Supporting Information to

A multifunctional supramolecular self-assembly system for colorimetric detection of Fg^{2+}, Fe^{3+}, Cu^{2+} and continuous sensing of volatile acids and organic amine gases

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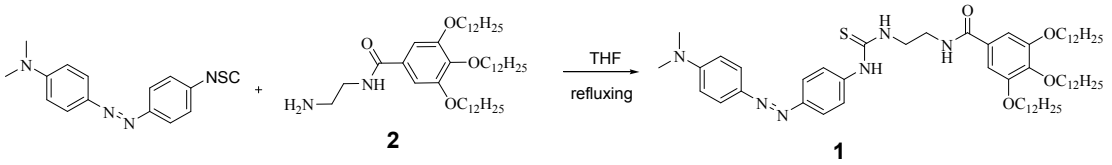

Compound 2 was synthesized according to literature 1.

Synthesis of 1: 4-(dimethylamino)-4'-isothiocyanatoazobenzene (1.0 g, 3.54 mmol) and compound **2** (2.54 g, 3.54mmol) were mixed in anhydrous THF (100 mL). The reaction mixture was stirred and refluxed for 12 h. After the reaction was over, THF was removed under reduced pressure and the residue was subjected to column chromatography (methanol/dichloromethane: 1/200, v/v as eluent) on silica gel to give **1** as a yellow powder. Yield 70.5 %; ^{1}HNMR (600 MHz, DMSO-d_6): 9.70 (s, 1H), 8.36 (s, 1H), 7.92 (s, 1H), 7.75 (d, J = 9.0 Hz, 2H), 7.69 (d, J = 9.0 Hz, 2H), 7.58 (d, J = 9.0 Hz, 2H), 7.15 (s, 2H), 6.82 (d, J = 9.0 Hz, 2H), 3.99 (t, J = 6.6 Hz, 4H), 3.91 (t, J = 6.6 Hz, 2H) 3.74 (d, J = 3.6 Hz, 2H), 3.50 (d, J = 3.6 Hz, 2H), 3.04 (s, 6H), 1.72-1.62 (m, 6H), 1.43-1.39 (m, 6H), 1.30-1.23 (m, 48H), 0.84 (t, J = 6.6 Hz, 9H); ^{13}CNMR (150 MHz, DMSO-d_6): 181.3, 166.7, 152.9, 152.8, 149.4, 143.4, 141.1, 140.7, 129.8, 1249., 123.4, 122.8, 112.1, 106.8, 73.1, 69.3, 44.2, 31.8, 30.3, 29.5, 29.3, 29.2, 26.1, 22.5, 14.3. HRMS calculated for $C_{60}H_{99}N_6O_4S$ $[M+H]^+$ 999.7449, found: 999.7474.

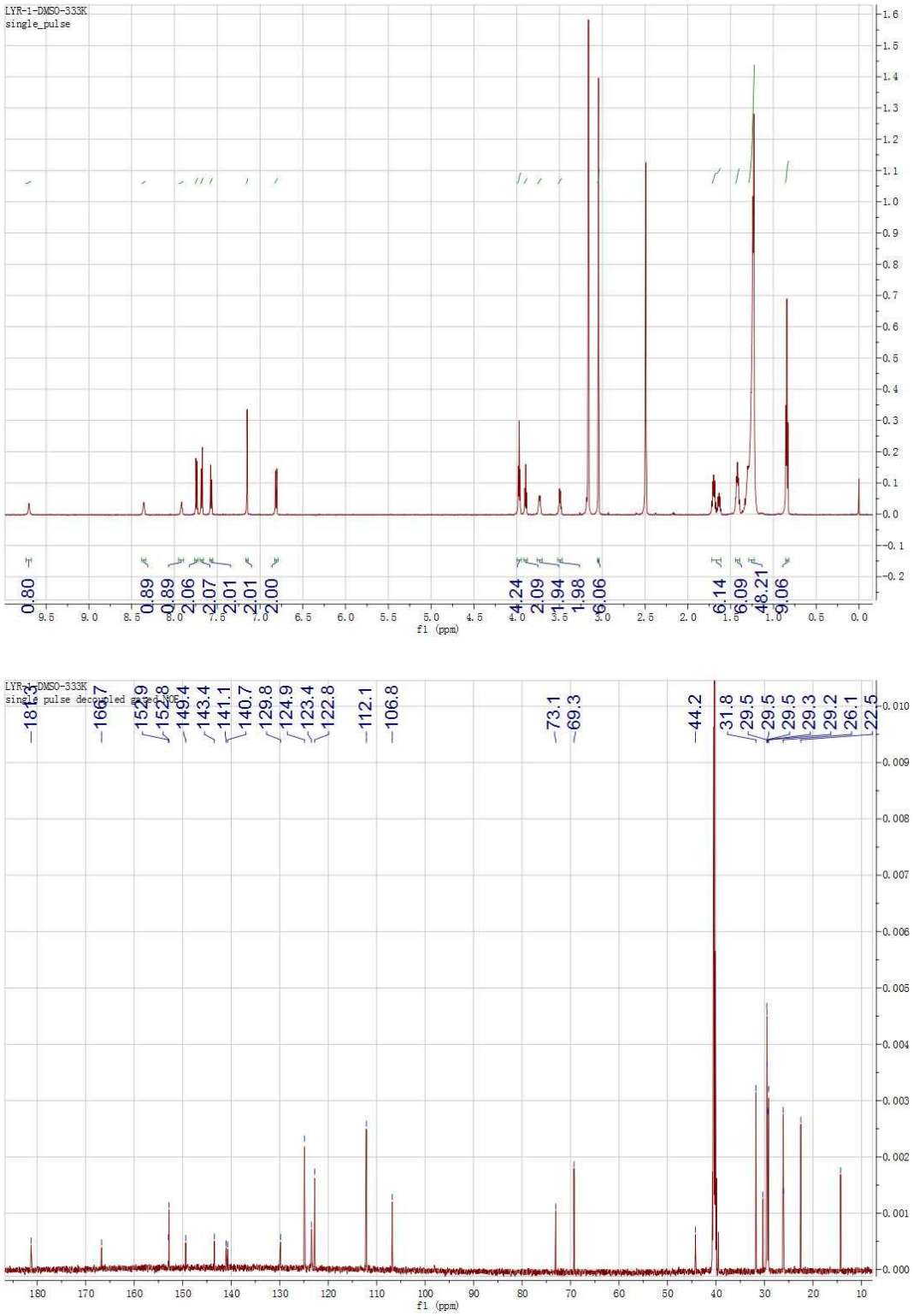

Figure S1 [1]HNMR and [13]CNMR of compound **1** in DMSO-d_6 at 60^{O}C

Table S1 Gelation ability of compound **1** in fourteen frequently-used organic solvents.

Solvent	**1**	Solvent	**1**
DMF	S	1,4-dioxane	S
hexane	G(1.9)	acetonitrile	G (12.5)
methanol	P	ethanol	G(25.0)
acetone	P	acetate ether	P
pertroleum ether	G(1.8)	toluene	S
DMSO	G(12.5)	THF	S
CH_2Cl_2	S	$CHCl_3$	S

P = precipitate; S = solution; G = gel; the values in the brackets denote the CGC with the unit of mg mL^{-1}.

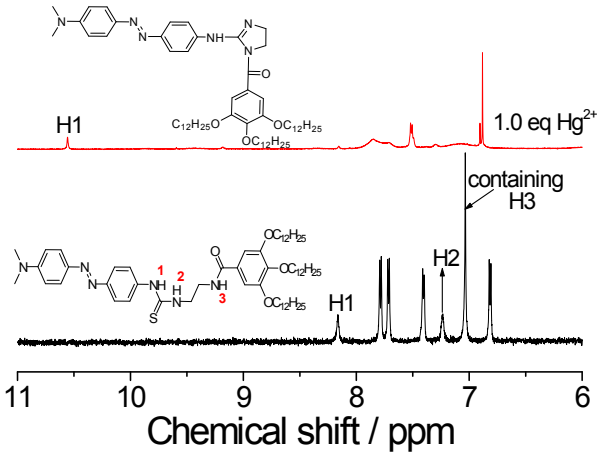

Figure S2 ^{1}HNMR of **1** before and after addition of 1.0 eq. Hg^{2+} in CD_3CN. Inset showing assigned protons of **1** for convenience.

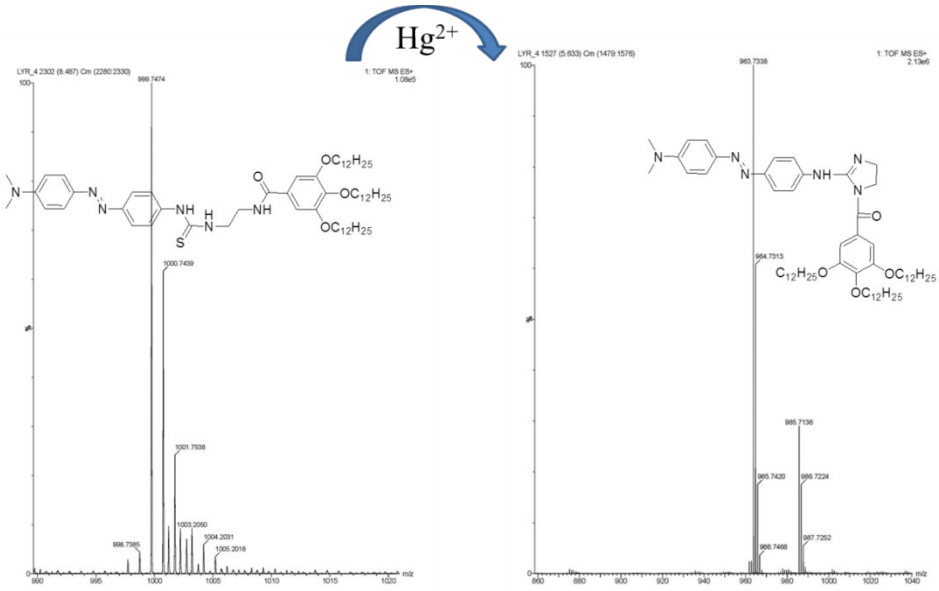

Figure S3 HRMS change of compound **1** before and after of Hg^{2+}.

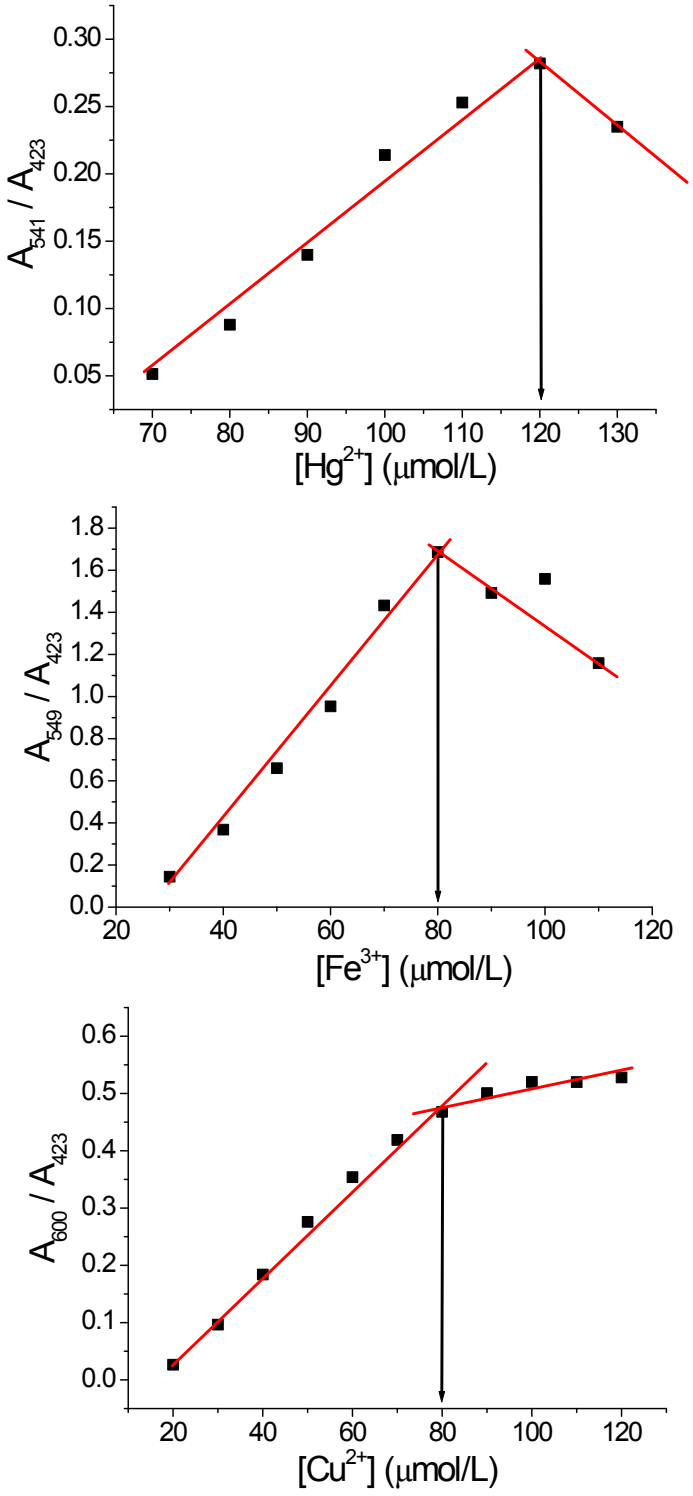

Figure S4 Plots of [A_{541}/ A_{423}], [A_{549}/ A_{423}] and [A_{600}/ A_{423}] v/s increasing concentration of Hg^{2+}, Fe^{3+} and Cu^{2+}.

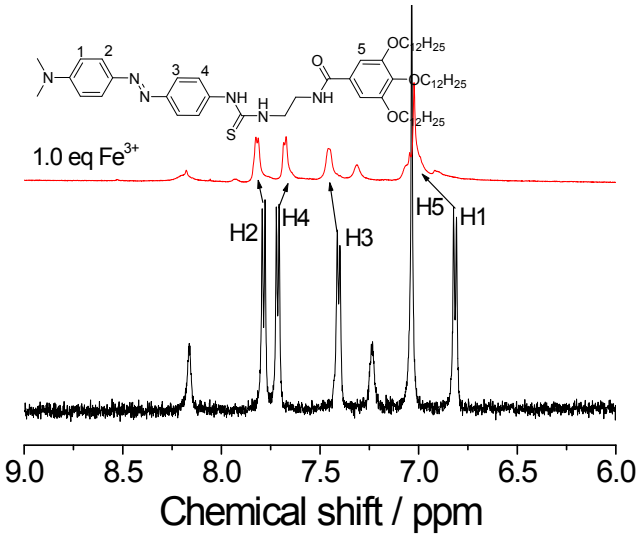

Figure S5 ^{1}HNMR of **1** before and after addition of 1.0 eq. Fe^{3+} in CD_3CN. Inset showing assigned protons of **1** for convenience.

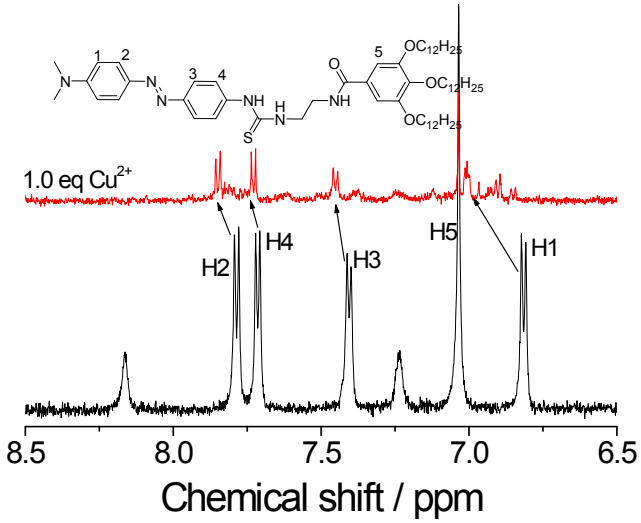

Figure S6 ^{1}HNMR of **1** before and after addition of 1.0 eq. Cu^{2+} in CD_3CN. Inset showing assigned protons of **1** for convenience.

Limit of detection calculation of solution 1 with the concentration of 10^{-4} M for Hg^{2+}, Fe^{3+} and Cu^{2+}

Table S2 Detection limit of compound **1** toward metal ions in acetonitrile by absorbance changes at 422 nm

n	1	2	3	4	5	6	7	8	9	10	11
Absorbance (Xn)	3.244	3.23	3.222	3.224	3.222	3.234	3.236	3.222	3.233	3.229	3.232

$X_{average}$= 3.230 σ_{wb}= sqrt($\sum(X_n-X_{average})^2/n$) = 4.454×10^{-5}

The limit of detection (LOD) was determined with the following equation: $LOD = 3\sigma/b$ [1]: where σ was the standard deviation (SD) of 10 blank samples(100 μmol/L of solution **1**) measurement and b was the slope of the linear fitusing the ratio of absorbance intensity versus Hg^{2+}, Fe^{3+}, Cu^{2+}, TFA or TEA concentration, respectively.

Limit of detection calculation of solution 1 with the concentration of 10^{-5} M for TFA and TEA

Table S3 Detection limit of compound **1** toward TFA and TEA in acetonitrile by absorbance changes at 422 nm

n	1	2	3	4	5	6	7	8	9	10	11
Absorbance (Xn)	0.329	0.330	0.329	0.329	0.329	0.328	0.329	0.330	0.327	0.328	0.327

$X_{average}$= 0.3286 σ_{wb}= sqrt($\sum(X_n-X_{average})^2/n$) = 9.636×10^{-7}

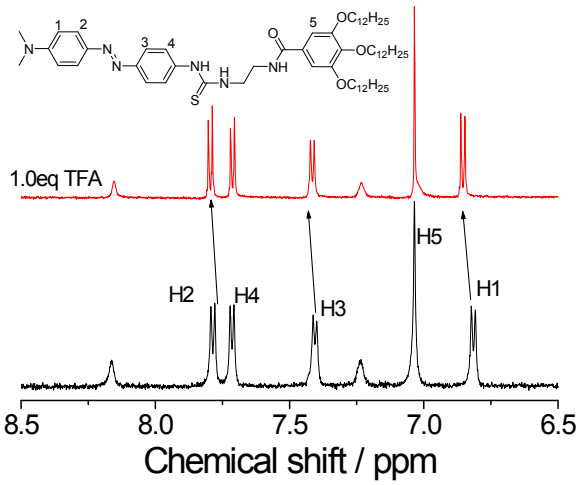

Figure S7 ^{1}HNMR of **1** before and after addition of 1.0 eq. TFA in CD_3CN. Inset showing assigned protons of **1** for convenience.

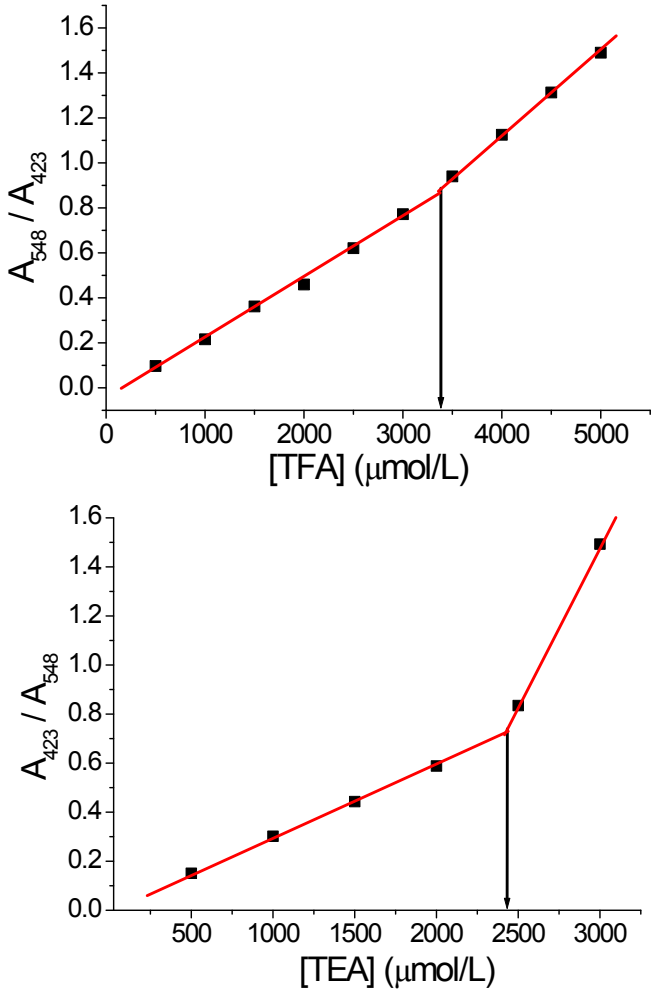

Figure S8 Plots of [A_{548}/ A_{423}], [A_{423}/ A_{548}] v/s increasing concentration of TFA and TEA.

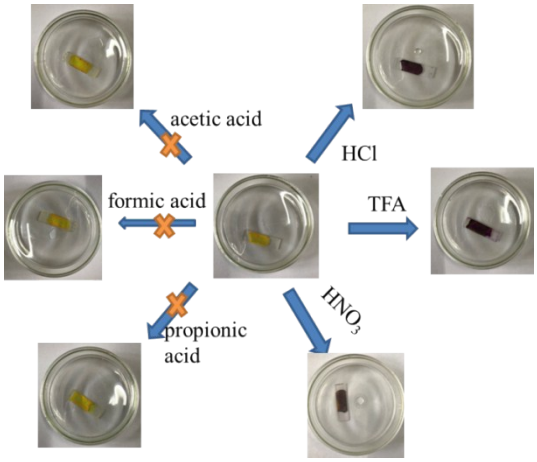

Figure S9 Images of film **1** with sensing different acids.

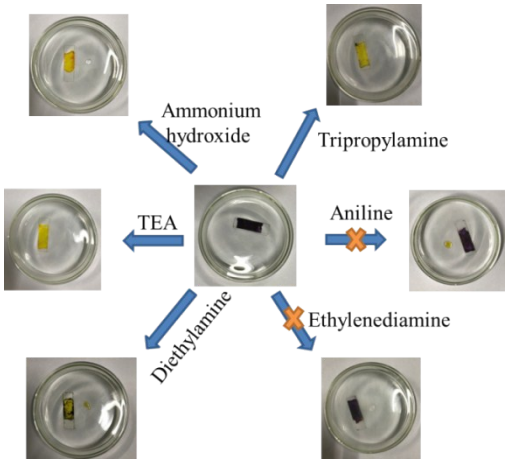

Figure S10 Images of film **1** with TFA contacting different amines.

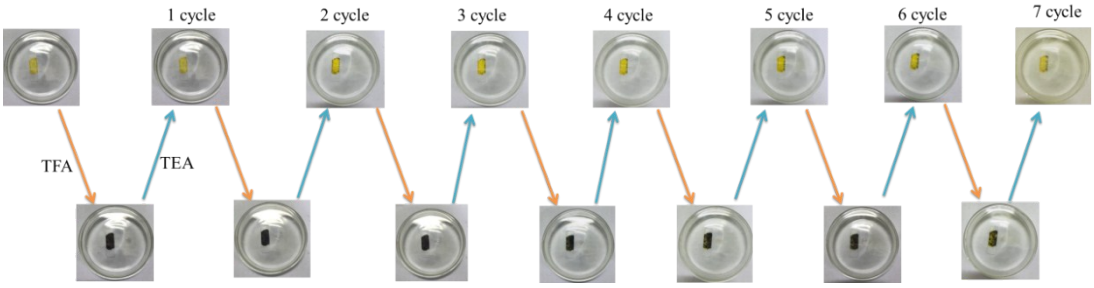

Figure S11 Images of film **1** with sensing TFA and TEA in turn for seven cycle times.

Limit of detection of film 1 towards TFA

Table S4 Detection limit of film **1** toward TFA gas by absorbance changes at 422 nm

n	1	2	3	4	5	6	7	8	9	10	11
Absorbance (Xn)	1.638	1.636	1.634	1.633	1.634	1.636	1.636	1.637	1.639	1.637	1.640

$X_{average}$= 1.636 σ_{wb}= sqrt($\sum(X_n-X_{average})^2/n$) = 4.36×10^{-6}

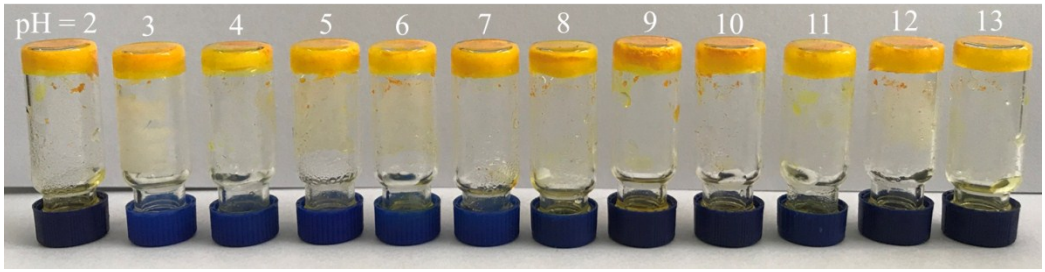

Figure S12 Images of gels **1** with addition of different pH buffer onto the top of gel surface.

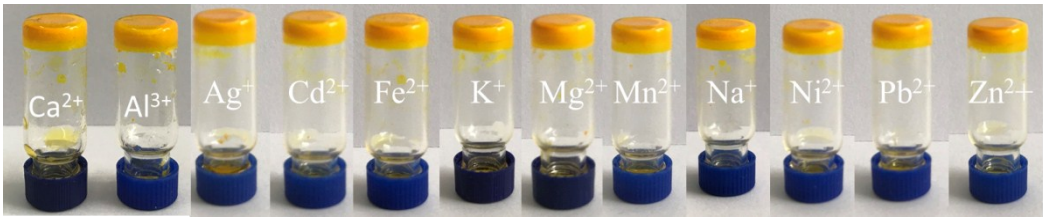

Figure S13 Photographs of color change of gels **1** in acetonitrile under addition of different metal ions (1.0 eq.).

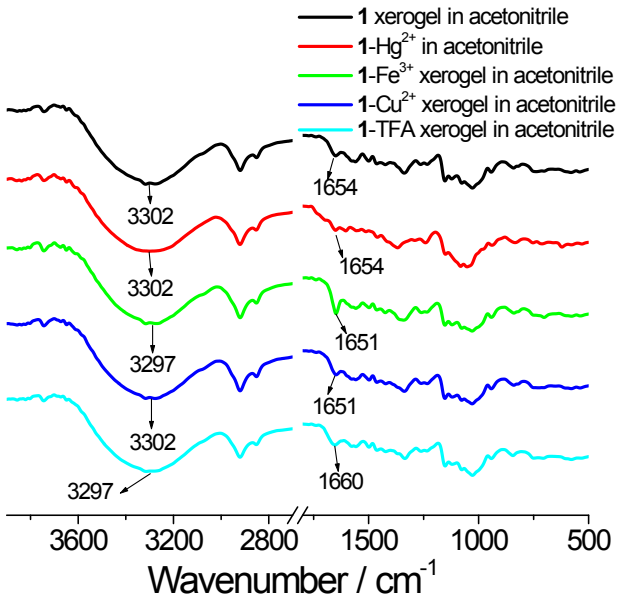

Figure S14 FTIR spectra of xerogels **1** formed in acetonitrile solution and the changes in the gel state of **1** upon addition of Hg^{2+} ion, Fe^{3+} ion**,** Cu^{2+} ion and TFA in acetonitrile solution.

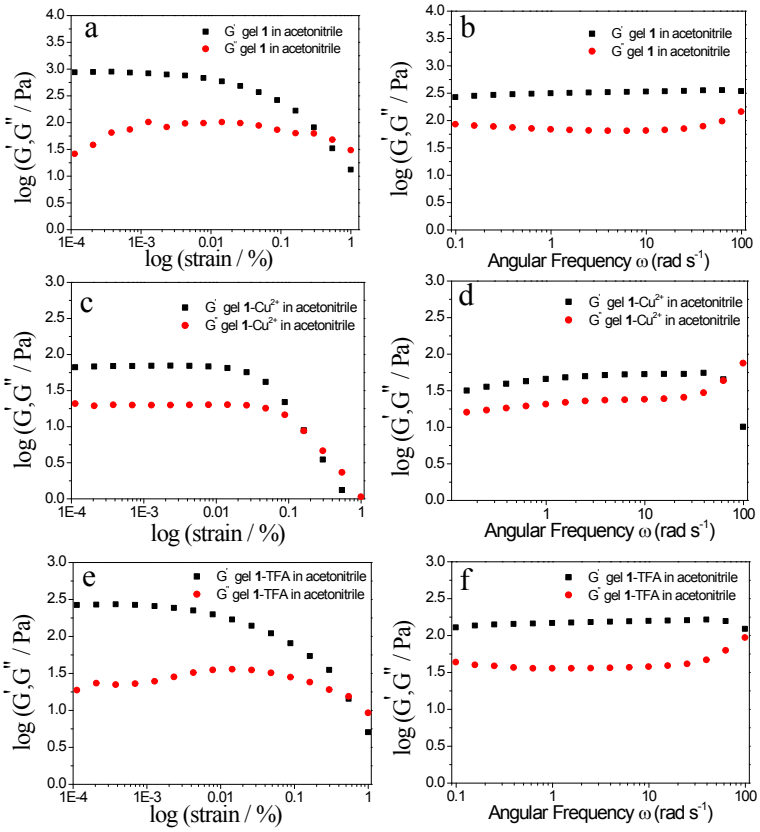

Figure S15 Rheological tests of gel **1**, gels **1** with 1.0 eq. Cu^{2+} and TFA at the CGC at 20°C. (a) Strain sweep at 6.28 rad s^{-1}, (b) frequency sweep at 0.1% amplitude within the linear regime.

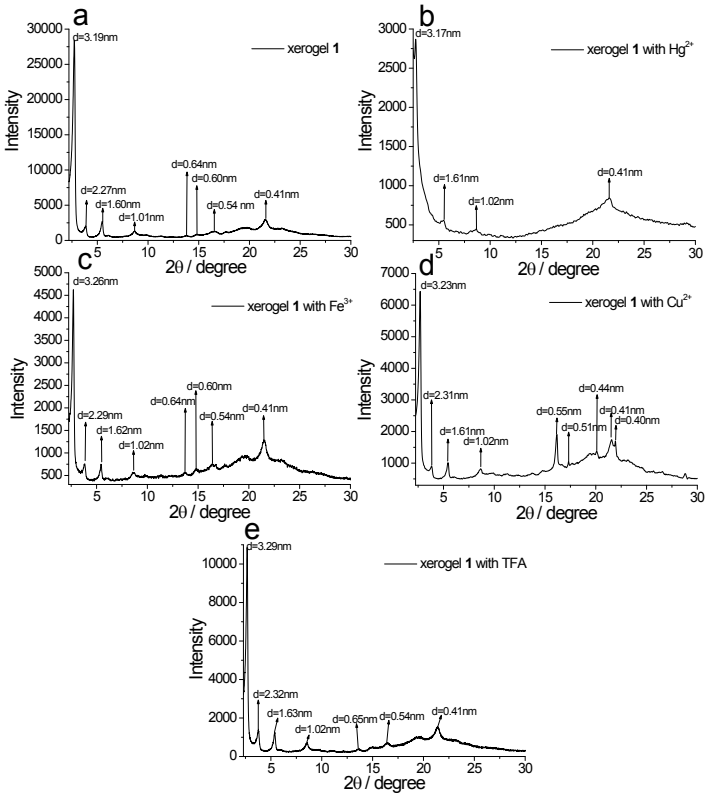

Figure S16 XRD patterns of xerogel **1** from acetonitrile (a) and xerogels **1** upon addition of 1.0 eq. (b) Hg^{2+}, (c) Fe^{3+}, (d) Cu^{2+} and (e) TFA.

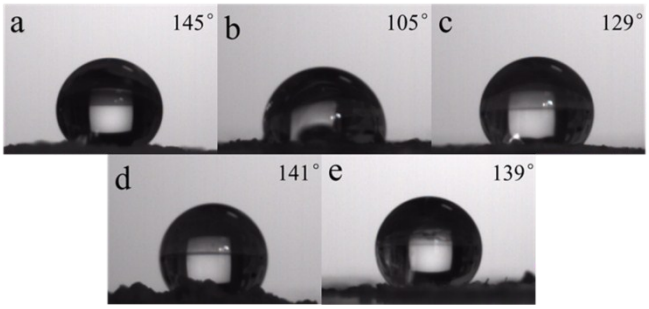

Figure S17 Water contact angle of xerogel **1** formed in acetonitrile (a) and xerogels **1** upon addition of 1.0 eq. (b) Hg^{2+}, (c) Fe^{3+}, (d) Cu^{2+} and (e) TFA.