Electronic Supplementary Information (ESI)

A thermo-sensitive supramolecular hydrogel derived from an onium salt with the property of solution-gel-crystal transition

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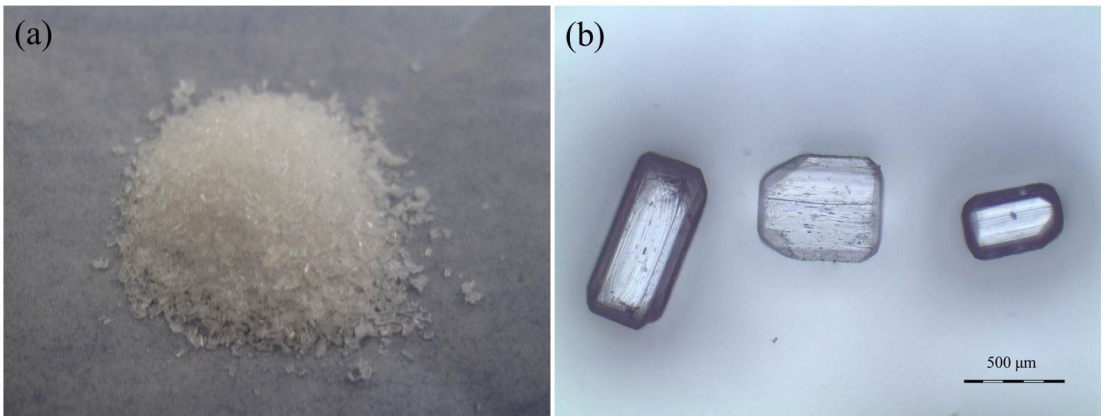

Fig. S1. (a) Photograph and (b) micrograph of the TTIBD crystals.

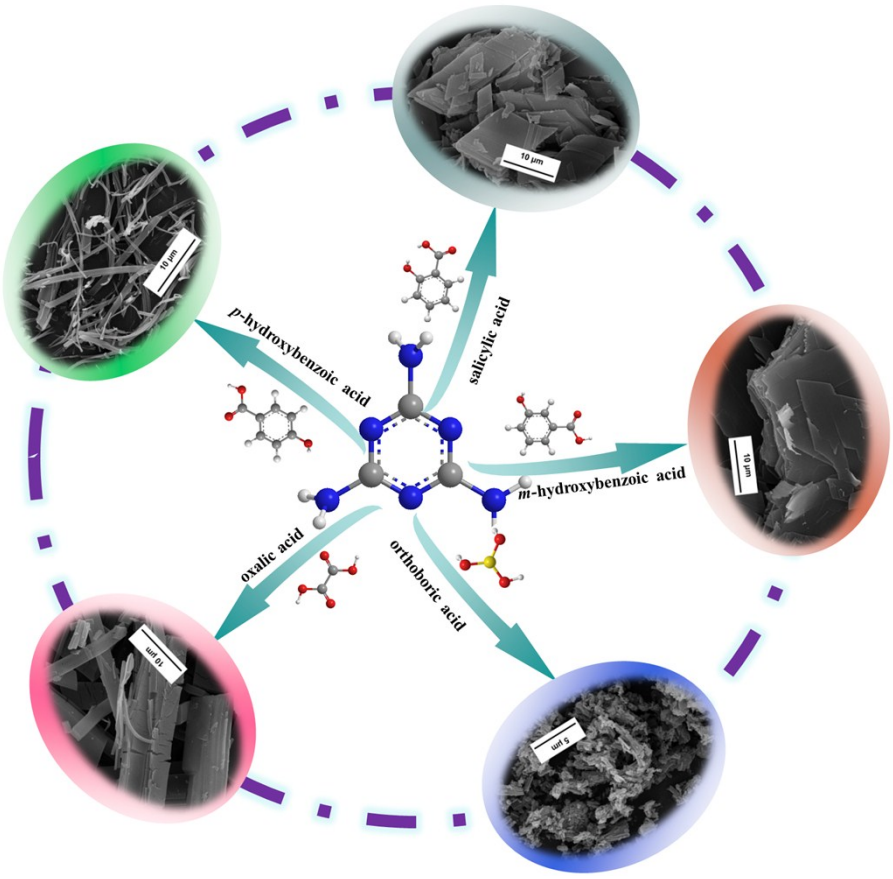

Fig. S2. Morphology of the xerogels formed from melamine with salicylic acid, *p*-hydroxybenzoic acid, *m*-hydroxybenzoic acid, orthoboric acid and oxalic acid.

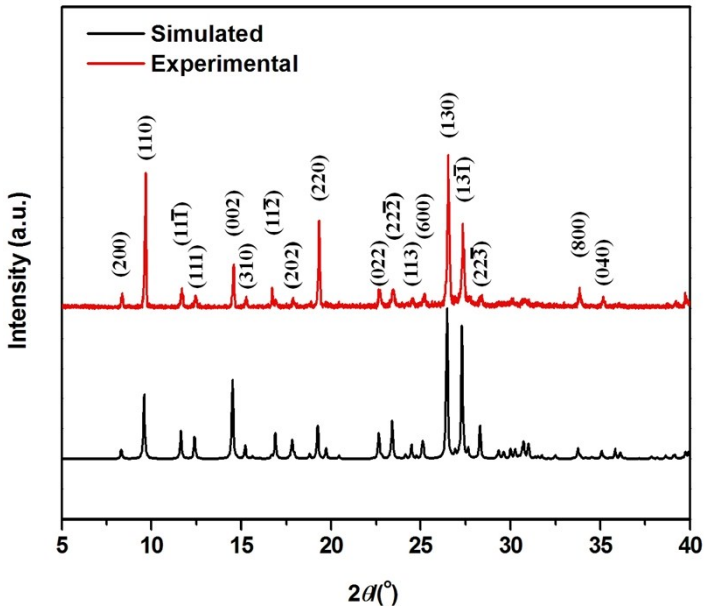

Fig. S3. Simulated and experimental PXRD patterns for the TTIBD crystals.

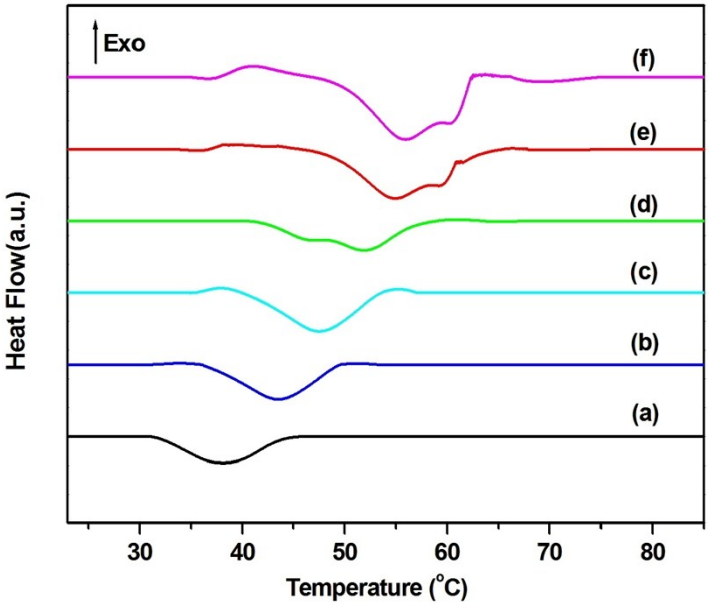

Fig. S4. DSC thermograms of the TTIBD hydrogels formed at different gelator concentrations: (a) 0.06 mol·L^{-1}, (b) 0.08 mol·L^{-1}, (c) 0.10 mol·L^{-1}, (d) 0.12 mol·L^{-1}, (e) 0.14 mol·L^{-1} and (f) 0.16 mol·L^{-1}.

Table S1. Crystal data and structure refinement for TTIBD.

Compound	**TTIBD**
Formula	$C_{10}H_{16}N_6O_4$
F.W.	284.29
T (K)	298 (2)
Crystal system	Monoclinic
Space group	$C2/c$
a (Å)	21.477 (3)
b (Å)	10.2253 (14)
c (Å)	12.3312 (17)
β (°)	98.717 (3)
V (Å^3)	2676.8 (6)
Z	8
D_c (g cm^{-3})	1.411
μ (mm^{-1})	0.111
Data collected/uniq. (R_{int})	7250/2351 (0.0249)
R_1, wR_2 [$I > 2\sigma(I)$]	0.0393, 0.1096
R_1, wR_2 (all data)	0.0445, 0.1158
GOF	1.027
Residues (e Å^{-3})	0.138, -0.235

[a] $R_1 = \Sigma \mid\mid F_o \mid - \mid F_c \mid\mid / \Sigma \mid F_o \mid$. [b] $wR_2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma w(F_o^2)^2]^{1/2}$, $w = 1/[\square^2 (F_o)^2 + (aP)^2 + bP]$, where $P = [(F_o^2) + 2F_c^2]/3$.

Table S2. Selected bond lengths (Å) and angles (°) for TTIBD.

C1—O1	1.2497 (17)	C9—N4	1.3149 (17)
C1—O2	1.2545 (17)	C9—N2	1.3245 (17)
C1—C2	1.5039 (19)	C9—N1	1.3519 (17)
C2—C7	1.377 (2)	C10—N5	1.3211 (17)
C2—C3	1.379 (2)	C10—N2	1.3501 (17)
C3—C4	1.388 (2)	C10—N3	1.3512 (17)
C3—H3	0.9300	N1—H1	0.8600
C4—C5	1.359 (2)	N4—H4A	0.8600
C4—H4	0.9300	N4—H4B	0.8600
C5—C6	1.374 (2)	N5—H5A	0.8600
C5—H5	0.9300	N5—H5B	0.8600
C6—C7	1.380 (2)	N6—H6A	0.8600
C6—H6	0.9300	N6—H6B	0.8600
C7—H7	0.9300	O1W—H1WA	0.879 (14)
C8—N6	1.3137 (18)	O1W—H1WB	0.880 (14)
C8—N3	1.3301 (17)	O2W—H2WA	0.874 (15)
C8—N1	1.3610 (17)	O2W—H2WB	0.860 (15)
O1—C1—O2	123.27 (12)	N3—C8—N1	121.38 (12)
O1—C1—C2	119.10 (12)	N4—C9—N2	120.41 (12)

O2—C1—C2	117.57 (12)	N4—C9—N1	117.79 (12)
C7—C2—C3	119.06 (13)	N2—C9—N1	121.80 (11)
C7—C2—C1	120.22 (13)	N5—C10—N2	116.76 (12)
C3—C2—C1	120.71 (13)	N5—C10—N3	117.34 (12)
C2—C3—C4	120.09 (14)	N2—C10—N3	125.90 (11)
C2—C3—H3	120.0	C9—N1—C8	119.46 (11)
C4—C3—H3	120.0	C9—N1—H1	120.3
C5—C4—C3	120.47 (15)	C8—N1—H1	120.3
C5—C4—H4	119.8	C9—N2—C10	115.73 (11)
C3—C4—H4	119.8	C8—N3—C10	115.63 (11)
C4—C5—C6	119.74 (14)	C9—N4—H4A	120.0
C4—C5—H5	120.1	C9—N4—H4B	120.0
C6—C5—H5	120.1	H4A—N4—H4B	120.0
C5—C6—C7	120.27 (16)	C10—N5—H5A	120.0
C5—C6—H6	119.9	C10—N5—H5B	120.0
C7—C6—H6	119.9	H5A—N5—H5B	120.0
C2—C7—C6	120.34 (15)	C8—N6—H6A	120.0
C2—C7—H7	119.8	C8—N6—H6B	120.0
C6—C7—H7	119.8	H6A—N6—H6B	120.0
N6—C8—N3	121.27 (12)	H1WA—O1W—H1WB	104.2 (14)
N6—C8—N1	117.34 (12)	H2WA—O2W—H2WB	106.2 (16)