

Supplementary Information for

Supramolecular gels based on monopyrrolotetrathiafulvalene and its TCNQ charge-transfer complex

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1. FT-IR spectra of compounds **1c** with TCNQ

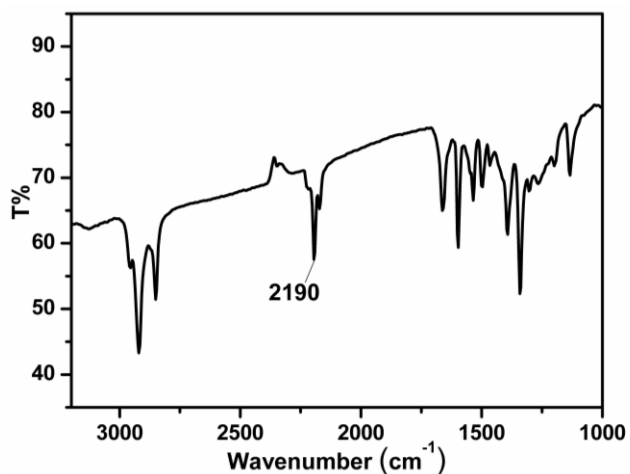


Figure S1 FT-IR spectra of the mixture of **1c** with TCNQ (1:1) in CHCl₃.

2. Gels photograph

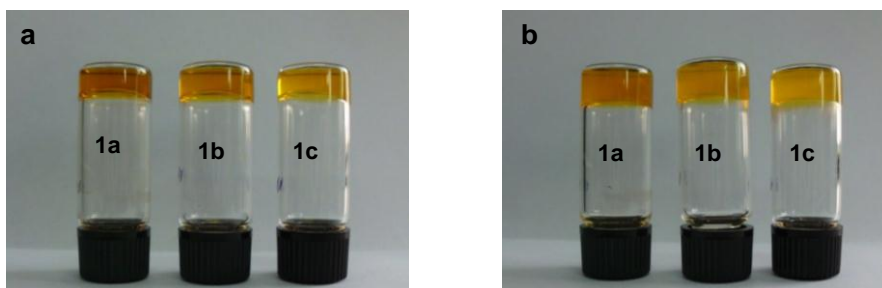


Figure S2 The photographs of gelators **1a-c** in (a) cyclohexane; (b) *n*-hexane.

3. Gelation properties of the compounds

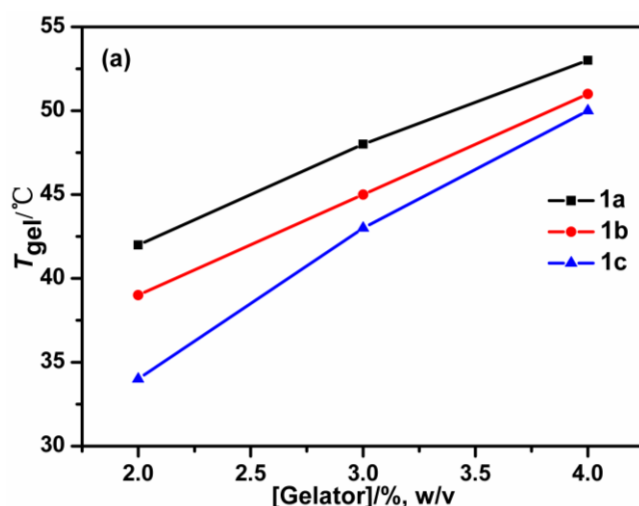
Table S1 Gelation properties of **1a-c** in various solvents.

Solvent	1a	1b	1c
Cyclohexane	TG ^a (3.9) ^b	TG(2.9)	TG(2.5)
<i>n</i> -Hexane	OG(1.4)	OG(1.5)	OG (1.9)
<i>n</i> -Heptane	OG(1.3)	OG (1.4)	OG (1.85)
<i>n</i> -Octane	OG(1.25)	OG (1.35)	OG (1.82)
CH ₃ CN	P	P	P
Methanol	P	P	P
Ethanol	OG(28)	OG(5.28)	OG(3.83)
<i>n</i> -Buthanol	S	OG(18.3)	OG(12.8)
<i>n</i> -Pathanol	S	OG(34)	OG(20.4)
EtOAc	S	S	S
Toluene	S	S	S
CH ₂ Cl ₂	S	S	S
CHCl ₃	S	S	S
Acetone	S	S	S
DMF	S	S	S
THF	S	S	S

^aTG: transparent gel, OG: opaque gel, S: soluble, P:precipitate.

^bCGC is the critical gelation concentration at which gelation was observed to restrict the flow of the medium at room temperature.

4. Gel-sol transition temperature



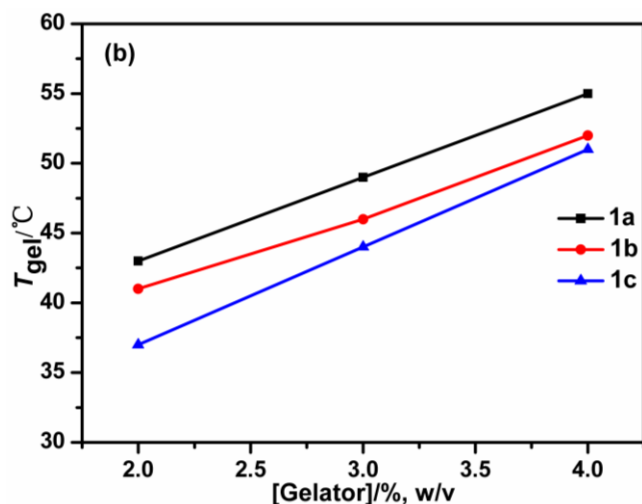


Figure S3 Plots of T_{gel} versus the concentration of **1a-c** in (a) *n*-heptane and (b) *n*-octane.

5. Gelation properties of the CT complexes

Table S2 Gelation properties of CT complexes.

Solvent	1a	1b	1c
Cyclohexane	OG(5.4)	OG(3.53)	OG(3.24)
<i>n</i> -Hexane	OG(3.97)	OG(4.15)	OG (4.22)
<i>n</i> -Heptane	OG(3.95)	OG (4.1)	OG (4.15)
<i>n</i> -Octane	OG(3.95)	OG (4.08)	OG (4.12)

6. XRD of gel **1c** and **1c**/TCNQ CT complex gel

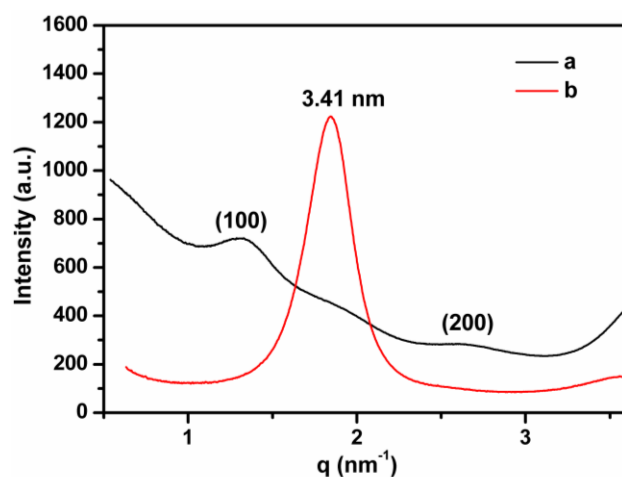


Figure S4 XRD patterns of xerogel **1c** from *n*-hexane (a) and xerogel **1c**/TCNQ (mole ratio = 1:1) from *n*-hexane (b).

7. FT-IR of the gels

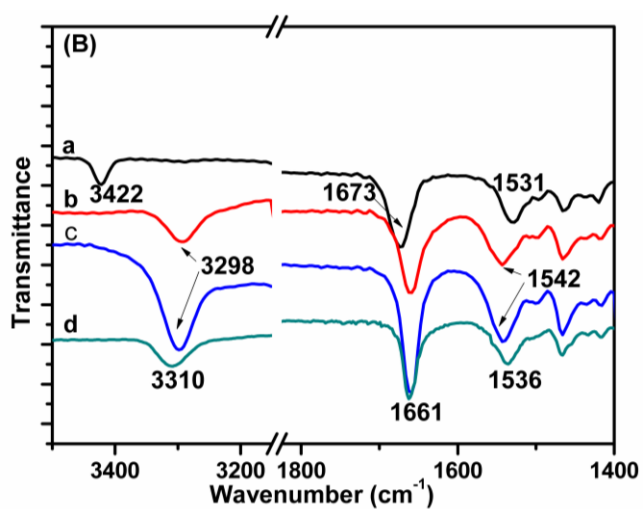
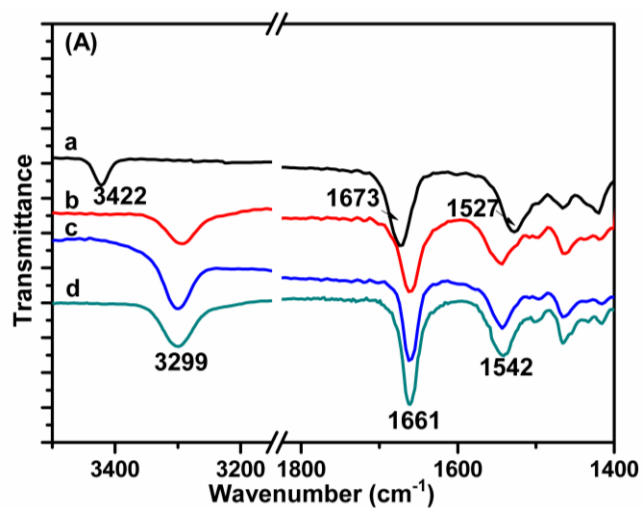
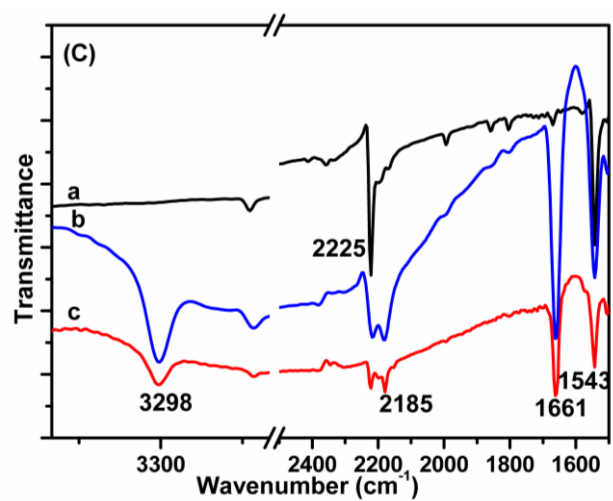


Figure S5 FT-IR spectra of **1a** (A) and **1b** (B) (a) in CHCl_3 solution; (b) cyclohexane gel; (c) *n*-hexane gel; (d) powder.



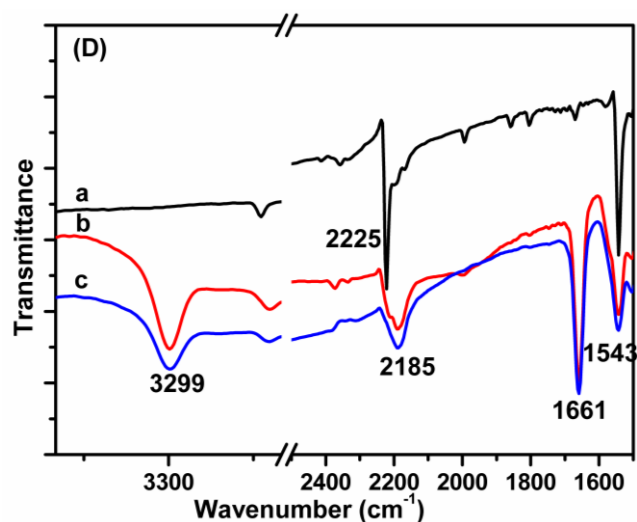


Figure S6 FT-IR spectra of xerogel of (C) **1a**; (D) **1b** and TCNQ 1: 1 CT complex (a) TCNQ; (b) from cyclohexane; (c) from *n*-hexane, which were measured by using KBr pellet.

8. Anions responsive

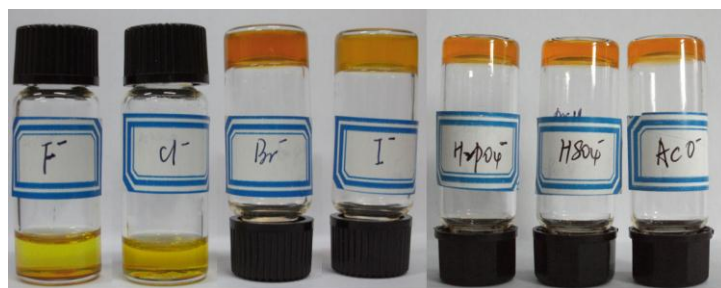


Figure S7 The variety of the gel **1c** in cyclohexane or *n*-hexane by anions stimulation.

9. ¹H NMR spectra

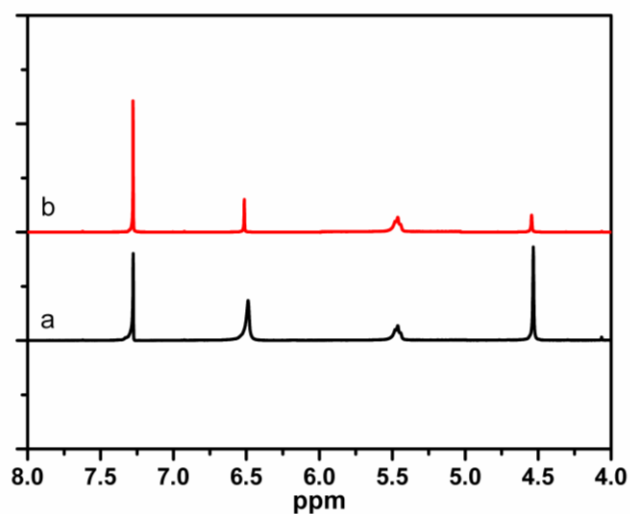


Figure S8 Partial ¹H NMR spectra of **1c** (2mM) in CDCl₃ upon the addition of AcO⁻ : (a) free; (b) 1.0 equiv.