Supplementary Information for

Solvent-dependent Photophysical and Anion Responsive Properties of One Glutamide Gelator

Pengchong Xue,^{*a} Yuan Zhang,^b Junhui Jia, ^a Defang Xu, ^a Xiaofei Zhang,^a Xingliang Liu, ^a Huipeng Zhou,^a Peng Zhang,^a Ran Lu,^{* a} Makoto Takafuji,^c Hirotaka Ihara^c

^a State Key Laboratory of Supramolecular Structure and Materials College of Chemistry, Jilin University, 2699# Changchun, China. E-mail: xuepengchong@jlu.edu.cn luran@jlu.edu.cn ^b College of Chemistry, Beijing Normal University, Beijing 100875, China

^c Department of Applied Chemistry and Biochemistry, Kumamoto University, 2-39-1 Kurokami, Kumamoto, Japan



Fig. S1. Frontier orbitals (AM1) of the aromatic moiety of 1.

To calculate easily, only aromatic moiety of **1** was chosen. Firstly, the geometric optimization of gelator molecule was estimated by AM1 force field, and then HOMO and LUMO could be obtained. As shown in Fig. S1, at the HOMO of **1**, electrons are mainly distributed in the p-conjugated phenylenevinylene unit and the amide moiety. However, at the LUMO level, with electronic excitation, intramolecular charge transfer induced electron movement from the donor site to the acceptor moiety (nitro group) of **1**. Therefore, the chromophores of **1** is typical D– π –A molecular structure.



Fig. S2. FT-IR spectra of solvents (DMSO and ODCB), the hot solution of 1 in DMSO and ODCB mixture (v/v = 1:3) and wet DMSO and ODCB gels.



Fig. S3 The gelator 1 after the geometric optimization by AM1 force field.



Fig. S4 concentration-dependent absorption and fluorescence spectra of **1** in DMF (a, c) and anisole (b, d).



Fig. S5 SEM and TEM images of xerogels of 1 from DMF (a and b) and anisole (c and d), respectively.



Fig. S6 Fluorescence spectral change of **1** in DMSO (a, 6.6 mM; b, 3.3 mM; c, 2.2 mM; d, 1.65 mM) with decreasing temperature from 90 to 20 °C. Inset in Fig. S6a is enlarged fluorescence spectrum of DMSO gel at 20 °C.



Fig. S7 Fluorescence spectral change of **1** in *o*-dichlorobenzene (a, 4.0 mM; b, 1.3 mM; c, 1.0 mM; d, 0.8 mM) with decreasing temperature from 160 to 20 °C.



Fig. S8 Fluorescence spectra of ODCB gels (1 mM) before and after the addition of DMSO.



Fig. S9 Photos of **1** in different solvents with and without anions. (a) 10 equiv anions were added in DMSO and ODCB, (b) 5 equiv TBAF was added in DMSO and (c) 5 equiv TBAF was added in ODCB.



Fig. S10 Absorption spectra of 1 in DMSO (0.5 mM) upon the addition of 10 equiv TABF, TBAOAc, $TBAH_2PO_4$.



Fig. S11 The absorption changes observed for **1** (0.5 mM) upon the addition of fluoride anion in DMSO/ODCB (v/v = 1/6). Inset shows the absorbance at 560 nm as a function of fluoride concentration.

As shown in Figure S11, **1** showed good affinity for fluoride because the linear dependence of thier absorbance vs. fluordie concentration which reached a plateaux after 4 equivlents of F^- had been added. This result suggests that 1: 4 bind stoichiometry, indicating that all NH units participate in the binding with F^- .



Fig. S12 Absorption spectra of **1** in ODCB upon the addition of 10 equiv anions as TBA salts.