

## Supplementary Information

### **A smart organic gel template as metal cation and inorganic anions sensor**

Novina Malviya,<sup>a</sup> Mriganka Das,<sup>a</sup> Poulami Mandal,<sup>a</sup> and Suman Mukhopadhyay<sup>\*a,b</sup>

<sup>a</sup>*Department of Chemistry, School of Basic Sciences, Indian Institute of Technology Indore, Simrol 453552 Indore, India.*

<sup>b</sup>*Center for Bioscience and Biomedical Engineering, Indian Institute of Technology Indore, Simrol 453552 Indore, India.*

*Email: [suman@iiti.ac.in](mailto:suman@iiti.ac.in)*

## Table of Contents

**Fig. S1.** FT-IR spectrum of gelator (**G1**).

**Fig. S2.**  $^1\text{H}$  NMR spectrum of gelator (**G1**).

**Fig. S3.**  $^{13}\text{C}$  NMR spectrum of gelator (**G1**).

**Fig. S4.** ESI- Mass spectrum of gelator (**G1**).

**Fig. S5.** "Inversion of a test tube" method

**Fig. S6.** FT-IR spectra of xerogel of **G1**.

**Fig. S7.** Partial  $^1\text{H}$  NMR spectra of **G1** in DMSO  $d_6$  at different concentrations:(a) 20 mM; (b) 100 mM; (c) 150 mM.

**Fig. S8.** Photographs of Sol-Gel of gelator **G1** in DMF and **G1** in the presence of various metal ions (using their perchlorate salts as the sources, **G1**: cation =2:1) under day light.

**Fig. S9-S13.** FT-IR spectra of xerogel of **ZnG1**, **NiG1**, **CuG1**, **Fe<sup>II</sup>G1**, **Fe<sup>III</sup>G1**.

**Fig. S14-S17.** FT-IR spectra of xerogel of **ZnG1+Br<sup>-</sup>**, **NiG1+CN<sup>-</sup>**, **CuG1+SCN<sup>-</sup>**, **Fe<sup>II</sup>G1+S<sup>2-</sup>**.

**Fig. S18.** Fluorescence spectra of (a) **ZnG1** (b) **NiG1** (c) **CuG1** (d) **FeG1** in the presence of mixture of anions at room temperature.

**Fig. S19.** (a) Fluorescence spectra of **ZnG1** with increasing concentration of **Br<sup>-</sup>** (using 0.01M **KBr** water solution as the **Br<sup>-</sup>** sources); (b) Fluorescence spectra of **NiG1** with increasing concentration of **CN<sup>-</sup>** (using 0.01M **NaCN** water solution as the **CN<sup>-</sup>** sources),(c) Fluorescence spectra of **CuG1** with increasing concentration of **SCN<sup>-</sup>** (using 0.01M **NaSCN** water solution as the **SCN<sup>-</sup>** sources); (d) Fluorescence spectra of **FeG1** with increasing concentration of **S<sup>2-</sup>**(using 0.01M **Na<sub>2</sub>S** water solution as the **S<sup>2-</sup>** sources),  $\lambda_{\text{exc}} = 350 \text{ nm}$ .

**Fig. S20-S23.** Linear viscoelastic (LSV) and Frequency sweep (FS) rheometry of **ZnG1**, **CuG1**, **NiG1**, **FeG1** The angular frequency (rad/s), storage modulus  $G'$  (Pa) and loss modulus  $G''$  (Pa) are shown as log scale.

**Fig. S24-S27.** SEM images of xerogel of **ZnG1**, **NiG1**, **FeG1**, **CuG1**.

**Fig. S28.** Powder XRD patterns of xerogel of **ZnG1**, **CuG1**, **NiG1**, **FeG1**.

**Fig. S29.** Powder XRD patterns of xerogel of **ZnG1+Br<sup>-</sup>**, **CuG1+SCN<sup>-</sup>**, **NiG1+CN<sup>-</sup>**, **FeG1+S<sup>2-</sup>**.

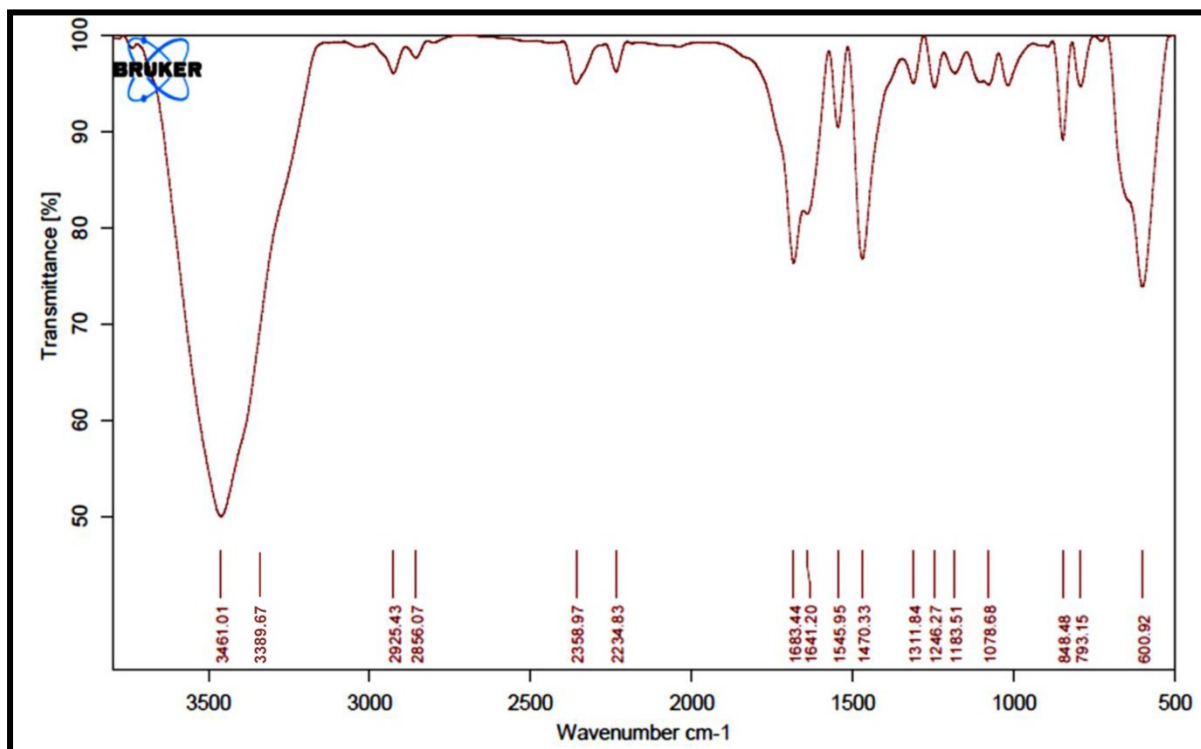
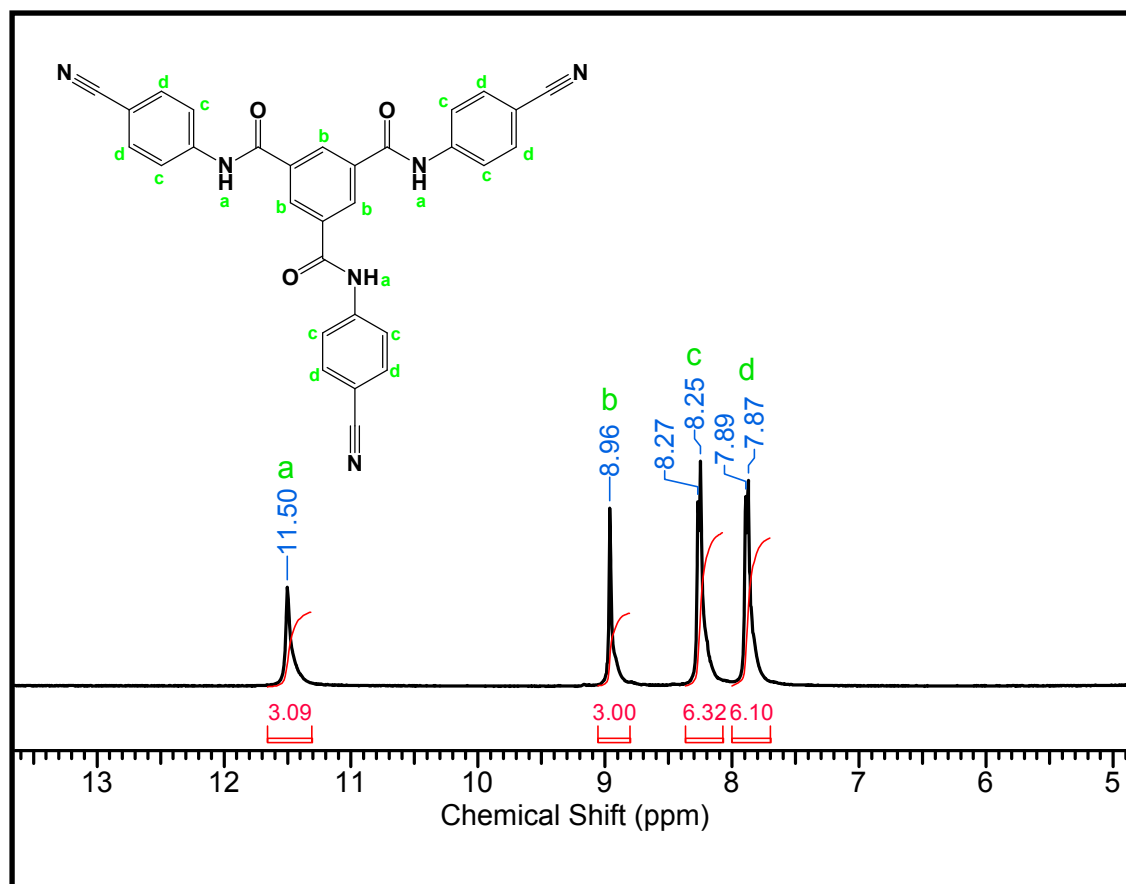
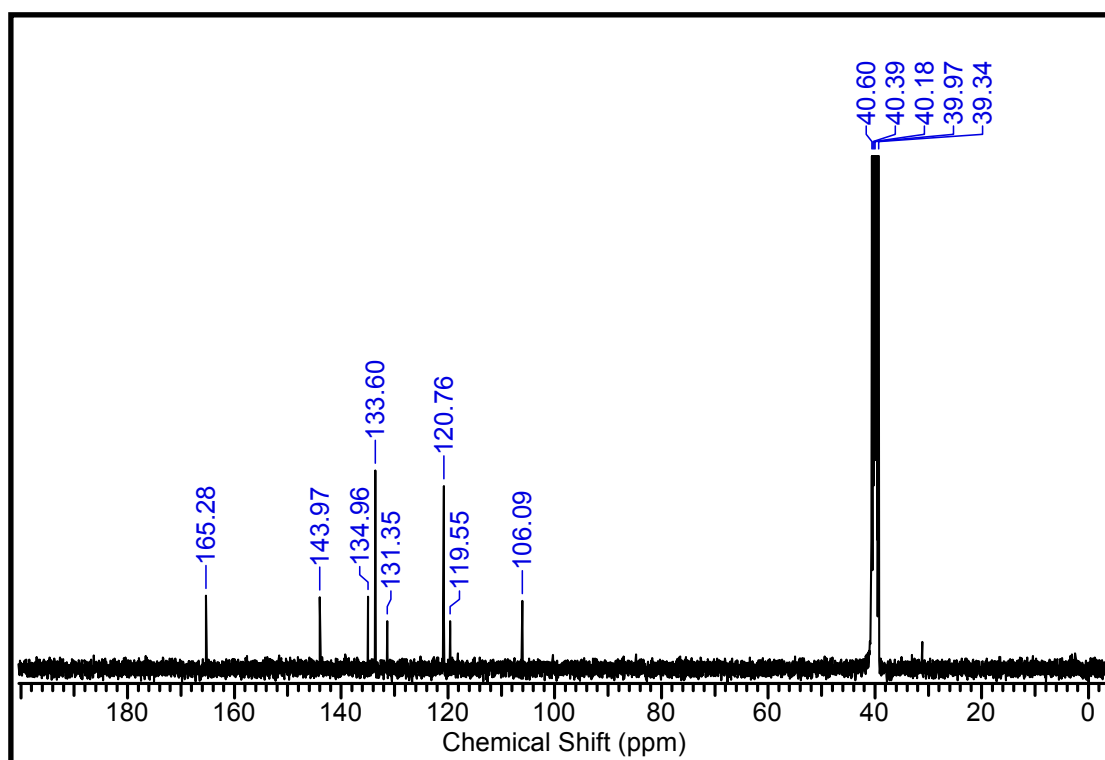


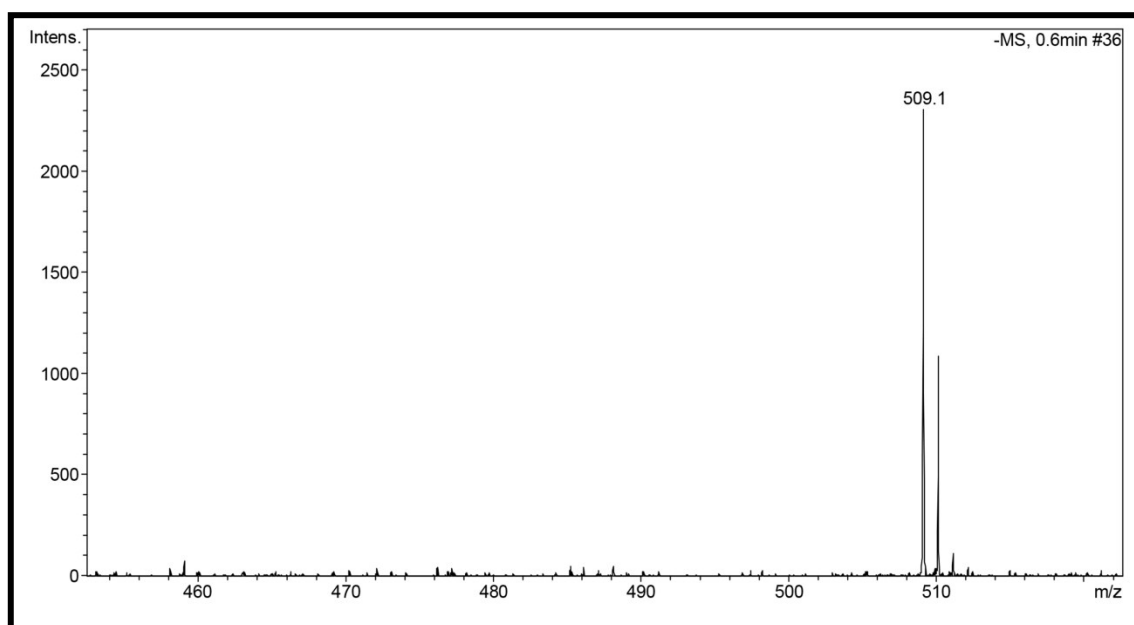
Fig. S1 FT-IR spectrum of gelator molecule **G1**.



**Fig. S2**  $^1\text{H}$  NMR spectrum of gelator molecule **G1**.



**Fig. S3**  $^{13}\text{C}$  NMR spectrum of gelator molecule **G1**.



**Fig. S4** ESI- Mass spectrum of gelator molecule **G1**.

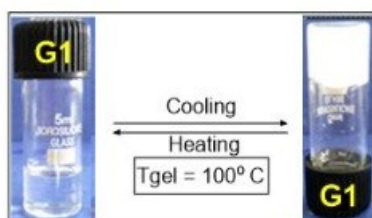


Fig. S5 "Inversion of a test tube" method.

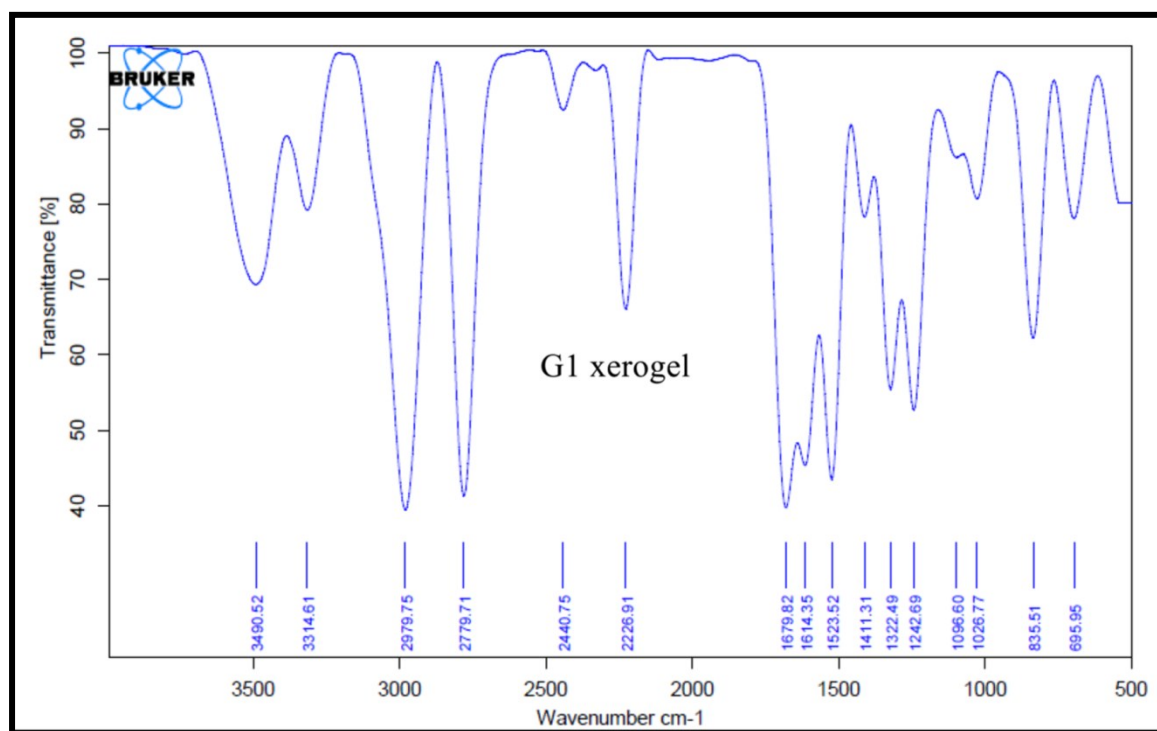
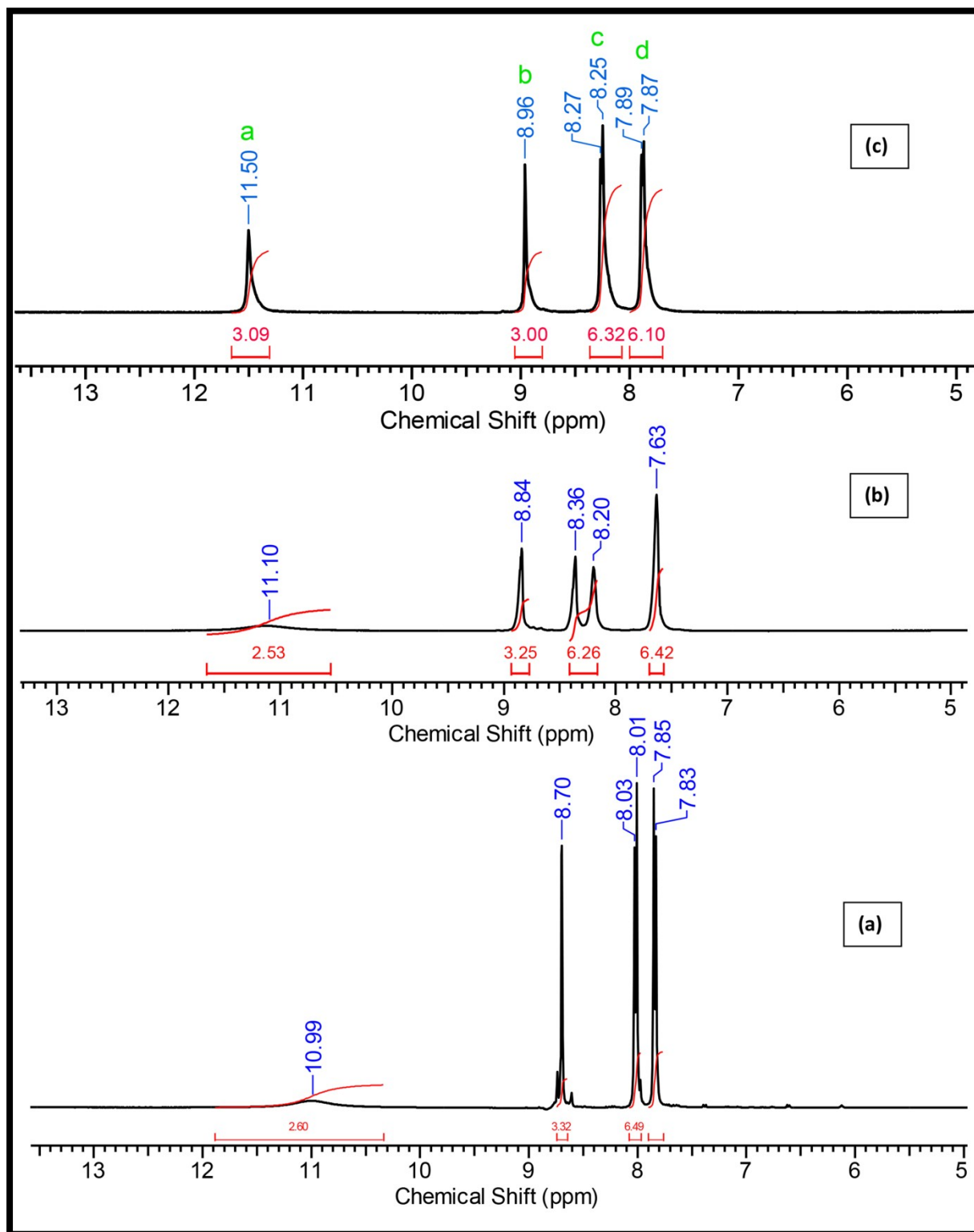
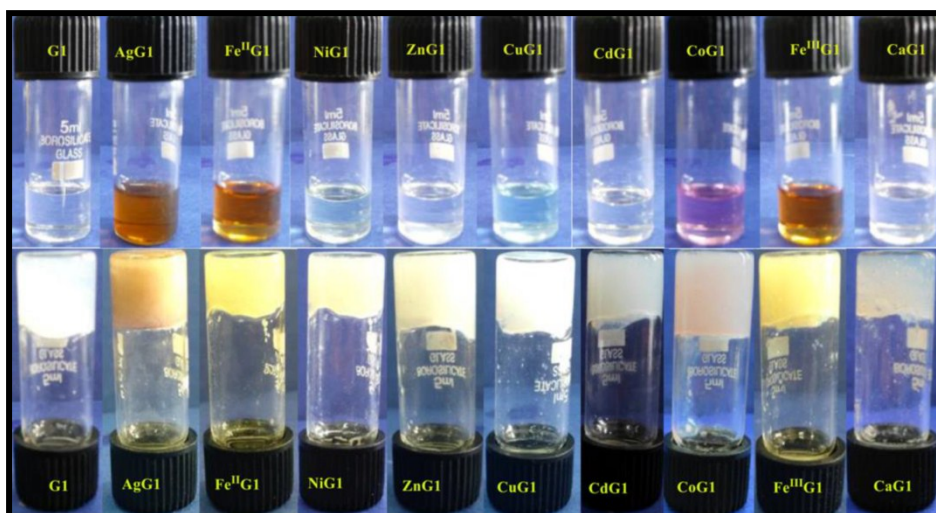


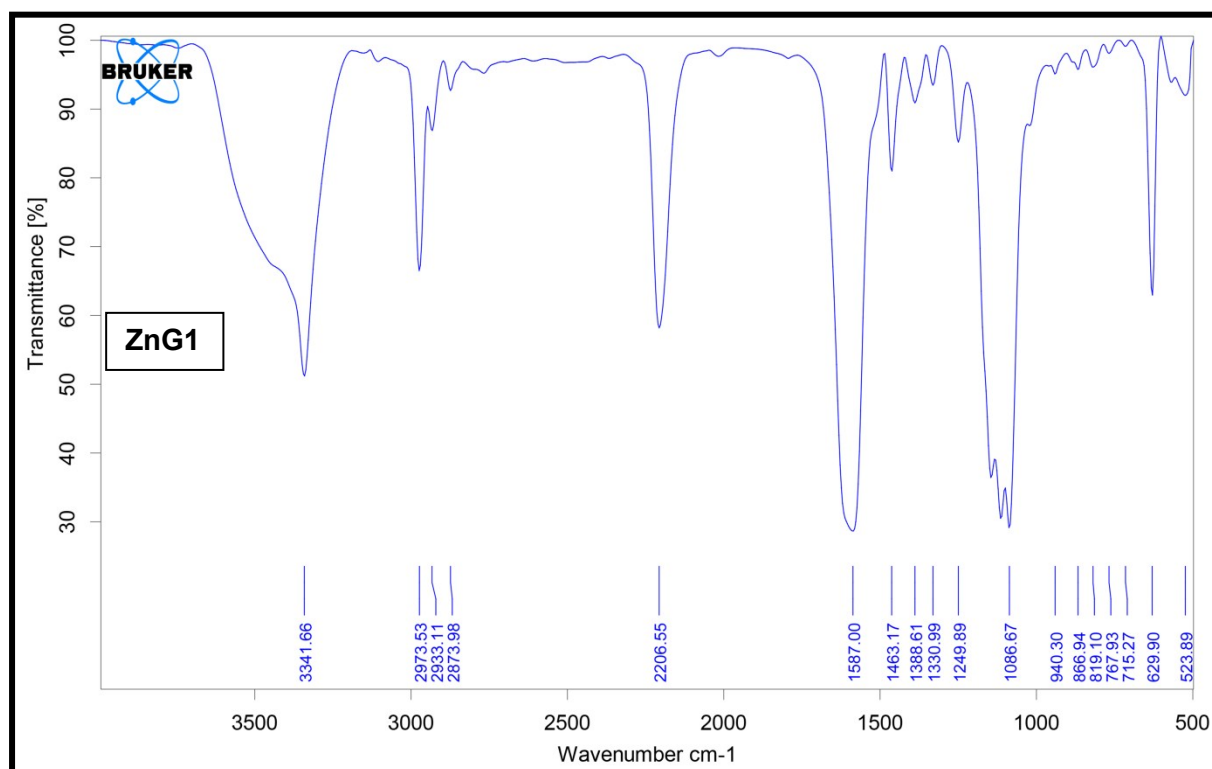
Fig. S6 FT-IR spectra of xerogel of G1 .

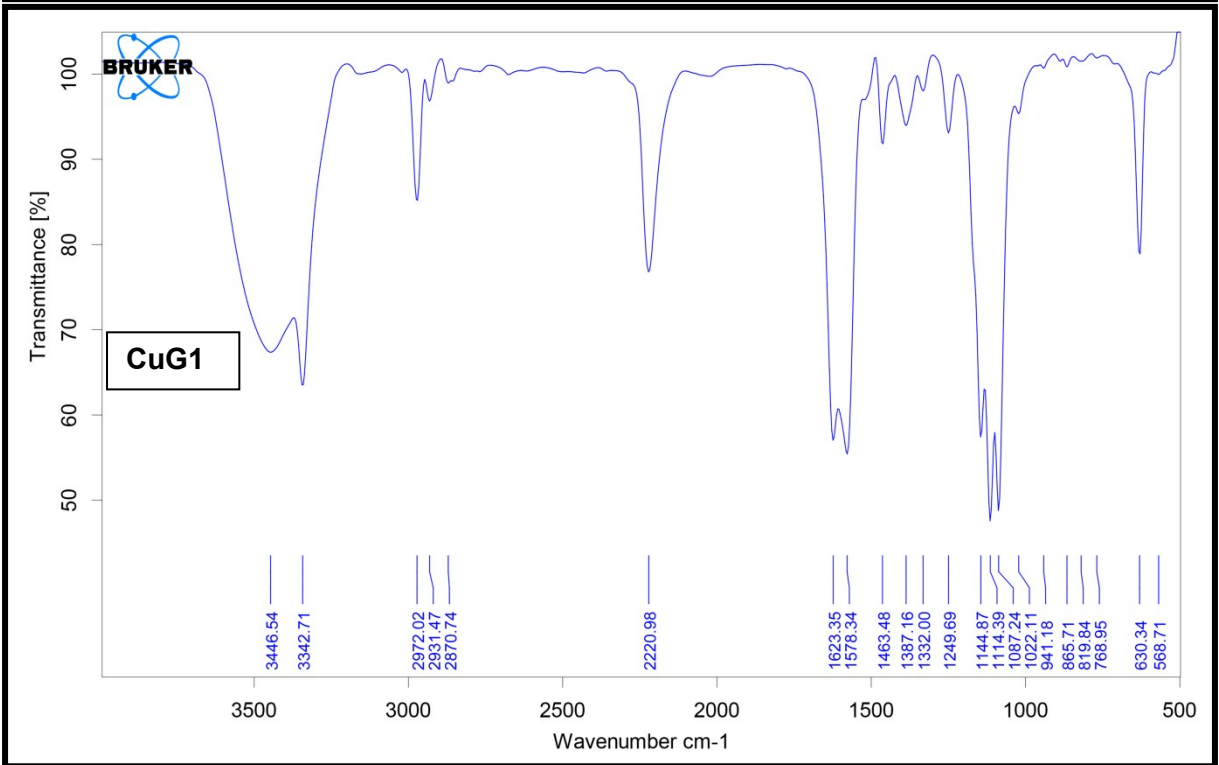
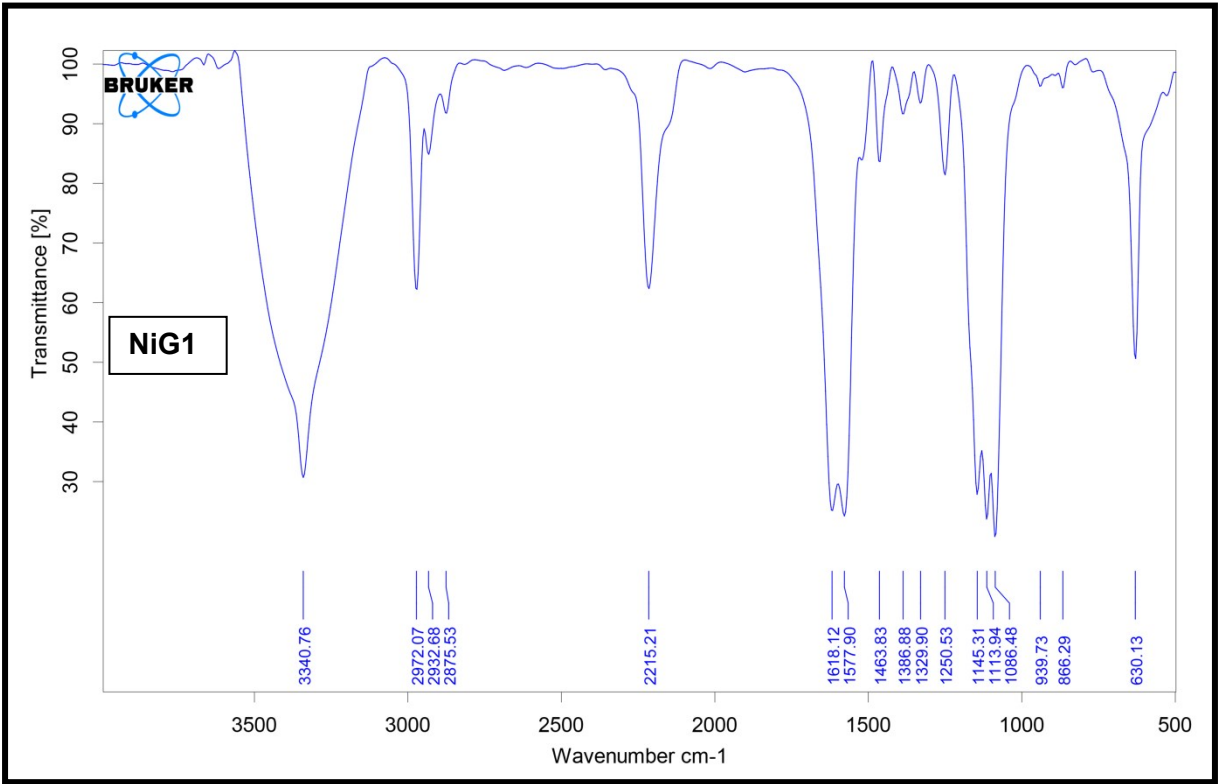


**Fig. S7** Partial  $^1\text{H}$  NMR spectra of G1 in  $\text{DMSO-}d_6$  at different concentrations: (a) 20 mM (b) 100 mM (c) 150 mM.



**Fig. S8** Photographs of Sol-Gel of gelator **G1** in DMF and **G1** in the presence of various metal ions (using their perchlorate salts as the sources, **G1** : cation = 2:1) under day light.







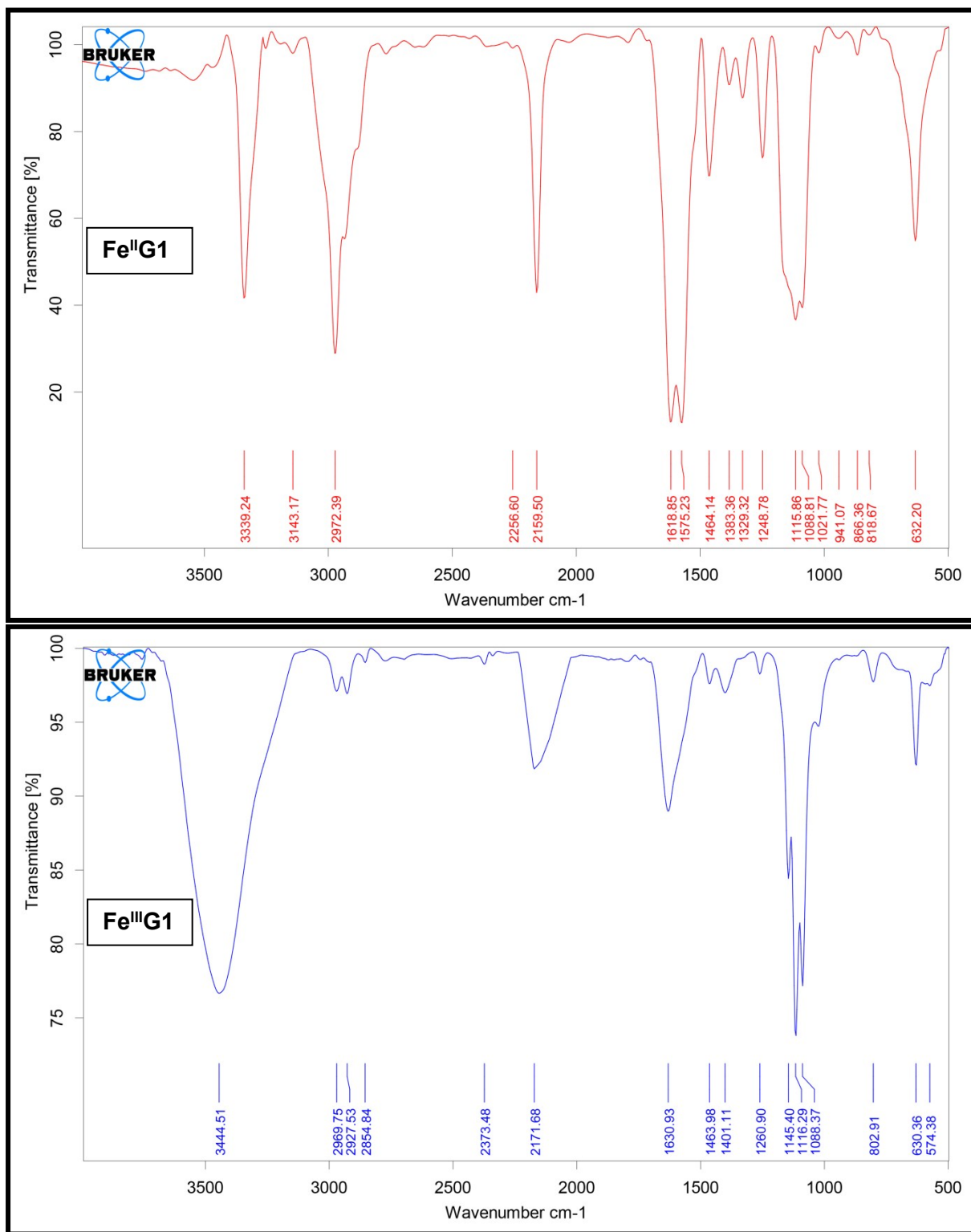
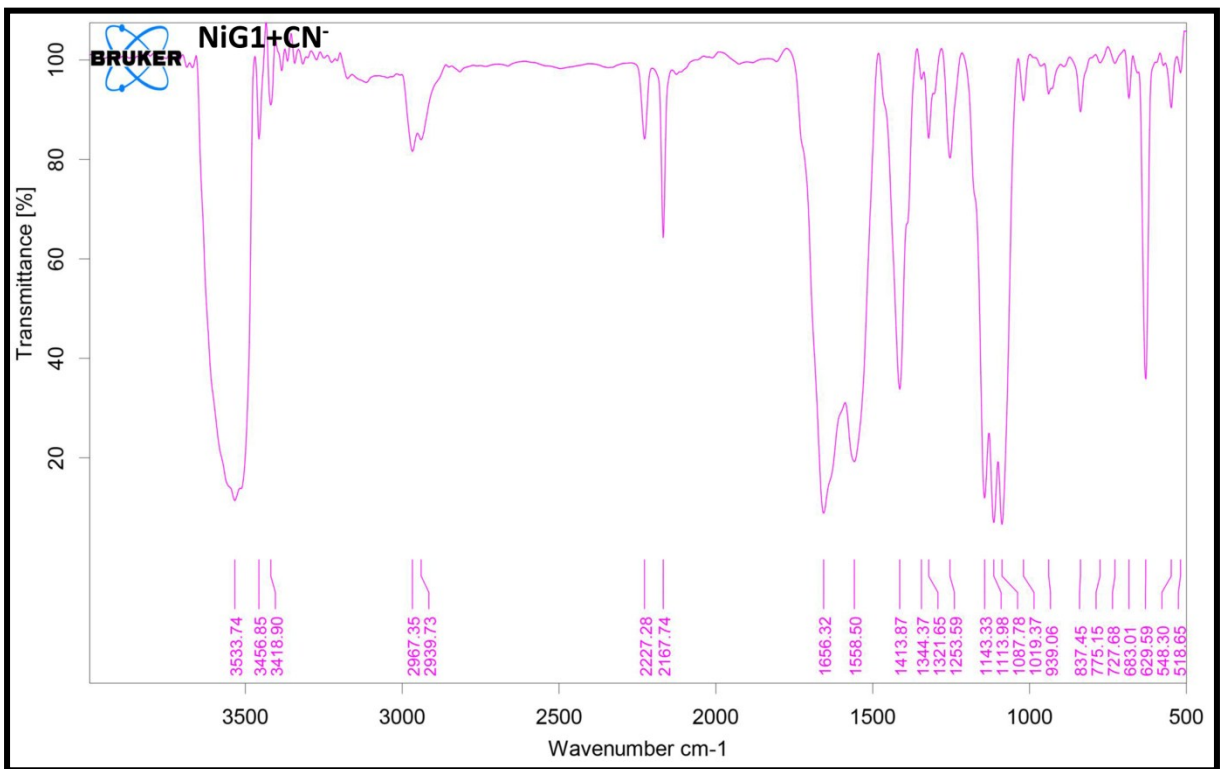
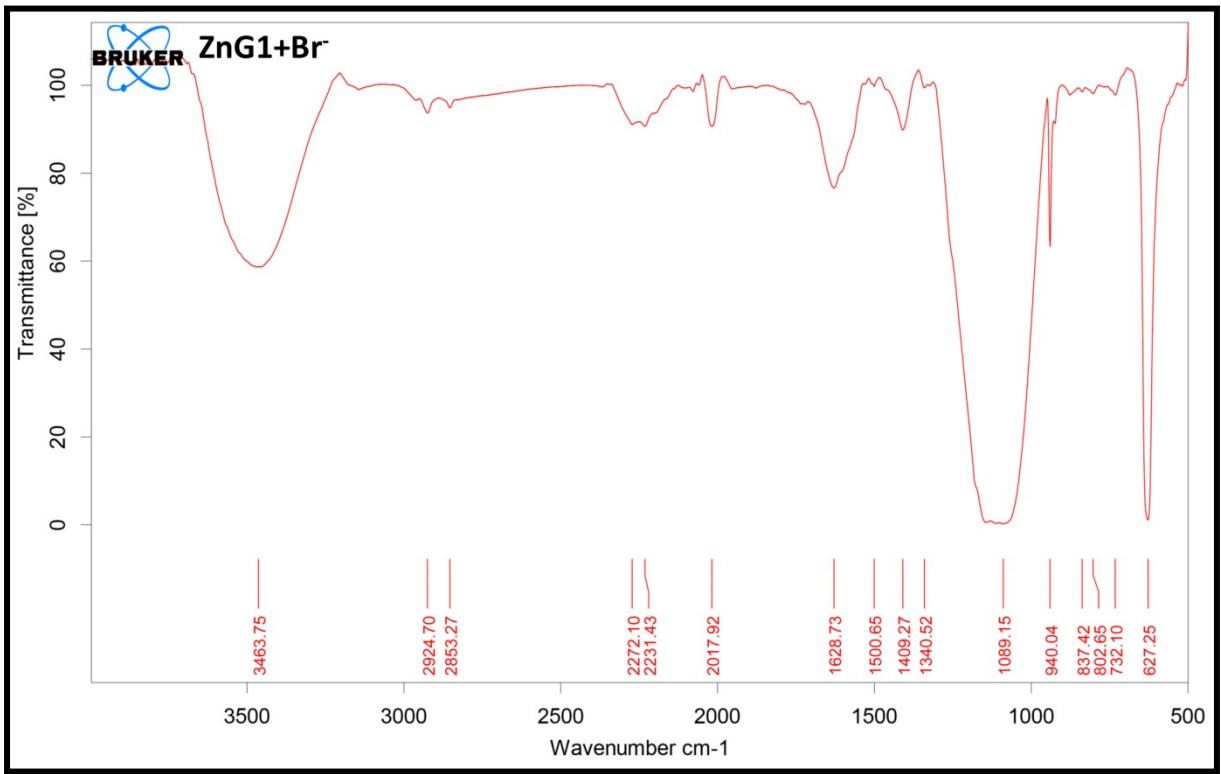


Fig. S9-S13 FT-IR spectra of xerogel of ZnG1, NiG1, CuG1, Fe<sup>II</sup>G1, Fe<sup>III</sup>G1.



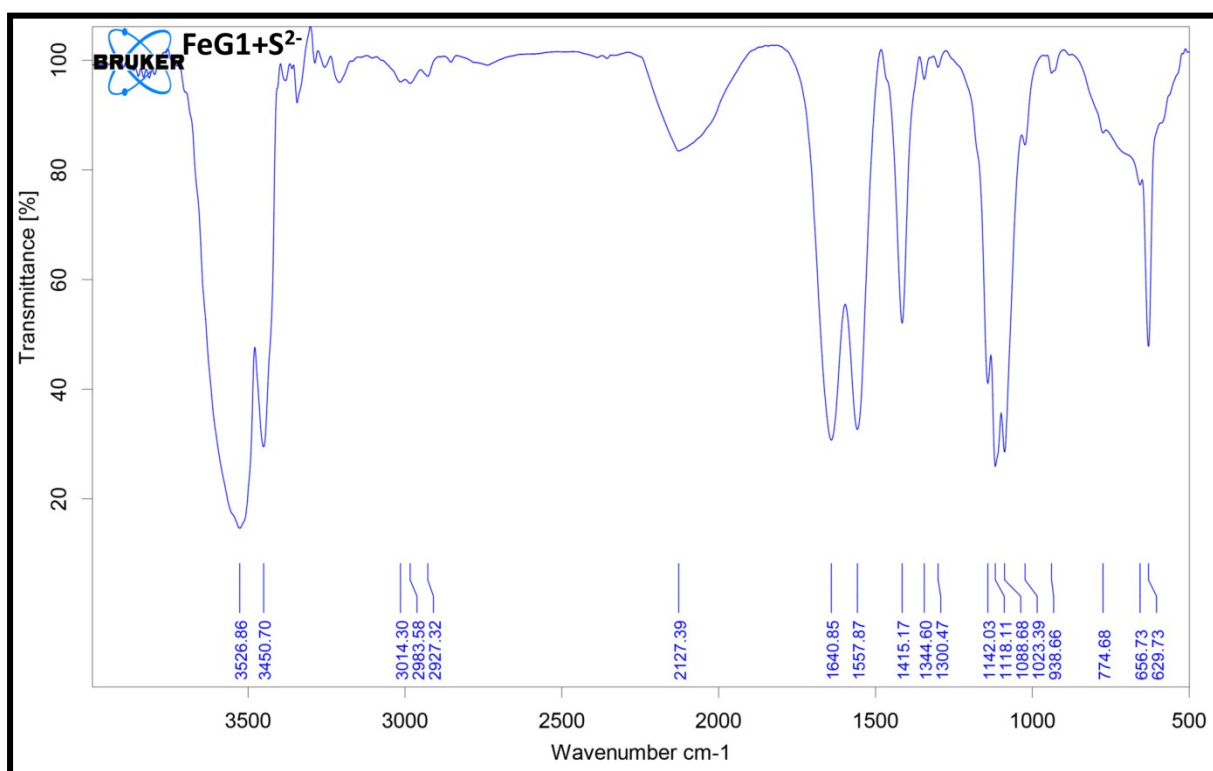
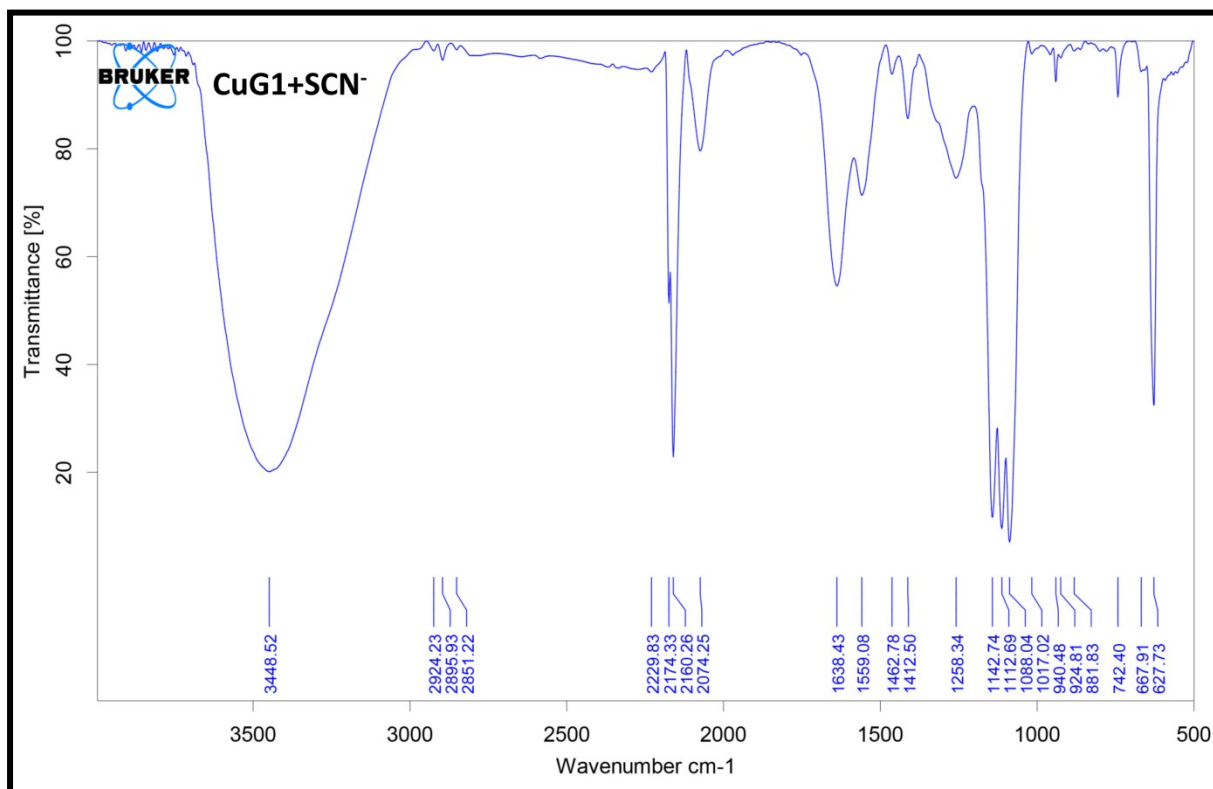
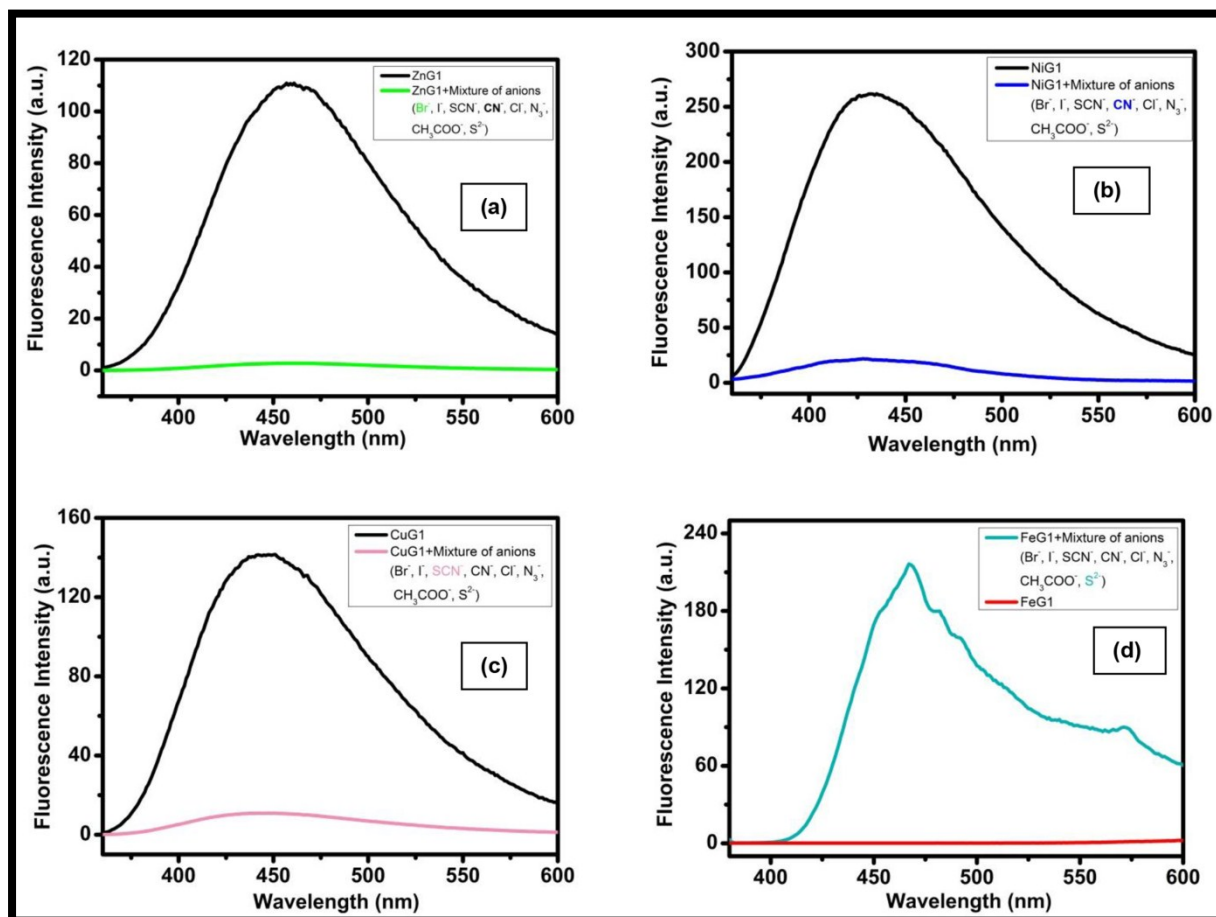


Fig. S14-S17. FT-IR spectra of xerogel of ZnG1+Br<sup>-</sup>, NiG1+CN<sup>-</sup>, CuG1+SCN<sup>-</sup>, Fe<sup>II</sup>G1+S<sup>2-</sup>.



**Fig. S18** Fluorescence spectra of (a) **ZnG1** (b) **NiG1** (c) **CuG1** (d) **FeG1** in the presence of mixture of anions at room temperature.

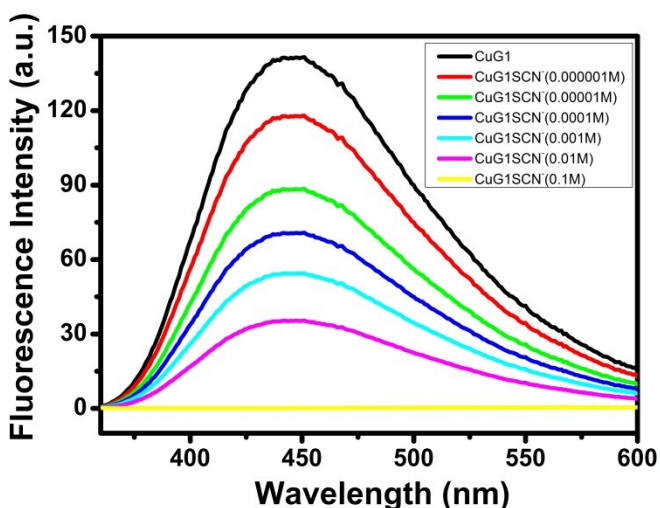
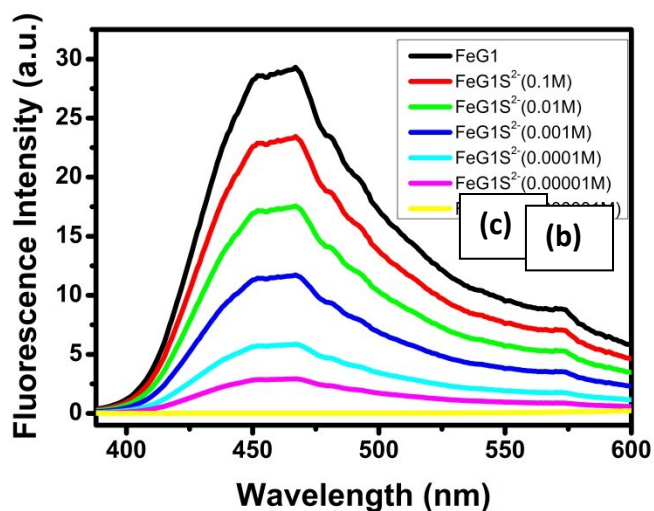
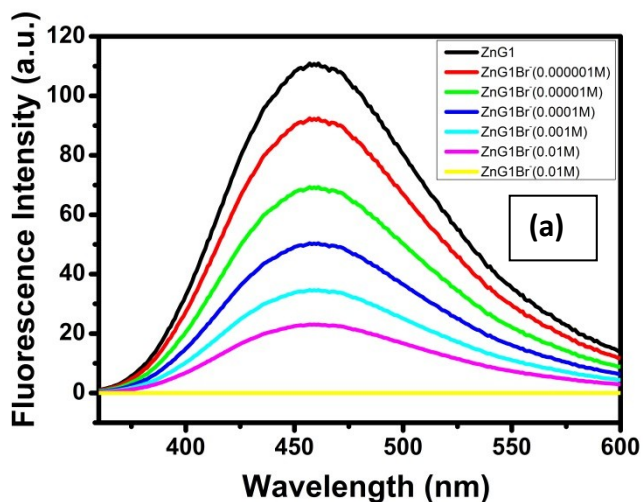


Fig. S19 (a) Fluorescence spectra of ZnG1 with increasing concentration of Br<sup>-</sup> (using 0.01M KBr water solution as the Br<sup>-</sup> sources); (b) Fluorescence spectra of NiG1 with increasing concentration of CN<sup>-</sup> (using 0.01M NaCN water solution as the CN<sup>-</sup> sources), (c) Fluorescence spectra of CuG1 with increasing concentration of SCN<sup>-</sup> (using 0.01M NaSCN water solution as the SCN<sup>-</sup> sources); (d) Fluorescence spectra of FeG1 with increasing concentration of S<sup>2-</sup> (using 0.01M Na<sub>2</sub>S water solution as the S<sup>2-</sup> sources),  $\lambda_{exc} = 350$  nm.

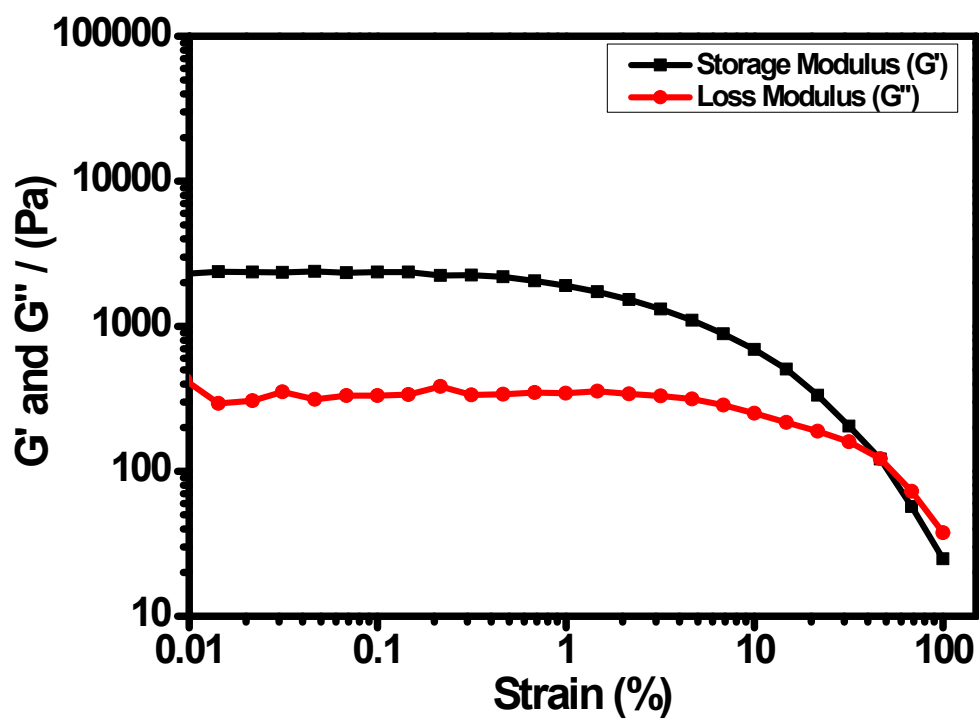


Fig. S20(a) Linear viscoelastic (LVE) property of FeG1.

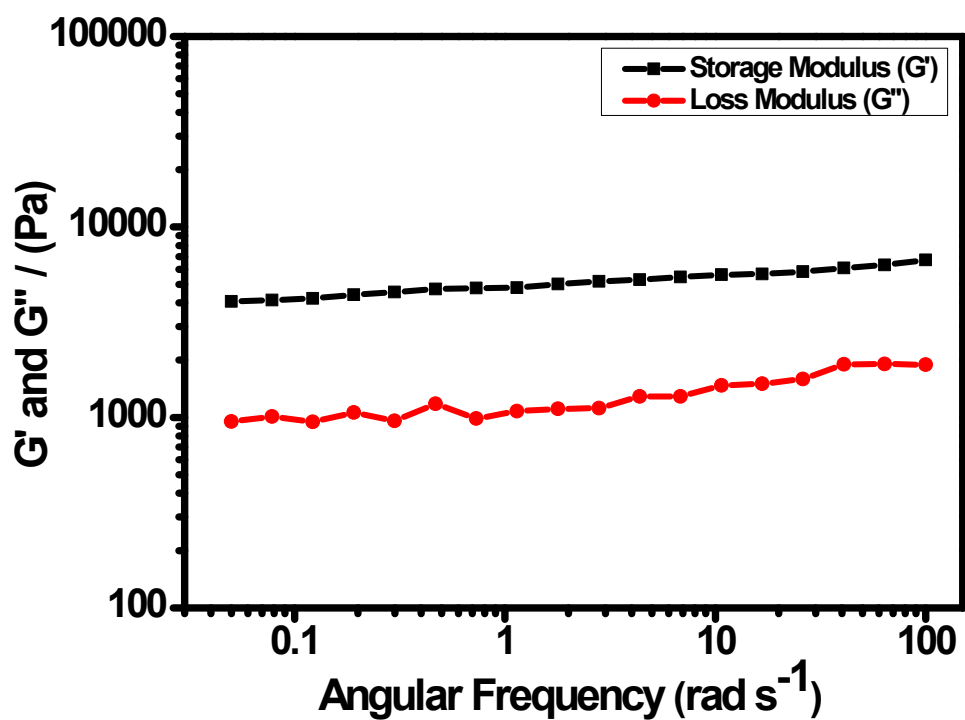


Fig. S20(b) The dynamic frequency sweep rheometry of FeG1. (Storage modulus  $G'$  is higher than the loss modulus  $G''$ ).

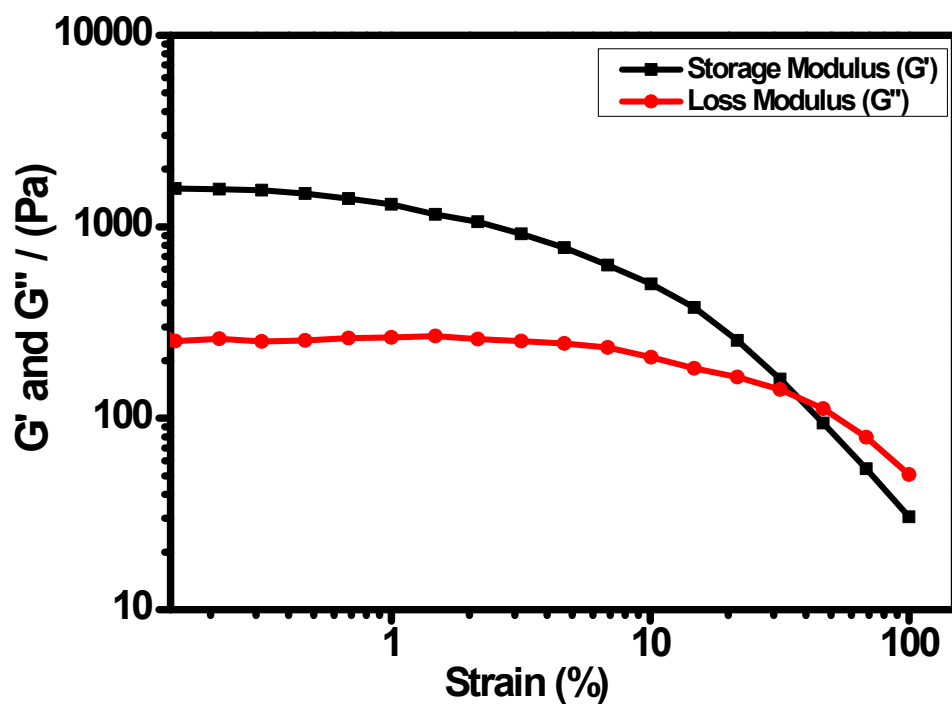


Fig. S21(a) Linear viscoelastic (LVE) property of CuG1.

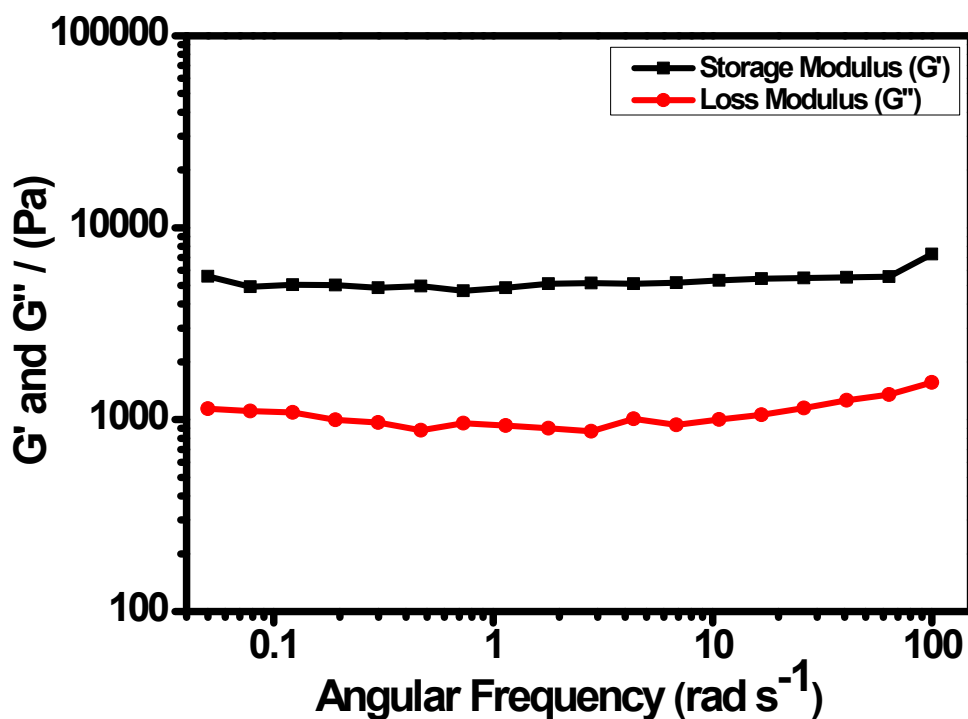


Fig. S21(b) The dynamic frequency sweep rheometry of CuG1. (Storage modulus  $G'$  is higher than the loss modulus  $G''$ ).

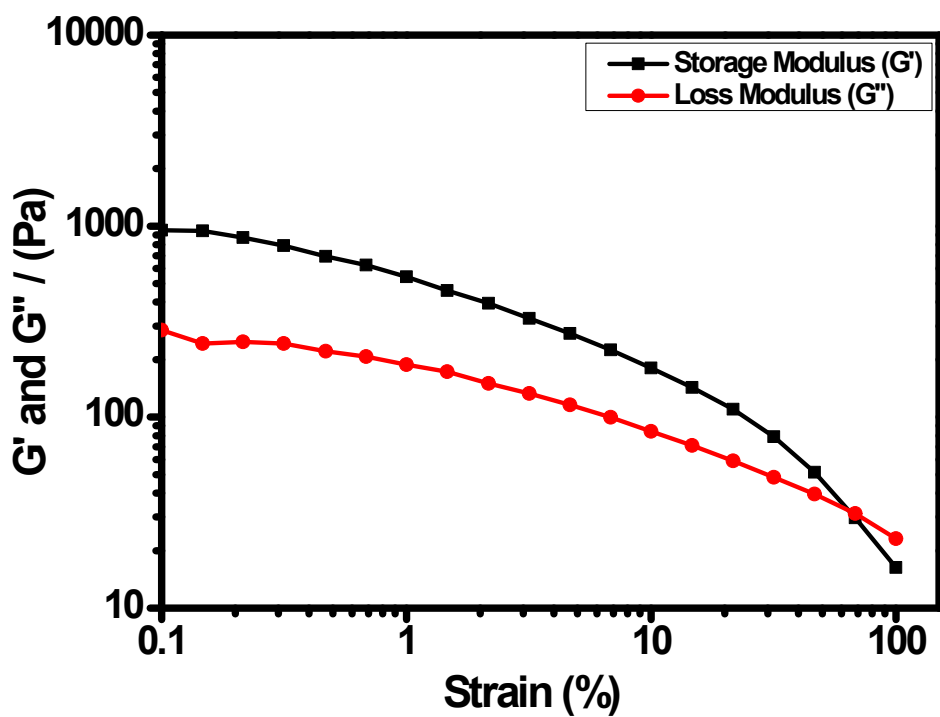


Fig. S22(a) Linear viscoelastic (LVE) property of ZnG1.

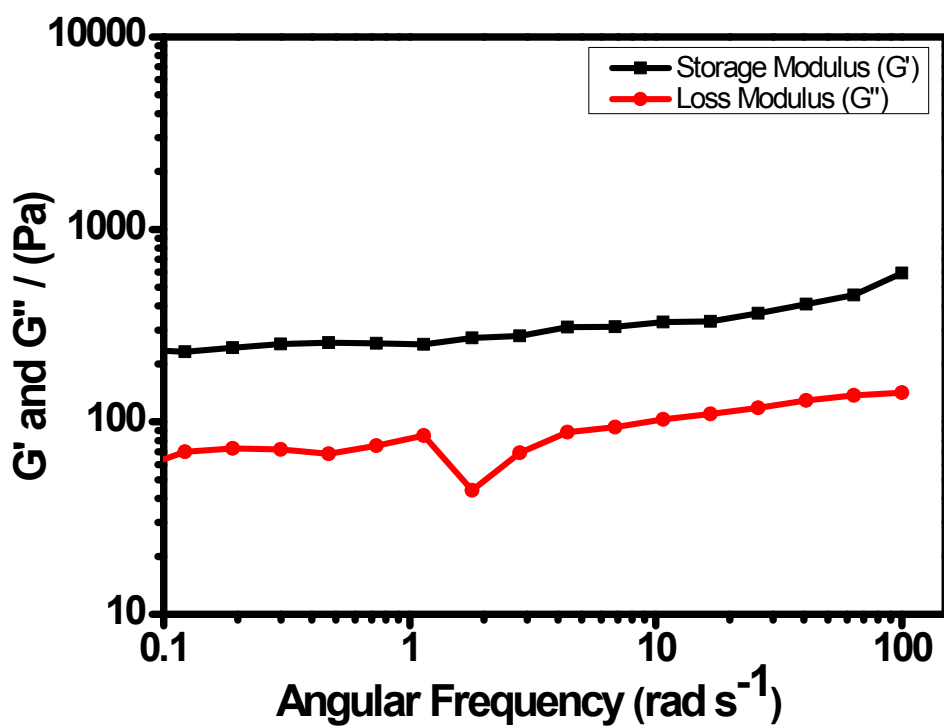


Fig. S22(b) The dynamic frequency sweep rheometry of ZnG1. (Storage modulus  $G'$  is higher than the loss modulus  $G''$ ).



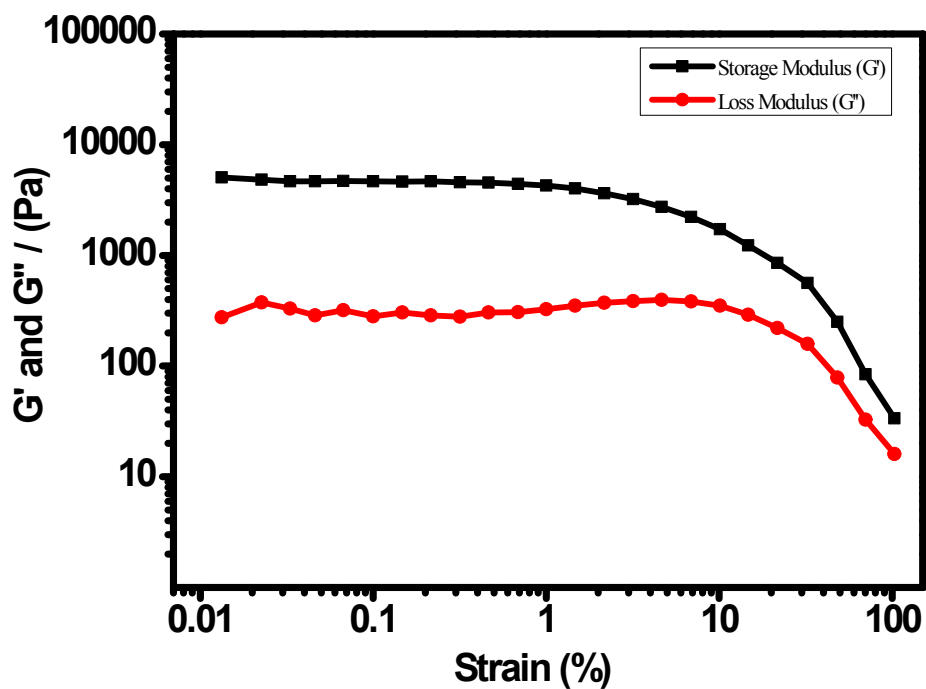


Fig. S23(a) Linear viscoelastic (LVE) property of NiG1.

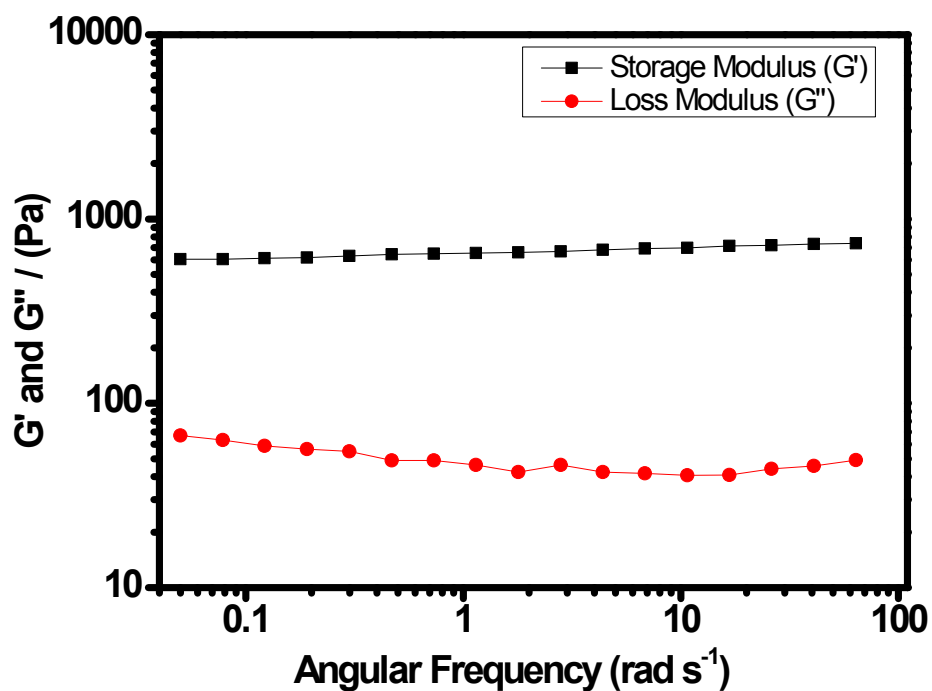


Fig. S23(b) The dynamic frequency sweep rheometry of NiG1. (Storage modulus  $G'$  is higher than the loss modulus  $G''$ ).

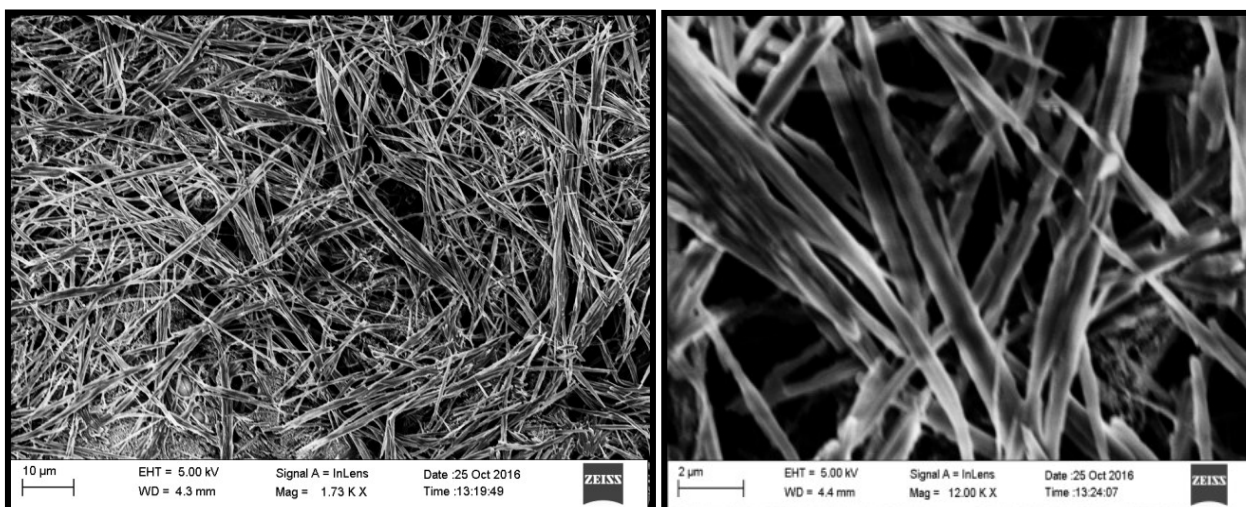


Fig. S24 SEM images of xerogel of ZnG1.

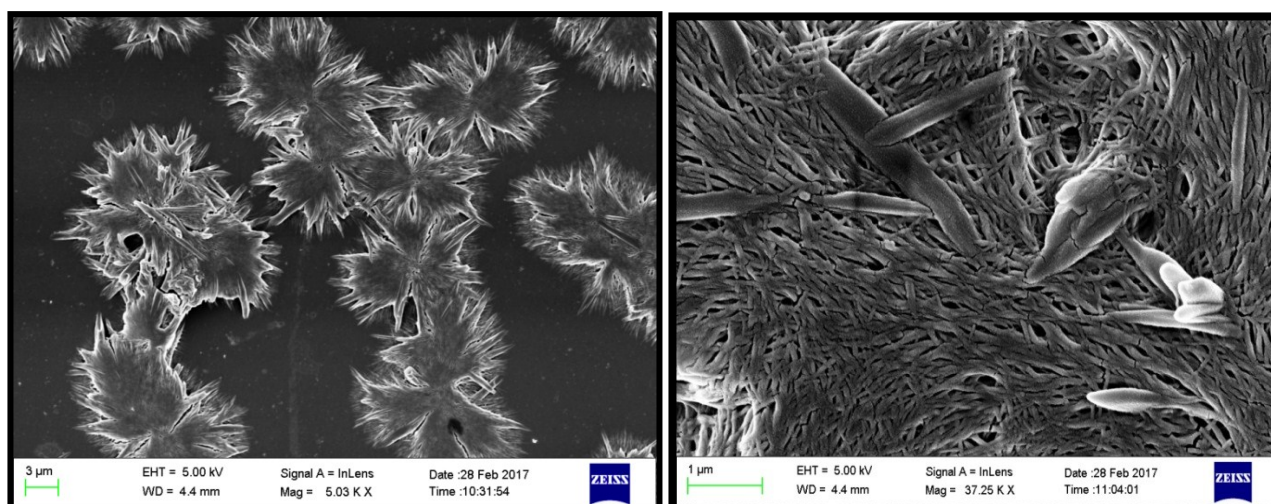
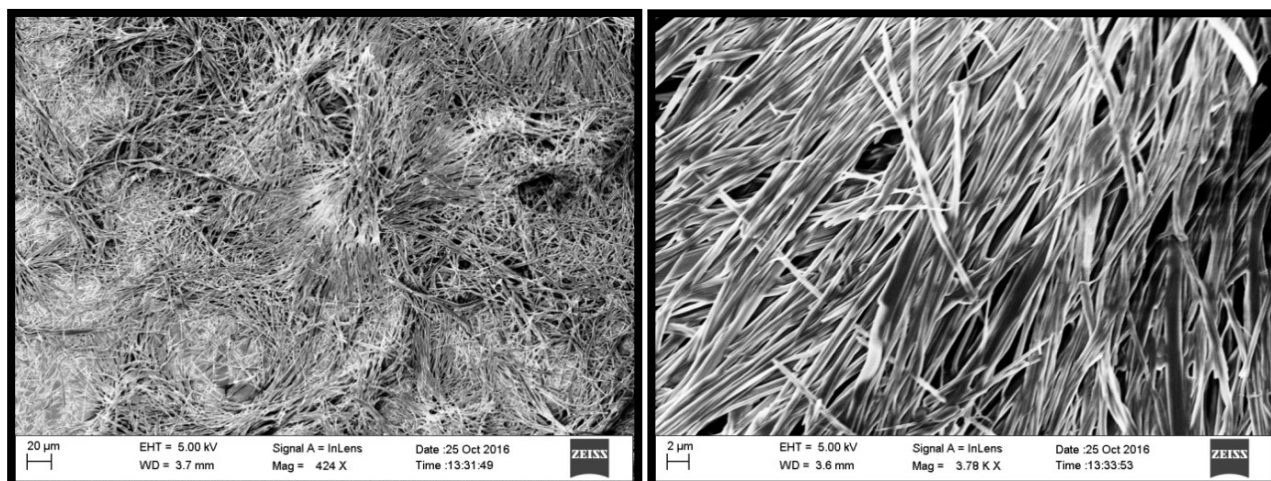
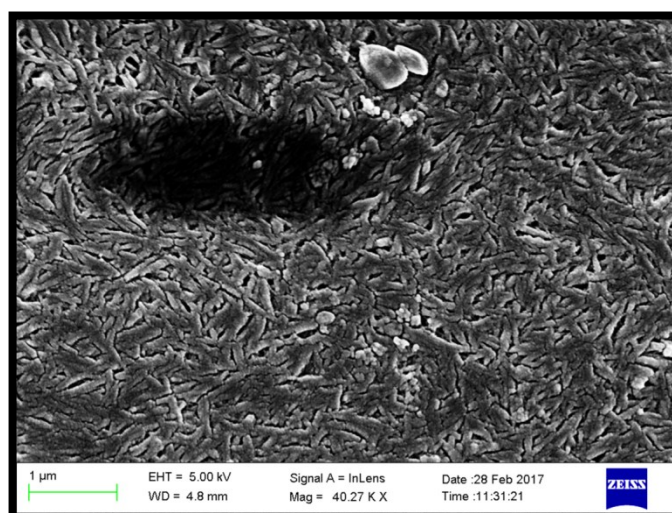


Fig. S25 SEM images of xerogel of NiG1.



**Fig. S26** SEM images of xerogel of **FeG1**.



**Fig. S27** SEM images of xerogel of **CuG1**.

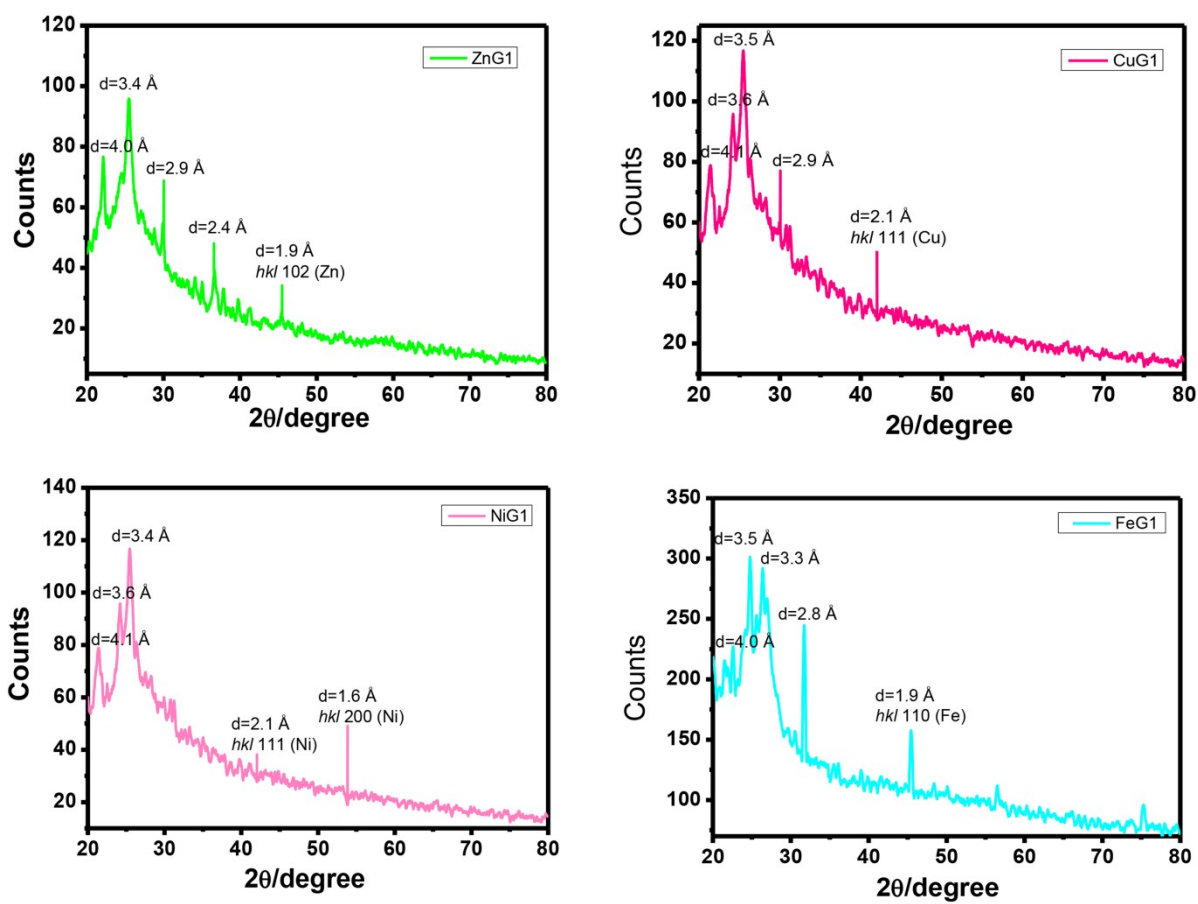


Fig. S28 Powder XRD patterns of xerogel of FeG1, CuG1, ZnG1, NiG1.

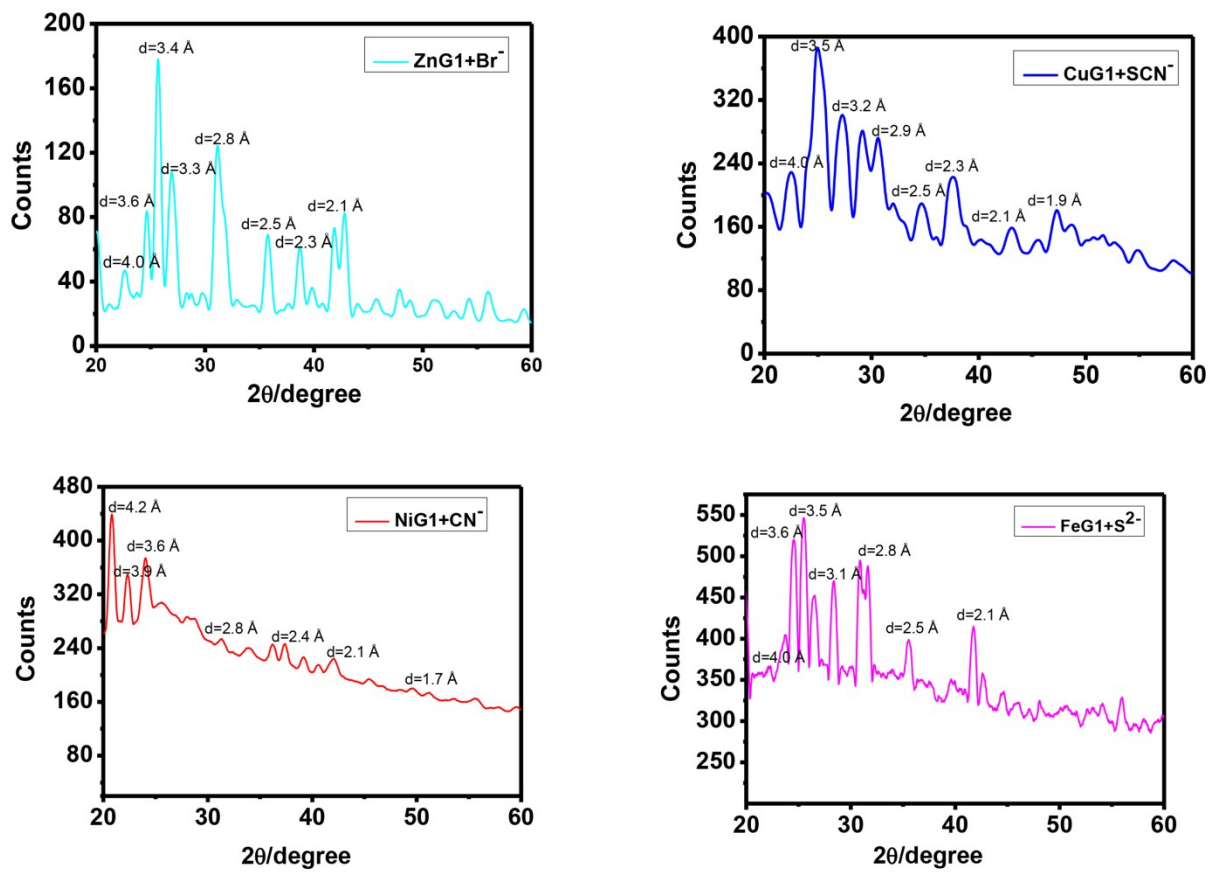


Fig. S29. Powder XRD patterns of xerogel of ZnG1+Br<sup>-</sup>, CuG1+SCN<sup>-</sup>, NiG1+CN<sup>-</sup>, FeG1+S<sup>2-</sup>.