Supplementary Material (ESI) for New Journal of Chemistry

Electronic Supplementary Information (ESI)

Metal-organic framework gel with Cd^{2+} derived from only coordination bonds without intermolecular interactions and its catalytic ability

Hyo hee Lee, Sung Ho Jung, Sunghong Park, Ki-Min Park and Jong Hwa Jung*[a]

Department of Chemistry and Research Institute of Natural Science, Gyeongsang National University, Jinju 660-701 (Korea); E-mail: jonghwa@gnu.ac.kr

Table S1. Gelation test of ligand **1** with metal ions (3.0 equiv) in organic solvents.

Entry	solvent	$ZnSO_4$	$CdSO_4$	$Cd(NO_3)_2$	$Cd(ClO_4)_2$	$CdBr_2$	$CdCl_2$	CdI_2
1	MeOH	P	P	P	P	P	P	P
2	DCM	P	P	P	P	P	P	P
3	THF	P	P	P	P	P	P	P
4	Toluene	P	P	P	P	P	P	P
5	AN	P	P	P	P	P	P	P
6	EA	P	P	P	P	P	P	P
7	$CHCl_3$	P	P	P	P	P	P	P
8	Ethanol	P	P	P	P	P	P	P
9	H_2O	G	G	G	G	P	P	P
10	DMF	S	S	S	S	S	S	S
11	DMSO	S	S	S	S	S	S	S
12	H_2O: DMSO	P	P	P	P	P	P	P

P: precipitate, G: stable gel, S: solution

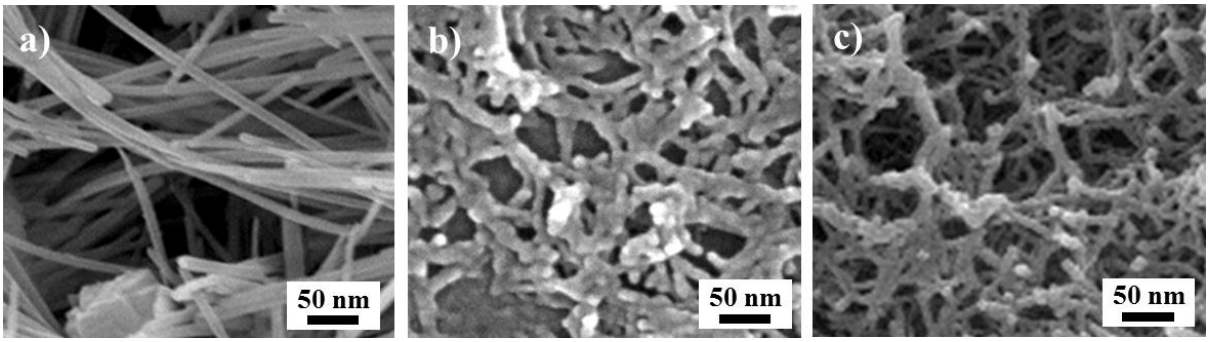

Fig. S1 SEM images of Cd^{2+} coordination polymer gel **1** with different anions; (a) $CdSO_4$, (b) $Cd(NO_3)_2$ and (c) $Cd(ClO_4)_2$.

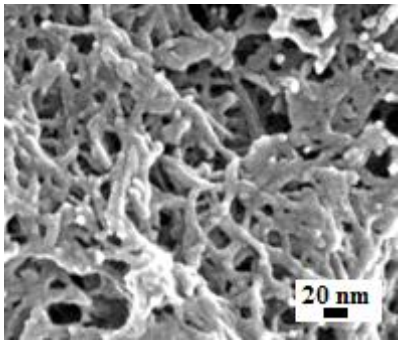

Fig. S2 SEM images of Cd^{2+} coordination polymer gel **1** with $ZnSO_4$

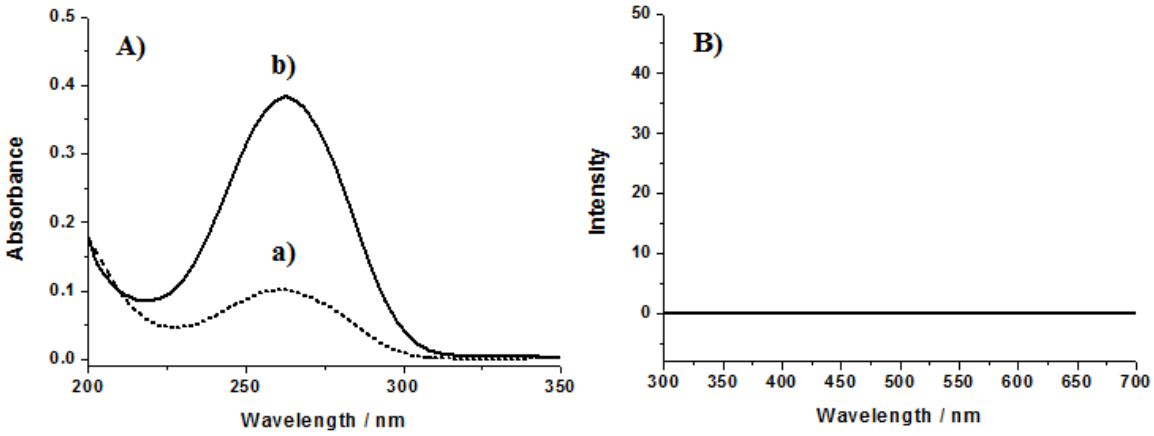

Fig. S3 (A) UV-vis spectra of (a) sol **1** (0.01 mM) and (b) coordination polymer gel **1** (0.01 mM) with $CdSO_4$ (3.0 equiv) in H_2O. (B) Fluorescence spectrum of coordination polymer gel **1** (0.01 mM) with $CdSO_4$ (3.0 equiv) upon excitation at λ=262 nm.

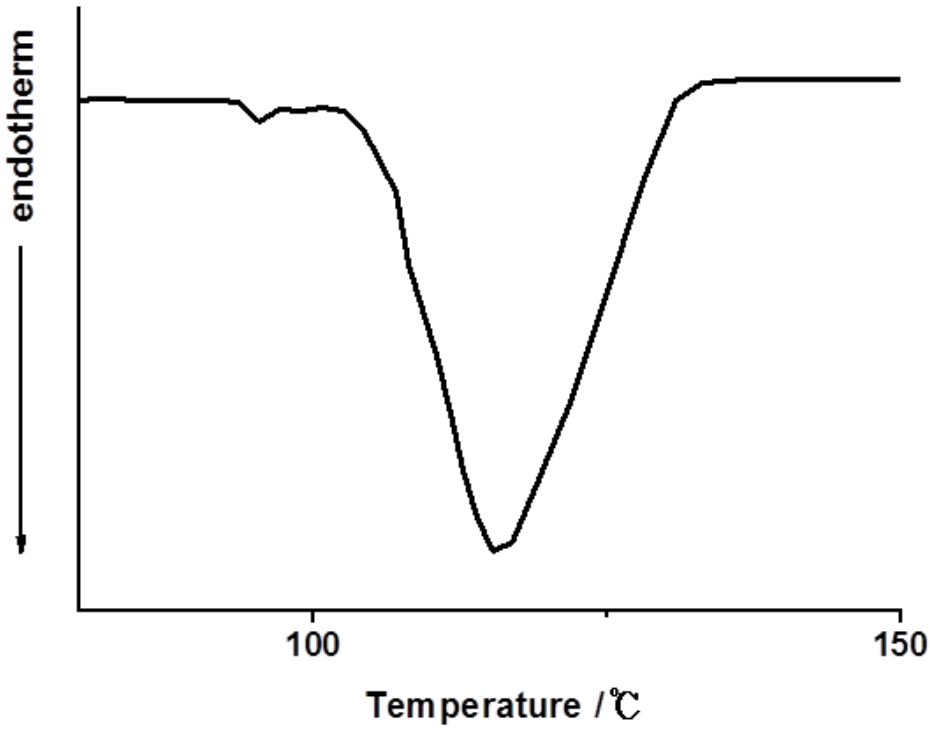

Fig. S4 DSC thermogram of coordination polymer gel **1** with $CdSO_4$ (3.0 equiv) in H_2O.

Table S2. Crystal and experimental data.

	1a
Formula	$C_{27}\ H_{40}\ Cd_{0.5}\ N_7\ O_{12}\ S$
Formula weight	742.92
Temperature (K)	173(2)
Crystal system	Monoclinic
Space group	*C2/c*
Z	8
F(000)	3096
a (Å)	15.7778(4)
b (Å)	14.6264(4)
c (Å)	29.5827(7)
β (º)	97.5540(10)
V (Å^3)	6767.6(3)
D_x (g/cm^3)	1.458
$2\theta_{max}$ (º)	53
R	0.0322
wR	0.0845
No. of reflection used [> 2σ(*I*)]	29691
Diffractometer	Bruker SMART CCD system
Structure determination	SHELXTL
Refinement	Full-matrix

Table S3. Selected bond lengths (Å) and bond angles (º) for **1**, $\{[Cd(H\mathbf{1})_2(SO_4)_2]\cdot DMF\cdot 4H_2O\}_n$

Cd1-O4	2.277 (1)	Cd1-N2	2.330 (1)
Cd1-N6A	2.348(2)		
O4B-Cd1-O4	176.98(7)	O4B-Cd1-N2B	92.45(5)
O4-Cd1-N2B	85.35(5)	O4-Cd1-N2	92.44(5)
N2B-Cd1-N2	86.41(8)	O4B-Cd1-N6A	96.34(5)
O4-Cd1-N6A	85.89(5)	N2B-Cd1-N6A	93.91(6)
N2-Cd1-N6A	178.27(5)		

Symmetry code: A) -*x*+1,*y*-1,-*z*+3/2; B) -*x*+1,*y*,-*z*+3/2