Electronic Supplementary Information (ESI)

A cyanurate gel derived by unusual hydrogen-bonding interaction in binary system

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Experimental Section

Preparation of gel 1. Tris(2-carboxyethyl) isocyanurate (**1**) and 4,4'-bipyridine (**2**) is dissolved in aqueous solution [200 μL, 1~5 wt % in H_2O] in vial by heating. Interestingly, it turns into gel-type phase upon cooling, and the gel-like phase is regenerated by heating and cooling process. The gelation state of the material was evaluated by "stable-to-inversion" of the test tube.

Preparation of crystal structure for $\mathbf{1}\cdot(\mathbf{2})_{1.5}$.

A mixture of Tris(2-carboxyethyl) isocyanurate (10 mg, 0.029 mmol) and 4,4'-bipyridine (9 mg, 0.059 mmol) is added in water (5 mL) in a 10 mL vial. The vial was kept at 80 ºC for 4h, followed by cooling to room temperature over 6h. The colorless crystals, $\mathbf{1}\cdot(\mathbf{2})_{1.5}$ suitable for X-ray amalysis were obtained.

Reference

1) Bruker, APEX2 Version 2009.1-0 Data Collection and Processing Software; Bruker AXS Inc., Madison, Wisconsin, U.S.A. **2008**.

2) Bruker, SHELXTL-PC Version 6.22 Program for Solution and Refinement of Crystal Structures; Bruker AXS Inc., Madison, Wisconsin, U.S.A. **2001**.

Table S1. Crystal data and structural refinement for **1**·(**2**)$_{1.5}$

Empirical formula	$C_{27}H_{27}N_6O_9$
Fw	579.55
Crystal system	Triclinic
Space group	*P*-1
Temperature (K)	173(2)
a /Å	8.3257(7)
b /Å	11.2037(9)
c /Å	15.5132(13)
α /°	70.668(4)
β /°	75.604(4)
γ /°	84.442(4)
V /Å^3	1322.42(19)
Z	2
D_{calc} / g cm^{-3}	1.455
F(000)	606
μ /mm^{-1}	0.112
θ range /°	1.43 to 26.50
Reflns collected	27241
Independent reflns	5476
R_1; wR_2 [$I > 2\sigma(I)$]	0.0488, 0.1392
R_1; wR_2 (all data)	0.0549,0.1459
GOF (F^2)	1.047

Table S2. Geometrical parameters of hydrogen bonds in crystal **1**·(**2**)$_{1.5}$.

D-H···A	D-H(Å)	H···A (Å)	D···A (Å)	D-H···A (deg)	Symmetry –for-A
O5-H5A···N5	0.82	1.91	2.696(5)	160	-*x*, 1-*y*, 1-*z*
O7-H5A ···N4	0.82	1.85	2.661(4)	167	1+*x*, -1+*y*, *z*
O8-H5A ···N6	0.82	1.80	2.624(1)	174	*x*, 1+*y*, *z*
C16-H16A···O6	0.93	2.63	3.528(0)	162	*x*, 1+*y*, *z*
C17-H17A···O2	0.93	2.30	3.197(6)	162	*x*, 1+*y*, *z*
C19-H19A···O4	0.93	2.36	3.286(3)	171	*x*, *y*, *z*
C20-H20A···O4	0.93	2.46	3.222(8)	123	-*x*, 1-*y*, 1-*z*
C22-H22A···O6	0.93	2.59	3.516(2)	177	*x*, 1+*y*, *z*
C23-H23A···O1	0.93	2.44	3.306(5)	155	1+*x*, -1+*y*, *z*
C24-H24A···O9	0.93	2.30	3.174(7)	157	1+*x*, -1+*y*, *z*

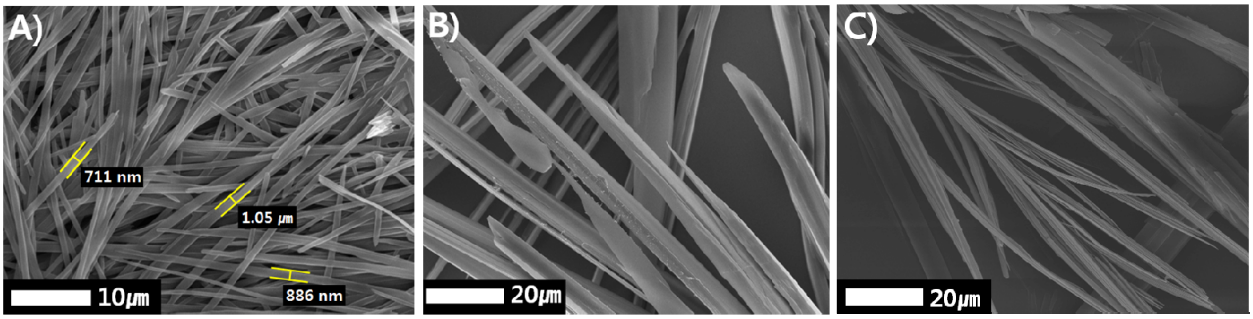

Fig. S1 Photographs of gels **1** with (a) 1eq, (b) 2eq and (c) 3eq of **2** in water.

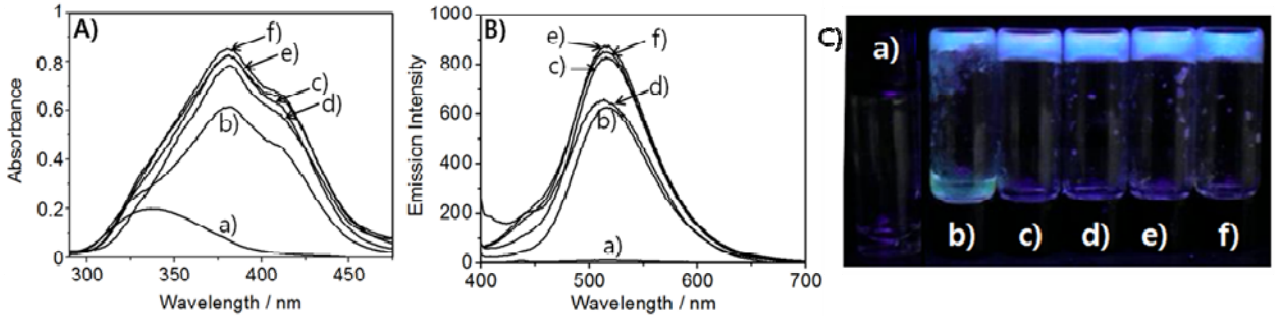

Fig. S2 (A) UV-vis and (B) fluorescence spectra (excitation at λ=380 nm) of (a) sol **1** (9.4 mM) and gel **1** (9.4 mM) and with (b) 1.0 equiv, (c) 2.0 equiv (d) 3.0 equiv, (e) 4.0 equiv and (f) 5.0 equiv of **2** in H_2O. (C) The photograph of (a) sol **1** (9.4 mM) and gel **1** (9.4 mM) and with (b) 1.0 equiv, (c) 2.0 equiv (d) 3.0 equiv, (e) 4.0 equiv and (f) 5.0 equiv of **2** in H_2O by irradiation of UV lamp.

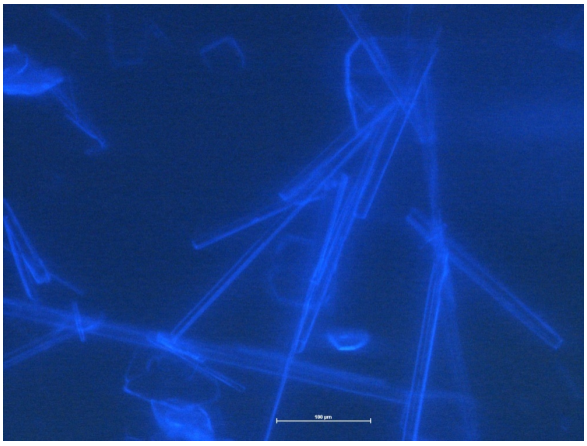

Figure S3. Fluorescence micrograph of gel **1** with 1.0 equiv of **2**.

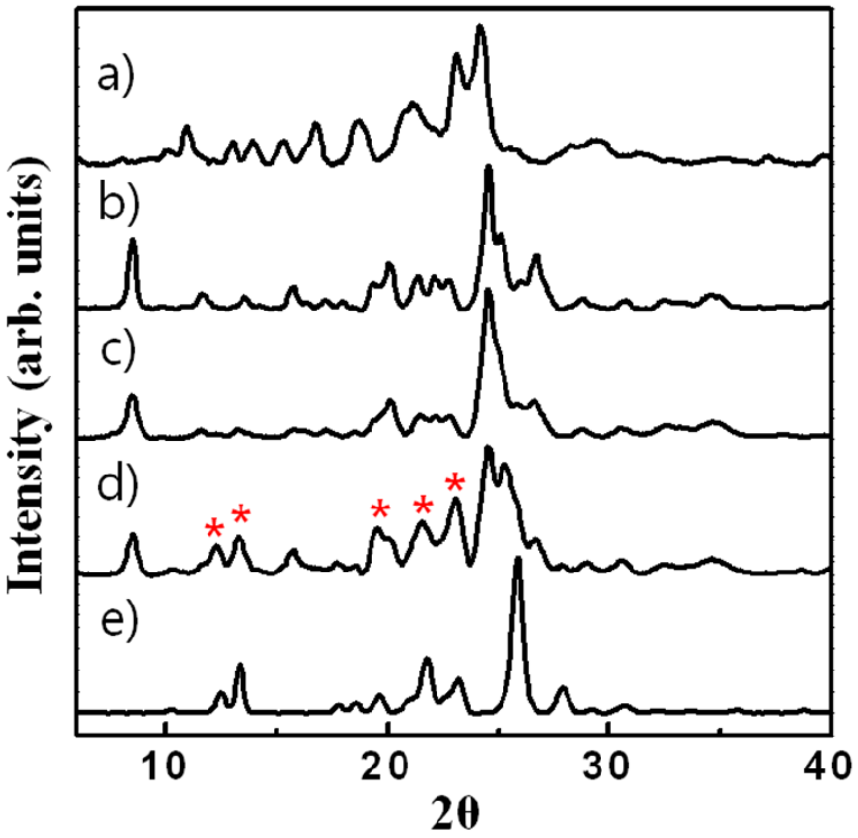

Fig. S4 Powder X-ray diffraction pattern of (a) xerogel **1** with 1.0 equiv of **2** and (b) crystal **1** obtained from 2.0 equivalent of **2**, xerogel **1** with (c) 2.0 and (d) 3.0 equiv of **2**, and (e) free **2** (4,4-bipyridine): *The pattern was originated from non-hydrogen-bonded 4,4-bipyridine

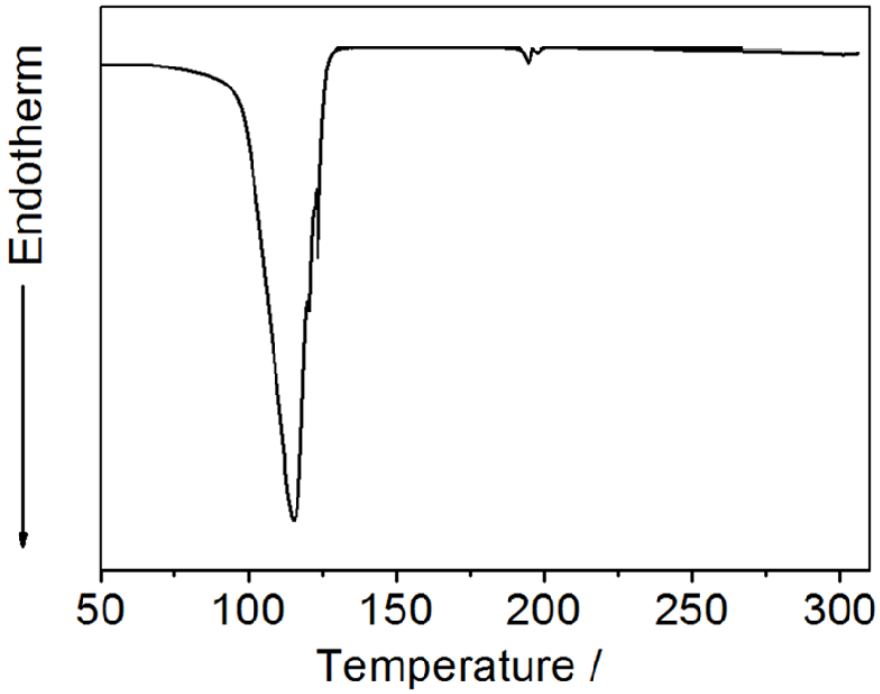

Fig. S5 DSC thermogram of gel **1** with 1.0 eqivalent of **2**.

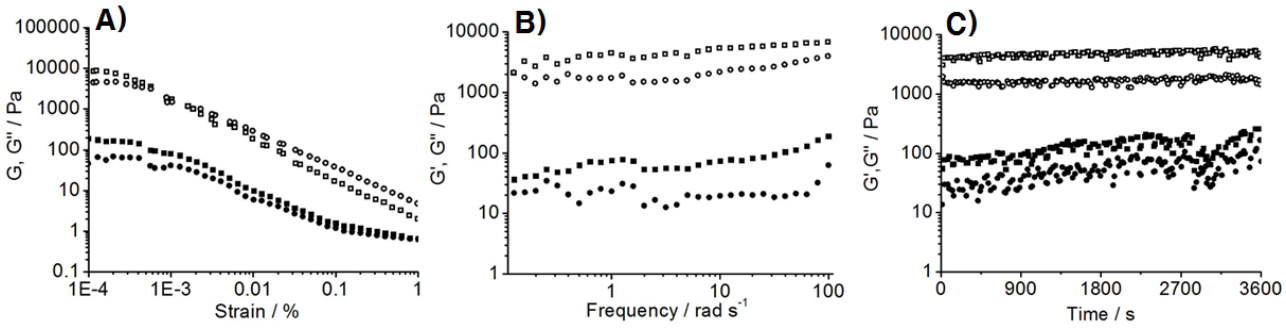

Figure S6. Dynamic oscillatory and steady shear measurements of gel **1** at different concentration of **2** at 25 ^{o}C: A) strain sweep at a frequency of 1 rad s^{-1}; B) frequency sweep at a strain of 0.01%; C) time sweep at a strain of 0.01% and frequency of 1 rad s^{-1}; **1**: **2**=1:1 ■: G′,●: G″; **1**: **2**=1:3 □: G′, ○: G″.