P[5]A**. Moreover, based on the competition of host-guest interactions, the network structure can be destroyed by external stimuli, including competitive molecules and heating. This work is the marriage of supramolecular chemistry and polymer science, we hope this supramolecular network system may give a new way to develop novel multi stimuli-responsive materials in the future. Further exploring of functional supramolecular network systems based on pillar[5]arenes and sulfonium salts derivatives is now ongoing in our laboratory.

#### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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#### Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.ccl.2022.03.103.

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